Novel Design and Development of Isochronous Time Integration Architectures for Ordinary Differential Equations and Differential-Algebraic Equations: Computational Science and Engineering Applications

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Masao Shimada

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Dedication

To my parents and sister

Abstract

Recently, the novel designs and developments encompassing *i*sochronous integrators [*i*Integrators] for systems of ordinary differential equations (ODE-*i*Integrators) have been invented [1] that entail most of the research to-date developed over the past fifty years or so including new and novel optimal schemes for both second-order and first-order transient systems. This present thesis next takes upon the daunting challenges for the extensions of the ODE *i*Integrators to systems of differential-algebraic equations (DAEs). The *i*Integrators for DAEs (DAE-*i*Integrators) is an extremely powerful time integration toolkit with new and contemporary schemes that are novel and suitable to DAEs of any index which can be applied both for second- and first-order systems; and it includes most single step single solve implicit/semi-explicit schemes which preserve second-order time accuracies in all the variables (this is the novelty and it is not trivial and is not readily achievable with current state of the art for the differential and algebraic quantities to-date due to lack of fundamental understanding, poor or improper designs and implementation). Sub-cases include the classical algorithms in second-order systems such as Newmark, HHT-α, WBZ methods and many others, including mechanical integrators, and more new and optimal algorithms and designs for second-order systems; and this very same computational framework (hence, the name *i*sochronous integration) readily adapts to the simulation of first-order systems as well as an added bonus and includes most of the classical developments such as Crank-Nicholson method, Gear's method, MacCormack's method and so on including more

new and optimal designs encompassing both implicit and explicit schemes for first-order systems as well under the umbrella of a single unified toolkit. The new and novel DAE-*i*Integration architecture is envisioned as the next generation toolkit, and can also be widely used, for example, as an added bonus for applicability to multi-physics problems such as fluid-structure, thermal-structure interaction problems. Additional studies on the multiple subdomain DAE simulations and model order reduction by the proper orthogonal decomposition (POD) for ODE systems are also investigated.

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Chapter 1

Introduction

In dealing with the *Time Dimension*, time discretized operators or those commonly referred to as to as time integrators, play a crucial role for linear or nonlinear transient/-dynamic applications in various fields such as mechanical, aerospace, civil, biomedical, electrical, chemical, economics and allied fields. This thesis provides the theoretical investigations on the design and developments and recent state-of-the-art with regards to pragmatic computer-aided modeling and simulation technologies applicable for a wide variety of transient science and engineering applications.

Suppose we have the governing mathematical models with or without constraints. First, numerical discretization in space is conducted with space discretization techniques such as finite elements, differences, volumes, meshless/particle type methods, etc, which gives rise to a system of ordinary differential equations (ODEs) in a continuous time system. Next, numerical discretization in time is performed to numerically track the evolution of the underlying physics of the original models in the fully-discrete sense. In discrete time systems, various numerical problems, such as accuracy, stability, robustness, and so on, come into the picture. Dealing with these problems have been of paramount importance in developing time integrators, and numerous efforts have been made over the past several decades; however, a sound, optimal resolution does not exist.

A fundamentally different concept of developing time integrators came into play by adopting the view point of *Algorithms by Design* [3]. The theoretical basis, methodology, and highlights of the concept of *Algorithms by Design* may be succinctly described as follows. In modern science and engineering design and analysis, each engineering application has its own emphasis and analysis requirements; wishful thinking is that a wish list of desired attributes by the analyst to meet certain required analysis needs is desirable. Optimal designs of algorithms are not usually trivial; and alternately, how to foster such optimal designs and how to determine whether an algorithm design is optimal for a selected application is a desirable goal and challenging task. The theoretical basis of *Algorithms by Design* emanates from a generalized time weighted residual philosophy. It comprises of three principal essentials: (1) it first utilizes a unified theory underlying computational algorithms for time dependent problems that fundamentally explain the underlying principles of the evolution, classification, relationships, and design of time discretized operators, unlike all previous representations and various frameworks existing in the literature; (2) it also utilizes the design spaces and algorithmic measures and metrics for evaluation and comparison, and for qualifying the optimality of an algorithm with respect to a particular application; and (3) it finally provides an educated design procedure and guidelines to the analyst utilizing the concepts, fundamental principles, and ideas described in (1) and (2) above for developing algorithms naturally endowed with the particular qualifications.

In general, time discretized operators can be categorized into Type 1, Type 2, and Type 3 classifications; see Fig. 1.1 for a pictorial description of the classifications.

Each classification pertains to distinct design spaces for time integrators; and all classifications can theoretically attain up to n^{th} degree time accuracy. Second-order time accuracy is the most practical and preferred in most research and commercial software.

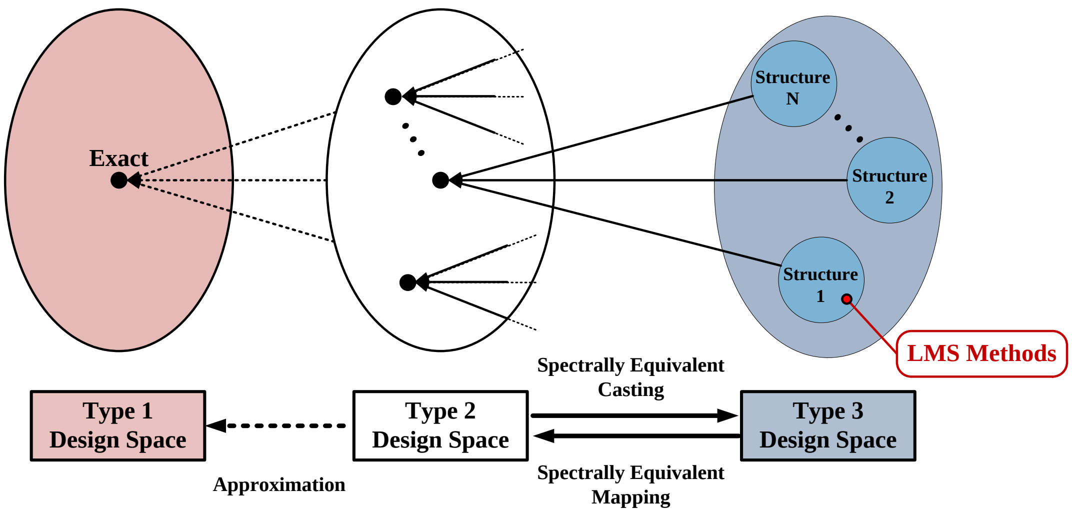


Figure 1.1: Design Spaces of Time Integrators

Type 1 classification entails an exact amplification matrix (such as an exponential matrix or its equivalent in the modal space such as the Duhamel integral), and how the load vector is treated can yield either exact or up to n^{th}-degree time accuracy; on the other hand, Type 2 classification is simply an approximation of the exact amplification matrix, but involves from first power to increasingly higher and higher powers of the amplification matrix that approximates (such as Pade, Norsett, etc.) the exact amplification matrix in Type 1; and lastly Type 3 classification is the design that only entails the first power of the approximate amplification matrix (there exists a mapping relation for each Type 3 algorithm to the corresponding Type 2 classification of algorithms which can be readily cast as Type 3 classifications).

Based on the concept of *Algorithms by Design*, inventing a novel next generation unified algorithmic architecture that encompasses not only most techniques being used over the past half century or so for first/second-order ODE/DAE systems, but also new, optimal algorithms and designs with attractive numerical features and significant improvements over current state-of-the-art is the main objective an contribution of this thesis.

Such an algorithmic architecture is termed *isochronous integrators* (or *iIntegrators*) because this same unified and single simulation environment can now also be readily applied concurrently to either second and/or first order-transient systems, just by controlling its variables and algorithmic parameters (isochronous adaptation process); simply put, only three algorithmic free parameters together with additional parameters that controls implicit/explicit features need to be adjusted to cover a wide range of practically useful new and optimal implicit or explicit algorithms and designs. It also includes most past efforts that have been derived from various other viewpoints over the past decades as sub-cases which continue to be employed in various commercial/research software but inherit several drawbacks/deficiencies mentioned previously. Besides the unified formalism with new and improved attributes, an added bonus is that only a single unified framework and family of algorithms originally designed for second-order transient ODE/DAE systems can also automatically generate and cover schemes applicable also to first-order transient ODE/DAE systems as well; maintaining important attributes such as desired numerical features.

Main Contributions of This Thesis

- Design and develop for the first time unified general time integration frameworks to solve ODE and DAE systems of any index and/or formulations for second- and first-order problems with particular attention to ensuring second-order time accuracy in all unknowns.

- Applications to multiple subdomain problems: Various combinations of numerically non-dissipative and dissipative algorithms WITHOUT losing second-order time accuracy of algorithms. Theory/design guidelines addressed for the first time.

- Applications to model order reduction by Proper orthogonal decomposition (POD): Employ POD model reduction to reduce problem size such that we can bypass the severe energy dissipation of numerically dissipative schemes through new avenues.

Chapter 2

The Isochronous Time Integration Architecture for Systems of Ordinary Differential Equations

2.1 Introduction

In this chapter, an overview of the ***isochronous time integration architecture*** (***i*Integrators**) for solving a system of ordinary differential equations (ODEs) of second and/or first order in time is presented. In essence, the *i*Integrators consist of two algorithmic frameworks; namely, the generalized single step single solve family of algorithms for a system of second order ODEs (***GS4-2 family of algorithms***) and the generalized single step single solve family of algorithms for a system of first order ODEs (***GS4-1 family of algorithms***). The main idea of the *i*Integrators is that the same GS4-2 family of algorithms can be readily reduced to the GS4-1 family of algorithms via the so-called ***adaptation process*** through a simple selection of algorithmic parameters; therefore, we, as users, only need to program the GS4-2 family of algorithms to solve not only hyperbolic or parabolic-hyperbolic problems, but also parabolic problems as well. This feature is indeed significant from a pragmatic point of view. It is also to be remarked that most widely-used implicit or explicit time integration schemes of second order-time accuracies, such as implicit Newmark method (average acceleration method), explicit central difference method, WBZ method, HHT-α method, the three parameter optimal method and so on for second-order systems, and Crank-Nicolson method, Gear's method and so on for first-order systems.

ODEs: Various science and engineering problems can be modeled by an explicit second-order ODEs of the form

$$\ddot{\mathbf{q}} = \mathbf{g}(\mathbf{q}, \dot{\mathbf{q}}, t) \ \ \forall t \in \mathbb{I} \subset \mathbb{R}_+ \quad \text{with} \ \ (\mathbf{q}, \dot{\mathbf{q}})(t_0) = (\mathbf{q}^0, \mathbf{v}^0) \tag{2.1}$$

where $\mathbf{q}(t) : \mathbb{I} \to \mathbb{R}^{N_2}$ is referred to be as a state variable of the system, and $\mathbf{g} \in C^2(\mathcal{B}, \mathbb{R}^{N_2})$ in which the set $\mathcal{B}$ is open in $\mathbb{R}^{N_2}$; or explicit first-order ODEs of the form

$$\dot{\mathbf{s}} = \mathbf{h}(\mathbf{s}, t) \ \ \forall t \in \mathbb{I} \subset \mathbb{R}_+ \quad \text{with} \ \ \mathbf{s}(t_0) = \mathbf{s}^0 \tag{2.2}$$

where $\mathbf{s}(t) : \mathbb{I} \to \mathbb{R}^{N_1}$ is referred to be as state variable of the system, and $\mathbf{h} \in C^1(\mathcal{A}, \mathbb{R}^{N_1})$ in which the set $\mathcal{A}$ is open in $\mathbb{R}^{N_1}$. Assume $(\mathbf{q}, \dot{\mathbf{q}})$ and $\mathbf{s}$ at the initial time $t = t_0$ are known, which forms the initial-value problems shown above. Let the time interval of interest be $T = t_L - t_0$ where t_0 and t_L denote the the initial and final time, and suppose it is divided into n_{steps} sub-intervals such that $\mathbb{I} = [t_0, t_L] = \bigcup_{n=0}^{n_{\text{steps}}-1} [t_n, t_{n+1}]$, assuming $0 \le t_0 < t_1 < t_2 < \cdots < t_{n_{\text{steps}}} \equiv t_L$. Define the time step size as $\Delta t_n := t_{n+1} - t_n > 0$ for $n \in \{0, 1, \cdots, n_{\text{steps}} - 1\}$ so we have $t_n = t_0 + \sum_{i=0}^{n_{\text{steps}}-1} \Delta t_i$. Hereafter, we assume the time step size is constant during the simulation for the sake of simplicity, i.e., $\Delta t = \Delta t_n$; therefore, we have $t_n = t_0 + n\Delta t$ and the number of time steps can be expressed as $n_{\text{steps}} = T/\Delta t$.

The GS4-2 family of algorithms was originally developed for the linearized Eq. (2.1) with constant coefficients $\mathbf{M}$, $\mathbf{C}$, and $\mathbf{K}$, represented by

$$\mathbf{M}\ddot{\mathbf{q}}(t) + \mathbf{C}\dot{\mathbf{q}}(t) + \mathbf{K}\mathbf{q}(t) = \mathbf{f}(t) \ \ \forall t \in \mathbb{I} \subset \mathbb{R}_+ \quad \text{with} \ \ (\mathbf{q}, \dot{\mathbf{q}})(t_0) = (\mathbf{q}^0, \mathbf{v}^0) \tag{2.3}$$

In structural dynamics, this is a familiar semi-discrete equation of motion of second order in time: $\mathbf{q}(t) : \mathbb{I} \to\in \mathbb{R}^{N_2}$, $\dot{\mathbf{q}}(t) : \mathbb{I} \to\in \mathbb{R}^{N_2}$, $\ddot{\mathbf{q}}(t) : \mathbb{I} \to\in \mathbb{R}^{N_2}$ are the nodal displacement, velocity, and acceleration vectors; $\mathbf{M} \in \mathbb{R}^{N_2 \times N_2}$, $\mathbf{C} \in \mathbb{R}^{N_2 \times N_2}$, and $\mathbf{K} \in \mathbb{R}^{N_2 \times N_2}$ are the mass, damping, and stiffness matrices; and $\mathbf{f}(t) : \mathbb{I} \to\in \mathbb{R}^{N_2}$ is the time-dependent external load vector. The mass matrix is symmetric, i.e., $\mathbf{M}^T = \mathbf{M}$, and positive-definite, i.e., $(\mathbf{a}, \mathbf{M}\mathbf{a}) > 0 \ \forall \mathbf{a} \in \mathbb{R}^{N_2}$; while the damping and stiffness matrices are symmetric, i.e., $\mathbf{C}^T = \mathbf{C}$ and $\mathbf{K}^T = \mathbf{K}$, positive-semidefinite, i.e., $(\mathbf{a}, \mathbf{C}\mathbf{a}) \geq 0$ and $(\mathbf{a}, \mathbf{K}\mathbf{a}) \geq 0 \ \forall \mathbf{a} \in \mathbb{R}^{N_2}$.

Similarly, the GS4-1 family of algorithms was originally developed for the linearized Eq. (2.2) with constant coefficients $\mathbf{Q}$ and $\mathbf{P}$, represented by

$$\mathbf{Q}\dot{\mathbf{s}}(t) + \mathbf{P}\mathbf{s}(t) = \mathbf{r}(t) \ \ \forall t \in \mathbb{I} \subset \mathbb{R}_+ \quad \text{with} \ \ \mathbf{s}(t_0) = \mathbf{s}^0 \tag{2.4}$$

In heat transfer problems, Eq. (2.4) is viewed as the semidiscrete heat equation of first order in time: $\mathbf{s}(t) : \mathbb{I} \to \mathbb{R}^{N_1}$ is the nodal temperature vector, and $\dot{\mathbf{s}}(t) : \mathbb{I} \to \mathbb{R}^{N_1}$ is the time derivative of $\mathbf{s}$; $\mathbf{Q} \in \mathbb{R}^{N_1 \times N_1}$, and $\mathbf{P} \in \mathbb{R}^{N_1 \times N_1}$ are capacity and conductivity matrices; and $\mathbf{r}(t) : \mathbb{I} \to\in \mathbb{R}^{N_1}$ is the time-dependent heat supply vector. The matrix $\mathbf{Q}$ is symmetric, i.e., $\mathbf{Q}^T = \mathbf{Q}$, and positive-definite, i.e., $(\mathbf{b}, \mathbf{Q}\mathbf{b}) > 0 \ \forall \mathbf{b} \in \mathbb{R}^{N_1}$; and $\mathbf{P}$ is also symmetric, i.e., $\mathbf{P}^T = \mathbf{P}$, but, positive-semidefinite, i.e., $(\mathbf{b}, \mathbf{P}\mathbf{b}) \geq 0 \ \forall \mathbf{b} \in \mathbb{R}^{N_1}$ in general.

2.2 Isochronous Time Integration: GS4-2 family of algorithms

2.2.1 Algorithmic Structure

The GS4-2 Family of algorithms consists of two branches of families: the ***U0 family*** and ***V0 family***. The names U0 and V0 are based upon the overshoot analysis of the algorithms in the *linear* system; which is to say, any schemes in the U0 family exhibit at least zeroth-order overshoot behaviors in $\mathbf{q}^n$, while any schemes in the V0 family exhibit at least zeroth-order overshoot behaviors in $\mathbf{v}^n$, as will be explained more closely in the next subsection. Overshoot is important and can effect completion of the analysis.

The algorithmic structure of the GS4-2 family of algorithms, which serves as the basic algorithmic framework through this thesis, is stated as follows:

Algorithm 2.2.1 (GS4-2 Family of Algorithms)

Suppose the initial conditions are given as $(\mathbf{q}, \dot{\mathbf{q}})(t_0) = (\mathbf{q}^0, \mathbf{v}^0)$, *so* $\mathbf{a}^0$ *can be obtained by* $\mathbf{a}^0 = \mathbf{g}(\mathbf{q}^0, \mathbf{v}^0, t_0)$. *Then, evaluate* $(\mathbf{q}^n, \mathbf{v}^n, \mathbf{a}^n)$ *for* $n \in \{1, 2, \cdots, n_{\text{steps}}\}$ *from the following integrator and associated updates:*

$$\tilde{\mathbf{a}}^n = \mathbf{g}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n, t_{n+W_1}) \tag{2.5a}$$

where $t_{n+W_1} := (1 - W_1)t_n + W_1 t_{n+1}$ *and*

$$\tilde{\mathbf{q}}^n = \mathbf{q}^n + W_1\Lambda_1\mathbf{v}^n\Delta t + W_2\Lambda_2\mathbf{a}^n\Delta t^2 + W_3\Lambda_3\Delta\mathbf{a}^n\Delta t^2 \tag{2.5b}$$

$$\tilde{\mathbf{v}}^n = \mathbf{v}^n + W_1\Lambda_4\mathbf{a}^n\Delta t + W_2\Lambda_5\Delta\mathbf{a}^n\Delta t \tag{2.5c}$$

$$\tilde{\mathbf{a}}^n = \mathbf{a}^n + W_1\Lambda_6\Delta\mathbf{a}^n =: \mathbf{a}^{n+W_1\Lambda_6} \tag{2.5d}$$

The updates are given as:

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \lambda_1 \mathbf{v}^n \Delta t + \lambda_2 \mathbf{a}^n \Delta t^2 + \lambda_3 \Delta \mathbf{a}^n \Delta t^2 \tag{2.5e}$$

$$\mathbf{v}^{n+1} = \mathbf{v}^n + \lambda_4 \mathbf{a}^n \Delta t + \lambda_5 \Delta \mathbf{a}^n \Delta t \tag{2.5f}$$

$$\mathbf{a}^{n+1} = \mathbf{a}^n + \Delta \mathbf{a}^n \tag{2.5g}$$

The algorithmic scalar parameters which characterize the U0 and V0 families are defined as follows:

$$\begin{aligned}
W_1 &= \frac{1}{1+\rho_\infty^{\mathrm{s}}} \quad , \quad \lambda_1 = \Lambda_1 = \lambda_4 = \Lambda_4 = 1 \\
W_2\Lambda_2 &= \frac{1}{2(1+\rho_\infty^{\mathrm{s}})} \quad , \quad \lambda_2 = \frac{1}{2} \\
W_3\Lambda_3 &= \frac{1}{(1+\rho_\infty^{\mathrm{min}})(1+\rho_\infty^{\mathrm{max}})(1+\rho_\infty^{\mathrm{s}})} \quad , \quad \lambda_3 = \frac{1}{(1+\rho_\infty^{\mathrm{min}})(1+\rho_\infty^{\mathrm{max}})} \\
W_2\Lambda_5 &= \frac{3+\rho_\infty^{\mathrm{min}}+\rho_\infty^{\mathrm{max}}-\rho_\infty^{\mathrm{min}}\rho_\infty^{\mathrm{max}}}{2(1+\rho_\infty^{\mathrm{min}})(1+\rho_\infty^{\mathrm{max}})(1+\rho_\infty^{\mathrm{s}})} \quad , \quad \lambda_5 = \frac{3+\rho_\infty^{\mathrm{min}}+\rho_\infty^{\mathrm{max}}-\rho_\infty^{\mathrm{min}}\rho_\infty^{\mathrm{max}}}{2(1+\rho_\infty^{\mathrm{min}})(1+\rho_\infty^{\mathrm{max}})} \\
W_1\Lambda_6 &= \frac{2+\rho_\infty^{\mathrm{min}}+\rho_\infty^{\mathrm{max}}+\rho_\infty^{\mathrm{s}}-\rho_\infty^{\mathrm{min}}\rho_\infty^{\mathrm{max}}\rho_\infty^{\mathrm{s}}}{(1+\rho_\infty^{\mathrm{min}})(1+\rho_\infty^{\mathrm{max}})(1+\rho_\infty^{\mathrm{s}})}
\end{aligned}$$

*for the **U0 family-based schemes**, and*

$$\begin{aligned}
W_1 &= \frac{3+\rho_\infty^{\mathrm{min}}+\rho_\infty^{\mathrm{max}}-\rho_\infty^{\mathrm{min}}\rho_\infty^{\mathrm{max}}}{2(1+\rho_\infty^{\mathrm{min}})(1+\rho_\infty^{\mathrm{max}})} \quad , \quad \lambda_1 = \Lambda_1 = \lambda_4 = \Lambda_4 = 1 \\
W_2\Lambda_2 &= \frac{1}{(1+\rho_\infty^{\mathrm{min}})(1+\rho_\infty^{\mathrm{max}})} \quad , \quad \lambda_2 = \frac{1}{2} \\
W_3\Lambda_3 &= \frac{1}{(1+\rho_\infty^{\mathrm{min}})(1+\rho_\infty^{\mathrm{max}})(1+\rho_\infty^{\mathrm{s}})} \quad , \quad \lambda_3 = \frac{1}{2(1+\rho_\infty^{\mathrm{s}})} \\
W_2\Lambda_5 &= \frac{2}{(1+\rho_\infty^{\mathrm{min}})(1+\rho_\infty^{\mathrm{max}})(1+\rho_\infty^{\mathrm{s}})} \quad , \quad \lambda_5 = \frac{1}{1+\rho_\infty^{\mathrm{s}}} \\
W_1\Lambda_6 &= \frac{2+\rho_\infty^{\mathrm{min}}+\rho_\infty^{\mathrm{max}}+\rho_\infty^{\mathrm{s}}-\rho_\infty^{\mathrm{min}}\rho_\infty^{\mathrm{max}}\rho_\infty^{\mathrm{s}}}{(1+\rho_\infty^{\mathrm{min}})(1+\rho_\infty^{\mathrm{max}})(1+\rho_\infty^{\mathrm{s}})}
\end{aligned}$$

*for the **V0 family-based schemes**.*

Remark 2.2.1 (Algorithm 2.2.1)

1. *The GS4-2 family of algorithms, which firstly appeared in [4], can be written in the* ***one-step, three-value form*** *in linear systems, shown in the next section, and the spectral roots* $(\rho_\infty^{\text{min}}, \rho_\infty^{\text{max}}, \rho_\infty^{\text{s}})$ *are the absolute values of the eigenvalues of the amplification matrix* $\mathbf{A} \in \mathbb{R}^{3\times3}$ *appearing in the representation; see Eq.* (2.38). ρ_∞^{max} *and* ρ_∞^{min} *are the higher and lower* ***principal roots*** *at infinity, respectively; and* ρ_∞^{s} *is the so-called* ***spurious root****, i.e., the absolute value of the lowest eigenvalue at infinity out of three eigenvalues; see Eq.* (2.47). ρ_∞^{max} *is also known as the* ***spectral radius*** *at infinity of the schemes; and it must be less than or equal to unity to guarantee the* ***unconditional stability***[1] *of any scheme within the GS4-2 family; see Eq.* (2.46). *That is, the spectral roots* $(\rho_\infty^{\text{min}}, \rho_\infty^{\text{max}}, \rho_\infty^{\text{s}})$ *must satisfy:*

$$0 \leq \rho_\infty^{\text{s}} \leq \rho_\infty^{\text{min}} \leq \rho_\infty^{\text{max}} \leq 1 \tag{2.6}$$

2. *The values of the algorithmic parameters* W_1, $W_1\Lambda_6$, $W_2\Lambda_2$, $W_2\Lambda_5$, $W_3\Lambda_3$, λ_3, *and* λ_5 *are determined by the spectral roots; and they are symmetric in* ρ_∞^{max} *and* ρ_∞^{min}. *They are called the* ***discrete numerical assigned (DNA)*** *parameters, together with the constant parameters,* $\lambda_1 = \Lambda_1 = \lambda_4 = \Lambda_4 = 1$ *and* $\lambda_2 = \frac{1}{2}$. *It is noteworthy to mention that every scheme within the GS4-2 family essentially possesses distinct values of the DNA parameters. That is, no two algorithms can have the same DNA.*

3. *Schemes in the GS4-2 family possess zeroth-order overshoot in both* $\mathbf{q}^n$ *and* $\mathbf{v}^n$*, i.e., U0V0 in the U0 family, and V0U0 in the V0 family, if and only if* $\rho_\infty^{\text{max}} = 1$ *in linear systems. For* $\rho_\infty^{\text{max}} \neq 1$*, any schemes in the U0 and V0 families become*

[1] *The unconditional stability is also called as the* ***absolute stability*** *or* ***A-stability****.*

U0V1 (zeroth-order overshoot in $\mathbf{q}^n$*, and first-order overshoot in* $\mathbf{v}^n$*) and V0U1 (zeroth-order overshoot in* $\mathbf{v}^n$*, and first-order overshoot in* $\mathbf{q}^n$*), respectively. Note that no scheme of higher order overshoots such as U1V1-, U0V2-, V0U2-, and V0U2-schemes, are essentially not included in the GS4-2 family. Such scheme with a higher order overshoot behavior is not competitive due to problematic issues with overshoot. For example, the Wilson-*θ *method which actually belongs to the U0V2 family is not discussed.*

4. *Schemes in the GS4-2 family are numerically non-dissipative in linear systems if and only if* $\rho_\infty^{\min} = \rho_\infty^{\max} = 1$*; otherwise, the resulting algorithms are numerically dissipative, i.e., the numerical damping is introduced.*

5. *Schemes within the U0 family become identical to the schemes within the V0 family if and only if* $\rho_\infty^{\max} = 1$ *and* $\rho_\infty^{\min} = \rho_\infty^{\mathrm{s}} \in [0,1]$*. The resulting family of algorithms are called the* ***U0V0/V0U0 Optimal Schemes****. For* $\rho_\infty^{\min} = \rho_\infty^{\mathrm{s}} \in [0,1)$*, the schemes become numerically dissipative; while, for* $\rho_\infty^{\min} = \rho_\infty^{\mathrm{s}} = 1$*, we recover the MPR-EPA method which is numerically non-dissipative.*

6. ***Time Accuracies and Time Level Shifting:*** $\mathbf{q}^n$ *and* $\mathbf{v}^n$ *obtained by any time integration scheme within the GS4-2 family are a priori second-order accurate in time. This is because the following second-order time accurate conditions for* $\mathbf{q}^n$ *and* $\mathbf{v}^n$ *were imposed during the derivation of the U0 and V0 families of schemes:*

$$\begin{aligned} &\lambda_1 = \Lambda_1 = \lambda_4 = \Lambda_4 = 1, \quad \lambda_2 = \tfrac{1}{2} \\ &\lambda_5 = \frac{1}{2} + W_1\Lambda_6 - W_1 \end{aligned} \tag{2.7}$$

$\mathbf{q}^n$ *and* $\mathbf{v}^n$ *are the approximations of* $\mathbf{q}(t_n)$ *and* $\dot{\mathbf{q}}(t_n)$*, respectively; whilst* $\mathbf{a}^n$ *is the approximation of* $\ddot{\mathbf{q}}(t_{n-\phi})$ *where* $\phi := W_1(\Lambda_6 - 1)$ *is the so-called* ***shifting***

parameter. *It is immensely important to note the* ***time level shifting*** *by* $\phi\Delta t$ *for* $\mathbf{a}^n$. *Without this shifting, the second order-time accuracies in* $\mathbf{a}^n$ *as well as in* $\mathbf{q}^n$ *and* $\mathbf{v}^n$ *are not guaranteed. The shifting parameter* ϕ *yields*

$$\phi = \frac{1-\rho_\infty^{\min}\rho_\infty^{\max}}{(1+\rho_\infty^{\min})(1+\rho_\infty^{\max})} \qquad \text{for the U0 family} \tag{2.8}$$

$$\phi = \frac{1-\rho_\infty^{s}}{2(1+\rho_\infty^{s})} \qquad \text{for the V0 family} \tag{2.9}$$

Refer to Section 2.2.5 for a detailed discussion on the algorithmic time level.

7. ***Combined Form:*** *Substituting the updates, Eqs.* (2.5e)-(2.5g), *the time integrators, Eqs.* (2.5b)-(2.5d), *yields the following expressions:*

$$\begin{aligned}\tilde{\mathbf{q}}^n &= \left(1-\frac{W_3\Lambda_3}{\lambda_3}\right)\mathbf{q}^n + \frac{W_3\Lambda_3}{\lambda_3}\mathbf{q}^{n+1} \\ &\quad +\Delta t\mathbf{v}^n\left(W_1\Lambda_1 - \lambda_1\frac{W_3\Lambda_3}{\lambda_3}\right) + \Delta t^2\mathbf{a}^n\left(W_2\Lambda_2 - \lambda_2\frac{W_3\Lambda_3}{\lambda_3}\right) \qquad (2.10a)\\ \tilde{\mathbf{v}}^n &= \left(1-\frac{W_2\Lambda_5}{\lambda_5}\right)\mathbf{v}^n + \frac{W_2\Lambda_5}{\lambda_5}\mathbf{v}^{n+1} + \Delta t\mathbf{a}^n\left(W_1\Lambda_4 - \lambda_4\frac{W_2\Lambda_5}{\lambda_5}\right) \qquad (2.10b)\\ \tilde{\mathbf{a}}^n &= (1-W_1\Lambda_6)\mathbf{a}^n + W_1\Lambda_6\mathbf{a}^{n+1} =: \mathbf{a}^{n+W_1\Lambda_6} \qquad (2.10c)\end{aligned}$$

We usually assume $\lambda_2 = \Lambda_2$, $\lambda_3 = \Lambda_3$, *and* $\lambda_5 = \Lambda_5$; *that is, we have* $W_2 = W_3$ *in the V0 family, which leads to*

$$\begin{aligned}\tilde{\mathbf{q}}^n &= (1-W_2)\mathbf{q}^n + W_2\mathbf{q}^{n+1} + \Delta t\mathbf{v}^n(W_1 - W_2)\\ &=: \mathbf{q}^{n+W_2} + \Delta t\mathbf{v}^n(W_1 - W_2) \qquad (2.11a)\\ \tilde{\mathbf{v}}^n &= (1-W_2)\mathbf{v}^n + W_2\mathbf{v}^{n+1} + \Delta t\mathbf{a}^n(W_1 - W_2)\\ &=: \mathbf{v}^{n+W_2} + \Delta t\mathbf{a}^n(W_1 - W_2) \qquad (2.11b)\\ \tilde{\mathbf{a}}^n &= (1-W_1\Lambda_6)\mathbf{a}^n + W_1\Lambda_6\mathbf{a}^{n+1} =: \mathbf{a}^{n+W_1\Lambda_6} \qquad (2.11c)\end{aligned}$$

Likewise, for the U0 family,

$$\tilde{\mathbf{q}}^n = (1 - W_1)\mathbf{q}^n + W_1\mathbf{q}^{n+1} =: \mathbf{q}^{n+W_1} \quad (2.12a)$$

$$\tilde{\mathbf{v}}^n = (1 - W_1)\mathbf{v}^n + W_1\mathbf{v}^{n+1} =: \mathbf{v}^{n+W_1} \quad (2.12b)$$

$$\tilde{\mathbf{a}}^n = (1 - W_1\Lambda_6)\mathbf{a}^n + W_1\Lambda_6\mathbf{a}^{n+1} =: \mathbf{a}^{n+W_1\Lambda_6} \quad (2.12c)$$

since we have $W_1 = W_2 = W_3$*.*

8. *The GS4-2 family of algorithms represented in the form* (2.5) *is called the* ***incremental a-form****. In this representation, one first solves for the primary increment* $\Delta\mathbf{a}^n$*, and then compute for* $(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}, \mathbf{a}^{n+1})$*, using the updates, Eqns.* (2.5e)-(2.5g)*. For linear systems, the incremental a-form can be written as:*

$$\begin{aligned}\overline{\mathbf{M}}\Delta\mathbf{a}^n = &- \mathbf{M}\mathbf{a}^n - \mathbf{C}\left[\mathbf{v}^n + W_1\Lambda_4\mathbf{a}^n\Delta t\right] \\ &- \mathbf{K}\left[\mathbf{q}^n + W_1\Lambda_1\mathbf{v}^n\Delta t + W_2\Lambda_2\mathbf{a}^n\Delta t^2\right] + \mathbf{f}(t_{n+W_1})\end{aligned} \quad (2.13)$$

where $\overline{\mathbf{M}} := W_1\Lambda_6\mathbf{M} + \Delta t W_2\Lambda_5\mathbf{C} + \Delta t^2 W_3\Lambda_3\mathbf{K}$*, and the updates are given in Eq.* (2.5e)-*Eq.* (2.5g)*. Likewise, the* ***incremental v-form*** and ***incremental d-form*** *yield the primary increments* $\Delta\mathbf{v}^n$ *and* $\Delta\mathbf{q}^n$*, respectively; and we can easily construct them from the time integrators, Eq.* (2.108a)-*Eq.* (2.5d)*, and the updates.*

On the other hand, we can write Eq. (2.5) *for linear systems as:*

$$\begin{aligned}\overline{\mathbf{M}}\mathbf{a}^{n+1} &= -(1 - W_1\Lambda_6)\mathbf{M}\mathbf{a}^n - \mathbf{C}\left[\mathbf{v}^n + \Delta t(W_1\Lambda_4 - W_2\Lambda_5)\mathbf{a}^n\right] \\ &\quad -\mathbf{K}\left[\mathbf{q}^n + \Delta t W_1\Lambda_1\mathbf{v}^n + \Delta t^2(W_2\Lambda_2 - W_3\Lambda_3)\mathbf{a}^n\right] + \mathbf{f}(t_{n+W_1})\end{aligned} \quad (2.14a)$$

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \lambda_1\mathbf{v}^n\Delta t + (\lambda_2 - \lambda_3)\mathbf{a}^n\Delta t^2 + \lambda_3\mathbf{a}^{n+1}\Delta t^2 \quad (2.14b)$$

$$\mathbf{v}^{n+1} = \mathbf{v}^n + (\lambda_4 - \lambda_5)\mathbf{a}^n\Delta t + \lambda_5\mathbf{a}^{n+1}\Delta t \quad (2.14c)$$

In this representation, one first solves for $\mathbf{a}^{n+1}$ *from Eq.* (2.14a)*, and then compute* $(\mathbf{q}^{n+1}, \mathbf{v}^{n+1})$*, using Eqns. 2.14b and 2.14c, respectively. This representation is* *called the **total a-form**. Similarly, we can easily construct the **total v-form**, i.e., solve for* $\mathbf{v}^{n+1}$*, and then compute* $(\mathbf{q}^{n+1}, \mathbf{a}^{n+1})$*, and the **total d-form**, i.e., solve for* $\mathbf{q}^{n+1}$*, and then compute* $(\mathbf{v}^{n+1}, \mathbf{a}^{n+1})$.

2.2.2 Three Important Branches within the GS4-2 Family: U0V0/V0U0 Numerically Non-dissipative/Dissipative and Optimal Schemes

Although there exist numerous schemes within the GS4-2 family of algorithms presented above, the following three subgroups are of special importance in light of the fact that they are numerically non-dissipative or numerically dissipative schemes belonging to the U0V0 and/or V0U0 families.

U0V0 Numerically Non-dissipative Family of Algorithms

This subgroup of the GS4-2 family can be obtained by setting $\rho_\infty^{\min} = \rho_\infty^{\max} = 1$ and $\rho_\infty^{\mathrm{s}} \in [0, 1]$ in the **U0 family**. Let $\rho := \rho_\infty^{\mathrm{s}} \in [0, 1]$.

Algorithm 2.2.2 (U0V0 Non-dissipative Family of Algorithms ⊂ Algorithm 2.2.1) *Suppose the initial conditions are given as* $(\mathbf{q}, \dot{\mathbf{q}})(t_0) = (\mathbf{q}^0, \mathbf{v}^0)$*, so* $\mathbf{a}^0$ *can be obtained by* $\mathbf{a}^0 = \mathbf{g}(\mathbf{q}^0, \mathbf{v}^0, t_0)$*. Then, evaluate* $(\mathbf{q}^n, \mathbf{v}^n, \mathbf{a}^n)$ *for* $n \in \{1, 2, \cdots, n_{\text{steps}}\}$ *from the following integrator and associated updates:*

$$\tilde{\mathbf{a}}^n = \mathbf{g}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n, t_{n+W}) \tag{2.15a}$$

where $t_{n+W} := (1 - W)t_n + Wt_{n+1}$ *and*

$$\begin{aligned} \tilde{\mathbf{q}}^n &= (1 - W)\mathbf{q}^n + W\mathbf{q}^{n+1} = \mathbf{q}^{n+W}, \quad \tilde{\mathbf{v}}^n = (1 - W)\mathbf{v}^n + W\mathbf{v}^{n+1} = \mathbf{v}^{n+W} \\ \tilde{\mathbf{a}}^n &= \mathbf{a}^n + W\Delta\mathbf{a}^n = \mathbf{a}^{n+W} \end{aligned} \tag{2.15b}$$

The updates are given as:

$$\begin{aligned}\mathbf{q}^{n+1} &= \mathbf{q}^n + \Delta t\mathbf{v}^n + \frac{\Delta t^2}{2}\mathbf{a}^{n+1/2}, \quad \mathbf{v}^{n+1} = \mathbf{v}^n + \Delta t\mathbf{a}^{n+1/2} \\ \mathbf{a}^{n+1} &= \mathbf{a}^n + \Delta\mathbf{a}^n\end{aligned} \tag{2.15c}$$

where

$$W := W_1 = W_2 = W_3 = W_1\Lambda_6 = \frac{1}{1+\rho} \in [\tfrac{1}{2}, 1] \tag{2.15d}$$

Remark 2.2.2 (Algorithm 2.2.2)

1. *For any* $\rho \in [0, 1]$,

$$\frac{\mathbf{q}^{n+1} - \mathbf{q}^n}{\Delta t} = \frac{\mathbf{v}^n + \mathbf{v}^{n+1}}{2} = \mathbf{v}^{n+1/2} \quad \textit{and} \quad \frac{\mathbf{v}^{n+1} - \mathbf{v}^n}{\Delta t} = \frac{\mathbf{a}^n + \mathbf{a}^{n+1}}{2} = \mathbf{a}^{n+1/2} \tag{2.16}$$

2. *The shifting parameter is given as*

$$\phi = W_1\Lambda_6 - W_1 = 0 \tag{2.17}$$

That is, the time level shifting is not necessary for any $\rho \in [0, 1]$.

V0U0 Numerically Non-dissipative Family of Algorithms

This subgroup of the GS4-2 family can be obtained by $\rho_\infty^{\mathrm{min}} = \rho_\infty^{\mathrm{max}} = 1$ and $\rho_\infty^{\mathrm{s}} \in [0, 1]$ in the **V0 family**. Let $\rho := \rho_\infty^{\mathrm{s}} \in [0, 1]$.

Algorithm 2.2.3 (V0U0 Non-dissipative Family of Algorithms ⊂ Algorithm 2.2.1)
Suppose the initial conditions are given as $(\mathbf{q}, \dot{\mathbf{q}})(t_0) = (\mathbf{q}^0, \mathbf{v}^0)$, *so* $\mathbf{a}^0$ *can be obtained by* $\mathbf{a}^0 = \mathbf{g}(\mathbf{q}^0, \mathbf{v}^0, t_0)$. *Then, evaluate* $(\mathbf{q}^n, \mathbf{v}^n, \mathbf{a}^n)$ *for* $n \in \{1, 2, \cdots, n_{\mathrm{steps}}\}$ *from the following integrator and associated updates:*

$$\tilde{\mathbf{a}}^n = \mathbf{g}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n, t_{n+W}) \tag{2.18a}$$

where $t_{n+W} := (1-W)t_n + Wt_{n+1}$ *and*

$$\begin{aligned} \tilde{\mathbf{q}}^n &= \frac{\mathbf{q}^n + \mathbf{q}^{n+1}}{2} = \mathbf{q}^{n+1/2}, \quad \tilde{\mathbf{v}}^n = \frac{\mathbf{v}^n + \mathbf{v}^{n+1}}{2} = \mathbf{v}^{n+1/2} \\ \tilde{\mathbf{a}}^n &= \mathbf{a}^n + W\Delta\mathbf{a}^n = \mathbf{a}^{n+W} \end{aligned} \tag{2.18b}$$

The updates are given as:

$$\begin{aligned} \mathbf{q}^{n+1} &= \mathbf{q}^n + \Delta t\mathbf{v}^n + \frac{\Delta t^2}{2}\mathbf{a}^{n+W}, \quad \mathbf{v}^{n+1} = \mathbf{v}^n + \Delta t\mathbf{a}^{n+W} \\ \mathbf{a}^{n+1} &= \mathbf{a}^n + \Delta\mathbf{a}^n \end{aligned} \tag{2.18c}$$

where

$$W := W_1\Lambda_6 = \lambda_5 = 2\lambda_3 = \frac{1}{1+\rho} \in [\tfrac{1}{2}, 1] \tag{2.18d}$$

Remark 2.2.3 (Algorithm 2.2.3)

1. *For any* $\rho \in [0, 1]$,

$$\frac{\mathbf{q}^{n+1} - \mathbf{q}^n}{\Delta t} = \frac{\mathbf{v}^n + \mathbf{v}^{n+1}}{2} = \mathbf{v}^{n+1/2} \quad \textit{and} \quad \frac{\mathbf{v}^{n+1} - \mathbf{v}^n}{\Delta t} = \mathbf{a}^{n+W} \tag{2.19}$$

2. *The shifting parameter is given as*

$$\phi = W_1\Lambda_6 - W_1 = \frac{1-\rho}{2(1+\rho)} \in [0, \tfrac{1}{2}] \tag{2.20}$$

The time level of the discrete balance equation (2.18a) *is* $t_{n+1/2}$ *or* $W_1 = 1/2$ *for any* $\rho \in [0, 1]$.

U0V0/V0U0 Optimal Family of Algorithms

This subgroup of the GS4-2 family can be obtained by $\rho_\infty^{\max} = 1$ and $\rho_\infty^{\min} = \rho_\infty^{s} \in [0, 1]$ in ***either*** the **U0 or V0 family**. Let $\rho := \rho_\infty^{\min} = \rho_\infty^{s} \in [0, 1]$.

Algorithm 2.2.4 (U0V0/V0U0 Optimal Family of Algorithms $\subset$ Algorithm 2.2.1)
Suppose the initial conditions are given as $(\mathbf{q}, \dot{\mathbf{q}})(t_0) = (\mathbf{q}^0, \mathbf{v}^0)$*, so* $\mathbf{a}^0$ *can be obtained by* $\mathbf{a}^0 = \mathbf{g}(\mathbf{q}^0, \mathbf{v}^0, t_0)$*. Then, evaluate* $(\mathbf{q}^n, \mathbf{v}^n, \mathbf{a}^n)$ *for* $n \in \{1, 2, \cdots, n_{\text{steps}}\}$ *from the following integrator and associated updates:*

$$\tilde{\mathbf{a}}^n = \mathbf{g}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n, t_{n+W}) \tag{2.21a}$$

where $t_{n+W} := (1 - W)t_n + W t_{n+1}$ *and*

$$\begin{aligned} &\tilde{\mathbf{q}}^n = (1 - W)\mathbf{q}^n + W\mathbf{q}^{n+1} = \mathbf{q}^{n+W}, \quad \tilde{\mathbf{v}}^n = (1 - W)\mathbf{v}^n + W\mathbf{v}^{n+1} = \mathbf{v}^{n+W} \\ &\tilde{\mathbf{a}}^n = \mathbf{a}^n + W\Lambda_6\Delta\mathbf{a}^n = \mathbf{a}^{n+W\Lambda_6} \end{aligned} \tag{2.21b}$$

The updates are given as:

$$\begin{aligned} &\mathbf{q}^{n+1} = \mathbf{q}^n + \Delta t\mathbf{v}^n + \frac{\Delta t^2}{2}\mathbf{a}^{n+W}, \quad \mathbf{v}^{n+1} = \mathbf{v}^n + \Delta t\mathbf{a}^{n+W} \\ &\mathbf{a}^{n+1} = \mathbf{a}^n + \Delta\mathbf{a}^n \end{aligned} \tag{2.21c}$$

where

$$W := W_1 = W_2 = W_3 = \lambda_5 = 2\lambda_3 = \frac{1}{1 + \rho} \in [\tfrac{1}{2}, 1] \tag{2.21d}$$

Remark 2.2.4 (Algorithm 2.2.4)

1. *For any* $\rho \in [0, 1]$,

$$\frac{\mathbf{q}^{n+1} - \mathbf{q}^n}{\Delta t} = \frac{\mathbf{v}^n + \mathbf{v}^{n+1}}{2} = \mathbf{v}^{n+1/2} \quad \text{and} \quad \frac{\mathbf{v}^{n+1} - \mathbf{v}^n}{\Delta t} = \mathbf{a}^{n+W} \tag{2.22}$$

2. *The shifting parameter for Algorithm 2.2.4 is the same as the one for Algorithm 2.2.3:*

$$\phi = W_1\Lambda_6 - W_1 = \frac{3 - \rho}{2(1 + \rho)} - \frac{1}{1 + \rho} = \frac{1 - \rho}{2(1 + \rho)} \in [0, \tfrac{1}{2}] \tag{2.23}$$

The time level of the discrete balance equation (2.21a) *is* t_{n+W_1} *where* $W_1 = 1/(1+\rho)$.

2.2.3 Various Expressions of Algorithm 2.2.1 in Linear Dynamical Systems

Modal Decomposition

Consider a system of linear, homogeneous, second-order ODEs without the damping term, i.e., $\mathbf{f} = \mathbf{0}$ and $\mathbf{C} = \mathbf{0}$ in Eq. (2.3): $\mathbf{M}\ddot{\mathbf{q}} + \mathbf{K}\mathbf{q} = \mathbf{0}$ $\forall t \in \mathbb{I}$. Postulating $\mathbf{q}(t) = \boldsymbol{\upsilon}\sin(\omega t) \in \mathbb{R}^{N_2}$ as a solution of this equation leads to the generalized eigenvalue problem,

$$(\mathbf{K} - \omega_i^2\mathbf{M})\boldsymbol{\upsilon}_i = \mathbf{0} \tag{2.24}$$

so that $(\omega_i^2, \boldsymbol{\upsilon}_i)$ (for $i = 1, 2, \cdots, N_2$) are its eigenpairs; the eigenvalues ω_i^2 are the roots of the characteristic equation

$$\det(\mathbf{K} - \omega_i^2\mathbf{M}) = 0 \tag{2.25}$$

and $\boldsymbol{\upsilon}_i$ are the corresponding eigenvectors which satisfy the orthonormality condition (**M-*orthonormality condition***),

$$(\boldsymbol{\upsilon}_i, \mathbf{M}\boldsymbol{\upsilon}_j) = \boldsymbol{\upsilon}_i^T\mathbf{M}\boldsymbol{\upsilon}_j = \delta_{ij} \tag{2.26}$$

Premultiplying Eq. (2.24) by $\boldsymbol{\upsilon}_j$, we get the **K-*orthogonality condition***,

$$(\boldsymbol{\upsilon}_i, \mathbf{K}\boldsymbol{\upsilon}_j) = \omega_i^2(\boldsymbol{\upsilon}_i, \mathbf{M}\boldsymbol{\upsilon}_j) = \omega_i^2\delta_{ij} \tag{2.27}$$

and suppose the eigenvalues ω_i^2 are ordered as

$$0 \leq |\omega_1^2| \leq |\omega_2^2| \leq \cdots \leq |\omega_{N_2}^2| \tag{2.28}$$

Defining $\mathbf{V} = [\boldsymbol{\upsilon}_1, \boldsymbol{\upsilon}_2, \cdots, \boldsymbol{\upsilon}_{N_2}] = [\boldsymbol{\upsilon}_i]$ (i.e., the columns in $\mathbf{V}$ are the eigenvectors), Eqs. (2.26) and (2.27) may be written as

$$(\mathbf{V}, \mathbf{M}\mathbf{V}) = \mathbf{I} \ \text{ and } \ (\mathbf{V}, \mathbf{K}\mathbf{V}) = \boldsymbol{\Omega}^2 \tag{2.29}$$

where $\mathbf{\Omega}^2 = \text{diag}(\omega_1^2, \omega_2^2, \cdots, \omega_{N_2}^2)$ is the diagonal matrix of the eigenvalues.

Using the projection of $\mathbf{q}$ parallel to $\boldsymbol{\upsilon}_i$, i.e.,

$$\mathbf{q}(t) = (\mathbf{q}(t), \boldsymbol{\upsilon}_i)\boldsymbol{\upsilon}_i = \boldsymbol{\upsilon}_i x_i = \mathbf{V}\mathbf{x} \tag{2.30}$$

where $\mathbf{x} = [x_1, x_2, \cdots, x_{N_2}]^T := (\mathbf{q}, \boldsymbol{\upsilon}_i) = \mathbf{V}^T\mathbf{q}$, Eq. (2.3) becomes

$$\mathbf{MV}\ddot{\mathbf{x}} + \mathbf{CV}\dot{\mathbf{x}} + \mathbf{KV}\mathbf{x} - \mathbf{f}(t) = \mathbf{0} \tag{2.31}$$

Therefore, premultiplying Eq. (2.31) by $\mathbf{V}^T$,

$$(\mathbf{V}, \mathbf{MV})\ddot{\mathbf{x}}(t) + (\mathbf{V}, \mathbf{CV})\dot{\mathbf{x}}(t) + (\mathbf{V}, \mathbf{KV})\mathbf{x}(t) = (\mathbf{V}, \mathbf{f}(t)) \tag{2.32}$$

yields

$$\ddot{\mathbf{x}}(t) + (\mathbf{V}, \mathbf{CV})\dot{\mathbf{x}}(t) + \mathbf{\Omega}^2\mathbf{x}(t) = \mathbf{g}(t) \tag{2.33}$$

where $\mathbf{g}(t) := (\mathbf{V}, \mathbf{f}(t))$. Similarly, the initial conditions for Eq. (2.33) may be given as

$$\mathbf{x}(t_0) = (\mathbf{V}, \mathbf{M}\mathbf{q}^0) \;\text{ and }\; \dot{\mathbf{x}}(t_0) = (\mathbf{V}, \mathbf{M}\mathbf{v}^0) \tag{2.34}$$

If we assume the eigenvectors satisfy the **C-*orthogonality condition*** in addition,

$$(\boldsymbol{\upsilon}_i, \mathbf{C}\boldsymbol{\upsilon}_j) = 2\omega_i\xi_i\delta_{ij} \tag{2.35}$$

where ξ_i is a modal damping parameter, Eq. (2.33) becomes the system of N_2 numbers of decoupled equations:

$$\boxed{\ddot{x}_i(t) + 2\omega_i\xi_i\dot{x}_i(t) + \omega_i^2 x_i(t) = g_i(t)} \tag{2.36}$$

(no sum on i) with the initial conditions:

$$\begin{aligned} x_i(t_0) &= V_{ji}M_{jk}q_k^0 = [\boldsymbol{\upsilon}_i]_j M_{jk}q_k^0 \\ \dot{x}_i(t_0) &= V_{ji}M_{jk}v_k^0 = [\boldsymbol{\upsilon}_i]_j M_{jk}v_k^0 \end{aligned} \tag{2.37}$$

GS4-2 Family of Algorithms in the One-step, Three-value Form

Apply Algorithm 2.2.1, i.e., the GS4-2 family of algorithms, to the SDOF governing equation (2.36); then, defining $\mathbf{y}^n := [x^n, \Delta t x_v^n, \Delta t^2 x_a^n]^T \in \mathbb{R}^3$, we can cast it into the following form:

$$\boxed{\mathbf{y}^{n+1} = \mathbf{A}\mathbf{y}^n + \mathbf{L}(t_{n+W_1})} \tag{2.38}$$

where $\mathbf{A} \in \mathbb{R}^{3\times3}$ is the amplification matrix given as

$$\mathbf{A} = \begin{bmatrix} 1 & \lambda_1 & \lambda_2 \\ 0 & 1 & \lambda_4 \\ 0 & 0 & 1 \end{bmatrix} + \begin{bmatrix} \lambda_3 \\ \lambda_5 \\ 1 \end{bmatrix} \begin{bmatrix} \alpha_1 & \alpha_2 & \alpha_3 \end{bmatrix} \tag{2.39}$$

in which

$$\begin{aligned} &\alpha_1 = -\frac{\Omega^2}{D}, \quad \alpha_2 = -\frac{2\xi\Omega + W_1\Lambda_1\Omega^2}{D}, \quad \alpha_3 = -\frac{1 + 2W_1\Lambda_4\xi\Omega + W_2\Lambda_2\Omega^2}{D} \\ &D = W_1\Lambda_6 + 2W_2\Lambda_5\xi\Omega + W_3\Lambda_3\Omega^2, \quad \Omega = \omega\Delta t \end{aligned} \tag{2.40}$$

and $\mathbf{L}(t_{n+W_1}) \in \mathbb{R}^3$ is the algorithmic external load vector given as

$$\mathbf{L}(t_{n+W_1}) = \frac{\Delta t^2}{D} \begin{bmatrix} \lambda_3 \\ \lambda_5 \\ 1 \end{bmatrix} g(t_{n+W_1}) \tag{2.41}$$

The characteristic polynomial of the amplification matrix $\mathbf{A}$ yields

$$-\det(\zeta\mathbf{I}_3 - \mathbf{A}) = \zeta^3 - A_1\zeta^2 + A_2\zeta - A_3 = 0 \tag{2.42}$$

where ζ are the eigenvalues of $\mathbf{A}$, $\mathbf{I}_3 \in \mathbb{R}^{3\times3}$ is the identity matrix; and $A_i \in \mathbb{R}$ $(i = 1, 2, 3)$ are defined as

$$A_1 = \mathrm{tr}(\mathbf{A}) = \zeta_1 + \zeta_2 + \zeta_3 \tag{2.43}$$

$$A_2 = \frac{1}{2}\left[(\mathrm{tr}(\mathbf{A}))^2 - \mathrm{tr}(\mathbf{A}^2)\right] = \zeta_1\zeta_2 + \zeta_2\zeta_3 + \zeta_3\zeta_1 \tag{2.44}$$

$$A_3 = \det(\mathbf{A}) = \zeta_1\zeta_2\zeta_3 \tag{2.45}$$

Remark 2.2.5 (Eq. (2.38))

1. *The spectral roots* $(\rho_\infty^{\min}, \rho_\infty^{\max}, \rho_\infty^{\mathrm{s}})$ *appearing in Algorithm 2.2.1 are defined as the absolute values of the eigenvalues of the amplification matrix* $\mathbf{A}$*: The* ***spectral radius*** *or higher* ***principal root*** *is defined as*

$$\rho_\infty^{\max} := \max\left(\left|\lim_{\Omega\to\infty} \zeta_1(\mathbf{A}(\Omega))\right|, \left|\lim_{\Omega\to\infty} \zeta_2(\mathbf{A}(\Omega))\right|, \left|\lim_{\Omega\to\infty} \zeta_3(\mathbf{A}(\Omega))\right|\right) \tag{2.46}$$

and the ***spurious root*** *is defined as*

$$\rho_\infty^{\mathrm{s}} := \min\left(\left|\lim_{\Omega\to\infty} \zeta_1(\mathbf{A}(\Omega))\right|, \left|\lim_{\Omega\to\infty} \zeta_2(\mathbf{A}(\Omega))\right|, \left|\lim_{\Omega\to\infty} \zeta_3(\mathbf{A}(\Omega))\right|\right) \tag{2.47}$$

The intermediate root is defined as the lower principal root $\rho_\infty^{\min}$.

GS4-2 Family of Algorithms in the Linear Three-step (Three-step LMS) Form

Employing the Cayley-Hamilton theorem, Eq. (2.42) yields

$$\mathbf{A}^3 - A_1\mathbf{A}^2 + A_2\mathbf{A} - A_3\mathbf{I}_3 = \mathbf{0} \tag{2.48}$$

Using Eq. (2.38) recursively, we obtain

$$\begin{aligned} \mathbf{y}^{n+1} &= \mathbf{A}\mathbf{y}^n + \mathbf{L}(t_{n+W_1}) \\ &= \mathbf{A}^2\mathbf{y}^{n-1} + \mathbf{A}\mathbf{L}(t_{n-1+W_1}) + \mathbf{L}(t_{n+W_1}) \\ &= \mathbf{A}^3\mathbf{y}^{n-2} + \mathbf{A}^2\mathbf{L}(t_{n-2+W_1}) + \mathbf{A}\mathbf{L}(t_{n-1+W_1}) + \mathbf{L}(t_{n+W_1}) \end{aligned} \tag{2.49}$$

Substituting Eq. (2.48) into Eq. (2.49) yields

$$\begin{aligned} \mathbf{y}^{n+1} &= \left[A_1\mathbf{A}^2 - A_2\mathbf{A} + A_3\mathbf{I}_3\right]\mathbf{y}^{n-2} + \mathbf{A}^2\mathbf{L}(t_{n-2+W_1}) + \mathbf{A}\mathbf{L}(t_{n-1+W_1}) + \mathbf{L}(t_{n+W_1}) \\ &= A_1\mathbf{A}^2\mathbf{y}^{n-2} - A_2\mathbf{A}\mathbf{y}^{n-2} + A_3\mathbf{y}^{n-2} + \mathbf{A}^2\mathbf{L}(t_{n-2+W_1}) + \mathbf{A}\mathbf{L}(t_{n-1+W_1}) + \mathbf{L}(t_{n+W_1}) \\ &= A_1\left[\mathbf{y}^n - \mathbf{A}\mathbf{L}(t_{n-2+W_1})\right] - A_2\left[\mathbf{y}^{n-1} - \mathbf{L}(t_{n-2+W_1})\right] + A_3\mathbf{y}^{n-2} \\ &\quad + \mathbf{A}^2\mathbf{L}(t_{n-2+W_1}) + \mathbf{A}\mathbf{L}(t_{n-1+W_1}) + \mathbf{L}(t_{n+W_1}) \end{aligned} \tag{2.50}$$

That is, the difference equation for the GS4-2 family of algorithms is obtained as:

$$\boxed{\begin{aligned} &\mathbf{y}^{n+1} - A_1\mathbf{y}^n + A_2\mathbf{y}^{n-1} - A_3\mathbf{y}^{n-2} \\ =& \left[\mathbf{A}^2 - A_1\mathbf{A} + A_2\mathbf{I}_3\right]\mathbf{L}(t_{n-2+W_1}) + [\mathbf{A} - A_1\mathbf{I}]\,\mathbf{L}(t_{n-1+W_1}) + \mathbf{L}(t_{n+W_1}) \end{aligned}} \tag{2.51}$$

This is the ***linear three-step (three-step LMS) form*** of Algorithm 2.2.1. For the homogeneous case, i.e., $\mathbf{y}_{n+1} = \mathbf{A}\mathbf{y}_n$ ($\mathbf{L} = \mathbf{0}\ \forall t \in \mathbb{I}$), Eq. (2.51) reduces to

$$\boxed{\mathbf{y}^{n+1} - A_1\mathbf{y}^n + A_2\mathbf{y}^{n-1} - A_3\mathbf{y}^{n-2} = \mathbf{0}} \tag{2.52}$$

Since $\mathbf{y}^n = [x^n, \Delta t x_v^n, \Delta t^2 x_a^n]^T$, the x-difference equation is given as

$$x^{n+1} - A_1 x^n + A_2 x^{n-1} - A_3 x^{n-2} = 0 \tag{2.53}$$

Linear Multistep (LMS) Methods for Second-order ODEs: Consider the second-order linear ODEs, Eqn. (2.3), and write it as

$$\ddot{\mathbf{q}}(t) = \mathbf{G}_{\mathrm{C}}\dot{\mathbf{q}}(t) + \mathbf{G}_{\mathrm{K}}\mathbf{q}(t) + \mathbf{G}_{\mathrm{f}}(t) \tag{2.54}$$

where $\mathbf{G}_{\mathrm{C}} := -\mathbf{M}^{-1}\mathbf{C} \in \mathbb{R}^{N_2\times N_2}$, $\mathbf{G}_{\mathrm{K}} := -\mathbf{M}^{-1}\mathbf{K} \in \mathbb{R}^{N_2\times N_2}$, and $\mathbf{G}_{\mathrm{f}}(t) := \mathbf{M}^{-1}\mathbf{f}(t) \in \mathbb{R}^{N_2}$. The ***linear k-step (k-step LMS) methods*** for Eq. (2.54), are given as follows:

$$\sum_{i=0}^{k}\left[\alpha_i\mathbf{q}^{n+1-i} + \Delta t\beta_i\mathbf{G}_{\mathrm{C}}\mathbf{q}^{n+1-i} + \Delta t^2\gamma_i\left(\mathbf{G}_{\mathrm{f}}(t_{n+1-i}) + \mathbf{G}_{\mathrm{K}}\mathbf{q}^{n+1-i}\right)\right] = \mathbf{0} \tag{2.55}$$

The k-step LMS methods are explicit if $\beta_0 = \gamma_0 = 0$. Employing the modal decomposition for the homogeneous case leads to

$$\sum_{i=0}^{k}\left[\alpha_i - 2\xi\Omega\beta_i - \Omega^2\gamma_i\right]x^{n+1-i} = \mathbf{0} \tag{2.56}$$

Therefore, Eq. (2.53) can be directly compared with the linear three-step methods, i.e., $k = 3$ in Eq. (2.56), and we get

$$\begin{aligned} A_1 &= -\frac{\alpha_1 - 2\xi\Omega\beta_1 - \Omega^2\gamma_1}{\alpha_0 - 2\xi\Omega\beta_0 - \Omega^2\gamma_0} \\ A_2 &= \frac{\alpha_2 - 2\xi\Omega\beta_2 - \Omega^2\gamma_2}{\alpha_0 - 2\xi\Omega\beta_0 - \Omega^2\gamma_0} \\ A_3 &= -\frac{\alpha_3 - 2\xi\Omega\beta_3 - \Omega^2\gamma_3}{\alpha_0 - 2\xi\Omega\beta_0 - \Omega^2\gamma_0} \end{aligned} \tag{2.57}$$

2.2.4 Explicit GS4-2 Family of Algorithms

Introduce new three parameters η_1, η_2, and η_3 that take either 0 or 1 in such a way that

$$W_3\Lambda_3 \to W_3\Lambda_3\eta_1, \quad W_2\Lambda_5 \to W_2\Lambda_5\eta_2, \quad \text{and} \quad \lambda_3 \to \lambda_3\eta_3 \tag{2.58}$$

in Algorithm 2.2.1. Obviously, the modified Algorithm 2.2.1 with η_i (for $i = 1, 2, 3$) recovers the original implicit GS4-2 family of algorithms whenever we select $\eta_1 = \eta_2 = \eta_3 = 1$; however, it becomes fully explicit for $\eta_1 = \eta_2 = 0$. Selecting $\eta_1 = 0$ but $\eta_2 = 1$ results in the so-called explicit GS4-2 family of algorithms with implicit treatment for velocity terms. Parameter η_3 influences some basic features of the algorithm, such as stability, numerical dissipation, and so on; see [1, 5] for details. For the explicit GS4-2 family of algorithms, we usually take $\eta_3 = 0$ since the explicit algorithms with $\eta_3 = 1$ always inherit numerical dissipation; in contrast to the case of the explicit algorithms with $\eta_3 = 0$. For $\hat{\eta} := \eta_1 = \eta_2 = \eta_3 = 0$,

$$\begin{aligned} (\rho_\infty^{\min}, \rho_\infty^{\max}, 0), \quad (1, 1, \rho_\infty^{s}), \quad \text{and;} \quad (1, 1, 1) \quad &\text{in the U0-based family} \\ (\rho_\infty^{\min}, 1, 1) \ \text{ and } \ (1, \rho_\infty^{\max}, 1) \quad &\text{in the V0-based family} \end{aligned} \tag{2.59}$$

are the numerically nondissipative explicit schemes. It is noteworthy that η_i (for $i = 1, 2, 3$) do not influence the order of time accuracy of the kinematic unknowns of the algorithm. The explicit schemes that can be generated from Algorithm 2.2.1 with the additional parameters η_i no longer possess the zeroth-order overshoot behaviors in the $\mathbf{q}^n$ and $\mathbf{v}^n$, i.e., U0 and V0 features, respectively.

2.2.5 Time Level Analysis

Both the U0 and V0 based-family of algorithms shown above have been particularly designed to be of second-order time accuracy in the displacement, velocity, and external load vectors; however, we get only first-order accuracy in the acceleration vector if we assume $\mathbf{a}_n \approx \ddot{\mathbf{q}}(t_n)$ and $\mathbf{a}_{n+1} \approx \ddot{\mathbf{q}}(t_{n+1})$. In order to guarantee the second-order time accuracy in all the variables, one must be aware of the correct time level of approximations for $\mathbf{q}$, $\dot{\mathbf{q}}$, and $\ddot{\mathbf{q}}$ as

$$\begin{aligned} \mathbf{q}_n \approx \mathbf{q}(t_n) \ \text{ and } \ \mathbf{q}_{n+1} \approx \mathbf{q}(t_{n+1}) \\ \mathbf{v}_n \approx \dot{\mathbf{q}}(t_n) \ \text{ and } \ \mathbf{v}_{n+1} \approx \dot{\mathbf{q}}(t_{n+1}) \\ \mathbf{a}_n \approx \ddot{\mathbf{q}}(t_{n-\phi}) \ \text{ and } \ \mathbf{a}_{n+1} \approx \ddot{\mathbf{q}}(t_{n+1-\phi}) \end{aligned} \tag{2.60}$$

where $\phi := W_1(\Lambda_6 - 1) \in \mathbb{R}$.

Theorem 2.2.1 (Time Level of Acceleration)

In the U0 and V0 based-family of algorithms, the second-order time accuracy in $\ddot{\mathbf{q}}$, i.e.,

$$\mathbf{a}_{n+1} - \ddot{\mathbf{q}}(t_{n+1-\phi}) = \mathcal{O}(\Delta t^2) \ \textit{ with } \ \phi := W_1(\Lambda_6 - 1) \tag{2.61}$$

is obtained for a solution satisfying

$$\begin{aligned} \mathbf{q}_n - \mathbf{q}(t_n) = \mathcal{O}(\Delta t^2) \ \textit{ and } \ \mathbf{q}_{n+1} - \mathbf{q}(t_{n+1}) = \mathcal{O}(\Delta t^2) \\ \mathbf{v}_n - \dot{\mathbf{q}}(t_n) = \mathcal{O}(\Delta t^2) \ \textit{ and } \ \mathbf{v}_{n+1} - \dot{\mathbf{q}}(t_{n+1}) = \mathcal{O}(\Delta t^2) \end{aligned} \tag{2.62}$$

if $\mathbf{a}_n - \ddot{\mathbf{q}}(t_{n-\phi}) = \mathcal{O}(\Delta t^2)$ is guaranteed.

Proof. In this proof, we only consider the V0 family-based algorithms since the proof for the U0 family-based algorithms is more straightforward, and we get the same result as stated in the theorem above. The V0 family-based algorithms can cast into

$$\mathbf{M}\tilde{\mathbf{a}} + \mathbf{C}\tilde{\mathbf{v}} + \mathbf{K}\tilde{\mathbf{q}} = \tilde{\mathbf{f}} \tag{2.63}$$

where the algorithmic $\ddot{\mathbf{q}}$, $\dot{\mathbf{q}}$, $\mathbf{q}$, and $\mathbf{f}$ are given by

$$\tilde{\mathbf{a}} = (1 - W_1\Lambda_6)\mathbf{a}_n + W_1\Lambda_6\mathbf{a}_{n+1} \tag{2.64}$$

$$\tilde{\mathbf{v}} = \mathbf{v}_n + W_2(\mathbf{v}_{n+1} - \mathbf{v}_n) + \Delta t(W_1 - W_2)\mathbf{a}_n \tag{2.65}$$

$$\tilde{\mathbf{q}} = \mathbf{q}_n + W_2(\mathbf{q}_{n+1} - \mathbf{q}_n) + \Delta t(W_1 - W_2)\mathbf{v}_n \tag{2.66}$$

$$\tilde{\mathbf{f}} = (1 - W_1)\mathbf{f}_n + W_1\mathbf{f}_{n+1} \tag{2.67}$$

Using Equation (2.62), we get

$$\begin{aligned}\tilde{\mathbf{v}} &= \dot{\mathbf{q}}(t_n) + W_2[\dot{\mathbf{q}}(t_{n+1}) - \dot{\mathbf{q}}(t_n)] + \Delta t(W_1 - W_2)\ddot{\mathbf{q}}(t_{n-\phi}) + \mathcal{O}(\Delta t^p) \\ &= \dot{\mathbf{q}}(t_n) + \Delta t W_1\ddot{\mathbf{q}}(t_n) + \mathcal{O}(\Delta t^p)\end{aligned} \tag{2.68}$$

where $p = 2$ and $p = 1$ for $s \geq 2$ and $s = 1$, respectively, in $\mathbf{a}_n - \ddot{\mathbf{q}}(t_{n-\phi}) = \mathcal{O}(\Delta t^s)$. Similarly,

$$\begin{aligned}\tilde{\mathbf{q}} &= \mathbf{q}(t_n) + W_2[\mathbf{q}(t_{n+1}) - \mathbf{q}(t_n)] + \Delta t(W_1 - W_2)\dot{\mathbf{q}}(t_{n-\phi}) + \mathcal{O}(\Delta t^2) \\ &= \mathbf{q}(t_n) + \Delta t W_1\dot{\mathbf{q}}(t_n) + \mathcal{O}(\Delta t^2)\end{aligned} \tag{2.69}$$

and

$$\tilde{\mathbf{f}} = \mathbf{f}(t_n) + W_1[\mathbf{f}(t_{n+1}) - \mathbf{f}(t_n)] + \mathcal{O}(\Delta t^2) = \mathbf{f}(t_n) + \Delta t W_1\dot{\mathbf{f}}(t_n) + \mathcal{O}(\Delta t^2) \tag{2.70}$$

Since the Taylor series expansions about time $t = t_n$ yields

$$\begin{aligned}\ddot{\mathbf{q}}(t_{n+1-\phi}) &= \ddot{\mathbf{q}}(t_n) + (1 - \phi)\Delta t\dddot{\mathbf{q}}(t_n) + \mathcal{O}(\Delta t^2) \\ \ddot{\mathbf{q}}(t_{n-\phi}) &= \ddot{\mathbf{q}}(t_n) - \phi\Delta t\dddot{\mathbf{q}}(t_n) + \mathcal{O}(\Delta t^2)\end{aligned} \tag{2.71}$$

we get

$$(1 - W_1\Lambda_6)\ddot{\mathbf{q}}(t_{n-\phi}) + W_1\Lambda_6\ddot{\mathbf{q}}(t_{n+1-\phi}) = \ddot{\mathbf{q}}(t_n) + \Delta t(W_1\Lambda_6 - \phi)\dddot{\mathbf{q}}(t_n) + O(\Delta t^2) \quad (2.72)$$

From Equations (2.63)-(2.72) with $\ddot{\mathbf{q}}(t) = -\mathbf{M}^{-1}[\mathbf{C}\dot{\mathbf{q}}(t) + \mathbf{K}\mathbf{q}(t) - \mathbf{f}(t)]$,

$$\begin{aligned}&(1 - W_1\Lambda_6)[\mathbf{a}_n - \ddot{\mathbf{q}}(t_{n-\phi})] + W_1\Lambda_6[\mathbf{a}_{n+1} - \ddot{\mathbf{q}}(t_{n+1-\phi})]\\ =&\Delta t(W_1 - W_1\Lambda_6 + \phi)\dddot{\mathbf{q}}(t_n) + O(\Delta t^p)\end{aligned} \quad (2.73)$$

Hence, $\mathbf{a}_{n+1} - \ddot{\mathbf{q}}(t_{n+1-\phi}) = O(\Delta t^2)$ is obtained when $\mathbf{a}_n - \ddot{\mathbf{q}}(t_{n-\phi}) = O(\Delta t^s)$ with $s \geq 2$ for $\phi = W_1(\Lambda_6 - 1)$. ∎

Remark 2.2.6 (Theorem 2.2.1)

1. *Choosing the initial value of* $\ddot{\mathbf{q}}$ *as* $\mathbf{a}_0 = \ddot{\mathbf{q}}(t_0) = -\mathbf{M}^{-1}[\mathbf{C}\dot{\mathbf{q}}(t_0) + \mathbf{K}\mathbf{q}(t_0) - \mathbf{f}(t_0)]$, *actually still gives the second-order accuracy in* $\ddot{\mathbf{q}}$.

2. *It is important to note that* $\mathbf{a}_n \approx \ddot{\mathbf{q}}(t_{n-\phi})$ *and* $\mathbf{a}_{n+1} \approx \ddot{\mathbf{q}}(t_{n+1-\phi})$ *are not the approximations of* $\ddot{\mathbf{q}}$ *at time* $t = t_n$ *and* $t = t_{n+1}$*, respectively. Therefore, to plot the* ***true acceleration*** *time history, one must use*

$$\ddot{\mathbf{q}}(t_1) \approx \frac{1}{1-\phi}\mathbf{a}_1 - \frac{\phi}{1-\phi}\mathbf{a}_0 =: \hat{\mathbf{a}}_1 \quad (2.74)$$

at the first time step and

$$\ddot{\mathbf{q}}(t_{n+1}) \approx (1+\phi)\mathbf{a}_{n+1} - \phi\mathbf{a}_n =: \hat{\mathbf{a}}_{n+1} \quad (2.75)$$

for $n \in \{1, 2, \cdots, n_t - 1\}$. *This is illustrated in Fig. 2.1.*

3. *The spectral condition V0*$\{1.0, 1.0, \rho_\infty^s\}$ *with* ρ_∞^s *in the V0 family-based algorithms leads to*

$$\mathbf{M}\tilde{\mathbf{a}} + \mathbf{C}\left[\mathbf{v}_n + \frac{\Delta t}{2}\tilde{\mathbf{a}}\right] + \mathbf{K}\left[\mathbf{q}_n + \frac{\Delta t}{2}\mathbf{v}_n + \frac{\Delta t^2}{4}\tilde{\mathbf{a}}\right] = \tilde{\mathbf{f}} \quad (2.76)$$

with

$$\begin{aligned}\mathbf{q}_{n+1} &= \mathbf{q}_n + \Delta t\mathbf{v}_n + \frac{\Delta t}{2}\tilde{\mathbf{a}} \\ \mathbf{v}_{n+1} &= \mathbf{v}_n + \Delta t\tilde{\mathbf{a}}\end{aligned} \tag{2.77}$$

where

$$\tilde{\mathbf{a}} = \mathbf{a}_n + \frac{1}{1+\rho_\infty^{\mathrm{s}}}(\mathbf{a}_{n+1} - \mathbf{a}_n) \tag{2.78}$$

Note that we have

$$W_1 = \frac{1}{2} \quad and \quad \phi = \frac{1-\rho_\infty^{\mathrm{s}}}{2(1+\rho_\infty^{\mathrm{s}})} \tag{2.79}$$

for V0:$\{(\rho_\infty^{\min}, \rho_\infty^{\max}, \rho_\infty^{\mathrm{s}}) = (1.0, 1.0, \rho_\infty^{\mathrm{s}})\}$ *with* ρ_∞^{s}. *We call U0/V0:*$\{(\rho_\infty^{\min}, \rho_\infty^{\max}, \rho_\infty^{\mathrm{s}}) = (1.0, 1.0, 1.0)\}$, *i.e.*, $\mathbf{a}_{n+1} \approx \ddot{\mathbf{q}}(t_{n+1})$, *and* *V0:*$\{(\rho_\infty^{\min}, \rho_\infty^{\max}, \rho_\infty^{\mathrm{s}}) = (1.0, 1.0, 0.0)\}$, *i.e.*, $\mathbf{a}_{n+1} \approx \ddot{\mathbf{q}}(t_{n+1/2})$, *the* ***midpoint rule with the endpoint acceleration (MRP-EPA)****, which is the classical midpoint rule, and the new* ***midpoint rule with the midpoint acceleration (MRP-MPA)****, respectively. Notice that the difference between MPR-EPA and MPR-MPA is*

$$\frac{\mathbf{v}_{n+1} - \mathbf{v}_n}{\Delta t} = \tilde{\mathbf{a}} = \begin{cases} \mathbf{a}_{n+1/2} \approx \frac{1}{2}[\ddot{\mathbf{q}}(t_{n+1}) + \ddot{\mathbf{q}}(t_n)] & for \ \ MPR\text{-}EPA \\ \mathbf{a}_{n+1} \approx \ddot{\mathbf{q}}(t_{n+1/2}) & for \ \ MPR\text{-}MPA \end{cases} \tag{2.80}$$

Note that the information regarding the acceleration at the previous time step is not required to evaluate the current acceleration, and consequently, the new MPR-MPA provides a robust computational algorithm for general dynamics applications. By eliminating the acceleration, Eq. (2.76)*- Eq.*(2.78) *can be reduced to the classical symplectic midpoint rule which takes the form*

$$\begin{aligned}\mathbf{M}\frac{\mathbf{v}_{n+1} - \mathbf{v}_n}{\Delta t} + \mathbf{C}\frac{\mathbf{v}_{n+1} + \mathbf{v}_n}{2} + \mathbf{K}\frac{\mathbf{q}_{n+1} + \mathbf{q}_n}{2} &= \tilde{\mathbf{f}} \\ \frac{\mathbf{v}_{n+1} + \mathbf{v}_n}{2} &= \frac{\mathbf{q}_{n+1} - \mathbf{q}_n}{\Delta t}\end{aligned} \tag{2.81}$$

where $\tilde{\mathbf{f}} = \mathbf{f}(t_{n+1/2})$ *can be used for the algorithmic time-dependent external force instead of* $\tilde{\mathbf{f}} = (\mathbf{f}_n + \mathbf{f})/2$ *since* $\mathbf{f}(t_{n+\alpha}) - \mathbf{f}_{n+\alpha} = O(\Delta t^2)$ *for* $\alpha \in [0, 1]$.

4. *In the derivation of the GSSSS family of algorithms, the conditions of the second-order time accuracy were imposed following the* algorithms by design *concept; see [6]. From the truncation error analysis, the necessary and sufficient conditions of second-order time accuracy for the displacement and velocity are given as:*

$$\begin{aligned} &\lambda_1 = \lambda_4 = 1, \\ &\lambda_2 = \tfrac{1}{2}, \quad \lambda_5 = \tfrac{1}{2} + W_1(\Lambda_6 - \Lambda_4) \end{aligned} \tag{2.82}$$

and $\Lambda_1 = \Lambda_4$ *for a homogeneous case (*$\mathbf{f} = \mathbf{0}$*), and* $\Lambda_1 = \Lambda_4 = 1$ *for a non-homogeneous case (*$\mathbf{f} \neq \mathbf{0}$*). Notice that the above conditions (for the non-homogeneous case) are* a priori *for the U0 and V0 family-based algorithms. In addition to the conditions, Eq.* (2.82)*, we must introduce* $\phi := W_1(\Lambda_6 - 1)$ *to guarantee the second-order time accuracy not only of the displacement and velocity, but also of the acceleration. Note that we can never obtain second order-time accuracy of the acceleration if we break the conditions, Eq.* (2.82)*, and the orders of accuracy of the displacement and velocity are always dependent upon each other in this algorithmic framework. However, the second order-time accuracy of the acceleration is not the necessary condition for the second order-time accuracy of the displacement and velocity.*

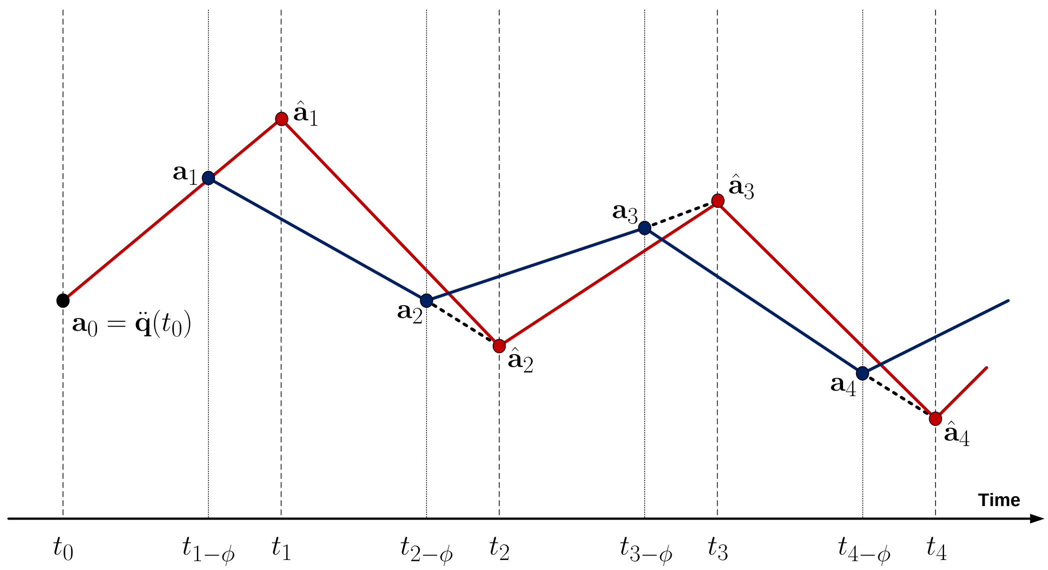


Figure 2.1: Illustration of the True Acceleration History (red line)

Theorem 2.2.2 (Time Level Consistency)

In order to guarantee the second-order time accuracy in all time-dependent variables, such as $\mathbf{q}(t)$, $\dot{\mathbf{q}}(t)$, $\ddot{\mathbf{q}}(t)$, *and* $\mathbf{f}(t)$, *in the discrete equation of motion, they must be evaluated at the same time level* $t = t^* = t_{n+W_1}$ *as*

$$\mathbf{0} = \mathbf{M}\tilde{\mathbf{a}} + \mathbf{C}\tilde{\mathbf{v}} + \mathbf{K}\tilde{\mathbf{q}} - \tilde{\mathbf{f}} + O(\Delta t^2) = \mathbf{M}\ddot{\mathbf{q}}(t^*) + \mathbf{C}\dot{\mathbf{q}}(t^*) + \mathbf{K}\mathbf{q}(t^*) - \mathbf{f}(t^*) \tag{2.83}$$

Proof. By using the Taylor series expansions about time $t = t_n$, we get

$$\begin{aligned}\tilde{\mathbf{a}} &= (1 - W_1\Lambda_6)\ddot{\mathbf{q}}(t_{n-\phi}) + W_1\Lambda_6\ddot{\mathbf{q}}(t_{n+1-\phi}) + O(\Delta t^2)\\ &= \ddot{\mathbf{q}}(t_n) + \Delta t W_1 \dddot{\mathbf{q}}(t_n) + O(\Delta t^2)\\ &= \ddot{\mathbf{q}}(t_{n+W_1})\end{aligned} \tag{2.84}$$

when $\mathbf{a}_n - \ddot{\mathbf{q}}(t_{n-\phi}) = \mathcal{O}(\Delta t^2)$. Similarly, we get

$$\tilde{\mathbf{v}} = \dot{\mathbf{q}}(t_n) + \Delta t W_1 \ddot{\mathbf{q}}(t_n) + \mathcal{O}(\Delta t^2) = \dot{\mathbf{q}}(t_{n+W_1}) \tag{2.85}$$

$$\tilde{\mathbf{q}} = \mathbf{q}(t_n) + \Delta t W_1 \dot{\mathbf{q}}(t_n) + \mathcal{O}(\Delta t^2) = \mathbf{q}(t_{n+W_1}) \tag{2.86}$$

$$\tilde{\mathbf{f}} = \mathbf{f}(t_n) + \Delta t W_1 \dot{\mathbf{f}}(t_n) + \mathcal{O}(\Delta t^2) = \mathbf{f}(t_{n+W_1}) \tag{2.87}$$

Therefore, the discrete equation of motion is evaluated at the time level $t = t_{n+W_1}$ when the second-order time accuracy in $\mathbf{q}$, $\dot{\mathbf{q}}$, $\ddot{\mathbf{q}}$, and $\mathbf{f}$ are guaranteed. The time level $t^* = t_{n+W_1}$ is called the ***algorithmic time level***. If the algorithmic balance equation is satisfied at the time level $t^* = t_{n+W_1}$ with the error $\mathcal{O}(\Delta t^2)$, the acceleration, velocity, and configuration are of second-order time accuracy. The algorithmic time level consistency at time $t = t_{n+W_1}$ in the balance equation is illustrated in Fig. 2.2. ∎

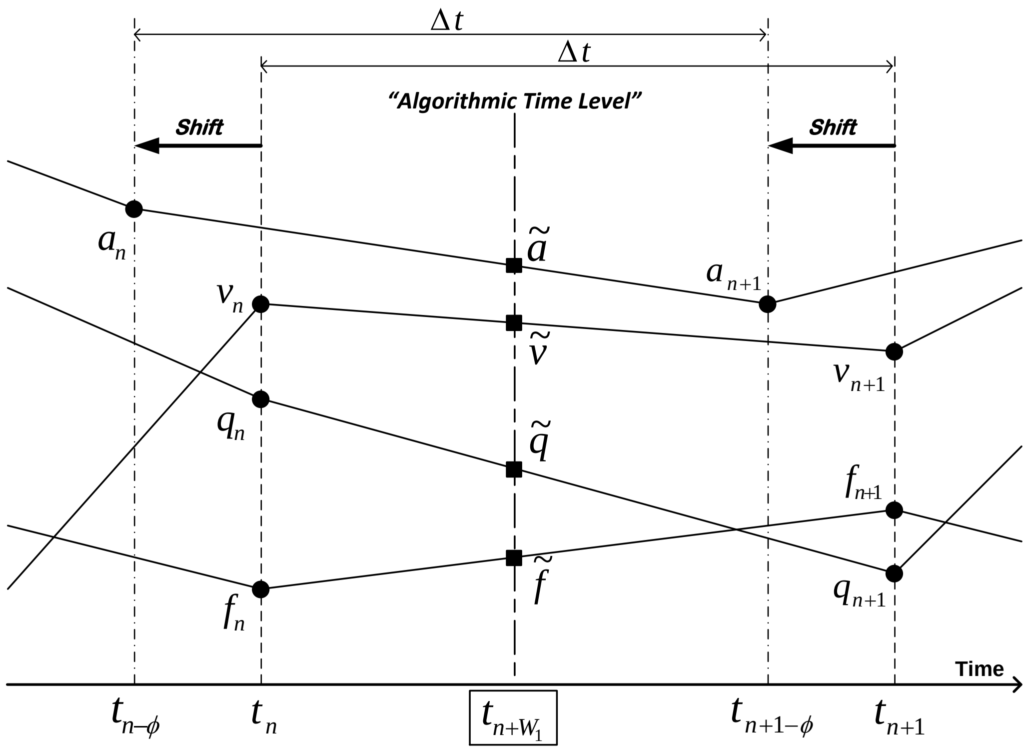


Figure 2.2: Illustration of the Algorithmic Time Level

Remark 2.2.7 (Theorem 2.2.2)

1. ***Extension to nonlinear systems:*** *The time level consistency theorem plays a fundamental role when applying the GSSSS family of algorithms to nonlinear dynamical systems. The basic strategy is that we develop time integration schemes which satisfy the algorithmic time level consistency theorem at time level of* t_{n+W_1} *in order to guarantee the second order-time accuracy in all variables that appear in discrete balance equations. See [7, 8, 9] for detailed discussions.*

2. ***First order systems:*** *The time level consistency theorem still holds for first-order systems generally represented as* $\dot{\mathbf{q}} = \mathbf{F}(\mathbf{q}, t)\ \forall t \in \mathbb{I}$ *with given initial condition* $\mathbf{q}_0 = \mathbf{q}(t_0)$*. That is, we discretize the balance equation with the* algorithms by design *concept such that the time level consistency at time* $t = t_{n+W_1}$ *is guaranteed as follows:*

$$\mathbf{0} = \tilde{\mathbf{v}} - \mathbf{F}(\tilde{\mathbf{q}}, t_{n+W_1}) + O(\Delta t^2) = \dot{\mathbf{q}}(t_{n+W_1}) - \mathbf{F}(\mathbf{q}(t_{n+W_1}), t_{n+W_1}) \tag{2.88}$$

where $\tilde{\mathbf{q}}$ *and* $\tilde{\mathbf{v}} = \mathbf{v}_{n+W_1\Lambda_6} := (1 - W_1\Lambda_6)\mathbf{v}_n + W_1\Lambda_6\mathbf{v}_{n+1}$ *in the above equation denote the algorithmic* $\mathbf{q}$ *and* $\mathbf{v}$ *for the first-order system. The time level of* $\mathbf{v}_n$ *must satisfy* $\mathbf{v}_n \approx \dot{\mathbf{q}}(t_{n-\phi})$ *for* $n \in \{1, 2, \cdots, \bar{n}\}$ *with* $\phi = W_1(\Lambda_6 - 1)$*. The resulting algorithm is known as the GSSSS-1 (or GS4-1) family of algorithms; see [10] for the detailed derivations and applications to linear transient first-order systems.*

2.2.6 Relations to Some Commonly-used Algorithms

Newmark Family of Algorithms [11]

Perhaps, one of the most popular algorithms, especially in structural dynamics, may be the Newmark family of algorithms. The basic structure of this family reads:

$$\mathbf{a}^{n+1} = \mathbf{g}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}, t_{n+1}) \tag{2.89a}$$

with the updates are given as:

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \mathbf{v}^n\Delta t + \mathbf{a}^n\frac{\Delta t^2}{2} + \beta\Delta\mathbf{a}^n\Delta t^2 \tag{2.89b}$$

$$\mathbf{v}^{n+1} = \mathbf{v}^n + \mathbf{a}^n\Delta t + \gamma\Delta\mathbf{a}^n\Delta t \tag{2.89c}$$

$$\mathbf{a}^{n+1} = \mathbf{a}^n + \Delta\mathbf{a}^n \tag{2.89d}$$

As can be seen, the two parameters β and γ defines the schemes within the Newmark family. Schemes are second-order time accurate if and only if $\gamma = 1/2$. Comparing Eq. (2.89) with the GS4-2 family of algorithms, Algorithm 2.2.1, we readily obtain the following relations:

$$\begin{aligned}
&W_1 = W_2 = W_3 = 1 \\
&\beta = \lambda_3 = \Lambda_3 \\
&\gamma = \lambda_5 = \Lambda_5 \\
&\tfrac{1}{2} = \Lambda_2 (= \lambda_2)
\end{aligned} \tag{2.90}$$

Three Parameter Optimal Method [12, 13]

Since numerical damping could not be introduced with most classic second-order accurate time integration schemes such as implicit Newmark method (average acceleration method), implicit velocity-based method (MPR-MPA method), and so on, without reducing the order of accuracy, there have been proposed several numerically dissipative schemes such as the three parameter optimal method. These schemes are not only unconditionally stable (in linear systems) and second order-time accurate, but also numerically dissipative, i.e., controllable numerical damping can be introduced. The three parameter optimal method includes some popular schemes such as the HHT-α method [14] and WBZ method [15], and the Generalized-α method [16] is identical to it. Point of fact is that these schemes are also constituent elements of the GS4-2 family of algorithms.

Here, we show a direct comparison between the GS4-2 family of algorithms and the three parameter optimal method. The three parameter optimal method applied for the nonlinear ODEs may be cast in the following form:

$$\tilde{\mathbf{a}}^n = \mathbf{g}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n, t_{n+1-\alpha_\mathrm{f}}) \tag{2.91a}$$

where $t_{n+1-\alpha_\mathrm{f}} := (1-\alpha_\mathrm{f})t_{n+1} + \alpha_\mathrm{f} t_n$ and

$$\tilde{\mathbf{q}}^n = \mathbf{q}_{n+1-\alpha_\mathrm{f}} := (1-\alpha_\mathrm{f})\mathbf{q}^{n+1} + \alpha_\mathrm{f}\mathbf{q}^n \tag{2.91b}$$

$$\tilde{\mathbf{v}}^n = \mathbf{v}_{n+1-\alpha_\mathrm{f}} := (1-\alpha_\mathrm{f})\mathbf{v}^{n+1} + \alpha_\mathrm{f}\mathbf{v}^n \tag{2.91c}$$

$$\tilde{\mathbf{a}}^n = \mathbf{a}_{n+1-\alpha_\mathrm{m}} := (1-\alpha_\mathrm{m})\mathbf{a}^{n+1} + \alpha_\mathrm{m}\mathbf{a}^n \tag{2.91d}$$

The updates are given as:

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \mathbf{v}^n\Delta t + \mathbf{a}^n\frac{\Delta t^2}{2} + \beta\Delta\mathbf{a}^n\Delta t^2 \tag{2.91e}$$

$$\mathbf{v}^{n+1} = \mathbf{v}^n + \mathbf{a}^n\Delta t + \gamma\Delta\mathbf{a}^n\Delta t \tag{2.91f}$$

$$\mathbf{a}^{n+1} = \mathbf{a}^n + \Delta\mathbf{a}^n \tag{2.91g}$$

The algorithmic parameters $(\alpha_\mathrm{m}, \alpha_\mathrm{f}, \beta, \gamma)$ must satisfy

$$\alpha_\mathrm{m} \leq \alpha_\mathrm{f} \leq \tfrac{1}{2}, \quad 0 \leq \alpha_\mathrm{f}, \quad 2\beta \geq \gamma = \tfrac{1}{2} - \alpha, \quad \alpha := \alpha_\mathrm{m} - \alpha_\mathrm{f} \tag{2.92}$$

so as to guarantee the unconditionally stable (in linear systems) and second order-time accurate features of the algorithm.

If we define the algorithmic parameters as

$$\begin{gathered}\alpha_\mathrm{m} = \frac{2\rho_\infty - 1}{1+\rho_\infty}, \quad \alpha_\mathrm{f} = \frac{\rho_\infty}{1+\rho_\infty}, \\ \beta = \frac{(1-\alpha)^2}{4}, \quad \gamma = \frac{1}{2} - \alpha, \quad \alpha := \alpha_\mathrm{m} - \alpha_\mathrm{f}\end{gathered} \tag{2.93}$$

in terms of the spectral radius at infinity, $\rho_\infty \in [0,1] \subset \mathbb{R}$, such that the conditions in Eq. (2.92) are met, the resulting algorithm is commonly known as the Generalized-α method [16] (note that the exact same scheme appeared much earlier in [12, 13]).

Comparing Eqs. (2.91b)-(2.91d) with (2.10) , we readily get the following relations:

$$1 - \alpha_{\mathrm{m}} = W_1 \Lambda_6 \tag{2.94}$$

$$1 - \alpha_{\mathrm{f}} = W_1 = 2W_2\Lambda_2 = \frac{W_2\Lambda_5}{\lambda_5} = \frac{W_3\Lambda_3}{\lambda_3} \tag{2.95}$$

(here, we used the relation $\lambda_1 = \Lambda_1 = \lambda_4 = \Lambda_4 = 1$). On the other hand, the comparisons of the updates readily lead to

$$\beta = \lambda_3, \quad \gamma = \lambda_5 \tag{2.96}$$

Hence, the following conditions for recovering the three parameter optimal method are obtained:

$$\boxed{\begin{array}{ll} \rho_\infty := \rho_\infty^{\mathrm{min}} = \rho_\infty^{\mathrm{max}} = \rho_\infty^{\mathrm{s}} \in [0,1] & \\ \quad \beta = \lambda_3 = \Lambda_3 & \\ \quad \gamma = \lambda_5 = \Lambda_5 & \textbf{in the U0 family} \\ \quad \frac{1}{2} = \Lambda_2 (= \lambda_2) & \end{array}} \Longrightarrow \boxed{\textbf{3 Para. Optimal Method}} \tag{2.97}$$

Remark 2.2.8

1. *The three parameter optimal method belongs to the U0V1 family for* $\rho_\infty \in [0,1)$*, and the MPR-EPA method, which belongs to the U0V0/V0U0 family, is recovered when* $\rho_\infty = 1$*. If we select the above conditions (Eq.* (2.97)*) in the V0 family, we can obtain the counterpart of the three parameter optimal method which belongs to the V0U1 family for* $\rho_\infty \in [0,1)$ *(this new scheme is spectrally equivalent to the traditional three parameter optimal method with regards to overshoot in linear systems; however, it is not well-known). It should be noted that the U0V0/V0U0 optimal method within the GS4-2 family is superior (with improved properties) to the three parameter optimal methods in either the U0 and V0 families with regards to overshoot.*

WBZ Method [15]. If we define the algorithmic parameters as

$$\begin{aligned}&\alpha_{\mathrm{m}} \le 0, \quad \alpha_{\mathrm{f}} = 0,\\ &\beta = \frac{(1-\alpha)^2}{4}, \quad \gamma = \frac{1}{2} - \alpha, \quad \alpha := \alpha_{\mathrm{m}} - \alpha_{\mathrm{f}} = \alpha_{\mathrm{m}}\end{aligned} \tag{2.98}$$

such that the conditions in Eq. (2.92) are satisfied for the same algorithmic structure given in Eq. (2.91), the resulting algorithm is known as the WBZ method [15]. The comparison with the GS4-2 family of algorithms leads to

$$\begin{aligned}&1 - \alpha_{\mathrm{m}} = W_1\Lambda_6\\ &W_1 = W_2 = W_3 = 1\\ &\beta = \lambda_3 = \Lambda_3, \quad \gamma = \lambda_5 = \Lambda_5, \quad \lambda_2 = \Lambda_2 = \tfrac{1}{2}\end{aligned} \tag{2.99}$$

together with $\lambda_1 = \Lambda_1 = \lambda_4 = \Lambda_4 = 1$. Therefore, the conditions for the GS4-2 family to recover the WBZ method are:

$$\boxed{\begin{array}{ll}\rho_\infty := \rho_\infty^{\mathrm{min}} = \rho_\infty^{\mathrm{max}} \in [0,1], \quad \rho_\infty^{\mathrm{s}} = 0 & \\ \quad \beta = \lambda_3 = \Lambda_3 & \\ \quad \gamma = \lambda_5 = \Lambda_5 & \textbf{in the U0 family} \\ \quad \frac{1}{2} = \Lambda_2 (= \lambda_2) & \end{array}} \implies \boxed{\textbf{WBZ Method}} \tag{2.100}$$

Remark 2.2.9

1. *The WBZ method belongs to the U0 family; however, we also have the new V0-based counterpart WBZ method which can be generated by imposing the same conditions given above in the V0 family. These two algorithms are spectrally equivalent. The only member which is numerically non-dissipative within the traditional (U0-based) WBZ method is the implicit Newmark method given by* $\rho_\infty := \rho_\infty^{\mathrm{min}} = \rho_\infty^{\mathrm{max}} = 1$*. For the V0-based WBZ counterpart, it is the MPR-MPA*

method. For $\rho_\infty \in [0,1)$, schemes are U0V1 and V0U1 numerically dissipative for the U0-based and V0-based WBZ methods, respectively.

2. *The algorithmic parameter α_m for the (U0-based) WBZ method can be expressed in terms of the spectral radius as*

$$\alpha_\mathrm{m} = -\frac{1-\rho_\infty}{1+\rho_\infty} \in [-1,0] \tag{2.101}$$

for $\rho_\infty := \rho_\infty^{\min} = \rho_\infty^{\max} \in [0,1]$.

HHT-α Method [14]. If we define the algorithmic parameters as

$$\begin{aligned} &\alpha_\mathrm{m} = 0, \quad 0 \le \alpha_\mathrm{f} \le \frac{1}{3}, \\ &\beta = \frac{(1-\alpha)^2}{4}, \quad \gamma = \frac{1}{2} - \alpha, \quad \alpha := \alpha_\mathrm{m} - \alpha_\mathrm{f} = -\alpha_\mathrm{f} \end{aligned} \tag{2.102}$$

such that the conditions in Eq. (2.92) are satisfied for the same algorithmic structure given in Eq. (2.91), the resulting algorithm is known as the HHT-α method [14]. Again, comparing with the GS4-2 family of algorithms, we get

$$\begin{aligned} &W_1\Lambda_6 = 1 \\ &1 - \alpha_\mathrm{f} = W_1 = W_2 = W_3 \\ &\beta = \lambda_3 = \Lambda_3, \quad \gamma = \lambda_5 = \Lambda_5, \quad \lambda_2 = \Lambda_2 = \tfrac{1}{2} \end{aligned} \tag{2.103}$$

together with $\lambda_1 = \Lambda_1 = \lambda_4 = \Lambda_4 = 1$. Therefore, the conditions to recover the HHT-α method from the GS4-2 family of algorithms are:

$$\boxed{\begin{aligned} &\rho_\infty := \rho_\infty^{\min} = \rho_\infty^{\max} \in [\tfrac{1}{2}, 1] \\ &\rho_\infty^{\mathrm{s}} = \frac{1-\rho_\infty}{2\rho_\infty} \in [0, \tfrac{1}{2}] \\ &\quad \beta = \lambda_3 = \Lambda_3 \qquad\qquad\qquad \textbf{in the U0 family} \\ &\quad \gamma = \lambda_5 = \Lambda_5 \\ &\quad \tfrac{1}{2} = \Lambda_2 (= \lambda_2) \end{aligned}} \implies \boxed{\textbf{HHT-}\boldsymbol{\alpha}\textbf{ Method}} \tag{2.104}$$

Remark 2.2.10

1. *The HHT-α method belongs to the U0 family. We can generate the spectrally-equivalent V0-based counterpart of the HHT-α method by imposing the same conditions given above within the V0 family. The implicit Newmark is the only numerically non-dissipative member in the U0-based HHT-α method; and the MPR-MPA method is the one for the V0-based HHT-α method.*

2. *The algorithmic parameter of the traditional (U0-based) HHT-α method can be expressed in terms of the spectral radius as*

$$\alpha_{\mathrm{f}} = 1 - W_1 = \frac{\rho_\infty^{\mathrm{s}}}{1 + \rho_\infty^{\mathrm{s}}} \in [-\tfrac{1}{3}, 0] \tag{2.105}$$

for $\rho_\infty^{\mathrm{s}} \in [0, \frac{1}{2}]$.

Algorithms	Spectral Conditions
3PO	$\rho_\infty := \rho_\infty^{\text{min}} = \rho_\infty^{\text{max}} = \rho_\infty^{\text{s}} \in [0, 1]$
WBZ	$\rho_\infty := \rho_\infty^{\text{min}} = \rho_\infty^{\text{max}} \in [0, 1],\ \ \rho_\infty^{\text{s}} = 0$
HHT-α	$\rho_\infty := \rho_\infty^{\text{min}} = \rho_\infty^{\text{max}} \in [\frac{1}{2}, 1],\ \ \rho_\infty^{\text{s}} \in [0, \frac{1}{2}]$

Table 2.1: Spectral Conditions for the Three Parameter Optimal Method (3PO), WBZ Method, and HHT-α Method in terms of the GS4-2 Family of Algorithms (used for both the U0- and V0-based cases)

Algorithmic Framework for the U0-based Family of Algorithms:

Integrator:

$$\tilde{\mathbf{a}}^n = \mathbf{g}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n, t_{n+1-\alpha_{\mathrm{f}}})$$

where

$$\begin{aligned}
t_{n+1-\alpha_{\mathrm{f}}} &:= (1-\alpha_{\mathrm{f}})t_{n+1} + \alpha_{\mathrm{f}} t_n \\
\tilde{\mathbf{q}}^n &= \mathbf{q}_{n+1-\alpha_{\mathrm{f}}} := (1-\alpha_{\mathrm{f}})\mathbf{q}^{n+1} + \alpha_{\mathrm{f}}\mathbf{q}^n \\
\tilde{\mathbf{v}}^n &= \mathbf{v}_{n+1-\alpha_{\mathrm{f}}} := (1-\alpha_{\mathrm{f}})\mathbf{v}^{n+1} + \alpha_{\mathrm{f}}\mathbf{v}^n \\
\tilde{\mathbf{a}}^n &= \mathbf{a}_{n+1-\alpha_{\mathrm{m}}} := (1-\alpha_{\mathrm{m}})\mathbf{a}^{n+1} + \alpha_{\mathrm{m}}\mathbf{a}^n
\end{aligned}$$

Updates:

$$\begin{aligned}
\mathbf{q}^{n+1} &= \mathbf{q}^n + \mathbf{v}^n\Delta t + \mathbf{a}^n\frac{\Delta t^2}{2} + \beta\Delta\mathbf{a}^n\Delta t^2 \\
\mathbf{v}^{n+1} &= \mathbf{v}^n + \mathbf{a}^n\Delta t + \gamma\Delta\mathbf{a}^n\Delta t \\
\mathbf{a}^{n+1} &= \mathbf{a}^n + \Delta\mathbf{a}^n
\end{aligned}$$

Algorithmic Parameters:

$$\begin{aligned}
\alpha_{\mathrm{m}} &= \frac{\rho_\infty^{\min} + \rho_\infty^{\max} + 2\rho_\infty^{\min}\rho_\infty^{\max}}{1 + \rho_\infty^{\min} + \rho_\infty^{\max} + \rho_\infty^{\min}\rho_\infty^{\max}} - \frac{1}{1+\rho_\infty^{\mathrm{s}}} \\
\alpha_{\mathrm{f}} &= \frac{\rho_\infty^{\mathrm{s}}}{1+\rho_\infty^{\mathrm{s}}} \\
\beta &= \frac{1}{1 + \rho_\infty^{\min} + \rho_\infty^{\max} + \rho_\infty^{\min}\rho_\infty^{\max}} \\
\gamma &= \frac{3 + \rho_\infty^{\min} + \rho_\infty^{\max} - \rho_\infty^{\min}\rho_\infty^{\max}}{2(1+\rho_\infty^{\min})(1+\rho_\infty^{\max})}
\end{aligned}$$

Algorithmic Framework for the V0-based Family of Algorithms:

Integrator:

$$\tilde{\mathbf{a}}^n = \mathbf{g}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n, t_{n+1-\alpha_\mathrm{f}})$$

where

$$\begin{aligned}
t_{n+1-\alpha_\mathrm{f}} &:= (1-\alpha_\mathrm{f})t_{n+1} + \alpha_\mathrm{f} t_n \\
\tilde{\mathbf{q}}^n &= \mathbf{q}_{n+1-\alpha_\mathrm{f}} + \kappa \mathbf{v}^n \Delta t := (1-\alpha_\mathrm{f})\mathbf{q}^{n+1} + \alpha_\mathrm{f}\mathbf{q}^n + \kappa \mathbf{v}^n \Delta t \\
\tilde{\mathbf{v}}^n &= \mathbf{v}_{n+1-\alpha_\mathrm{k}} + \kappa \mathbf{v}^n \Delta t := (1-\alpha_\mathrm{k})\mathbf{v}^{n+1} + \alpha_\mathrm{k}\mathbf{v}^n + \kappa \mathbf{a}^n \Delta t \\
\tilde{\mathbf{a}}^n &= \mathbf{a}_{n+1-\alpha_\mathrm{m}} := (1-\alpha_\mathrm{m})\mathbf{a}^{n+1} + \alpha_\mathrm{m}\mathbf{a}^n
\end{aligned}$$

Updates:

$$\begin{aligned}
\mathbf{q}^{n+1} &= \mathbf{q}^n + \mathbf{v}^n \Delta t + \mathbf{a}^n \frac{\Delta t^2}{2} + \beta \Delta \mathbf{a}^n \Delta t^2 \\
\mathbf{v}^{n+1} &= \mathbf{v}^n + \mathbf{a}^n \Delta t + \gamma \Delta \mathbf{a}^n \Delta t \\
\mathbf{a}^{n+1} &= \mathbf{a}^n + \Delta \mathbf{a}^n
\end{aligned}$$

Algorithmic Parameters:

$$\begin{aligned}
\alpha_\mathrm{m} &= \frac{\rho_\infty^{\min} + \rho_\infty^{\max} + 2\rho_\infty^{\min}\rho_\infty^{\max}}{1 + \rho_\infty^{\min} + \rho_\infty^{\max} + \rho_\infty^{\min}\rho_\infty^{\max}} - \frac{1}{1+\rho_\infty^\mathrm{s}} \\
\alpha_\mathrm{f} &= \frac{\rho_\infty^{\min} + \rho_\infty^{\max} + 3\rho_\infty^{\min}\rho_\infty^{\max} - 1}{2(1+\rho_\infty^{\min})(1+\rho_\infty^{\max})} \\
\alpha_\mathrm{k} &= \frac{\rho_\infty^{\min} + \rho_\infty^{\max} + \rho_\infty^{\min}\rho_\infty^{\max} - 1}{\rho_\infty^{\min} + \rho_\infty^{\max} + \rho_\infty^{\min}\rho_\infty^{\max} + 1} \\
\kappa &= -\frac{(\rho_\infty^{\min} - 1)(\rho_\infty^{\max} - 1)}{2(1+\rho_\infty^{\min})(1+\rho_\infty^{\max})} \\
\beta &= \frac{1}{2(1+\rho_\infty^\mathrm{s})} \\
\gamma &= \frac{1}{1+\rho_\infty^\mathrm{s}}
\end{aligned}$$

GS4-2: U0 Family				
Method	α_{m}	α_{f}	β	γ
3PO	$\frac{2\rho_\infty-1}{1+\rho_\infty} \in [-1, \frac{1}{2}]$	$\frac{\rho_\infty}{1+\rho_\infty} \in [0, \frac{1}{2}]$	$\frac{1}{(1+\rho_\infty)^2} \in [\frac{1}{4}, 1]$	$\frac{3-\rho_\infty}{2(1+\rho_\infty)} \in [\frac{1}{2}, \frac{3}{2}]$
WBZ	$-\frac{1-\rho_\infty}{1+\rho_\infty} \in [-1, 0]$	0	$\frac{1}{(1+\rho_\infty)^2} \in [\frac{1}{4}, 1]$	$\frac{3-\rho_\infty}{2(1+\rho_\infty)} \in [\frac{1}{2}, \frac{3}{2}]$
HHT-α	0	$\frac{\rho_\infty^s}{1+\rho_\infty^s} \in [-\frac{1}{3}, 0]$	$\frac{1}{(1+\rho_\infty)^2} \in [\frac{1}{4}, \frac{4}{9}]$	$\frac{3-\rho_\infty}{2(1+\rho_\infty)} \in [\frac{1}{2}, \frac{5}{6}]$

Table 2.2: Algorithmic Parameters of the Three Parameter Optimal Method (3PO), WBZ Method, and HHT-α Method (traditional; ***U0-based***) in terms of the GS4-2 Family of Algorithms

GS4-2: V0 Family						
Method	α_{m}	α_{f}	α_{k}	κ	β	γ
3PO	$\frac{2\rho_\infty-1}{1+\rho_\infty} \in [-1, \frac{1}{2}]$	$\frac{3\rho_\infty-1}{2(1+\rho_\infty)} \in [-\frac{1}{2}, \frac{1}{2}]$	$\frac{\rho_\infty(\rho_\infty+2)}{(1+\rho_\infty)^2} \in [0, \frac{3}{4}]$	$\frac{1+2\rho_\infty-\rho_\infty^2}{2(1+\rho_\infty)^2} \in [\frac{1}{4}, \frac{1}{2}]$	$\frac{1}{2(1+\rho_\infty)} \in [\frac{1}{4}, \frac{1}{2}]$	$\frac{1}{1+\rho_\infty} \in [\frac{1}{2}, 1]$
WBZ	$\frac{\rho_\infty-1}{1+\rho_\infty} \in [-1, 0]$	$\frac{3\rho_\infty-1}{2(1+\rho_\infty)} \in [-\frac{1}{2}, \frac{1}{2}]$	$\frac{\rho_\infty^2+2\rho_\infty-1}{(1+\rho_\infty)^2} \in [-1, \frac{1}{2}]$	$-\frac{(\rho_\infty-1)^2}{2(1+\rho_\infty)^2} \in [-\frac{1}{2}, 0]$	$\frac{1}{2}$	1
HHT-α	0	$\frac{3\rho_\infty-1}{2(1+\rho_\infty)} \in [-\frac{1}{2}, \frac{1}{2}]$	$\frac{\rho_\infty^2+2\rho_\infty-1}{(1+\rho_\infty)^2} \in [-1, \frac{1}{2}]$	$-\frac{(\rho_\infty-1)^2}{2(1+\rho_\infty)^2} \in [-\frac{1}{2}, 0]$	$\frac{\rho_\infty}{(1+\rho_\infty)} \in [0, \frac{1}{2}]$	$\frac{2\rho_\infty}{(1+\rho_\infty)} \in [0, 1]$

Table 2.3: Algorithmic Parameters of the ***V0-based*** Three Parameter Optimal Method (3PO), ***V0-based*** WBZ Method, and ***V0-based*** HHT-α Method in terms of the GS4-2 Family of Algorithms

Implementation with the Full Newton Method

■ **Step 1: Predictor** ($k \leftarrow 0$)

$${}^{(k)}\mathbf{q}^{n+1} = \Xi^{q}_{P_1}\,\mathbf{q}^n + \Xi^{q}_{P_2}\,\mathbf{v}^n + \Xi^{q}_{P_3}\,\mathbf{a}^n$$

$${}^{(k)}\mathbf{v}^{n+1} = \Xi^{v}_{P_1}\,\mathbf{q}^n + \Xi^{v}_{P_2}\,\mathbf{v}^n + \Xi^{v}_{P_3}\,\mathbf{a}^n$$

$${}^{(k)}\mathbf{a}^{n+1} = \Xi^{a}_{P_1}\,\mathbf{q}^n + \Xi^{a}_{P_2}\,\mathbf{v}^n + \Xi^{a}_{P_3}\,\mathbf{a}^n$$

■ **Step 2: Iteration** ($k \leftarrow k+1$)

Solve for the increment ${}^{(k)}\delta\boldsymbol{\vartheta}$ from:

$${}^{(k)}\mathbf{J}^n\ {}^{(k)}\delta\boldsymbol{\vartheta}^n = -{}^{(k)}\mathbf{R}^n$$

with the residual vector,

$${}^{(k)}\mathbf{R}^n = \mathbf{F}({}^{(k)}\tilde{\mathbf{q}}^n, {}^{(k)}\tilde{\mathbf{v}}^n, {}^{(k)}\tilde{\mathbf{a}}^n, t_{n+W_1})$$

where

$${}^{(k)}\tilde{\mathbf{a}}^n = {}^{(k)}\mathbf{a}^n + W_1\Lambda_6\,{}^{(k)}\Delta\mathbf{a}^n \quad ({}^{(k)}\Delta\mathbf{a}^n := {}^{(k)}\mathbf{a}^{n+1} - {}^{(k)}\mathbf{a}^n)$$

$${}^{(k)}\tilde{\mathbf{v}}^n = {}^{(k)}\mathbf{v}^n + W_1\Lambda_4\,{}^{(k)}\mathbf{a}^n\Delta t + W_2\Lambda_5\,{}^{(k)}\Delta\mathbf{a}^n\Delta t$$

$${}^{(k)}\tilde{\mathbf{q}}^n = {}^{(k)}\mathbf{q}^n + W_1\Lambda_1\,{}^{(k)}\mathbf{v}^n\Delta t + W_2\Lambda_2\,{}^{(k)}\mathbf{a}^n\Delta t^2 + W_3\Lambda_3\,{}^{(k)}\Delta\mathbf{a}^n\Delta t^2$$

and the associated Jacobian matrix,

$${}^{(k)}\mathbf{J}^n := \frac{\partial\mathbf{F}}{\partial\,{}^{(k)}\delta\boldsymbol{\vartheta}^n} = \Xi_{C_1}\,{}^{(k)}\mathbf{M}^n_T + \Xi_{C_2}\,{}^{(k)}\mathbf{C}^n_T + \Xi_{C_3}\,{}^{(k)}\mathbf{K}^n_T$$

■ **Step 3: Corrector**

$${}^{(k)}\tilde{\mathbf{a}}^n = {}^{(k-1)}\tilde{\mathbf{a}}^n + \Xi_{C_1}\,{}^{(k)}\delta\boldsymbol{\vartheta}^n$$

$${}^{(k)}\tilde{\mathbf{v}}^n = {}^{(k-1)}\tilde{\mathbf{v}}^n + \Xi_{C_2}\,{}^{(k)}\delta\boldsymbol{\vartheta}^n$$

$${}^{(k)}\tilde{\mathbf{q}}^n = {}^{(k-1)}\tilde{\mathbf{q}}^n + \Xi_{C_3}\,{}^{(k)}\delta\boldsymbol{\vartheta}^n$$

Convergence Criteria:

If $\sqrt{({}^{(k)}\mathbf{R}^n)^{T\,(k)}\mathbf{R}^n} > \epsilon\sqrt{({}^{(0)}\mathbf{R}^n)^{T\,(0)}\mathbf{R}^n}$,

repeat for the next iteration; else, go to **Step 4**.

■ **Step 4: Update**

$$\mathbf{a}^{n+1} = \mathbf{a}^n + \frac{{}^{(k)}\tilde{\mathbf{a}}^n - \mathbf{a}^n}{W_1\Lambda_6}$$

$$\mathbf{v}^{n+1} = \mathbf{v}^n + \lambda_4\mathbf{a}^n\Delta t + \lambda_5(\mathbf{a}^{n+1} - \mathbf{a}^n)\Delta t$$

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \lambda_1\mathbf{v}^n\Delta t + \lambda_2\mathbf{a}^n\Delta t^2 + \lambda_3(\mathbf{a}^{n+1} - \mathbf{a}^n)\Delta t^2$$

Set $n \leftarrow n+1$ and go to **Step 1**.

	a-form	v-form	d-form
$\Xi^q_{\mathrm{P}_1}$	1	1	1
$\Xi^q_{\mathrm{P}_2}$	$\lambda_1 \Delta t$	$\lambda_1 \Delta t$	0
$\Xi^q_{\mathrm{P}_3}$	$\lambda_2 \Delta t^2$	$\left(\lambda_2 - \frac{\lambda_3 \lambda_4}{\lambda_5}\right) \Delta t^2$	0
$\Xi^v_{\mathrm{P}_1}$	0	0	0
$\Xi^v_{\mathrm{P}_2}$	1	1	$1 - \frac{\lambda_1 \lambda_5}{\lambda_3}$
$\Xi^v_{\mathrm{P}_3}$	$\lambda_4 \Delta t$	0	$\left(\lambda_4 - \frac{\lambda_2 \lambda_5}{\lambda_3}\right) \Delta t$
$\Xi^a_{\mathrm{P}_1}$	0	0	0
$\Xi^a_{\mathrm{P}_2}$	0	0	$-\frac{\lambda_1}{\lambda_3 \Delta t}$
$\Xi^a_{\mathrm{P}_3}$	1	$1 - \frac{\lambda_4}{\lambda_5}$	$1 - \frac{\lambda_2}{\lambda_3}$
Ξ_{C_1}	$W_1 \Lambda_6$	$\frac{W_1 \Lambda_6}{\lambda_5 \Delta t}$	$\frac{W_1 \Lambda_6}{\lambda_3 \Delta t^2}$
Ξ_{C_2}	$W_2 \Lambda_5 \Delta t$	$\frac{W_2 \Lambda_5}{\lambda_5}$	$\frac{W_2 \Lambda_5}{\lambda_3 \Delta t}$
Ξ_{C_3}	$W_3 \Lambda_3 \Delta t^2$	$\frac{W_3 \Lambda_3 \Delta t}{\lambda_5}$	$\frac{W_3 \Lambda_3}{\lambda_3}$

Table 2.4: Predictor-corrector Coefficients for the Incremental a-,v-, and d-form Representations

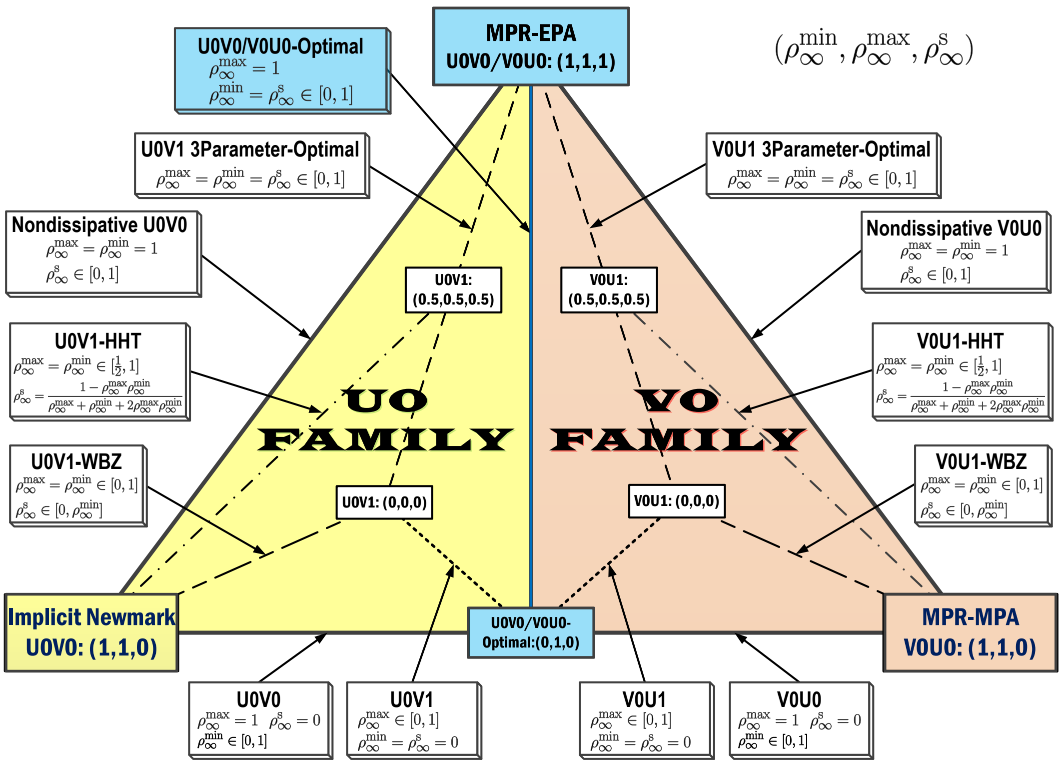


Figure 2.3: The Framework of the GSSSS Family of Algorithms

2.3 Isochronous Time Integration: Adaptation Process - Generation of GS4-1 Family of Algorithms from GS4-2 Family of Algorithms

The GS4-2 family of algorithms shown in the foregoing section is used for solving a system of ODEs of second-order in time. However, the *same* algorithmic framework can actually be applied to a system of ODEs of first order in time via the so-called v***adaptation process***, summarized in Table 2.3. In other words, due to the adaptation process, the GS4-2 family of algorithms is readily reduced to the GS4-1 family of algorithms: this is the key concept and feature of the isochronous time integration. But, it should be noted that the GS4-1 family was originally independently derived for the ODEs of first order in linear systems through a sequence of imposing conditions of second order-time accuracy, unconditional stability, and zeroth-order overshoot behaviors, similar to the case of the GS4-2 family; see [17].

We will now show how to reduce the GS4-2 family to GS4-1 family. The adaptation process essentially takes two steps: **(1) Adaptation process for the unknowns**, and **(2) Adaptation process for the spectral parameters**. Procedures of these adaptation processes are summarized in Table 2.3.

- **Adaptation process for the unknowns:** As to **Step (1)**, consider $(\mathbf{q}^n, \mathbf{v}^n, \mathbf{a}^n)$ in Eq. (2.5). Treat $\mathbf{a}^n \approx \ddot{\mathbf{q}}(t_{n-\phi})$ and $\mathbf{v}^n \approx \dot{\mathbf{q}}(t_n)$ as $\boldsymbol{\nu}^n$ and $\mathbf{s}^n$, respectively, where $\boldsymbol{\nu}^n$ and $\mathbf{s}^n$ are the approximations of $\dot{\mathbf{s}}(t_{n-\phi})$ and $\mathbf{s}(t_n)$. $\mathbf{q}^n \approx \mathbf{q}(t_n)$ is treated as a *dummy* after the reduction. Utilizing $(\mathbf{s}^n, \boldsymbol{\nu}^n)\ \forall n$, Eq. (2.2) (first-order ODEs) may be temporally discretized such that the basic algorithmic structure of the so-called GS4-1 family, shown in Algorithm 2.3.1, is recovered.

- **Adaptation process for the spectral parameters:** Set the spectral parameters $(\rho_\infty^{\min}\rho_\infty^{\max}, \rho_\infty^{s})$ in Algorithm 2.2.1 as

$$\rho_\infty^{\max} = 1, \quad \rho_\infty^{\min} = \rho_\infty, \quad \text{and} \quad \rho_\infty^{\min} = \rho_\infty^{s} \tag{2.106}$$

  Then, the algorithmic parameters of the GS4-1 family, Algorithm 2.3.1, is readily recovered. Similar to the case of Algorithm 2.2.1, the spectral parameters for the GS4-1 family, $(\rho_\infty, \rho_\infty^{s})$ need to satisfy

$$0 \le \rho_\infty^{s} \le \rho_\infty \le 1 \tag{2.107}$$

for the implicit case, i.e., $\eta_i = 1$, but the relation no longer needs to be satisfied for an explicit case, $\eta_i = 0$.

For the unknown vectors $n \in \{0, 1, \cdots, n_{\text{steps}}\}$	Treat $\mathbf{a}^n$ in the GS4-2 framework as $\boldsymbol{\nu}^n$ in the first order system
	Treat $\mathbf{v}^n$ in the GS4-2 framework as $\mathbf{s}^n$ in the first order system
	Neglect $\mathbf{q}^n$ in the GS4-2 framework (dummy)
For the spectral parameters	Set ρ_∞^{s} in the GS4-2 framework as ρ_∞^{s} in the GS4-1 framework
	Set ρ_∞^{max} in the GS4-2 framework to equal to unity
	Set ρ_∞^{min} in the GS4-2 framework as ρ_∞ in the GS4-1 framework
In the U0-based Family	Additionally require $\rho_\infty^{\text{s}} = \rho_\infty^{\text{min}}$ and yield the GS4-1 framework without the selective control feature
In the V0-based Family	Choose $(\rho_\infty^{\text{s}}, \rho_\infty^{\text{min}})$ and yield the GS4-1 framework with/without the selective control feature

Table 2.5: Adaptation Process

Algorithm 2.3.1 (GS4-1 Family of Algorithms)

Given initial condition $\mathbf{s}(t_0) = \mathbf{s}^0$*. Find* $\mathbf{s}^n$ *and* $\boldsymbol{\nu}^n$ *(for* $n \in \{1, 2, \cdots, n_{\text{steps}}\}$*) from*

$$\tilde{\boldsymbol{\nu}}^n = \mathbf{h}(\tilde{\mathbf{s}}^n, t_{n+W_1}) \tag{2.108a}$$

where

$$\tilde{\mathbf{s}}^n = \mathbf{s}^n + W_1 \Lambda_4 \boldsymbol{\nu}^n \Delta t + W_2 \Lambda_5 \Delta \boldsymbol{\nu}^n \Delta t \tag{2.108b}$$

$$\tilde{\boldsymbol{\nu}}^n = \boldsymbol{\nu}^n + W_1 \Lambda_6 \Delta \boldsymbol{\nu}^n =: \boldsymbol{\nu}_{n+W_1\Lambda_6} \tag{2.108c}$$

And the associated updates are:

$$\mathbf{s}^{n+1} = \mathbf{s}^{n} + \lambda_4 \boldsymbol{\nu}^{n} \Delta t + \lambda_5 \Delta \boldsymbol{\nu}^{n} \Delta t \tag{2.108d}$$

$$\boldsymbol{\nu}^{n+1} = \boldsymbol{\nu}^{n} + \Delta \boldsymbol{\nu}^{n} \tag{2.108e}$$

The algorithmic parameters are defined by

$$\begin{aligned} W_1 &= \frac{1}{1+\rho_\infty} \quad , \quad \lambda_4 = \Lambda_4 = 1 \\ W_2\Lambda_5 &= \frac{1}{(1+\rho_\infty)(1+\rho_\infty^{\mathrm{s}})} \quad , \quad \lambda_5 = \frac{1}{1+\rho_\infty^{\mathrm{s}}} \\ W_1\Lambda_6 &= \frac{3+\rho_\infty+\rho_\infty^{\mathrm{s}}-\rho_\infty\rho_\infty^{\mathrm{s}}}{2(1+\rho_\infty)(1+\rho_\infty^{\mathrm{s}})} \end{aligned}$$

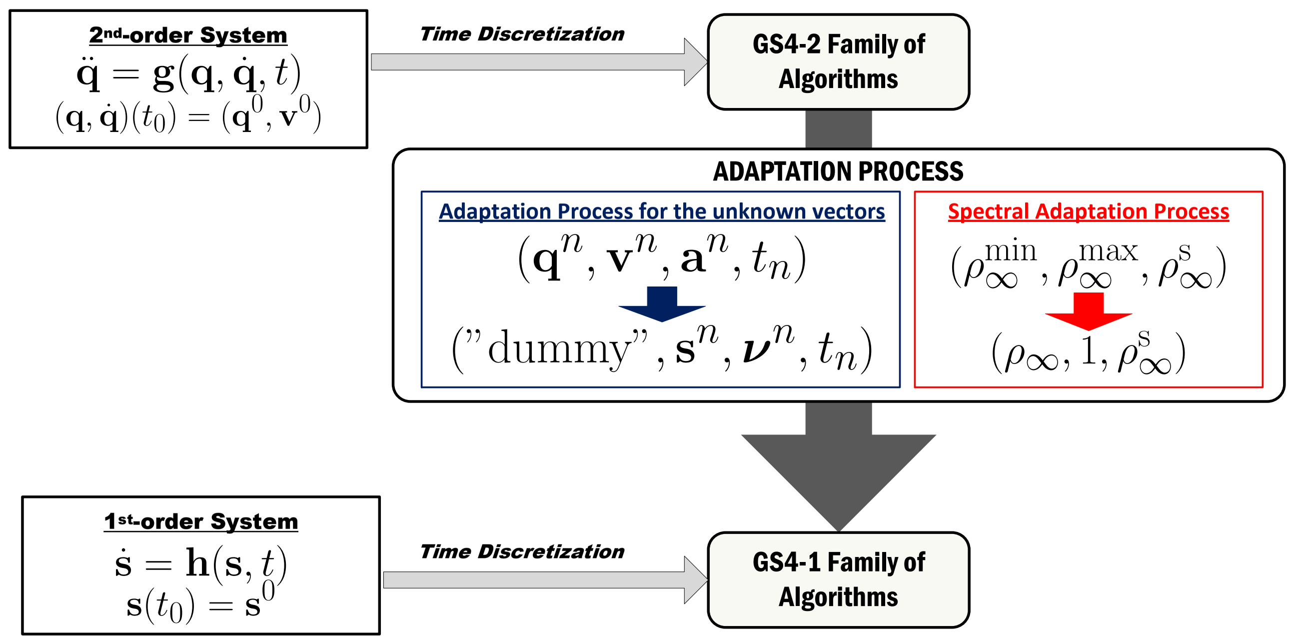


Figure 2.4: An Overview of the GS4-2 and GS4-1 Families of Algorithms and the Adaptation Process

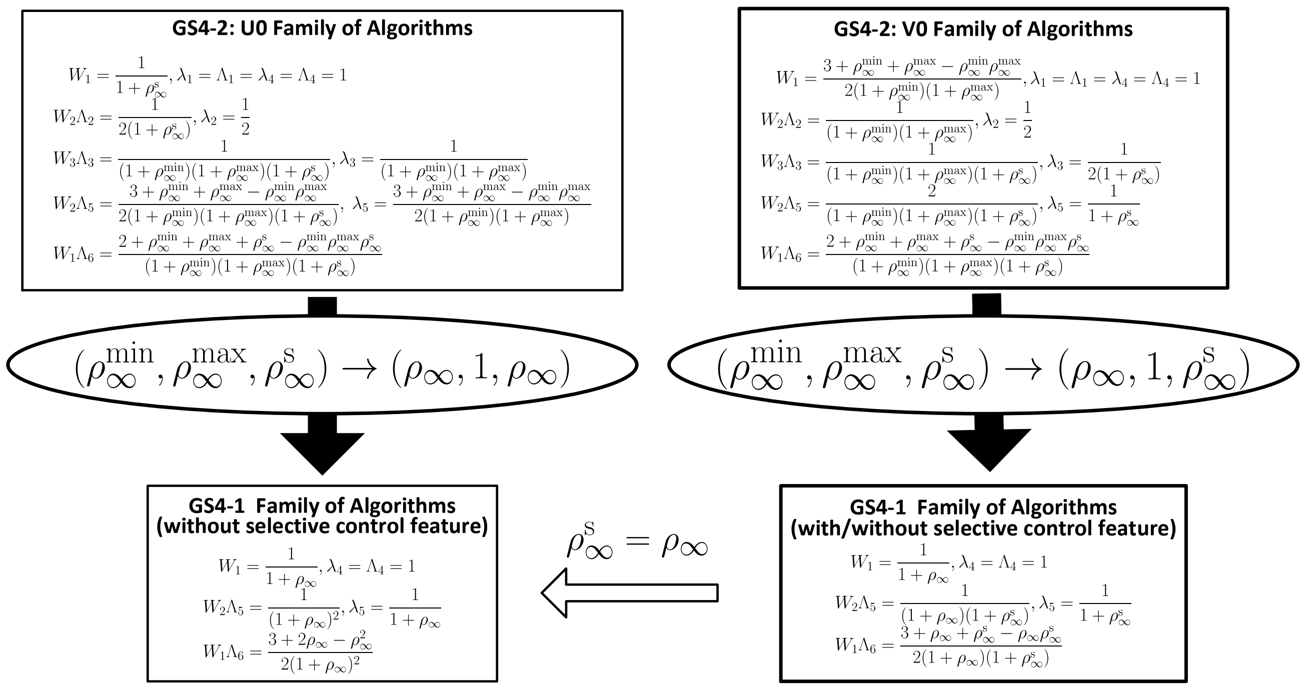


Figure 2.5: Spectral Relationship Between the GS4-2 and GS4-1 Families of Algorithms

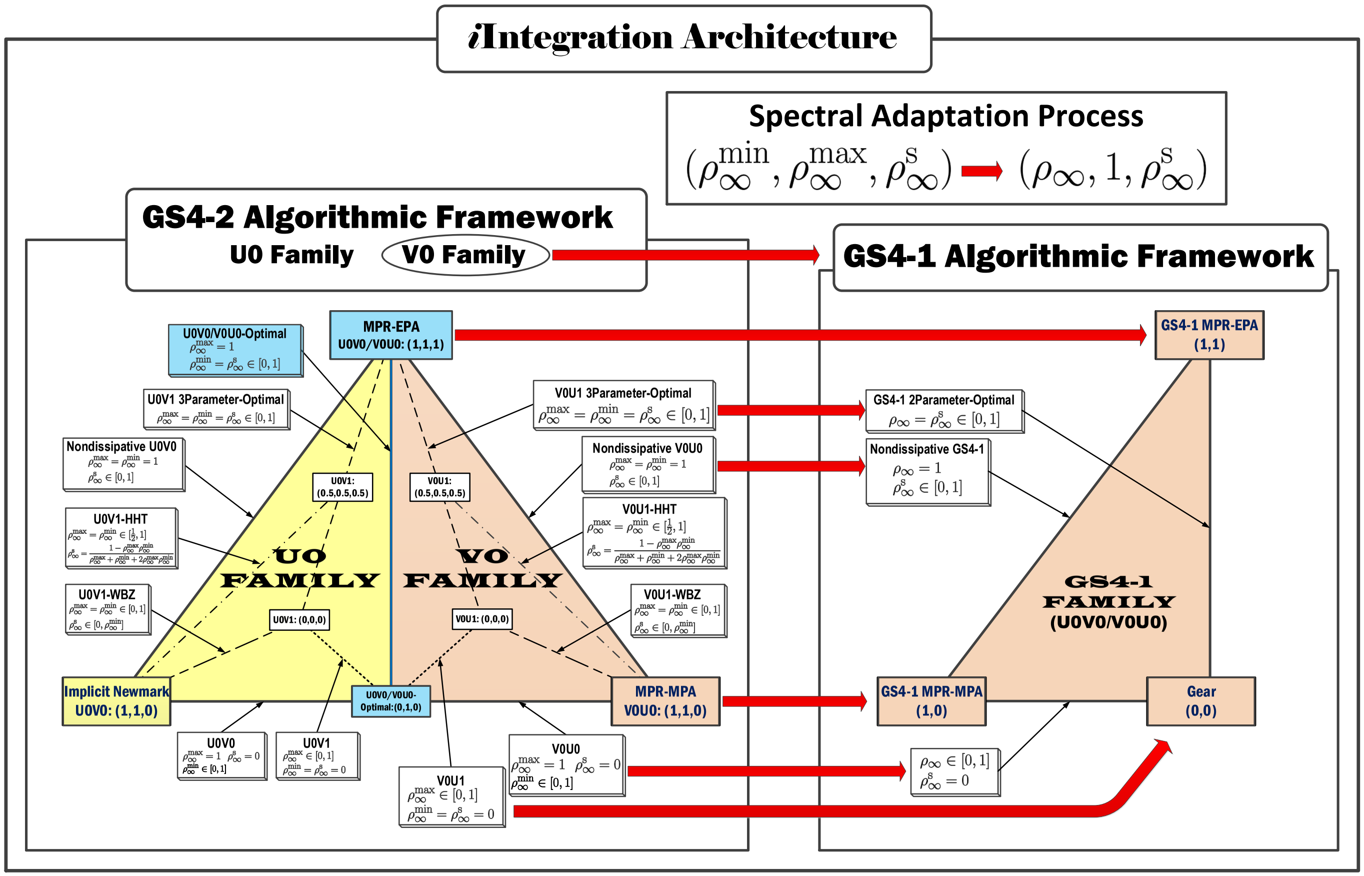


Figure 2.6: *i*Integration Architecture: Spectral Adaptation Process

2.3.1 Numerical Examples: Adaptation Process

Example 2.3.1 (Second-order ODE: The seven stars Pleiades problem [18])

Solve the seven stars problem, which is called the Pleiades problem, with Algorithm 2.2.1. Since this problem is described by second-order ODEs, as shown below, the adaptation process is not required. The governing equations for this problem are:

$$\begin{aligned} \ddot{x}_i &= \sum_{j \neq i} m_j \frac{x_j - x_i}{r_{ij}} \\ \ddot{y}_i &= \sum_{j \neq i} m_j \frac{y_j - y_i}{r_{ij}} \end{aligned} \tag{2.109}$$

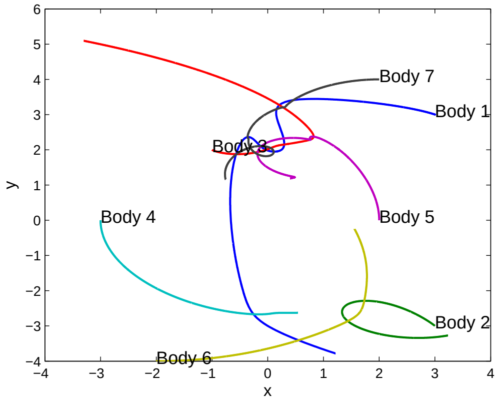
for $i, j = 1, 2, \cdots, 7$, where m_j denotes the mass of star j, and

$$r_{ij} := \left[(x_i - x_j)^2 + (y_i - y_j)^2 \right]^{(3/2)} \tag{2.110}$$

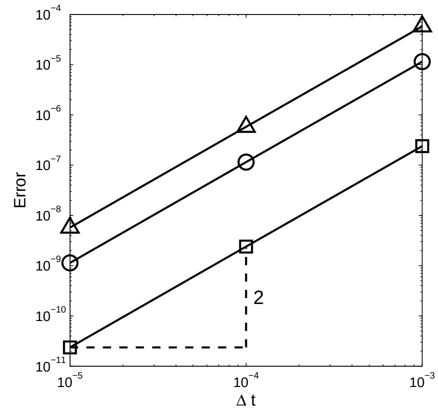
Fig. 2.7 shows the solutions of the system and time accuracy[2] of body 2 for three different integrators for $t \in [0, 3]$: U0V0/V0U0(1,1,1) method, i.e., MPR-EPA method, V0U0(1,1,0) method, i.e., MPR-MPA method, and U0V0/V0U0 optimal (0,1,0) method. The velocity and acceleration histories in the x- and y-dirctions for these three distinct algorithms are shown in Fig. 2.8 and Fig. 2.9, respectively. The masses of each star are assumed to be unity. The time step size is $\Delta t = 0.001$, and initial conditions used are:

$$\begin{aligned} \mathbf{x}(0) &= (x_1, x_2, x_3, x_4, x_5, x_6, x_7)^T(0) = (3, 3, -1, -3, 2, -2, 2)^T \\ \mathbf{y}(0) &= (y_1, y_2, y_3, y_4, y_5, y_6, y_7)^T(0) = (3, -3, 2, 0, 0, -4, 4)^T \\ \dot{\mathbf{x}}(0) &= (\dot{x}_1, \dot{x}_2, \dot{x}_3, \dot{x}_4, \dot{x}_5, \dot{x}_6, \dot{x}_7)^T(0) = (0, 0, 0, 0, 0, 1.75, -1.5)^T \\ \dot{\mathbf{y}}(0) &= (\dot{y}_1, \dot{y}_2, \dot{y}_3, \dot{y}_4, \dot{y}_5, \dot{y}_6, \dot{y}_7)^T(0) = (0, 0, 0, -1.25, 1, 0, 0)^T \end{aligned} \tag{2.111}$$

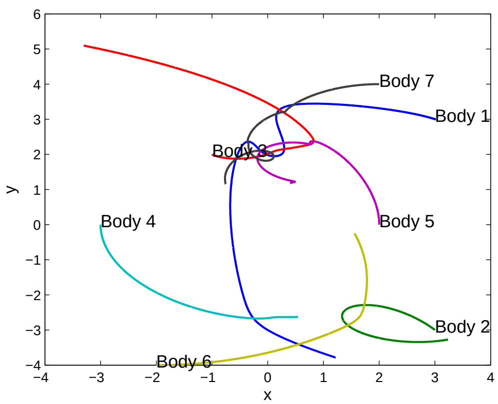
[2] *For the time accuracy plots, ○, □, and △ denotes the displacement, velocity, and acceleration data, respectively.*



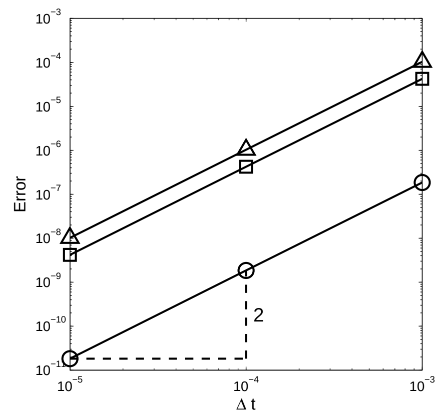
(a) MPR-EPA: Configuration



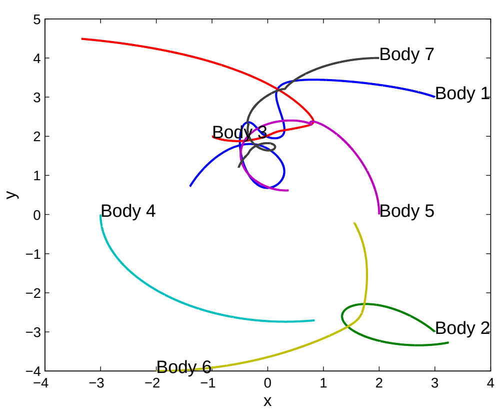
(b) MPR-EPA: Time Accuracy



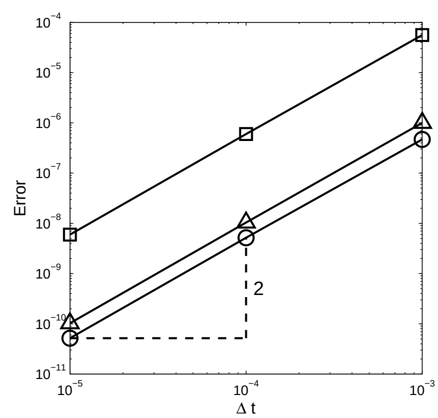
(c) MPR-MPA: Configuration



(d) MPR-MPA: Time Accuracy

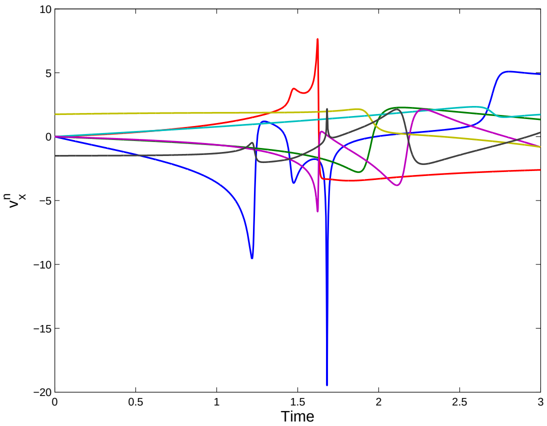


(e) U0V0/V0U0(0,1,0): Configuration

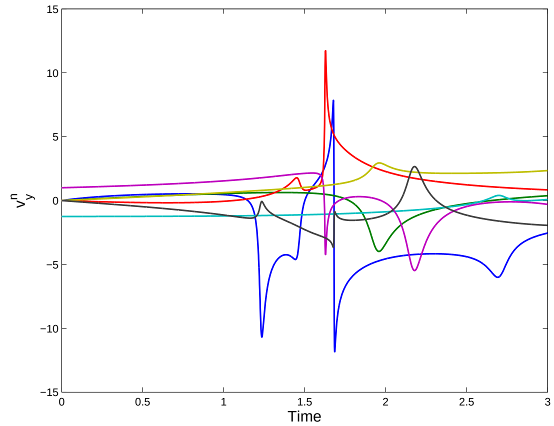


(f) U0V0/V0U0(0,1,0): Time Accuracy

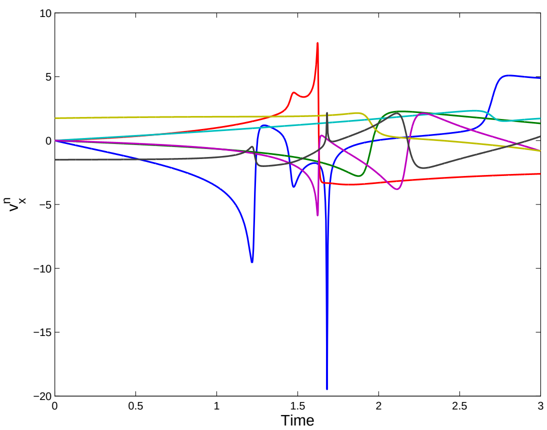
Figure 2.7: The Pleiades Problem: Solutions



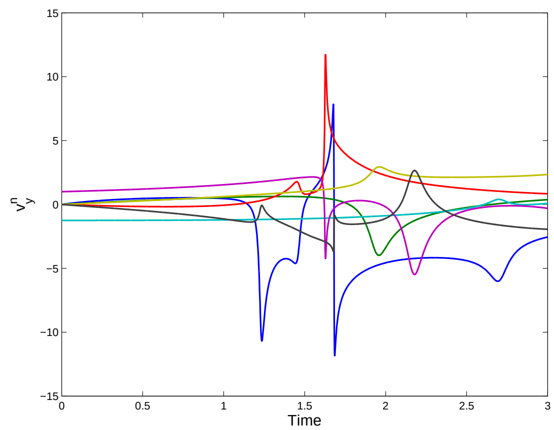
(a) MPR-EPA: v_x^n



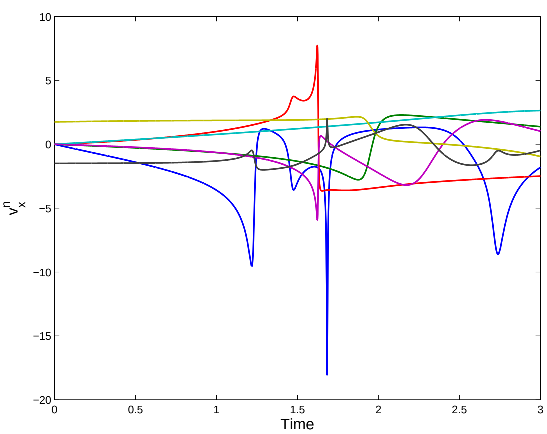
(b) MPR-EPA: v_y^n



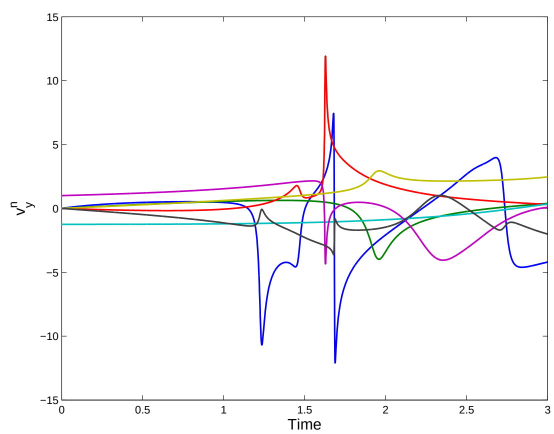
(c) MPR-MPA: v_x^n



(d) MPR-MPA: v_y^n

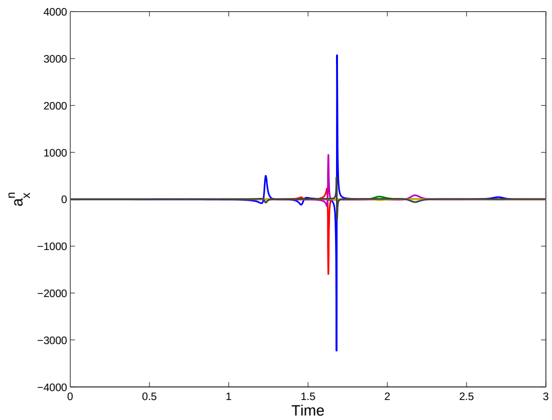


(e) U0V0/V0U0(0,1,0): v_x^n

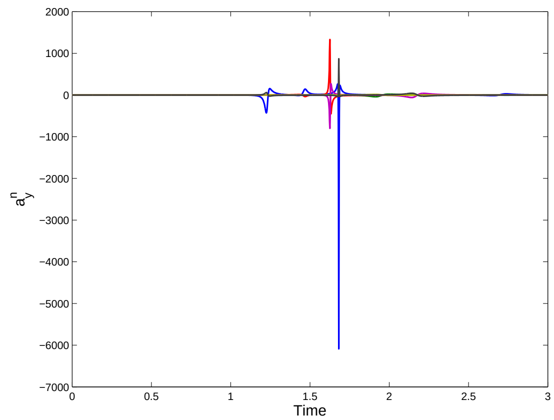


(f) U0V0/V0U0(0,1,0): v_y^n

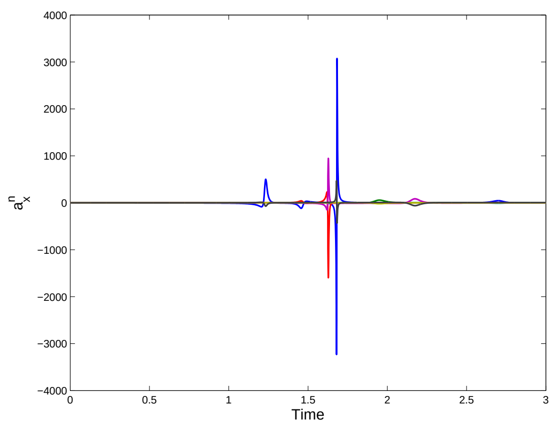
Figure 2.8: The Pleiades Problem: Velocity responses



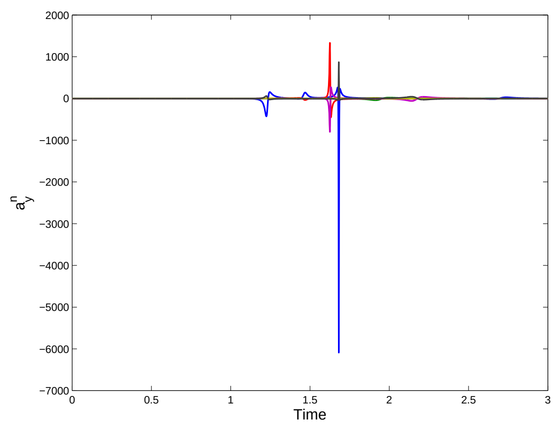
(a) MPR-EPA: a_x^n



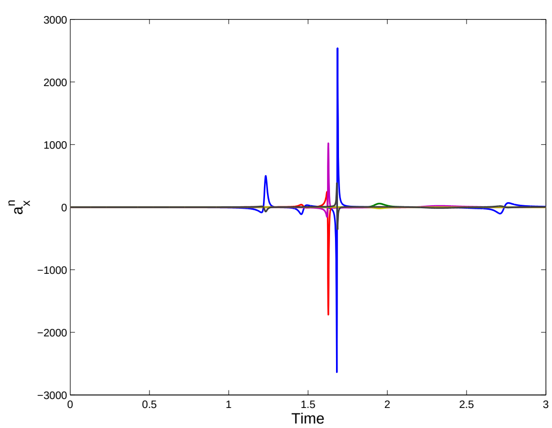
(b) MPR-EPA: a_y^n



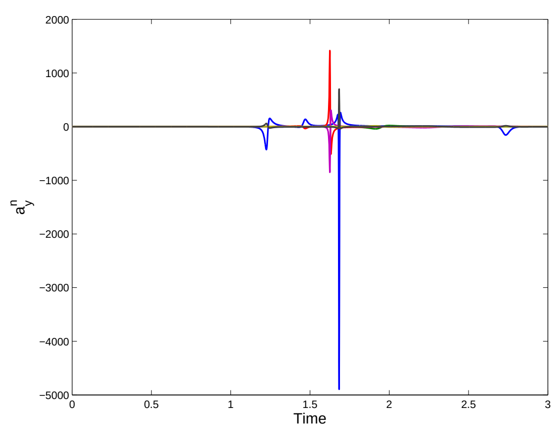
(c) MPR-MPA: a_x^n



(d) MPR-MPA: a_y^n



(e) U0V0/V0U0(0,1,0): a_x^n



(f) U0V0/V0U0(0,1,0): a_y^n

Figure 2.9: The Pleiades Problem: Acceleration Responses

Example 2.3.2 (First-order ODE: The Brusselator Chemical Reaction Problem) *A mathematical model for an autocatalystic chemical reaction is the* ***Brusselator*** *model. The chemical reaction*

$$\begin{aligned} A &\longrightarrow X \\ 2X + Y &\longrightarrow 3X \\ B + X &\longrightarrow Y + D \\ X &\longrightarrow E \end{aligned} \tag{2.112}$$

is modeled by the following first-order ODE:

$$\begin{aligned} \dot{X} &= A - (B+1)X + X^2Y \\ \dot{Y} &= BX - X^2Y \end{aligned} \tag{2.113}$$

for the case of no spatial diffusion. Eq. (2.113) *has a fixed point at* $(X, Y) = (A, B/A)$, *and this fixed point is unstable when* $B > 1 + A$. *Employ the following five distinct algorithms that can be generated from Algorithm 2.2.1 via the adaptation process:*

- *Algorithm 1: MPR-EPA method obtained from the V0/U0(1,1,1) method, i.e., MPR-EPA method for second-order systems*

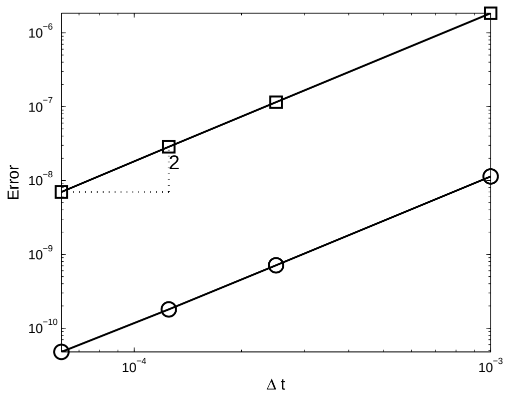
- *Algorithm 2: The GS4-1(1,0.5) method obtained from the V0(1,1,0.5) method for second-order systems*

- *Algorithm 3: MPR-MPA method obtained from the V0(1,1,0) method, i.e., MPR-MPA method for second-order systems*

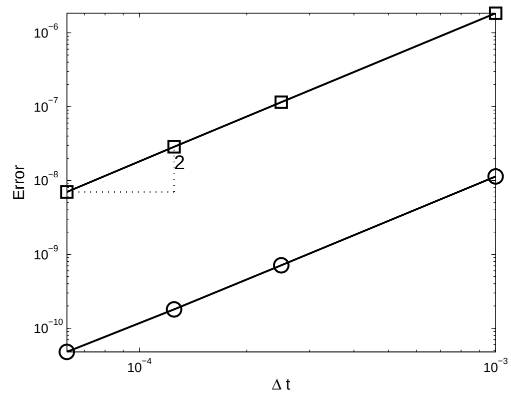
- *Algorithm 4: The GS4-1(0.5,0.5) method obtained from the V0/U0(0.5,1,0.5) method for second-order systems*

- *Algorithm 5: Gear's method obtained from the V0/U0(0,1,0) method for second-order systems*

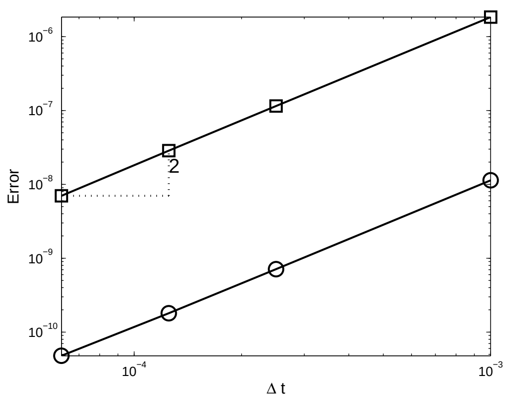
Fig. 2.10 shows that any scheme inherits second-order time accuracy in both X^n *(*$\circ$*) and* $V_X^n \approx \dot{X}(t_{n-\phi})$ *(*$\square$*). Fig. 2.11 and Fig. 2.12 show the limit circles and time histories of the Brusselator with given initial conditions* $\mathbf{s}(0) = (X_1, X_2)^T(t_0) = (1, 1)^T$ *and* $\boldsymbol{\nu}(0) = (V_X, V_Y)^T(t_0) = (0, 0)^T$ *with time step size* $\Delta t = 0.1$ *for the stable and unstable cases, respectively.*



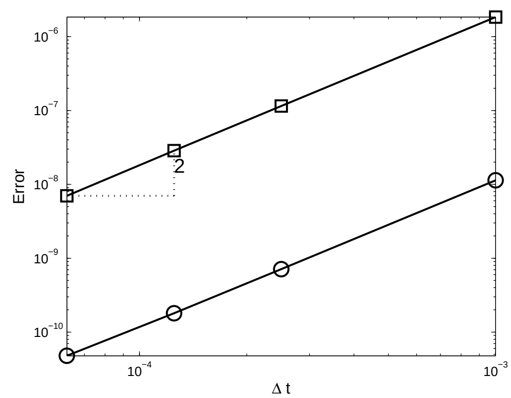
(a) Algorithm 1



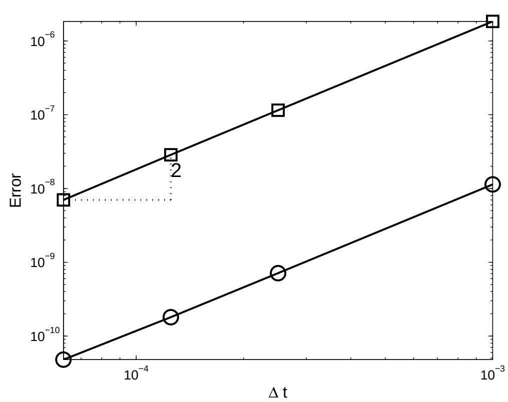
(b) Algorithm 2



(c) Algorithm 3

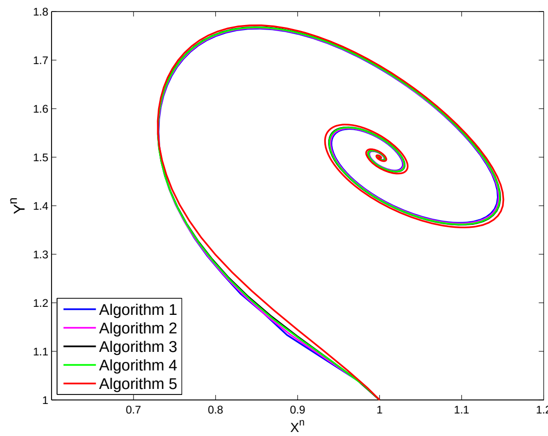


(d) Algorithm 4

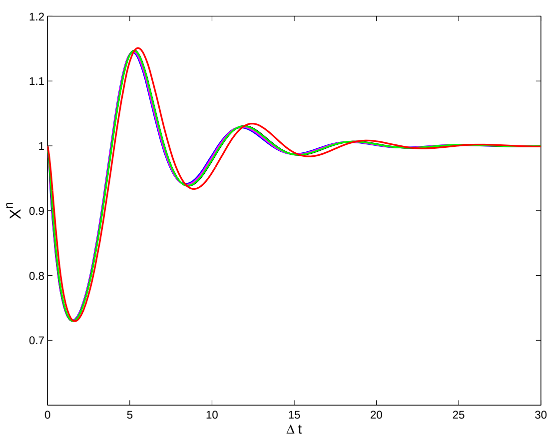


(e) Algorithm 5

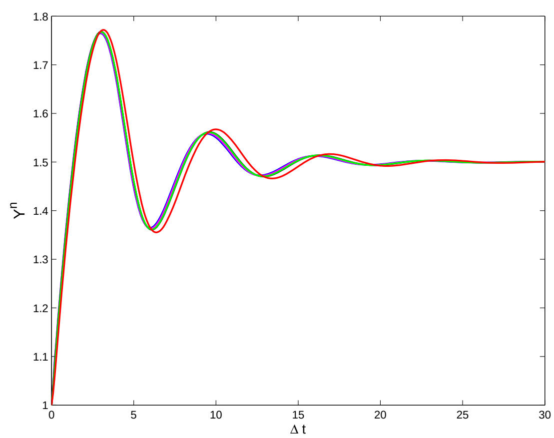
Figure 2.10: The Brusselator Problem: Time Accuracy of the Algorithms used for the Simulation



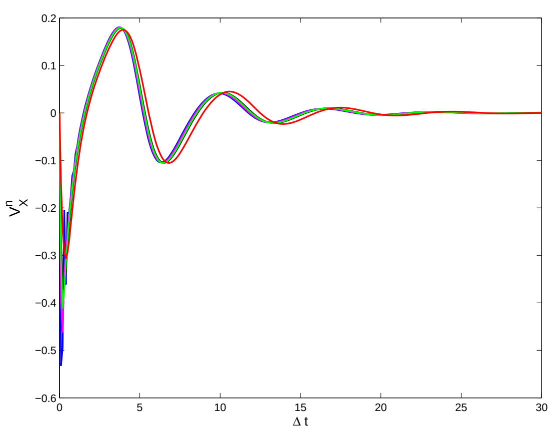
(a) Limit Circle



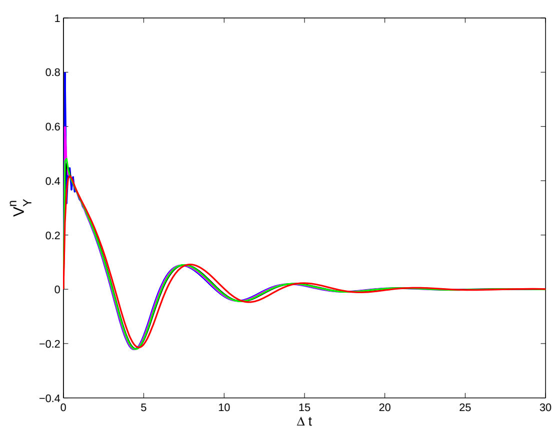
(b) X^n



(c) Y^n

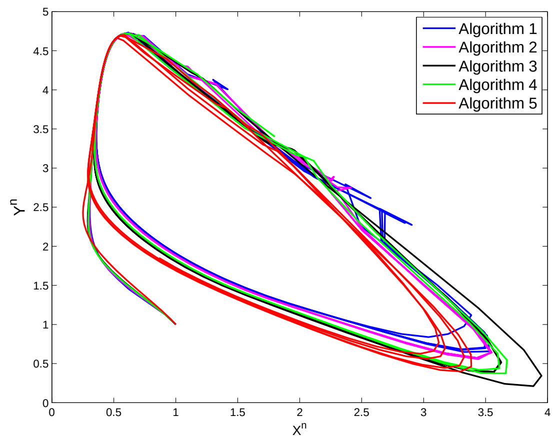


(d) V_X^n

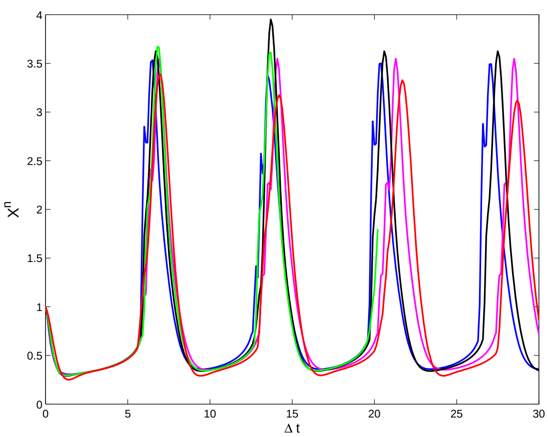


(e) V_Y^n

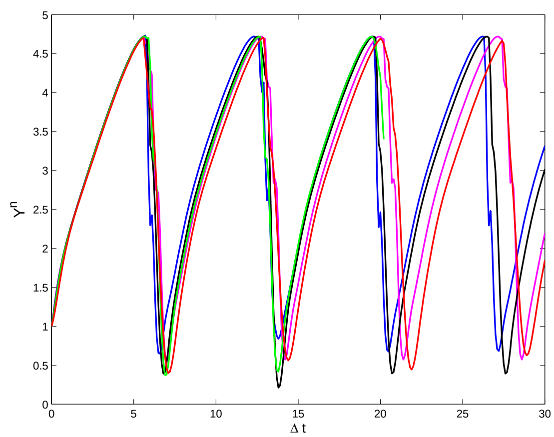
Figure 2.11: The Brusselator Problem: Numerical Results for Case 1 (stable): $(A, B) = (1, 1.5)$



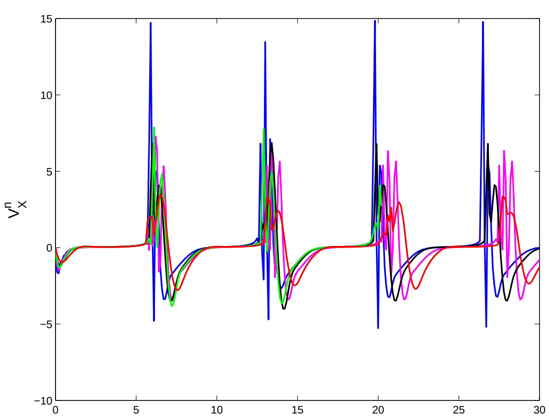
(a) Limit Circle



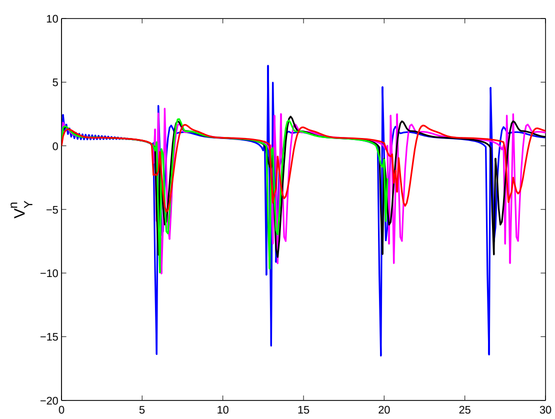
(b) X^n



(c) Y^n



(d) V_X^n



(e) V_Y^n

Figure 2.12: The Brusselator Problem: Numerical Results for Case 2 (unstable): $(A, B) = (1, 3)$

Example 2.3.3

(Second- and First-order Coupled/Uncoupled Thermal Stress Wave Propagation Problems)

Algorithm 2.2.1 can be efficiently applied to coupled problems of second- and first-order ODEs. See [19, 20] for the numerical results for the coupled and uncoupled thermal stress wave propagation problems with Algorithm 2.2.1 with implicit and explicit settings via the adaptation process.

2.4 Mechanical Integrators

2.4.1 Equations of Motion in the Lagrangian and Hamiltonian Formalisms for Conservative Systems

Lagrange's Equation of Motion: Consider an n_{g}-dimensional configuration manifold Q with local coordinates $\mathbf{q}(t) = (q_1, q_2, \cdots, q_{n_{\mathrm{g}}})^T(t) : \mathbb{I} := [t_0, t_L] \subset \mathbb{R} \to Q$. The corresponding velocity is defined as the time derivative of $\mathbf{q}(t)$, i.e., $\dot{\mathbf{q}}(t) = d\mathbf{q}/dt$, defined on the tangent space at $\mathbf{q}$: $\dot{\mathbf{q}}(t) : \mathbb{I} \to T_{\mathbf{q}}Q$. An autonomous Lagrangian function $\mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}) : TQ \to \mathbb{R}$ of a system is defined on the tangent bundle (also called as ***velocity phase space*** or ***state space***), TQ.

If initial conditions $(\mathbf{q}, \dot{\mathbf{q}})(t_0) = (\mathbf{q}^0, \mathbf{v}^0)$ are given, the ***Lagrange equation of motion***[3] of the form,

$$\boxed{\frac{d}{dt}\left(\frac{\partial \mathscr{L}(\mathbf{q}, \dot{\mathbf{q}})}{\partial \dot{\mathbf{q}}}\right) - \frac{\partial \mathscr{L}(\mathbf{q}, \dot{\mathbf{q}})}{\partial \mathbf{q}} = \mathbf{0}} \tag{2.114}$$

uniquely defines the dynamics of the n_{g}-dimensional system.

[3] The derivations of the Lagrangian equations of motion and Hamilton's canonical equations of motion for nonconservative constrained mechanical systems are shown in Chapter 7.

Theorem 2.4.1 (Total Energy Conservation)

The autonomous Jacobi integral of the system is defined by

$$(\mathbf{q}, \dot{\mathbf{q}}) := \dot{\mathbf{q}}^T \frac{\partial \mathscr{L}(\mathbf{q}, \dot{\mathbf{q}})}{\partial \dot{\mathbf{q}}} - \mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}) \tag{2.115}$$

and it is conserved, i.e., $d\mathscr{E}/dt = 0$*, along a solution of the Lagrange's equation of motion. When the autonomous Lagrangian function of the systems is defined as the difference between the kinetic energy function of the quadratic form in the velocity and potential energy function as a function of the configuration, i.e.,*

$$\mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}) = \mathscr{T}(\mathbf{q}, \dot{\mathbf{q}}) - \mathscr{U}(\mathbf{q}) = \frac{1}{2}\dot{\mathbf{q}}^T \mathbf{M}(\mathbf{q})\dot{\mathbf{q}} - \mathscr{U}(\mathbf{q}) \tag{2.116}$$

where $\mathbf{M}(\mathbf{q}) :\in \mathbb{R}^{n_g \times n_g}$ *is a symmetric, positive-definite matrix, is the total energy function of the system:*

$$(\mathbf{q}, \dot{\mathbf{q}}) = (\mathbf{q}, \dot{\mathbf{q}}) = \frac{1}{2}\dot{\mathbf{q}}^T \mathbf{M}(\mathbf{q})\dot{\mathbf{q}} + \mathscr{U}(\mathbf{q}) \tag{2.117}$$

Hamilton's Canonical Equations of Motion: In the Hamiltonian mechanics, a set of the generalized coordinates $\mathbf{q} \in Q$ and so-called canonical momentum $\mathbf{p} = \partial\mathscr{L}/\partial\dot{\mathbf{q}} : \mathbb{I} \to T^*_{\mathbf{q}}Q$, which is conjugate to the generalized velocity, $\dot{\mathbf{q}}(t) : \mathbb{I} \to T_{\mathbf{q}}Q$, is used as the primary variables to describe the dynamics of the system.

Proposition 2.4.1 (Fibre Derivative [21])

*The **fibre derivative*** $\mathbb{F}\mathscr{L} : TQ \to T^*Q$ *for a Lagrangian function* $\mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}) : TQ \to \mathbb{R}$ *is defined by*

$$\mathbb{F}\mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}) = \left(\mathbf{q}, \frac{\partial \mathscr{L}(\mathbf{q}, \dot{\mathbf{q}})}{\partial \dot{\mathbf{q}}}\right) = (\mathbf{q}, \mathbf{p}) \tag{2.118}$$

where T^*Q *is called the **phase space**, or the **cotangent bundle** to the configuration manifold,* Q*. The transformation* $TQ \to T^*Q : (\mathbf{q}, \dot{\mathbf{q}}) \mapsto (\mathbf{q}, \mathbf{p})$ *is known as the **Legendre transformation**.*

Employing the fibre derivative for the autonomous Lagrangian function, $\mathscr{L}(\mathbf{q}, \dot{\mathbf{q}})$, the autonomous Hamiltonian function, $\mathscr{H}(\mathbf{q}, \mathbf{p}) : T^*Q \to \mathbb{R}$, is defined as

$$\mathscr{H}(\mathbf{q}, \mathbf{p}) := \dot{\mathbf{q}}^T \mathbf{p} - \mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}) \tag{2.119}$$

If the Legendre transformation is invertible, the ***Hamilton's canonical equations of motion*** of the form,

$$\boxed{\dot{\mathbf{q}} = \frac{\partial \mathscr{H}(\mathbf{q}, \mathbf{p})}{\partial \mathbf{p}} \quad \text{and} \quad \dot{\mathbf{p}} = -\frac{\partial \mathscr{H}(\mathbf{q}, \mathbf{p})}{\partial \mathbf{q}}} \tag{2.120}$$

with given initial conditions $(\mathbf{q}, \mathbf{p})(t_0) = (\mathbf{q}^0, \mathbf{p}^0)$ uniquely defines the dynamics, which are equivalent to the ones for the Lagrange's equation of motion, on the phase space. Utilizing the Poisson's bracket (see Definition 2.4.2), Eq. (2.120) can be simply written as

$$\boxed{\dot{\mathbf{q}} = [\mathbf{q}, \mathscr{H}(\mathbf{q}, \mathbf{p})] \quad \text{and} \quad \dot{\mathbf{p}} = [\mathbf{p}, \mathscr{H}(\mathbf{q}, \mathbf{p})]} \tag{2.121}$$

respectively.

Defining $\mathbf{z}(t) := (\mathbf{q}^T, \mathbf{p}^T)^T : \mathbb{I} \to T^*Q$, Hamilton's canonical equations for the autonomous Hamiltonian function can be also written compactly as

$$\boxed{\dot{\mathbf{z}}(t) = \mathbb{J} D\mathscr{H}(\mathbf{z})} \tag{2.122}$$

where

$$\dot{\mathbf{z}} := \frac{d}{dt}(\mathbf{q}^T, \mathbf{p}^T)^T \quad \text{and} \quad D\mathscr{H}(\mathbf{z}) := \begin{bmatrix} \partial\mathscr{H}/\partial\mathbf{q} \\ \partial\mathscr{H}/\partial\mathbf{p} \end{bmatrix} \tag{2.123}$$

Matrix $\mathbb{J}$ is a skew-symmetric matrix, known as ***symplectic matrix***, and it is defined as

$$\mathbb{J} := \begin{bmatrix} \mathbf{0}_{n_g} & \mathbf{I}_{n_g} \\ -\mathbf{I}_{n_g} & \mathbf{0}_{n_g} \end{bmatrix} \in \mathbb{R}^{2n_g \times 2n_g} \tag{2.124}$$

with the zero and identity matrices, $\mathbf{0}_{n_g} \in \mathbb{R}^{n_g \times n_g}$ and $\mathbf{I}_{n_g} \in \mathbb{R}^{n_g \times n_g}$, respectively. Notice that $\mathbb{J}$ has unit determinant, i.e., $\det(\mathbb{J}) = +1$, and

$$\mathbb{J}^{-1} = \mathbb{J}^T = -\mathbb{J} \tag{2.125}$$

Proposition 2.4.2 (Poisson's Bracket)

Poisson's bracket is defined as:

$$\boxed{[A, B] := \frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i}} \tag{2.126}$$

for arbitrary functions, $A(\mathbf{q}, \mathbf{p}, t)$ and $B(\mathbf{q}, \mathbf{p}, t)$. In terms of $\mathbf{z}(t) = (\mathbf{q}^T, \mathbf{p}^T)^T(t)$, Poisson's bracket for the functions $A(\mathbf{z}, t)$ and $B(\mathbf{z}, t)$ can be expressed as

$$\boxed{[A, B] = (D_1 A(\mathbf{z}, t))^T \, \mathbb{J} \, (D_1 B(\mathbf{z}, t))} \tag{2.127}$$

where $D_i A$ denotes the partial derivative of A with respect to its i^{th} slot (argument) [4] .

Remark 2.4.1

1. *We can verify the following properties of Poisson's bracket (proof omitted):*

$$\begin{aligned}
&[A, \alpha_1 B + \alpha_2 C] = \alpha_1 [A, B] + \alpha_2 [A, C] \ (\textit{Linearlity}) \\
&[A, B] = -[B, A] \ (\textit{Skew-symmetry}) \\
&[A + B, C] = [A, C] + [B, C] \\
&[A, BC] = [A, B]C + B[A, C] \\
&[AB, C] + [BC, A] + [CA, B] \\
&[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0 \ (\textit{Jacobi identity})
\end{aligned} \tag{2.129}$$

[4] *For $A(\mathbf{z}, t) = A(\mathbf{q}, \mathbf{p}, t)$,*

$$D_1 A(\mathbf{z}, t) = \nabla A(\mathbf{z}, t) = \frac{\partial A(\mathbf{z}, t)}{\partial \mathbf{z}} = \begin{bmatrix} \frac{\partial A(\mathbf{z}, t)}{\partial \mathbf{q}} \\ \frac{\partial A(\mathbf{z}, t)}{\partial \mathbf{p}} \end{bmatrix} \tag{2.128}$$

for arbitrary functions, $A(\mathbf{q},\mathbf{p},t)$, $B(\mathbf{q},\mathbf{p},t)$, *and* $C(\mathbf{q},\mathbf{p},t)$; *and* $\alpha_1, \alpha_2 \in \mathbb{R}$.[5]

2. *For arbitrary functions,* $\mathbf{u} = \mathbf{u}(\mathbf{q},\mathbf{p},t)$ *and* $\mathbf{w} = \mathbf{w}(\mathbf{q},\mathbf{p},t)$, *the derivatives with respect to* q_i *and* p_i *are given as*

$$\begin{aligned} \frac{\partial}{\partial q_i}[\mathbf{u},\mathbf{w}] &= \left[\frac{\partial \mathbf{u}}{\partial q_i}, \mathbf{w}\right] + \left[\mathbf{u}, \frac{\partial \mathbf{w}}{\partial q_i}\right] \\ \frac{\partial}{\partial p_i}[\mathbf{u},\mathbf{w}] &= \left[\frac{\partial \mathbf{u}}{\partial p_i}, \mathbf{w}\right] + \left[\mathbf{u}, \frac{\partial \mathbf{w}}{\partial p_i}\right] \end{aligned} \tag{2.131}$$

respectively (proof omitted).

3. *Evaluating Poisson's bracket for* q_i *and* p_i, *we get*[6]

$$\begin{aligned} [q_i, p_j] &= \delta_{ij} \\ [q_i, q_j] &= [p_i, p_j] = 0 \end{aligned} \tag{2.133}$$

4. *Let* $X_j = X_j(\mathbf{q},\mathbf{p},t)$ *be an arbitrary function. Taking the total time derivative of* X_j, *we obain*

$$\frac{d}{dt}X_j = \frac{\partial X_j}{\partial q_i}\dot{q}_i + \frac{\partial X_j}{\partial p_i}\dot{p}_i + \frac{\partial X_j}{\partial t} \tag{2.134}$$

Substituting Hamilton's canonical equations yields

$$\begin{aligned} \frac{d}{dt}X_j(\mathbf{q},\mathbf{p},t) &= \frac{\partial X_j}{\partial q_i}\frac{\partial \mathscr{H}}{\partial p_i} - \frac{\partial X_j}{\partial p_i}\frac{\partial \mathscr{H}}{\partial q_i} + \frac{\partial X_j}{\partial t} \\ &= \left[X_j, \mathscr{H}\right] + \frac{\partial X_j}{\partial t} \end{aligned} \tag{2.135}$$

---

[5] *From the skew-symmetry of Posson's bracket, we have*

$$[A, A] = 0 \tag{2.130}$$

[6] $\delta_{ij} = [\mathbf{I}]_{ij}$ *denotes the Kronecker delta symbol defined by*

$$\delta_{ij} = \begin{cases} 1 & \textit{if } i = j \\ 0 & \textit{if } i \neq j \end{cases} \tag{2.132}$$

for $i, j = 1, 2, \cdots, n$.

If $\mathbf{X}$ *is autonomous, i.e.,* $X_j = X_j(\mathbf{q}, \mathbf{p})$*, Eq.* (2.135) *can be written as*

$$\frac{d}{dt}X_j(\mathbf{q}, \mathbf{p}) = \left[X_j(\mathbf{q}, \mathbf{p}), \mathscr{H}\right] \tag{2.136}$$

Notice that, from Eq. (2.136)*,* X_i *is constant (in time) along the solution of Hamilton's canonical equations with* $\mathscr{H}$ *if and only if* $\left[X_j, \mathscr{H}\right] = 0$*.*

Theorem 2.4.2 (Total Energy (Hamiltonian) Conservation)

The autonomous Hamiltonian $\mathscr{H}(\mathbf{q}, \mathbf{p}) = \mathscr{E}(\mathbf{q}, \dot{\mathbf{q}})$ *is conserved,*

$$\frac{d}{dt}\mathscr{H}(\mathbf{q}, \mathbf{p}) = [\mathscr{H}(\mathbf{q}, \mathbf{p}), \mathscr{H}(\mathbf{q}, \mathbf{p})] = 0 \tag{2.137}$$

along a solution of the Hamilton's canonical equations of motion. When the Lagrangian function is given as in Eq. (2.116)*, the Hamiltonian is the system total energy.*

2.4.2 Symplectic Transformations and Symplectic Integrators within the *i*Integrators

Symplectic Transformations

Definition 2.4.1 (Symplectic Map)

A mapping $\mathbf{h} : U \subset \mathbb{R}^{2n_g} \to \mathbb{R}^{2n_g}$ *is called* ***symplectic*** *if its Jacobian matrix* $D\mathbf{h} \in \mathbb{R}^{2n_g \times 2n_g}$ *satisfies*

$$(D\mathbf{h})^T\ \mathbb{J}\ (D\mathbf{h}) = \mathbb{J} \tag{2.138}$$

where $\mathbb{J}$ *is the symplectic matrix, defined in Eq.* (2.124)*.*

In an autonomous Hamiltonian system, the ***Hamiltonian flow*** $\boldsymbol{\varphi}_t$ is defined as the mapping that advances the solution in time from $(\mathbf{q}, \mathbf{p})(t_0) = (\mathbf{q}^0, \mathbf{p}^0) \in T^*Q$ onto $(\mathbf{q}, \mathbf{p})(t) = (\mathbf{q}, \mathbf{p}) \in T^*Q$ as

$$\boldsymbol{\varphi}_t(\mathbf{q}^0, \mathbf{p}^0) = \left(\mathbf{q}(t; \mathbf{q}^0, \mathbf{p}^0), \mathbf{p}(t; \mathbf{q}^0, \mathbf{p}^0)\right) \tag{2.139}$$

At $t = t_0$, the flow, i.e., $\boldsymbol{\varphi}_{t_0}$ is the identity map.

Theorem 2.4.3 (Symplectic Transformation)

Assume $\mathscr{H}(\mathbf{q}, \mathbf{p})$ is twice continuously differentiable on $U \subset T^*Q$. Then, the ***Hamiltonian flow*** *$\boldsymbol{\varphi}_t$ is a* ***symlectic transformation****.*

Proof. Since matrix $\partial\boldsymbol{\varphi}_t/\partial\mathbf{z}^0$ satisfies

$$\frac{d}{dt}\left(\frac{\partial\boldsymbol{\varphi}_t}{\partial\mathbf{z}^0}\right) = \mathbb{J}^{-1}\mathbf{H}\left(\frac{\partial\boldsymbol{\varphi}_t}{\partial\mathbf{z}^0}\right) \tag{2.140}$$

where $\mathbf{H} := D^2\mathscr{H}(\boldsymbol{\varphi}_t(\mathbf{z}^0))$ is the symmetric Hessian matrix, the following relation is valid:

$$\begin{aligned} \frac{d}{dt}\left[\left(\frac{\partial\boldsymbol{\varphi}_t}{\partial\mathbf{z}^0}\right)^T \mathbb{J}\left(\frac{\partial\boldsymbol{\varphi}_t}{\partial\mathbf{z}^0}\right)\right] &= \left[\frac{d}{dt}\left(\frac{\partial\boldsymbol{\varphi}_t}{\partial\mathbf{z}^0}\right)\right]^T \mathbb{J}\left(\frac{\partial\boldsymbol{\varphi}_t}{\partial\mathbf{z}^0}\right) + \left(\frac{\partial\boldsymbol{\varphi}_t}{\partial\mathbf{z}^0}\right)^T \mathbb{J}\left[\frac{d}{dt}\left(\frac{\partial\boldsymbol{\varphi}_t}{\partial\mathbf{z}^0}\right)\right] \\ &= \left(\frac{\partial\boldsymbol{\varphi}_t}{\partial\mathbf{z}^0}\right)^T \underbrace{\mathbf{H}^T}_{\mathbf{H}} \underbrace{\mathbb{J}^{-T}\mathbb{J}}_{-\mathbf{I}}\left(\frac{\partial\boldsymbol{\varphi}_t}{\partial\mathbf{z}^0}\right) + \left(\frac{\partial\boldsymbol{\varphi}_t}{\partial\mathbf{z}^0}\right)^T \underbrace{\mathbb{J}\mathbb{J}^{-1}}_{\mathbf{I}}\mathbf{H}\left(\frac{\partial\boldsymbol{\varphi}_t}{\partial\mathbf{z}^0}\right) \\ &= \mathbf{0} \end{aligned} \tag{2.141}$$

Since

$$\left(\frac{\partial\boldsymbol{\varphi}_{t_0}}{\partial\mathbf{z}^0}\right)^T \mathbb{J}\left(\frac{\partial\boldsymbol{\varphi}_{t_0}}{\partial\mathbf{z}^0}\right) = \mathbb{J} \quad \text{at} \quad t = t_0 \tag{2.142}$$

the relation

$$\left(\frac{\partial\boldsymbol{\varphi}_t}{\partial\mathbf{z}^0}\right)^T \mathbb{J}\left(\frac{\partial\boldsymbol{\varphi}_t}{\partial\mathbf{z}^0}\right) = \mathbb{J} \tag{2.143}$$

holds for $\mathscr{H}(\boldsymbol{\varphi}_t(\mathbf{z}^0))$ for $t \in \mathbb{I}$; hence, the Hamiltonian flow is a symplectic transformation. ∎

Symplectic Integrators within the *i*Integrators

Since the *i*Integrators essentially include numerous one-step schemes of second-order time accuracy, we need to investigate the conditions of the algorithmic parameters that guarantee the symplecticity of the algorithms. For brevity of exposition, we assume the Lagrangian function is autonomous and given as in Eq. (2.116) with a constant $\mathbf{M}$.

Theorem 2.4.4 (Symplectic Integrators within the GS4-2 Family of Algorithms) *In conservative systems, the symplectic condition for the GS4-2 family of algorithms (Algorithm 2.2.1) is given by:*

$$\boxed{W_1\Lambda_1 = \lambda_1 - \frac{\lambda_3}{\lambda_5}} \tag{2.144}$$

Therefore, the symplectic spectral conditions for the U0- and V0-based families are given by

$$\rho_\infty^{s}(1+\rho_\infty^{\min}+\rho_\infty^{\max}-\rho_\infty^{\min}\rho_\infty^{\max}) = 2 \qquad \textit{for U0-based Family} \tag{2.145}$$

$$\rho_\infty^{\min}\rho_\infty^{\max} = 1 \qquad \textit{for V0-based Family} \tag{2.146}$$

respectively.

Proof. To prove this theorem, without loss of generality, let the positive-definite mass matrix be the identity matrix for simplicity of the exposition: $\mathbf{M} = \mathbf{I}$. Therefore, the momentum update is simply given as

$$\mathbf{p}^{n+1} = \mathbf{p}^n + \lambda_4\mathbf{a}^n\Delta t + \lambda_5\Delta\mathbf{a}^n\Delta t \tag{2.147}$$

Substituting

$$\Delta\mathbf{a} = \frac{1}{W_1\Lambda_6}\left[\mathbf{g}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n) - \mathbf{a}^n\right] \tag{2.148}$$

we have

$$\mathbf{p}^{n+1} = \mathbf{p}^n + \left(\lambda_4 - \frac{\lambda_5}{W_1\Lambda_6}\right)\mathbf{a}^n\Delta t + \frac{\lambda_5}{W_1\Lambda_6}\mathbf{g}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n)\Delta t \tag{2.149}$$

Hence, the differential of $\mathbf{p}^{n+1}$ obeys

$$\begin{aligned} d\mathbf{p}^{n+1} &= d\mathbf{p}^n + \Delta t\left(\lambda_4 - \frac{\lambda_5}{W_1\Lambda_6}\right)d\mathbf{a}^n + \frac{\Delta t\lambda_5}{W_1\Lambda_6}d\mathbf{g}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n) \\ &= d\mathbf{p}^n + \Delta t\left(\lambda_4 - \frac{\lambda_5}{W_1\Lambda_6}\right)d\mathbf{a}^n + \frac{\Delta t\lambda_5}{W_1\Lambda_6}\left[\tilde{\mathbf{K}}_T^n d\tilde{\mathbf{q}}^n + \tilde{\mathbf{C}}_T^n d\tilde{\mathbf{v}}^n\right] \end{aligned} \tag{2.150}$$

where

$$\tilde{\mathbf{K}}_T^n := \mathfrak{D}_1\, \mathbf{g}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n) = \frac{\partial \mathbf{g}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n)}{\partial \tilde{\mathbf{q}}^n} \tag{2.151}$$

$$\tilde{\mathbf{C}}_T^n := \mathfrak{D}_2\, \mathbf{g}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n) = \frac{\partial \mathbf{g}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n)}{\partial \tilde{\mathbf{v}}^n} \tag{2.152}$$

Therefore,

$$\frac{\partial \mathbf{p}^{n+1}}{\partial \mathbf{p}^n} = \mathbf{I} + \frac{\Delta t\lambda_5}{W_1\Lambda_6}\tilde{\mathbf{K}}_T^n\frac{\partial \tilde{\mathbf{q}}^n}{\partial \mathbf{p}^n} + \frac{\Delta t\lambda_5}{W_1\Lambda_6}\tilde{\mathbf{C}}_T^n\frac{\partial \tilde{\mathbf{p}}^n}{\partial \mathbf{p}^n} \tag{2.153a}$$

$$\frac{\partial \mathbf{p}^{n+1}}{\partial \mathbf{q}^n} = \frac{\Delta t\lambda_5}{W_1\Lambda_6}\tilde{\mathbf{K}}_T^n\frac{\partial \tilde{\mathbf{q}}^n}{\partial \mathbf{q}^n} + \frac{\Delta t\lambda_5}{W_1\Lambda_6}\tilde{\mathbf{C}}_T^n\frac{\partial \tilde{\mathbf{p}}^n}{\partial \mathbf{q}^n} \tag{2.153b}$$

Since $\tilde{\mathbf{q}}^n$ and $\tilde{\mathbf{v}}^n$ can be written in the forms

$$\begin{aligned} \tilde{\mathbf{q}}^n &= \mathbf{q}^n + W_1\Lambda_1\mathbf{v}^n\Delta t + W_2\Lambda_2\mathbf{a}^n\Delta t^2 + W_3\Lambda_3\Delta\mathbf{a}^n\Delta t^2 \\ &= \mathbf{q}^n + W_1\Lambda_1\mathbf{v}^n\Delta t + W_2\Lambda_2\mathbf{a}^n\Delta t^2 + \frac{W_3\Lambda_3}{\lambda_3}\left[\mathbf{q}^{n+1} - \mathbf{q}^n - \Delta t\lambda_1\mathbf{p}^n - \Delta t^2\lambda_2\mathbf{a}^n\right] \\ &= \left(1 - \frac{W_3\Lambda_3}{\lambda_3}\right)\mathbf{q}^n + \frac{W_3\Lambda_3}{\lambda_3}\mathbf{q}^{n+1} \\ &\quad + \Delta t\left(W_1\Lambda_1 - \frac{\lambda_1 W_3\Lambda_3}{\lambda_3}\right)\mathbf{p}^n + \Delta t^2\left(W_2\Lambda_2 - \frac{\lambda_2 W_3\Lambda_3}{\lambda_3}\right)\mathbf{a}^n \end{aligned} \tag{2.154}$$

$$\begin{aligned} \tilde{\mathbf{p}}^n &= \mathbf{p}^n + W_1\Lambda_4\mathbf{a}^n\Delta t + W_2\Lambda_5\Delta\mathbf{a}^n\Delta t \\ &= \mathbf{p}^n + W_1\Lambda_4\mathbf{a}^n\Delta t + \frac{W_2\Lambda_5}{\lambda_5}\left[\mathbf{p}^{n+1} - \mathbf{p}^n - \Delta t\lambda_4\mathbf{a}^n\right] \\ &= \left(1 - \frac{W_2\Lambda_5}{\lambda_5}\right)\mathbf{p}^n + \frac{W_2\Lambda_5}{\lambda_5}\mathbf{p}^{n+1} + \Delta t\left(W_1\Lambda_4 - \frac{\lambda_4 W_2\Lambda_5}{\lambda_5}\right)\mathbf{a}^n \end{aligned} \tag{2.155}$$

respectively; the differentials obey

$$\begin{aligned} d\tilde{\mathbf{q}}^n &= \left(1 - \frac{W_3\Lambda_3}{\lambda_3}\right) d\mathbf{q}^n + \frac{W_3\Lambda_3}{\lambda_3} d\mathbf{q}^{n+1} \\ &\quad + \Delta t \left(W_1\Lambda_1 - \frac{\lambda_1 W_3\Lambda_3}{\lambda_3}\right) d\mathbf{p}^n + \Delta t^2 \left(W_2\Lambda_2 - \frac{\lambda_2 W_3\Lambda_3}{\lambda_3}\right) d\mathbf{a}^n \end{aligned} \tag{2.156}$$

$$d\tilde{\mathbf{p}}^n = \left(1 - \frac{W_2\Lambda_5}{\lambda_5}\right) d\mathbf{p}^n + \frac{W_2\Lambda_5}{\lambda_5} d\mathbf{p}^{n+1} + \Delta t \left(W_1\Lambda_4 - \frac{\lambda_4 W_2\Lambda_5}{\lambda_5}\right) d\mathbf{a}^n \tag{2.157}$$

and therefore, we get

$$\begin{aligned} \frac{\partial \tilde{\mathbf{q}}^n}{\partial \mathbf{p}^n} &= \frac{W_3\Lambda_3}{\lambda_3} \frac{\partial \mathbf{q}^{n+1}}{\partial \mathbf{p}^n} + \Delta t \left(W_1\Lambda_1 - \frac{\lambda_1 W_3\Lambda_3}{\lambda_3}\right) \mathbf{I} \\ \frac{\partial \tilde{\mathbf{p}}^n}{\partial \mathbf{p}^n} &= \frac{W_2\Lambda_5}{\lambda_5} \frac{\partial \mathbf{p}^{n+1}}{\partial \mathbf{p}^n} + \left(1 - \frac{W_2\Lambda_5}{\lambda_5}\right) \mathbf{I} \end{aligned} \tag{2.158a}$$

and

$$\begin{aligned} \frac{\partial \tilde{\mathbf{q}}^n}{\partial \mathbf{q}^n} &= \frac{W_3\Lambda_3}{\lambda_3} \frac{\partial \mathbf{q}^{n+1}}{\partial \mathbf{q}^n} + \left(1 - \frac{W_3\Lambda_3}{\lambda_3}\right) \mathbf{I} \\ \frac{\partial \tilde{\mathbf{p}}^n}{\partial \mathbf{q}^n} &= \frac{W_2\Lambda_5}{\lambda_5} \frac{\partial \mathbf{p}^{n+1}}{\partial \mathbf{q}^n} \end{aligned} \tag{2.158b}$$

Next, from the update equation for $\mathbf{q}$,

$$\begin{aligned} \mathbf{q}^{n+1} &= \mathbf{q}^n + \lambda_1 \mathbf{p}^n \Delta t + \lambda_2 \mathbf{a}^n \Delta t^2 + \lambda_3 \Delta \mathbf{a}^n \Delta t^2 \\ &= \mathbf{q}^n + \lambda_1 \mathbf{p}^n \Delta t + \lambda_2 \mathbf{a}^n \Delta t^2 + \Delta t^2 \lambda_3 \frac{\mathbf{p}^{n+1} - \mathbf{p}^n - \Delta t \lambda_4 \mathbf{a}^n}{\Delta t \lambda_5} \end{aligned} \tag{2.159}$$

the differential of $\mathbf{q}^{n+1}$ is obtined as

$$d\mathbf{q}^{n+1} = d\mathbf{q}^n + \Delta t \left(\lambda_1 - \frac{\lambda_3}{\lambda_5}\right) d\mathbf{p}^n + \Delta t \frac{\lambda_3}{\lambda_5} d\mathbf{p}^{n+1} + \Delta t^2 \left(\lambda_2 - \frac{\lambda_3\lambda_4}{\lambda_5}\right) d\mathbf{a}^n \tag{2.160}$$

Therefore,

$$\frac{\partial \mathbf{q}^{n+1}}{\partial \mathbf{p}^n} = \Delta t \left(\lambda_1 - \frac{\lambda_3}{\lambda_5}\right) \mathbf{I} + \Delta t \frac{\lambda_3}{\lambda_5} \frac{\partial \mathbf{p}^{n+1}}{\partial \mathbf{p}^n} \tag{2.161a}$$

$$\frac{\partial \mathbf{q}^{n+1}}{\partial \mathbf{q}^n} = \mathbf{I} + \Delta t \frac{\lambda_3}{\lambda_5} \frac{\partial \mathbf{p}^{n+1}}{\partial \mathbf{q}^n} \tag{2.161b}$$

Since we can cast Eq. (2.153) (together with Eq. (2.158)) and Eq. (2.161) into the following form,

$$\underbrace{\begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}}_{\mathbf{A}} \underbrace{\begin{bmatrix} \frac{\partial \mathbf{p}^{n+1}}{\partial \mathbf{p}^n} & \frac{\partial \mathbf{p}^{n+1}}{\partial \mathbf{q}^n} \\ \frac{\partial \mathbf{q}^{n+1}}{\partial \mathbf{p}^n} & \frac{\partial \mathbf{q}^{n+1}}{\partial \mathbf{p}^n} \end{bmatrix}}_{\frac{\partial(\mathbf{p}^{n+1},\mathbf{q}^{n+1})}{\partial(\mathbf{p}^n,\mathbf{q}^n)}} = \underbrace{\begin{bmatrix} \mathbf{B}_{11} & \mathbf{B}_{12} \\ \mathbf{B}_{21} & \mathbf{B}_{22} \end{bmatrix}}_{\mathbf{B}} \tag{2.162}$$

where

$$\begin{aligned} \mathbf{A}_{11} &= \mathbf{I} - \Delta t \frac{W_2\Lambda_5}{W_1\Lambda_6}\tilde{\mathbf{C}}_T^n \\ \mathbf{A}_{12} &= -\Delta t \frac{\lambda_5}{\lambda_3}\frac{W_3\Lambda_3}{W_1\Lambda_6}\tilde{\mathbf{K}}_T^n \\ \mathbf{A}_{21} &= \Delta t \frac{\lambda_3}{\lambda_5} \\ \mathbf{A}_{22} &= -\mathbf{I} \end{aligned} \tag{2.163}$$

and

$$\begin{aligned} \mathbf{B}_{11} &= \mathbf{I} + \Delta t \frac{\lambda_5}{W_1\Lambda_6}\left(1 - \frac{W_2\Lambda_5}{\lambda_5}\right)\tilde{\mathbf{C}}_T^n + \Delta t^2 \frac{\lambda_5}{W_1\Lambda_6}\left(W_1\Lambda_1 - \frac{\lambda_1}{\lambda_3}W_3\Lambda_3\right)\tilde{\mathbf{K}}_T^n \\ \mathbf{B}_{12} &= \Delta t \frac{\lambda_5}{W_1\Lambda_6}\left(1 - \frac{W_3\Lambda_3}{\lambda_3}\right)\tilde{\mathbf{K}}_T^n \\ \mathbf{B}_{21} &= \Delta t\left(\frac{\lambda_3}{\lambda_5} - \lambda_1\right)\mathbf{I} \\ \mathbf{B}_{22} &= -\mathbf{I} \end{aligned} \tag{2.164}$$

it is straightforward to check the symplectic condition of the family of algorithms,

$$\left[\frac{\partial(\mathbf{p}^{n+1},\mathbf{q}^{n+1})}{\partial(\mathbf{p}^n,\mathbf{q}^n)}\right]^T \mathbb{J} \left[\frac{\partial(\mathbf{p}^{n+1},\mathbf{q}^{n+1})}{\partial(\mathbf{p}^n,\mathbf{q}^n)}\right] = \mathbb{J} \tag{2.165}$$

with the skew-symmetric symplectic matrix. Since Eq. (2.165) leads to

$$\begin{aligned} &W_1\Lambda_6 - \Delta t W_2\Lambda_5\tilde{\mathbf{C}}_T^n - \Delta t^2 W_3\Lambda_3\tilde{\mathbf{K}}_T^n \\ =&W_1\Lambda_6 + \Delta t(\lambda_5 - W_2\Lambda_5)\tilde{\mathbf{C}}_T^n + \Delta t^2(\lambda_3 - W_3\Lambda_3 + W_1\Lambda_1\lambda_5 - \lambda_1\lambda_5)\tilde{\mathbf{K}}_T^n \end{aligned} \tag{2.166}$$

The symplectic condition for the GS4-2 family of algorithms yields:

$$\lambda_5 = 0 \ \text{ and } \ W_1\Lambda_1 = \lambda_1 - \frac{\lambda_3}{\lambda_5} \tag{2.167}$$

Therefore, when $\tilde{\mathbf{C}}_T^n = \mathbf{0}$, the symplectic condition is simply given by

$$W_1\Lambda_1 = \lambda_1 - \frac{\lambda_3}{\lambda_5} \tag{2.168}$$

Substituting the spectral parameters in the U0- and V0-based families, Eq. (2.168) yields Eq. (2.145) and Eq. (2.146), respectively. ∎

Remark 2.4.2

1. *When $\tilde{\mathbf{C}}_T^n = \mathbf{0}$, the only scheme that is symplectic within the **implicit** GS4-2 U0-based family of algorithms is: $(\rho_\infty^{\min}, \rho_\infty^{\max}, \rho_\infty^{s}) = (1, 1, 1)$, i.e., the MPR-EPA method. Within the **implicit** GS4-2 V0-based family of algorithms, any scheme that satisfies $\rho_\infty^{\min} = \rho_\infty^{\max} = 1$ and $\rho_\infty^{s} \in [0, 1]$ is symplectic. These symplectic schemes are also momentum-conserving; and they are actually energy-momentum conserving symplectic schemes for linear dynamical systems; see [7, 1]. For nonlinear dynamical systems, it is well-known that the symplectic-momentum conserving schemes and energy-momentum conserving schemes cannot coexist; see [22] for example.*

   Note that the spectral parameters need to satisfy the condition:

$$0 \le \rho_\infty^{s} \le \rho_\infty^{\min} \le \rho_\infty^{\max} \le 1 \tag{2.169}$$

2. ***Relations to Variational Integrators [23, 24, 25, 26, 27, 28] :***[7] *Any scheme in the U0V0 numerically nondissipative and V0U0 numerically nondissipative*

[7] *For the original works on the variational integrators, see [29, 30]*

*families are **variational** although this feature is not easy to observe since most variational schemes within the nondissipative GS4-2 family are not symplectic-momentum conserving at time grids, t_n. For example, as reported in [31], the implicit Newmark method, i.e., U0(1,1,0) with $\hat{\eta} = 1$, is actually a symplectic-momentum conserving scheme although it does not satisfy the symplectic condition, given in Eq.* (2.145)*, at t_n $\forall n$.*

Corollary 2.4.1 (Symplectic Conditions for Explicit GS4-2 Algorithms)

For the explicit version of the GS4-2 family, as discussed in Section 2.2.4, we employ the replacements, given in Eq. (2.58)*; therefore, the symplectic condition for the explicit case is modified as*

$$\boxed{W_1 \Lambda_1 = \lambda_1 - \frac{\lambda_3 \eta_3}{\lambda_5}} \tag{2.170}$$

in the case of $\tilde{\mathbf{C}}_T^n = \mathbf{0}$. Since parameter η_3 is allowed to take either 0 *or* 1*, the condition is readily reduced to Eq.* (2.144) *when $\eta_3 = 1$, and the spectral conditions are therefore given as Eq.* (2.145) *and Eq.* (2.146) *for the U0- and V0-based families; however, the spectral condition* (2.169) *no longer need to be satisfied for the explicit families.*

When $\eta_3 = 0$, the symplectic condition, given in Eq. (2.170)*, is readily reduced to*

$$\boxed{W_1 \Lambda_1 = \lambda_1} \tag{2.171}$$

and it leads to the symplectic spectral conditions

$$\rho_\infty^{\text{min}} \in \mathbb{R},\ \ \rho_\infty^{\text{max}} \in \mathbb{R},\ \ \rho_\infty^{\text{s}} = 0 \qquad \textit{for the U0-based family} \tag{2.172a}$$

$$\rho_\infty^{\text{min}} = \frac{1-\rho_\infty^{\text{max}}}{1+3\rho_\infty^{\text{max}}},\ \ \rho_\infty^{\text{s}} \in \mathbb{R} \qquad \textit{for the V0-based family} \tag{2.172b}$$

Remark 2.4.3

When $\eta_3 = 0$ and $(\rho_\infty^{\text{min}}, \rho_\infty^{\text{max}}, \rho_\infty^{\text{s}}) = (1, 1, 0)$ in the U0-based family, the resulting algorithm is the central difference method (equivalently, the Velocity-Verlet method [32]), *and it is symplectic since Eq.* (2.172a) *is satisfied. However, when we select* $\eta_3 = 1$ *with* $(\rho_\infty^{\mathrm{min}}, \rho_\infty^{\mathrm{max}}, \rho_\infty^{\mathrm{s}}) = (1, 1, 0)$ *in the U0-based family, the resulting algorithm is not symplectic since the symplectic condition, given in Eq.* (2.145), *is not satisfied.*

Next, we investigate the symplectic conditions for the GS4-1 family of algorithms, which can be generated from the GS4-2 family of algorithms via the *i*Integration adaptation process, when it is applied to a $2n_{\mathrm{g}}$-dimensional system of the first-order differential equations. For symplicity, consider the Hamilton's canonical equations of motion of the form,

$$\dot{\mathbf{z}} = \mathbb{J}D\mathscr{H}(\mathbf{z}), \quad \mathbf{z} = \begin{Bmatrix} \mathbf{q} \\ \mathbf{p} \end{Bmatrix} : \mathbb{I} \to T^*Q \tag{2.173}$$

or equivalently,

$$\begin{aligned} \dot{\mathbf{q}} &= [\mathbf{q}, \mathscr{H}(\mathbf{q}, \mathbf{p})] = \mathbf{M}^{-1}\mathbf{p} \\ \dot{\mathbf{p}} &= [\mathbf{p}, \mathscr{H}(\mathbf{q}, \mathbf{p})] = -\mathfrak{D}_1 \mathscr{H}(\mathbf{q}, \mathbf{p}) = -\frac{\partial \mathscr{H}(\mathbf{q}, \mathbf{p})}{\partial \mathbf{q}} \end{aligned} \tag{2.174a}$$

with the positive definite, symmetric, constant mass matrix $\mathbf{M}$. Without loss of generality, let us assume $\mathbf{M} = \mathbf{I}$; hence, $\dot{\mathbf{q}} = \mathbf{p}$. Applying the *i*Integrators to the system given in Eq. (2.173) via the adaptation process, we get

$$\textbf{[Integrator]} \quad \tilde{\mathbf{w}}^n = \mathbb{J}D\mathscr{H}(\tilde{\mathbf{z}}^n) \tag{2.175a}$$

$$\begin{aligned} \text{where} \quad \tilde{\mathbf{w}}^n &= \mathbf{w}^n + W_1\Lambda_6\Delta\mathbf{w}^n \quad (\mathbf{w}^n \approx \dot{\mathbf{z}}(t_{n-\phi})) \\ \tilde{\mathbf{z}}^n &= \mathbf{z}^n + \Delta t W_1\Lambda_4\mathbf{w}^n + \Delta t W_2\Lambda_5\Delta\mathbf{w}^n \end{aligned}$$

$$\begin{aligned} \textbf{[Update]} \quad \mathbf{z}^{n+1} &= \mathbf{z}^n + \Delta t\lambda_4\mathbf{w}^n + \Delta t\lambda_5\Delta\mathbf{w}^n \\ \mathbf{w}^{n+1} &= \mathbf{w}^n + \Delta\mathbf{w}^n \end{aligned} \tag{2.175b}$$

together with initial condition $\mathbf{z}(t_0) = \mathbf{z}^0 = (\mathbf{q}^0, \mathbf{p}^0)^T$. Let $\mathbf{w}^n = (\mathbf{v}^n, \mathbf{a}^n)^T$ and $\mathbf{z}^n = (\mathbf{q}^n, \mathbf{p}^n)^T$; then, the algorithm for Eq. (2.174) (with $\mathbf{M} = \mathbf{I}$) may be written as

$$\begin{aligned}
\textbf{[Integrator]}\quad \tilde{\mathbf{v}}^n &= \tilde{\mathbf{p}}^n && (2.176a)\\
\tilde{\mathbf{a}}^n &= -\mathfrak{D}_1 \mathscr{H}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{p}}^n)\\
\text{where}\quad \tilde{\mathbf{v}}^n &= \mathbf{v}^n + W_1\Lambda_6\Delta\mathbf{v}^n, \quad \tilde{\mathbf{a}}^n = \mathbf{a}^n + W_1\Lambda_6\Delta\mathbf{a}^n\\
\tilde{\mathbf{q}}^n &= \mathbf{q}^n + \Delta t W_1\Lambda_4\mathbf{v}^n + \Delta t W_2\Lambda_5\Delta\mathbf{v}^n\\
\tilde{\mathbf{p}}^n &= \mathbf{p}^n + \Delta t W_1\Lambda_4\mathbf{a}^n + \Delta t W_2\Lambda_5\Delta\mathbf{a}^n\\
\textbf{[Update]}\quad \mathbf{q}^{n+1} &= \mathbf{q}^n + \Delta t\lambda_4\mathbf{v}^n\Delta t\lambda_5\Delta\mathbf{v}^n && (2.176b)\\
\mathbf{p}^{n+1} &= \mathbf{p}^n + \Delta t\lambda_4\mathbf{a}^n\Delta t\lambda_5\Delta\mathbf{a}^n\\
\mathbf{v}^{n+1} &= \mathbf{v}^n + \Delta\mathbf{v}^n, \quad \mathbf{a}^{n+1} = \mathbf{a}^n + \Delta\mathbf{a}^n
\end{aligned}$$

together with initial condition $(\mathbf{q}, \mathbf{p})(t_0) = (\mathbf{q}^0, \mathbf{p}^0)^T$.

Theorem 2.4.5 (Symplectic Integrators within the GS4-1 Family of Algorithms) *Unless otherwise we artificially set $\lambda_5 = 0$, no scheme within the GS4-1 family of algorithms is symplectic. If we artificially set $\lambda_5 = 0$, every scheme within this algorithmic framework is symplectic.*

Proof. After tedious, but straightforward work (similar to the procedure for the GS4-2 family), the GS4-1 family of algorithms (Eq. (2.176)) can be written in the form,

$$\underbrace{\begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}}_{\mathbf{A}} \underbrace{\begin{bmatrix} \frac{\partial \mathbf{p}^{n+1}}{\partial \mathbf{p}^n} & \frac{\partial \mathbf{p}^{n+1}}{\partial \mathbf{q}^n} \\ \frac{\partial \mathbf{q}^{n+1}}{\partial \mathbf{p}^n} & \frac{\partial \mathbf{q}^{n+1}}{\partial \mathbf{p}^n} \end{bmatrix}}_{\frac{\partial(\mathbf{p}^{n+1}, \mathbf{q}^{n+1})}{\partial(\mathbf{p}^n, \mathbf{q}^n)}} = \underbrace{\begin{bmatrix} \mathbf{B}_{11} & \mathbf{B}_{12} \\ \mathbf{B}_{21} & \mathbf{B}_{22} \end{bmatrix}}_{\mathbf{B}} \qquad (2.177)$$

where

$$
\begin{aligned}
\mathbf{A}_{11} &= \mathbf{I} \\
\mathbf{A}_{12} &= -\frac{W_1\Lambda_6}{\Delta t W_2\Lambda_5}\mathbf{I} \\
\mathbf{A}_{21} &= -\Delta t^2 \frac{(W_2\Lambda_5)^2}{(W_1\Lambda_6)^2}\tilde{\mathbf{C}}_T^n \\
\mathbf{A}_{22} &= \mathbf{I} - \Delta t^2 \frac{(W_2\Lambda_5)^2}{(W_1\Lambda_6)^2}\tilde{\mathbf{K}}_T^n
\end{aligned}
\tag{2.178}
$$

and

$$
\begin{aligned}
\mathbf{B}_{11} &= \left(1 - \frac{\lambda_5}{W_2\Lambda_5}\right)\mathbf{I} \\
\mathbf{B}_{12} &= -\frac{W_1\Lambda_6}{\Delta t W_2\Lambda_5}\mathbf{I} \\
\mathbf{B}_{21} &= \frac{\Delta t \lambda_5}{W_1\Lambda_6}\mathbf{I} + \Delta t^2 \frac{W_2\Lambda_5\lambda_5}{(W_1\Lambda_6)^2}\left(1 - \frac{W_2\Lambda_5}{\lambda_5}\right)\tilde{\mathbf{C}}_T^n \\
\mathbf{B}_{22} &= \mathbf{I} + \Delta t^2 \frac{W_2\Lambda_5\lambda_5}{(W_1\Lambda_6)^2}\left(1 - \frac{W_2\Lambda_5}{\lambda_5}\right)\tilde{\mathbf{K}}_T^n
\end{aligned}
\tag{2.179}
$$

where $\tilde{\mathbf{C}}_T^n := -\partial(\mathfrak{D}_1\mathscr{H}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{p}}^n))/\partial\tilde{\mathbf{p}}^n$ and $\tilde{\mathbf{K}}_T^n := -\partial(\mathfrak{D}_1\mathscr{H}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{p}}^n))/\partial\tilde{\mathbf{q}}^n$. The GS4-1 family of algorithms is symplectic if the following relation holds,

$$
\left[\frac{\partial(\mathbf{p}^{n+1}, \mathbf{q}^{n+1})}{\partial(\mathbf{p}^n, \mathbf{q}^n)}\right]^T \mathbb{J} \left[\frac{\partial(\mathbf{p}^{n+1}, \mathbf{q}^{n+1})}{\partial(\mathbf{p}^n, \mathbf{q}^n)}\right] = \mathbb{J}
\tag{2.180}
$$

After tedious and straightforward work, it leads to

$$
\begin{aligned}
&-(W_1\Lambda_6)^2 + \Delta t W_1\Lambda_6(W_2\Lambda_5 - \lambda_5)\tilde{\mathbf{C}}_T^n + \Delta t^2(W_2\Lambda_5 - \lambda_5)^2\tilde{\mathbf{K}}_T^n \\
=& -(W_1\Lambda_6)^2 + \Delta t W_1\Lambda_6(W_2\Lambda_5)\tilde{\mathbf{C}}_T^n + \Delta t^2(W_2\Lambda_5)^2\tilde{\mathbf{K}}_T^n
\end{aligned}
\tag{2.181}
$$

Hence, the symplectic condition for the GS4-1 family of algorithms yields:

$$
\lambda_5 = 0
\tag{2.182}
$$

However, it contradicts with $\lambda_5 = 1/(1+\rho_\infty^s)$; therefore, no scheme is symplectic within the original GS4-1 family of algorithms. ∎

Remark 2.4.4

Second-order time accuracy of the kinematic unknowns can be maintained even by setting $\lambda_5 = 0$ in the GS4-1 family of algorithms. The second-order time accurate, explicit, symplectic GS4-1 family of algorithms is generated via the adaptation process from the GS4-2 family of algorithms with $\eta_2 = 0$ (in $W_2\Lambda_5\eta_2$) and the enforcement $\lambda_5 = 0$.

2.4.3 Energy Conserving Integrators

A large amount of research on developing the exact ***energy-momentum conserving methods*** (EMM) for various cases in mechanics can be found in literature. The pioneering works may be traced back to [33, 34, 35], and the more details work can be found in [22, 36, 37, 38, 39, 40], particularly for N-body systems and hyperelastic material models. The comparisons and discussions on the EMM and GS4-2 family for N-body and nonlinear elastic models; refer to [7, 41, 8].

Example 2.4.1 (Invariants in the Discrete System: The Kepler Problem)

The Hamiltonian for the famous Kepler problem is given by [42]

$$\mathscr{H}(\mathbf{q}, \mathbf{p}) = \frac{p_1^2 + p_2^2}{2} - \frac{1}{\sqrt{q_1^2 + q_2^2}} \tag{2.183}$$

Hence, the Hamilton's canonical equation yields,

$$\begin{aligned} \dot{q}_1 &= [q_1, \mathscr{H}] = p_1, \quad \dot{q}_2 = [q_2, \mathscr{H}] = p_2 \\ \dot{p}_1 &= [p_1, \mathscr{H}] = -\frac{q_1}{(q_1^2 + q_2^2)^{(3/2)}}, \quad \dot{p}_2 = [p_2, \mathscr{H}] = -\frac{q_2}{(q_1^2 + q_2^2)^{(3/2)}} \end{aligned} \tag{2.184}$$

Initial conditions are given as

$$\mathbf{q}(0) = \begin{bmatrix} q_1(0) \\ q_2(0) \\ 0 \end{bmatrix} = \begin{bmatrix} 1-e \\ 0 \\ 0 \end{bmatrix} \quad \textit{and} \quad \dot{\mathbf{q}}(0) = \begin{bmatrix} \dot{q}_1(0) \\ \dot{q}_2(0) \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ \sqrt{(1+e)/(1-e)} \\ 0 \end{bmatrix} \tag{2.185}$$

where e denotes the eccentricity. The orbital period is 2π. This system has three invariants, namely, the Hamiltonian, angular momentum, and the so-called Laplace-Runge-Lenz vector. The angular momentum is given as a quadratic invariant of the form

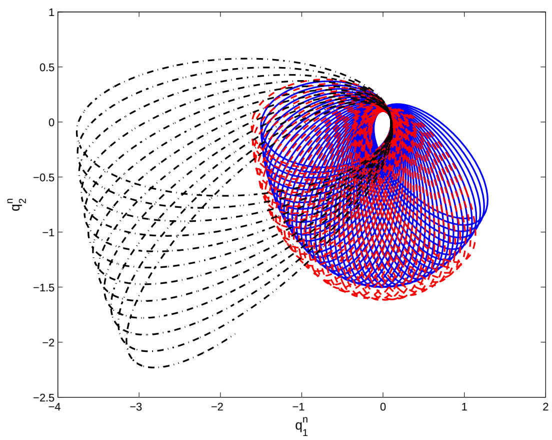
$$\mathbf{J}^T = \begin{bmatrix} 0, 0, q_1 p_2 - q_2 p_1 \end{bmatrix} \tag{2.186}$$

The Laplace-Runge-Lenz vector $\mathbf{A} \in \mathbb{R}^3$ is defined as

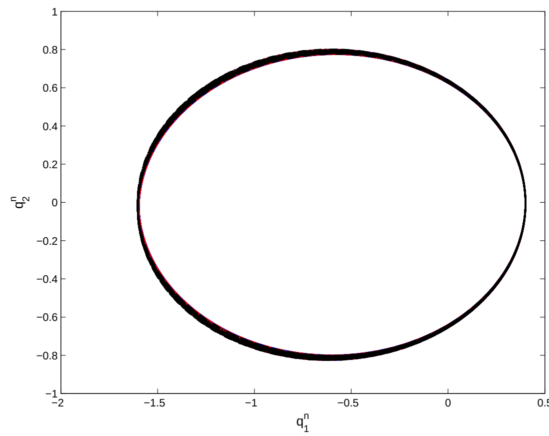
$$\begin{aligned} \mathbf{A} &:= \widetilde{\mathbf{p}}\mathbf{J} - \frac{\mathbf{q}}{||\mathbf{q}||} \\ &= \begin{bmatrix} 0 & 0 & p_2 \\ 0 & 0 & -p_1 \\ -p_2 & p_1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ q_1 p_2 - q_2 p_1 \end{bmatrix} - \frac{1}{||\mathbf{q}||} \begin{bmatrix} q_1 \\ q_2 \\ 0 \end{bmatrix} \\ &= \begin{bmatrix} p_2(q_1 p_2 - q_2 p_1) - q_1 / ||\mathbf{q}|| \\ -p_1(q_1 p_2 - q_2 p_1) - q_2 / ||\mathbf{q}|| \\ 0 \end{bmatrix} \end{aligned} \tag{2.187}$$

Fig. 2.13- Fig. 2.15 show the numerical solutions obtained by several schemes from Algorithm 2.2.1 with time step size $\Delta t = 0.01$ and two different eccentricity values $e = 0.9$ and $e = 0.6$. The tolerance for the Newton-type iteration is 10^{-6}. The angular momentum is conserved within a time step in the sense of $\mathbf{J}_n = \mathbf{J}_{n+1}$ for V0-based (1,1,ρ_∞^s) family of algorithms (for $\rho_\infty^s \in [0,1]$. The energy is not conserved within a time step for any scheme within Algorithm 2.2.1 presented; however, the modified version

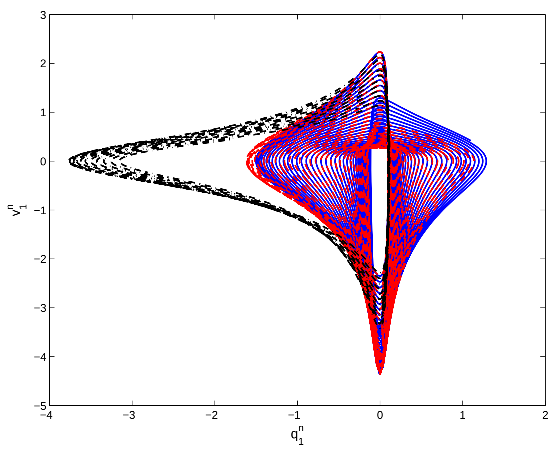
of Algorithm 2.2.1 that includes the exact energy-momentum conserving schemes of second-order time accuracy is shown in [1]. Note that the trajectory in discrete time system is not closed since the Laplace-Runge-Lenz vector within a time step is no longer conserved not only for Algorithm 2.2.1, but also for the EMM.



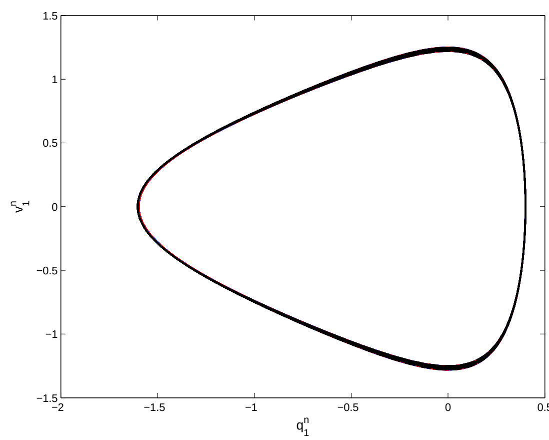
(a) Configuration: $e = 0.9$



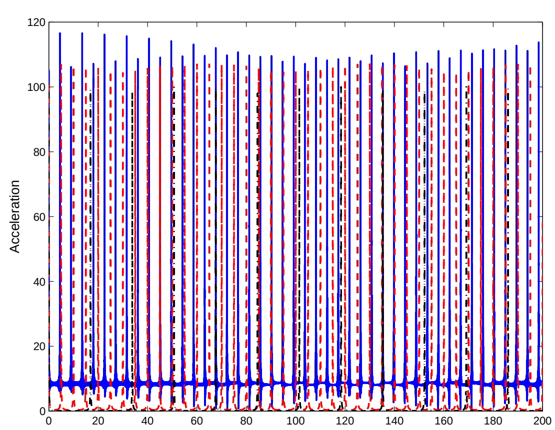
(b) Configuration: $e = 0.6$



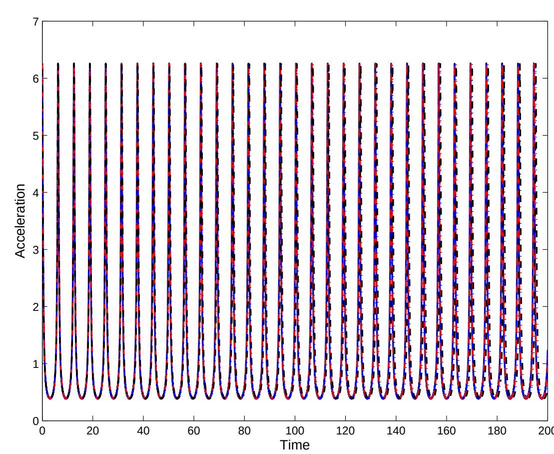
(c) Phase Space: $e = 0.9$



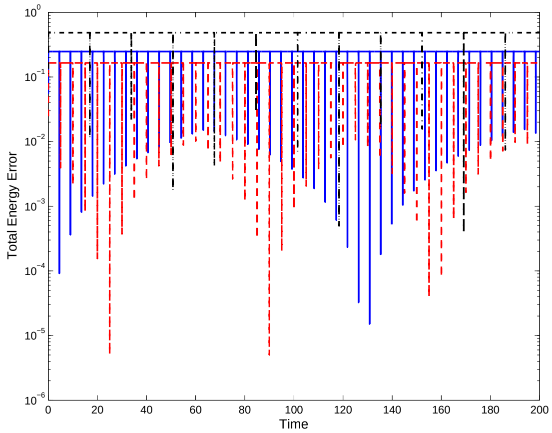
(d) Phase Space: $e = 0.6$



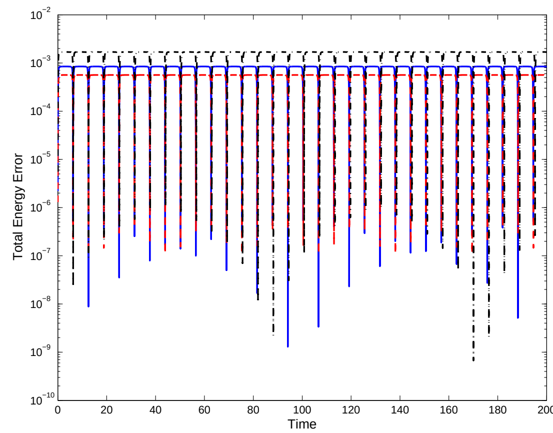
(e) Acceleration: $e = 0.9$



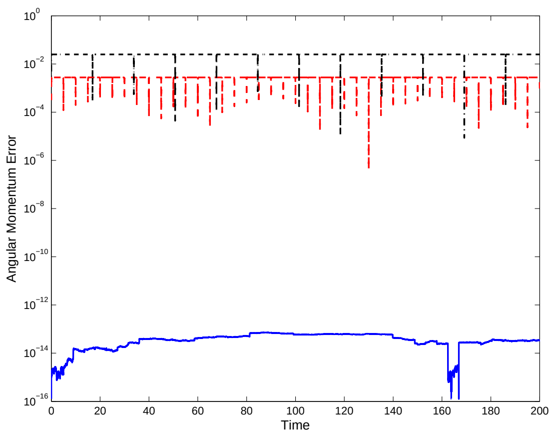
(f) Acceleration: $e = 0.6$



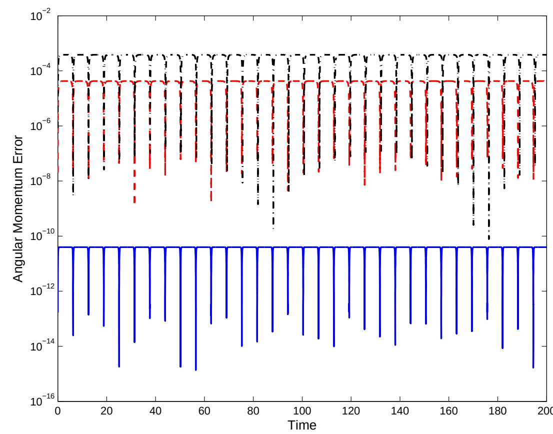
(g) Total Energy Error: $e = 0.9$



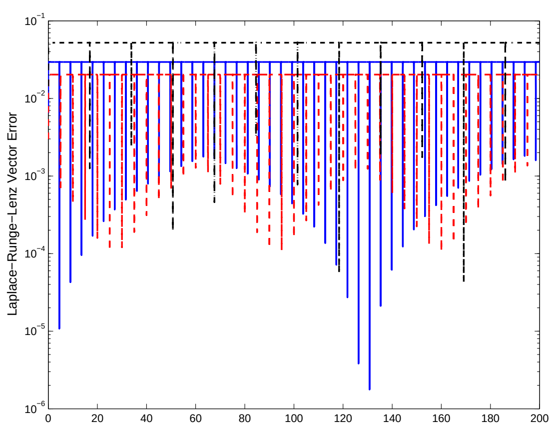
(h) Total Energy Error: $e = 0.6$



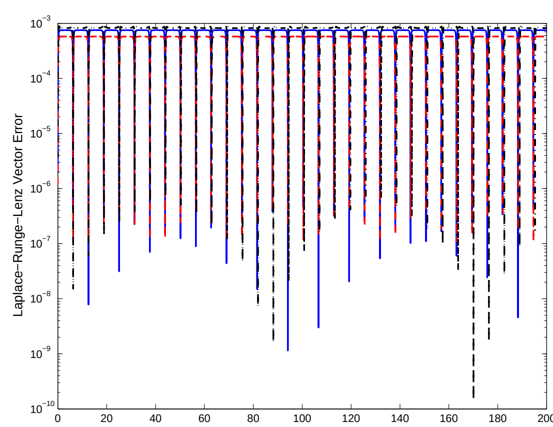
(i) Angular Momentum Error: $e = 0.9$



(j) Angular Momentum Error: $e = 0.6$

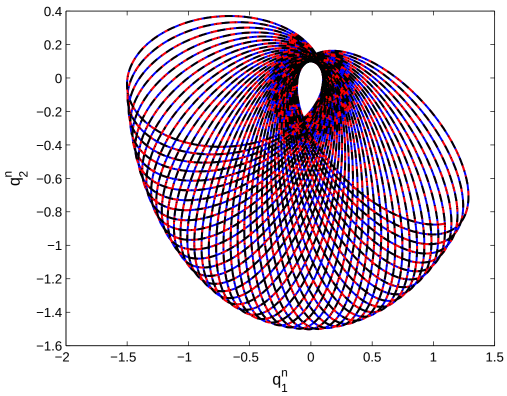


(k) Laplace-Runge-Lenz Vector Error: $e = 0.9$

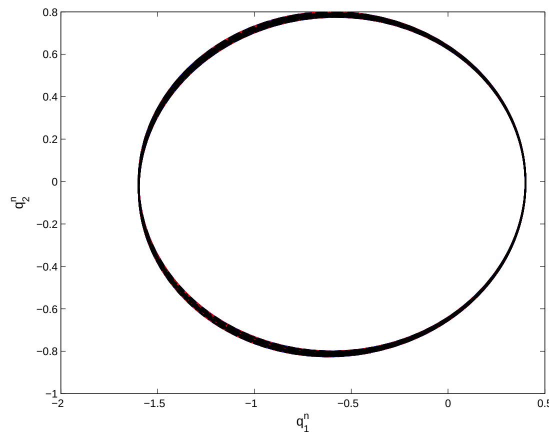


(l) Laplace-Runge-Lenz Vector Error: $e = 0.6$

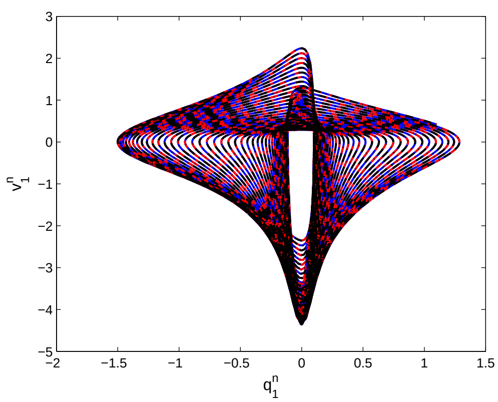
Figure 2.13: The Kepler Problem: The (1,1,1) [blue], (1,1,0.5) [red], and (1,1,0) [black] Schemes from the U0 Family of Algorithms for $e = 0.9$ and $e = 0.6$



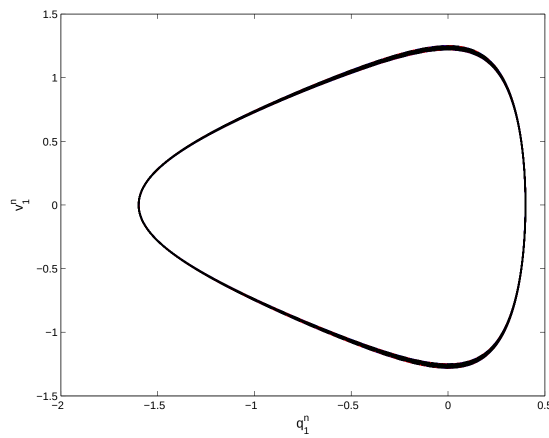
(a) Configuration: $e = 0.9$



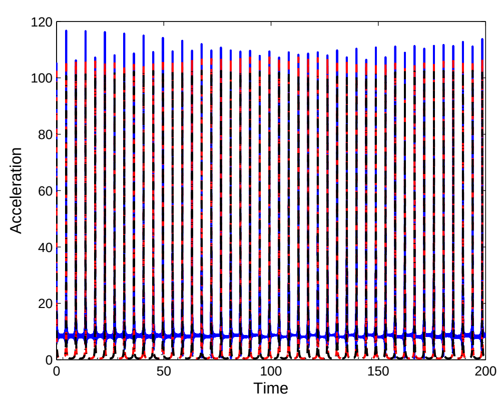
(b) Configuration: $e = 0.6$



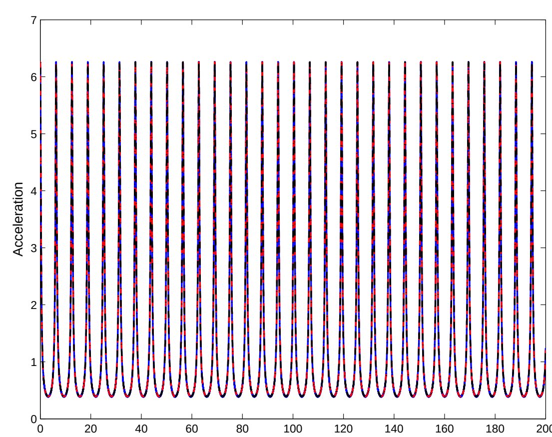
(c) Phase Space: $e = 0.9$



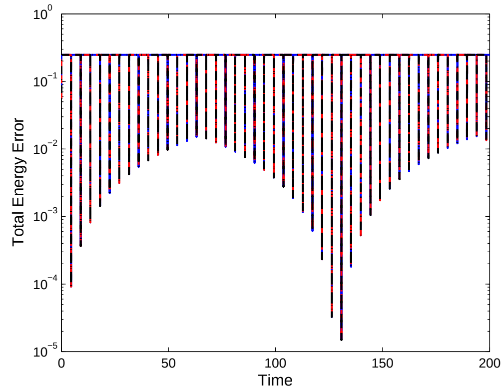
(d) Phase Space: $e = 0.6$



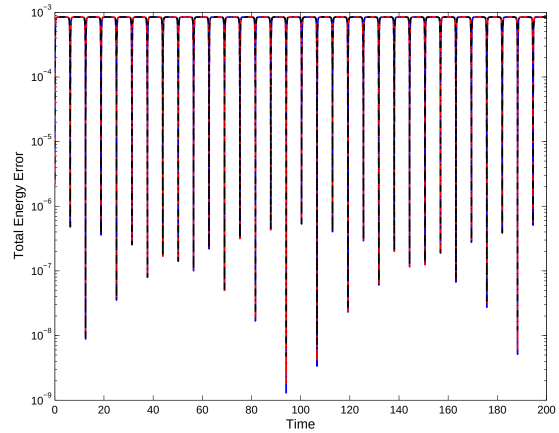
(e) Acceleration: $e = 0.9$



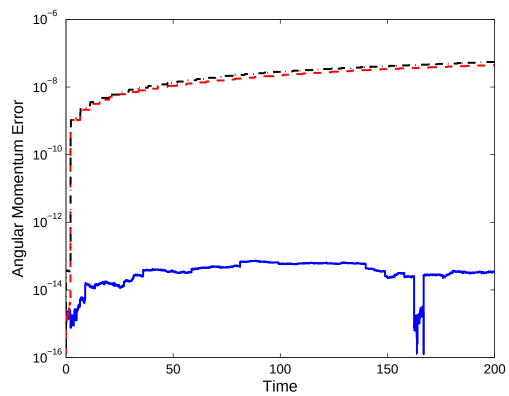
(f) Acceleration: $e = 0.6$



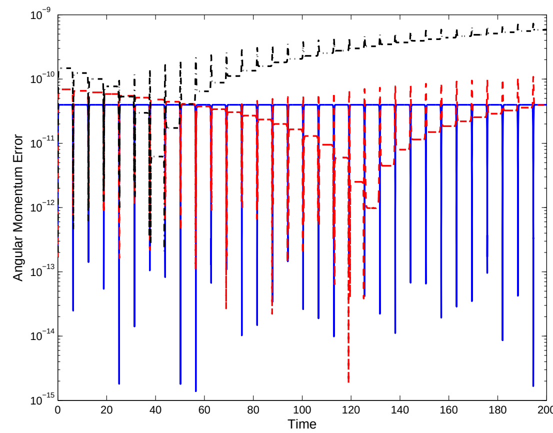
(g) Total Energy Error: $e = 0.9$



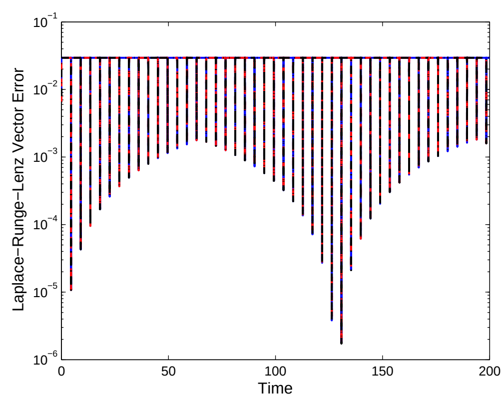
(h) Total Energy Error: $e = 0.6$



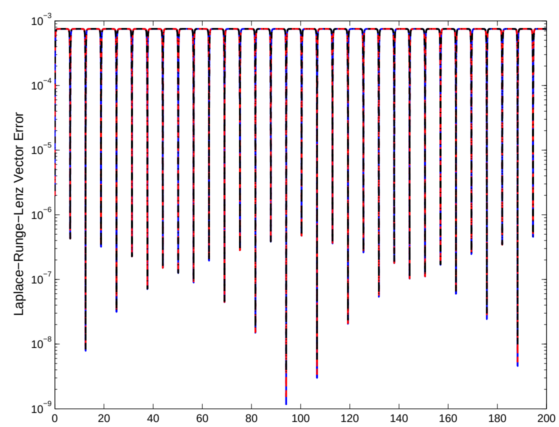
(i) Angular Momentum Error: $e = 0.9$



(j) Angular Momentum Error: $e = 0.6$

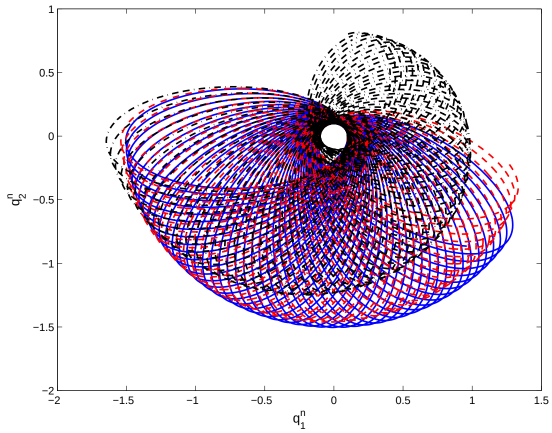


(k) Laplace-Runge-Lenz Vector Error: $e = 0.9$

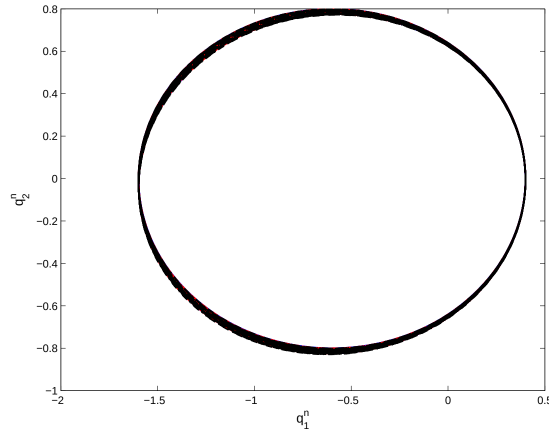


(l) Laplace-Runge-Lenz Vector Error: $e = 0.6$

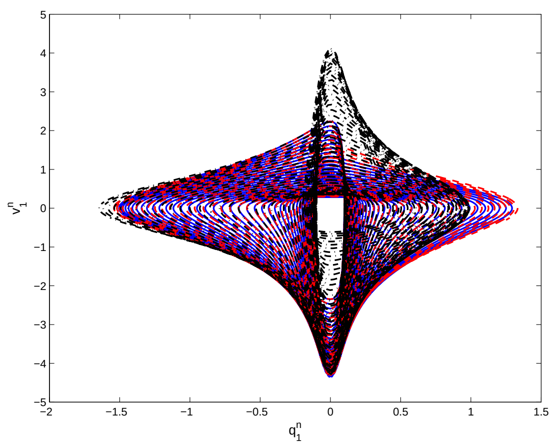
Figure 2.14: The Kepler Problem: The (1,1,1) [blue], (1,1,0.5) [red], and (1,1,0) [black] Schemes from the V0 Family of Algorithms for $e = 0.9$ and $e = 0.6$



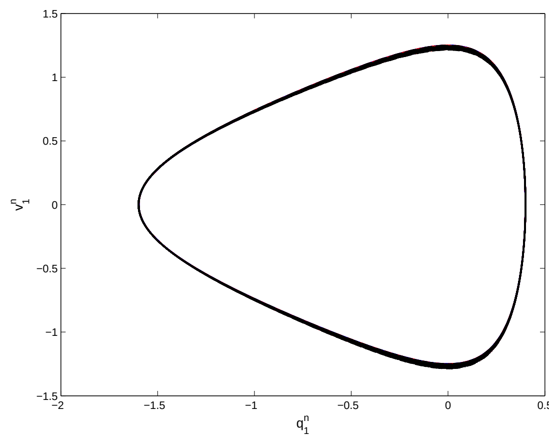
(a) Configuration: $e = 0.9$



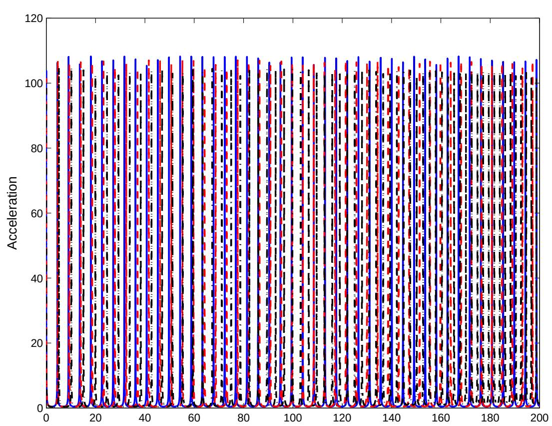
(b) Configuration: $e = 0.6$



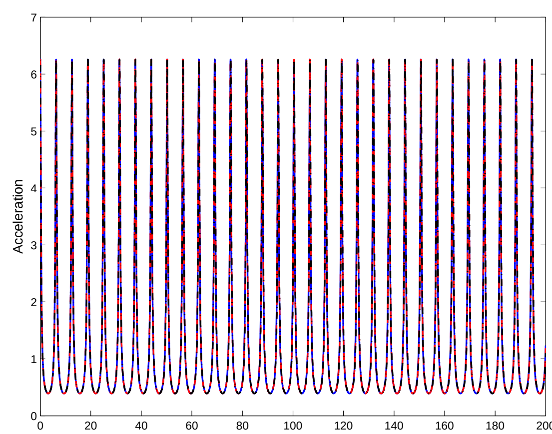
(c) Phase Space: $e = 0.9$



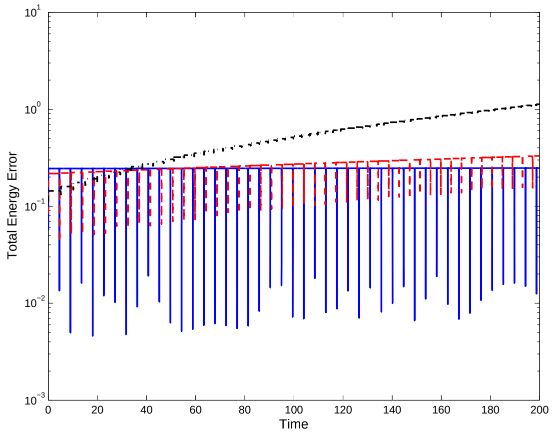
(d) Phase Space: $e = 0.6$



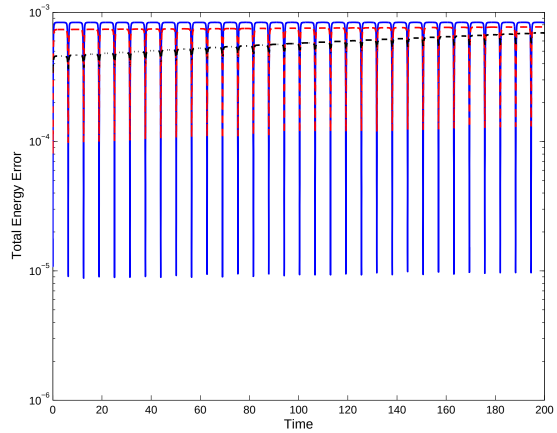
(e) Acceleration: $e = 0.9$



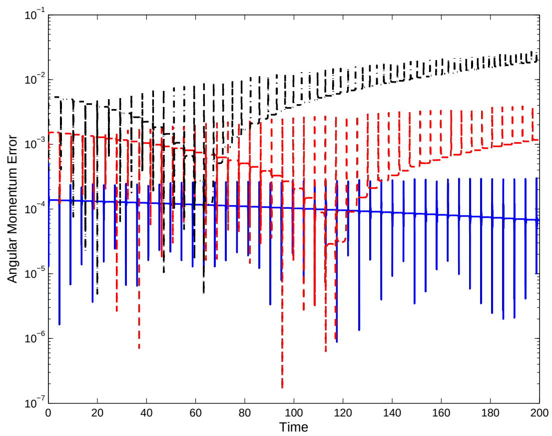
(f) Acceleration: $e = 0.6$



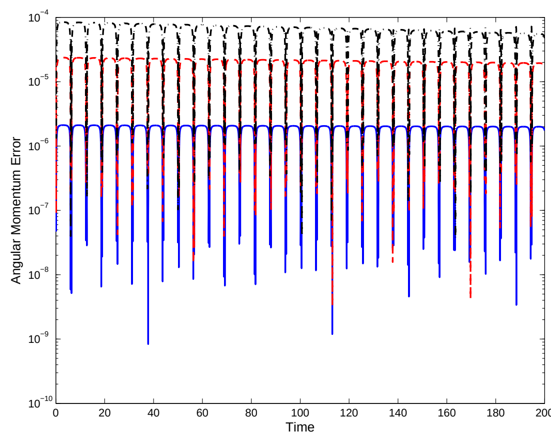
(g) Total Energy Error: $e = 0.9$



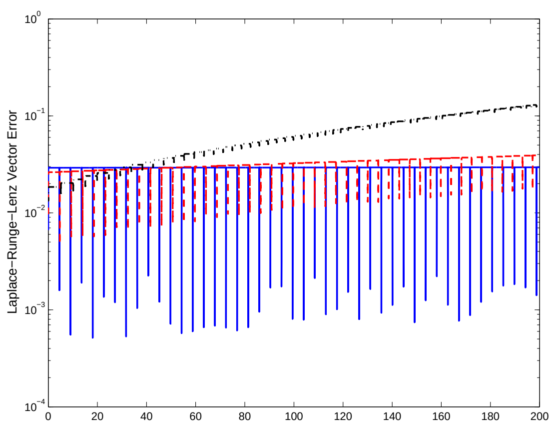
(h) Total Energy Error: $e = 0.6$



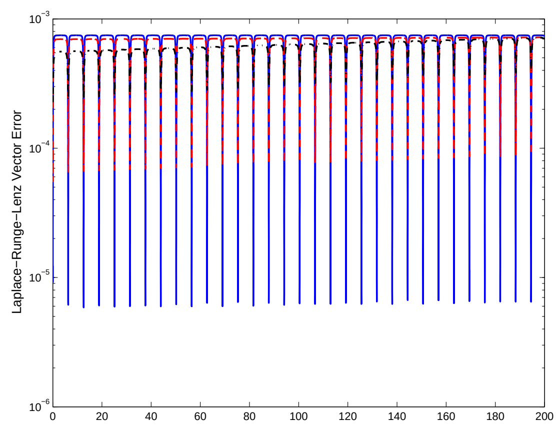
(i) Angular Momentum Error: $e = 0.9$



(j) Angular Momentum Error: $e = 0.6$



(k) Laplace-Runge-Lenz Vector Error: $e = 0.9$



(l) Laplace-Runge-Lenz Vector Error: $e = 0.6$

Figure 2.15: The Kepler Problem: The (0.9,1.0,0.9) [blue], (0.7,1.0,0.7) [red], and (0.5,1.0,0.5) [black] Schemes from the U0/V0 Optimal Family of Algorithms for $e = 0.9$ and $e = 0.6$

Chapter 3

The Isochronous Time Integration Architecture for Systems of Differential-Algebraic Equations

3.1 Introduction

In this chapter, the ***isochronous time integration architecture*** specially developed for solving systems of differential-algebraic equations is presented. This newly developed time integration architecture, also referred to as the ***DAE-iIntegrator***, is a powerful single or unified simulation toolkit and package that can be applied to wide variety of science and engineering problems, including multibody dynamics, electrical circuits, chemical reactions, and so on. The DAE-*i*Integrators can be used not only to the second-order DAE systems, but also to the first-order DAE systems, in a similar manner as for the ODE-*i*Integrators, discussed in the previous chapter.

3.2 Differential-Algebraic Equations

In this section, some basic theories and concepts of differential-algebraic equations (DAEs) are succinctly summarized.

3.2.1 Morphology of DAEs

Definition 3.2.1 (Fully-implicit DAEs)

The most general form of a differential algebraic equation (DAE) is of the form of a set of implicit differential equations,

$$\boxed{\mathbf{F}(t, \mathbf{x}, \dot{\mathbf{x}}) = \mathbf{0}} \tag{3.1}$$

where $\mathbf{x}(t) : \mathbb{I} = [t_0, T] \subset \mathbb{R} \to \mathbb{R}^{n_\mathrm{x}}$ *and* $\dot{\mathbf{x}}(t) := d\mathbf{x}/dt \in T_{\mathbf{x}}\mathbb{R}^{n_\mathrm{x}} = \mathbb{R}^{n_\mathrm{x}}$ *denote state variables and the time derivative of* $\mathbf{x}$*, respectively.* $[\mathbf{F}]_i = F_i(t, \mathbf{x}, \dot{\mathbf{x}}) : \mathbb{I} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \to \mathbb{R}$ *for* $i = 1, 2, \cdots, n_\mathrm{x}$ *is a nonlinear function, and* $\mathbf{F} = (F_1, F_2, \cdots, F_{n_\mathrm{x}})^T$ *is assumed to be a smooth map from* $\mathbb{I} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$ *into* $\mathbb{R}^{n_x}$*. Eq.* (3.1) *is a nonlinear fully-implicit DAE.*

Remark 3.2.1

1. *If the Jacobian,* $\mathbf{J}_{\dot{\mathbf{x}}} := \partial\mathbf{F}/\partial\dot{\mathbf{x}} \in \mathbb{R}^{n_\mathrm{x} \times n_\mathrm{x}}$*, is isomorphism at some solution of* $\mathbf{F}(t, \mathbf{x}, \dot{\mathbf{x}}) = \mathbf{0}$*; then, it is possible to* locally *transform Eq.* (3.1) *into a system of* ***explicit ordinary differential equations*** *via the* ***implicit function theorem*** *(see Theorem 3.2.1), and we can locally solve for* $\dot{\mathbf{x}}$*. Eq.* (3.1) *is called a system of* ***fully-implicit differential-algebraic equations*** *only if*

$$\mathrm{rank}\,(\mathbf{J}_{\dot{\mathbf{x}}}) < n_x \tag{3.2}$$

   on the domain of interest.

2. *If input variables* $\mathbf{u}(t)$ *to a system appear, Eq.* (3.1) *can be modified as*

$$\mathbf{F}(t, \mathbf{x}, \dot{\mathbf{x}}, \mathbf{u}) = \mathbf{0} \tag{3.3}$$

This situation often happens, for example, in system dynamics problems.

3. *The nonlinear fully-implicit DAE of the form given in Eq.* (3.1) *is the most general form of DAEs; however, in a particular case, it can be written in the form*

$$\mathbf{B}(t, \mathbf{x})\dot{\mathbf{x}} = \boldsymbol{\varphi}(t, \mathbf{x}) \tag{3.4}$$

with $\mathbf{B}(t, \mathbf{x}) : \mathbb{I} \times \mathbb{R}^{n_x} \to \mathbb{R}^{n_x \times n_x}$ *and* $\boldsymbol{\varphi}(t, \mathbf{x})\mathbb{I} \times \mathbb{R}^{n_x} \to \mathbb{R}^{n_x}$.

4. ***Linear Fully-implicit DAEs:*** *Eq.* (3.1) *is the general form of the fully-implicit DAEs, but in linear systems, it can be written as*

$$\mathbf{B}\dot{\mathbf{x}} + \mathbf{A}\mathbf{x} = \mathbf{c}(t) \tag{3.5}$$

with constant matrices $\mathbf{B} \in \mathbb{R}^{n_x \times n_x}$ *and* $\mathbf{A} \in \mathbb{R}^{n_x \times n_x}$ *and a time-dependent function* $\mathbf{c}(t) : \mathbb{I} \to n_x$. *If these matrices depend on time* t, *i.e.,*

$$\mathbf{B}(t)\dot{\mathbf{x}} + \mathbf{A}(t)\mathbf{x} = \mathbf{c}(t) \tag{3.6}$$

it is called the time-varying *linear fully-implicit DAEs.*

Theorem 3.2.1 (Implicit Function Theorem)

Let $\mathbf{F}(t, \mathbf{x}, \dot{\mathbf{x}}) : \mathbb{I} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_x} \to \mathbb{R}^{n_x}$ *be a set of continuously differentiable functions defined in a neighborhood* $U \subset \mathbb{R}^{2n_x} = \mathbb{R}^{n_x} \times \mathbb{R}^{n_x}$ *of* $(\mathbf{x}^*, \dot{\mathbf{x}}^*)$ *at time* $t = t^*$, *i.e.,* $(\mathbf{x}, \dot{\mathbf{x}})(t^*) = (\mathbf{x}^*, \dot{\mathbf{x}}^*)$, *such that*

$$\mathbf{F}(t^*, \mathbf{x}^*, \dot{\mathbf{x}}^*) = \mathbf{0} \tag{3.7}$$

Suppose we wish to solve $\mathbf{F} = \mathbf{0}$ *for* $\dot{\mathbf{x}}$ *in terms of* t *and* $\mathbf{x}$ *in* U. *If the following Jacobian matrix*

$$\mathbf{J}_{\dot{\mathbf{x}}}(t^*, \mathbf{x}^*, \dot{\mathbf{x}}^*) = \frac{\partial \mathbf{F}}{\partial \dot{\mathbf{x}}}(t^*, \mathbf{x}^*, \dot{\mathbf{x}}^*), \tag{3.8}$$

is invertible, or $\mathbf{J}_{\dot{\mathbf{x}}}$ *is isomorphism at* $(t^*, \mathbf{x}^*, \dot{\mathbf{x}}^*)$*, and continuous in* U*; then, there exists a set of continuously differentiable unique functions* $\boldsymbol{\varphi}(t, \mathbf{x}) \in \mathbb{R}^{n_x}$ *in a neighborhood of* $(t^*, \mathbf{x}^*)$ *such that* $\dot{\mathbf{x}}^* = \boldsymbol{\varphi}(t^*, \mathbf{x}^*)$ *and*

$$\{(t, \mathbf{x}, \dot{\mathbf{x}}) : \mathbf{F}(t, \mathbf{x}, \dot{\mathbf{x}}) = \mathbf{0}\} = \{(t, \mathbf{x}, \boldsymbol{\varphi}(t, \mathbf{x}))\} \tag{3.9}$$

for all t *and* $\mathbf{x}$ *in a neighborhood of* t^* *and a neighborhood of* $\mathbf{x}^*$*, respectively.*

Consider the system of non-autonomous, linear-implicit DAEs of the form,

$$\mathbf{B}\dot{\mathbf{x}} = \boldsymbol{\varphi}(t, \mathbf{x}) \tag{3.10}$$

where $\mathbf{B} \in \mathbb{R}^{n_x \times n_x}$ is a singular matrix. By Gaussian elimination with total pivoting, for example, we can readily show that there exist regular matrices $\mathbf{S}_i$ (for $i = 1, 2$) such that

$$\mathbf{S}_1\mathbf{B}\mathbf{S}_2 = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \tag{3.11}$$

Premultiplying Eq. (3.10) by $\mathbf{S}_1$, we have

$$\mathbf{S}_1\mathbf{B}\dot{\mathbf{x}} = \mathbf{S}_1\boldsymbol{\varphi}(t, \mathbf{x}) \tag{3.12}$$

Employing the transformation

$$\mathbf{S}_2^{-1}\mathbf{x} =: \begin{pmatrix} \mathbf{y} \\ \mathbf{w} \end{pmatrix} \tag{3.13}$$

we obtain

$$\frac{d}{dt}\begin{pmatrix} \mathbf{y} \\ \mathbf{w} \end{pmatrix} = \mathbf{S}_1\boldsymbol{\varphi}\left(t, \mathbf{S}_2\begin{pmatrix} \mathbf{y} \\ \mathbf{w} \end{pmatrix}\right) =: \boldsymbol{\theta}(t, \mathbf{y}, \mathbf{w}) \tag{3.14}$$

where we used Eq. (3.11). By adding $\dot{t} = 1$, we can obtain the autonomous form:

$$\begin{aligned} \dot{\mathbf{y}} &= \mathbf{f}(\mathbf{y}, \mathbf{w}) \\ \mathbf{0} &= \mathbf{h}(\mathbf{y}, \mathbf{w}) \end{aligned} \tag{3.15}$$

Eq. (3.15) is called an autonomous semi-explicit DAE, and $\mathbf{y}$ and $\mathbf{w}$ are the differential and algebraic variables of the system.

The semi-explicit DAEs are generally defined as follows:

Definition 3.2.2 (Semi-explicit DAEs)

The general semi-explicit DAEs in nonlinear systems are of the form

$$\boxed{\begin{aligned} \bar{\mathbf{f}}(t, \mathbf{y}, \dot{\mathbf{y}}, \mathbf{w}) &= \mathbf{0} \\ \mathbf{h}(t, \mathbf{y}, \mathbf{w}) &= \mathbf{0} \end{aligned}} \tag{3.16}$$

where $\mathbf{y} \in \mathbb{R}^{\mathrm{y}}$ *is the differential variable,* $\dot{\mathbf{y}} := d\mathbf{y}/dt \in \mathbb{R}^{n_{\mathrm{y}}}$ *is the time derivative of* $\mathbf{y}$, *and* $\mathbf{w} \in \mathbb{R}^{n_{\mathrm{w}}}$ *is the algebraic variable of the system. In a special case, Eq.* (3.16) *can be written in the form*

$$\boxed{\begin{aligned} \dot{\mathbf{y}} &= \mathbf{f}(t, \mathbf{y}, \mathbf{w}) \\ \mathbf{0} &= \mathbf{h}(t, \mathbf{y}, \mathbf{w}) \end{aligned}} \tag{3.17}$$

A wide-variety of problems in science and engineering can be formulated in this expression.

Remark 3.2.2

1. ***Linear Semi-explicit DAEs:*** *In linear systems, the semi-explicit DAEs may be written in the form*

$$\begin{aligned} \dot{\mathbf{y}} + \mathbf{A}_{11}\mathbf{y} + \mathbf{A}_{12}\mathbf{w} &= \mathbf{f}_1(t) \\ \mathbf{h}(t, \mathbf{y}, \mathbf{w}) &= \mathbf{A}_{21}\mathbf{y} + \mathbf{A}_{22}\mathbf{w} + \mathbf{f}_2(t) \end{aligned} \tag{3.18}$$

with $\mathbf{A}_{i1} \in \mathbb{R}^{n_{\mathrm{y}} \times n_{\mathrm{y}}}$ *and* $\mathbf{A}_{i2} \in \mathbb{R}^{n_{\mathrm{y}} \times n_{\mathrm{w}}}$ *(for* $i = 1, 2$*). If* $\mathbf{A}_{ij}$ *depends on time* t*, i.e.,*

$$\begin{aligned} \dot{\mathbf{y}} + \mathbf{A}_{11}(t)\mathbf{y} + \mathbf{A}_{12}(t)\mathbf{w} &= \mathbf{f}_1(t) \\ \mathbf{h}(t, \mathbf{y}, \mathbf{w}) &= \mathbf{A}_{21}(t)\mathbf{y} + \mathbf{A}_{22}(t)\mathbf{w} + \mathbf{f}_2(t) \end{aligned} \tag{3.19}$$

it is called the linear semi-explicit DAE with time-varying coefficients.

Definition 3.2.3 (Hessenberg Form of Size r of a DAE)

The Hessenberg form of size s of a DAE is defined as:

$$\begin{aligned}
\dot{\mathbf{x}}_1 &= \mathbf{F}_1(t, \mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_{s-1}, \mathbf{x}_s) \\
\dot{\mathbf{x}}_2 &= \mathbf{F}_2(t, \mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_{s-1}) \\
&\vdots \\
\dot{\mathbf{x}}_{s-2} &= \mathbf{F}_{s-2}(t, \mathbf{x}_{s-3}, \mathbf{x}_{s-2}, \mathbf{x}_{s-1}) \\
\dot{\mathbf{x}}_{s-1} &= \mathbf{F}_{s-1}(t, \mathbf{x}_{s-2}, \mathbf{x}_{s-1}) \\
\mathbf{0} &= \mathbf{F}_s(t, \mathbf{x}_{s-1})
\end{aligned} \tag{3.20}$$

with $\mathbf{x} = [\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_{s-2}, \mathbf{x}_{s-1}, \mathbf{x}_s]^T$, *and the assumption that matrix*

$$\left(\frac{\partial \mathbf{F}_s}{\partial \mathbf{x}_{s-1}}\right)\left(\frac{\partial \mathbf{F}_{s-1}}{\partial \mathbf{x}_{s-2}}\right)\left(\frac{\partial \mathbf{F}_{s-2}}{\partial \mathbf{x}_{s-3}}\right)\cdots\left(\frac{\partial \mathbf{F}_2}{\partial \mathbf{x}_1}\right)\left(\frac{\partial \mathbf{F}_1}{\partial \mathbf{x}_s}\right) \tag{3.21}$$

is invertible.

Remark 3.2.3

1. ***Semi-explicit DAEs in the Hessenberg Form of Size 1 (Hessenberg Index-1 Form):*** *When* $s = 1$, *Eq.* (3.20) *yields:*

$$\dot{\mathbf{x}}_1 = \mathbf{F}_1(t, \mathbf{x}_1) \tag{3.22}$$

with the assumption that

$$\left(\frac{\partial \mathbf{F}_1}{\partial \mathbf{x}_1}\right) \tag{3.23}$$

is invertible. If $\mathbf{x} = \mathbf{x}_1 = [\mathbf{y}^T, \mathbf{w}^T]^T$, *Eq.* (3.22) *can be written in the form*

$$\begin{aligned}
\dot{\mathbf{y}} &= \mathbf{f}(t, \mathbf{y}, \mathbf{w}) \\
\mathbf{0} &= \mathbf{h}(t, \mathbf{y}, \mathbf{w})
\end{aligned} \tag{3.24}$$

with matrix $\partial \mathbf{h}/\partial \mathbf{w}$ *being invertible, where* $\mathbf{y} \in \mathbb{R}^{n_y}$ *and* $\mathbf{w} \in \mathbb{R}^{n_w}$ *are the differential and algebraic variables, respectively.*

2. ***Semi-explicit DAEs in the Hessenberg Form of Size 2 (Hessenberg Index-2 Form):*** *When* $s = 2$, *Eq.* (3.20) *yields:*

$$\begin{aligned} \dot{\mathbf{x}}_1 &= \mathbf{F}_1(t, \mathbf{x}_1, \mathbf{x}_2) \\ \mathbf{0} &= \mathbf{F}_2(t, \mathbf{x}_1) \end{aligned} \tag{3.25}$$

with the assumption that

$$\left(\frac{\partial \mathbf{F}_2}{\partial \mathbf{x}_1}\right)\left(\frac{\partial \mathbf{F}_1}{\partial \mathbf{x}_2}\right) \tag{3.26}$$

is invertible.

3. ***Semi-explicit DAEs in the Hessenberg Form of Size 3 (Hessenberg Index-3 Form):*** *When* $s = 3$, *Eq.* (3.20) *yields:*

$$\begin{aligned} \dot{\mathbf{x}}_1 &= \mathbf{F}_1(t, \mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) \\ \dot{\mathbf{x}}_2 &= \mathbf{F}_2(t, \mathbf{x}_1, \mathbf{x}_2) \\ \mathbf{0} &= \mathbf{F}_3(t, \mathbf{x}_2) \end{aligned} \tag{3.27}$$

with the assumption that

$$\left(\frac{\partial \mathbf{F}_3}{\partial \mathbf{x}_2}\right)\left(\frac{\partial \mathbf{F}_2}{\partial \mathbf{x}_1}\right)\left(\frac{\partial \mathbf{F}_1}{\partial \mathbf{x}_3}\right) \tag{3.28}$$

is invertible. Most mechanical problems can be expressed in the Hessenberg form. For example, governing equations following the DAE approach in mechanical systems can be written in the Hessenberg form of size three.

4. *The semi-explicit DAEs in the Hessenberg form of any size can be written in the form*

$$\mathbf{B}\dot{\mathbf{x}} = \boldsymbol{\varphi}(t, \mathbf{x}) \tag{3.29}$$

where $\mathbf{B}$ *is a diagonal matrix with entries* 1 *and* 0.

3.2.2 Index Concepts of DAEs

Nilpotency Index

Consider linear DAEs with constant coefficients of the form

$$\mathbf{B}\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{c}(t), \quad \mathbf{x}(t_0) = \mathbf{x}_0 \tag{3.30}$$

where $\mathbf{B} \in \mathbb{R}^{n_x \times n_x}$ and $\mathbf{A} \in \mathbb{R}^{n_x \times n_x}$ are constant. If $\mathbf{B}$ is regular, it is clearly possible to solve for $\dot{\mathbf{x}}$ by premultiplying $\mathbf{B}^{-1}$ in Eq. (3.30), i.e., the ODE case; however, $\mathbf{B}$ is singular for the DAE case. In looking for the solution, $\mathbf{x}(t) = e^{\mu t}\mathbf{x}_0$ where $\mathbf{x}_0 = \mathbf{x}(t_0)$, assuming $\mathbf{c} \equiv \mathbf{0}$, we may define the ***matrix pencil***, $\mathbf{A} + \mu\mathbf{B}$. If the matrix pencil is singular for any μ, Eq. (3.30) has either no solution or infinitely many solutions. If the matrix pencil is regular, there exist some μ such that $\mathbf{A} + \mu\mathbf{B}$ is regular.

Assume the matrix pencil is regular; that is there exist some υ such that $\mathbf{A} + \upsilon\mathbf{B}$ is regular. Consider

$$\mathbf{A} + \mu\mathbf{B} = (\mathbf{A} + \upsilon\mathbf{B}) + (\mu - \upsilon)\mathbf{B} \tag{3.31}$$

Premultiplying $(\mathbf{A} + \upsilon\mathbf{B})^{-1}$, we have

$$\begin{aligned} (\mathbf{A} + \upsilon\mathbf{B})^{-1}(\mathbf{A} + \mu\mathbf{B}) &= \mathbf{I} + (\mu - \upsilon)(\mathbf{A} + \upsilon\mathbf{B})^{-1}\mathbf{B} \\ &= \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} + (\mu - \upsilon)\begin{bmatrix} \mathbf{J}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{J}_2 \end{bmatrix} \end{aligned} \tag{3.32}$$

where $\mathbf{I}$ denotes the identity matrix, and $\mathbf{J}_1$ and $\mathbf{J}_2$ are the matrices which contain the Jordan blocks with non-zero eigenvalues and zero eigenvalues, respectively. From Eq.

(3.32), we obtain

$$\begin{aligned}&\begin{bmatrix}\mathbf{J}_1^{-1} & \mathbf{0}\\ \mathbf{0} & (\mathbf{I}-\upsilon\mathbf{J}_2)^{-1}\end{bmatrix}(\mathbf{A}+\upsilon\mathbf{B})^{-1}(\mathbf{A}+\mu\mathbf{B})\\ &=\begin{bmatrix}\mathbf{J}_1^{-1}(\mathbf{I}-\upsilon\mathbf{J}_1) & \mathbf{0}\\ \mathbf{0} & \mathbf{I}\end{bmatrix}+\upsilon\begin{bmatrix}\mathbf{I} & \mathbf{0}\\ \mathbf{0} & (\mathbf{I}-\upsilon\mathbf{J}_2)^{-1}\mathbf{J}_2\end{bmatrix}\end{aligned} \tag{3.33}$$

Notice that $\mathbf{J}_1^{-1}(\mathbf{I}-\upsilon\mathbf{J}_1)$ and $(\mathbf{I}-\upsilon\mathbf{J}_2)^{-1}\mathbf{J}_2$ in the right-hand side of the above equation are in Jordan canonical forms. Since all eigenvalues of $(\mathbf{I}-\upsilon\mathbf{J}_2)^{-1}\mathbf{J}_2$ are zero, we may conclude that there exist non-singular $\mathbf{P}$ and $\mathbf{Q}$ such that

$$\mathbf{PBQ}=\begin{bmatrix}\mathbf{I} & \mathbf{0}\\ \mathbf{0} & \mathbf{N}\end{bmatrix},\quad \mathbf{PAQ}=\begin{bmatrix}\mathbf{C} & \mathbf{0}\\ \mathbf{0} & \mathbf{I}\end{bmatrix} \tag{3.34}$$

where $\mathbf{C}$ can be assumed to be in Jordan canonical form, and $\mathbf{N}$ is a nilpotent matrix of the form,

$$\mathbf{N}=\begin{bmatrix}\mathbf{N}_1 & & & & & \\ & \mathbf{N}_2 & & & & \\ & & \ddots & & & \\ & & & \mathbf{N}_i & & \\ & & & & \ddots & \\ & & & & & \mathbf{N}_\ell\end{bmatrix},\quad \mathbf{N}_i=\begin{bmatrix}0 & 1 & & & \\ & 0 & 1 & & \\ & & 0 & \ddots & \\ & & & \ddots & 1\\ & & & & 0\end{bmatrix} \tag{3.35}$$

The transformations, Eq. (3.34), are called the ***Kronecker canonical forms*** of $\mathbf{B}$ and $\mathbf{A}$, respectively. Consider the transformations,

$$\mathbf{Q}^{-1}\mathbf{x}=:\begin{pmatrix}\mathbf{y}\\ \mathbf{z}\end{pmatrix},\quad \mathbf{Pc}(t)=:\begin{pmatrix}\boldsymbol{\varrho}\\ \boldsymbol{\vartheta}\end{pmatrix}(t) \tag{3.36}$$

Premultiplying Eq. (3.30) by $\mathbf{P}$ and using the above transformations, we obtain

$$\mathbf{PBQ}\begin{pmatrix}\dot{\mathbf{y}}\\ \dot{\mathbf{z}}\end{pmatrix}=\mathbf{PAQ}\begin{pmatrix}\mathbf{y}\\ \mathbf{z}\end{pmatrix}+\begin{pmatrix}\boldsymbol{\varrho}\\ \boldsymbol{\vartheta}\end{pmatrix} \tag{3.37}$$

Using Eq. (3.34), the above equation yields the following decoupled system of DAEs:

$$\dot{\mathbf{y}} + \mathbf{C}\mathbf{y} = \boldsymbol{\varrho}(t) \tag{3.38}$$

$$\mathbf{N}\dot{\mathbf{z}} + \mathbf{z} = \boldsymbol{\vartheta}(t) \tag{3.39}$$

Eq. (3.38) is an ordinary differential equation for $\mathbf{y}(t)$; therein, we can readily solve for $\mathbf{y}(t)$ by integration. On the other hand, we can solve for $\mathbf{z}(t)$ recursively from Eq. (3.39) by differentiating with respect to time and premultiplying by $\mathbf{N}$ repeatedly as

$$\begin{aligned}
\mathbf{N}^2\frac{d^2\mathbf{z}}{dt^2} &= -\mathbf{N}\frac{d\mathbf{z}}{dt} + \mathbf{N}\frac{d\boldsymbol{\vartheta}}{dt} = \mathbf{z} - \boldsymbol{\vartheta} + \mathbf{N}\frac{d\boldsymbol{\vartheta}}{dt} \\
\mathbf{N}^3\frac{d^3\mathbf{z}}{dt^3} &= -\mathbf{N}^2\frac{d^2\mathbf{z}}{dt^2} + \mathbf{N}^2\frac{d^2\boldsymbol{\vartheta}}{dt^2} = -\mathbf{z} + \boldsymbol{\vartheta} - \mathbf{N}\frac{d\boldsymbol{\vartheta}}{dt} + \mathbf{N}^2\frac{d^2\boldsymbol{\vartheta}}{dt^2} \\
\mathbf{N}^4\frac{d^4\mathbf{z}}{dt^4} &= -\mathbf{N}^3\frac{d^3\mathbf{z}}{dt^3} + \mathbf{N}^3\frac{d^3\boldsymbol{\vartheta}}{dt^3} = \mathbf{z} - \boldsymbol{\vartheta} + \mathbf{N}\frac{d\boldsymbol{\vartheta}}{dt} - \mathbf{N}^2\frac{d^2\boldsymbol{\vartheta}}{dt^2} + \mathbf{N}^3\frac{d^3\boldsymbol{\vartheta}}{dt^3} \\
&\vdots \\
\mathbf{N}^\ell\frac{d^\ell\mathbf{z}}{dt^\ell} &= (-1)^\ell\mathbf{z} + \sum_{i=0}^{\ell-1}(-1)^{\ell-1-i}\mathbf{N}^i\frac{d^i\boldsymbol{\vartheta}}{dt^i}
\end{aligned} \tag{3.40}$$

Therefore, assuming $\boldsymbol{\vartheta}(t)$ is differentiable $\ell - 1$ times, we can obtain the explicit expression of $\mathbf{z}$ as

$$\boxed{\mathbf{z} = \sum_{i=0}^{\ell-1}(-1)^i\mathbf{N}^i\frac{d^i\boldsymbol{\vartheta}}{dt^i}} \tag{3.41}$$

Definition 3.2.4 (Nilpotency Index)

The integer ℓ in Eq. (3.41) *is called the* ***degree of nilpotency*** *of the regular matrix pencil,* $\mathbf{A}+\mu\mathbf{B}$, *and denotes the* ***nilpotency index*** *of the initial value problem represented by the linear DAE systems, Eq.* (3.30), *with the regular matrix pencil.*

Remark 3.2.4

The nilpotency index can be defined only for linear DAE systems. The nilpotency index and the differentiation index (see Definition 3.2.5) are the same for the linear DAE system with constant coefficient matrices with a regular matrix pencil.

Differentiation Index and Perturbation Index

Definition 3.2.5 (Differentiation Index)

The ***differentiation index*** ℓ_{d} *of the fully-implicit nonlinear equation, Eq.* (3.1), *is defined as the minimal nonnegative integer of analytical differentiations,*

$$\begin{aligned} \mathbf{F}(\mathbf{x}, \dot{\mathbf{x}}, t) &= \mathbf{0} \\ \frac{d}{dt}\mathbf{F}(\mathbf{x}, \dot{\mathbf{x}}, t) &= \mathbf{0} \\ &\vdots \\ \frac{d^{\ell_{\mathrm{d}}}}{dt^{\ell_{\mathrm{d}}}}\mathbf{F}(\mathbf{x}, \dot{\mathbf{x}}, t) &= \mathbf{0} \end{aligned} \tag{3.42}$$

such that we can extract an ordinary differential equation, the ***underlying ODE*** $\dot{\mathbf{x}} = \mathbf{\Psi}(\mathbf{x}, t)$, *from the system of equations (****derivative array****), Eq.* (3.42), *only by algebraic manipulations. Note that if the Jacobian,* $\partial\mathbf{F}/\partial\dot{\mathbf{x}}$, *is regular, we readily have* $\ell_{\mathrm{d}} = 0$; *that is, the differentiation index is* 0.

Definition 3.2.6 (Perturbation Index)

The ***perturbation index*** ℓ_{p} *of the fully-implicit nonlinear equation, Eq.* (3.1), *along a solution* $\mathbf{x}(t) : \mathbb{I} \to \mathbb{R}^{n_{\mathrm{x}}}$ *is defined as the minimal integer such that there exists an estimate, with constant* C, *on* $\mathbb{I}$,

$$\|\hat{\mathbf{x}}(t) - \mathbf{x}(t)\| \le C\left(\|\hat{\mathbf{x}}(t_0) - \mathbf{x}(t_0)\| + \max_{t_0 \le \varepsilon \le t}\|\boldsymbol{\delta}(\varepsilon)\| + \cdots + \max_{t_0 \le \varepsilon \le t}\left\|\frac{d^{(\ell_{\mathrm{p}}-1)}}{dt^{(\ell_{\mathrm{p}}-1)}}\boldsymbol{\delta}(\varepsilon)\right\|\right) \tag{3.43}$$

whenever the right-hand side of Eq. (3.43) *is sufficiently small for all* $\hat{\mathbf{x}}(t) : \mathbb{I} \to \mathbb{R}^{n_{\mathrm{x}}}$ *which have the perturbation* $\boldsymbol{\delta}$ *as* $\mathbf{F}(\hat{\mathbf{x}}, \dot{\hat{\mathbf{x}}}, t) = \boldsymbol{\delta}(t)$.

Remark 3.2.5

1. *The differential index and perturbation index are equal, i.e.,* $\ell_{\mathrm{d}} = \ell_{\mathrm{p}}$, *when DAEs are of the form*

$$\mathbf{B}\dot{\mathbf{x}} = \boldsymbol{\varphi}(t, \mathbf{x}) \tag{3.44}$$

with constant matrix $\mathbf{B}$*. For example, the differential index of a semi-explicit DAE in the Hessenberg form is equal to its perturbation index.*

In general, ℓ_d *and* ℓ_p *are not always the same, and* $\ell_\mathrm{d} \leq \ell_\mathrm{p} \leq \ell_\mathrm{d} + 1$*; see [43].*

2. *The size* (s) *of Hessenberg form of semi-explicit DAEs, defined in Definition 3.2.3, is equal to the differential/perturbation index:* $s = \ell_\mathrm{d} = \ell_\mathrm{p}$*.*

Underlying ODEs, Consistent Initial Conditions, and Hidden Constraint Equations

As mentioned in Definition 3.2.5, the ***underlying ODE***, $\dot{\mathbf{x}} = \mathbf{\Psi}(\mathbf{x}, t)$ with initial condition $\mathbf{x}_0 = \mathbf{x}(t_0)$, of a DAE system is obtained by taking the total time derivative(s) of all or part of $\mathbf{F}(t, \mathbf{x}, \dot{\mathbf{x}}) = \mathbf{0}$. The solution of a DAE system becomes identical to the one of the underlying ODE if initial conditions of the DAE system are ***consistent***. A consistent initial condition of the DAE system must satisfy not only the dynamical and algebraic equations, which explicitly appear, but also the ***hidden*** equations derivable from the time derivative(s) of the algebraic equation. For an illustration purpose only, the ideas of underlying ODEs and consistent initial conditions for semi-explicit DAEs in the Hessenberg forms of size $s = 1, 2, 3$ are shown below.

Example 3.2.1 (A Hessenberg Index-1 System)

Consider the following semi-explicit DAEs in the Hessenberg form of size $s = 1$*:*

$$\dot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y}, \mathbf{w}) \tag{3.45a}$$

$$\mathbf{0} = \mathbf{h}(t, \mathbf{y}, \mathbf{w}) \tag{3.45b}$$

Taking the total time derivative of Eq. (3.45b) *leads to*

$$\begin{aligned} \mathbf{0} &= \dot{\mathbf{h}} = \frac{\partial \mathbf{h}}{\partial t} + \frac{\partial \mathbf{h}}{\partial \mathbf{y}}\dot{\mathbf{y}} + \frac{\partial \mathbf{h}}{\partial \mathbf{w}}\dot{\mathbf{w}} \\ &= \frac{\partial \mathbf{h}}{\partial t} + \frac{\partial \mathbf{h}}{\partial \mathbf{y}}\mathbf{f}(t,\mathbf{y},\mathbf{w}) + \frac{\partial \mathbf{h}}{\partial \mathbf{w}}\dot{\mathbf{w}} \end{aligned} \tag{3.46}$$

Hence, the ODE for $\mathbf{w}$ *is obtained as*

$$\dot{\mathbf{w}} = -\left(\frac{\partial \mathbf{h}}{\partial \mathbf{w}}\right)^{-1}\left[\frac{\partial \mathbf{h}}{\partial t} + \frac{\partial \mathbf{h}}{\partial \mathbf{y}}\mathbf{f}(t,\mathbf{y},\mathbf{w})\right] \tag{3.47}$$

if matrix $\partial\mathbf{h}/\partial\mathbf{w}$ *is invertible in a neighborhood of the solution. The set of Eq.* (3.45a) *and Eq.* (3.47) *is called the* ***underlying ODE*** *of the DAE system given in Eq.* (3.45)*. Since only one differentiation is required to obtain the underlying ODE, the DAE system is of (differential) index* 1*. Initial condition* $(\mathbf{y}_0, \mathbf{w}_0)$ *is said to be* ***consistent*** *if it satisfies*

$$\mathbf{h}(t_0, \mathbf{y}_0, \mathbf{w}_0) = \mathbf{0} \tag{3.48}$$

Example 3.2.2 (A Hessenberg Index-2 System)

Consider the following semi-explicit DAEs in the Hessenberg form of size $s = 2$*:*

$$\dot{\mathbf{y}} = \mathbf{f}(t,\mathbf{y},\mathbf{w}) \tag{3.49a}$$

$$\mathbf{0} = \mathbf{h}(t,\mathbf{y}) \tag{3.49b}$$

Taking the total time derivative of Eq (3.49b) *leads to*

$$\mathbf{0} = \dot{\mathbf{h}} = \frac{\partial \mathbf{h}}{\partial t} + \frac{\partial \mathbf{h}}{\partial \mathbf{y}}\dot{\mathbf{y}} = \frac{\partial \mathbf{h}}{\partial t} + \frac{\partial \mathbf{h}}{\partial \mathbf{y}}\mathbf{f}(t,\mathbf{y},\mathbf{w}) =: \mathbf{h}_v(t,\mathbf{y},\mathbf{w}) \tag{3.50}$$

Differentiating Eq. (3.50) *in time again, we get*

$$\begin{aligned} \mathbf{0} = \ddot{\mathbf{h}} &= \frac{\partial^2 \mathbf{h}}{\partial t^2} + \frac{d}{dt}\left(\frac{\partial \mathbf{h}}{\partial \mathbf{y}}\right)\mathbf{f}(t,\mathbf{y},\mathbf{w}) \\ &\quad + \frac{\partial \mathbf{h}}{\partial \mathbf{y}}\left[\frac{\partial \mathbf{f}}{\partial t} + \frac{\partial \mathbf{f}}{\partial \mathbf{y}}\mathbf{f}(t,\mathbf{y},\mathbf{w}) + \frac{\partial \mathbf{f}}{\partial \mathbf{w}}\dot{\mathbf{w}}\right] \end{aligned} \tag{3.51}$$

Hence, the ODE for $\mathbf{w}$ *is obtained as*

$$\dot{\mathbf{w}} = -\left(\frac{\partial \mathbf{h}}{\partial \mathbf{y}}\frac{\partial \mathbf{f}}{\partial \mathbf{w}}\right)^{-1}\left[\frac{\partial^2 \mathbf{h}}{\partial t^2} + \frac{d}{dt}\left(\frac{\partial \mathbf{h}}{\partial \mathbf{y}}\right)\mathbf{f} + \frac{\partial \mathbf{h}}{\partial \mathbf{y}}\frac{\partial \mathbf{f}}{\partial t} + \frac{\partial \mathbf{h}}{\partial \mathbf{y}}\frac{\partial \mathbf{f}}{\partial \mathbf{y}}\mathbf{f}\right] \tag{3.52}$$

if matrix

$$\left(\frac{\partial \mathbf{h}}{\partial \mathbf{y}}\right)\left(\frac{\partial \mathbf{f}}{\partial \mathbf{w}}\right) \tag{3.53}$$

is invertible in a neighborhood of the solution. Therefore, the ***underlying ODE*** *of the DAE system given in Eq.* (3.50) *is Eq.* (3.49a) *together with Eq.* (3.52)*. Since we need to differentiate Eq.* (3.49b) *twice, the DAE system is of (differential) index* 2*. A* ***consistent*** *initial condition* $(\mathbf{y}_0, \mathbf{w}_0)$ *must satisfy*

$$\mathbf{h}(t_0, \mathbf{y}_0) = \mathbf{0} \ \ \textit{and} \ \ \mathbf{h}_{\mathrm{v}}(t_0, \mathbf{y}_0, \mathbf{w}_0) = \mathbf{0} \tag{3.54}$$

where $\mathbf{h}_{\mathrm{v}}(t, \mathbf{y}, \mathbf{w}) := d\mathbf{h}/dt = \mathbf{0}$ *is called the* ***hidden constraint equation*** *of the DAE system.*

Example 3.2.3 (A Hessenberg Index-3 System)

Consider the following semi-explicit DAEs in the Hessenberg form of size $s = 3$*:*

$$\dot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y}, \mathbf{v}) \tag{3.55a}$$

$$\dot{\mathbf{v}} = \mathbf{g}(t, \mathbf{y}, \mathbf{v}, \mathbf{w}) \tag{3.55b}$$

$$\mathbf{0} = \mathbf{h}(t, \mathbf{y}) \tag{3.55c}$$

where $\mathbf{y} \in \mathbb{R}^{n_{\mathrm{y}}}$ *and* $\mathbf{v} \in \mathbb{R}^{n_{\mathrm{y}}}$ *are the differential variables, and* $\mathbf{w} \in \mathbb{R}^{n_{\mathrm{w}}}$ *is the algebraic variable of the DAE system. Taking the total time derivative of Eq.* (3.55c) *three times,* *we have*

$$
\begin{aligned}
\mathbf{0} &= \dot{\mathbf{h}} = \frac{\partial \mathbf{h}}{\partial t} + \frac{\partial \mathbf{h}}{\partial \mathbf{y}}\mathbf{f}(t, \mathbf{y}, \mathbf{v}) =: \mathbf{h}_{\mathrm{v}}(t, \mathbf{y}, \mathbf{v}) && (3.56)\\
\mathbf{0} &= \ddot{\mathbf{h}} = \frac{\partial^2 \mathbf{h}}{\partial t^2} + \frac{d}{dt}\left(\frac{\partial \mathbf{h}}{\partial \mathbf{y}}\right)\mathbf{f} \\
&\quad + \frac{\partial \mathbf{h}}{\partial \mathbf{y}}\left[\frac{\partial \mathbf{f}}{\partial t} + \frac{\partial \mathbf{f}}{\partial \mathbf{y}}\mathbf{f} + \frac{\partial \mathbf{f}}{\partial \mathbf{v}}\mathbf{g}\right] =: \mathbf{h}_{\mathrm{a}}(t, \mathbf{y}, \mathbf{v}, \mathbf{w}) && (3.57)\\
\mathbf{0} &= \dddot{\mathbf{h}} = \frac{\partial^3 \mathbf{h}}{\partial t^3} + \frac{d^2}{dt^2}\left(\frac{\partial \mathbf{h}}{\partial \mathbf{y}}\right)\mathbf{f} + \frac{d}{dt}\left(\frac{\partial \mathbf{h}}{\partial \mathbf{y}}\right)\dot{\mathbf{f}} \\
&\quad + \frac{d}{dt}\left(\frac{\partial \mathbf{h}}{\partial \mathbf{y}}\right)\left[\frac{\partial \mathbf{f}}{\partial t} + \frac{\partial \mathbf{f}}{\partial \mathbf{y}}\mathbf{f} + \frac{\partial \mathbf{f}}{\partial \mathbf{v}}\mathbf{g}\right] \\
&\quad + \frac{\partial \mathbf{h}}{\partial \mathbf{y}}\left[\frac{\partial^2 \mathbf{f}}{\partial t^2} + \frac{d}{dt}\left(\frac{\partial \mathbf{f}}{\partial \mathbf{y}}\right)\mathbf{f} + \frac{\partial \mathbf{f}}{\partial \mathbf{y}}\dot{\mathbf{f}} + \frac{d}{dt}\left(\frac{\partial \mathbf{f}}{\partial \mathbf{v}}\right)\mathbf{g} + \frac{\partial \mathbf{f}}{\partial \mathbf{v}}\dot{\mathbf{g}}\right] && (3.58)
\end{aligned}
$$

with

$$
\dot{\mathbf{g}} = \frac{\partial \mathbf{g}}{\partial t} + \frac{\partial \mathbf{g}}{\partial \mathbf{y}}\mathbf{f} + \frac{\partial \mathbf{g}}{\partial \mathbf{v}}\mathbf{g} + \frac{\partial \mathbf{g}}{\partial \mathbf{w}}\dot{\mathbf{w}} \tag{3.59}
$$

Hence, the ODE for $\mathbf{w}$ *is obtained as* $\dot{\mathbf{w}} = \boldsymbol{\psi}(t, \mathbf{y}, \mathbf{v}, \mathbf{w})$ *if matrix*

$$
\left(\frac{\partial \mathbf{h}}{\partial \mathbf{y}}\right)\left(\frac{\partial \mathbf{f}}{\partial \mathbf{v}}\right)\left(\frac{\partial \mathbf{g}}{\partial \mathbf{w}}\right) \tag{3.60}
$$

is invertible in a neighborhood of the solution. The ***underlying ODE*** *of the DAE system is therefore given as* $\dot{\mathbf{w}} = \boldsymbol{\psi}(t, \mathbf{y}, \mathbf{v}, \mathbf{w})$ *and Eq. (3.55a). A* ***consistent*** *initial condition* $(\mathbf{y}_0, \mathbf{v}_0, \mathbf{w}_0)$ *must satisfy*

$$
\begin{aligned}
\mathbf{h}(t_0, \mathbf{y}_0) &= \mathbf{0} \\
\mathbf{h}_{\mathrm{v}}(t_0, \mathbf{y}_0, \mathbf{v}_0) &= \mathbf{0} \\
\mathbf{h}_{\mathrm{a}}(t_0, \mathbf{y}_0, \mathbf{v}_0, \mathbf{w}_0) &= \mathbf{0}
\end{aligned} \tag{3.61}
$$

where $\mathbf{h}_{\mathrm{v}} = \mathbf{0}$ *and* $\mathbf{h}_{\mathrm{a}} = \mathbf{0}$ *are the* ***hidden constant equations*** *of the system.*

3.2.3 DAEs and Differential Equations with Invariants

Consider the ODE for $\mathbf{y}(t) : \mathbb{I} \rightarrow \mathbb{R}^{n_y}$,

$$\dot{\mathbf{y}} = \mathbf{g}(\mathbf{y}) \tag{3.62a}$$

with initial condition $\mathbf{y}_0 = \mathbf{y}(t_0)$, and suppose the solution $\mathbf{y}(t)$ satisfies the ***invariant***,

$$\mathbf{\Gamma}(\mathbf{y}) = \mathbf{0} \tag{3.62b}$$

The invariant $\mathbf{\Gamma}(\mathbf{y}) = \mathbf{0} \in \mathbb{R}^{n_\Gamma}$ is called a ***first integral*** if the solution also satisfies

$$\mathbf{0} \equiv \dot{\mathbf{\Gamma}} = \frac{\partial \mathbf{\Gamma}}{\partial \mathbf{y}} \mathbf{g}(\mathbf{y}) \tag{3.63}$$

in a neighborhood of the solution. In order to treat the invariant given in Eq. (3.62b) as the constraint, reformulate Eq. (3.62) with algebraic variable $\mathbf{w} \in \mathbb{R}^{n_\Gamma}$ as

$$\dot{\mathbf{y}} = \mathbf{g}(\mathbf{y}) - \left(\frac{\partial \mathbf{\Gamma}}{\partial \mathbf{y}}\right)^T \mathbf{w} \tag{3.64a}$$

$$\mathbf{0} = \mathbf{\Gamma}(\mathbf{y}) \tag{3.64b}$$

Note that the ODE system, Eq. (3.62), has turned into the DAE system, Eq. (3.64); and $\mathbf{\Gamma}(\mathbf{y}) = \mathbf{0}$ given in Eq. (3.64b) is now viewed as the constraint equation of the system. The solution of the DAE system is identical to the one of the ODE system if and only if the algebraic variable is $\mathbf{w} \equiv \mathbf{0}$, and it is actually true in the continuous time system if matrix $\partial \mathbf{\Gamma} / \partial \mathbf{y}$ has full rank[1] since

$$\mathbf{0} \equiv \dot{\mathbf{\Gamma}} = \frac{\partial \mathbf{\Gamma}}{\partial \mathbf{y}} \mathbf{g}(\mathbf{y}) - \frac{\partial \mathbf{\Gamma}}{\partial \mathbf{y}} \left(\frac{\partial \mathbf{\Gamma}}{\partial \mathbf{y}}\right)^T \mathbf{w} = \underbrace{\dot{\mathbf{\Gamma}}}_{=\mathbf{0}} - \frac{\partial \mathbf{\Gamma}}{\partial \mathbf{y}} \left(\frac{\partial \mathbf{\Gamma}}{\partial \mathbf{y}}\right)^T \mathbf{w} = -\frac{\partial \mathbf{\Gamma}}{\partial \mathbf{y}} \left(\frac{\partial \mathbf{\Gamma}}{\partial \mathbf{y}}\right)^T \mathbf{w} \tag{3.65}$$

[1] If matrix $\partial \mathbf{\Gamma} / \partial \mathbf{y}$ has full rank, the DAE system, given in Eq. (3.64), is in the Hessenberg Index-2 form.

Example 3.2.4 (GGL and Overdetermined Formulations)

An example of turning a system invariant into the constraint can be found in the formulation of the stabilized Index-2 (GGL) DAE system from the Index-2 DAE system in constrained mechanical system; see Eq. (3.93) *in the next subsection. Similar idea is applied for the formulation of the overdetermined DAE system; see Eq.* (3.99) *and* (3.100).

3.2.4 Formulations of DAEs in Constrained Mechanical Systems

In order to illustrate the concepts of the formulations of DAEs, consider the semi-discrete equation of motion for constrained dynamical problems with holonomic constraints, as an example. It is generally written in the following DAE form

$$\boxed{\begin{array}{c} \mathbf{Q}^{\text{iner}}(\mathbf{q}, \dot{\mathbf{q}}, \ddot{\mathbf{q}}) + \mathbf{G}^T \boldsymbol{\lambda} + \mathbf{Q}^{\text{int}}(\mathbf{q}) = \mathbf{Q}^{\text{appl}}(\mathbf{q}, \dot{\mathbf{q}}, t) \\ \boldsymbol{\Phi} = \mathbf{0} \end{array} \quad \forall t \in \mathbb{I} := [t_0, t_{\text{L}}] \subset \mathbb{R}} \tag{3.66}$$

where $\mathbf{q}(t) : \mathbb{I} \to Q$ and $\boldsymbol{\lambda}(t) : \mathbb{I} \to \mathbb{R}^{n_{\text{c}}}$ are the configuration of the system and the Lagrange multiplier, respectively [2] ; and $\mathbf{Q}^{\text{iner}}$, $\mathbf{Q}^{\text{int}}$, and $\mathbf{Q}^{\text{appl}}$ are the generalized inertia, internal, and applied forces, respectively[3] . The second equation in Eq. (3.66), i.e., $\boldsymbol{\Phi} = \mathbf{0} \in \mathbb{R}^{n_{\text{c}}}$, is the ***geometric constraint equation*** (or the ***constraint equation at***

[2] Q is an n_{g}-dimensional real differentiable configuration manifold of the system defined as

$$Q := \left\{ \mathbf{q} = (q_1, q_2, \cdots, q_{n_{\text{g}}}) \in \mathbb{R}^{n_{\text{g}}} \mid \boldsymbol{\Phi} = \mathbf{0} \right\} \tag{3.67}$$

where $\mathbf{q}(t) : \mathbb{I} = [t_0, t_L] \subset \mathbb{R} \to Q$ are the local coordinates with at least twice differentiable function $q_i(t) = [\mathbf{q}(t)]_i : \mathbb{I} \to \mathbb{R}$ (for $i = 1, 2, \cdots, n_{\text{g}}$). The tangent space at $\mathbf{q} \in Q$: $\dot{\mathbf{q}}(t) : \mathbb{I} \to T_{\mathbf{q}}Q$ is therefore defined as

$$T_{\mathbf{q}}Q := \left\{ \dot{\mathbf{q}} \in \mathbb{R}^{n_{\text{g}}} \mid \dot{\boldsymbol{\Phi}} = \mathbf{G}\dot{\mathbf{q}} = \mathbf{0} \right\} \tag{3.68}$$

[3] See Chapter 6 for the classifications of the generalized force vectors.

position level), and matrix $\mathbf{G}$ is defined as the derivative of $\mathbf{\Phi}$ with respect to $\mathbf{q}$:

$$\mathbf{G} := \frac{\partial \mathbf{\Phi}}{\partial \mathbf{q}} \in \mathbb{R}^{n_c \times n_g} \tag{3.69}$$

If the geometric constraint equation depends only on $\mathbf{q}$, i.e., $\mathbf{\Phi}(\mathbf{q}) = \mathbf{0}$, it is called ***holonomic-scleronomic***; while, $\mathbf{\Phi}(\mathbf{q}) = \mathbf{0}$ is called the ***holonomic-rheonomic***; see Definition 6.1.1.

For simplicity of the exposition, we adopt the following assumptions without loss of generality in this and following sections:

- The generalized inertia force is given as a linear function in the generalized acceleration vector in the form,

$$\mathbf{Q}^{\text{iner}} = \mathbf{M}(\mathbf{q})\ddot{\mathbf{q}} \tag{3.70}$$

  where $\mathbf{M} : Q \to \mathbb{R}^{n_g \times n_g}$ is the symmetric, positive-definite mass matrix.

- The generalized internal force does not appear, i.e., $\mathbf{Q}^{\text{int}}(\mathbf{q}) = \mathbf{0}$.

- The constraint equation is holonomic-schleronomic.

Hence, Eq. (3.66) may be reduced to [4]

$$\left.\begin{aligned} \mathbf{M}(\mathbf{q})\ddot{\mathbf{q}} + \mathbf{G}^T(\mathbf{q})\boldsymbol{\lambda} &= \mathbf{Q}^{\text{appl}}(\mathbf{q}, \dot{\mathbf{q}}, t) \\ \mathbf{\Phi}(\mathbf{q}) &= \mathbf{0} \end{aligned}\right\} \quad \forall t \in \mathbb{I} \tag{3.71}$$

Index-3 Formulation

The system of equations given in Eq. (3.71) is classified as a Index 3 formulation:

$$\boxed{\begin{aligned} \mathbf{M}(\mathbf{q})\ddot{\mathbf{q}} &= \mathbf{Q}^{\text{appl}}(\mathbf{q}, \dot{\mathbf{q}}, t) - \mathbf{G}^T\boldsymbol{\lambda} \\ \mathbf{\Phi}(\mathbf{q}) &= \mathbf{0} \end{aligned} \quad \forall t \in \mathbb{I}} \tag{3.72}$$

[4] see Chapter 7 for the details of the derivation and discussions of Eq. (3.71).

Eq. (3.72) together with initial conditions $(\mathbf{q}, \dot{\mathbf{q}}, \lambda)(t_0) = (\mathbf{q}_0, \mathbf{v}_0, \lambda_0)$ is the system of second-order differential-algebraic equations in $\mathbf{q} \in Q$. By introducing velocity variable $\mathbf{v}(t) : \mathbb{I} \to T_{\mathbf{q}}Q$, [5] Eq. (3.72) can be written in the Hessenberg form of size three as

$$\boxed{\begin{aligned} \mathbf{M}(\mathbf{q})\dot{\mathbf{v}} &= \mathbf{Q}^{\text{appl}}(\mathbf{q}, \mathbf{v}, t) - \mathbf{G}^T \boldsymbol{\lambda} \\ \dot{\mathbf{q}} &= \mathbf{v} \qquad\qquad\qquad\qquad \forall t \in \mathbb{I} \\ \boldsymbol{\Phi}(\mathbf{q}) &= \mathbf{0} \end{aligned}} \tag{3.74}$$

Remark 3.2.6

1. ***Hidden Constraints:*** *The* ***constraint equations at the velocity level****, also called the* ***velocity constraint equations****, can be obtained by simply differentiating the geometric constraint equations,* $\boldsymbol{\Phi}(\mathbf{q})$ *as*

$$0 = \frac{d}{dt}\Phi_i(\mathbf{q}) = G_{ij}(\mathbf{q})\dot{q}_j = G_{ij}(\mathbf{q})v_j \quad \forall t \in \mathbb{I} \tag{3.75}$$

or, in the vector-matrix notation,

$$\boxed{\mathbf{0} = \dot{\boldsymbol{\Phi}} = \mathbf{G}(\mathbf{q})\dot{\mathbf{q}} = \mathbf{G}(\mathbf{q})\mathbf{v}} \tag{3.76}$$

Taking the time derivative of Eq. (3.75)*, the* ***constraint equations at the acceleration level****, also called the* ***acceleration constraint equations****, can be obtained as*

$$\begin{aligned} 0 &= \frac{d^2}{dt^2}\Phi_i(\mathbf{q}) \\ &= G_{ij}(\mathbf{q})\ddot{q}_j + \dot{G}_{ij}(\mathbf{q})\dot{q}_j = G_{ij}(\mathbf{q})\dot{v}_j + \dot{G}_{ij}(\mathbf{q})v_j \end{aligned} \qquad \forall t \in \mathbb{I} \tag{3.77}$$

[5] The tangent space at $\mathbf{q} \in Q$: $\dot{\mathbf{q}}(t) : \mathbb{I} \to T_{\mathbf{q}}Q$ for the system of Eq. (3.74) is

$$T_{\mathbf{q}}Q := \left\{ \dot{\mathbf{q}} \in \mathbb{R}^{n_g} \mid \dot{\boldsymbol{\Phi}} = \mathbf{G}\mathbf{v} = \mathbf{0} \right\} \tag{3.73}$$

in which the time derivative of G_{ij} is given by

$$\dot{G}_{ij}(\mathbf{q}) = \dot{q}_\ell \partial G_{ij}/\partial q_\ell = v_\ell \partial G_{ij}/\partial q_\ell \tag{3.78}$$

In the vector-matrix notation, Eq. (3.77) *can be written as*

$$\boxed{\mathbf{0} = \ddot{\mathbf{\Phi}} = \mathbf{G}(\mathbf{q})\ddot{\mathbf{q}} + \mathfrak{D}\mathbf{G}(\mathbf{q})(\dot{\mathbf{q}}, \dot{\mathbf{q}}) = \mathbf{G}(\mathbf{q})\dot{\mathbf{v}} + \mathfrak{D}\mathbf{G}(\mathbf{q})(\mathbf{v}, \mathbf{v})} \tag{3.79}$$

with $\mathfrak{D}\mathbf{G}(\mathbf{q}) = \nabla\mathbf{G}(\mathbf{q}) = \partial\mathbf{G}(\mathbf{q})/\partial\mathbf{q}$. *For the system of Eq.* (3.72) *or Eq.* (3.74), *the velocity and acceleration constraint equations, given in Eq.* (3.75) *and Eq.* (3.77), *respectively, are the* ***hidden*** *constraint equations to be additionally satisfied. Combining Eq.* $(3.74)_1$ *and Eq.* (3.79) *yields the linear form*

$$\underbrace{\begin{bmatrix} \mathbf{M} & \mathbf{G}^T \\ \mathbf{G} & \mathbf{0} \end{bmatrix}}_{=:\mathbf{H}} \begin{bmatrix} \dot{\mathbf{v}} \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathbf{Q}^{\text{appl}}(\mathbf{q}, \mathbf{v}, t) \\ -\mathfrak{D}\mathbf{G}(\mathbf{q})(\mathbf{v}, \mathbf{v}) \end{bmatrix} \tag{3.80}$$

We assume matrix $\mathbf{G}$ *is invertible, i.e.,* $\mathbf{G}$ *is of full rank,* $\text{rank}(\mathbf{G}) = n_\text{c}$; *hence, the symmetric matrix* $\mathbf{H}$ *is invertible since* $\mathbf{M}$ *is symmetric and positive-definite.*[6]

It is worth mentioning that numerical solutions, given from a time integration scheme, do not satisfy the hidden constraints in general at time grids $t_n \in \mathbb{I}$.

2. ***Underlying ODE:*** *According to the definition of the differential index, introduced in the previous section, the* ***underlying ordinary differential equations*** *of the Index-3 DAE system may be obtained after taking the time derivative of the*

[6] *A symmetric, square matrix which can be written in the form*

$$\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix} \tag{3.81}$$

where $\mathbf{A}$ *is a square positive semi-definite matrix, and* $\mathbf{B}$ *has full rank, is called the* ***saddle-point matrix***.

constraint equation three times. Substituting Eq. $(3.72)_1$ *or Eq.* $(3.74)_1$ *into Eq.* (3.79)*, we get*

$$\left[\mathbf{G}\mathbf{M}^{-1}\mathbf{G}^T\right]\lambda = \mathbf{G}\mathbf{M}^{-1}\mathbf{Q}^{\mathrm{appl}}(\mathbf{q},\mathbf{v},t) + \mathfrak{D}\mathbf{G}(\mathbf{q})(\mathbf{v},\mathbf{v}) \tag{3.82}$$

Since matrix $\mathbf{G}\mathbf{M}^{-1}\mathbf{G}^T$ *is invertible, we can express the Lagrange multiplier as a function of* $\mathbf{q}$, $\mathbf{v}$, *and* t*:*

$$\lambda = \mathbf{\Lambda}(\mathbf{q},\mathbf{v},t) = \left[\mathbf{G}\mathbf{M}^{-1}\mathbf{G}^T\right]^{-1}\left[\mathbf{G}\mathbf{M}^{-1}\mathbf{Q}^{\mathrm{appl}}(\mathbf{q},\mathbf{v},t) + \mathfrak{D}\mathbf{G}(\mathbf{q})(\mathbf{v},\mathbf{v})\right] \tag{3.83}$$

Substituting Eq. (3.83) *into Eq.* $(3.72)_1$ *leads to an ordinary differential equation in* $(\mathbf{q},\mathbf{v}) : \mathbb{I} \to TQ$ *as*

$$\boxed{\frac{d}{dt}\begin{bmatrix}\mathbf{q}\\ \mathbf{v}\end{bmatrix} = \begin{bmatrix}\mathbf{v}\\ \mathbf{M}^{-1}\left[\mathbf{Q}^{\mathrm{appl}}(\mathbf{q},\mathbf{v},t) - \mathbf{G}^T\mathbf{\Lambda}(\mathbf{q},\mathbf{v},t)\right]\end{bmatrix} \quad \forall t \in \mathbb{I}} \tag{3.84}$$

Eq. (3.84) *is called the **state space form ODE** of the system for* $(\mathbf{q},\mathbf{v})$*. In the single-field form, the ordinary differential equation of the system in* $\mathbf{q}(t) : \mathbb{T} \to Q$ *is given in the form*

$$\boxed{\ddot{\mathbf{q}} = \mathbf{M}^{-1}\left[\mathbf{Q}^{\mathrm{appl}}(\mathbf{q},\dot{\mathbf{q}},t) - \mathbf{G}^T\mathbf{\Lambda}(\mathbf{q},\dot{\mathbf{q}},t)\right] \quad \forall t \in \mathbb{I}} \tag{3.85}$$

where

$$\lambda = \mathbf{\Lambda}(\mathbf{q},\dot{\mathbf{q}},t) = \left[\mathbf{G}\mathbf{M}^{-1}\mathbf{G}^T\right]^{-1}\left[\mathbf{G}\mathbf{M}^{-1}\mathbf{Q}^{\mathrm{appl}}(\mathbf{q},\dot{\mathbf{q}},t) + \mathfrak{D}\mathbf{G}(\mathbf{q})(\dot{\mathbf{q}},\dot{\mathbf{q}})\right] \tag{3.86}$$

By taking the time derivative of $\mathbf{\Lambda}(\mathbf{q},\mathbf{v},t)$*, given in Eq.* (3.83)*, or* $\mathbf{\Lambda}(\mathbf{q},\dot{\mathbf{q}},t)$*, given in Eq.* (3.86)*, we finally obtain the differential equation in the Lagrange multiplier, also referred to as the algebraic variable. As we can see, the Index-3 system requires three-time differentiation steps in order to obtain the **underlying ODEs** of the system; in other words, the system, given in Eq.* (3.74)*/Eq.* (3.72)*, are Index-3 if* $\mathbf{H}$ *is invertible.*

3. ***Consistent Initial Conditions:*** *Initial conditions that satisfy both the geometric constraint and the hidden constraints, i.e.,*

$$\begin{aligned}
\mathbf{0} &= \boldsymbol{\Phi}(\mathbf{q}_0) \\
\mathbf{0} &= \dot{\boldsymbol{\Phi}} = \mathbf{G}(\mathbf{q}_0)\mathbf{v}_0 =: \boldsymbol{\Phi}_{\mathrm{v}}(\mathbf{q}_0, \mathbf{v}_0) \\
\mathbf{0} &= \ddot{\boldsymbol{\Phi}} = \mathbf{G}(\mathbf{q}_0)\mathbf{a}_0 + \mathfrak{D}\mathbf{G}(\mathbf{q}_0)(\mathbf{v}_0, \mathbf{v}_0) =: \boldsymbol{\Phi}_{\mathrm{a}}(\mathbf{q}_0, \mathbf{v}_0, \mathbf{a}_0)
\end{aligned} \tag{3.87}$$

*are called the **consistent initial conditions**. In other words, the initial acceleration and Lagrange multiplier vectors,* $\mathbf{a}_0 = \dot{\mathbf{v}}(t_0)$ *and* $\lambda_0 = \lambda(t_0)$*, need to be evaluated from* [7]

$$\begin{bmatrix} \mathbf{M}(\mathbf{q}_0) & \mathbf{G}^T(\mathbf{q}_0) \\ \mathbf{G}(\mathbf{q}_0) & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{a}_0 \\ \lambda_0 \end{bmatrix} = \begin{bmatrix} \mathbf{Q}^{\mathrm{appl}}(\mathbf{q}_0, \mathbf{v}_0, t_0) \\ -\mathfrak{D}\mathbf{G}(\mathbf{q}_0)(\mathbf{v}_0, \mathbf{v}_0) \end{bmatrix} \tag{3.88}$$

with the initial conditions $(\mathbf{q}, \mathbf{v})(t_0) = (\mathbf{q}_0, \mathbf{v}_0)$ *that satisfy the geometric and velocity constraints, i.e.,*

$$\mathbf{0} = \boldsymbol{\Phi}(\mathbf{q}_0) = \boldsymbol{\Phi}_{\mathrm{v}}(\mathbf{q}_0, \mathbf{v}_0) \tag{3.89}$$

With the consistent initial conditions, $(\mathbf{q}_0, \mathbf{v}_0)$*, solutions from Eq.* (3.74) *and Eq.* (3.84) *become identical in* $t \in \mathbb{I}$*. In the sense of the second-order system, Eq.* (3.72) *and Eq.* (3.85) *with consistent initial conditions* $(\mathbf{q}, \dot{\mathbf{q}})(t_0) = (\mathbf{q}_0, \mathbf{v}_0)$ *yield the same solutions in* $t \in \mathbb{I}$*.*

The following alternative formulations, i.e., Index-2, stabilized Index-2, Index-1, and overdetermined formulations, are mathematically equivalent if initial conditions are consistent.

---

[7] *The initial condition of the Lagrange multiplier is therefore obtained from Eq.* (3.83) *as* $\lambda_0 = \lambda(\mathbf{q}_0, \mathbf{v}_0, t_0)$.

Index-2 Formulation

Replacing the geometric constraint, $\mathbf{\Phi} = \mathbf{0}$, in the Index-3 formulation with the velocity constraint leads to the ***Index-2*** formulation:

$$\boxed{\begin{aligned} \mathbf{M}(\mathbf{q})\ddot{\mathbf{q}} &= \mathbf{Q}^{\text{appl}}(\mathbf{q}, \dot{\mathbf{q}}, t) - \mathbf{G}^T \boldsymbol{\lambda} \\ \dot{\mathbf{\Phi}} &= \mathbf{G}(\mathbf{q})\dot{\mathbf{q}} = \mathbf{0} \end{aligned} \quad \forall t \in \mathbb{I}} \tag{3.90}$$

in $\mathbf{q}$, or

$$\boxed{\begin{aligned} \mathbf{M}(\mathbf{q})\dot{\mathbf{v}} &= \mathbf{Q}^{\text{appl}}(\mathbf{q}, \mathbf{v}, t) - \mathbf{G}^T \boldsymbol{\lambda} \\ \dot{\mathbf{q}} &= \mathbf{v} \\ \dot{\mathbf{\Phi}} &= \mathbf{G}(\mathbf{q})\mathbf{v} = \mathbf{0} \end{aligned} \quad \forall t \in \mathbb{I}} \tag{3.91}$$

in $(\mathbf{q}, \mathbf{v})$.

Remark 3.2.7

1. ***Hidden Constraints:*** *In the Index-2 system given above, we have only one hidden constraint: the acceleration constraint, which can be derived by taking the time derivative of* $\dot{\mathbf{\Phi}} = \mathbf{0}$, *i.e.,*

$$\boxed{\mathbf{0} = \ddot{\mathbf{\Phi}} = \mathbf{G}(\mathbf{q})\ddot{\mathbf{q}} + \mathfrak{D}\mathbf{G}(\mathbf{q})(\dot{\mathbf{q}}, \dot{\mathbf{q}}) = \mathbf{G}(\mathbf{q})\dot{\mathbf{v}} + \mathfrak{D}\mathbf{G}(\mathbf{q})(\mathbf{v}, \mathbf{v}),} \tag{3.92}$$

   which is identical to Eq. (3.79).

2. ***Underlying ODE:*** *The underlying ODE for the system formulated in Index 2 is of course the same as the one for the Index-3 case. With the assumption that matrix* $\mathbf{H}$, *defined in Eq.* (3.80), *is invertible, the system given in Eq.* (3.90)*/Eq.* (3.91) *are "Index 2" since twice time derivatives are required to obtain the underlying ODE of the system.*

3. ***Drift-off Phenomenon and Invariant:*** *Obviously, the Index-2 formulation defined in Eq.* (3.90) *and Eq.* (3.91) *lacks the information of the geometric constraint equation,* $\mathbf{\Phi}(\mathbf{q}) = \mathbf{0}$*; therefore, the so-called* ***drift-off*** *phenomenon may occur when we solving with a numerical scheme. The numerical solutions of Eq.* (3.90)*/Eq.* (3.91) *are not restricted to be on the curve on* Q*, and they no longer satisfy* $\mathbf{\Phi}(\mathbf{q}) = \mathbf{0}$ *in general, which leads to a numerical instability issue, especially during the Newton-type iteration process. As will be discussed later, the violation of the geometric constraint in this Index-2 formulation grows linearly in time step size* Δt.

   In order to resolve this issue, the so-called ***stabilized Index-2 formulation****, also known as the* ***Gear-Gupta-Leimkuhler (GGL) formulation*** *has been proposed. In this formulation, the geometric constraint equation is viewed as a* ***invariant*** *of the system*[8] *and included in the formation, introducing an additional Lagrange multiplier* $\boldsymbol{\mu} : \mathbb{I} \to \mathbb{R}^{n_c}$*; see the following.*

Stabilized Index-2 Formulation (or GGL formulation)

The stabilized Index-2 (GGL) formulation for the system reads [44]:

$$\boxed{\begin{aligned} \mathbf{M}(\mathbf{q})\dot{\mathbf{v}} &= \mathbf{Q}^{\mathrm{appl}}(\mathbf{q}, \mathbf{v}, t) - \mathbf{G}^T \boldsymbol{\lambda} \\ \mathbf{S}\dot{\mathbf{q}} &= \mathbf{S}\mathbf{v} - \mathbf{G}^T \boldsymbol{\mu} \\ \mathbf{\Phi}(\mathbf{q}) &= \mathbf{0} \\ \dot{\mathbf{\Phi}} &= \mathbf{G}(\mathbf{q})\mathbf{v} = \mathbf{0} \end{aligned} \qquad \forall t \in \mathbb{I}} \tag{3.93}$$

[8] *It is important to note that* $\mathbf{\Phi}(\mathbf{q}) = \mathbf{0}$ *is NOT a hidden constraint! The only hidden constraint for the system given in Eq.* (3.90)*/Eq.* (3.91) *is the acceleration constraint.*

where $\boldsymbol{\lambda} : \mathbb{I} \to \mathbb{R}^{n_c}$ and $\boldsymbol{\mu} : \mathbb{I} \to \mathbb{R}^{n_c}$ are the Lagrange multipliers, and $\mathbf{S} \in \mathbb{R}^{n_g \times n_g}$ is the ***scaling matrix***.

Remark 3.2.8

1. ***Scaling Matrix:*** *Taking the time derivative of Eq.* (3.93)$_3$ *yields*

$$\begin{aligned} \mathbf{0} &= \dot{\boldsymbol{\Phi}} = \mathbf{G}\dot{\mathbf{q}} \\ &= \mathbf{G}\left[\mathbf{v} - \mathbf{S}^{-1}\mathbf{G}^T\boldsymbol{\mu}\right] \quad \because \ \textit{Eq.}\,(3.93)_2 \\ &= \underbrace{\mathbf{G}\mathbf{v}}_{\mathbf{0}} - \mathbf{G}\mathbf{S}^{-1}\mathbf{G}^T\boldsymbol{\mu} \quad \because \ \textit{Eq.}\,(3.93)_4 \\ &= -\mathbf{G}\mathbf{S}^{-1}\mathbf{G}^T\boldsymbol{\mu} \end{aligned} \tag{3.94}$$

Therefore, if matrix $\mathbf{G}\mathbf{S}^{-1}\mathbf{G}^T \in \mathbb{R}^{n_c \times n_c}$ *is invertible, i.e., if scaling matrix* $\mathbf{S}$ *is symmetric and positive-definite, the Lagrange multiplier* $\boldsymbol{\mu}$ *actually vanishes:*

$$\boxed{\boldsymbol{\mu} \equiv \mathbf{0} \ \ \forall t \in \mathbb{I}} \tag{3.95}$$

This is why the stabilized Index-2 formulation is equivalent to other formulations, such as Index-2, Index-3, and so on, if the initial conditions are consistent. The mass matrix $\mathbf{M}(\mathbf{q})$ *(or corresponding diagonalized damped mass matrix) is usually adopted as the scaling matrix, i.e.,* $\mathbf{S} = \mathbf{M}$*, since it possesses the symmetric and positive-definite properties.*

2. *The Lagrange multiplier* $\boldsymbol{\mu}$ *are introduced in Eq.* (3.93) *so as to enforce the velocity constraint equation,* $\dot{\boldsymbol{\Phi}} = \mathbf{0}$*; however, the velocity constraint equation is always satisfied whenever the geometric constraint equation is satisfied when* $\mathbf{v} = \dot{\mathbf{q}}$*. In other words, since the velocity constraint is redundant in the continuous time system, Eq.* (3.95) *is trivial. However, Eq.* (3.95) *becomes no longer trivial in general, i.e.,* $\boldsymbol{\mu}(t_n) \approx \boldsymbol{\mu}^n \neq \mathbf{0}$ *at time level* t_n*, once the system given in Eq.* (3.93)

is discretized in time because the satisfaction of the geometric constraint equation does not always imply the satisfaction of the velocity constraint equation within a time step with most numerical techniques.

3. *A disadvantage of the stabilized Index-2 formulation, given in Eq.* (3.93), *is that the inverse of the mass matrix needs to be evaluated every step when it is discretized in time. This can become computationally very expensive, especially when tackling large size problems. In order to remedy it, the following formulation was developed without losing any benefit in the original stabilized Index-2 formulation; refer to [45]:*

$$\boxed{\begin{aligned} \mathbf{0} &= -\mathbf{M}(\mathbf{q})\mathbf{w} + \mathbf{Q}^{\text{appl}}(\mathbf{q}, \mathbf{v}, t) - \mathbf{G}^T \boldsymbol{\lambda} \\ \dot{\mathbf{v}} &= \mathbf{w} \\ \mathbf{S}\dot{\mathbf{q}} &= \mathbf{S}\mathbf{v} - \mathbf{G}^T \boldsymbol{\mu} & \forall t \in \mathbb{I} \\ \mathbf{\Phi}(\mathbf{q}) &= \mathbf{0} \\ \dot{\mathbf{\Phi}} &= \mathbf{G}(\mathbf{q})\mathbf{v} = \mathbf{0} \end{aligned}} \tag{3.96}$$

with additional acceleration variables $\mathbf{w} : \mathbb{I} \to \mathbb{R}^{n_g}$.

Index-1 Formulation

Replacing the geometric constraint, $\mathbf{\Phi} = \mathbf{0}$, in the Index-3 formulation with the acceleration constraint leads to the ***Index-1*** formulation:

$$\boxed{\begin{aligned} \mathbf{M}(\mathbf{q})\ddot{\mathbf{q}} &= \mathbf{Q}^{\text{appl}}(\mathbf{q}, \dot{\mathbf{q}}, t) - \mathbf{G}^T \boldsymbol{\lambda} & \forall t \in \mathbb{I} \\ \ddot{\mathbf{\Phi}} &= \mathbf{G}(\mathbf{q})\ddot{\mathbf{q}} + \mathfrak{D}\mathbf{G}(\mathbf{q})(\dot{\mathbf{q}}, \dot{\mathbf{q}}) = \mathbf{0} \end{aligned}} \tag{3.97}$$

in $\mathbf{q}$, or

$$\boxed{\begin{aligned} \mathbf{M}(\mathbf{q})\dot{\mathbf{v}} &= \mathbf{Q}^{\mathrm{appl}}(\mathbf{q}, \mathbf{v}, t) - \mathbf{G}^T \boldsymbol{\lambda} & \\ \dot{\mathbf{q}} &= \mathbf{v} & \forall t \in \mathbb{I} \\ \ddot{\mathbf{\Phi}} &= \mathbf{G}(\mathbf{q})\dot{\mathbf{v}} + \mathfrak{D}\mathbf{G}(\mathbf{q})(\mathbf{v}, \mathbf{v}) = \mathbf{0} & \end{aligned}} \tag{3.98}$$

in $(\mathbf{q}, \mathbf{v})$.

Remark 3.2.9

1. ***Drift-off Phenomena and Invariants:*** *There exists no hidden constraint in the Index-1 formulation given in Eq.* (3.97)*/Eq.* (3.98)*; however, the geometric and velocity constraints, which do not explicitly appear in the formulation, are now treated as invariants of the system. Those two invariants are no longer satisfied along the solution curve at time grids t_n in general once the system is discretized in time. Violations of the geometric and velocity constraint equations in this Index-1 formulation grows* quadratically *and* linearly *in time step size Δt, respectively. As remedies for these issues, several techniques have been proposed; see Section 3.4.*

2. ***Underlying ODE:*** *Only one time derivative is required (for $\mathbf{\Lambda}(\mathbf{q}, \dot{\mathbf{q}}, t)$) to derive the underlying ODE for the system, with the assumption of the invertible matrix* $\mathbf{H}$*, defined in Eq.* (3.80).

Overdetermined Formulation

The ***overdetermined formulation*** includes all constraint equations at position, velocity, and acceleration levels:

$$\boxed{\begin{aligned} \mathbf{M}(\mathbf{q})\ddot{\mathbf{q}} &= \mathbf{Q}^{\text{appl}}(\mathbf{q}, \dot{\mathbf{q}}, t) - \mathbf{G}^T \boldsymbol{\lambda} \\ \boldsymbol{\Phi} &= \mathbf{0} \\ \dot{\boldsymbol{\Phi}} &= \mathbf{G}(\mathbf{q})\dot{\mathbf{q}} = \mathbf{0} \\ \ddot{\boldsymbol{\Phi}} &= \mathbf{G}(\mathbf{q})\ddot{\mathbf{q}} + \mathfrak{D}\mathbf{G}(\mathbf{q})(\dot{\mathbf{q}}, \dot{\mathbf{q}}) = \mathbf{0} \end{aligned} \quad \forall t \in \mathbb{I}} \tag{3.99}$$

in $\mathbf{q}$, and

$$\boxed{\begin{aligned} \mathbf{M}(\mathbf{q})\dot{\mathbf{v}} &= \mathbf{Q}^{\text{appl}}(\mathbf{q}, \mathbf{v}, t) - \mathbf{G}^T \boldsymbol{\lambda} \\ \dot{\mathbf{q}} &= \mathbf{v} \\ \boldsymbol{\Phi} &= \mathbf{0} \\ \dot{\boldsymbol{\Phi}} &= \mathbf{G}(\mathbf{q})\mathbf{v} = \mathbf{0} \\ \ddot{\boldsymbol{\Phi}} &= \mathbf{G}(\mathbf{q})\dot{\mathbf{v}} + \mathfrak{D}\mathbf{G}(\mathbf{q})(\mathbf{v}, \mathbf{v}) = \mathbf{0} \end{aligned} \quad \forall t \in \mathbb{I}} \tag{3.100}$$

in $(\mathbf{q}, \mathbf{v})$. The system given in Eq. (3.99)/Eq. (3.100) is obviously *overdetermined*: it possesses more numbers of equations than the ones of unknowns.

3.2.5 Lagrangian and Hamiltonian Formalisms in Constrained Mechanical Systems

In this section, the various DAE formulations, discussed so far, are exposited from the view point of the Lagrangian and Hamiltonian formalisms; see [21] for more details.

Lagrangian Formalism: Consider a constrained mechanical system in an n_{g}-dimensional configuration manifold Q subject to holonomic-scleronomic constraint equations, $\mathbf{0} =$

$\mathbf{\Phi}(\mathbf{q}) : Q \to \mathbb{R}^{n_c}$. A so-called $(n_g - n_c)$-dimensional ***constraint manifold*** C is defined as

$$C := \mathbf{\Phi}^{-1}(\mathbf{0}) = \{\mathbf{q}|\ \mathbf{q}(t) : \mathbb{I} := [t_0, t_L] \subset \mathbb{R} \to Q,\ \mathbf{\Phi}(\mathbf{q}) = \mathbf{0}\} \subset Q \tag{3.101}$$

for a regular value $\mathbf{0}$ of $\mathbf{\Phi}(\mathbf{q}) = \mathbf{0}$.

Theorem 3.2.2 (Hamilton's Principle with an Augmented Lagrangian)

Define the augmented *Lagrangian function* $\widetilde{\mathscr{L}} : T(Q \times \mathbb{R}^{n_c}) \to \mathbb{R}$ *as*

$$\widetilde{\mathscr{L}}(\mathbf{q}, \dot{\mathbf{q}}, \boldsymbol{\lambda}, \dot{\boldsymbol{\lambda}}) := \mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}) - \boldsymbol{\lambda}^T \mathbf{\Phi}(\mathbf{q}) \tag{3.102}$$

where $\mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}) : TQ \to \mathbb{R}$ *is an autonomous Lagrangian function of the system, and* $\boldsymbol{\lambda} : \mathbb{I} \to \mathbb{R}^{n_c}$ *is the Lagrangian multiplier vector. Then,* $(\mathbf{q}, \boldsymbol{\lambda}) \in C(Q \times \mathbb{R}^{n_c})$*, where the set* $C(Q \times \mathbb{R}^{n_c}) = C(\mathbb{I}, Q \times \mathbb{R}^{n_c}, \mathbf{q}^0, \mathbf{q}^L)$ *denotes the space of* $(\mathbf{q}, \boldsymbol{\lambda})$ *with*

$$\mathbf{q}(t_0) = \mathbf{q}^0 \ \text{ and } \ \mathbf{q}(t_L) = \mathbf{q}^L, \tag{3.103}$$

extremise the action integral defined by

$$\widetilde{\mathscr{I}}(\mathbf{q}, \boldsymbol{\lambda}) := \int_{t_0}^{t_L} \mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}) dt - \boldsymbol{\lambda}^T \mathbf{\Phi}(\mathbf{q}) \tag{3.104}$$

That is,

$$\boxed{\delta \widetilde{\mathscr{I}} = 0} \tag{3.105}$$

From Eq. (3.105)*, the following* ***Euler-Lagrange*** *equation of motion is obtained:*

$$\frac{d}{dt}\left(\frac{\partial \mathscr{L}(\mathbf{q}, \dot{\mathbf{q}})}{\partial \dot{\mathbf{q}}}\right) - \frac{\partial \mathscr{L}(\mathbf{q}, \dot{\mathbf{q}})}{\partial \mathbf{q}} + \mathbf{G}^T(\mathbf{q})\boldsymbol{\lambda} = \mathbf{0} \tag{3.106}$$

where $\mathbf{G} := D\Phi(\mathbf{q}) \in \mathbb{R}^{n_c \times n_g}$*, with the subsidiary equation,*

$$\mathbf{\Phi}(\mathbf{q}) = \mathbf{0} \tag{3.107}$$

Proof. The proof of this theorem is straightforward, so it is omitted. See Chapter 7 for some discussions.

Remark 3.2.10

1. *The system of equations comprising Eq.* (3.105) *and Eq.* (3.107) *constitutes* $(n_c + n_g)$ *numbers of second-order differential-algebraic equations of index* 3*, which are equivalent to the system given in Eq.* (3.72)*. The other formulations, i.e., index-2, stabilized index-2, index-1, and overdetermined formulations, can be obtained by replacing/adding the constraint equations together with additional algebraic variables if necessary, following a similar manner discussed in the previous subsection.*

Hamiltonian Formalism: The augmented Lagrangian $\widetilde{\mathscr{L}}$, defined in Theorem 3.2.2, is defined on the extended tangent bundle $T(Q \times \mathbb{R}^{n_c})$. The fibre derivative (see Proposition 2.4.1) of $\widetilde{\mathscr{L}}$ allows us to define the momentum $\mathbf{p}$ that is conjugate to $\mathbf{q}$ as

$$\mathbf{p} = \frac{\partial \widetilde{\mathscr{L}}}{\partial \dot{\mathbf{q}}} = \frac{\partial \mathscr{L}}{\partial \dot{\mathbf{q}}} = \mathbf{M}(\mathbf{q})\dot{\mathbf{q}} \tag{3.108}$$

However, momentum $\boldsymbol{\zeta}$ that is conjugate to the Lagrange multiplier $\boldsymbol{\lambda}$ becomes

$$\boldsymbol{\zeta} = \frac{\partial \widetilde{\mathscr{L}}}{\partial \dot{\boldsymbol{\lambda}}} = \mathbf{0} \tag{3.109}$$

This means the augmented Lagrangian function $\widetilde{\mathscr{L}}$ is ***degenerate*** in $\boldsymbol{\lambda}$, and therefore the Legendre transform is not invertible. Viewing $\boldsymbol{\zeta} = \mathbf{0}$ as an invariant of the system, the corresponding augmented Hamiltonian function $\widetilde{\mathcal{H}}(\mathbf{q}, \mathbf{p}, \boldsymbol{\lambda}, \boldsymbol{\zeta}) : T^*(Q \times \mathbb{R}^{n_c}) \to \mathbb{R}$ may be defined on the extended cotangent bundle $T^*(Q \times \mathbb{R}^{n_c})$ as

$$\widetilde{\mathcal{H}}(\mathbf{q}, \mathbf{p}, \boldsymbol{\lambda}, \boldsymbol{\zeta}) := \mathscr{H}(\mathbf{q}, \dot{\mathbf{q}}) + \boldsymbol{\lambda}^T \boldsymbol{\Phi}(\mathbf{q}) + \boldsymbol{\mu}^T \boldsymbol{\zeta} \tag{3.110}$$

where $\boldsymbol{\mu}(t) : \mathbb{I} \to \mathbb{R}^{n_c}$ is an additional Lagrange multiplier vector.

Proposition 3.2.1 (Poisson's Bracket on $T^*(Q \times \mathbb{R}^{n_c})$)

Define Poisson's bracket on the extended cotangent bundle $T^*(Q \times \mathbb{R}^{n_c})$ as

$$\boxed{\begin{aligned}[A, B]_P &:= \frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i} + \frac{\partial A}{\partial \lambda_k}\frac{\partial B}{\partial \zeta_k} - \frac{\partial A}{\partial \zeta_k}\frac{\partial B}{\partial \lambda_k} \\ &= \frac{\partial A}{\partial \mathbf{q}}\frac{\partial B}{\partial \mathbf{p}} - \frac{\partial A}{\partial \mathbf{p}}\frac{\partial B}{\partial \mathbf{q}} + \frac{\partial A}{\partial \boldsymbol{\lambda}}\frac{\partial B}{\partial \boldsymbol{\zeta}} - \frac{\partial A}{\partial \boldsymbol{\zeta}}\frac{\partial B}{\partial \boldsymbol{\lambda}}\end{aligned}} \tag{3.111}$$

(for $i = 1, 2, \cdots, n_g$ and $k = 1, 2, \cdots, n_c$) for arbitrary functions, $A(\mathbf{q}, \mathbf{p}, \boldsymbol{\lambda}, \boldsymbol{\zeta}, t)$ and $B(\mathbf{q}, \mathbf{p}, \boldsymbol{\lambda}, \boldsymbol{\zeta}, t)$.

Making use of the Poisson's bracket defined in Proposition 3.2.1, the canonical equations of the system for the autonomous augmented Hamiltonian function on $T^*(Q \times \mathbb{R}^{n_c})$ may be obtained from:

$$\dot{\mathbf{q}} = [\mathbf{q}, \widetilde{\mathcal{H}}]_P = \frac{\partial \widetilde{\mathcal{H}}}{\partial \mathbf{p}} = \mathbf{M}^{-1}(\mathbf{q})\mathbf{p} \tag{3.112a}$$

$$\dot{\mathbf{p}} = [\mathbf{p}, \widetilde{\mathcal{H}}]_P = -\frac{\partial \widetilde{\mathcal{H}}}{\partial \mathbf{q}} = -\frac{\partial \mathscr{H}}{\partial \mathbf{q}} - \mathbf{G}^T(\mathbf{q})\boldsymbol{\lambda} \tag{3.112b}$$

$$\dot{\boldsymbol{\lambda}} = [\boldsymbol{\lambda}, \widetilde{\mathcal{H}}]_P = \frac{\partial \widetilde{\mathcal{H}}}{\partial \boldsymbol{\zeta}} = \boldsymbol{\mu} \tag{3.112c}$$

$$\dot{\boldsymbol{\zeta}} = [\boldsymbol{\zeta}, \widetilde{\mathcal{H}}]_P = -\frac{\partial \widetilde{\mathcal{H}}}{\partial \boldsymbol{\lambda}} = -\frac{\partial \mathscr{H}}{\partial \boldsymbol{\lambda}} = -\boldsymbol{\Phi}(\mathbf{q}) \tag{3.112d}$$

The system of equations (3.112) constitutes $2(n_g+n_c)$ numbers of first-order differential equations. It is important to note that $\mathbf{0} = \dot{\boldsymbol{\zeta}}$ is valid only on the cotangent bundle defined by $\boldsymbol{\zeta} = \mathbf{0}$. To emphasize this point, write it as $\boldsymbol{\zeta} \approx \mathbf{0}$, called the ***weak equation*** [46]. Hence, the consistency conditions for $\boldsymbol{\zeta} \approx \mathbf{0}$ may be written as:

$$\mathbf{0} \approx \dot{\boldsymbol{\zeta}} = [\boldsymbol{\zeta}, \widetilde{\mathcal{H}}]_P = -\boldsymbol{\Phi} \tag{3.113}$$

$$\mathbf{0} \approx \ddot{\boldsymbol{\zeta}} = [\dot{\boldsymbol{\zeta}}, \widetilde{\mathcal{H}}]_P = -\mathbf{G}\frac{\partial \mathscr{H}}{\partial \mathbf{p}} \tag{3.114}$$

$$\begin{aligned}\mathbf{0} &\approx \dddot{\boldsymbol{\zeta}} = [\ddot{\boldsymbol{\zeta}}, \widetilde{\mathcal{H}}]_P \\ &= -\frac{\partial}{\partial \mathbf{q}}\left(\mathbf{G}\frac{\partial \mathscr{H}}{\partial \mathbf{p}}\right)\frac{\partial \mathscr{H}}{\partial \mathbf{p}} + \mathbf{G}\frac{\partial^2 \mathscr{H}}{\partial \mathbf{p}^2}\frac{\partial \mathscr{H}}{\partial \mathbf{q}} + \left[\mathbf{G}\frac{\partial^2 \mathscr{H}}{\partial \mathbf{p}^2}\mathbf{G}^T\right]\boldsymbol{\lambda}\end{aligned} \tag{3.115}$$

Assuming $\mathbf{G}$ has full rank,

$$\boldsymbol{\lambda} \approx \left[\mathbf{G}\frac{\partial^2 \mathscr{H}}{\partial \mathbf{p}^2}\mathbf{G}^T\right]^{-1}\left[\frac{\partial}{\partial \mathbf{q}}\left(\mathbf{G}\frac{\partial \mathscr{H}}{\partial \mathbf{p}}\right)\frac{\partial \mathscr{H}}{\partial \mathbf{p}} - \mathbf{G}\frac{\partial^2 \mathscr{H}}{\partial \mathbf{p}^2}\frac{\partial \mathscr{H}}{\partial \mathbf{q}}\right] =: \mathbf{\Lambda}_{\mathrm{H}}(\mathbf{q}, \mathbf{p}) \tag{3.116}$$

Therefore, Eq. (3.112c) yields

$$\dot{\boldsymbol{\lambda}} = \boldsymbol{\mu} \approx \dot{\mathbf{\Lambda}}_{\mathrm{H}}(\mathbf{q}, \mathbf{p}) \tag{3.117}$$

Eq. (3.112a), Eq. (3.112b) with $\boldsymbol{\lambda} \approx \mathbf{\Lambda}_{\mathrm{H}}(\mathbf{q}, \mathbf{p})$, and Eq. (3.117) consist the ***underlying ODE*** of the system. From Eq. (3.112a), Eq. (3.112b), and Eq. (3.112d), the Hamilton's canonical equations for the constrained system on T^*C are obtained:

$$\begin{aligned}
\dot{\mathbf{q}} &= [\mathbf{q}, \mathscr{H}] = \frac{\partial \widetilde{\mathcal{H}}}{\partial \mathbf{p}} = \mathbf{M}^{-1}(\mathbf{q})\mathbf{p} \\
\dot{\mathbf{p}} &= [\mathbf{p}, \mathscr{H}] = -\frac{\partial \widetilde{\mathcal{H}}}{\partial \mathbf{q}} = -\frac{\partial \mathscr{H}}{\partial \mathbf{q}} - \mathbf{G}^T(\mathbf{q})\boldsymbol{\lambda} \\
\mathbf{0} &= \mathbf{\Phi}(\mathbf{q})
\end{aligned} \tag{3.118}$$

The system of Eq. (3.118), which is equivalent to the system formed by Eq. (3.74), constitutes $(2n_{\mathrm{g}} + n_{\mathrm{c}})$ first-order differential-algebraic equations of Index 3. Since the constraint equations at the momentum ($\mathbf{p}$) and $\dot{\mathbf{p}}$ levels are defined on T^*C as

$$\mathbf{0} \;=\; \dot{\mathbf{\Phi}} = \mathbf{G}\frac{\partial \mathscr{H}}{\partial \mathbf{p}} =: \mathbf{\Phi}_{\mathrm{p}}(\mathbf{q}, \mathbf{p}) \tag{3.119}$$

$$\mathbf{0} \;=\; \ddot{\mathbf{\Phi}} = \dot{\mathbf{G}}\frac{\partial \mathscr{H}}{\partial \mathbf{p}} + \frac{d}{dt}\left(\frac{\partial \mathscr{H}}{\partial \mathbf{p}}\right) =: \mathbf{\Phi}_{\dot{\mathrm{p}}}(\mathbf{q}, \mathbf{p}, \dot{\mathbf{q}}, \dot{\mathbf{p}}) \approx \mathbf{0} \tag{3.120}$$

$(2n_{\mathrm{g}} + n_{\mathrm{c}})$ first-order differential-algebraic equations of Index-2 and Index-1, which are equivalent to Eq. (3.91) and Eq. (3.98), respectively, can be obtained in the Hamiltonian formalism.

Including the constraint equation at the momentum level in the Hamiltonian function with an additional Lagrange multiplier $\boldsymbol{\eta} : \mathbb{I} \to \mathbb{R}^{n_{\mathrm{c}}}$ as

$$\widetilde{\mathcal{H}}'(\mathbf{q}, \mathbf{p}, \boldsymbol{\lambda}, \boldsymbol{\zeta}, \boldsymbol{\eta}, \boldsymbol{\vartheta}) := \mathscr{H}(\mathbf{q}, \dot{\mathbf{q}}) + \boldsymbol{\lambda}^T\mathbf{\Phi}(\mathbf{q}) + \boldsymbol{\eta}^T\mathbf{\Phi}_{\mathrm{p}}(\mathbf{q}, \mathbf{p}) \tag{3.121}$$

where $\boldsymbol{\vartheta}$ is the momentum vector conjugate to $\boldsymbol{\eta}$, we can derive the augmented formulation introduced in [47]. That is, for the modified Hamiltonian $\widetilde{\mathcal{H}}'(\mathbf{q},\mathbf{p},\boldsymbol{\lambda},\boldsymbol{\zeta},\boldsymbol{\eta},\boldsymbol{\vartheta}) : T^*(Q\times\mathbb{R}^{n_c}\times\mathbb{R}^{n_c})\to\mathbb{R}$,

$$\begin{aligned}
\dot{\mathbf{q}} &= [\mathbf{q},\widetilde{\mathcal{H}}']_{P'} = \frac{\partial\mathscr{H}}{\partial\mathbf{p}} + \boldsymbol{\eta}^T\frac{\partial\boldsymbol{\Phi}_{\mathrm{p}}}{\partial\mathbf{p}}\\
\dot{\mathbf{p}} &= [\mathbf{p},\widetilde{\mathcal{H}}']_{P'} = -\frac{\partial\mathscr{H}}{\partial\mathbf{q}} - \mathbf{G}^T\boldsymbol{\lambda} - \boldsymbol{\eta}^T\frac{\partial\boldsymbol{\Phi}_{\mathrm{p}}}{\partial\mathbf{q}}\\
\dot{\boldsymbol{\zeta}} &= [\boldsymbol{\zeta},\widetilde{\mathcal{H}}']_{P'} = -\boldsymbol{\Phi} = \mathbf{0}\\
\dot{\boldsymbol{\vartheta}} &= [\boldsymbol{\vartheta},\widetilde{\mathcal{H}}']_{P'} = -\boldsymbol{\Phi}_{\mathrm{p}} = \mathbf{0}
\end{aligned} \tag{3.122}$$

on T^*C with an assumption that

$$\mathbf{G}\left(\frac{\partial\boldsymbol{\Phi}_{\mathrm{p}}}{\partial\mathbf{p}}\right)^T \tag{3.123}$$

is invertible.

Theorem 3.2.3 (Conservation of Hamiltonian)

Consider the system given in Eq. (3.118). *The Hamiltonian function* $\widetilde{\mathscr{H}}(\mathbf{q},\mathbf{p},\boldsymbol{\lambda}) := \mathscr{H}(\mathbf{q},\mathbf{p})+\boldsymbol{\lambda}^T\boldsymbol{\Phi}$, *or equivalently,* $\widetilde{\mathcal{H}}(\mathbf{q},\mathbf{p},\boldsymbol{\lambda},\boldsymbol{\zeta})$ *on the cotangent bundle defined by* $\boldsymbol{\zeta}=\mathbf{0}$, *is conserved along a solution:*

$$0 = \frac{d\widetilde{\mathscr{H}}}{dt} = \frac{d\mathscr{H}}{dt} \quad \forall t\in\mathbb{I} \tag{3.124}$$

if $\boldsymbol{\lambda}^T\dot{\boldsymbol{\Phi}}=\mathbf{0}$, *i.e., the workless constraint condition is fulfilled.*

Proof. For the autonomous Hamiltonian functions, $\widetilde{\mathscr{H}}(\mathbf{q},\mathbf{p},\boldsymbol{\lambda})$, the following relations can be readily obtained due to the skew-symmetry of the Poisson's bracket:

$$\begin{aligned}
\frac{d\widetilde{\mathscr{H}}}{dt} &= [\widetilde{\mathscr{H}},\mathscr{H}] = \frac{\partial\widetilde{\mathscr{H}}}{\partial\mathbf{q}}\frac{\partial\mathscr{H}}{\partial\mathbf{p}} - \frac{\partial\widetilde{\mathscr{H}}}{\partial\mathbf{p}}\frac{\partial\mathscr{H}}{\partial\mathbf{q}}\\
&= \left[\frac{\partial\mathscr{H}}{\partial\mathbf{q}} + \mathbf{G}^T(\mathbf{q})\lambda\right]\frac{\partial\mathscr{H}}{\partial\mathbf{p}} - \frac{\partial\mathscr{H}}{\partial\mathbf{p}}\frac{\partial\mathscr{H}}{\partial\mathbf{q}}\\
&= \underbrace{[\mathscr{H},\mathscr{H}]}_{\dot{\mathscr{H}}} + \mathbf{G}^T(\mathbf{q})\lambda\frac{\partial\mathscr{H}}{\partial\mathbf{p}}\\
&= \lambda^T\dot{\boldsymbol{\Phi}}
\end{aligned} \tag{3.125}$$

Hence, we have $\dot{\widetilde{\mathscr{H}}} = \dot{\mathscr{H}} = 0$ if $\lambda^T \dot{\mathbf{\Phi}} = \mathbf{0}$. ∎

Remark 3.2.11

Note that $\boldsymbol{\eta} \equiv \mathbf{0}$ if

$$\mathbf{G}\left(\frac{\partial \mathbf{\Phi}_{\mathrm{p}}}{\partial \mathbf{p}}\right)^T \quad \textit{has full rank} \tag{3.126}$$

$\forall t \in \mathbb{I}$ in continuous time systems; however, in discrete time systems, $\boldsymbol{\eta} \neq \mathbf{0}$ in general. In other words, $\boldsymbol{\eta}(t)$ plays the role of a Lagrange multiplier to enforce $\mathbf{\Phi}_{\mathrm{p}} = \mathbf{0}$. The following both workless constraint condition and the workless projection condition, i.e.,

$$\mathbf{0} = \lambda^T \frac{d\mathbf{\Phi}}{dt} \tag{3.127}$$

$$\mathbf{0} = \boldsymbol{\eta}^T \mathbf{\Phi}_{\mathrm{p}} \tag{3.128}$$

respectively, need to be carefully taken into account when we discretize the system, Eq. (3.122), *in time in order to fulfill the discrete energy conservation condition within a time step: $\mathscr{H}(\mathbf{q}^{n+1}, \mathbf{p}^{n+1}) = \mathscr{H}(\mathbf{q}^n, \mathbf{p}^n)$.*

The above system of equations, Eq. (3.122), can be written in the following compact form,

$$\boxed{\begin{aligned} \dot{\mathbf{z}} &= \mathbb{J}\left[\mathfrak{D}\mathscr{H}(\mathbf{z}) + \chi \mathfrak{D}\mathbf{\Theta}(\mathbf{z})\right] \\ \mathbf{0} &= \mathbf{\Theta}(\mathbf{z}) \end{aligned}} \tag{3.129}$$

where $\mathbf{z}(t) := (\mathbf{q}^T, \mathbf{p}^T)^T$, $\chi(t) := (\lambda^T, \boldsymbol{\eta}^T)^T$, and $\mathbf{\Theta}(\mathbf{z}) := (\mathbf{\Phi}^T, \mathbf{\Phi}_{\mathrm{p}}^T)^T$. Matrix $\mathbb{J}$ is the symplectic matrix defined as in Eq. (2.124).

3.3 The DAE-*i*Integrator: Algorithmic Structures

In this section, the algorithmic structure of the isochronous time integration for the DAE systems (***DAE-iIntegrator***) is stated. For illustration purpose only, we first focus on the various DAE formulations in constrained mechanical systems, as presented in the previous section, and then show how those algorithmic structure can be directly used for first-order systems in time.

Let the time interval of interest be $T = t_L - t_0$ where t_0 and t_L denote the the initial and final time, and suppose it is divided into n_{steps} sub-intervals such that $\mathbb{I} = [t_0, t_L] = \bigcup_{n=0}^{n_{\text{steps}}-1}[t_n, t_{n+1}]$, assuming $0 \leq t_0 < t_1 < t_2 < \cdots < t_{n_{\text{steps}}} \equiv t_L$. Define the time step size as $\Delta t_n := t_{n+1} - t_n > 0$ for $n \in \{0, 1, \cdots, n_{\text{steps}} - 1\}$ so we have $t_n = t_0 + \sum_{i=0}^{n_{\text{steps}}-1} \Delta t_i$. Hereafter, we assume the time step size is constant during the simulation for the sake of simplicity, i.e., $\Delta t = \Delta t_n$; therefore, we have $t_n = t_0 + n\Delta t$ and the number of time steps can be expressed as $n_{\text{steps}} = T/\Delta t$.

3.3.1 Algorithmic Structures of the DAE-*i*Integrator for Constrained Mechanical Systems

Just like the previous section, we assume the geometric constraint equation is holonomic-scleronomic for brevity of the exposition: $\mathbf{\Phi}(\mathbf{q}) = \mathbf{0}$. Every scheme within the *i*Integrator is designed in such a way that it uniquely inherits second-order time accuracy in all differential and algebraic variables and possesses a one-step (or single-step single-solve) form, i.e.,

$$\boxed{(\mathbf{q}_{n+1}, \mathbf{v}_{n+1}, \mathbf{a}_{n+1}, \boldsymbol{\lambda}_{n+1}) = \mathcal{G}_2(\mathbf{q}_n, \mathbf{v}_n, \mathbf{a}_n, \boldsymbol{\lambda}_n)} \tag{3.130}$$

for $n \in \{0, 1, 2, \cdots, n_{\text{steps}} - 1\}$. Throughout this section, initial conditions are considered to be consistent unless otherwise specially mentioned. The algorithmic parameters for the algorithms introduced in this subsection are defined as follows:

$$\begin{aligned}
W_1 &= \frac{1}{1+\rho_\infty^{\text{s}}} \quad &, \quad \lambda_1 &= \Lambda_1 = \lambda_4 = \Lambda_4 = 1 \\
W_2\Lambda_2 &= \frac{1}{2(1+\rho_\infty^{\text{s}})} \quad &, \quad \lambda_2 &= \frac{1}{2} \\
W_3\Lambda_3 &= \frac{1}{(1+\rho_\infty^{\text{min}})(1+\rho_\infty^{\text{max}})(1+\rho_\infty^{\text{s}})} \quad &, \quad \lambda_3 &= \frac{1}{(1+\rho_\infty^{\text{min}})(1+\rho_\infty^{\text{max}})} \\
W_2\Lambda_5 &= \frac{3+\rho_\infty^{\text{min}}+\rho_\infty^{\text{max}}-\rho_\infty^{\text{min}}\rho_\infty^{\text{max}}}{2(1+\rho_\infty^{\text{min}})(1+\rho_\infty^{\text{max}})(1+\rho_\infty^{\text{s}})} \quad &, \quad \lambda_5 &= \frac{3+\rho_\infty^{\text{min}}+\rho_\infty^{\text{max}}-\rho_\infty^{\text{min}}\rho_\infty^{\text{max}}}{2(1+\rho_\infty^{\text{min}})(1+\rho_\infty^{\text{max}})} \\
W_1\Lambda_6 &= \frac{2+\rho_\infty^{\text{min}}+\rho_\infty^{\text{max}}+\rho_\infty^{\text{s}}-\rho_\infty^{\text{min}}\rho_\infty^{\text{max}}\rho_\infty^{\text{s}}}{(1+\rho_\infty^{\text{min}})(1+\rho_\infty^{\text{max}})(1+\rho_\infty^{\text{s}})}
\end{aligned}$$

for the ***U0 family-based schemes***, and

$$\begin{aligned}
W_1 &= \frac{3+\rho_\infty^{\text{min}}+\rho_\infty^{\text{max}}-\rho_\infty^{\text{min}}\rho_\infty^{\text{max}}}{2(1+\rho_\infty^{\text{min}})(1+\rho_\infty^{\text{max}})} \quad &, \quad \lambda_1 &= \Lambda_1 = \lambda_4 = \Lambda_4 = 1 \\
W_2\Lambda_2 &= \frac{1}{(1+\rho_\infty^{\text{min}})(1+\rho_\infty^{\text{max}})} \quad &, \quad \lambda_2 &= \frac{1}{2} \\
W_3\Lambda_3 &= \frac{1}{(1+\rho_\infty^{\text{min}})(1+\rho_\infty^{\text{max}})(1+\rho_\infty^{\text{s}})} \quad &, \quad \lambda_3 &= \frac{1}{2(1+\rho_\infty^{\text{s}})} \\
W_2\Lambda_5 &= \frac{2}{(1+\rho_\infty^{\text{min}})(1+\rho_\infty^{\text{max}})(1+\rho_\infty^{\text{s}})} \quad &, \quad \lambda_5 &= \frac{1}{1+\rho_\infty^{\text{s}}} \\
W_1\Lambda_6 &= \frac{2+\rho_\infty^{\text{min}}+\rho_\infty^{\text{max}}+\rho_\infty^{\text{s}}-\rho_\infty^{\text{min}}\rho_\infty^{\text{max}}\rho_\infty^{\text{s}}}{(1+\rho_\infty^{\text{min}})(1+\rho_\infty^{\text{max}})(1+\rho_\infty^{\text{s}})}
\end{aligned}$$

for the ***V0 family-based schemes***. These are employed from Algorithm 2.2.1 as an extension of the ODE-*i*Integrator to the DAE systems.

Algorithm 3.3.1 (Index-3 Formulation)

Starting with initial conditions, $(\mathbf{q}^n, \mathbf{v}^n, \mathbf{a}^n, \lambda^n)$ *is evaluated for* $n \in \{1, 2, \cdots, n_{\text{steps}}\}$ *from:*

$$\mathbf{M}(\tilde{\mathbf{q}}^n)\tilde{\mathbf{a}}^n = \mathbf{Q}^{\text{appl}}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n, t_{n+W_1}) - \mathbf{G}^T(\tilde{\mathbf{q}}^n)\tilde{\lambda}^n \tag{3.131a}$$

$$\mathbf{0} = \mathbf{\Phi}(\mathbf{q}^{n+1}) \tag{3.131b}$$

where $t_{n+W_1} := (1 - W_1)t_n + W_1 t_{n+1}$ *and*

$$\begin{aligned}
\tilde{\mathbf{q}}^n &= \mathbf{q}^n + W_1\Lambda_1\mathbf{v}^n\Delta t + W_2\Lambda_2\mathbf{a}^n\Delta t^2 + W_3\Lambda_3\Delta\mathbf{a}^n\Delta t^2 && (3.131c)\\
\tilde{\mathbf{v}}^n &= \mathbf{v}^n + W_1\Lambda_4\mathbf{a}^n\Delta t + W_2\Lambda_5\Delta\mathbf{a}^n\Delta t && (3.131d)\\
\tilde{\mathbf{a}}^n &= \mathbf{a}^n + W_1\Lambda_6\Delta\mathbf{a}^n =: \mathbf{a}^{n+W_1\Lambda_6} && (3.131e)\\
\tilde{\boldsymbol{\lambda}}^n &= (1 - W_1)\boldsymbol{\lambda}^n + W_1\boldsymbol{\lambda}^{n+1} =: \boldsymbol{\lambda}^{n+W_1} && (3.131f)
\end{aligned}$$

The updates are given as:

$$\begin{aligned}
\mathbf{q}^{n+1} &= \mathbf{q}^n + \lambda_1\mathbf{v}^n\Delta t + \lambda_2\mathbf{a}^n\Delta t^2 + \lambda_3\Delta\mathbf{a}^n\Delta t^2 && (3.131g)\\
\mathbf{v}^{n+1} &= \mathbf{v}^n + \lambda_4\mathbf{a}^n\Delta t + \lambda_5\Delta\mathbf{a}^n\Delta t && (3.131h)\\
\mathbf{a}^{n+1} &= \mathbf{a}^n + \Delta\mathbf{a}^n && (3.131i)
\end{aligned}$$

Remark 3.3.1

1. ***Linearized Correction Equation:*** *Defining the algorithmic residual vector by*

$$\mathbf{R}^{(3)} = \begin{bmatrix} \mathbf{R}_1 \\ \mathbf{R}_2^{(3)} \end{bmatrix} := \begin{bmatrix} \mathbf{M}(\tilde{\mathbf{q}}^n)\tilde{\mathbf{a}}^n + \mathbf{G}^T(\tilde{\mathbf{q}}^n)\tilde{\boldsymbol{\lambda}}^n - \mathbf{Q}^{\mathrm{appl}}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n, t_{n+W_1}) \\ \boldsymbol{\Phi}(\mathbf{q}^{n+1}) \end{bmatrix} \equiv \mathbf{0} \tag{3.132}$$

the linearized correction equation may be written in the form

$$\mathbf{J}^{(3)} \underbrace{\begin{bmatrix} \Delta\boldsymbol{\vartheta}^n \\ \Delta\boldsymbol{\lambda}^n \end{bmatrix}}_{\Delta\boldsymbol{\chi}^n} \simeq -\mathbf{R}^{(3)} \tag{3.133}$$

with $\Delta\boldsymbol{\vartheta}^n := \boldsymbol{\vartheta}^{n+1} - \boldsymbol{\vartheta}^n$ *and* $\Delta\boldsymbol{\lambda}^n := \boldsymbol{\lambda}^{n+1} - \boldsymbol{\lambda}^n$. *The associated Jacobian matrix is obtained as*

$$\mathbf{J}^{(3)} := \frac{\partial\mathbf{R}_3}{\partial\Delta\boldsymbol{\chi}^n} = \begin{bmatrix} \mathbf{J}_{11} & \mathbf{J}_{12} \\ \mathbf{J}_{21}^{(3)} & \mathbf{J}_{22}^{(3)} \end{bmatrix} \tag{3.134}$$

where matrix entries $\mathbf{J}_{11} \in \mathbb{R}^{n_g \times n_g}$, $\mathbf{J}_{12} \in \mathbb{R}^{n_g \times n_c}$, $\mathbf{J}_{21}^{(3)} \in \mathbb{R}^{n_c \times n_g}$, *and* $\mathbf{J}_{22}^{(3)} \in \mathbb{R}^{n_c \times n_c}$ *are defined as*

$$\begin{aligned}
\mathbf{J}_{11} &:= \frac{\partial \mathbf{R}_1}{\partial \Delta \boldsymbol{\vartheta}^n} = \underbrace{\frac{\partial \mathbf{R}_1}{\partial \tilde{\mathbf{q}}^n}}_{=:\mathbf{K}_T} \frac{\partial \tilde{\mathbf{q}}^n}{\partial \Delta \boldsymbol{\vartheta}^n} + \underbrace{\frac{\partial \mathbf{R}_1}{\partial \tilde{\mathbf{v}}^n}}_{=:\mathbf{C}_T} \frac{\partial \tilde{\mathbf{v}}^n}{\partial \Delta \boldsymbol{\vartheta}^n} + \underbrace{\frac{\partial \mathbf{R}_1}{\partial \tilde{\mathbf{a}}^n}}_{\mathbf{M}} \frac{\partial \tilde{\mathbf{a}}^n}{\partial \Delta \boldsymbol{\vartheta}^n} \\
&= \Xi_{C_1} \mathbf{K}_T + \Xi_{C_2} \mathbf{C}_T + \Xi_{C_3} \mathbf{M} && (3.135) \\
\mathbf{J}_{12} &:= \frac{\partial \mathbf{R}_1}{\partial \Delta \boldsymbol{\lambda}^n} = \frac{\partial \mathbf{R}_1}{\partial \tilde{\boldsymbol{\lambda}}^n} \frac{\partial \tilde{\boldsymbol{\lambda}}^n}{\partial \Delta \boldsymbol{\lambda}^n} = W_1 \mathbf{G}^T(\tilde{\mathbf{q}}^n) && (3.136) \\
\mathbf{J}_{21}^{(3)} &:= \frac{\partial \mathbf{R}_2^{(3)}}{\partial \Delta \boldsymbol{\vartheta}^n} = \frac{\partial \mathbf{R}_2^{(3)}}{\partial \mathbf{q}^{n+1}} \frac{\partial \mathbf{q}^{n+1}}{\partial \Delta \boldsymbol{\vartheta}^n} = \Xi^{q} \mathbf{G}(\mathbf{q}^{n+1}) && (3.137) \\
\mathbf{J}_{22}^{(3)} &:= \frac{\partial \mathbf{R}_2^{(3)}}{\partial \Delta \boldsymbol{\lambda}^n} = \mathbf{0} && (3.138)
\end{aligned}$$

respectively. Depending on the choice of the (incremental) a-,v-, and d-forms, the definition of $\boldsymbol{\vartheta}^{n+1}$ *changes as* $\boldsymbol{\vartheta}^{n+1} = \mathbf{a}^{n+1}$, $\boldsymbol{\vartheta}^{n+1} = \mathbf{v}^{n+1}$, *and* $\boldsymbol{\vartheta}^{n+1} = \mathbf{q}^{n+1}$, *respectively. The coefficients* Ξ_{C_1}, Ξ_{C_2}, *and* Ξ_{C_3} *are defined in Table 2.4 for the (incremental) a-,v-, and d-form representations. The coefficient* Ξ^{q} *is defined in Table 3.1.*

2. *It is well-known that the numerical solutions from this algorithmic framework are prone to numerical instabilities; see [48, 49].*

Algorithm 3.3.2 (Index-2 Formulation)

Starting with initial conditions, $(\mathbf{q}^n, \mathbf{v}^n, \mathbf{a}^n, \boldsymbol{\lambda}^n)$ *is evaluated for* $n \in \{1, 2, \cdots, n_{\text{steps}}\}$ *from:*

$$\begin{aligned}
\mathbf{M}(\tilde{\mathbf{q}}^n)\tilde{\mathbf{a}}^n &= \mathbf{Q}^{\text{appl}}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n, t_{n+W_1}) - \mathbf{G}^T(\tilde{\mathbf{q}}^n)\tilde{\boldsymbol{\lambda}}^n && (3.139a) \\
\mathbf{0} &= \mathbf{G}(\mathbf{q}^{n+1})\mathbf{v}^{n+1} =: \boldsymbol{\Phi}_{\text{v}}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}) && (3.139b)
\end{aligned}$$

The algorithmic configuration, velocity, acceleration, and Lagrange multiplier vectors are as defined in Eq. (3.131c)*-Eq.* (3.131f)*, respectively. The associated updates are as given in Eq.* (3.131g)*-Eq.* (3.131i).

Remark 3.3.2

1. *Define the algorithmic residual vector for Algorithm 3.3.2 as*

$$\mathbf{R}^{(2)} = \begin{bmatrix} \mathbf{R}_1 \\ \mathbf{R}_2^{(2)} \end{bmatrix} := \begin{bmatrix} \mathbf{M}(\tilde{\mathbf{q}}^n)\tilde{\mathbf{a}}^n + \mathbf{G}^T(\tilde{\mathbf{q}}^n)\tilde{\boldsymbol{\lambda}}^n - \mathbf{Q}^{\text{appl}}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n, t_{n+W_1}) \\ \boldsymbol{\Phi}_{\text{v}}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}) \end{bmatrix} \equiv \mathbf{0} \tag{3.140}$$

Then, the linearized correction equation for Algorithm 3.3.2 can be written in the form

$$\underbrace{\begin{bmatrix} \mathbf{J}_{11} & \mathbf{J}_{12} \\ \mathbf{J}_{21}^{(2)} & \mathbf{0} \end{bmatrix}}_{=:\mathbf{J}^{(2)}} \underbrace{\begin{bmatrix} \Delta\boldsymbol{\vartheta}^n \\ \Delta\boldsymbol{\lambda}^n \end{bmatrix}}_{\Delta\boldsymbol{\chi}^n} \simeq - \underbrace{\begin{bmatrix} \mathbf{R}_1 \\ \mathbf{R}_2^{(2)} \end{bmatrix}}_{=:\mathbf{R}^{(2)}} \tag{3.141}$$

where the entries $\mathbf{J}_{11} \in \mathbb{R}^{n_{\text{g}} \times n_{\text{g}}}$, $\mathbf{J}_{12} \in \mathbb{R}^{n_{\text{g}} \times n_{\text{c}}}$ *in Jacobian* $\mathbf{J}^{(2)}$ *are as given in Eq.* (3.135) *and Eq.* (3.136), *respectively, since vector* $\mathbf{R}_1$ *for Algorithm 3.3.2 is identical to the one for Algorithm 3.3.1; and* $\mathbf{J}_{21}^{(2)} \in \mathbb{R}^{n_{\text{c}} \times n_{\text{g}}}$ *is defined as*

$$\begin{aligned} \mathbf{J}_{21}^{(2)} &:= \frac{\partial \mathbf{R}_2^{(2)}}{\partial \Delta\boldsymbol{\vartheta}^n} = \frac{\partial \mathbf{R}_2^{(2)}}{\partial \mathbf{q}^{n+1}} \frac{\partial \mathbf{q}^{n+1}}{\partial \Delta\boldsymbol{\vartheta}^n} + \frac{\partial \mathbf{R}_2^{(2)}}{\partial \mathbf{v}^{n+1}} \frac{\partial \mathbf{v}^{n+1}}{\partial \Delta\boldsymbol{\vartheta}^n} \\ &= \Xi^{\text{q}} \frac{\partial \mathbf{R}_2^{(2)}}{\partial \mathbf{q}^{n+1}} + \Xi^{\text{v}} \mathbf{G}(\mathbf{q}^{n+1}) \end{aligned} \tag{3.142}$$

where

$$\frac{\partial \mathbf{R}_2^{(2)}}{\partial \mathbf{q}^{n+1}} = \frac{\partial \boldsymbol{\Phi}_{\text{v}}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1})}{\partial \mathbf{q}^{n+1}} = \mathfrak{D}\mathbf{G}(\mathbf{q}^{n+1})(\mathbf{v}^{n+1}, \mathbf{v}^{n+1}) \tag{3.143}$$

for the holonomic-scleronomic constraint. See Table 3.1 for the coefficients Ξ^{q} *and* Ξ^{v} *for (incremental) a-, v-, and d-forms.*

Algorithm 3.3.3 (Index-1 Formulation)

Starting with initial conditions, $(\mathbf{q}^n, \mathbf{v}^n, \mathbf{a}^n, \boldsymbol{\lambda}^n)$ *is evaluated for* $n \in \{1, 2, \cdots, n_{\text{steps}}\}$ *from:*

$$\mathbf{M}(\tilde{\mathbf{q}}^n)\tilde{\mathbf{a}}^n = \mathbf{Q}^{\text{appl}}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n, t_{n+W_1}) - \mathbf{G}^T(\tilde{\mathbf{q}}^n)\tilde{\boldsymbol{\lambda}}^n \tag{3.144a}$$

$$\begin{aligned} \mathbf{0} &= \mathbf{G}(\mathbf{q}^{n+1})\hat{\mathbf{a}}^{n+1} + \mathfrak{D}\mathbf{G}(\mathbf{q}^{n+1})(\mathbf{v}^{n+1}, \mathbf{v}^{n+1}) \\ &=: \boldsymbol{\Phi}_{\text{a}}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}, \hat{\mathbf{a}}^{n+1}) \end{aligned} \tag{3.144b}$$

where

$$\hat{\mathbf{a}}^1 := \frac{1}{1-\phi}\mathbf{a}^1 - \frac{\phi}{1-\phi}\mathbf{a}^0 \tag{3.145a}$$

at the first time step ($n = 0$) and

$$\hat{\mathbf{a}}^{n+1} := (1+\phi)\mathbf{a}^{n+1} - \phi\mathbf{a}^n \tag{3.145b}$$

for $n \in \{1, 2, \cdots, n_{\text{steps}} - 1\}$, with

$$\phi := W_1\Lambda_6 - W_1 \tag{3.146}$$

The algorithmic configuration, velocity, acceleration, and Lagrange multiplier vectors are as defined in Eq. (3.131c)*-Eq.* (3.131f)*, respectively. The associated updates are as given in Eq.* (3.131g)*-Eq.* (3.131i).

Remark 3.3.3

1. *The feature of paramount importance in Algorithm 3.3.3 is the numerical acceleration vector denoted by $\hat{\mathbf{a}}^{n+1}$ in contrast to $\mathbf{a}^{n+1}$. The definition of $\hat{\mathbf{a}}^{n+1}$, given in Eq.* (3.145)*, was distilled from the concept that the time level of $\mathbf{a}^{n+1}$ is actually $t_{n+1-\phi}$. Herein, the vector $\hat{\mathbf{a}}^{n+1}$ is designed in such a way that its time level is t_{n+1} in the sense of $\hat{\mathbf{a}}^{n+1} - \ddot{\mathbf{q}}(t_{n+1}) = \mathcal{O}(\Delta t^2)$. Although, at the first step, adopting the definition given in Eq.* (3.145a) *seems reasonable, as in Fig. 2.1, it cannot be defined when $\phi = 1$, or $\Lambda_6 = 1$. In order to obviate this disadvantage, we employ $\hat{\mathbf{a}}^{n+1} := (1+\phi)\mathbf{a}^{n+1} - \phi\mathbf{a}^n$, i.e., Eq.* (3.145b)*, for every step, $n \in \{0, 1, 2, \cdots, n_{\text{steps}}\}$, since it does not influence the order of time accuracy of the algorithm due to the fact that the error of the initial acceleration at $t = t_0$ is of $\mathcal{O}(\Delta t^2)$; refer to Theorem 2.2.1.*

2. *With the residual vector being defined as*

$$\mathbf{R}^{(1)} = \begin{bmatrix} \mathbf{R}_1 \\ \mathbf{R}_2^{(1)} \end{bmatrix} := \begin{bmatrix} \mathbf{M}(\tilde{\mathbf{q}}^n)\tilde{\mathbf{a}}^n + \mathbf{G}^T(\tilde{\mathbf{q}}^n)\tilde{\lambda}^n - \mathbf{Q}^{\mathrm{appl}}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n, t_{n+W_1}) \\ \mathbf{\Phi}_{\mathrm{a}}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}, \hat{\mathbf{a}}^{n+1}) \end{bmatrix} \equiv \mathbf{0} \tag{3.147}$$

the linearized correction equation for Algorithm 3.3.3 can be written in the form

$$\underbrace{\begin{bmatrix} \mathbf{J}_{11} & \mathbf{J}_{12} \\ \mathbf{J}_{21}^{(1)} & \mathbf{0} \end{bmatrix}}_{=:\mathbf{J}^{(1)}} \underbrace{\begin{bmatrix} \Delta\boldsymbol{\vartheta}^n \\ \Delta\lambda^n \end{bmatrix}}_{\Delta\chi^n} \simeq - \underbrace{\begin{bmatrix} \mathbf{R}_1 \\ \mathbf{R}_2^{(1)} \end{bmatrix}}_{=:\mathbf{R}^{(1)}} \tag{3.148}$$

where the entries $\mathbf{J}_{11} \in \mathbb{R}^{n_{\mathrm{g}}\times n_{\mathrm{g}}}$, $\mathbf{J}_{12} \in \mathbb{R}^{n_{\mathrm{g}}\times n_{\mathrm{c}}}$ *in Jacobian* $\mathbf{J}^{(2)}$ *are the same for Algorithm 3.3.3/Algorithm 3.3.2, and* $\mathbf{J}_{21}^{(1)} \in \mathbb{R}^{n_{\mathrm{c}}\times n_{\mathrm{g}}}$ *is defined as*

$$\begin{aligned} \mathbf{J}_{21}^{(1)} &:= \frac{\partial \mathbf{R}_2^{(1)}}{\partial \Delta\boldsymbol{\vartheta}^n} = \frac{\partial \mathbf{R}_2^{(1)}}{\partial \mathbf{q}^{n+1}}\frac{\partial \mathbf{q}^{n+1}}{\partial \Delta\boldsymbol{\vartheta}^n} + \frac{\partial \mathbf{R}_2^{(1)}}{\partial \mathbf{v}^{n+1}}\frac{\partial \mathbf{v}^{n+1}}{\partial \Delta\boldsymbol{\vartheta}^n} + \frac{\partial \mathbf{R}_2^{(1)}}{\partial \hat{\mathbf{a}}^{n+1}}\frac{\partial \hat{\mathbf{a}}^{n+1}}{\partial \mathbf{a}^{n+1}}\frac{\partial \mathbf{a}^{n+1}}{\partial \Delta\boldsymbol{\vartheta}^n} \\ &= \Xi^{\mathrm{q}}\frac{\partial \mathbf{R}_2^{(1)}}{\partial \mathbf{q}^{n+1}} + \Xi^{\mathrm{v}}\frac{\partial \mathbf{R}_2^{(1)}}{\partial \mathbf{v}^{n+1}} + \Xi^{\mathrm{a}}(1+\phi)\mathbf{G}(\mathbf{q}^{n+1}) \end{aligned} \tag{3.149}$$

in the case of $\hat{\mathbf{a}}^{n+1} := (1+\phi)\mathbf{a}^{n+1} - \phi\mathbf{a}^n$. *See Table 3.1 for the coefficients* Ξ^{q} *and* Ξ^{v} *for (incremental) a-, v-, and d-forms.*

	a-form	**v-form**	**d-form**
Ξ^{q}	$\lambda_3\Delta t^2$	$\frac{\lambda_3\Delta t}{\lambda_5}$	1
Ξ^{v}	$\lambda_5\Delta t$	1	$\frac{\lambda_5}{\lambda_3\Delta t}$
Ξ^{a}	1	$\frac{1}{\lambda_5\Delta t}$	$\frac{1}{\lambda_3\Delta t^2}$

Table 3.1: Coefficients for the Incremental a-,v-, and d-form Representations

3.3.2 Algorithmic Time Level Consistency

Algorithms shown above for Index-3, Index-2, and Index-1 systems, i.e. Algorithms 3.3.1, 3.3.2, and 3.3.3, respectively, were designed in such a way that the algorithmic time level of the discrete dynamical equation is consistently at t_{n+W_1}, which implies that they inherit second-order time accuracy in all the differential and algebraic variables.

Consider Algorithm 3.3.3, as an illustration of the concept. Premultiplying Eq. (3.144b) by $\mathbf{G}^T(\mathbf{q}^{n+1})$, we get

$$\begin{aligned}\mathbf{0} &= \mathbf{G}^T(\mathbf{q}^{n+1})\mathbf{\Phi}_{\mathrm{a}}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}, \hat{\mathbf{a}}^{n+1}) \\ &= \mathbf{G}^T(\mathbf{q}^{n+1})\mathbf{G}(\mathbf{q}^{n+1})\hat{\mathbf{a}}^{n+1} + \mathbf{G}^T(\mathbf{q}^{n+1})\boldsymbol{\kappa}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1})\end{aligned} \tag{3.150}$$

where $\boldsymbol{\kappa}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}) := \mathfrak{D}\mathbf{G}(\mathbf{q}^{n+1})(\mathbf{v}^{n+1}, \mathbf{v}^{n+1})$. Since $\mathbf{G}(\mathbf{q}^{n+1})$ is assumed to have full rank, matrix $\mathbf{G}^T(\mathbf{q}^{n+1})\mathbf{G}(\mathbf{q}^{n+1})$ is invertible; therefore,

$$\hat{\mathbf{a}}^{n+1} = -\left[\mathbf{G}^T(\mathbf{q}^{n+1})\mathbf{G}(\mathbf{q}^{n+1})\right]^{-1} \mathbf{G}^T(\mathbf{q}^{n+1})\boldsymbol{\kappa}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}) \tag{3.151}$$

As we assume the configuration and velocity vectors $\mathbf{q}^{n+1}$ and $\mathbf{v}^{n+1}$ are the approximations at time t_{n+1} in the sense of

$$\mathbf{q}^{n+1} - \mathbf{q}(t_{n+1}) = \mathcal{O}(\Delta t^2) \text{ and } \mathbf{v}^{n+1} - \dot{\mathbf{q}}(t_{n+1}) = \mathcal{O}(\Delta t^2) \tag{3.152}$$

respectively, the algorithmic time level of the right-hand side of Eq. (3.151) must be also t_{n+1}. Therefore, the numerical acceleration $\hat{\mathbf{a}}^{n+1}$ should be designed such that

$$\hat{\mathbf{a}}^{n+1} - \ddot{\mathbf{q}}(t_{n+1}) = \mathcal{O}(\Delta t^2) \tag{3.153}$$

By linearly extrapolating at time t_{n+1} for $\mathbf{a}^{n+1} \approx \ddot{\mathbf{q}}(t_{n+1-\phi})$ and $\mathbf{a}^n \approx \ddot{\mathbf{q}}(t_{n-\phi})$, we get the expression,

$$\hat{\mathbf{a}}^{n+1} := (1+\phi)\mathbf{a}^{n+1} - \phi\mathbf{a}^n \tag{3.154}$$

Hence, the algorithmic acceleration $\tilde{\mathbf{a}}^n := (1 - W_1\Lambda_6)\mathbf{a}^n + W_1\Lambda_6\mathbf{a}^{n+1}$ yields

$$\begin{aligned}\tilde{\mathbf{a}}^n &= (1 - W_1)\mathbf{a}^n - \frac{W_1\Lambda_6}{1+\phi}\left[\mathbf{G}^T(\mathbf{q}^{n+1})\mathbf{G}(\mathbf{q}^{n+1})\right]^{-1}\mathbf{G}^T(\mathbf{q}^{n+1})\boldsymbol{\kappa}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}) \\ &\approx \ddot{\mathbf{q}}(t_{n+W_1})\end{aligned} \tag{3.155}$$

and therefore the algorithmic time level of the algorithm is consistently at t_{n+W_1}, which implied the second-order time accurcy in all the kinematic and algebraic quantities in the system.

3.3.3 Conditioning of the Algorithms

The algorithms for the DAE systems usually suffer from the so-called ***conditioning*** issues, especially when a sufficiently small time step size is used since the Jacobian matrices $\mathbf{J}^\ell$ tend to become close to singular as $\Delta t \to 0$. Such Jacobian matrices are termed ***ill-conditioned***.

As already shown, the Jacobian matrices (for Algorithms 3.3.1,3.3.2, and 3.3.3) are given as

$$\mathbf{J}^{(\ell)} = \begin{bmatrix} \mathbf{J}_{11} & \mathbf{J}_{12} \\ \mathbf{J}_{21}^{(\ell)} & \mathbf{0} \end{bmatrix} \tag{3.156a}$$

(for $\ell = 1, 2, 3$) where

$$\begin{aligned}\mathbf{J}_{11} &= \Xi_{C_1}\mathbf{K}_T + \Xi_{C_2}\mathbf{C}_T + \Xi_{C_3}\mathbf{M} \\ \mathbf{J}_{12} &= W_1\mathbf{G}^T(\tilde{\mathbf{q}}^n) =: W_1\hat{\mathbf{G}}^T\end{aligned} \tag{3.156b}$$

and

$$\mathbf{J}_{21}^{(3)} = \Xi^{\mathrm{q}}\mathbf{G}(\mathbf{q}^{n+1}) \tag{3.156c}$$

$$\mathbf{J}_{21}^{(2)} = \Xi^{\mathrm{q}}\frac{\partial\mathbf{R}_2^{(2)}}{\partial\mathbf{q}^{n+1}} + \Xi^{\mathrm{v}}\mathbf{G}(\mathbf{q}^{n+1}) \tag{3.156d}$$

$$\mathbf{J}_{21}^{(1)} = \Xi^{\mathrm{q}}\frac{\partial\mathbf{R}_2^{(1)}}{\partial\mathbf{q}^{n+1}} + \Xi^{\mathrm{v}}\frac{\partial\mathbf{R}_2^{(1)}}{\partial\mathbf{v}^{n+1}} + \Xi^{\mathrm{a}}(1+\phi)\mathbf{G}(\mathbf{q}^{n+1}) \tag{3.156e}$$

Using the Gauss-Jordan elimination, the inverse of the Jacobian $\mathbf{J}^{(\ell)}$ can be written (after a tedious work) as

$$\left(\mathbf{J}^{(\ell)}\right)^{-1} =: \mathbf{\Pi}^{(\ell)} = \begin{bmatrix} \mathbf{\Pi}_{11}^{(\ell)} & \mathbf{\Pi}_{12}^{(\ell)} \\ \mathbf{\Pi}_{21}^{(\ell)} & \mathbf{\Pi}_{22}^{(\ell)} \end{bmatrix} \tag{3.157a}$$

where

$$\mathbf{\Pi}_{11}^{(\ell)} = \mathbf{J}_{11}^{-1} - \mathbf{J}_{11}^{-1}\hat{\mathbf{G}}^T\mathbf{\Psi}_{(\ell)}^{-1}\mathbf{J}_{21}^{(\ell)}\mathbf{J}_{11}^{-1} \tag{3.157b}$$

$$\mathbf{\Pi}_{12}^{(\ell)} = \mathbf{J}_{11}^{-1}\hat{\mathbf{G}}^T\mathbf{\Psi}_{(\ell)}^{-1} \tag{3.157c}$$

$$\mathbf{\Pi}_{21}^{(\ell)} = W_1^{-1}\mathbf{\Psi}_{(\ell)}^{-1}\mathbf{J}_{21}^{(\ell)}\mathbf{J}_{11}^{-1} \tag{3.157d}$$

$$\mathbf{\Pi}_{22}^{(\ell)} = -W_1^{-1}\mathbf{\Psi}_{(\ell)}^{-1} \tag{3.157e}$$

where $\mathbf{\Psi}_{(\ell)} := \mathbf{J}_{21}^{(\ell)}\mathbf{J}_{11}^{-1}\hat{\mathbf{G}}^T$. Without loss of generality of the discussion for the conditioning problem, let us assume $\mathbf{C}_T = \mathbf{0}$ for simplicity; thereby, $\mathbf{J}_{11} = \Xi_{\mathrm{C}_1}\mathbf{K}_T + \Xi_{\mathrm{C}_3}\mathbf{M}$ can be written as

$$\mathbf{J}_{11} = \Xi_{\mathrm{C}_3}\mathbf{M}_{\mathrm{L}}\left[\mathbf{I} + \frac{\Xi_{\mathrm{C}_1}}{\Xi_{\mathrm{C}_3}}\mathbf{M}_{\mathrm{L}}^{-1}\mathbf{K}_T\mathbf{M}_{\mathrm{U}}^{-1}\right]\mathbf{M}_{\mathrm{U}} \tag{3.158}$$

where $\mathbf{M} = \mathbf{M}_{\mathrm{L}}\mathbf{M}_{\mathrm{U}}$ (LU-factorization of $\mathbf{M}$). Then, the inverse of $\mathbf{J}_{11}$ can be written as

$$\begin{aligned}\mathbf{J}_{11}^{-1} &= \Xi_{\mathrm{C}_3}^{-1}\mathbf{M}_{\mathrm{U}}^{-1}\left[\mathbf{I} + \frac{\Xi_{\mathrm{C}_1}}{\Xi_{\mathrm{C}_3}}\mathbf{M}_{\mathrm{L}}^{-1}\mathbf{K}_T\mathbf{M}_{\mathrm{U}}^{-1}\right]^{-1}\mathbf{M}_{\mathrm{L}}^{-1} \\ &= \Xi_{\mathrm{C}_3}^{-1}\mathbf{M}_{\mathrm{U}}^{-1}\sum_{k=0}^{\infty}\left[-\frac{\Xi_{\mathrm{C}_1}}{\Xi_{\mathrm{C}_3}}\mathbf{M}_{\mathrm{L}}^{-1}\mathbf{K}_T\mathbf{M}_{\mathrm{U}}^{-1}\right]^k\mathbf{M}_{\mathrm{L}}^{-1} \\ &= \frac{1}{\Xi_{\mathrm{C}_3}}\mathbf{M}^{-1} - \frac{\Xi_{\mathrm{C}_1}}{\Xi_{\mathrm{C}_3}^2}\mathbf{M}^{-1}\mathbf{K}_T\mathbf{M}^{-1} + \cdots\end{aligned} \tag{3.159}$$

Likewise, for $\mathbf{\Psi}_{(\ell)}^{-1}$,

$$\begin{aligned}\mathbf{\Psi}_{(\ell)}^{-1} &= \left(\mathbf{J}_{21}^{(\ell)}\mathbf{J}_{11}^{-1}\hat{\mathbf{G}}^T\right)^{-1} \\ &= \left(\Xi_{\mathrm{C}_3}^{-1}\mathbf{J}_{21}^{(\ell)}\mathbf{M}_{\mathrm{U}}^{-1}\sum_{k=0}^{\infty}\left[-\frac{\Xi_{\mathrm{C}_1}}{\Xi_{\mathrm{C}_3}}\mathbf{M}_{\mathrm{L}}^{-1}\mathbf{K}_T\mathbf{M}_{\mathrm{U}}^{-1}\right]^k\mathbf{M}_{\mathrm{L}}^{-1}\hat{\mathbf{G}}^T\right)^{-1} \\ &= \Xi_{\mathrm{C}_3}\mathbf{N}_{(\ell)}^{-1} + \Xi_{\mathrm{C}_1}\mathbf{N}_{(\ell)}^{-1}\left[\mathbf{J}_{21}^{(\ell)}\mathbf{K}_T\hat{\mathbf{G}}^T\right]\mathbf{N}_{(\ell)}^{-1} + \cdots\end{aligned} \tag{3.160}$$

where $\mathbf{N}_{(\ell)} := \mathbf{J}_{21}^{(\ell)}\mathbf{M}^{-1}\hat{\mathbf{G}}^T$. Since we have

$$\Xi_{\mathrm{C}_1} = \begin{cases} W_1\Lambda_6 & \text{for a-form} \\ \Delta t^{-1}(W_1\Lambda_6/\lambda_5) & \text{for v-form} \\ \Delta t^{-2}(W_1\Lambda_6/\lambda_3) & \text{for d-form} \end{cases} \quad \text{and} \quad \Xi_{\mathrm{C}_3} = \begin{cases} \Delta t^2 W_3\Lambda_3 & \text{for a-form} \\ \Delta t(W_3\Lambda_3/\lambda_5) & \text{for v-form} \\ W_3\Lambda_3/\lambda_3 & \text{for d-form} \end{cases} \tag{3.161}$$

the orders of $\mathbf{J}_{11}^{-1}$ and $\mathbf{\Psi}_{(\ell)}^{-1}$ are readily obtained with the help of Table 3.1. Let $\mathbf{J}_{21}^{(\ell)} = \mathcal{O}(\Delta t^{r_\ell})$, $\mathbf{J}_{11}^{-1} = \mathcal{O}(\Delta t^{a})$, and $\mathbf{\Psi}_{(\ell)}^{-1} = \mathcal{O}(\Delta t^{b})$ (note that the order values r_ℓ, a, and b are different for DAE index orders and algorithmic forms (a-, v-, and d-forms). From these order values, the order of matrix $\mathbf{\Pi}^{(\ell)}$ is determined. Suppose

$$\mathbf{\Pi}^{(\ell)} = \begin{bmatrix} \mathcal{O}(\Delta t^{d_1}) & \mathcal{O}(\Delta t^{d_2}) \\ \mathcal{O}(\Delta t^{d_3}) & \mathcal{O}(\Delta t^{d_4}) \end{bmatrix} \tag{3.162}$$

where d_i depends on r_ℓ; then, the ***condition number*** of the iteration matrix finally given from:

$$K(\mathbf{J}^{(\ell)}) = \left\|\mathbf{J}^{(\ell)}\right\| \left\|\mathbf{\Pi}^{(\ell)}\right\| \tag{3.163}$$

3.3.4 Newton-type Iteration

In general, the Newton-type iteration techniques need to be employed to obtain numerical solutions from the algorithms introduced. As an example, as the basis of various quasi-Newton methods, the procedures for the full-Newton method for Algorithms 3.3.1,3.3.2, and 3.3.3 are summarized overleaf.

■ **Step 1: Predictor ($k \leftarrow 0$)**

$$^{(k)}\mathbf{q}^{n+1} = \Xi^{q}_{\mathrm{P}_1}\mathbf{q}^n + \Xi^{q}_{\mathrm{P}_2}\mathbf{v}^n + \Xi^{q}_{\mathrm{P}_3}\mathbf{a}^n, \quad {}^{(k)}\mathbf{v}^{n+1} = \Xi^{v}_{\mathrm{P}_1}\mathbf{q}^n + \Xi^{v}_{\mathrm{P}_2}\mathbf{v}^n + \Xi^{v}_{\mathrm{P}_3}\mathbf{a}^n$$

$$^{(k)}\mathbf{a}^{n+1} = \Xi^{a}_{\mathrm{P}_1}\mathbf{q}^n + \Xi^{a}_{\mathrm{P}_2}\mathbf{v}^n + \Xi^{a}_{\mathrm{P}_3}\mathbf{a}^n, \quad {}^{(k)}\boldsymbol{\lambda}^{n+1} = \boldsymbol{\lambda}^n$$

■ **Step 2: Iteration ($k \leftarrow k + 1$)**

Solve for the increment ${}^{(k)}\delta\boldsymbol{\chi}^n := (({}^{(k)}\delta\boldsymbol{\vartheta}^n)^T, ({}^{(k)}\delta\boldsymbol{\lambda}^n)^T)^T$ from:

$$^{(k)}\mathbf{J}^n \, {}^{(k)}\delta\boldsymbol{\chi}^n = -{}^{(k)}\mathbf{R}^n$$

with the residual vector,

$$^{(k)}\mathbf{R}^n = \mathbf{F}({}^{(k)}\tilde{\mathbf{q}}^n, {}^{(k)}\tilde{\mathbf{v}}^n, {}^{(k)}\tilde{\mathbf{a}}^n, {}^{(k)}\tilde{\boldsymbol{\lambda}}^n, t_{n+W_1})$$

where

$$^{(k)}\tilde{\mathbf{a}}^n = {}^{(k)}\mathbf{a}^n + W_1\Lambda_6 {}^{(k)}\Delta\mathbf{a}^n, \quad {}^{(k)}\tilde{\boldsymbol{\lambda}}^n = {}^{(k)}\boldsymbol{\lambda}^n + W_1 {}^{(k)}\Delta\boldsymbol{\lambda}^n$$

$$^{(k)}\tilde{\mathbf{v}}^n = {}^{(k)}\mathbf{v}^n + W_1\Lambda_4 {}^{(k)}\mathbf{a}^n\Delta t + W_2\Lambda_5 {}^{(k)}\Delta\mathbf{a}^n\Delta t$$

$$^{(k)}\tilde{\mathbf{q}}^n = {}^{(k)}\mathbf{q}^n + W_1\Lambda_1 {}^{(k)}\mathbf{v}^n\Delta t + W_2\Lambda_2 {}^{(k)}\mathbf{a}^n\Delta t^2 + W_3\Lambda_3 {}^{(k)}\Delta\mathbf{a}^n\Delta t^2$$

$$({}^{(k)}\Delta\mathbf{a}^n := {}^{(k)}\mathbf{a}^{n+1} - {}^{(k)}\mathbf{a}^n, \; {}^{(k)}\Delta\boldsymbol{\lambda}^n := {}^{(k)}\boldsymbol{\lambda}^{n+1} - {}^{(k)}\boldsymbol{\lambda}^n),$$

and the Jacobian matrix,

$$^{(k)}\mathbf{J}^n := \frac{\partial\mathbf{F}}{\partial {}^{(k)}\delta\boldsymbol{\chi}^n}$$

■ **Step 3: Corrector**

$$^{(k)}\tilde{\mathbf{a}}^n = {}^{(k-1)}\tilde{\mathbf{a}}^n + \Xi_{\mathrm{C}_1} {}^{(k)}\delta\boldsymbol{\vartheta}^n, \quad {}^{(k)}\tilde{\mathbf{v}}^n = {}^{(k-1)}\tilde{\mathbf{v}}^n + \Xi_{\mathrm{C}_2} {}^{(k)}\delta\boldsymbol{\vartheta}^n, \quad {}^{(k)}\tilde{\mathbf{q}}^n = {}^{(k-1)}\tilde{\mathbf{q}}^n + \Xi_{\mathrm{C}_3} {}^{(k)}\delta\boldsymbol{\vartheta}^n$$

$$^{(k)}\tilde{\boldsymbol{\lambda}}^n = {}^{(k-1)}\tilde{\boldsymbol{\lambda}}^n + W_1 {}^{(k)}\delta\boldsymbol{\lambda}^n$$

Convergence Criteria:

If $\sqrt{({}^{(k)}\mathbf{R}^n)^{T\,(k)}\mathbf{R}^n} > \epsilon\sqrt{({}^{(0)}\mathbf{R}^n)^{T\,(0)}\mathbf{R}^n}$,

repeat for the next iteration; else, go to **Step 4**.

■ **Step 4: Update**

$$\mathbf{a}^{n+1} = \mathbf{a}^n + \frac{{}^{(k)}\tilde{\mathbf{a}}^n - \mathbf{a}^n}{W_1\Lambda_6}, \quad \boldsymbol{\lambda}^{n+1} = \boldsymbol{\lambda}^n + \frac{{}^{(k)}\tilde{\boldsymbol{\lambda}}^n - \boldsymbol{\lambda}^n}{W_1}$$

$$\mathbf{v}^{n+1} = \mathbf{v}^n + \lambda_4\mathbf{a}^n\Delta t + \lambda_5(\mathbf{a}^{n+1} - \mathbf{a}^n)\Delta t$$

$$\mathbf{q}^{n+1} = \mathbf{q}^n + \lambda_1\mathbf{v}^n\Delta t + \lambda_2\mathbf{a}^n\Delta t^2 + \lambda_3(\mathbf{a}^{n+1} - \mathbf{a}^n)\Delta t^2$$

Set $n \leftarrow n + 1$ and go to **Step 1**.

3.4 Remedies for the Drift-off Phenomenon

3.4.1 Drift-off Phenomenon

Algorithm 3.3.2 and Algorithm 3.3.3 usually suffer from the so-called ***drift-off*** issues.

Theorem 3.4.1

For Algorithm 3.3.3 (for Index 1), the drift-off from the configuration and velocity constraints grows quadratically *and* linearly*, respectively, with the simulation time interval at t_n, i.e., $t_n - t_0$:*

$$\begin{aligned} \|\mathbf{\Phi}(\mathbf{q}^n)\| &\leq \Delta t^2 \left[A(t_n - t_0) + B(t_n - t_0)^2\right] \\ \|\mathbf{\Phi}_\mathrm{v}(\mathbf{q}^n, \mathbf{v}^n)\| = \|\mathbf{G}(\mathbf{q}^n)\mathbf{v}^n\| &\leq \Delta t C(t_n - t_0) \end{aligned} \tag{3.164}$$

For Algorithm 3.3.2 (for Index 2), the drift-off from the configuration constraints grows linearly *with $t_n - t_0$, but there is no drift-off in the velocity constraints:*

$$\begin{aligned} \|\mathbf{\Phi}(\mathbf{q}^n)\| &\leq \Delta t \left[D(t_n - t_0)\right] \\ \|\mathbf{\Phi}_\mathrm{v}(\mathbf{q}^n, \mathbf{v}^n)\| = \|\mathbf{G}(\mathbf{q}^n)\mathbf{v}^n\| &= \mathbf{0} \end{aligned} \tag{3.165}$$

Proof. See [50] for an analogous proof.

Remark 3.4.1

Algorithm 3.3.3 suffers from a more severe drift-off from the configuration constraints, comparing to Algorithm 3.3.2. Because of this reason, it is well-known that Algorithm 3.3.3 without employing the Baumgarte stabilization method or the projection method, which will be discussed below, is prone to numerical instabilities. In contrast, Algorithm 3.3.2 inherits a significantly more stable feature due to its weaker violation of the system invariant.

3.4.2 Baumgarte Stabilization Method [2]

The Baumgarte stabilization method for the Index-1 formulation is based on a system obtained by replacing the acceleration constraint equation with the linear combination of the acceleration, velocity, and geometric constraint equations of the form,

$$\boxed{\begin{aligned}\mathbf{0} &= \ddot{\mathbf{\Phi}} + 2\alpha\dot{\mathbf{\Phi}} + \beta\mathbf{\Phi} \\ &= \mathbf{\Phi}_{\mathrm{a}}(\mathbf{q},\dot{\mathbf{q}},\ddot{\mathbf{q}}) + 2\alpha\mathbf{\Phi}_{\mathrm{v}}(\mathbf{q},\dot{\mathbf{q}}) + \beta^2\mathbf{\Phi}(\mathbf{q}) =: \mathbf{\Phi}_{\mathrm{B}}(\mathbf{q},\dot{\mathbf{q}},\ddot{\mathbf{q}})\end{aligned}} \tag{3.166}$$

where $\alpha \in \mathbb{R}$ and $\beta \in \mathbb{R}$ are known as the ***Baumgarte parameters***. The Baumgarte parameters need to be selected such that differential equation

$$\ddot{y} + 2\alpha\dot{y} + \beta^2 y = 0 \tag{3.167}$$

for scalar $y(t) : \mathbb{I} \to \mathbb{R}$ possesses an asymptotically stable solution. The solutions of Eq. (3.167) are given as

$$y(t) = C_1 \exp\left[t\left(-\alpha - \sqrt{\alpha^2 - \beta^2}\right)\right] + C_2 \exp\left[t\left(-\alpha + \sqrt{\alpha^2 - \beta^2}\right)\right] \tag{3.168}$$

where the coefficients are

$$\begin{aligned} C_1 &= -\frac{u_0 + y_0(\alpha - \sqrt{\alpha^2 - \beta^2})}{2\sqrt{\alpha^2 - \beta^2}} \\ C_2 &= \frac{u_0 + y_0(\alpha + \sqrt{\alpha^2 - \beta^2})}{2\sqrt{\alpha^2 - \beta^2}} \end{aligned} \tag{3.169}$$

if $y(0) = y_0$ and $\dot{y}(0) = u_0$. Taking the Laplace transform[9] of Eq. (3.167), we get the following characteristic equation:

$$s^2 + 2\alpha s + \beta^2 = 0 \tag{3.171}$$

[9] Recall the Laplace transform of n^{th}-derivative of $y(t)$:

$$\mathcal{L}\left[y^{(n)}\right] = s^n F(s) - s^{n-1} y(0) - \cdots - f^{(n-1)}(0) \tag{3.170}$$

where $s \in \mathbb{C}$ is a complex parameter and $F(s) = \mathcal{L}\left[f(t)\right]$.

if $y(0) = y_0 = 0$ and $\dot{y}(0) = u_0 = 0$. Since the Laplace transform is related to the Z-transform through

$$z := \mathrm{e}^{st} = \exp\left[\mathrm{Re}(s)t\right] \ \angle \mathrm{Im}(s)t \tag{3.172}$$

where $t = 1/f_\mathrm{s}$ is the sampling period, and f_s is the sampling rate. From Eq. (3.172), we see that the system is stable if $|z| < 1$ and marginally stable if $|z| = 1$. That is, the roots of the characteristic equation (Eq. (3.171)), i.e.,

$$s = -\alpha \pm \sqrt{\alpha^2 - \beta^2} \tag{3.173}$$

must have negative real parts so that the system is stable.

Remark 3.4.2

1. *The equation of motion with the Baumgarte stabilization method may be written in the single field-form as*

$$\begin{bmatrix} \mathbf{M}(\mathbf{q}) & \mathbf{G}^T(\mathbf{q}) \\ \mathbf{G}(\mathbf{q}) & \mathbf{0} \end{bmatrix} \begin{bmatrix} \ddot{\mathbf{q}} \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathbf{Q}^{\mathrm{appl}}(\mathbf{q}, \dot{\mathbf{q}}, t) \\ -\mathfrak{D}\mathbf{G}(\mathbf{q})(\dot{\mathbf{q}}, \dot{\mathbf{q}}) - 2\alpha\mathbf{G}(\mathbf{q})\dot{\mathbf{q}} - \beta^2\mathbf{\Phi}(\mathbf{q})\lambda \end{bmatrix} \tag{3.174}$$

2. *Consider the following perturbed system with deviations in Eq.* (3.167) *and the initial conditions:*

$$\ddot{y} + 2\alpha\dot{y} + \beta^2 y = \sigma \tag{3.175}$$

with $y(0) = y_0 + \sigma_\mathrm{x}$ *and* $\dot{y}(0) = u_0 + \sigma_\mathrm{u}$.

3. *For first-order systems, the Baumgarte stabilization method replaces the constraint equation with*

$$\boxed{\mathbf{\Phi}_\mathrm{B}(\mathbf{q}, \dot{\mathbf{q}}) := \mathbf{\Phi}_\mathrm{v}(\mathbf{q}, \dot{\mathbf{q}}) + \alpha\mathbf{\Phi}(\mathbf{q}) = \mathbf{G}(\mathbf{q})\dot{\mathbf{q}} + \alpha\mathbf{\Phi}(\mathbf{q}) = \mathbf{0}} \tag{3.176}$$

with the Baumgarte parameter $\alpha \in \mathbb{R}$. *Parameter* α *is selected such that the solution of*

$$\dot{y} + \alpha y = 0 \tag{3.177}$$

is asymptotically stable. With the initial condition $y(0) = y_0$, the solution is given as

$$y(t) = y_0 \mathrm{e}^{-\alpha t} \tag{3.178}$$

Therein, $y(t) \to 0$ as $t \to \infty$ if $\alpha > 0$. Consider the perturbed system,

$$\dot{y} + \alpha y = \sigma \tag{3.179}$$

with $y(0) = y_0 + \sigma_{\mathrm{y}}$ where σ and σ_{y} are deviations in Eq. (3.177) and the initial condition, respectively. In this case, the solution is

$$y(t) = \frac{\sigma}{\alpha} + \mathrm{e}^{-\alpha t}\left[y_0 + \sigma_{\mathrm{y}} - \frac{\sigma}{\alpha}\right] \tag{3.180}$$

Hence, we can see that the deviation σ_{y} can be damped out by taking $\alpha > 0$. From the characteristic equation of Eq. (3.177) with $y(0) = y_0 = 0$, obtained from the Laplace transform, we have

$$s = -\alpha \tag{3.181}$$

Hence, $\alpha > 0$ guarantees the stability of the system analytically *(not numerically).*

Algorithm 3.4.1

(GS4-2 Family of Algorithms with Baumgarte Stabilization Method)

The unified family of algorithms with the Baumgarte Stabilization Method may be stated as:

$$\boxed{\begin{aligned}&\mathbf{M}(\tilde{\mathbf{q}}^n)\tilde{\mathbf{a}}^n + \mathbf{G}^T(\tilde{\mathbf{q}}^n)\tilde{\lambda}^n = \mathbf{Q}^{\mathrm{appl}}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n, t_{n+W_1})\\ &\mathbf{\Phi}_{\mathrm{B}}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}, \hat{\mathbf{a}}^{n+1}) = \mathbf{\Phi}_{\mathrm{a}}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}, \hat{\mathbf{a}}^{n+1}) + 2\alpha\mathbf{\Phi}_{\mathrm{v}}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}) + \beta^2\mathbf{\Phi}(\mathbf{q}^{n+1}) = \mathbf{0}\end{aligned}} \tag{3.182}$$

together with the updates for the normal GS4-2 family of algorithms where the algorithmic configuration, velocity, and acceleration vectors, i.e., $\tilde{\mathbf{q}}^n$, $\tilde{\mathbf{v}}^n$, and $\tilde{\mathbf{a}}^n$, respectively, are defined in the same manner.

Remark 3.4.3

1. *The Jacobian matrix in the linearized equation is*

$$\begin{aligned}\mathbf{J}_{21} &= \Xi^{\mathrm{a}}(1+\phi)\mathbf{G}(\mathbf{q}^{n+1}) + \Xi^{\mathrm{v}}\frac{\partial \mathbf{\Phi}_{\mathrm{a}}^{n+1}}{\partial \mathbf{v}^{n+1}} + \Xi^{\mathrm{q}}\frac{\partial \mathbf{\Phi}_{\mathrm{a}}^{n+1}}{\partial \mathbf{q}^{n+1}} \\ &+ 2\alpha\left[\Xi^{\mathrm{v}}\mathbf{G}(\mathbf{q}^{n+1}) + \Xi^{\mathrm{q}}\frac{\partial \mathbf{\Phi}_{\mathrm{v}}^{n+1}}{\partial \mathbf{q}^{n+1}}\right] \\ &+ \beta^2\Xi^{\mathrm{q}}\mathbf{G}(\mathbf{q}^{n+1})\end{aligned} \tag{3.183}$$

   with $\mathbf{\Phi}_{\mathrm{v}}^{n+1} := \mathbf{\Phi}_{\mathrm{v}}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1})$ *and* $\mathbf{\Phi}_{\mathrm{a}}^{n+1} := \mathbf{\Phi}_{\mathrm{a}}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}, \hat{\mathbf{a}}^{n+1})$.

2. *Unless otherwise time step size Δt is not too small, selecting $\alpha = 1/\Delta t$ and $\beta = \sqrt{2}/\Delta t$, which are based on the Taylor expansion of $\mathbf{\Phi}_{\mathrm{B}}$ at time t_{n+1} in time about time t_n, reasonably work well. When Δt is too small or a selection of the parameters is not good, the system tends to become stiff easily, which leads to a serious numerical instability issue.*

3.4.3 Projection Method

An alternative way for the stabilization of constraints is the ***projection method***. This method requires a Newton-type iterative process with additional Lagrange multipliers so as to satisfy constraint equations.

Let $(\mathbf{q}^n, \mathbf{v}^n, \mathbf{a}^n)$ be the configuration, velocity, and acceleration vectors obtained from the Index-1 GSSSS family of algorithms at time level $t = t_n$. In the case of the Index-1 formulation, the geometric and velocity constraint equations within a time step are not satisfied in general, i.e.,

$$\boldsymbol{\Phi}(\mathbf{q}^n) \neq \mathbf{0} \;\text{ and }\; \boldsymbol{\Phi}_{\mathrm{v}}(\mathbf{q}^n, \mathbf{v}^n) = \mathbf{G}(\mathbf{q}^n)\mathbf{v}^n \neq \mathbf{0} \tag{3.184}$$

in contrast to the acceleration constraint equation, which is enforced to be satisfied at every time step t_n as

$$\boldsymbol{\Phi}_{\mathrm{a}}(\mathbf{q}^n, \mathbf{v}^n, \hat{\mathbf{a}}^n) = \mathbf{0} \tag{3.185}$$

The projection method for a two-stage method. For the Index-1 formulation, we first project numerical solution $\mathbf{q}^n$ onto the configuration manifold, where the geometric constraint equation is valid; then, project $\mathbf{v}^n$ onto the manifold so that both the geometric and velocity constraint equations are satisfied.

- **(Stage 1) Stabilization of the Geometric Constraint:** In order to satisfy the geometric constraint, project the numerical configuration at t_n onto the configuration manifold Q by solving the minimization problem,[10]

$$\boxed{\min \|\check{\mathbf{q}}^n - \mathbf{q}^n\|_{\mathbf{S}} \quad \text{s.t.} \;\; \boldsymbol{\Phi}(\check{\mathbf{q}}^n) = \mathbf{0}} \tag{3.186}$$

  where $\check{\mathbf{q}}^n \in \mathbb{R}^{n_{\mathrm{g}}}$ is the projected numerical configuration vector at t_n, and $\mathbf{S} \in \mathbb{R}^{n_{\mathrm{g}} \times n_{\mathrm{g}}}$ is a symmetric and positive-definite matrix. The mass matrix (or the corresponding diagonalized mass matrix) is usually adopted for $\mathbf{S}$. With Lagrange multiplier $\boldsymbol{\mu} \in \mathbb{R}^{n_{\mathrm{c}}}$, the necessary condition for the minimization problem as given in Eq. (3.186)

$$\boxed{\begin{aligned} \mathbf{M}(\check{\mathbf{q}}^n)\left[\check{\mathbf{q}}^n - \mathbf{q}^n\right] + \mathbf{G}^T(\check{\mathbf{q}}^n)\boldsymbol{\mu} = \mathbf{0} \\ \boldsymbol{\Phi}(\check{\mathbf{q}}^n) = \mathbf{0} \end{aligned}} \tag{3.187}$$

[10] The norm is defined by $\|\boldsymbol{\xi}\|_{\mathbf{S}} := \sqrt{\boldsymbol{\xi}^T \mathbf{S} \boldsymbol{\xi}}$ for an arbitrary vector $\boldsymbol{\xi} \in \mathbb{R}^{n_{\mathrm{g}}}$.

Solving Eq. (3.187) for $(\check{\mathbf{q}}^n, \boldsymbol{\mu})$ by means of the Newton-type iterative method, we can obtain $\check{\mathbf{q}}^n$ and replace the old data $\mathbf{q}^n$ with the updated one as

$$(\mathbf{q}^n, \mathbf{v}^n, \mathbf{a}^n) \longrightarrow (\check{\mathbf{q}}^n, \mathbf{v}^n, \mathbf{a}^n) \tag{3.188}$$

- **(Stage 2) Stabilization of the Velocity Constraint:** Next, the numerical velocity vector at t_n is projected onto the tangent space at $\check{\mathbf{q}}^n$ to satisfy the velocity constraint at this time level by solving the following minimization problem:

$$\boxed{\min \|\check{\mathbf{v}}^n - \mathbf{v}^n\|_{\mathbf{S}} \quad \text{s.t.} \;\; \boldsymbol{\Phi}_{\mathrm{v}}(\check{\mathbf{q}}^n, \check{\mathbf{v}}^n) = \mathbf{G}(\check{\mathbf{q}}^n)\check{\mathbf{v}}^n = \mathbf{0}} \tag{3.189}$$

With the Lagrange multiplier vector $\boldsymbol{\varsigma} \in \mathbb{R}^{n_c}$, the necessary condition for the problem is given by

$$\boxed{\begin{aligned} \mathbf{M}(\check{\mathbf{q}}^n)\,[\check{\mathbf{v}}^n - \mathbf{v}^n] + \mathbf{G}^T(\check{\mathbf{q}}^n)\boldsymbol{\varsigma} = \mathbf{0} \\ \boldsymbol{\Phi}_{\mathrm{v}}(\check{\mathbf{q}}^n, \check{\mathbf{v}}^n) = \mathbf{G}(\check{\mathbf{q}}^n)\check{\mathbf{v}}^n = \mathbf{0} \end{aligned}} \tag{3.190}$$

for $\mathbf{S} = \mathbf{M}$. We can solved for $(\check{\mathbf{v}}^n, \boldsymbol{\varsigma})$ without adopting the Newton-type iterative process from the following linear equation:

$$\begin{bmatrix} \mathbf{M}(\check{\mathbf{q}}^n) & \mathbf{G}^T(\check{\mathbf{q}}^n) \\ \mathbf{G}(\check{\mathbf{q}}^n) & \mathbf{0} \end{bmatrix} \begin{bmatrix} \check{\mathbf{v}}^n \\ \boldsymbol{\varsigma} \end{bmatrix} = \begin{bmatrix} \mathbf{M}(\check{\mathbf{q}}^n)\mathbf{v}^n \\ \mathbf{0} \end{bmatrix} \tag{3.191}$$

Hence, from Eq. (3.190) (after solving Eq. (3.187)), the updated numerical configuration and velocity vectors are obtained:

$$(\check{\mathbf{q}}^n, \mathbf{v}^n, \mathbf{a}^n) \longrightarrow (\check{\mathbf{q}}^n, \check{\mathbf{v}}^n, \mathbf{a}^n) \tag{3.192}$$

Remark 3.4.4

1. *As can be seen from Eq.* (3.186) *and Eq.* (3.189), *the projected numerical values* $(\check{\mathbf{q}}^n, \check{\mathbf{v}}^n)$ *are the points on the tangent bundle* TQ, *and they have the minimum distance from the original points* $(\mathbf{q}^n, \mathbf{v}^n)$ *in the induced metric sense with* $\mathbf{S} = \mathbf{M}$.

2. *The order of convergence of the time-stepping algorithm is not affected by the projection method above since* $\|\check{\mathbf{q}}^n - \mathbf{q}^n\| = \mathcal{O}(\Delta t^2)$ *and* $\|\check{\mathbf{v}}^n - \mathbf{v}^n\| = \mathcal{O}(\Delta t^2)$*. That is,* $\|\check{\mathbf{q}}^n - \mathbf{q}(t_n)\| = \mathcal{O}(\Delta t^2)$ *and* $\|\check{\mathbf{v}}^n - \dot{\mathbf{q}}(t_n)\| = \mathcal{O}(\Delta t^2)$ *since the orders of convergence of the configuration and velocity in the GSSSS family of algorithms are two. Of course, those of acceleration and the Lagrange multiplier* $\boldsymbol{\lambda}^n$ *also remain as two.*

3. *For real-time simulation purpose, only one iterative step is sufficient for stabilizing the geometric constraint at* ***stage 1****; see [51]. Although the geometric constraint equation may not be exactly satisfied within the time step, we can get reasonably accurate projected solutions without reducing the order of convergence of a time integration scheme.*

3.4.4 Penalty Method

Another approach to stabilizing the geometric and velocity constraints in the Index-1 formulation is the ***penalty method***. Introduce the kinetic and potential energy functions in terms of $\dot{\mathbf{\Phi}}$ and $\mathbf{\Phi}$ as

$$\mathscr{T}_{\mathrm{PM}} := \frac{1}{2}\dot{\mathbf{\Phi}}^T \mathbf{W} \dot{\mathbf{\Phi}} \quad \text{and} \quad \mathscr{U}_{\mathrm{PM}} := \frac{1}{2}\mathbf{\Phi}^T \mathbf{W} \mathbf{\Omega}^2 \mathbf{\Phi} \tag{3.193}$$

respectively, where matrix $\mathbf{W} \in \mathbb{R}^{n_c \times n_c}$ and $\mathbf{\Omega}^2 \in \mathbb{R}^{n_c \times n_c}$ are given by

$$\mathbf{W} = (1/p)\mathbf{I} \quad \text{and} \quad \mathbf{\Omega}^2 = \omega^2 \mathbf{I} \tag{3.194}$$

with the ***penalty coefficient*** $p \in \mathbb{R}$ and the frequency $\omega \in \mathbb{R}$. The constants p and ω need to be selected by analysts.

In the penalty method, the equation of equation is modified as

$$\boxed{\mathbf{M}(\mathbf{q})\ddot{\mathbf{q}} + \mathbf{Q}_2^{\mathrm{PM}}(\mathbf{q}, \dot{\mathbf{q}}) + \mathbf{Q}_1^{\mathrm{PM}}(\mathbf{q}, \dot{\mathbf{q}}) = \mathbf{Q}^{\mathrm{appl}}(\mathbf{q}, \dot{\mathbf{q}}, t)} \tag{3.195}$$

where $\mathbf{Q}_1^{\mathrm{PM}}$ and $\mathbf{Q}_2^{\mathrm{PM}}$ are defined by

$$\begin{aligned}
\mathbf{Q}_1^{\mathrm{PM}} &:= \frac{d}{dt}\left(\frac{\partial \mathscr{L}_{\mathrm{PM}}}{\partial \dot{\mathbf{q}}}\right) - \frac{\partial \mathscr{L}_{\mathrm{PM}}}{\partial \mathbf{q}} \\
&= \mathbf{G}^T\mathbf{W}\mathbf{G}\ddot{\mathbf{q}} + \mathbf{G}^T\mathbf{W}\dot{\mathbf{G}}\dot{\mathbf{q}} + \mathbf{G}^T\mathbf{W}\mathbf{\Omega}^2\mathbf{\Phi}
\end{aligned} \tag{3.196}$$

with Lagrangian function $\mathscr{L}_{\mathrm{PM}} = \mathscr{T}_{\mathrm{PM}} - \mathscr{U}_{\mathrm{PM}}$, and

$$\mathbf{Q}_2^{\mathrm{PM}} := \frac{\partial \Theta_{\mathrm{R}}}{\partial \dot{\mathbf{q}}} = \mathbf{C}_{\mathrm{R}}\dot{\mathbf{q}} = \gamma \mathbf{G}^T\mathbf{W}\mathbf{\Omega}\mathbf{G}\dot{\mathbf{q}} \tag{3.197}$$

with the Rayleigh dissipative function defined by

$$\Theta_{\mathrm{R}} := \frac{1}{2}\dot{\mathbf{q}}^T\mathbf{C}_{\mathrm{R}}\dot{\mathbf{q}}, \quad \mathbf{C}_{\mathrm{R}} := \gamma\mathbf{G}^T\mathbf{W}\mathbf{\Omega}\mathbf{G} \in \mathbb{R}^{n_c \times n_c} \tag{3.198}$$

The scalar parameter $\gamma \in \mathbb{R}$ is selected by analysts. Therefore, Eq. (3.195) results in

$$\boxed{\left[\mathbf{M}(\mathbf{q}) + \mathbf{G}^T\mathbf{W}\mathbf{G}\right]\ddot{\mathbf{q}} + \gamma\mathbf{G}^T\mathbf{W}\mathbf{\Omega}\mathbf{G}\dot{\mathbf{q}} + \mathbf{G}^T\mathbf{W}\,\mathfrak{D}\mathbf{G}(\mathbf{q})(\dot{\mathbf{q}},\dot{\mathbf{q}}) + \mathbf{G}^T\mathbf{W}\mathbf{\Omega}^2\mathbf{\Phi} = \mathbf{Q}^{\mathrm{appl}}(\mathbf{q},\dot{\mathbf{q}},t)} \tag{3.199}$$

Eq. (3.199) is a ODE; therein, we can make use of ODE integrators, such as the ODE-GSSSS family of algorithms, stated in the previous chapter.

3.5 The DAE-*i*Integrator: Adaptation Process

3.5.1 Adaptation Process

The adaptation process of the *i*Integrators for DAE systems is similar to the one for the ODE case introduced in in section 2.3 in the previous chapter. Namely, it is the two step procedure: (1) Adaptation process for unknowns and (2) Adaptation process for the spectral parameters. The only difference from the ODE case is the appearance of algebraic unknowns. Actually, the adaptation process in step (1) is only for kinematic unknowns, and the rest is exactly the same as summarized in Table 2.3 for the ODE case. In order to demonstrate the concept, consider the following two general and practical cases for constrained mechanical systems with holonomic-scleronomic constraints.

Illustrations

Consider the fully discretized second-order DAE system given as

$$\mathbf{M}(\tilde{\mathbf{q}}^n)\tilde{\mathbf{a}}^n = \mathbf{Q}^{\text{appl}}(\tilde{\mathbf{q}}^n, \tilde{\mathbf{v}}^n, t_{n+W_1}) - \mathbf{G}^T(\tilde{\mathbf{q}}^n)\tilde{\boldsymbol{\lambda}}^n \tag{3.200a}$$

$$\mathbf{0} = \boldsymbol{\Sigma}_{(2)}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}, \hat{\mathbf{a}}^{n+1}) \tag{3.200b}$$

Let us defined

$$\boldsymbol{\Sigma}_{(2)}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}, \hat{\mathbf{a}}^{n+1}) := \gamma_3^{(2)}\boldsymbol{\Phi}_{\text{a}}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}, \hat{\mathbf{a}}^{n+1}) + \gamma_2^{(2)}\boldsymbol{\Phi}_{\text{v}}(\mathbf{q}^{n+1}, \mathbf{v}^{n+1}) + \gamma_1^{(2)}\boldsymbol{\Phi}(\mathbf{q}^{n+1}) \tag{3.201}$$

such that: when $(\gamma_1^{(2)}, \gamma_2^{(2)}, \gamma_3^{(2)}) = (\beta^2, 2\alpha, 1)$, Eq. (3.200) recovers Algorithm 3.4.1 with the Baumgarte Stabilization Method. When $(\gamma_1^{(2)}, \gamma_2^{(2)}, \gamma_3^{(2)}) = (0, 0, 1)$, Eq. (3.200) readily recovers Algorithm 3.3.3. Likewise, Algorithms 3.3.2 and 3.3.1 can be also recovered by $(\gamma_1^{(2)}, \gamma_2^{(2)}, \gamma_3^{(2)}) = (0, 1, 0)$ and $(\gamma_1^{(2)}, \gamma_2^{(2)}, \gamma_3^{(2)}) = (1, 0, 0)$, respectively.

Via the adaptation process for the kinematic unknowns and the spectral parameters,

$$\begin{gathered}(\mathbf{q}^n, \mathbf{v}^n, \mathbf{a}^n) \longrightarrow (\text{“dummy”}, \mathbf{s}^n, \boldsymbol{\nu}^n) \\ \boldsymbol{\lambda}^n \longrightarrow \boldsymbol{\varsigma}^n \\ (\rho_\infty^{\text{min}}, \rho_\infty^{\text{max}}, \rho_\infty^{\text{s}}) \longrightarrow (\rho, 1, \rho_\infty^{\text{s}})\end{gathered} \tag{3.202}$$

respectively, the analogous application of the GS4-1 family of algorithms to first-order

DAE systems of the form,

$$\begin{aligned}\dot{\mathbf{s}} &= \mathbf{h}(\mathbf{s}, \boldsymbol{\varsigma}, t)\\ \mathbf{0} &= \boldsymbol{\Sigma}_{(1)}(\mathbf{s}, \dot{\mathbf{s}})\end{aligned} \tag{3.203}$$

where $\mathbf{s}(t)$ and $\dot{\mathbf{s}}(t) := d\mathbf{s}/dt$ are the kinematic variables, and $\boldsymbol{\varsigma}(t)$ is the algebraic variable of the system, yields:

Algorithm 3.5.1 (GS4-1 Family of Algorithms for First-order DAE Systems)
Given (consistent) initial condition $(\mathbf{s}, \dot{\mathbf{s}}, \boldsymbol{\varsigma})(t_0) = (\mathbf{s}^0, \boldsymbol{\nu}^0, \boldsymbol{\varsigma}^0)$. *Find* $\mathbf{s}^n$ *and* $\boldsymbol{\nu}^n$ *(for* $n \in \{1, 2, \cdots, n_{\text{steps}}\}$*) from*

$$\tilde{\boldsymbol{\nu}}^n = \mathbf{h}(\tilde{\mathbf{s}}^n, \tilde{\boldsymbol{\varsigma}}^n, t_{n+W_1}) \tag{3.204a}$$

$$\mathbf{0} = \boldsymbol{\Sigma}_{(1)}(\mathbf{s}^{n+1}, \hat{\boldsymbol{\nu}}^{n+1}) \tag{3.204b}$$

where

$$t_{n+W_1} := (1 - W_1)t_n + W_1 t_{n+1} \tag{3.204c}$$

$$\tilde{\mathbf{s}}^n := \mathbf{s}^n + W_1\Lambda_4\boldsymbol{\nu}^n\Delta t + W_2\Lambda_5\Delta\boldsymbol{\nu}^n\Delta t \tag{3.204d}$$

$$\tilde{\boldsymbol{\nu}}^n := \boldsymbol{\nu}^n + W_1\Lambda_6\Delta\boldsymbol{\nu}^n =: \boldsymbol{\nu}_{n+W_1\Lambda_6} \tag{3.204e}$$

$$\tilde{\boldsymbol{\varsigma}}^n := (1 - W_1)\boldsymbol{\varsigma}^n + W_1\boldsymbol{\varsigma}^{n+1} \tag{3.204f}$$

and

$$\hat{\boldsymbol{\nu}}^{n+1} := (1 + \phi)\boldsymbol{\nu}^{n+1} - \phi\boldsymbol{\nu}^n \tag{3.204g}$$

The associated updates are:

$$\mathbf{s}^{n+1} = \mathbf{s}^n + \lambda_4\boldsymbol{\nu}^n\Delta t + \lambda_5\Delta\boldsymbol{\nu}^n\Delta t \tag{3.204h}$$

$$\boldsymbol{\nu}^{n+1} = \boldsymbol{\nu}^n + \Delta\boldsymbol{\nu}^n \tag{3.204i}$$

The algorithmic parameters are defined by

$$\begin{aligned} W_1 &= \frac{1}{1+\rho_\infty} \quad , \quad \lambda_4 = \Lambda_4 = 1 \\ W_2\Lambda_5 &= \frac{1}{(1+\rho_\infty)(1+\rho_\infty^{\mathrm{s}})} \quad , \quad \lambda_5 = \frac{1}{1+\rho_\infty^{\mathrm{s}}} \\ W_1\Lambda_6 &= \frac{3+\rho_\infty+\rho_\infty^{\mathrm{s}}-\rho_\infty\rho_\infty^{\mathrm{s}}}{2(1+\rho_\infty)(1+\rho_\infty^{\mathrm{s}})} \end{aligned}$$

Remark 3.5.1

1. *The adaptation process naturally leads to* $\boldsymbol{\varsigma}^n \approx \boldsymbol{\varsigma}(t_n)$, $\mathbf{s}^n \approx \mathbf{s}(t_n)$ *and* $\boldsymbol{\nu}^n \approx \dot{\mathbf{s}}(t_{n-\phi})$ *with* $\phi := W_1\Lambda_6 - W_1$. *This direct adaptation guarantees the second-order time accuracy of the resulting algorithm for the kinematic and algebraic unknowns,* $(\mathbf{s}^n, \boldsymbol{\nu}^n, \boldsymbol{\varsigma}^n)$ *at time level* $t = t_n$. *The proof is similar to the one for the second-order systems. Note that* $\hat{\boldsymbol{\nu}}^{n+1}$ *defined in Eq.* (3.204g) *implies* $\hat{\boldsymbol{\nu}}^{n+1} \approx \boldsymbol{\nu}(t_{n+1})$.

2. *Suppose* $\boldsymbol{\Sigma}_{(1)}$ *is defined as*

$$\boldsymbol{\Sigma}_{(1)}(\mathbf{s}^{n+1}, \hat{\boldsymbol{\nu}}^{n+1}) := \gamma_2^{(1)}\boldsymbol{\varphi}_\nu(\mathbf{s}^{n+1}, \hat{\boldsymbol{\nu}}^{n+1}) + \gamma_1^{(1)}\boldsymbol{\varphi}(\mathbf{s}^{n+1}) \tag{3.205}$$

Then, Algorithm 3.5.1 leads to the GS4-1 family applied with the Baumgarte stabilization method when $(\gamma_1^{(1)}, \gamma_2^{(1)}) = (\alpha, 1)$. *When* $(\gamma_1^{(1)}, \gamma_2^{(1)}) = (1, 0)$ *and* $(\gamma_1^{(1)}, \gamma_2^{(1)}) = (0, 1)$, *Algorithm 3.5.1 recovers the GS4-1 family of algorithms for the Index-2 and Index-1 first-order DAEs, respectively.*

Applications to the First-order Mechanical Systems Algorithm 3.5.1 can be applied to the mechanical systems in the first-order DAE systems in the form of Eq. (3.98) (Index 3), Eq. (3.91) (Index 2), or Eq. (3.74) (Index 1), for instance. This class of algorithms is also suitable for the stabilized Index-2 (GGL) formulation, given in Eq. (3.93) or Eq. (3.96). For a practical purpose, we only show the family of algorithms for Eq. (3.129), as an application of Algorithm 3.5.1. The adaptation process for this case[11] , i.e.,

$$
\begin{aligned}
(\mathbf{q}^n, \mathbf{v}^n, \mathbf{a}^n) &\longrightarrow (\text{“dummy”}, \mathbf{z}^n, \mathbf{c}^n) \\
\lambda^n &\longrightarrow \chi^n \\
(\rho_\infty^{\min}, \rho_\infty^{\max}, \rho_\infty^{\mathrm{s}}) &\longrightarrow (\rho, 1, \rho_\infty^{\mathrm{s}})
\end{aligned}
\tag{3.206}
$$

with $(\mathbf{z}^n, \mathbf{c}^n, \chi^n) \approx (\mathbf{z}(t_n), \dot{\mathbf{z}}(t_{n-\phi}), \chi(t_n))$, gives rise to:

Algorithm 3.5.2 (GS4-1 Family for a Mechanical System)

Find $\mathbf{s}^n$ *and* $\boldsymbol{\nu}^n$ *(for* $n \in \{1, 2, \cdots, n_{\mathrm{steps}}\}$*) from*

$$\tilde{\mathbf{c}}^n = \mathbb{J}\left[\mathfrak{D}\mathscr{H}(\tilde{\mathbf{z}}^n) + \tilde{\chi}^n \mathfrak{D}\boldsymbol{\Theta}(\tilde{\mathbf{z}}^n)\right] \tag{3.207a}$$

$$\mathbf{0} = \boldsymbol{\Theta}(\mathbf{z}^{n+1}) \tag{3.207b}$$

where

$$t_{n+W_1} := (1 - W_1)t_n + W_1 t_{n+1} \tag{3.207c}$$

$$\tilde{\mathbf{z}}^n := \mathbf{z}^n + W_1\Lambda_4\mathbf{c}^n\Delta t + W_2\Lambda_5\Delta\mathbf{c}^n\Delta t \tag{3.207d}$$

$$\tilde{\mathbf{c}}^n := \mathbf{c}^n + W_1\Lambda_6\Delta\mathbf{c}^n =: \mathbf{c}_{n+W_1\Lambda_6} \tag{3.207e}$$

$$\tilde{\chi}^n := (1 - W_1)\chi^n + W_1\chi^{n+1} \tag{3.207f}$$

The associated updates are:

$$\mathbf{z}^{n+1} = \mathbf{z}^n + \lambda_4\mathbf{c}^n\Delta t + \lambda_5\Delta\mathbf{c}^n\Delta t \tag{3.207g}$$

$$\mathbf{c}^{n+1} = \mathbf{c}^n + \Delta\mathbf{c}^n \tag{3.207h}$$

[11] Eq. (3.129):

$$
\begin{aligned}
\dot{\mathbf{z}} &= \mathbb{J}\left[\mathfrak{D}\mathscr{H}(\mathbf{z}) + \chi\mathfrak{D}\boldsymbol{\Theta}(\mathbf{z})\right] \\
\mathbf{0} &= \boldsymbol{\Theta}(\mathbf{z})
\end{aligned}
$$

where $\mathbf{z}(t) := (\mathbf{q}^T, \mathbf{p}^T)^T$, $\chi(t) := (\boldsymbol{\lambda}^T, \boldsymbol{\eta}^T)^T$, and $\boldsymbol{\Theta}(\mathbf{z}) := (\boldsymbol{\Phi}^T, \boldsymbol{\Phi}_{\mathrm{p}}^T)^T$.

The algorithmic parameters are as defined in Algorithm 3.5.1.

Remark 3.5.2

Since the algorithmic time level is consistently at $t = t_{n+W_1}$, Algorithm 3.5.2 inherits the second-order time accuracy in all the kinematic and algebraic unknowns. Because of Eq. (3.207b), *the satisfactions of the constraint equations both at the configuration and momentum levels are fulfilled at the time grids t_n $\forall n$.*

3.5.2 Numerical Illustrations

Example 3.5.1 (Second-order DAE: Andrew's Squeezing Mechanism)

A classical detailed problem description of Andrew's squeezing mechanism [52] is provided in [53]. Here, we formulate this mechanical problem following the way shown in [54]; and numerical results from the second-order DAE algorithm for Index 3 formulation, i.e., Algorithm 3.3.1, and Algorithm 3.5.2 are shown in order to validate the performance of the adaptation process in DAE systems. The (expanded) generalized coordinates are given as

$$\mathbf{q} = [x_1, y_1, \beta, x_2, y_2, \theta, x_3, y_3, \gamma, x_4, y_4, \phi, x_5, y_5, \delta, x_6, y_6, \Omega, x_7, y_7, \epsilon]^T \in \mathbb{R}^{21} \tag{3.208}$$

where $(\beta, \theta, \gamma, \phi, \delta, \Omega, \epsilon)$ are the original generalized coordinates suggested in [53]. The equation of motion of the system is naturally given in the Index 3 format of the form

$$\begin{aligned} \mathbf{M}\ddot{\mathbf{q}} &= \mathbf{Q}^{\text{appl}}(\mathbf{q}) - \mathbf{G}^T(\mathbf{q}) \\ \mathbf{0} &= \mathbf{\Phi}(\mathbf{0}) \end{aligned} \tag{3.209}$$

where the mass matrix for this problem is defined as

$$\mathbf{M} = \text{diag}([m_1, m_1, 0, m_2, m_2, 0, ...m_7, m_7, 0]) \in \mathbb{R}^{21\times 21} \tag{3.210}$$

the nonzero components of the applied force vector $\mathbf{Q}^{\text{appl}} \in \mathbb{R}^{21}$ *are given as*

$$Q_3^{\text{appl}} = T, \quad Q_7^{\text{appl}} = F_x, \quad Q_8^{\text{appl}} = F_y, \quad Q_9^{\text{appl}} = F_x(x_d - x_3) - F_y(y_d - y_3) \tag{3.211}$$

The geometric constraint equations are defined as follows:

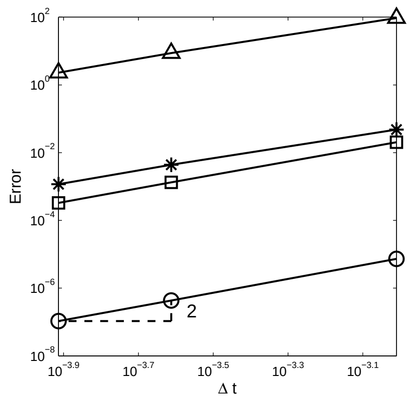
$$\Phi(\mathbf{u}) = \begin{bmatrix} x_1 - r_a \cos(\beta) \\ y_1 - r_a \sin(\beta) \\ x_2 - (r_r \cos(\beta) - da \cos(\theta)) \\ y_2 - (r_r \sin(\beta) - da \sin(\theta)) \\ x_3 - (x_b + s_a \sin(\gamma) + s_b \cos(\gamma)) \\ y_3 - (y_b - s_a \cos(\gamma) + s_b \sin(\gamma)) \\ x_4 - (x_a + z_t \cos(\delta) + (e - e_a) \sin(\phi)) \\ y_4 - (y_a + z_t \sin(\delta) - (e - e_a) \cos(\phi)) \\ x_5 - (x_a + t_a \cos(\delta) - t_b \sin(\delta)) \\ y_5 - (y_a + t_a \sin(\delta) + t_b \cos(\delta)) \\ x_6 - (x_a + u \sin(\epsilon) + (z_f - f_a) \cos(\Omega)) \\ y_6 - (y_a - u \cos(\epsilon) + (z_f - f_a) \sin(\Omega)) \\ x_7 - (x_a + u_a \sin(\epsilon) - u_b \cos(\epsilon)) \\ y_7 - (y_a - u_a \cos(\epsilon) - u_b \sin(\epsilon)) \\ r_r * \cos(\beta) - d \cos(\theta) - s_s \sin(\gamma) - x_b \\ r_r * \sin(\beta) - d \sin(\theta) + s_s \cos(\gamma) - y_b \\ r_r * \cos(\beta) - d \cos(\theta) - e \sin(\phi) - z_t \cos(\delta) - x_a \\ r_r * \sin(\beta) - d \sin(\theta) + e \cos(\phi) - z_t \sin(\delta) - y_a \\ r_r * \cos(\beta) - d \cos(\theta) - z_f \cos(\Omega) - u \sin(\epsilon) - x_a \\ r_r * \sin(\beta) - d \sin(\theta) - z_f \sin(\Omega) + u \cos(\epsilon) - y_a \end{bmatrix} \tag{3.212}$$

Fig. 3.1 and Fig. 3.2 show the numerical results obtained by directly applying Algorithm 3.3.1 to the Index 3 DAE system with the algorithmic parameters $(\rho_\infty^{\mathrm{min}}, \rho_\infty^{\mathrm{max}}, \rho_\infty^{\mathrm{s}}) = (1, 1, 0)$ *in the V0-based family and* $(\rho_\infty^{\mathrm{min}}, \rho_\infty^{\mathrm{max}}, \rho_\infty^{\mathrm{s}}) = (0, 1, 0)$ *in the U0V0/V0U0-based optimal family, respectively: the MPR-MPA method and numerically dissipative optimal (0,1,0) method. And Fig. 3.3 shows the numerical results obtained by the algorithms that can be generated by way of the adaptation process from these two distinct schemes applied to the reformulated system in the sense of Algorithm 3.5.2. The consistent initial conditions and other input data were directly employed from the ones shown in [54]. Note that second-order accuracy in kinematic and algebraic quantities for all cases is obtained*[12] *. The constraint equations at the position and momentum levels are exactly satisfied within a time step in Algorithm 3.5.2; whilst, Algorithm 3.5.2 can satisfy only the position constraint equation. Since there is no enforcement for the constraint equation at the* acceleration *level even in Algorithm 3.5.2, it is not satisfied at* t_n $\forall n$ *in general; therein, the projection method, shown in section 3.4.3, may be employed for the enforcement of* $\mathbf{\Phi}_{\mathrm{a}} = \mathbf{0}$. *That is, solve the following simple linear equation to obtain the projected acceleration data without influence the order of time accuracy:*

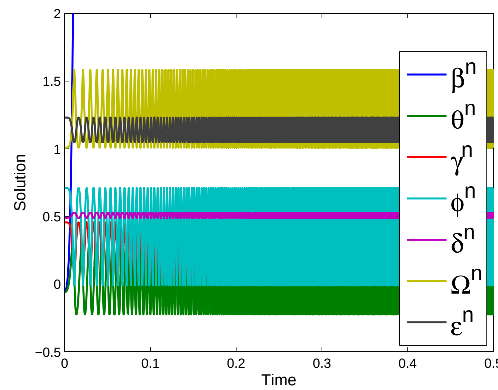
$$\begin{bmatrix} \mathbf{M} & \mathbf{G}^T(\check{\mathbf{q}}^n) \\ \mathbf{G}(\check{\mathbf{q}}^n) & \mathbf{0} \end{bmatrix} \begin{bmatrix} \check{\mathbf{a}}^n \\ \boldsymbol{\iota} \end{bmatrix} = \begin{bmatrix} \mathbf{M}\mathbf{a}^n \\ \mathbf{0} \end{bmatrix} \tag{3.213}$$

where $\boldsymbol{\iota}$ *is the additional Lagrange multiplier, and the acceleration* $\mathbf{a}^n$ *can be obtained directly from* $\mathbf{c}^n$ *since the mass matrix is constant for this example problem.*

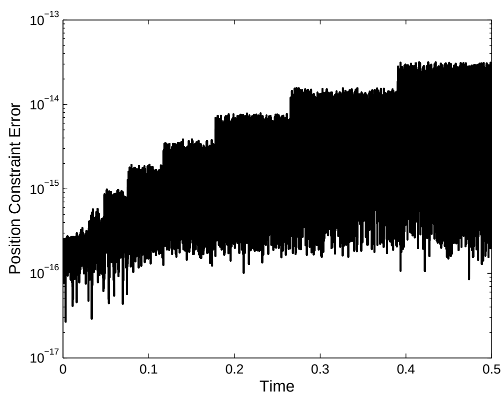
[12] $\circ$, $\square$, $\triangle$, *and* $*$ *in the time accuracy plots in Fig. 3.1 and Fig. 3.2 denote the data of the configuration, velocity, acceleration, and Lagrange multiplier, respectively.* $\circ$, $\square$, *and* $*$ *in the time accuracy plots in Fig. 3.3 denote the data for* $\mathbf{z}^n$, $\mathbf{c}^n$, *and* $\boldsymbol{\chi}^n$, *respectively.*



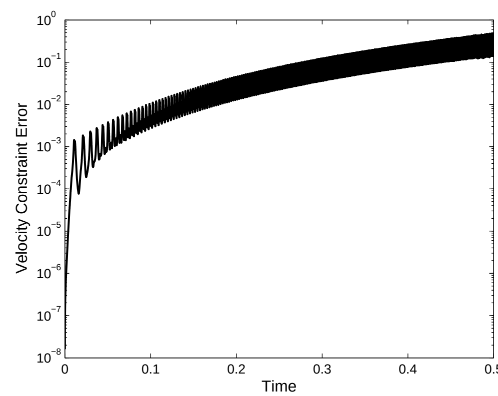
(a) Time Accuracy



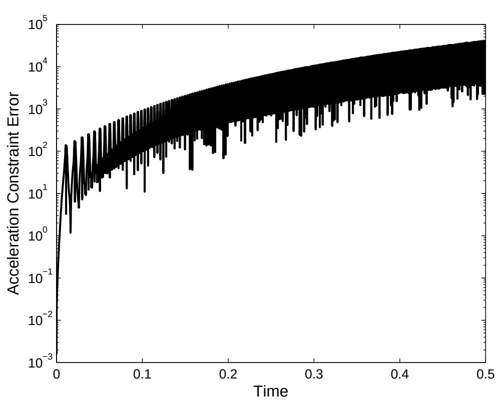
(b) Solution



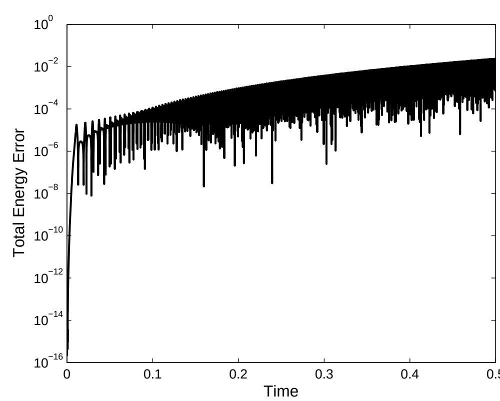
(c) Position Constraint Error



(d) Velocity Constraint Error

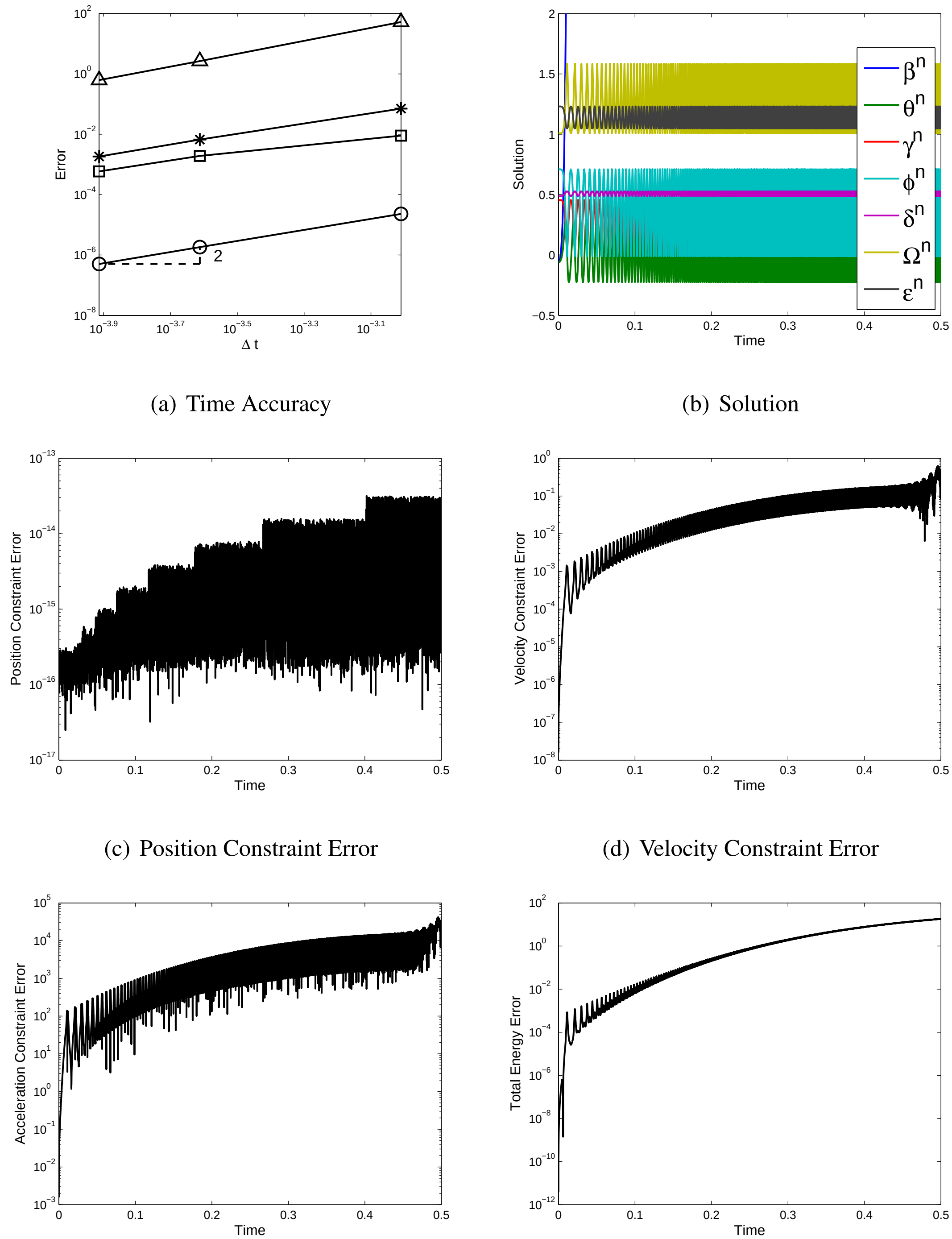


(e) Acceleration Constraint Error



(f) Total Energy Error

Figure 3.1: Example 3.5.1: The MPR-MPA Method (Index 3)



(a) Time Accuracy

(b) Solution

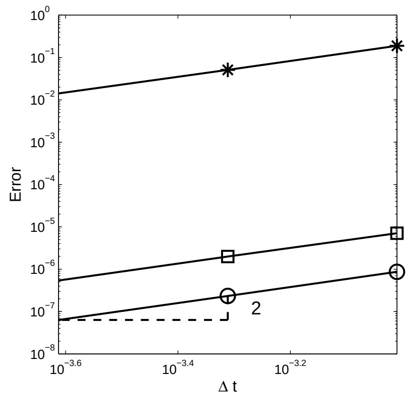
(c) Position Constraint Error

(d) Velocity Constraint Error

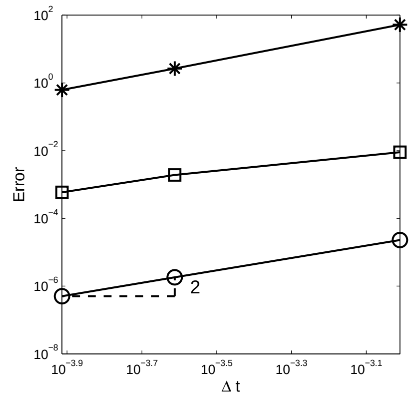
(e) Acceleration Constraint Error

(f) Total Energy Error

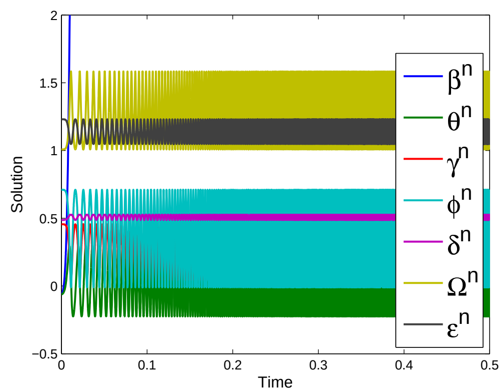
Figure 3.2: Example 3.5.1: U0V0/V0U0 Optimal (0,1,0) Method (Index 3)



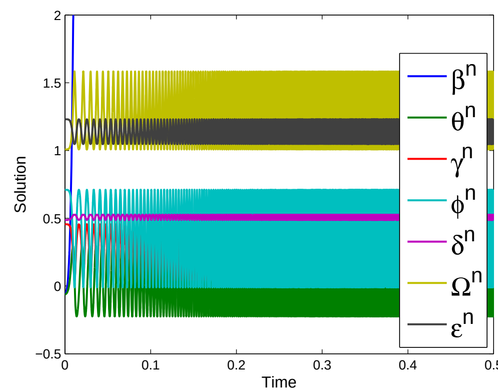
(a) Time Accuracy: MPR-MPA



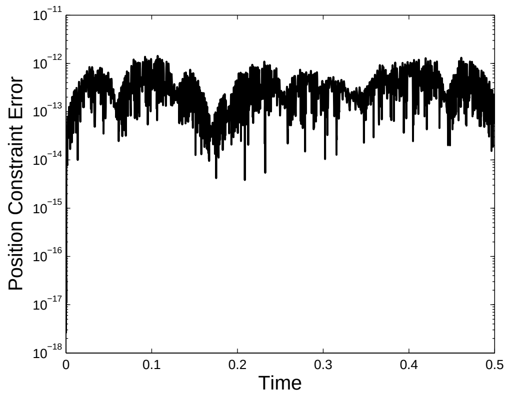
(b) Time Accuracy: Gear



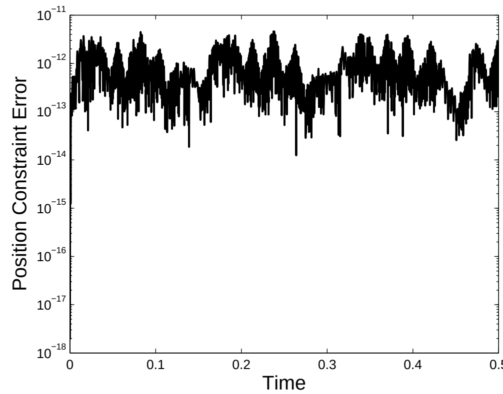
(c) Solution: MPR-MPA



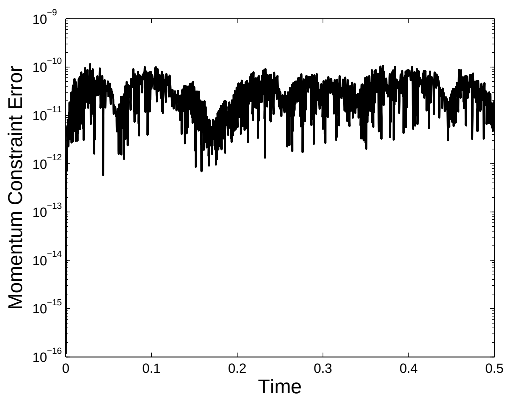
(d) Solution: Gear



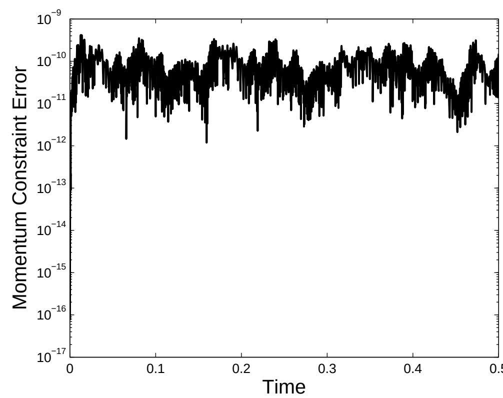
(e) Position Constraint Error: MPR-MPA



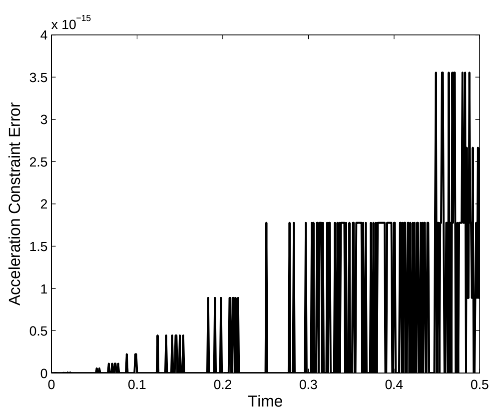
(f) Position Constraint Error: Gear



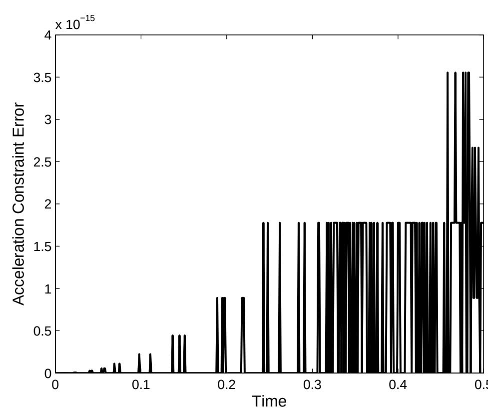
(g) Momentum Constraint Error: MPR-MPA



(h) Momentum Constraint Error: Gear



(i) Acceleration Constraint Error: MPR-MPA



(j) Acceleration Constraint Error: Gear

Figure 3.3: Example 3.5.1: Numerical Results by the MPR-MPA Method and Gear's Method in Algorithm 3.5.2

Example 3.5.2 (First-order DAE: Van der Pol's Equation)

Consider Van der Pol's equation,

$$\epsilon\ddot{q} + (q^2 - 1)\dot{q} + q = 0 \tag{3.214}$$

with parameter $\epsilon > 0$. *Due to the Lienhard's coordinates transformation,*

$$\eta := q, \quad s := \epsilon\dot{\eta} + \frac{\eta^2}{3} - \eta \tag{3.215}$$

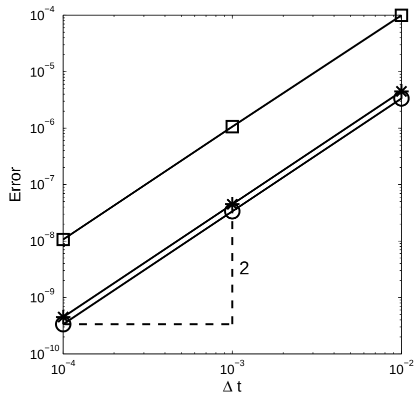
Eq. (3.214) *may be written as*

$$\begin{aligned} \dot{s} &= -\eta \\ \epsilon\dot{\eta} &= s - \frac{\eta^3}{3} + \eta \end{aligned} \tag{3.216}$$

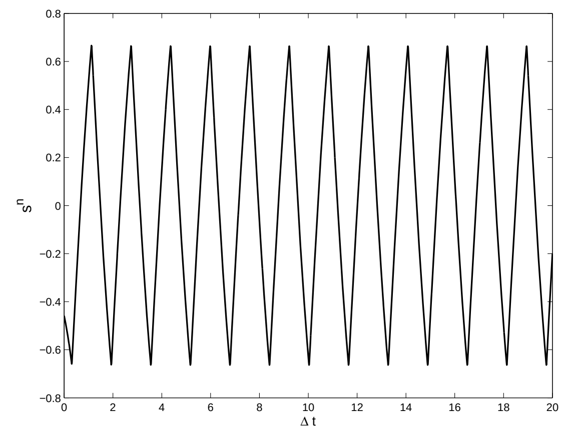
When $\epsilon = 0$, *this singularly perturbed system as in Eq.* (3.217) *yields the following semi-explicit DAE system:*

$$\begin{aligned} \dot{s} &= -\eta \\ 0 &= s - \frac{\eta^3}{3} + \eta \end{aligned} \tag{3.217}$$

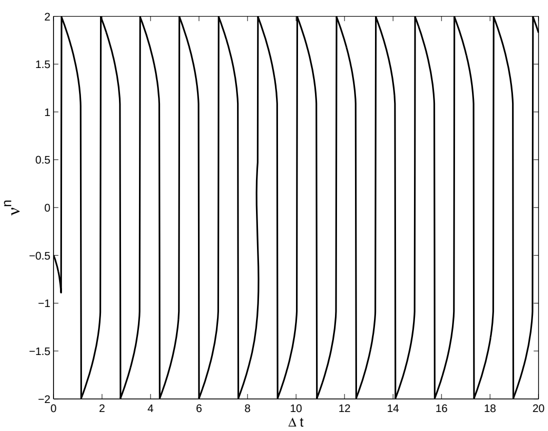
Fig. 3.4 and Fig. 3.5 the numerical results by Algorithm 3.3.1 via the adaptation process with $(\rho_\infty^{\mathrm{min}}, \rho_\infty^{\mathrm{max}}, \rho_\infty^{\mathrm{s}}) = (1, 1, 0)$ *in the V0-based family and* $(\rho_\infty^{\mathrm{min}}, \rho_\infty^{\mathrm{max}}, \rho_\infty^{\mathrm{s}}) = (0, 1, 0)$ *in the U0V0/V0U0-based optimal family, respectively. The simulation is based on selecting a time step size of* $\Delta t = 0.01$ *and* $\eta(0) = 0.5$.



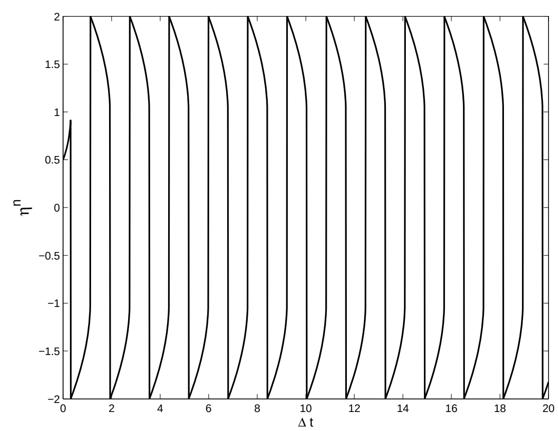
(a) Time Accuracy



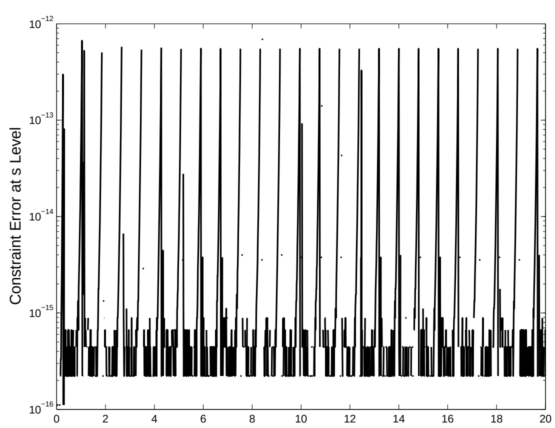
(b) s^n



(c) ν^n

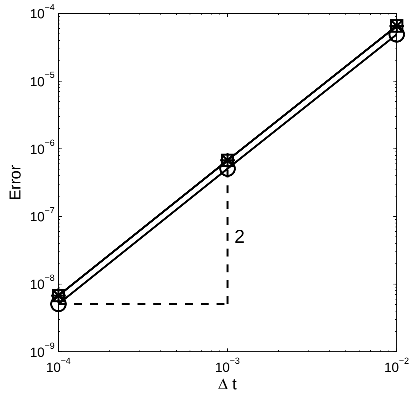


(d) η^n

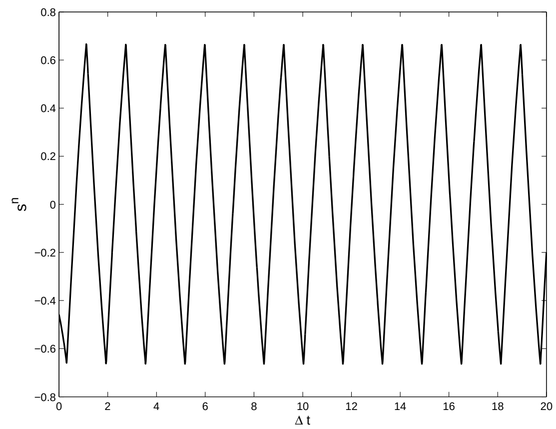


(e) Constraint Error

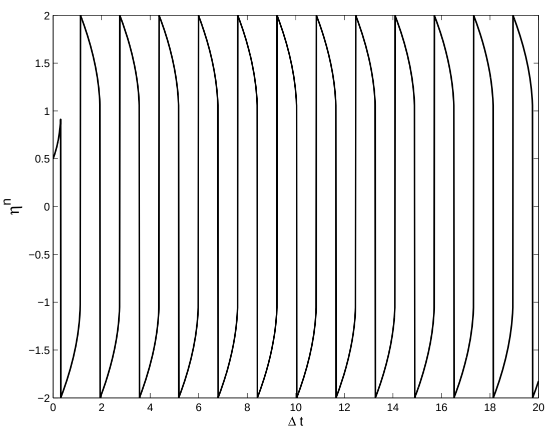
Figure 3.4: Example 3.5.2: MPR-MPA Method



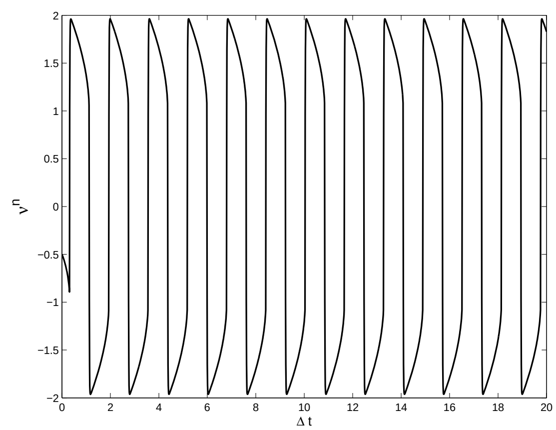
(a) Time Accuracy



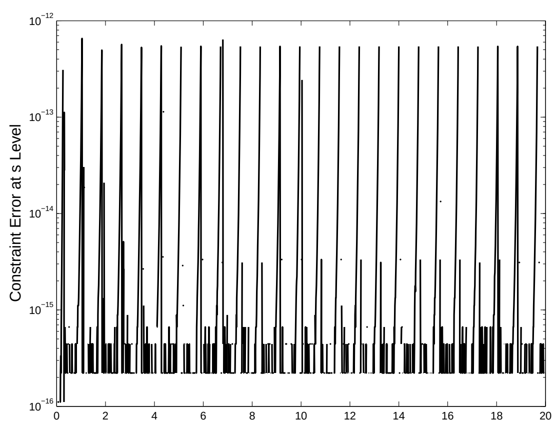
(b) s^n



(c) η^n



(d) ν^n



(e) Constraint Error

Figure 3.5: Example 3.5.2: Gear's Method

Example 3.5.3 (DAE: Spinning top in $\mathbb{E}^3$)

As will be thoroughly discussed in Chapters 5-7, multibody dynamics can be formulated as a system of DAEs. As an example of multibody simulation, consider a spinning top in the Eucledian 3-space. $\mathbb{E}^3$[13] *The governing equations are given as the Newton-Euler equations*[14] *in the form of Eq.* (7.55) *as*

$$\boxed{\begin{aligned} m\,{}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}) &= {}^{\mathcal{B}_0}\mathbf{f}^{\mathrm{ext}} \in \mathbb{R}^3 \\ \left({}^{\mathcal{B}_1}_{\mathbf{C}}\Im\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\omega}}\right) + \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\left({}^{\mathcal{B}_1}_{\mathbf{C}}\Im\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right) &= {}^{\mathcal{B}_1}_{\mathbf{C}}\mathcal{T}^{\mathrm{ext}} \in \mathbb{R}^3 \end{aligned}} \tag{3.218}$$

where m and ${}^{\mathcal{B}_1}_{\mathbf{C}}\Im$ are the mass of the top and moment of inertia about the point of center of mass $\mathbf{C} \in \mathbb{E}^3$, respectively; ${}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}$ is the angular velocity vector of the body-fixed frame $\mathcal{B}_1$ with respect to the reference frame $\mathcal{B}_0$ in the component form in terms of the body-fixed frame $\mathcal{B}_1$; ${}^{\mathcal{B}_0}\mathbf{f}^{\mathrm{ext}}$ denotes the external force vector in the component form with respect to $\mathcal{B}_0$; and ${}^{\mathcal{B}_1}_{\mathbf{C}}\mathcal{T}^{\mathrm{ext}}$ denotes the external torque vector in the component form with respect to $\mathcal{B}_1$. Fig. 3.6 illustrates the initial configuration of the top. The external force and torque vectors consist of two parts:

$$\begin{aligned} {}^{\mathcal{B}_0}\mathbf{f}^{\mathrm{ext}} &= {}^{\mathcal{B}_0}\mathbf{f}^{\mathrm{appl}} + {}^{\mathcal{B}_0}\mathbf{f}^{\mathrm{c}} \\ {}^{\mathcal{B}_1}_{\mathbf{C}}\mathcal{T}^{\mathrm{ext}} &= {}^{\mathcal{B}_1}_{\mathbf{C}}\mathcal{T}^{\mathrm{appl}} + {}^{\mathcal{B}_1}_{\mathbf{C}}\mathcal{T}^{\mathrm{c}} \end{aligned} \tag{3.219}$$

where ${}^{\mathcal{B}_0}\mathbf{f}^{\mathrm{appl}} = [0,0,-mg]^T = [0,0,-9.81m]^T$ and ${}^{\mathcal{B}_1}_{\mathbf{C}}\mathcal{T}^{\mathrm{appl}}$ are the applied force and torque vectors, respectively; and ${}^{\mathcal{B}_0}\mathbf{f}^{\mathrm{c}}$ and ${}^{\mathcal{B}_1}_{\mathbf{C}}\mathcal{T}^{\mathrm{c}}$ are the constraint force and torque vectors, respectively. As discussed carefully in chapter 7, the constraint force and torque vectors can be expressed with the Lagrange multipliers.

Assume the tip of the top $\mathbf{S} \in \mathbb{E}^3$ always coincides with the origin $\mathbf{O}$ of $\mathcal{B}_0$; therein,

---

[13] *See section A.1 in appendix*

[14] ***Refer to Chapter 7 for the notations used in this example and more detailed explanations of the derivations of the Newton-Euler equations.***

the geometric constraint equation is given as

$$\mathbf{\Phi} := {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{C}) + {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\,{}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{C},\mathbf{S}) \tag{3.220}$$

Hence, the constraint equations at the velocity and acceleration levels are obtained by differentiating Eq. (3.220). *It should be noted that the angular velocity vector* ${}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}$ *is holonomic; hence, we need to obtain the Euler angle vector* $\mathbf{\Theta}_{\mathrm{E}} := [\phi,\theta,\psi]^T$ *(see Sec. 5.2 in Chapter 5) from:*

$$\dot{\mathbf{\Theta}}_{\mathrm{E}} = \begin{bmatrix} \sin(\psi)/\sin(\theta) & \cos(\psi)/\sin(\theta) & 0 \\ \cos(\psi) & -\sin(\psi) & 0 \\ -\sin(\psi)\cos(\theta)/\sin(\theta) & -\cos(\psi)\cos(\theta)/\sin(\theta) & 1 \end{bmatrix} {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega} \tag{3.221}$$

Fig. 3.7 - Fig. 3.14 show the numerical results of the spinning top in the index-1 formulation and the Baumgarte stabilized index-1 formulation (in the Hamiltonian formalism) by Algorithm 3.3.1 via the adaptation process with $(\rho_\infty^{\min},\rho_\infty^{\max},\rho_\infty^{s}) = (0,1,0)$ *in the U0V0/V0U0-based optimal family. The simulation is based on the time step size used of* $\Delta t = 0.01$ *and the tolerance for the quasi-Newton iteration is* 10^{-5}. *The Baumgarte coefficients employed for the simulation are:* $\alpha = 1/\Delta t$ *and* $\beta = \sqrt{2}/\Delta t$. *The second-order time accuracies in configuration* ($\circ$)*, velocity* ($\square$)*, acceleration* ($\triangle$)*, and Lagrange multiplier* ($*$) *are achieved for both formulations; see Fig. 3.7.* [15] *As can be from the comparisons among Fig. 3.10- Fig. 3.14, the stabilized index-1 formulation remedies the violations of the constraint equations within time step at the configuration (position) and velocity levels well. The initial data for the Euler angles are:* $\mathbf{\Theta}_{\mathrm{E}}(0) = [\phi,\theta,\psi]^T(0) = [0,\pi/8,0]^T$ *rad, and* $\dot{\mathbf{\Theta}}_{\mathrm{E}}(0) = [\dot\phi,\dot\theta,\dot\psi]^T(0) = [2\pi,0,(1200/60)2\pi]^T$ *(i.e., 1200 rpm about z-axis).*

[15] *Note that this implies the second-order time accuracies in all kinematic and algebraic unknowns are achieved for the algorithms in any formulation are achieved.*

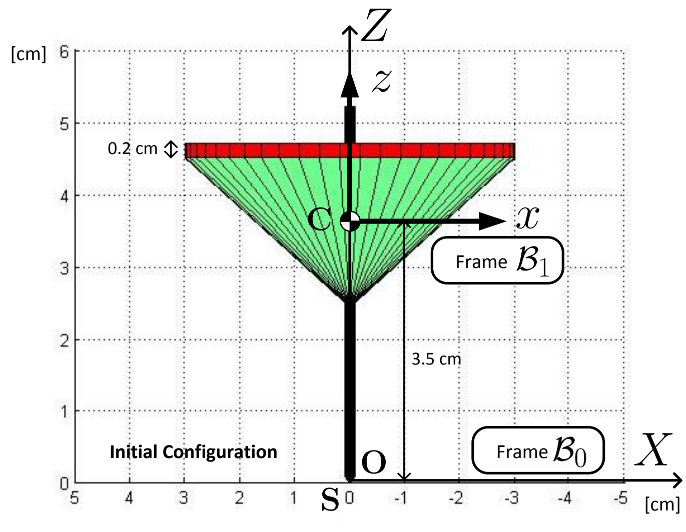
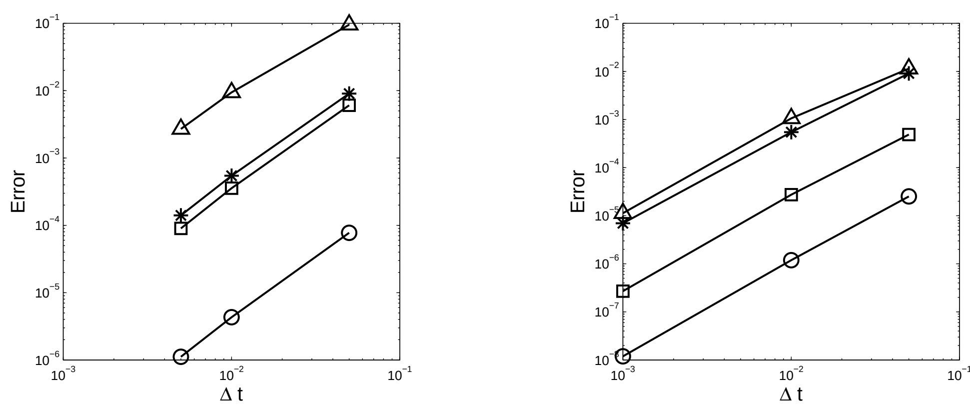


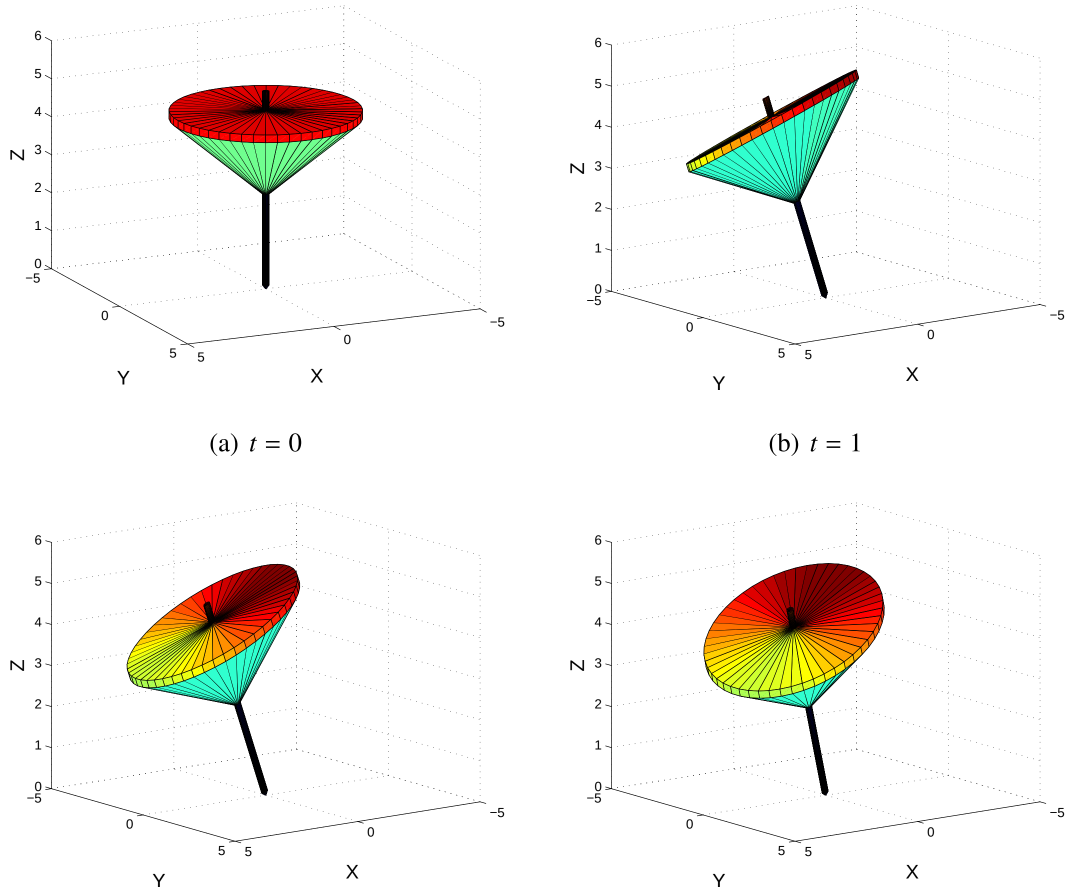
Figure 3.6: Example 3.5.3: Initial Configuration of the Top



(a) $t = 0$

(b) $t = 1$

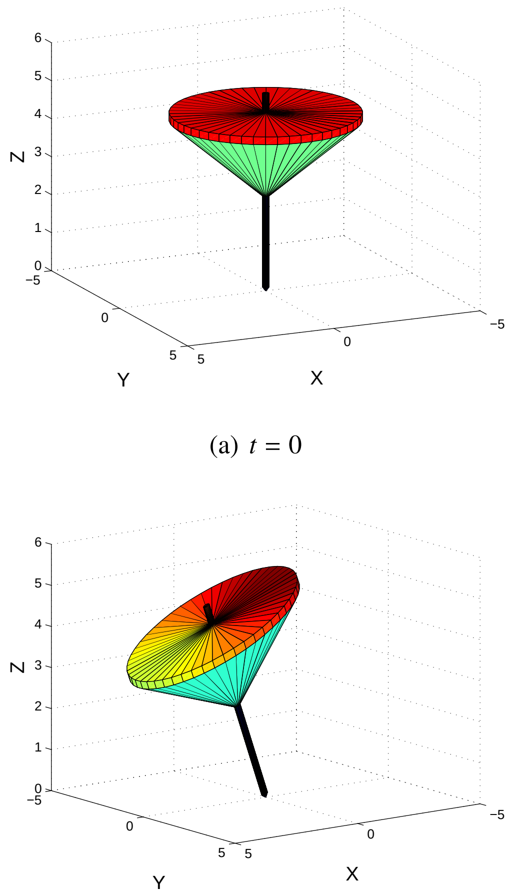
Figure 3.7: Example 3.5.3: Time Accuracy Plots for the Index-1 Formulation and the Stabilized Index-1 Formulation



(a) $t = 0$ (b) $t = 1$

(c) $t = 2$ (d) $t = 3$

Figure 3.8: Example 3.5.3: Configuration at Every One Second in the Index-1 Formulation



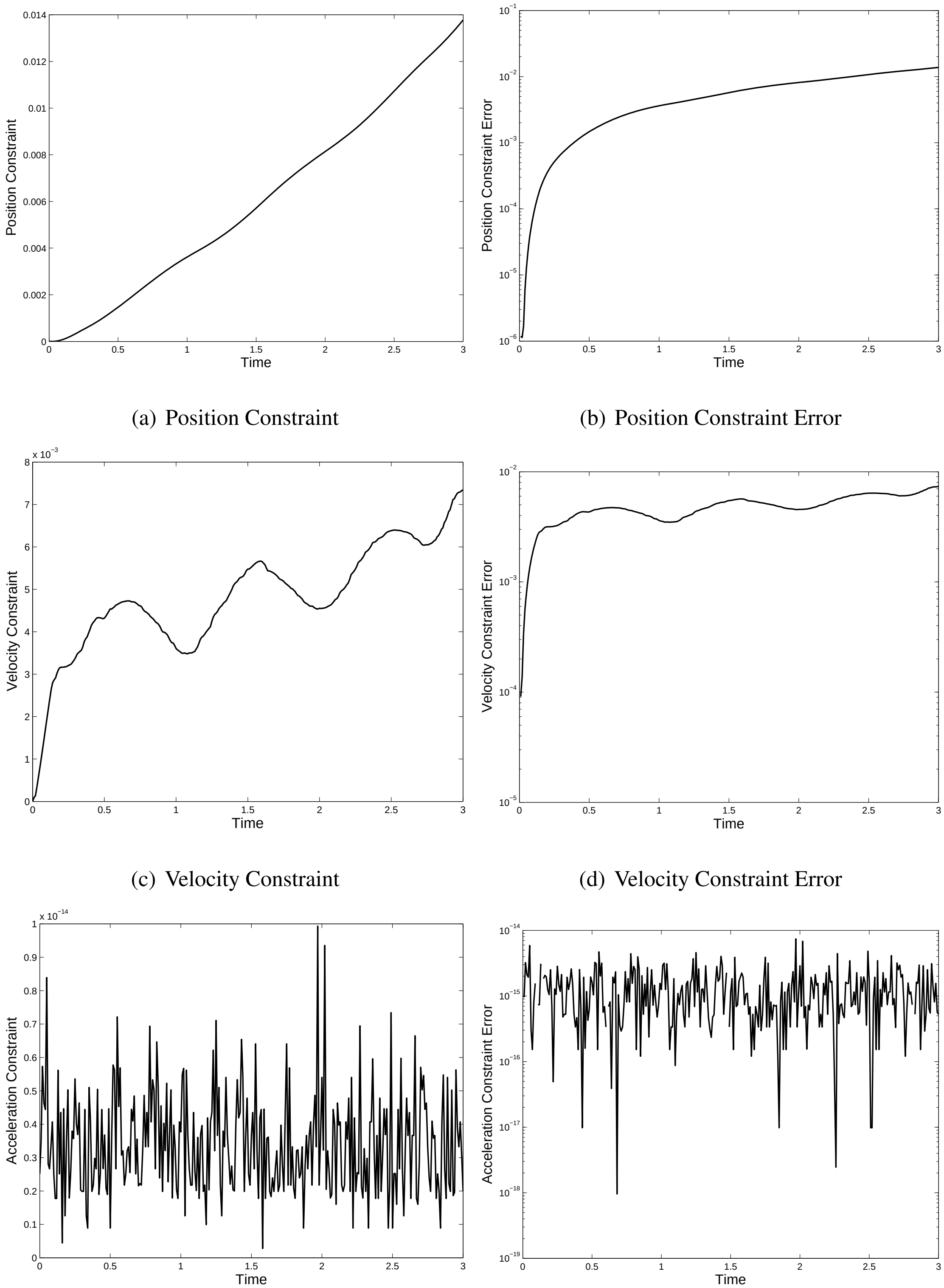
(a) $t = 0$

(b) $t = 1$

(c) $t = 2$

(d) $t = 3$

Figure 3.9: Example 3.5.3: Configuration at Every One Second in the Stabilized Index-1 Formulation



(a) Position Constraint

(b) Position Constraint Error

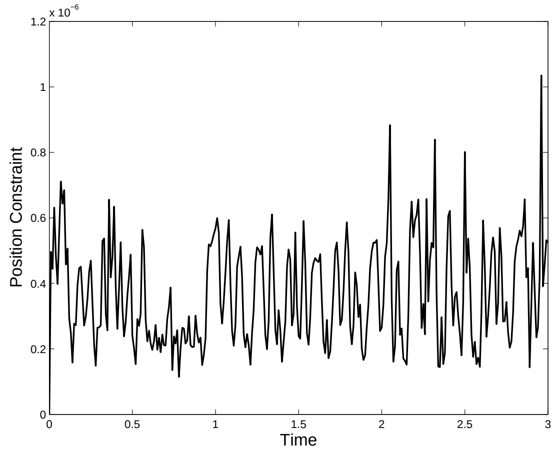
(c) Velocity Constraint

(d) Velocity Constraint Error

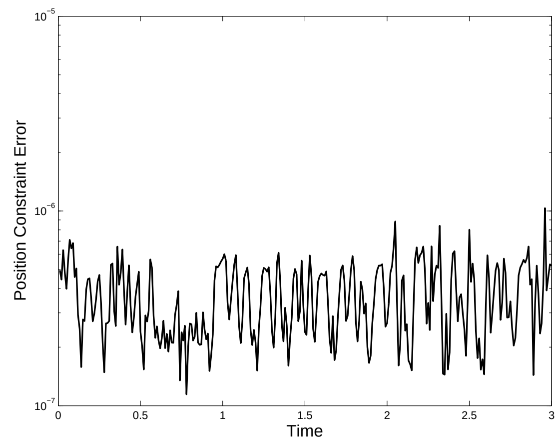
(e) Acceleration Constraint

(f) Acceleration Constraint Error

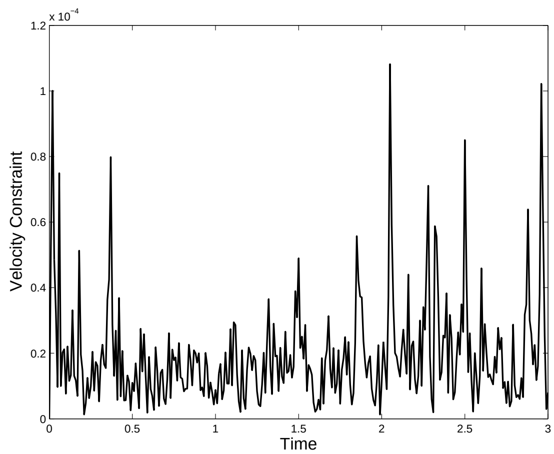
Figure 3.10: Example 3.5.3: Constraint Satisfactions for the Index-1 Formulation



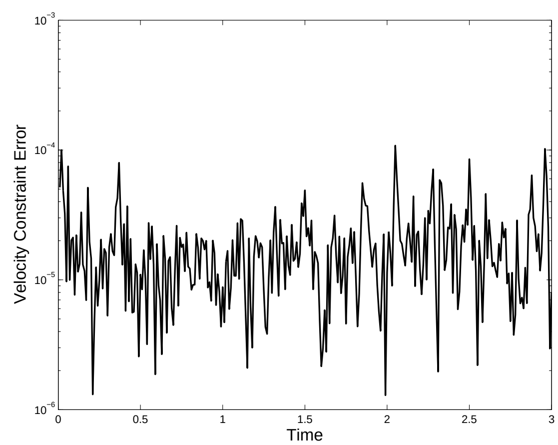
(a) Position Constraint



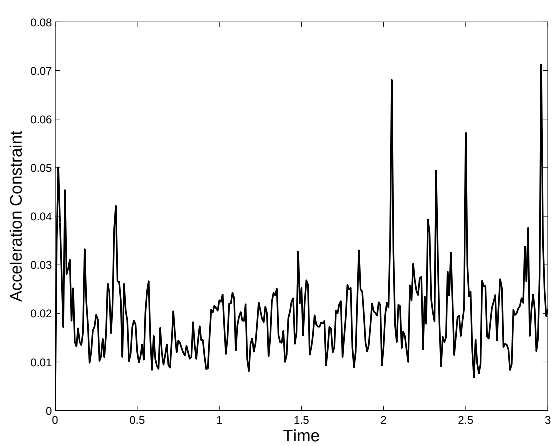
(b) Position Constraint Error



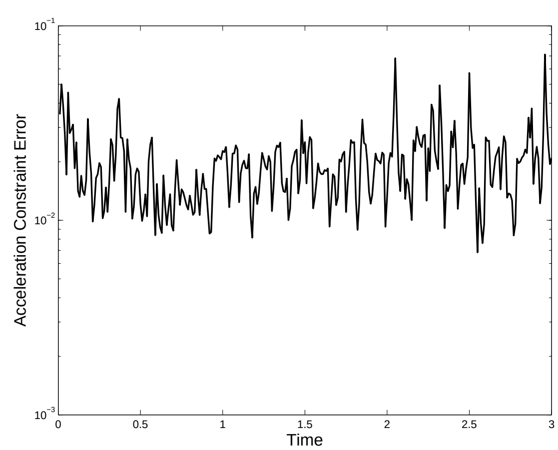
(c) Velocity Constraint



(d) Velocity Constraint Error

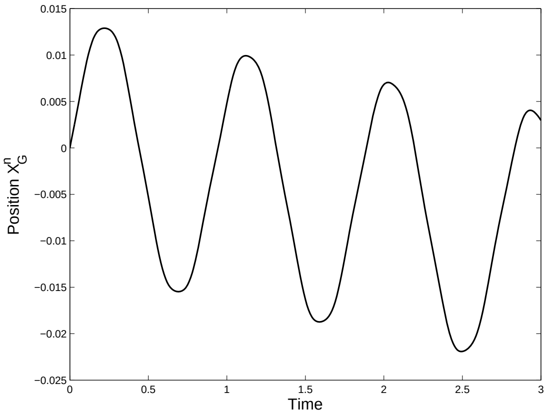


(e) Acceleration Constraint

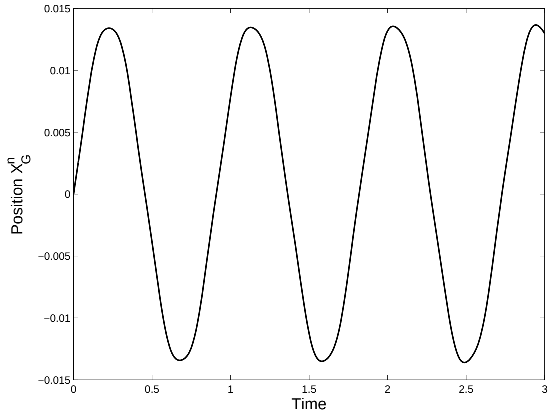


(f) Acceleration Constraint Error

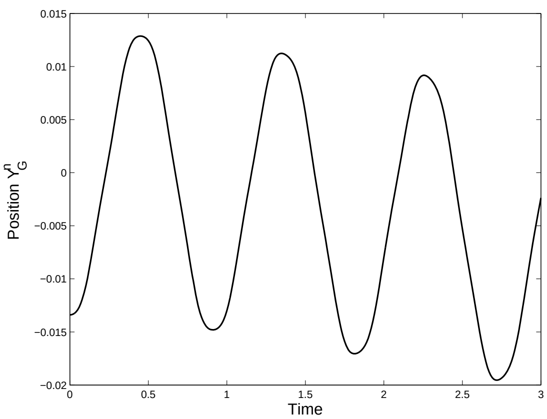
Figure 3.11: Example 3.5.3: Constraint Satisfactions for the Stabilized Index-1 Formulation



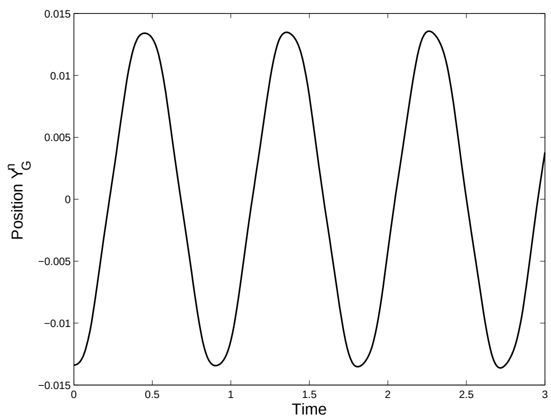
(a) X_G^n: Index 1



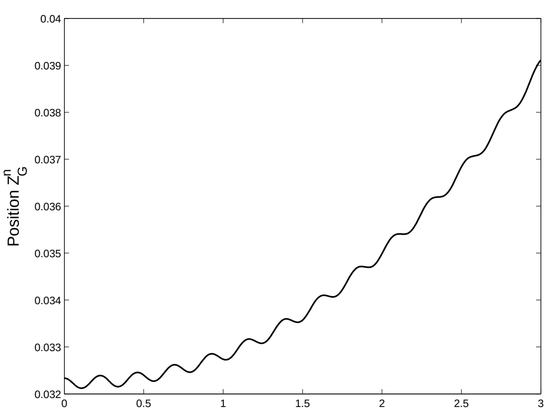
(b) X_G^n: Stabilized Index 1



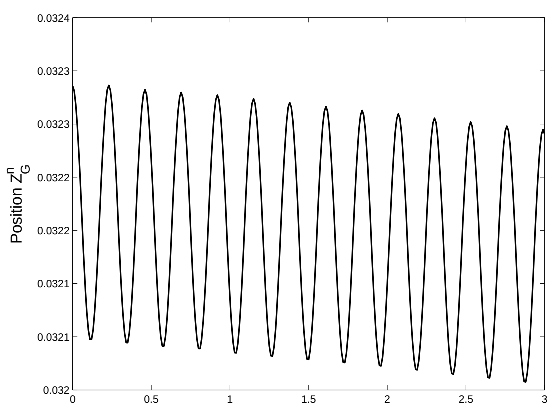
(c) Y_G^n: Index 1



(d) Y_G^n: Stabilized Index 1

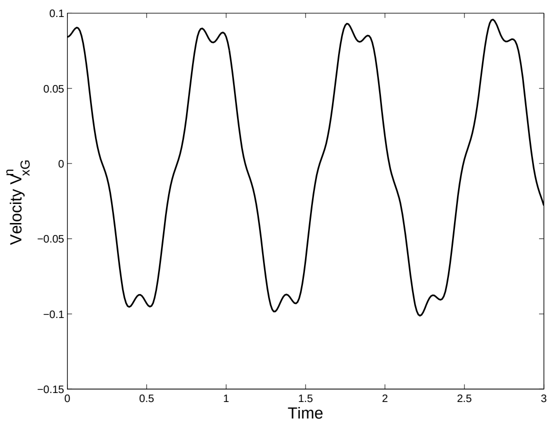


(e) Z_G^n: Index 1

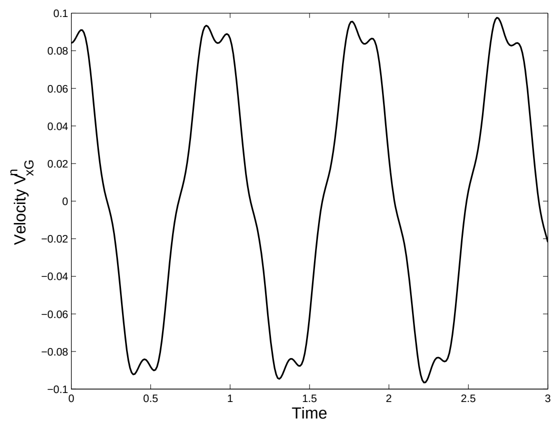


(f) Z_G^n: Stabilized Index 1

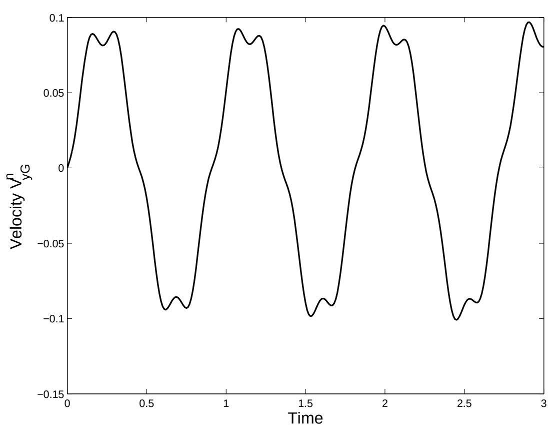
Figure 3.12: Example 3.5.3: Position Data of the Center of Gravity for the Index-1 and Stabilized Index-1 Formulations



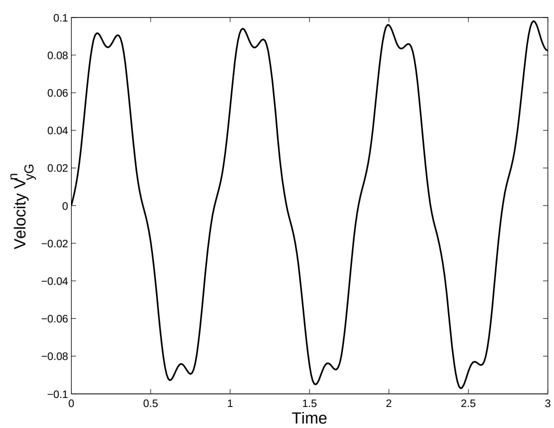
(a) V^n_{Gx}: Index 1



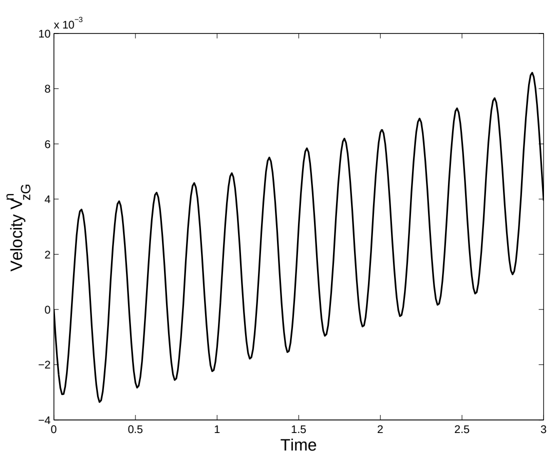
(b) V^n_{Gx}: Stabilized Index 1



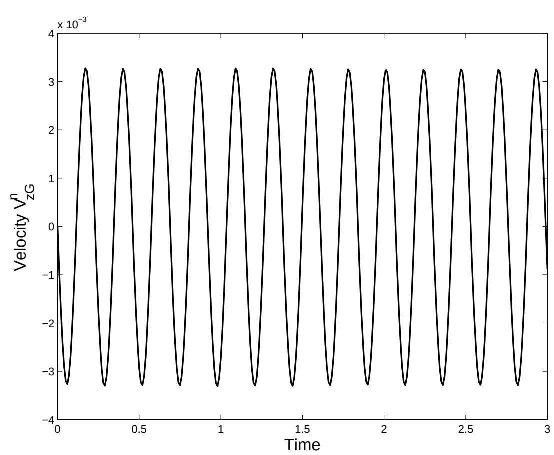
(c) V^n_{Gy}: Index 1



(d) V^n_{Gy}: Stabilized Index 1

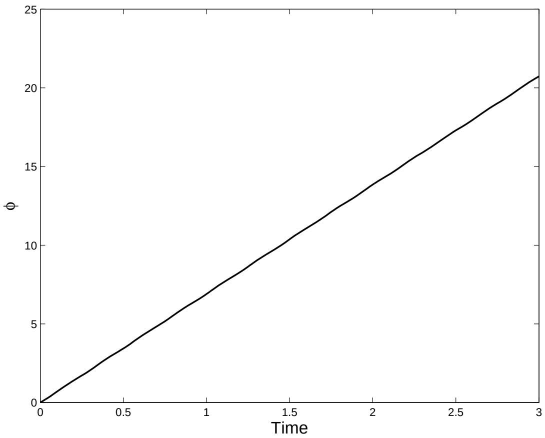


(e) V^n_{Gz}: Index 1

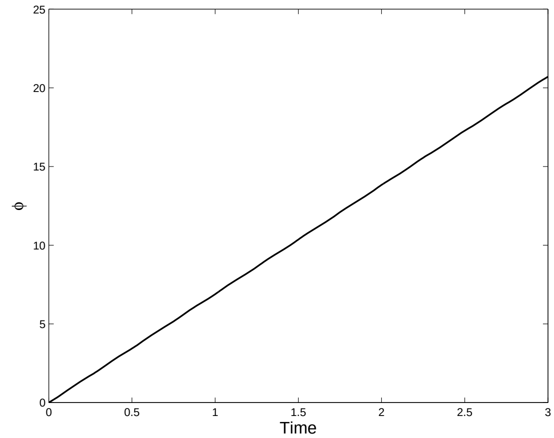


(f) V^n_{Gz}: Stabilized Index 1

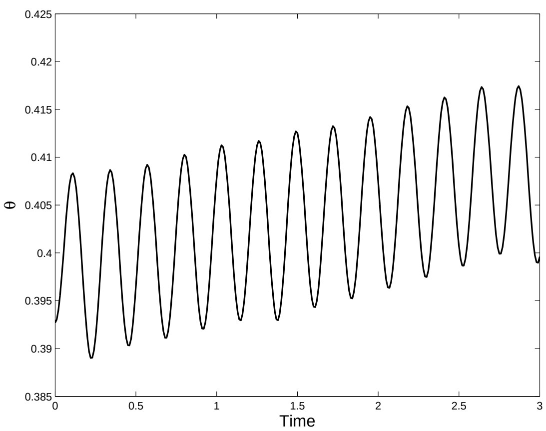
Figure 3.13: Example 3.5.3: Velocity Data of the Center of Gravity for the Index-1 and Stabilized Index-1 Formulations



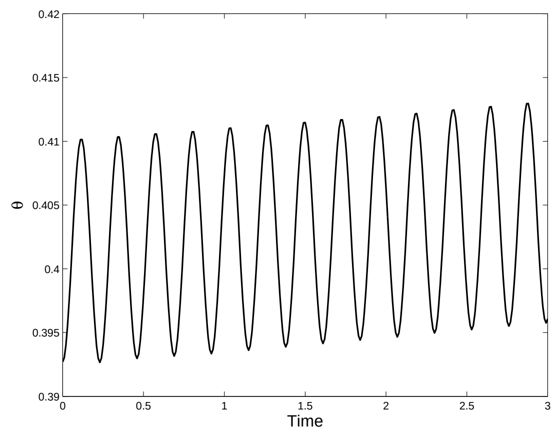
(a) ϕ^n: Index 1



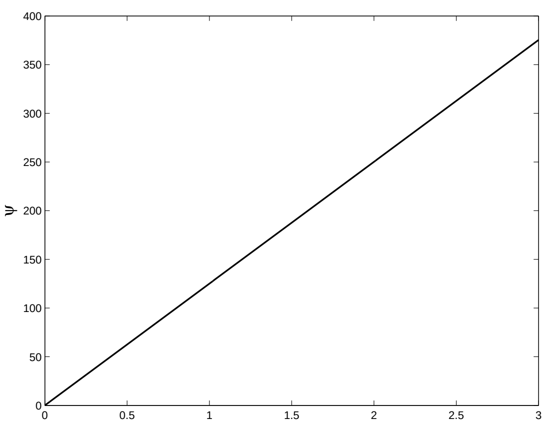
(b) ϕ^n: Stabilized Index 1



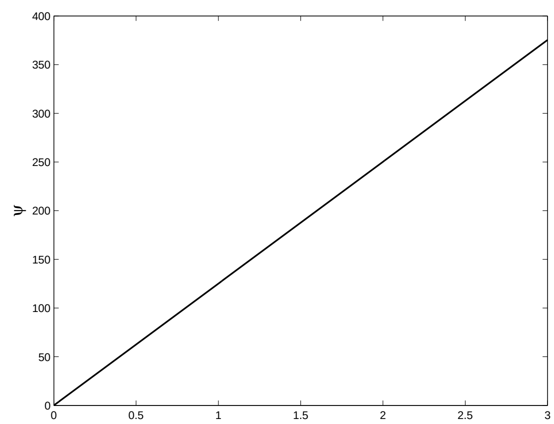
(c) θ^n: Index 1



(d) θ^n: Stabilized Index 1



(e) ψ^n: Index 1



(f) ψ^n: Stabilized Index 1

Figure 3.14: Example 3.5.3: Euler Angle Data for the Index-1 and Stabilized Index-1 Formulations

Chapter 4

Subdomain Time Integrators: A DAE Approach

4.1 Introduction

The use of different time integration algorithms within the *i*Integrators in different subdomains without reducing the time accuracy of order two in all the kinmatic and algebraic unknowns is of main interest in this chapter. Similar to some recent efforts in this area, for example, the GC method [55], PH method [56], and KN method [57], we employ the dual Schur domain decomposition approach [58].

4.2 Equations of Motion for a System of Multiple Subdomains

Consider a domain of interest Ω; and suppose that it can be divided into n_{dom} numbers of subdomains, Ω_ℓ (for $\ell = 1, 2, \cdots, n_{\mathrm{dom}}$), i.e., $\Omega = \bigcup_{\ell=1}^{n_{\mathrm{dom}}} \Omega_\ell$, and each subdomain is not allowed to overlap each other: $\Omega_i \cap \Omega_j = \emptyset$. The equation of motion for subdomain Ω_ℓ reads[1] : For $\ell = 1, 2, \cdots, n_{\mathrm{dom}}$,

$$\mathbf{M}_\ell \ddot{\mathbf{q}}_\ell = \mathbf{Q}_\ell^{\mathrm{int}}(\mathbf{q}_\ell) + \mathbf{Q}_\ell^{\mathrm{appl}}(\mathbf{q}_\ell, \dot{\mathbf{q}}_\ell, t) + \mathbf{G}_\ell^T \boldsymbol{\lambda}(t) \tag{4.1a}$$

$$\mathbf{0} = \sum_{\ell=1}^{n_{\mathrm{dom}}} \mathbf{G}_\ell \mathbf{q}_\ell \tag{4.1b}$$

($\forall t \in \mathbb{I} := [t_0, t_L] \subset \mathbb{R}$) together with given (consistent) initial conditions, where $\mathbf{q}_\ell(t) : \mathbb{I} \to \mathbb{R}^{n_\ell}$, $\dot{\mathbf{q}}_\ell(t) := d\mathbf{q}_\ell/dt : \mathbb{I} \to \mathbb{R}^{n_\ell}$, and $\ddot{\mathbf{q}}_\ell(t) := d^2\mathbf{q}_\ell/dt^2 : \mathbb{I} \to \mathbb{R}^{n_\ell}$ are the configuration, velocity, and acceleration vectors of the ℓ^{th}-subdomain, respectively; $\mathbf{M}_\ell \in \mathbb{R}^{n_\ell \times n_\ell}$ is the symmetric, positive-definite mass matrix of the ℓ^{th}-subdomain; and $\mathbf{Q}_\ell^{\mathrm{int}}(\mathbf{q}_\ell) \in \mathbb{R}^{n_\ell}$ and $\mathbf{Q}_\ell^{\mathrm{appl}}(\mathbf{q}_\ell, \dot{\mathbf{q}}_\ell, t) \in \mathbb{R}^{n_\ell}$ are the generalized internal and applied force vectors of the ℓ^{th}-subdomain, respectively. The algebraic variable vector $\boldsymbol{\lambda}(t) : \mathbb{I} \to \mathbb{R}^{n_{\mathrm{c}}}$, which plays a role as the Lagrange multiplier, is introduced in order to enforce the constraint equation (4.1b). Note that $\boldsymbol{\lambda}$ is defined not in the subdomain level, but in the system level. Matrix $\mathbf{G}_\ell \in \mathbb{R}^{n_{\mathrm{c}} \times n_\ell}$ is a signed Boolean matrix with entries either -1, 0, or $+1$, and it is defined based on the subdomain interface conditions among Ω_ℓ. The differential index of the DAE system given in Eq. (4.1) is three, and it is called the ***displacement-continuity*** formulation since the constraint equation at the configuration (displacement) level, Eq. (4.1b), enforces the displacement continuity along the interface among the subdomains in the system. Similar to the GC method [55], PH method

[1] No sum on ℓ in Eq. (4.1a)

[56], and KN method [57], we adopt the Index-2 formulation with the constraint equation at the velocity level, i.e.,

$$\mathbf{M}_\ell \ddot{\mathbf{q}}_\ell = \mathbf{Q}_\ell^{\text{int}}(\mathbf{q}_\ell) + \mathbf{Q}_\ell^{\text{appl}}(\mathbf{q}_\ell, \dot{\mathbf{q}}_\ell, t) + \mathbf{G}_\ell^T \lambda(t) \tag{4.2a}$$

$$\mathbf{0} = \sum_{\ell=1}^{n_{\text{dom}}} \mathbf{G}_\ell \dot{\mathbf{q}}_\ell \tag{4.2b}$$

and develop and analyze the time integrators for multiple subdomains since the index-3 DAE formulation or index-1 formulation, also called the ***acceleration-continuity*** formulation in this application, tend to suffer from severe numerical difficulties (see previous chapter for details). This DAE system is refered to as the ***velocity-continuity*** formulation since Eq. (4.2b) enforces the velocity continuity along the interface among the subdomains in the system.

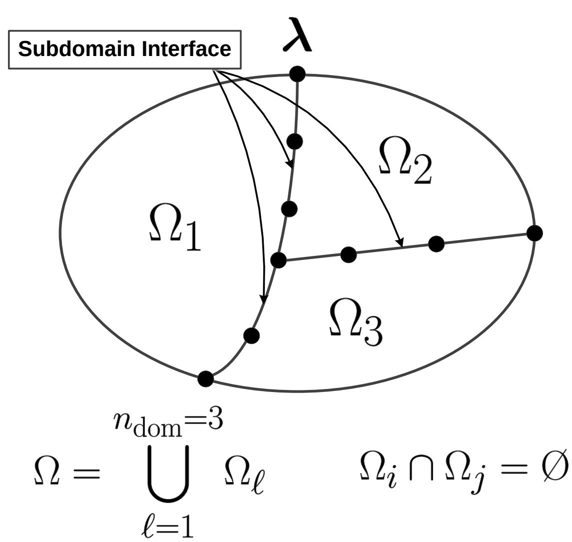


Figure 4.1: $n_{\text{dom}} = 3$

4.3 Application of the *i*Integrators for the Equations of Motion for a System of Multiple Subdomains

In this section, we discretize the DAE system given in Eq. (4.2) in time by dividing the time domain of interest, $\mathbb{I} = [t_0, t_L] \subset \mathbb{R}$, into n_{steps} sub-intervals, i.e., $\mathbb{I} = [t_0, t_L] = \bigcup_{n=0}^{n_{\text{steps}}-1} [t_n, t_{n+1}]$, with the *i*Integrators, following the idea of the KN method [57], originally employed with the Newmark family of algorithms [11].

Let Δt and Δt_ℓ be the ***system time step size*** and the ***subdomain time step size*** for Ω_ℓ, respectively, and define the ratio as $\tau_\ell := \Delta t / \Delta t_\ell$ with the assumption of $\Delta t \geq \Delta t_\ell$ for $\ell = 1, 2, \cdots, n_{\text{dom}}$. The system and subdomain time step sizes are defined as

$$\Delta t := t_{n+1} - t_n \quad \text{and} \quad \Delta t_\ell := t_{n+\frac{m+1}{\tau_\ell}} - t_{n+\frac{m}{\tau_\ell}} \tag{4.3}$$

respectively, for $n \in \{0, 1, 2, \cdots, n_{\text{steps}} - 1\}$ and $m \in \{0, 1, 2, \cdots, \tau_\ell - 1\}$.

Algorithm 4.3.1 (Subdomain GS4-2 Family of algorithms)

Given (consistent) initial conditions $(\mathbf{q}, \dot{\mathbf{q}}, \ddot{\mathbf{q}}, \lambda)(t_0) = (\mathbf{q}^0, \mathbf{v}^0, \mathbf{a}^0, \lambda^0)$. *Find the solutions for* $n \in \{1, 2, \cdots, n_{\text{steps}} - 1\}$ *and* $m \in \{1, 2, \cdots, \tau_\ell - 1\}$ *from:*

$$\begin{aligned}
\mathbf{M}_\ell \tilde{\mathbf{a}}_\ell^{(n,m)} &= \mathbf{Q}_\ell^{\text{int}}(\tilde{\mathbf{q}}_\ell^{(n,m)}) + \mathbf{Q}_\ell^{\text{appl}}(\tilde{\mathbf{q}}_\ell^{(n,m)}, \tilde{\mathbf{v}}_\ell^{(n,m)}, t_{n+\frac{m+W_1}{\tau_\ell}}) + \mathbf{G}_\ell^T \tilde{\boldsymbol{\lambda}}^{(n,m)} && \text{(4.4a)} \\
\mathbf{0} &= \sum_{\ell=1}^{n_{\text{dom}}} \mathbf{G}_\ell \mathbf{v}_\ell^{n+1} && \text{(4.4b)}
\end{aligned}$$

where

$$
\begin{aligned}
t_{n+\frac{m+W_1}{\tau_\ell}} &:= t_n + \left(\frac{m+W_1}{\tau_\ell}\right)\Delta t = t_0 + n\Delta t + (m+W_1)\Delta t_\ell && \text{(4.4c)}\\
\tilde{\lambda}^{(n,m)} &:= \lambda^n + \left(\frac{m+W_1}{\tau_\ell}\right)\left(\lambda^{n+1} - \lambda^n\right) && \text{(4.4d)}\\
\tilde{\mathbf{a}}_\ell^{(n,m)} &:= \mathbf{a}_\ell^{n+\frac{m}{\tau_\ell}} + W_1\Lambda_6\Delta\mathbf{a}_\ell^{(n,m)} && \text{(4.4e)}\\
\tilde{\mathbf{v}}_\ell^{(n,m)} &:= \mathbf{v}_\ell^{n+\frac{m}{\tau_\ell}} + \Delta t W_1\Lambda_4\mathbf{a}_\ell^{n+\frac{m}{\tau_\ell}} + \Delta t W_2\Lambda_5\Delta\mathbf{a}_\ell^{(n,m)} && \text{(4.4f)}\\
\tilde{\mathbf{q}}_\ell^{(n,m)} &:= \mathbf{q}_\ell^{n+\frac{m}{\tau_\ell}} + \Delta t W_1\Lambda_1\mathbf{v}_\ell^{n+\frac{m}{\tau_\ell}} + \Delta t^2 W_2\Lambda_2\mathbf{a}_\ell^{n+\frac{m}{\tau_\ell}} + \Delta t^2 W_3\Lambda_3\Delta\mathbf{a}_\ell^{(n,m)} && \text{(4.4g)}
\end{aligned}
$$

And the associated updates:

$$
\begin{aligned}
\mathbf{q}_\ell^{n+\frac{m+1}{\tau_\ell}} &= \mathbf{q}_\ell^{n+\frac{m}{\tau_\ell}} + \Delta t\lambda_1\mathbf{v}_\ell^{n+\frac{m}{\tau_\ell}} + \Delta t^2\lambda_2\mathbf{a}_\ell^{n+\frac{m}{\tau_\ell}} + \Delta t^2\lambda_3\Delta\mathbf{a}_\ell^{(n,m)} && \text{(4.4h)}\\
\mathbf{v}_\ell^{n+\frac{m+1}{\tau_\ell}} &= \mathbf{v}_\ell^{n+\frac{m}{\tau_\ell}} + \Delta t\lambda_4\mathbf{a}_\ell^{n+\frac{m}{\tau_\ell}} + \Delta t\lambda_5\Delta\mathbf{a}_\ell^{(n,m)} && \text{(4.4i)}\\
\mathbf{a}_\ell^{n+\frac{m+1}{\tau_\ell}} &= \mathbf{a}_\ell^{n+\frac{m}{\tau_\ell}} + \Delta\mathbf{a}_\ell^{(n,m)} && \text{(4.4j)}
\end{aligned}
$$

The algorithmic scalar parameters which characterize the U0- and V0-based families are defined as follows:

$$
\begin{aligned}
W_1 &= \frac{1}{1+\rho_\infty^{\mathrm{s}}} \quad , \quad \lambda_1 = \Lambda_1 = \lambda_4 = \Lambda_4 = 1\\
W_2\Lambda_2 &= \frac{1}{2(1+\rho_\infty^{\mathrm{s}})} \quad , \quad \lambda_2 = \frac{1}{2}\\
W_3\Lambda_3 &= \frac{1}{(1+\rho_\infty^{\min})(1+\rho_\infty^{\max})(1+\rho_\infty^{\mathrm{s}})} \quad , \quad \lambda_3 = \frac{1}{(1+\rho_\infty^{\min})(1+\rho_\infty^{\max})}\\
W_2\Lambda_5 &= \frac{3+\rho_\infty^{\min}+\rho_\infty^{\max}-\rho_\infty^{\min}\rho_\infty^{\max}}{2(1+\rho_\infty^{\min})(1+\rho_\infty^{\max})(1+\rho_\infty^{\mathrm{s}})} \quad , \quad \lambda_5 = \frac{3+\rho_\infty^{\min}+\rho_\infty^{\max}-\rho_\infty^{\min}\rho_\infty^{\max}}{2(1+\rho_\infty^{\min})(1+\rho_\infty^{\max})}\\
W_1\Lambda_6 &= \frac{2+\rho_\infty^{\min}+\rho_\infty^{\max}+\rho_\infty^{\mathrm{s}}-\rho_\infty^{\min}\rho_\infty^{\max}\rho_\infty^{\mathrm{s}}}{(1+\rho_\infty^{\min})(1+\rho_\infty^{\max})(1+\rho_\infty^{\mathrm{s}})}
\end{aligned}
$$

*for the **U0 family-based schemes**, and*

$$
\begin{aligned}
W_1 &= \frac{3+\rho_\infty^{\min}+\rho_\infty^{\max}-\rho_\infty^{\min}\rho_\infty^{\max}}{2(1+\rho_\infty^{\min})(1+\rho_\infty^{\max})} \quad &, \quad \lambda_1 = \Lambda_1 = \lambda_4 = \Lambda_4 = 1 \\
W_2\Lambda_2 &= \frac{1}{(1+\rho_\infty^{\min})(1+\rho_\infty^{\max})} \quad &, \quad \lambda_2 = \frac{1}{2} \\
W_3\Lambda_3 &= \frac{1}{(1+\rho_\infty^{\min})(1+\rho_\infty^{\max})(1+\rho_\infty^{\mathrm{s}})} \quad &, \quad \lambda_3 = \frac{1}{2(1+\rho_\infty^{\mathrm{s}})} \\
W_2\Lambda_5 &= \frac{2}{(1+\rho_\infty^{\min})(1+\rho_\infty^{\max})(1+\rho_\infty^{\mathrm{s}})} \quad &, \quad \lambda_5 = \frac{1}{1+\rho_\infty^{\mathrm{s}}} \\
W_1\Lambda_6 &= \frac{2+\rho_\infty^{\min}+\rho_\infty^{\max}+\rho_\infty^{\mathrm{s}}-\rho_\infty^{\min}\rho_\infty^{\max}\rho_\infty^{\mathrm{s}}}{(1+\rho_\infty^{\min})(1+\rho_\infty^{\max})(1+\rho_\infty^{\mathrm{s}})}
\end{aligned}
$$

*for the **V0 family-based schemes**.*

Remark 4.3.1

1. *As can be seen from Eq.* (4.4d), *the Lagrange multipliers are approximated linearly in time withing a* system *time step; whilst, the acceleration, velocity, and configuration vectors are approximated in linear, quadratic, and cubic senses, respectively, in time within a subdomain time step.*

2. *By introducing $\hat{\eta}$, which takes either zero or unity, as introduced in section 2.2.4, the algorithm can be easily switched between the implicit an explicit families.*

3. *In accordance with the **adaptation process** introduced in section 3.5 in chapter 3, we can generate the algorithmic framework that can be applied to first-order DAE systems with multiple subdomains.*

4.3.1 Implementation of Algorithm 4.3.1 in Linear Dynamical Systems

In linear dynamical systems, Eq. (4.2) may be written as

$$\mathbf{M}_\ell \ddot{\mathbf{q}}_\ell + \mathbf{C}_\ell \dot{\mathbf{q}}_\ell + \mathbf{K}_\ell \mathbf{q}_\ell = \mathbf{Q}_\ell(t) + \mathbf{G}_\ell^T \lambda(t) \tag{4.5a}$$

$$\mathbf{0} = \sum_{\ell=1}^{n_{\text{dom}}} \mathbf{G}_\ell \dot{\mathbf{q}}_\ell \tag{4.5b}$$

where $\mathbf{C}_\ell \in \mathbb{R}^{n_\ell \times n_\ell}$ and $\mathbf{K}_\ell \in \mathbb{R}^{n_\ell \times n_\ell}$ are the damping and stiffness matrices for Ω_ℓ, respectively; and $\mathbf{Q}_\ell(t) : \mathbb{I} \to \mathbb{R}^{n_\ell}$ is the generalized time-dependent external force vector for Ω_ℓ.

Eq. (4.5a)**:** Define a set of all kinematic unknowns, i.e., the acceleration, velocity, and configuration vectors, for Ω_ℓ for its subdomain time step as

$$\mathbf{X}_\ell^{n+\frac{m}{\tau_\ell}} := \begin{bmatrix} \mathbf{a}_\ell^{n+\frac{m}{\tau_\ell}} \\ \mathbf{v}_\ell^{n+\frac{m}{\tau_\ell}} \\ \mathbf{q}_\ell^{n+\frac{m}{\tau_\ell}} \end{bmatrix} \in \mathbb{R}^{3n_\ell} \tag{4.6}$$

Then, the discretized form of Eq. (4.5a) in time in the sense of Algorithm 4.3.1 may be written in the following compact form:

$$\boxed{\mathbb{L}_\ell \mathbf{X}_\ell^{n+\frac{m+1}{\tau_\ell}} - \left(\frac{m+W_1}{\tau_\ell}\right)\left(\hat{\mathbb{G}}_\ell^{(1)}\right)^T \left(\boldsymbol{\lambda}^{n+1} - \boldsymbol{\lambda}^n\right) = \mathbb{Q}_\ell^{n+\frac{m+W_1}{\tau_\ell}} + \left(\hat{\mathbb{G}}_\ell^{(1)}\right)^T \boldsymbol{\lambda}^n + \mathbb{R}_\ell \mathbf{X}_\ell^{n+\frac{m}{\tau_\ell}}} \tag{4.7}$$

where

$$\mathbb{L}_\ell := \begin{bmatrix} \mathbb{L}_\ell^* & \mathbf{O}_{n_\ell \times n_\ell} & \mathbf{O}_{n_\ell \times n_\ell} \\ -\Delta t_\ell \lambda_5 \mathbf{I}_{n_\ell \times n_\ell} & \mathbf{I}_{n_\ell \times n_\ell} & \mathbf{O}_{n_\ell \times n_\ell} \\ -\Delta t_\ell^2 \lambda_3 \mathbf{I}_{n_\ell \times n_\ell} & \mathbf{O}_{n_\ell \times n_\ell} & \mathbf{I}_{n_\ell \times n_\ell} \end{bmatrix} \in \mathbb{R}^{3n_\ell \times 3n_\ell} \tag{4.8a}$$

with

$$\mathbb{L}_\ell^* := W_1 \Lambda_6 \mathbf{M}_\ell + \Delta t_\ell W_2 \Lambda_5 \mathbf{C}_\ell + \Delta t_\ell^2 W_3 \Lambda_3 \mathbf{K}_\ell \in \mathbb{R}^{n_\ell \times n_\ell} \tag{4.8b}$$

$$\mathbb{R}_\ell := \begin{bmatrix} \mathbb{R}_\ell^* & -(1+\Delta t_\ell W_1 \Lambda_1)\mathbf{I}_{n_\ell \times n_\ell} & -\mathbf{I}_{n_\ell \times n_\ell} \\ \Delta t_\ell(\lambda 4 - \lambda 5)\mathbf{I}_{n_\ell \times n_\ell} & \mathbf{I}_{n_\ell \times n_\ell} & \mathbf{O}_{n_\ell \times n_\ell} \\ \Delta t_\ell^2(\lambda 2 - \lambda 3)\mathbf{I}_{n_\ell \times n_\ell} & \Delta t_\ell \lambda_1 \mathbf{I}_{n_\ell \times n_\ell} & \mathbf{I}_{n_\ell \times n_\ell} \end{bmatrix} \in \mathbb{R}^{3n_\ell \times 3n_\ell} \tag{4.9a}$$

with

$$\mathbb{R}_\ell^* := (W_1\Lambda_6 - 1)\mathbf{M}_\ell + \Delta t_\ell(W_2\Lambda_5 - W_1\Lambda_4)\mathbf{C}_\ell + \Delta t_\ell^2(W_3\Lambda_3 - W_2\Lambda_2)\mathbf{K}_\ell \in \mathbb{R}^{n_\ell \times n_\ell} \tag{4.9b}$$

$$\mathbb{Q}_\ell^{n+\frac{m+W_1}{\tau_\ell}} := \begin{bmatrix} \mathbf{Q}_\ell(t_{n+\frac{m+W_1}{\tau_\ell}}) \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} \in \mathbb{R}^{3n_\ell} \tag{4.10}$$

and

$$\hat{\mathbb{G}}_\ell^{(1)} := \begin{bmatrix} \mathbf{G}_\ell & \mathbf{O}_{n_c \times n_\ell} & \mathbf{O}_{n_c \times n_\ell} \end{bmatrix} \in \mathbb{R}^{n_c \times 3n_\ell} \tag{4.11}$$

Eq. (4.5b)**:** Define a set of all kinematic unknowns, i.e., the acceleration, velocity, and configuration vectors, for Ω_ℓ *over* its subdomain time step and a set of all kinematic unknowns of all subdomains in the system over a system time step as

$$\mathbb{X}_\ell^{(n+1)} := \begin{bmatrix} \mathbf{X}_\ell^{n+\frac{1}{\tau_\ell}} \\ \mathbf{X}_\ell^{n+\frac{2}{\tau_\ell}} \\ \vdots \\ \mathbf{X}_\ell^{n+\frac{\tau_\ell - 1}{\tau_\ell}} \\ \mathbf{X}_\ell^{n+1} \end{bmatrix} \in \mathbb{R}^{3n_\ell \tau_\ell} \quad \text{and} \quad \mathbb{X}^{(n+1)} := \begin{bmatrix} \mathbb{X}_1^{(n+1)} \\ \mathbb{X}_2^{(n+1)} \\ \vdots \\ \mathbb{X}_{n_{\mathrm{dom}}}^{(n+1)} \end{bmatrix} \in \mathbb{R}^{3n_\ell \tau_\ell n_{\mathrm{dom}}} \tag{4.12}$$

respectively. The constraint equation at the velocity level, i.e., Eq. (4.5b), can be compactly written in the form

$$\boxed{\mathbf{0} = \sum_{\ell=1}^{n_{\mathrm{dom}}} \mathbb{G}_\ell \mathbb{X}_\ell^{(n+1)} = \mathbb{G}\mathbb{X}^{(n+1)}} \tag{4.13}$$

where

$$\mathbb{G}_\ell := \begin{bmatrix} \mathbf{O}_{n_c \times 3n_\ell} & \mathbf{O}_{n_c \times 3n_\ell} & \cdots & \mathbf{O}_{n_c \times 3n_\ell} & \hat{\mathbb{G}}_\ell^{(2)} \end{bmatrix} \in \mathbb{R}^{n_c \times 3n_\ell \tau_\ell} \tag{4.14}$$

with

$$\hat{\mathbb{G}}_\ell^{(2)} := \begin{bmatrix} \mathbf{O}_{n_c \times n_\ell} & \mathbf{G}_\ell & \mathbf{O}_{n_c \times n_\ell} \end{bmatrix} \in \mathbb{R}^{n_c \times 3n_\ell} \tag{4.15}$$

and

$$\mathbb{G} := \begin{bmatrix} \mathbb{G}_1 & \mathbb{G}_2 & \cdots & \mathbb{G}_{n_{\mathrm{dom}}} \end{bmatrix} \in \mathbb{R}^{n_c \times \Sigma_\ell^{n_{\mathrm{dom}}} 3n_\ell \tau_\ell} \tag{4.16}$$

Linear Equation in the System Time Step Level

The solutions $(\mathbb{X}^{(n+1)}, \boldsymbol{\lambda}^{n+1})$ can be found by solving the following linear equation for $n = 0, 1, 2, \cdots, n_{\mathrm{steps}} - 1$:

$$\boxed{\begin{bmatrix} \mathbb{A} & \mathbb{B} \\ \mathbb{G} & \mathbb{O} \end{bmatrix} \begin{bmatrix} \mathbb{X}^{(n+1)} \\ \boldsymbol{\lambda}^{n+1} - \boldsymbol{\lambda}^{n} \end{bmatrix} = \begin{bmatrix} \mathbb{F}^{(n)} \\ \mathbf{0} \end{bmatrix}} \tag{4.17}$$

where

$$\mathbb{A} := \mathrm{diag}\left[\mathbb{A}_1, \mathbb{A}_2, \cdots, \mathbb{A}_{n_{\mathrm{dom}}}\right] \in \mathbb{R}^{(3n_\ell \tau_\ell n_{\mathrm{dom}}) \times (3n_\ell \tau_\ell n_{\mathrm{dom}})} \tag{4.18}$$

in which

$$\mathbb{A}_\ell := \begin{bmatrix} \mathbb{L}_\ell & & & & \\ -\mathbb{R}_\ell & \mathbb{L}_\ell & & & \\ & -\mathbb{R}_\ell & \mathbb{L}_\ell & & \\ & & \ddots & \ddots & \\ & & & -\mathbb{R}_\ell & \mathbb{L}_\ell \end{bmatrix} \in \mathbb{R}^{(3n_\ell \tau_\ell) \times (3n_\ell \tau_\ell)} \tag{4.19}$$

$$\mathbb{B} := \begin{bmatrix} \mathbb{B}_1 \\ \mathbb{B}_2 \\ \vdots \\ \mathbb{B}_{n_{\mathrm{dom}}} \end{bmatrix} \in \mathbb{R}^{(\Sigma_\ell^{n_{\mathrm{dom}}} 3n_\ell \tau_\ell) \times n_c} \tag{4.20}$$

in which

$$\mathbb{B}_\ell := \begin{bmatrix} -\frac{1}{\tau_\ell}\hat{\mathbb{G}}_\ell^{(1)} & -\frac{2}{\tau_\ell}\hat{\mathbb{G}}_\ell^{(1)} & \cdots & -\frac{\tau_\ell - 1}{\tau_\ell}\hat{\mathbb{G}}_\ell^{(1)} & -\hat{\mathbb{G}}_\ell^{(1)} \end{bmatrix}^T \in \mathbb{R}^{3n_\ell\tau_\ell \times n_c} \tag{4.21}$$

and

$$\mathbb{F}^{(n)} := \begin{bmatrix} \mathbb{F}_1^{(n)} \\ \mathbb{F}_2^{(n)} \\ \vdots \\ \mathbb{F}_{n_{\mathrm{dom}}}^{(n)} \end{bmatrix} \in \mathbb{R}^{3n_\ell\tau_\ell n_{\mathrm{dom}}} \tag{4.22}$$

in which

$$\mathbb{F}_\ell^{(n)} := \begin{bmatrix} \mathbb{Q}_\ell^{n+\frac{1+W_1}{\tau_\ell}} + \left(\hat{\mathbb{G}}_\ell^{(1)}\right)^T \boldsymbol{\lambda}^n + \mathbb{R}_\ell \mathbf{X}_\ell^n \\ \mathbb{Q}_\ell^{n+\frac{2+W_1}{\tau_\ell}} + \left(\hat{\mathbb{G}}_\ell^{(1)}\right)^T \boldsymbol{\lambda}^n \\ \vdots \\ \mathbb{Q}_\ell^{n+\frac{\tau_\ell+W_1}{\tau_\ell}} + \left(\hat{\mathbb{G}}_\ell^{(1)}\right)^T \boldsymbol{\lambda}^n \end{bmatrix} \in \mathbb{R}^{3n_\ell\tau_\ell} \tag{4.23}$$

4.4 Analysis of Algorithm 4.3.1

4.4.1 Time Accuracy

Theorem 4.4.1 (Time Accuracy of Algorithm 4.3.1)

Suppose a domain Ω is divided into n_{dom} numbers of subdomains, Ω_ℓ for $\ell = 1, 2, \cdots, n_{\mathrm{dom}}$; and different algorithms, generated from Algorithm 4.3.1, and different subdomain time step sizes, Δt_ℓ, are used for different subdomain. The ***second-order*** *time accuracy in all the kinematic and algebraic quantities can be achieved if W_1 are the same for all subdomains and $\tau_\ell = 1$ for $\ell = 1, 2, \cdots, n_{\mathrm{dom}}$, i.e., no subcycling; otherwise, only first-order time accuracy in all the kinematic and algebraic quantities. In order to guarantee the second-order time accuracy in the acceleration, the numerical acceleration $\mathbf{a}_\ell^{n+\frac{m}{\tau_\ell}}$ must* *be an approximation at time level t_n:*

$$\mathbf{a}_\ell^{n+\frac{m}{\tau_\ell}} \approx \ddot{\mathbf{q}}(t_n + (m - \phi_\ell)\Delta t_\ell) \tag{4.24}$$

where $\phi_\ell := W_1\Lambda_6 - W_1$ in which W_1 and $W_1\Lambda_6$ are the values used for subdomain Ω_ℓ. For the other kinematic unknowns, i.e., $\mathbf{q}_\ell^{n+\frac{m}{\tau_\ell}}$ and $\mathbf{v}_\ell^{n+\frac{m}{\tau_\ell}}$, and the algebraic unknown, i.e., $\boldsymbol{\lambda}^n$,

$$\begin{aligned} \mathbf{q}_\ell^{n+\frac{m}{\tau_\ell}} &\approx \mathbf{q}_\ell(t_n + m\Delta t_\ell) \\ \mathbf{v}_\ell^{n+\frac{m}{\tau_\ell}} &\approx \dot{\mathbf{q}}_\ell(t_n + m\Delta t_\ell) \\ \boldsymbol{\lambda}^n &\approx \boldsymbol{\lambda}(t_n) \end{aligned} \tag{4.25}$$

Remark 4.4.1

1. *When the same algorithm is applied for all subdomains with no subcycling, i.e., $\tau_\ell = 1$, the second-order time accuracy can be obtained.*

2. *Of special interest from the pragmatic point of view may be the applications of mixed time integration algorithms for different subdomains with implicit or/and explicit numerically dissipative schemes and numerically non-dissipative schemes. Table 2 summarizes two significantly important options for second-order time accurate mixed algorithms for subdomains Ω_i and Ω_j. Option (1) is the combinations of algorithms from the U0- and V0-based algorithms. Some typical examples of this option are:*

   - ***Implicit U0V0 numerically nondissipative schemes***, *i.e., U0$(1, 1, \rho)$ with $\hat{\eta} = 1$*, and ***implicit U0V0/V0U0 optimal numerically dissipative schemes***, *i.e., V0/U0$(\rho, 1, \rho)$ with $\hat{\eta} = 1$.*

   - ***Implicit Newmark method***, *i.e., U0$(1, 1, 0)$ with $\hat{\eta} = 1$*, and ***implicit U0V0/V0U0 optimal numerically dissipative scheme*** *V0/U0$(0, 1, 0)$ with $\hat{\eta} = 1$.*

- ***Explicit central difference method***, *i.e.,* $U0(1,1,0)$ *with* $\hat{\eta} = 0$, and ***implicit U0V0/V0U0 optimal numerically dissipative scheme*** $V0/U0(0,1,0)$ *with* $\hat{\eta} = 1$.

The spectral parameter $\hat{\rho}_1^j$ *in the table is defined as*

$$\hat{\rho}_1^j := \frac{1 - \rho_2^j + \rho(\rho_2^j + 3)}{1 + 3\rho_2^j + \rho(\rho_2^j - 1)} \tag{4.26}$$

Another suggestion is the U0-based and U0-based combinations; see option (2) *in the table. Some typical examples of this option are:*

- ***Implicit Newmark method***, *i.e.,* $U0(1,1,0)$ *with* $\hat{\eta} = 1$, and ***Explicit central difference method***, *i.e.,* $U0(1,1,0)$ *with* $\hat{\eta} = 0$.
- ***Implicit Newmark method*** or ***Explicit central difference method*** and ***implicit three parameter optimal scheme***[2] $U0(0,0,0)$ with $\hat{\eta} = 1$.

[2] *Implicit three parameter optimal scheme* $U0(0,0,0)$ *with* $\hat{\eta} = 1$ *is* *L-stable* in linear systems.

Option	Subdomain Ω_i	Subdomain Ω_j	W_1
(1)	$\mathrm{U0}(\rho_1^i, \rho_2^i, \rho)$	$\mathrm{V0}(\hat{\rho}_1^j, \rho_2^j, \rho_3^j)$	$\frac{1}{1+\rho}$
E.g.	$\mathrm{U0V0}(1, 1, \rho)$	$\mathrm{U0V0/V0U0}(\rho, 1, \rho)$	$\frac{1}{1+\rho}$
(2)	$\mathrm{U0}(\rho_1^i, \rho_2^i, \rho)$	$\mathrm{U0}(\rho_1^j, \rho_2^j, \rho)$	$\frac{1}{1+\rho}$
E.g.	$\mathrm{U0V0}(1, 1, \rho)$	$\mathrm{U0V0/V0U0}(\rho, 1, \rho)$	$\frac{1}{1+\rho}$
	$\mathrm{U0V0}(1, 1, \rho)$	$\mathrm{U0V1}(\rho, \rho, \rho)$	$\frac{1}{1+\rho}$

Table 4.1: Second-order Time Accurate Mixed Algorithms for Subdomains Ω_i and Ω_j. $\mathrm{U0}(\rho_\infty^{\mathrm{min}}, \rho_\infty^{\mathrm{max}}, \rho_\infty^{\mathrm{s}})$ and $\mathrm{V0}(\rho_\infty^{\mathrm{min}}, \rho_\infty^{\mathrm{max}}, \rho_\infty^{\mathrm{s}})$ Denote Algorithms which are Generated from the U0- and V0-based Families in Algorithm 4.3.1, Respectively. Parameter $\rho \in \mathbb{R}$ Must Obeys $0 \le \rho \le \min_\ell(\rho_1^\ell)$ for Implicit Cases.

4.4.2 Configuration and Acceleration Drifts in Interface

Algorithm 4.3.1 is based on the Index-2 velocity-continuity formulation, and therefore the velocities at the subdomain interface are enforced to be continuous in the sense of Eq. (4.13). However, the configurations and accelerations at the subdomain interface in the time-discrete system may suffer from drifts in general; that is, the constraint equations at the configuration and acceleration levels are not always satisfied once the system is discretized in time.

Theorem 4.4.2 (Displacement and Acceleration Drifts in Interface)

Suppose there is no subcycling, i.e., $\tau_\ell = 1$. Define the drifts in the displacement and acceleration at the subdomain interface as

$$\mathbf{q}_{\mathrm{drift}}^n := \mathbf{G}_\ell \mathbf{q}_\ell^n \neq \mathbf{0} \;\; \textit{and} \;\; \mathbf{a}_{\mathrm{drift}}^n := \mathbf{G}_\ell \mathbf{a}_\ell^n \neq \mathbf{0} \tag{4.27}$$

Then, the configuration and acceleration drifts within the system time step are given as

$$\mathbf{q}_{\mathrm{drift}}^{n+1} = \mathbf{q}_{\mathrm{drift}}^{n} + \Delta t^2 \left(\lambda_2 - \frac{\lambda_3 \lambda_4}{\lambda_5} \right) \mathbf{a}_{\mathrm{drift}}^{n} \tag{4.28}$$

$$\mathbf{a}_{\mathrm{drift}}^{n+1} = \left(\frac{\lambda_5 - \lambda_4}{\lambda_5} \right) \mathbf{a}_{\mathrm{drift}}^{n} \tag{4.29}$$

Proof. Eq (4.28) and Eq. (4.29) can be easily derived from the update equations of Algorithm 4.3.1 for the configuration and velocity vectors, i.e. Eq. (4.4h) and Eq. (4.4i), respectively, using

$$\mathbf{v}_{\mathrm{drift}}^{n} := \mathbf{G}_{\ell} \mathbf{v}_{\ell}^{n} = \mathbf{0} \tag{4.30}$$

and Eq. (4.27). ∎

Remark 4.4.2

1. *In terms of the spectral parameters, $(\rho_\infty^{\mathrm{min}}, \rho_\infty^{\mathrm{max}}, \rho_\infty^{\mathrm{s}})$, we have*

$$\lambda_2 - \frac{\lambda_3 \lambda_4}{\lambda_5} = \frac{-(1-\rho_\infty^{\mathrm{min}})(1-\rho_\infty^{\mathrm{max}})}{2(3+\rho_\infty^{\mathrm{min}}+\rho_\infty^{\mathrm{max}}-\rho_\infty^{\mathrm{min}}\rho_\infty^{\mathrm{max}})} \tag{4.31}$$

$$\frac{\lambda_5 - \lambda_4}{\lambda_5} = \frac{-1+\rho_\infty^{\mathrm{min}}+\rho_\infty^{\mathrm{max}}+3\rho_\infty^{\mathrm{min}}\rho_\infty^{\mathrm{max}}}{3+\rho_\infty^{\mathrm{min}}+\rho_\infty^{\mathrm{max}}-\rho_\infty^{\mathrm{min}}\rho_\infty^{\mathrm{max}}} \tag{4.32}$$

for the U0-based family, and

$$\lambda_2 - \frac{\lambda_3 \lambda_4}{\lambda_5} = 0 \tag{4.33}$$

$$\frac{\lambda_5 - \lambda_4}{\lambda_5} = -\rho_\infty^{\mathrm{s}} \tag{4.34}$$

for the V0-based family. The spectral conditions for the configuration and acceleration drifts in interface for the U0- and V0-based families are summarized in Table 4.4.2.

	U0-based Family: $(\rho_\infty^{\min}, \rho_\infty^{\max}, \rho_\infty^{s})$		V0-based Family: $(\rho_\infty^{\min}, \rho_\infty^{\max}, \rho_\infty^{s})$	
	Implicit ($\hat{\eta} = 1$)	Explicit ($\hat{\eta} = 0$)	Implicit ($\hat{\eta} = 1$)	Explicit ($\hat{\eta} = 0$)
$\mathbf{q}_{\text{drift}}^{n+1} = \mathbf{q}_{\text{drift}}^{n}$	$\rho_\infty^{\max} = 1$	Never	Any	Never
$\mathbf{a}_{\text{drift}}^{n+1} = \mathbf{0}$	$\rho_\infty^{\min} = \frac{1-\rho_\infty^{\max}}{1+3\rho_\infty^{\max}}$	$\rho_\infty^{\min} = \frac{1-\rho_\infty^{\max}}{1+3\rho_\infty^{\max}}$	$\rho_\infty^{s} = 0$	$\rho_\infty^{s} = 0$
$\left\lVert\mathbf{a}_{\text{drift}}^{n+1}\right\rVert \leq \left\lVert\mathbf{a}_{\text{drift}}^{n}\right\rVert$	$0 \leq \rho_\infty^{\min}\rho_\infty^{\max} \leq 1$	$\left\lVert\rho_\infty^{\min}\rho_\infty^{\max}\right\rVert \leq 1$	$0 \leq \rho_\infty^{s} \leq 1$	$\left\lVert\rho_\infty^{s}\right\rVert \leq 1$

Table 4.2: The Configuration and Acceleration Drifts at the Subdomain Interface for No-subcycling Case.

4.5 Numerical Illustration: Split Lumped Parameter System

Example 4.5.1 (Split Lumped Parameter System)

Consider a equation of motion for a spring-mass system in the form,

$$m\ddot{q}(t) + kq(t) = f \quad \forall t \in \mathbb{I} = [0, T] \tag{4.35}$$

with given initial conditions $q(0) = q^0$ *and* $\dot{q}(0) = v^0$*, where* m*,* k*, and* f *denote the mass of the body, stiffness of the spring(s), and the time-dependent external load, respectively. The analytical solution to the ODE* (4.35) *is given by*

$$q(t) = \frac{v^0}{\omega}\sin(\omega t) + \left(q^0 - \frac{f(t)}{k}\right)\cos(\omega t) + \frac{f(t)}{k} \tag{4.36}$$

where $\omega := \sqrt{k/m}$*. This problem can be split into two subdomains as shown in Fig. 4.2, and the governing equation can be written in the sense of the index-2 DAE system* *of the form,*

$$\begin{bmatrix} m_1 & 0 \\ 0 & m_2 \end{bmatrix} \begin{bmatrix} \ddot{q}_1 \\ \ddot{q}_2 \end{bmatrix} + \begin{bmatrix} k_1 & 0 \\ 0 & k_2 \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} + \begin{bmatrix} \lambda \\ -\lambda \end{bmatrix} \quad \text{and} \quad \dot{q}_1 - \dot{q}_2 = 0 \tag{4.37}$$

with $m = m_1 + m_2$, $k = k_1 + k_2$, *and* $f = f_1 + f_2$.

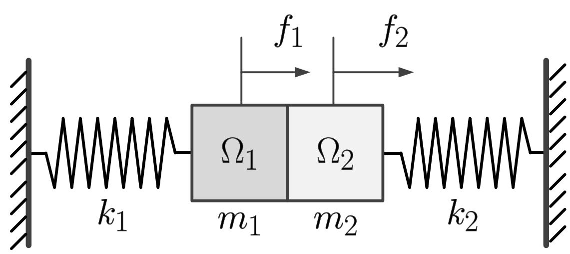
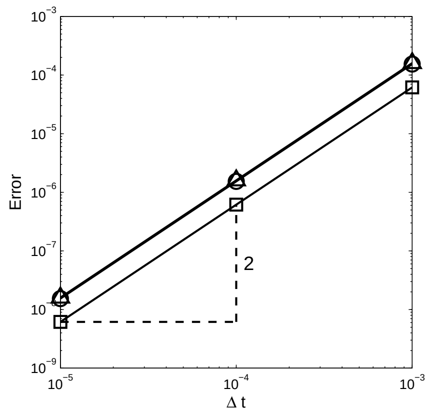


Figure 4.2: Split Lumped Parameter System

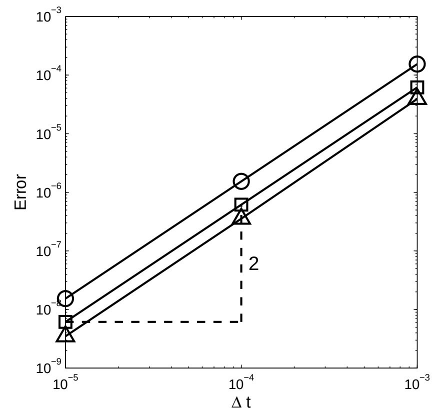
In Fig. 4.3 - Fig. 4.11, some examples of implicit-implicit/implicit-explicit/explicit-explicit mixed algorithms for Ω_ℓ (for $\ell = 1, 2$) with no subcycling with second-order time accuracy are shown with the time histories of the displacements, velocities, and accelerations of each split masses. The mass and stiffness for each Ω_ℓ are: $m_1 = 0.095$ and $k_1 = 5$; and $m_2 = 0.005$ and $k_2 = 45$, respectively. The system time step size is $\Delta t = 0.02$. For the time accuracy plots (a) for Ω_1 and (b) for Ω_2 in Fig. 4.3 - Fig. 4.11, the external loads are applied, $f_1(t) = f_2(t) = \sin(t)$; while for the displacement, velocity, and acceleration histories, given in (c), (d), and (e), respectively, no external load is applied, i.e., $f_1(t) = f_2(t) = 0$; therefore, the system is conservative. Note that the subdomain time step sizes for each Ω_ℓ are selected as $\Delta t_1 = 0.01$ and $\Delta t_2 = 0.005$, respectively, for the displacement, velocity, and acceleration time histories, i.e., $\tau_1 = 2$ and $\tau_2 = 4$; however, the time accuracy plots are based on no subcycling, i.e., $\tau_1 = \tau_2 =$

1. [3] Since every combination in Fig. 4.3 - Fig. 4.11 satisfy the condition given in Theorem 4.4.1, the second-order time accuracies in all the quantities are achieved; see (a) and (b). And note that the stable numerical displacement, velocity, and acceleration responses are observed for any combinations as shown in (c), (d), and (e) of the figures.

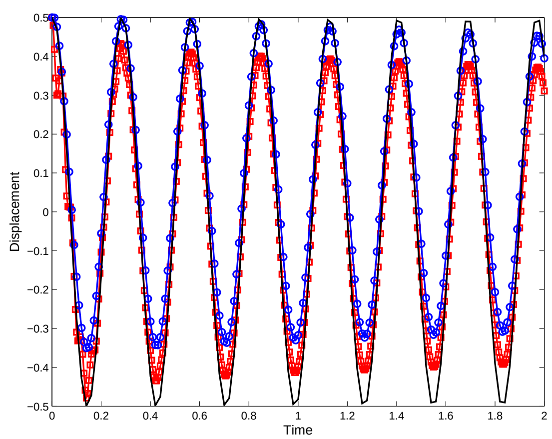
[3] In (a) and (b) in Fig. 4.3 - Fig. 4.11, ◯, □, and △ denotes the displacement, velocity, and acceleration data, respectively, for the time accuracy plots.
In (c)-(e) in Fig. 4.3 - Fig. 4.11, ◯ (in blue) and □ (in red) denote the data for subdomains Ω_1 and Ω_2, respectively. The black curves are the exact data.



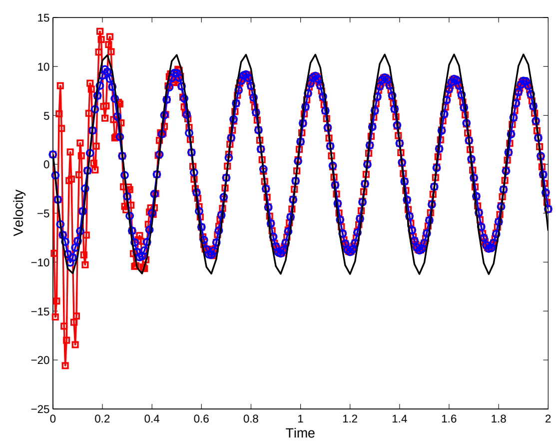
(a) Ω_1: I-U0(1,1,0)



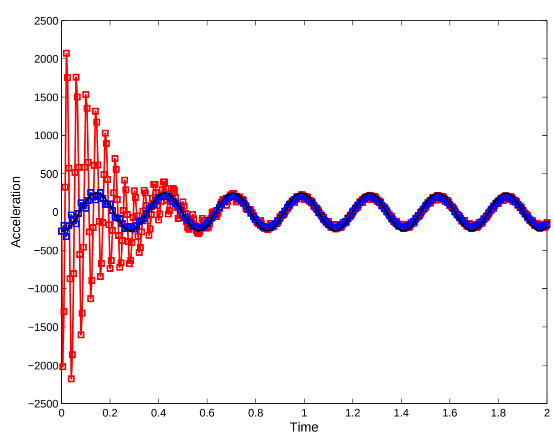
(b) Ω_2: I-U0/V0(0,1,0)



(c) Displacement

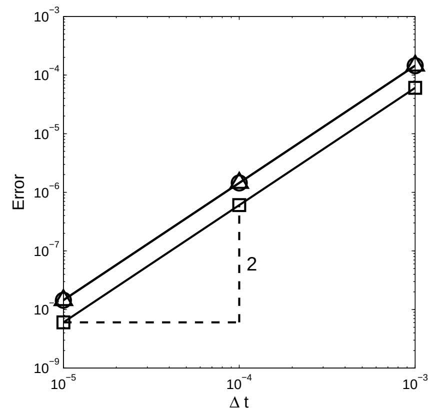


(d) Velocity

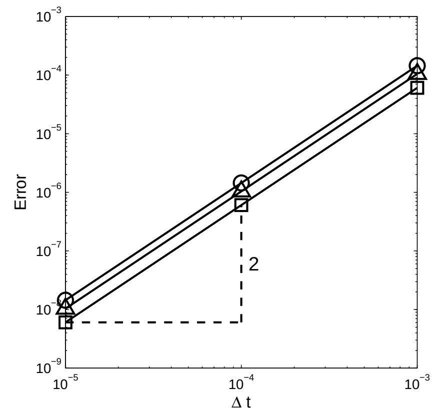


(e) Acceleration

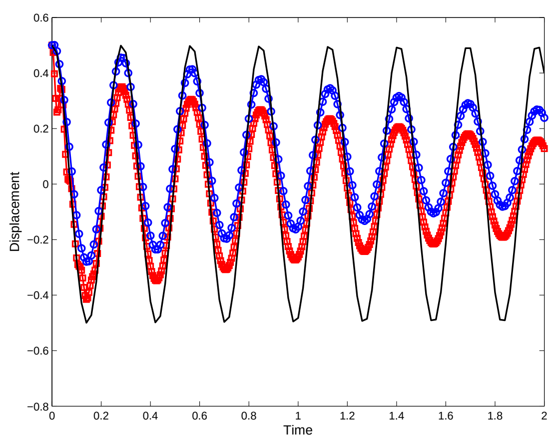
Figure 4.3: The Combination of the Implicit Numerically Nondissipative Algorithm I-U0(1,1,0) (Implicit Newmark) for Ω_1 and Implicit Numerically Dissipative Optimal Algorithm I-U0/V0(0,1,0) for Ω_2.



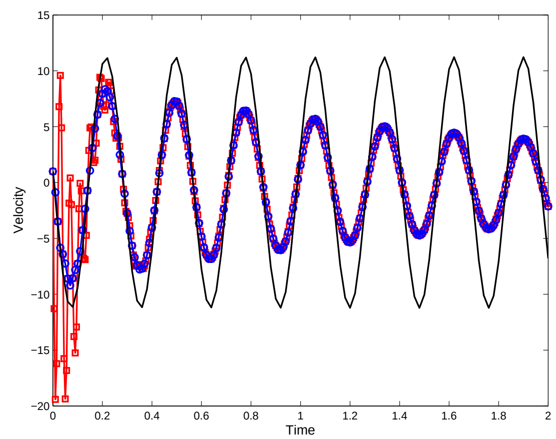
(a) Ω_1: I-U0(1,1,0.5)



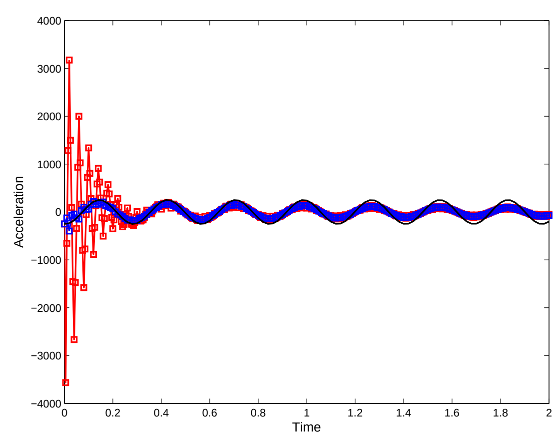
(b) Ω_2: I-U0/V0(0.5,1,0.5)



(c) Displacement

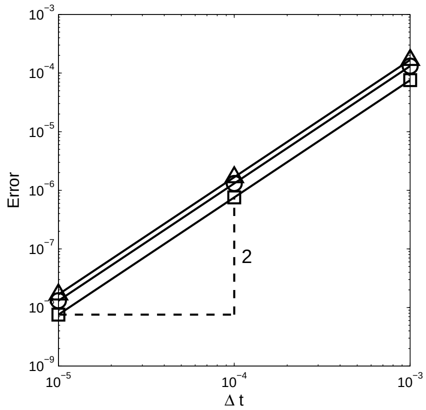


(d) Velocity

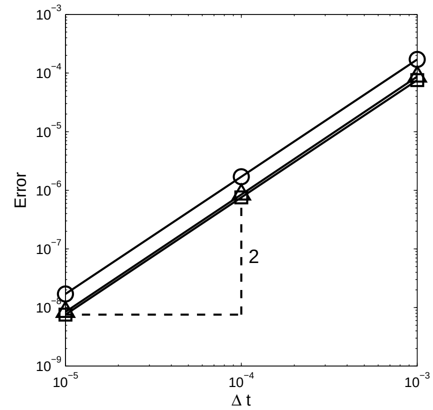


(e) Acceleration

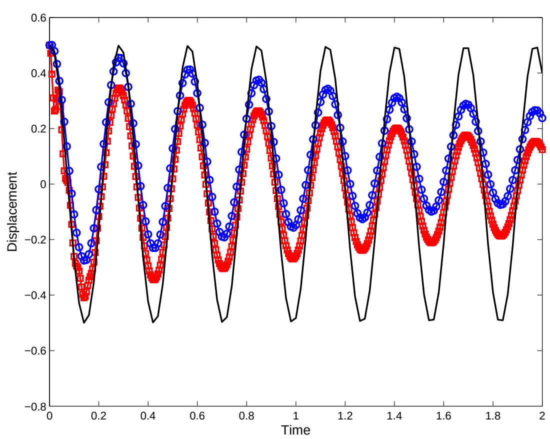
Figure 4.4: The Combination of the Implicit Numerically Nondissipative Algorithm I-U0(1,1,0.5) for Ω_1 and Implicit Numerically Dissipative Optimal Algorithm I-U0/V0(0.5,1,0.5) for Ω_2.



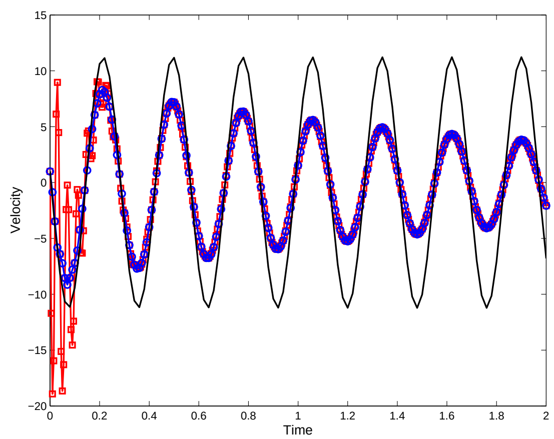
(a) Ω_1: I-U0(1,1,0.5)



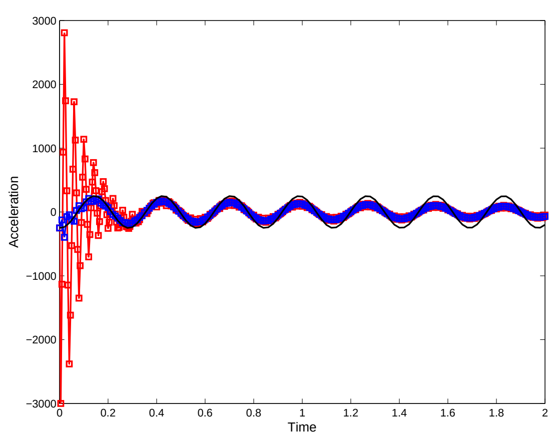
(b) Ω_2: I-U0/V0(0.5,0.5,0.5)



(c) Displacement

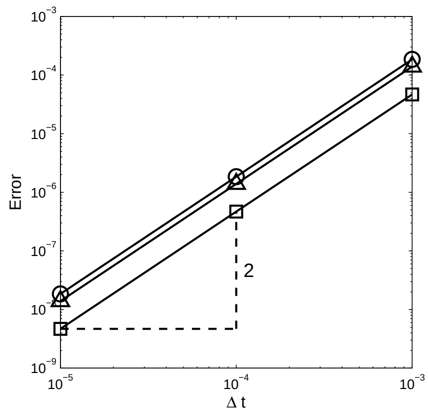


(d) Velocity

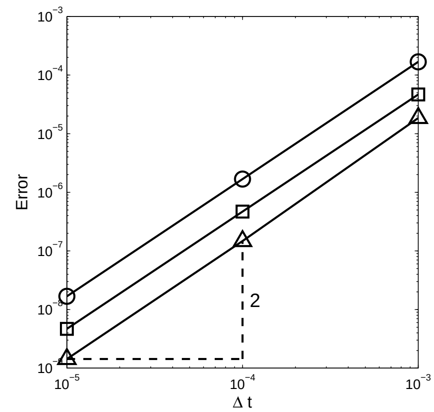


(e) Acceleration

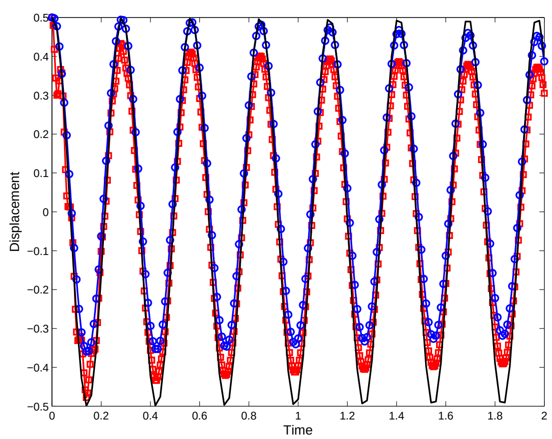
Figure 4.5: The Combination of the Implicit Numerically Nondissipative Algorithm I-U0(1,1,0.5) for Ω_1 and Implicit Numerically Dissipative Algorithm I-U0/V0(0.5,0.5,0.5) ($\in$ Three Parameter Optimal Method) for Ω_2.



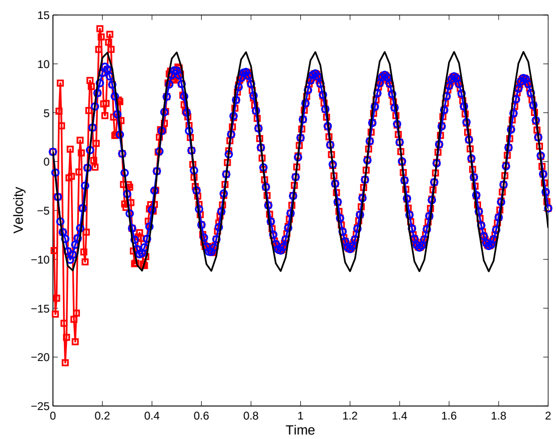
(a) Ω_1: E-U0(1,1,0)



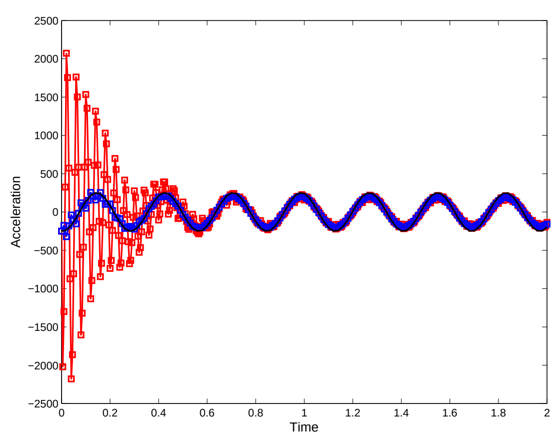
(b) Ω_2: I-U0/V0(0,1,0)



(c) Displacement

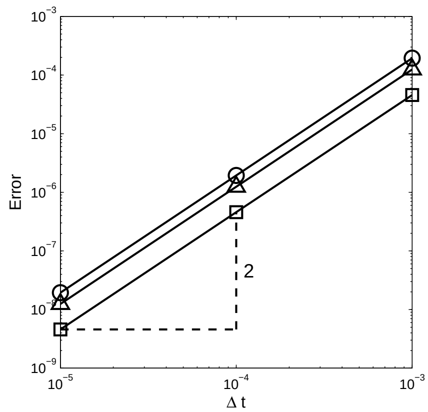


(d) Velocity

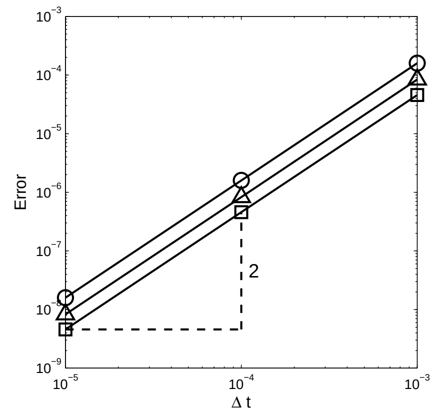


(e) Acceleration

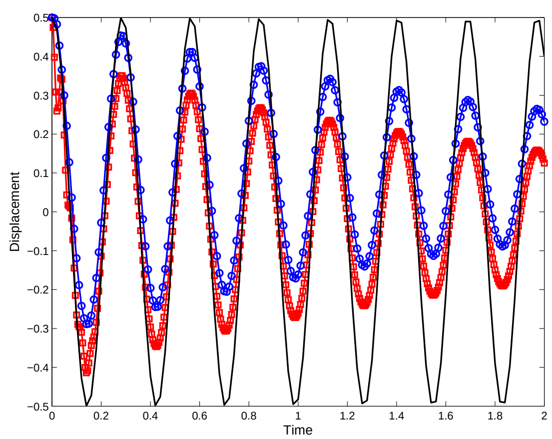
Figure 4.6: The Combination of the Explicit Numerically Nondissipative Algorithm E-U0(1,1,0) (Central difference) for Ω_1 and Implicit Numerically Dissipative Optimal Algorithm I-U0/V0(0,1,0) for Ω_2.



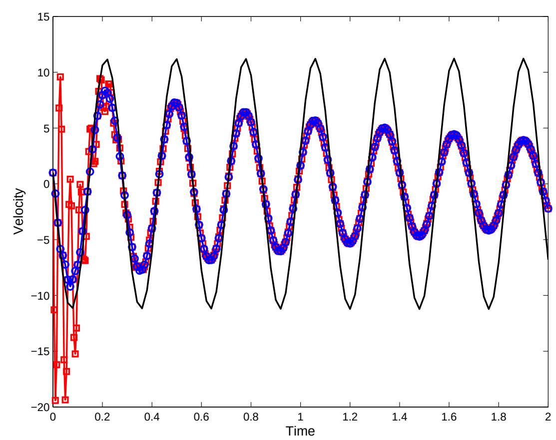
(a) Ω_1: E-U0(1,1,0.5)



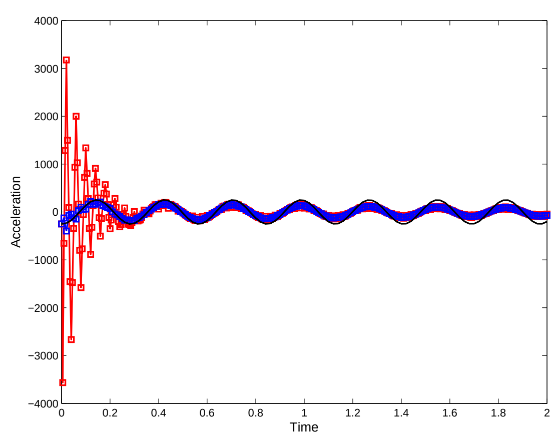
(b) Ω_2: I-U0/V0(0.5,1,0.5)



(c) Displacement

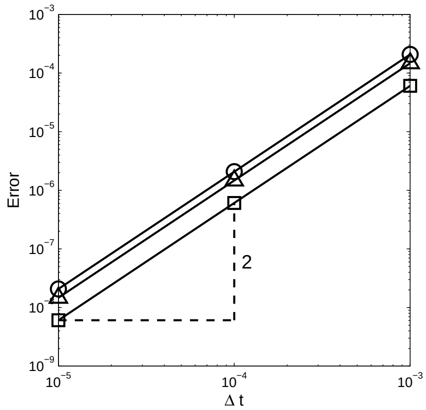


(d) Velocity

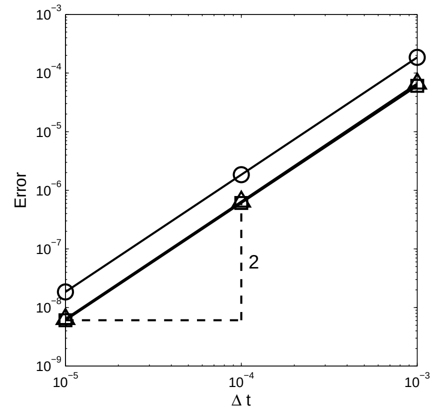


(e) Acceleration

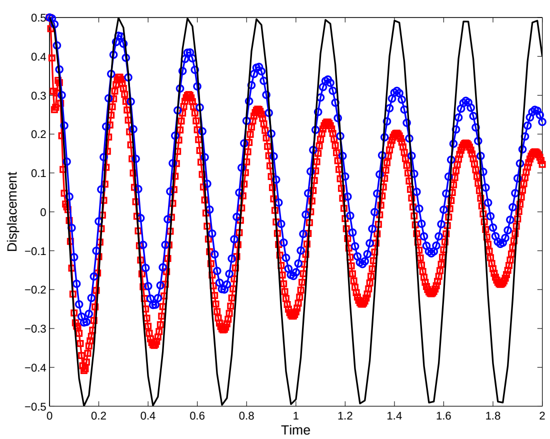
Figure 4.7: The Combination of the Explicit Numerically Nondissipative Algorithm E-U0(1,1,0.5) for Ω_1 and Implicit Numerically Dissipative Optimal Algorithm I-U0/V0(0.5,1,0.5) for Ω_2.



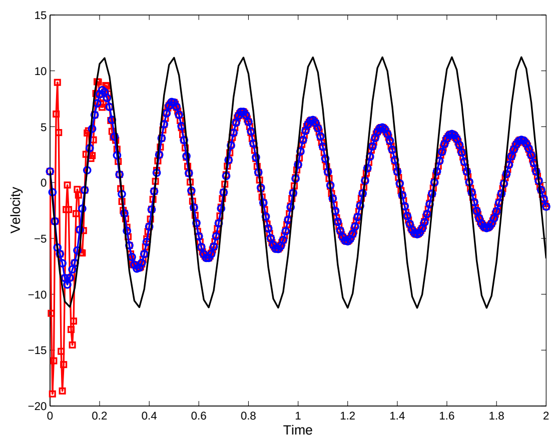
(a) Ω_1: E-U0(1,1,0.5)



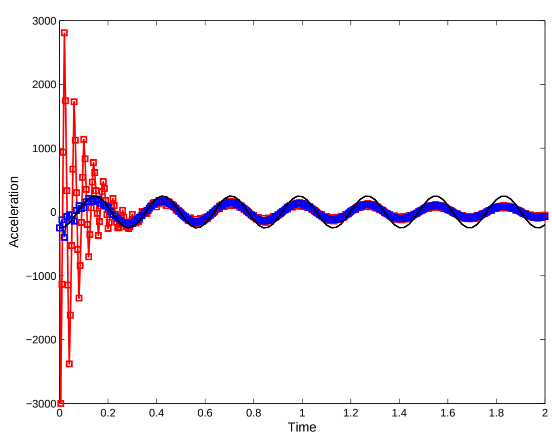
(b) Ω_2: I-U0/V0(0.5,0.5,0.5)



(c) Displacement

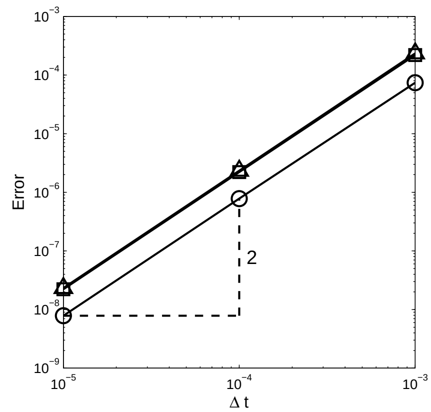


(d) Velocity

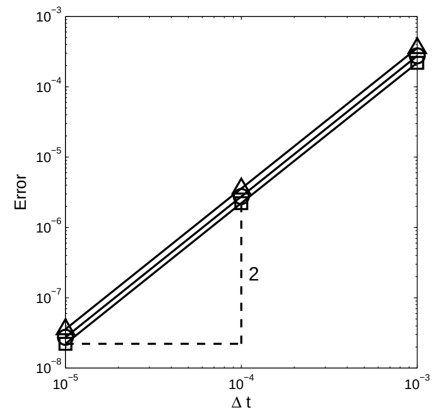


(e) Acceleration

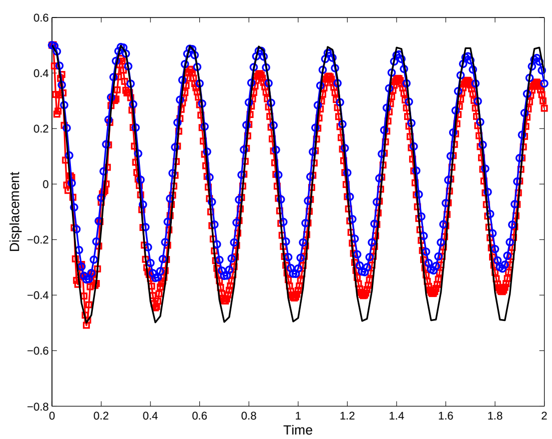
Figure 4.8: The Combination of the Explicit Numerically Nondissipative Algorithm E-U0(1,1,0.5) for Ω_1 and Implicit Numerically Dissipative Algorithm I-U0/V0(0.5,0.5,0.5) ($\in$ Three Parameter Optimal Method) for Ω_2.



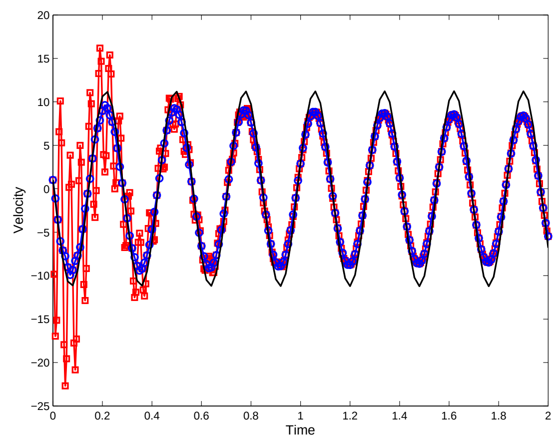
(a) Ω_1: E-U0(1,1,0)



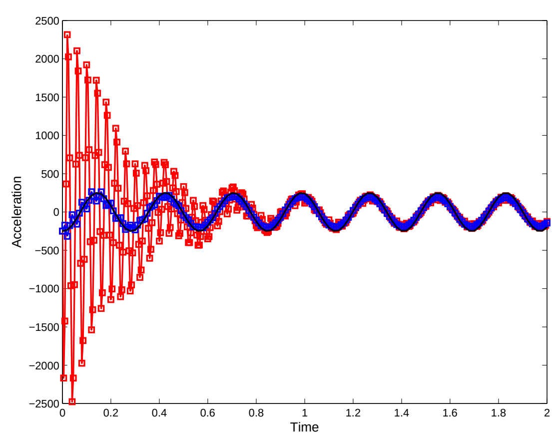
(b) Ω_2: E-U0/V0(0,1,0)



(c) Displacement

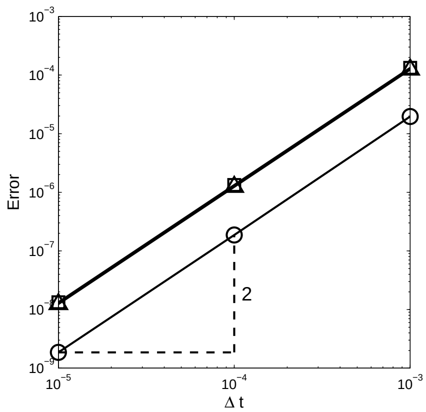


(d) Velocity

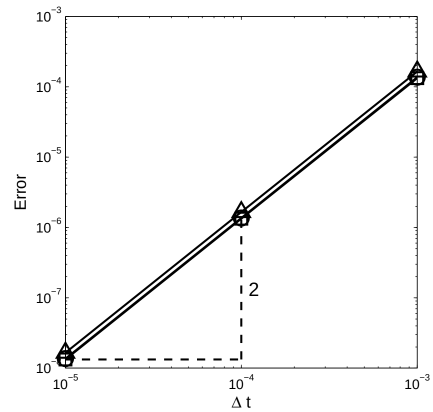


(e) Acceleration

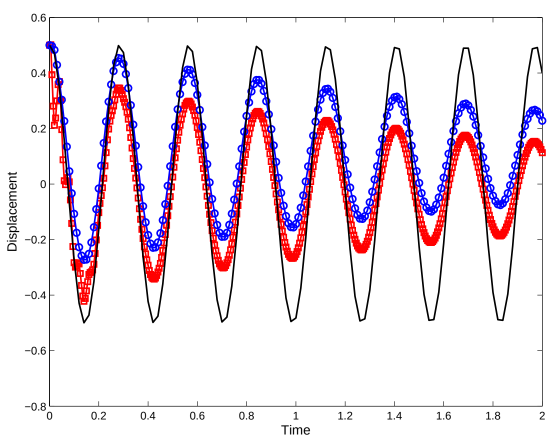
Figure 4.9: The Combination of the Explicit Numerically Nondissipative Algorithm E-U0(1,1,0) (Central Difference) for Ω_1 and Explicit Numerically Nondissipative Optimal Algorithm E-U0/V0(0,1,0) for Ω_2.



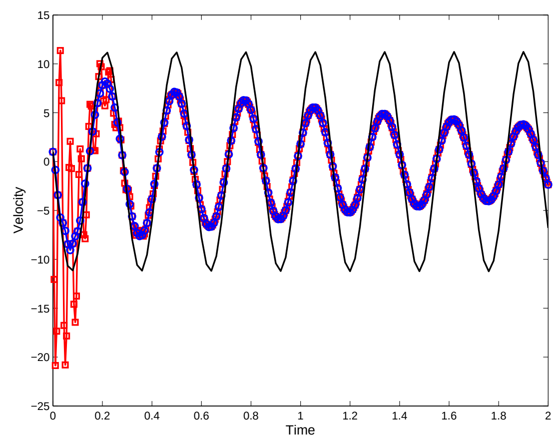
(a) Ω_1: E-U0(1,1,0.5)



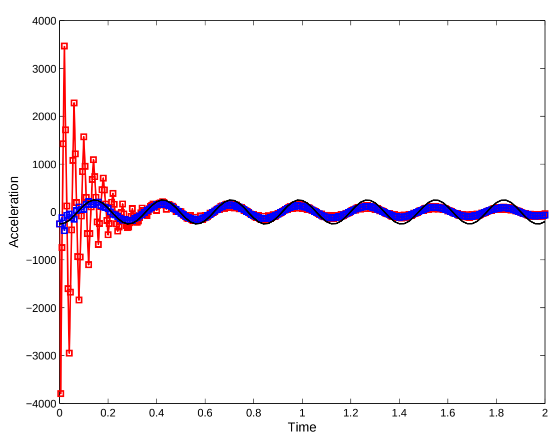
(b) Ω_2: E-U0/V0(0.5,1,0.5)



(c) Displacement

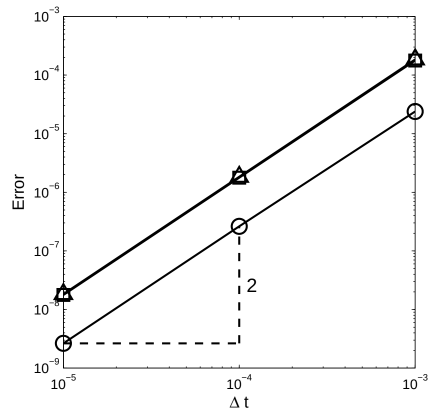


(d) Velocity

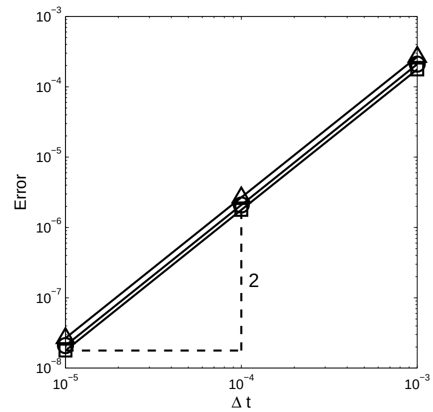


(e) Acceleration

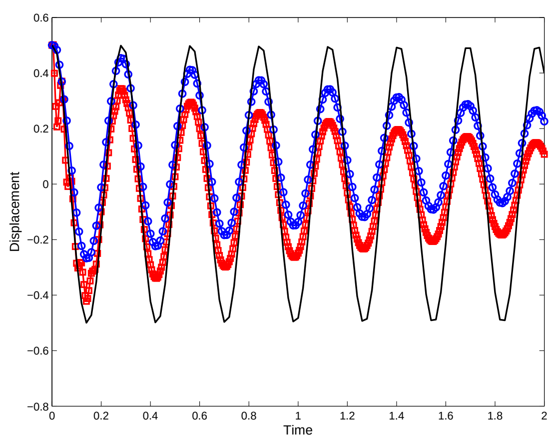
Figure 4.10: The Combination of the Explicit Numerically Nondissipative Algorithm E-U0(1,1,0.5) for Ω_1 and Explicit Numerically Dissipative Optimal Algorithm I-U0/V0(0.5,1,0.5) for Ω_2.



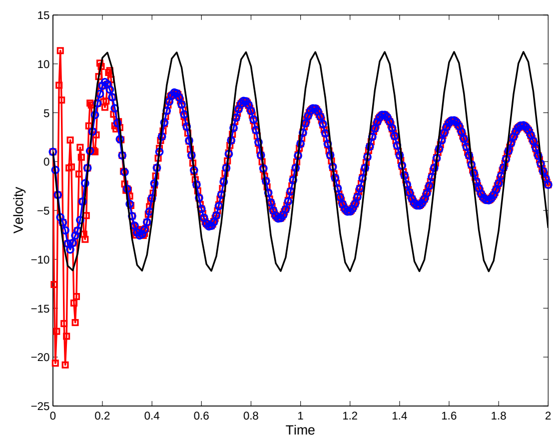
(a) Ω_1: E-U0(1,1,0.5)



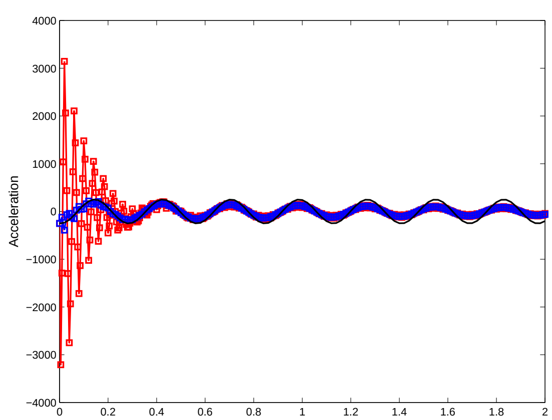
(b) Ω_2: E-U0/V0(0.5,0.5,0.5)



(c) Displacement



(d) Velocity



(e) Acceleration

Figure 4.11: The Combination of the Explicit Numerically Nondissipative Algorithm E-U0(1,1,0.5) for Ω_1 and Explicit Numerically Dissipative Algorithm I-U0/V0(0.5,0.5,0.5) ($\in$ Three Parameter Optimal Method) for Ω_2.

Example 4.5.2 (Plate under Tangential Load)

Next example is a thin plate under a tangential load with the plane stress assumption as shown in Fig. 4.12. Tangential load $f_y = 1 \times 10^6$ N/m^2 *is applied at one end in the* y*-direction, while the other end (at* $x = 0$*) is fully constrained. The whole domain* Ω *is divided into three subdomains* Ω_ℓ *(for* $\ell = 1, 2, 3$*), and each subdomain is meshed using eight quadrilateral elements with four nodes. Suppose the size of the plate be* $L_x = 6$ *m and* $L_x = 4$ *m with thickness* 0.1 *m. Fig. 4.13 shows the accuracy of two points* **A** *and* **B** *indicated in Fig. 4.12 for two different combinations of time integration schemes without* subcycling with $\Delta t = \Delta t_\ell = 0.01$ *sec (for* $\ell = 1, 2, 3$*).*

- ***Case 1:*** *Use the implicit U0(0.5,0.5,0.5) scheme, implicit U0(1,1,0.5) scheme, and implicit U0V0/V0U0(0.5,1,0.5) scheme for* Ω_1, Ω_2, *and* Ω_3, *respectively*

- ***Case 2:*** *Use the explicit U0(0.5,0.5,0.5) scheme, implicit U0(1,1,0.5) scheme, and explicit U0V0/V0U0(0.5,1,0.5) scheme for* Ω_1, Ω_2, *and* Ω_3, *respectively*

Young's modulus, Poisson's ratio, and density used are $E = 1 \times 10^8$ *psi,* $\nu = 0.3$*, and* $\rho = 1$ kg/m^3*, respectively. For both cases, the second-order time accuracy features of the algorithms are preserved, as expected.*

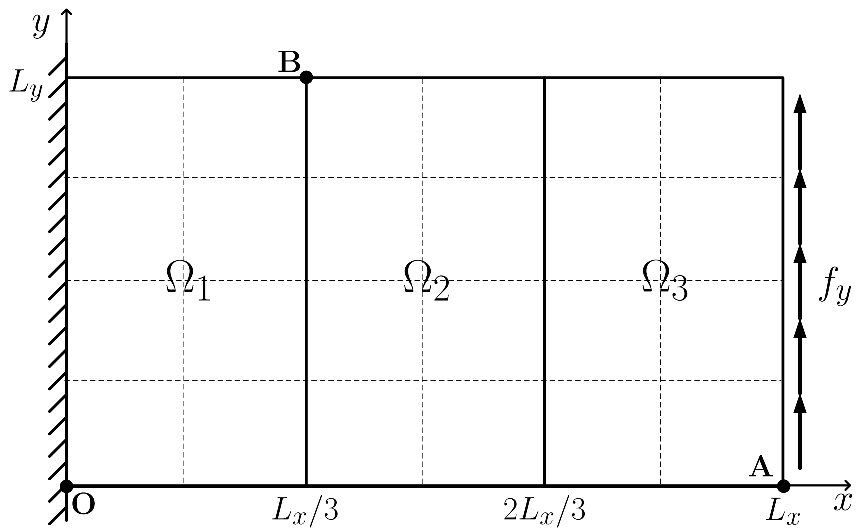
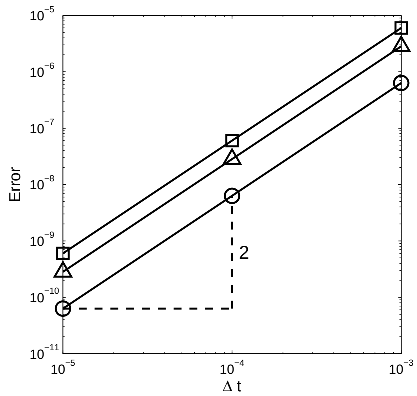
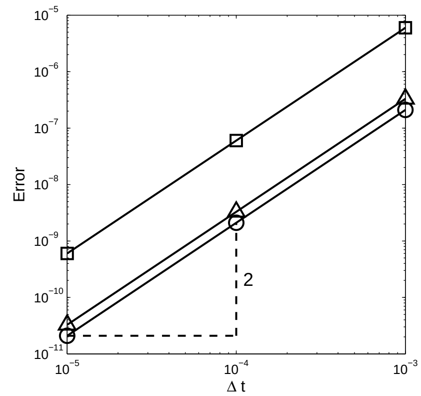


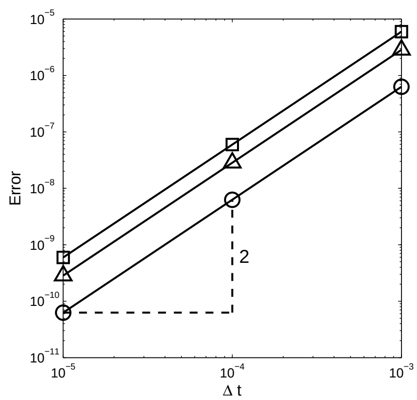
Figure 4.12: Problem Description of Example 4.5.2



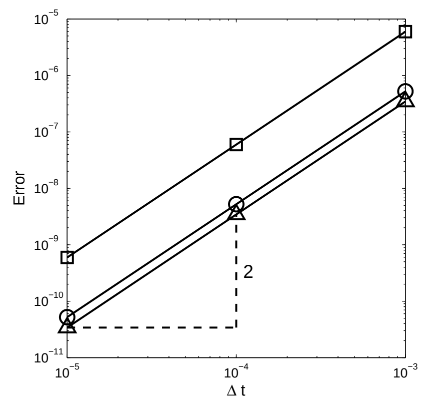
(a) Case 1: Point A



(b) Case 1: Point B



(c) Case 2: Point A



(d) Case 2: Point B

Figure 4.13: Time Accuracy Plots for Example 4.5.2

Chapter 5

RIGID-BODY KINEMATICS

5.1 Position Vectors

5.1.1 In the n-dimensional Euclidean Space

Consider an ***n-dimensional Euclidean space*** $\mathbb{E}^n$; see Section A.1. Suppose one defines a Cartesian frame $\mathcal{B}_1 : (\mathbf{O}_1; \{^{\mathcal{B}_1}\vec{\mathbf{e}}_i\}_{i=1}^n)$ by an origin $\mathbf{O}_1 \in \mathbb{E}^n$ and an *orthonormal* base vectors $\{^{\mathcal{B}_1}\vec{\mathbf{e}}_i\}_{i=1}^n = \{^{\mathcal{B}_1}\vec{\mathbf{e}}_1, {}^{\mathcal{B}_1}\vec{\mathbf{e}}_2, \cdots, {}^{\mathcal{B}_1}\vec{\mathbf{e}}_n\}$ defined in a real linear n-dimensional vector space (linear space) $\mathbb{V}^n$ endowed with the scalar product[1] . The orthonormal base vectors ${}^{\mathcal{B}_1}\vec{\mathbf{e}}_i \in \mathbb{V}^n$ satisfy

$$ {}^{\mathcal{B}_1}\vec{\mathbf{e}}_i \cdot {}^{\mathcal{B}_1}\vec{\mathbf{e}}_j = \delta_{ij} \tag{5.1} $$

[1] See Definition A.1.3 and Theorem A.1.1 for the definition and properties of the scalar product.

for $i, j = 1, 2, \cdots, n$, where δ_{ij} is the ***Kronecker delta*** symbol [2] . The ***position vector***, i.e., the ***radius vector*** about the origin $\mathbf{O}_1$, for every point $\mathbf{P} \in \mathbb{E}^n$ is defined as

$$\vec{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{P}) := \mathbf{P} - \mathbf{O}_1 \tag{5.3}$$

with a map $\vec{\boldsymbol{\pi}} : \mathbb{E}^n \times \mathbb{E}^n \to \mathbb{V}^n$ [3] . The position vector, $\vec{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{P})$, can be uniquely decomposed with respect to frame $\mathcal{B}_1$ as

$$\begin{aligned} \vec{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{P}) &= {}^{\mathcal{B}_1}\pi_1(\mathbf{O}_1, \mathbf{P})\, {}^{\mathcal{B}_1}\vec{\mathbf{e}}_1 + {}^{\mathcal{B}_1}\pi_2(\mathbf{O}_1, \mathbf{P})\, {}^{\mathcal{B}_1}\vec{\mathbf{e}}_2 + \cdots + {}^{\mathcal{B}_1}\pi_n(\mathbf{O}_1, \mathbf{P})\, {}^{\mathcal{B}_1}\vec{\mathbf{e}}_n \\ &= {}^{\mathcal{B}_1}\pi_i(\mathbf{O}_1, \mathbf{P})\, {}^{\mathcal{B}_1}\vec{\mathbf{e}}_i \end{aligned} \tag{5.4}$$

where the scalar quantities ${}^{\mathcal{B}_1}\pi_i(\mathbf{O}_1, \mathbf{P}) : \mathbb{E}^n \times \mathbb{E}^n \to \mathbb{R}$ (for $i = 1, 2, \cdots, n$) are called the ***components*** of $\vec{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{P})$ with respect to $\mathcal{B}_1$, or the ***coordinates*** of point $\mathbf{P} \in \mathbb{E}^3$ with respect to $\mathcal{B}_1$. Defining the component n-tuples, ${}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{P}) : \mathbb{E}^n \times \mathbb{E}^n \to \mathbb{R}^n$, as

$$\begin{aligned} {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{P}) &:= [{}^{\mathcal{B}_1}\pi_1(\mathbf{O}_1, \mathbf{P}), {}^{\mathcal{B}_1}\pi_2(\mathbf{O}_1, \mathbf{P}), \cdots, {}^{\mathcal{B}_1}\pi_n(\mathbf{O}_1, \mathbf{P})]^T \\ &= [{}^{\mathcal{B}_1}\pi_i(\mathbf{O}_1, \mathbf{P})] \in \mathbb{R}^n \end{aligned} \tag{5.5}$$

and the ***vectorix*** for frame $\mathcal{B}_1$ as

$${}^{\mathcal{B}_1}\mathbf{e} := [{}^{\mathcal{B}_1}\vec{\mathbf{e}}_1, {}^{\mathcal{B}_1}\vec{\mathbf{e}}_2, \cdots, {}^{\mathcal{B}_1}\vec{\mathbf{e}}_n]^T \tag{5.6}$$

vector $\vec{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{P})$ in Eq. (5.4) can be written in a compact form as

$$\vec{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{P}) = {}^{\mathcal{B}_1}\mathbf{e}^T\, {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{P}) = {}^{\mathcal{B}_1}\boldsymbol{\pi}^T(\mathbf{O}_1, \mathbf{P})\, {}^{\mathcal{B}_1}\mathbf{e} \tag{5.7}$$

[2] The Kronecker delta symbol is defined as:

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \tag{5.2}$$

for $i, j = 1, 2, \cdots, n$.

[3] See Theorem A.1.2 for the properties of the mapping map $\vec{\boldsymbol{\pi}} : \mathbb{E}^n \times \mathbb{E}^n \to \mathbb{V}^n$.

in which the exponent T denotes transposition, and ${}^{\mathcal{B}_1}\boldsymbol{\pi}^T(\mathbf{O}_1, \mathbf{P}) \equiv ({}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{P}))^T$.

Suppose we define another frame $\mathcal{B}_2 : (\mathbf{O}_2; \{{}^{\mathcal{B}_2}\vec{\mathbf{e}}_i\}_{i=1}^n)$ by an origin $\mathbf{O}_2 \in \mathbb{E}^n$ and an orthonormal base vectors ${}^{\mathcal{B}_2}\vec{\mathbf{e}}_i \in \mathbb{V}^n$ (for $i = 1, 2, \cdots, n$) which are related to ${}^{\mathcal{B}_1}\vec{\mathbf{e}}_i$ via a transformation matrix ${}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A} = [{}^{\mathcal{B}_2\mathcal{B}_1}A_{ij}] \in \mathbb{R}^{n\times n}$ as

$$ {}^{\mathcal{B}_2}\vec{\mathbf{e}}_i = {}^{\mathcal{B}_2\mathcal{B}_1}A_{ij}{}^{\mathcal{B}_1}\vec{\mathbf{e}}_j \quad \text{or} \quad {}^{\mathcal{B}_2}\mathbf{e} = {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}{}^{\mathcal{B}_1}\mathbf{e} \tag{5.8} $$

where ${}^{\mathcal{B}_2}\mathbf{e} := [{}^{\mathcal{B}_2}\vec{\mathbf{e}}_1, {}^{\mathcal{B}_2}\vec{\mathbf{e}}_2, \cdots, {}^{\mathcal{B}_2}\vec{\mathbf{e}}_n]^T$. Notice that the orthonormality of the base vectors (see Eq. (5.1)) yields

$$ {}^{\mathcal{B}_i}\mathbf{e} \cdot {}^{\mathcal{B}_i}\mathbf{e}^T = \mathbf{I}_n \tag{5.9} $$

for $i = 1, 2$ where $\mathbf{I}_n = [\delta_{ij}] \in \mathbb{R}^{n\times n}$ denotes the identity matrix of dimension n; therefore, we have

$$ \mathbf{I}_n = {}^{\mathcal{B}_2}\mathbf{e} \cdot {}^{\mathcal{B}_2}\mathbf{e}^T = ({}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}{}^{\mathcal{B}_1}\mathbf{e}) \cdot ({}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}{}^{\mathcal{B}_1}\mathbf{e})^T = {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}\underbrace{({}^{\mathcal{B}_1}\mathbf{e} \cdot {}^{\mathcal{B}_1}\mathbf{e}^T)}_{\mathbf{I}_n}{}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}^T = {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}{}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}^T \tag{5.10} $$

Hence, the *orthogonal* property of the transformation matrix ${}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}$ is revealed:

$$ {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}^{-1} = {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}^T \tag{5.11} $$

That is, ${}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A} \in O(n)$ where $O(n)$ denotes the ***orthogonal group***; see Definition A.2.3. Premultiplying Eq. (5.8) by ${}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}^{-1}$ (i.e., multiplication of Eq. (5.8) by ${}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}^{-1}$ from the left), we get

$$ {}^{\mathcal{B}_1}\mathbf{e} = {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}^{-1}{}^{\mathcal{B}_2}\mathbf{e} \tag{5.12} $$

In view of Eq. (5.11), Eq. (5.12) yields

$$ {}^{\mathcal{B}_1}\mathbf{e} = \underbrace{{}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}^T}_{=:{}^{\mathcal{B}_1\mathcal{B}_2}\mathbf{A}}{}^{\mathcal{B}_2}\mathbf{e} \tag{5.13} $$

Therefore, we have

$$ {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}^{-1} = {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}^T = {}^{\mathcal{B}_1\mathcal{B}_2}\mathbf{A} \tag{5.14} $$

Postmultiplying Eq. (5.8) by ${}^{\mathcal{B}_1}\mathbf{e}^T$ (i.e., multiplication of Eq. (5.8) by ${}^{\mathcal{B}_1}\mathbf{e}^T$ from the right), we can express ${}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}$, using ${}^{\mathcal{B}_1}\mathbf{e}$ and ${}^{\mathcal{B}_2}\mathbf{e}$:

$$ {}^{\mathcal{B}_2}\mathbf{e}\cdot{}^{\mathcal{B}_1}\mathbf{e}^T = {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}\,\underbrace{({}^{\mathcal{B}_1}\mathbf{e}\cdot{}^{\mathcal{B}_1}\mathbf{e}^T)}_{\mathbf{I}_n} = {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A} \tag{5.15} $$

The same vector $\vec{\pi}(\mathbf{O}_1,\mathbf{P})$ given in Eq. (5.7) can be also expressed with respect to $\mathcal{B}_2$ as

$$ \vec{\pi}(\mathbf{O}_1,\mathbf{P}) = {}^{\mathcal{B}_2}\mathbf{e}^T\,{}^{\mathcal{B}_2}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) = {}^{\mathcal{B}_2}\boldsymbol{\pi}^T(\mathbf{O}_1,\mathbf{P})\,{}^{\mathcal{B}_2}\mathbf{e} \tag{5.16} $$

where

$$ \begin{aligned} {}^{\mathcal{B}_2}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) &:= [{}^{\mathcal{B}_2}\pi_1(\mathbf{O}_1,\mathbf{P}), {}^{\mathcal{B}_2}\pi_2(\mathbf{O}_1,\mathbf{P}), \cdots, {}^{\mathcal{B}_2}\pi_n(\mathbf{O}_1,\mathbf{P})]^T \\ &= [{}^{\mathcal{B}_2}\pi_i(\mathbf{O}_1,\mathbf{P})] \in \mathbb{R}^n \end{aligned} \tag{5.17} $$

Note that we, in general, have

$$ {}^{\mathcal{B}_1}\pi_i(\mathbf{O}_1,\mathbf{P}) \neq {}^{\mathcal{B}_2}\pi_i(\mathbf{O}_1,\mathbf{P}) \tag{5.18} $$

for $i = 1, 2, \cdots, n$ unless otherwise the frame $\mathcal{B}_1$ tallies with $\mathcal{B}_2$. The vector ${}^{\mathcal{B}_\ell}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) = [{}^{\mathcal{B}_\ell}\pi_i(\mathbf{O}_1,\mathbf{P})] \in \mathbb{R}^n$ (for $\ell = 1, 2$) or the coefficients ${}^{\mathcal{B}_\ell}\pi_i(\mathbf{O}_1,\mathbf{P}) \in \mathbb{R}$ can be always explicitly expressed as

$$ \begin{aligned} {}^{\mathcal{B}_\ell}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) &= {}^{\mathcal{B}_\ell}\mathbf{e}\cdot\vec{\pi}(\mathbf{O}_1,\mathbf{P}) \\ {}^{\mathcal{B}_\ell}\pi_i(\mathbf{O}_1,\mathbf{P}) &= {}^{\mathcal{B}_\ell}\vec{\mathbf{e}}_i\cdot\vec{\pi}(\mathbf{O}_1,\mathbf{P}) \end{aligned} \tag{5.19} $$

Theorem 5.1.1 (Position Component Vector)

Consider a point, $\mathbf{P} \in \mathbb{E}^n$, and two Cartesian frames, $\mathcal{B}_1 : (\mathbf{O}_1; \{{}^{\mathcal{B}_1}\vec{\mathbf{e}}_i\}_{i=1}^n)$ and $\mathcal{B}_2 : (\mathbf{O}_2; \{{}^{\mathcal{B}_2}\vec{\mathbf{e}}_i\}_{i=1}^n)$, defined in the n-dimensional Euclidean space. The component vector of vector $\vec{\pi}(\mathbf{O}_1,\mathbf{P})$ in terms of frame $\mathcal{B}_1$ can be expressed as:

$$ \boxed{{}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) = {}^{\mathcal{B}_1\mathcal{B}_2}\mathbf{A}\,{}^{\mathcal{B}_2}\boldsymbol{\pi}(\mathbf{O}_2,\mathbf{P}) + {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{O}_2)} \tag{5.20} $$

Proof. We can define the position vectors, i.e., the radius vectors with respect to the origins of the two different frames, $\mathcal{B}_1$ and $\mathcal{B}_2$, as

$$\vec{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{P}) = \mathbf{P} - \mathbf{O}_1 \ \text{ and } \ \vec{\boldsymbol{\pi}}(\mathbf{O}_2, \mathbf{P}) = \mathbf{P} - \mathbf{O}_2 \tag{5.21}$$

and the radius vector between the origin points, $\mathbf{O}_1$ and $\mathbf{O}_2$, is given as

$$\vec{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{O}_2) = \mathbf{O}_2 - \mathbf{O}_1 \tag{5.22}$$

Thus, we can readily show

$$\vec{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{P}) = \vec{\boldsymbol{\pi}}(\mathbf{O}_2, \mathbf{P}) + \vec{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{O}_2) \tag{5.23}$$

Since vector $\vec{\boldsymbol{\pi}}(\mathbf{O}_2, \mathbf{P})$ can be expressed, using ${}^{\mathcal{B}_1}\mathbf{e}$, as

$$\begin{aligned}
\vec{\boldsymbol{\pi}}(\mathbf{O}_2, \mathbf{P}) &= {}^{\mathcal{B}_2}\mathbf{e}^T \, {}^{\mathcal{B}_2}\boldsymbol{\pi}(\mathbf{O}_2, \mathbf{P}) = ({}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}^{\mathcal{B}_1}\mathbf{e})^T \, {}^{\mathcal{B}_2}\boldsymbol{\pi}(\mathbf{O}_2, \mathbf{P}) \\
&= \left[{}^{\mathcal{B}_1}\mathbf{e}^T \, {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}^T\right] \, {}^{\mathcal{B}_2}\boldsymbol{\pi}(\mathbf{O}_2, \mathbf{P}) \\
&= {}^{\mathcal{B}_1}\mathbf{e}^T \underbrace{\left[{}^{\mathcal{B}_1\mathcal{B}_2}\mathbf{A} \, {}^{\mathcal{B}_2}\boldsymbol{\pi}(\mathbf{O}_2, \mathbf{P})\right]}_{{}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_2, \mathbf{P})}
\end{aligned} \tag{5.24}$$

Eq. (5.23) yields in terms of $\mathcal{B}_1$ as

$${}^{\mathcal{B}_1}\mathbf{e}^T \, {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{P}) = {}^{\mathcal{B}_1}\mathbf{e}^T \, \left[{}^{\mathcal{B}_1\mathcal{B}_2}\mathbf{A} \, {}^{\mathcal{B}_2}\boldsymbol{\pi}(\mathbf{O}_2, \mathbf{P}) + {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{O}_2)\right] \tag{5.25}$$

where ${}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{P}) \in \mathbb{R}^n$ and ${}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{O}_2) \in \mathbb{R}^n$ are the component n-tuples of the vectors $\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{P})$ and $\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{O}_2)$ with respect to the base vector ${}^{\mathcal{B}_1}\vec{\mathbf{e}}_i$ (for $i = 1, 2, \cdots, n$). Hence, we obtain the following relation:

$${}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{P}) = {}^{\mathcal{B}_1\mathcal{B}_2}\mathbf{A} \, {}^{\mathcal{B}_2}\boldsymbol{\pi}(\mathbf{O}_2, \mathbf{P}) + {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{O}_2) \tag{5.26}$$

5.1.2 In the three-dimensional Euclidean Space

In accordance with the discussion in the previous section, we confine our attention to a three dimensional Euclidean space $\mathbb{E}^3$. We can decompose a vector $\vec{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{P}) \in \mathbb{V}^3$ as

$$\begin{aligned}\vec{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{P}) &= {}^{\mathcal{B}_1}\pi_i(\mathbf{O}_1, \mathbf{P})\,{}^{\mathcal{B}_1}\vec{\mathbf{e}}_i \\ &= {}^{\mathcal{B}_1}\pi_1(\mathbf{O}_1, \mathbf{P})\,{}^{\mathcal{B}_1}\vec{\mathbf{e}}_1 + {}^{\mathcal{B}_1}\pi_2(\mathbf{O}_1, \mathbf{P})\,{}^{\mathcal{B}_1}\vec{\mathbf{e}}_2 + +{}^{\mathcal{B}_1}\pi_3(\mathbf{O}_1, \mathbf{P})\,{}^{\mathcal{B}_1}\vec{\mathbf{e}}_3 \\ &= {}^{\mathcal{B}_1}\mathbf{e}^T\,{}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{P}) = {}^{\mathcal{B}_1}\boldsymbol{\pi}^T(\mathbf{O}_1, \mathbf{P})\,{}^{\mathcal{B}_1}\mathbf{e}\end{aligned} \tag{5.27}$$

with respect to the Cartesian frame $\mathcal{B}_1 : (\mathbf{O}_1; \{{}^{\mathcal{B}_1}\vec{\mathbf{e}}_i\}_{i=1}^3)$; see Eq. (5.4) and Eq. (5.7). Note that the orthonormal base vectors satisfy [4]

$$|({}^{\mathcal{B}_1}\vec{\mathbf{e}}_1 \times {}^{\mathcal{B}_1}\vec{\mathbf{e}}_2) \cdot {}^{\mathcal{B}_1}\vec{\mathbf{e}}_3| = 1 \tag{5.29}$$

and, hereafter, we assume the base vectors always satisfy the ***right-handedness condition***:[5]

$$\boxed{({}^{\mathcal{B}_1}\vec{\mathbf{e}}_1 \times {}^{\mathcal{B}_1}\vec{\mathbf{e}}_2) \cdot {}^{\mathcal{B}_1}\vec{\mathbf{e}}_3 = +1} \tag{5.31}$$

so that the orthonormal base vectors are oriented in the sense of

$${}^{\mathcal{B}_1}\vec{\mathbf{e}}_i \times {}^{\mathcal{B}_1}\vec{\mathbf{e}}_j = \epsilon_{ijk}\,{}^{\mathcal{B}_1}\vec{\mathbf{e}}_k \tag{5.32}$$

---

[4] The ***cross product*** (or vector product) " $\times$ " is defined as

$$\vec{\mathbf{x}} \times \vec{\mathbf{y}} = (\|\vec{\mathbf{x}}\|\|\vec{\mathbf{y}}\| \sin\theta)\vec{\mathbf{e}} \quad \forall \vec{\mathbf{x}}, \vec{\mathbf{y}} \in \mathbb{V}^3 \tag{5.28}$$

where $\theta \in [0, \pi]$ is the (acute) angle between $\vec{\mathbf{x}}$ and $\vec{\mathbf{y}}$, and $\vec{\mathbf{e}}$ is a unit vector perpendicular to the plane containing $\vec{\mathbf{x}}$ and $\vec{\mathbf{y}}$.

[5] On the other hand, the left-handed base vectors satisfy

$$({}^{\mathcal{B}_1}\vec{\mathbf{e}}_1 \times {}^{\mathcal{B}_1}\vec{\mathbf{e}}_2) \cdot {}^{\mathcal{B}_1}\vec{\mathbf{e}}_3 = -1 \tag{5.30}$$

where ϵ_{ijk} is the ***Levi-Civita*** symbol [6] .

Remark 5.1.1 (Tilde Matrix)

1. *It is worth mentioning in this connection the following properties of* ${}^{\mathcal{B}_1}\mathbf{e} := [{}^{\mathcal{B}_1}\vec{\mathbf{e}}_1, {}^{\mathcal{B}_1}\vec{\mathbf{e}}_2, {}^{\mathcal{B}_1}\vec{\mathbf{e}}_3]^T$ *hold:*

$$\begin{aligned} {}^{\mathcal{B}_1}\mathbf{e}^T \times {}^{\mathcal{B}_1}\mathbf{e} &= \mathbf{0} && (5.34) \\ {}^{\mathcal{B}_1}\mathbf{e} \times {}^{\mathcal{B}_1}\mathbf{e}^T &= -{}^{\mathcal{B}_1}\widetilde{\mathbf{e}} && (5.35) \end{aligned}$$

where ${}^{\mathcal{B}_1}\widetilde{\mathbf{e}}$ *is the* ***tilde matrix*** *of* ${}^{\mathcal{B}_1}\mathbf{e}$ *defined by*

$${}^{\mathcal{B}_1}\widetilde{\mathbf{e}} := \begin{bmatrix} 0 & -{}^{\mathcal{B}_1}\vec{\mathbf{e}}_3 & {}^{\mathcal{B}_1}\vec{\mathbf{e}}_2 \\ {}^{\mathcal{B}_1}\vec{\mathbf{e}}_3 & 0 & -{}^{\mathcal{B}_1}\vec{\mathbf{e}}_1 \\ -{}^{\mathcal{B}_1}\vec{\mathbf{e}}_2 & {}^{\mathcal{B}_1}\vec{\mathbf{e}}_1 & 0 \end{bmatrix} \tag{5.36}$$

The tilde matrix plays an important role in multibody analysis; and it actually can be defined for any component vector ${}^{\mathcal{B}_1}\mathbf{a} = [{}^{\mathcal{B}_1}a_1, {}^{\mathcal{B}_1}a_2, {}^{\mathcal{B}_1}a_3]^T \in \mathbb{R}^3$ *as*

$${}^{\mathcal{B}_1}\widetilde{\mathbf{a}} := \begin{bmatrix} 0 & -{}^{\mathcal{B}_1}a_3 & {}^{\mathcal{B}_1}a_2 \\ {}^{\mathcal{B}_1}a_3 & 0 & -{}^{\mathcal{B}_1}a_1 \\ -{}^{\mathcal{B}_1}a_2 & {}^{\mathcal{B}_1}a_1 & 0 \end{bmatrix} \in \mathbb{R}^{3\times 3} \tag{5.37}$$

and it is always skew-symmetric, i.e., ${}^{\mathcal{B}_1}\widetilde{\mathbf{a}}^T = -{}^{\mathcal{B}_1}\widetilde{\mathbf{a}}$*. Notice that Eq. (5.36) and Eq. (5.37) are related to one another as*

$${}^{\mathcal{B}_1}\widetilde{\mathbf{a}} = {}^{\mathcal{B}_1}\widetilde{\mathbf{e}} \cdot \vec{\mathbf{a}} \tag{5.38}$$

---

[6] The Levi-Civita symbol in three dimensions is defined as:

$$\epsilon_{ijk} = \begin{cases} +1 & \text{if } (i,j,k) \text{ is } (1,2,3), (2,3,1), \text{ or } (3,1,2) \\ -1 & \text{if } (i,j,k) \text{ is } (3,2,1), (21,3,2), \text{ or } (2,1,3) \\ 0 & \text{if } i = j \text{ or } j = k \text{ or } k = i \end{cases} \tag{5.33}$$

for $i, j, k = 1, 2, 3$.

2. Suppose we define another Cartesian frame $\mathcal{B}_2 : (\mathbf{O}_2; \{{}^{\mathcal{B}_2}\vec{\mathbf{e}}_i\}_{i=1}^3)$*. Invoking Eq.* (5.13), *Eq.* (5.35) *yields*

$$\begin{aligned} {}^{\mathcal{B}_1}\widetilde{\mathbf{e}} &= -{}^{\mathcal{B}_1}\mathbf{e} \times {}^{\mathcal{B}_1}\mathbf{e}^T = -{}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}^T \underbrace{({}^{\mathcal{B}_2}\mathbf{e} \times {}^{\mathcal{B}_2}\mathbf{e}^T)}_{-{}^{\mathcal{B}_2}\widetilde{\mathbf{e}}} {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A} \\ &= {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}^T \, {}^{\mathcal{B}_2}\widetilde{\mathbf{e}} \, {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A} = {}^{\mathcal{B}_1\mathcal{B}_2}\mathbf{A} \, {}^{\mathcal{B}_2}\widetilde{\mathbf{e}} \, {}^{\mathcal{B}_1\mathcal{B}_2}\mathbf{A}^T \end{aligned} \tag{5.39}$$

Since ${}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}$ *is orthogonal, i.e.,* ${}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}^T = {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}^{-1}$*,we readily get*

$${}^{\mathcal{B}_2}\widetilde{\mathbf{e}} = {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A} \, {}^{\mathcal{B}_1}\widetilde{\mathbf{e}} \, {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}^T \tag{5.40}$$

Similarly, we can show

$$\begin{aligned} {}^{\mathcal{B}_1}\widetilde{\mathbf{a}} &= {}^{\mathcal{B}_1\mathcal{B}_2}\mathbf{A} \, {}^{\mathcal{B}_2}\widetilde{\mathbf{a}} \, {}^{\mathcal{B}_1\mathcal{B}_2}\mathbf{A}^T \\ {}^{\mathcal{B}_2}\widetilde{\mathbf{a}} &= {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A} \, {}^{\mathcal{B}_1}\widetilde{\mathbf{a}} \, {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}^T \end{aligned} \tag{5.41}$$

from Eq. (5.38)*. Summarizing, we have the following relations between two arbitrary Cartesian frames,* $\mathcal{B}_i$ *and* $\mathcal{B}_j$*:*

$${}^{\mathcal{B}_i/\mathcal{B}_j}\mathbf{A} \, {}^{\mathcal{B}_j}\widetilde{\mathbf{e}} = {}^{\mathcal{B}_i}\widetilde{\mathbf{e}} \, {}^{\mathcal{B}_i/\mathcal{B}_j}\mathbf{A} \tag{5.42}$$

$${}^{\mathcal{B}_i/\mathcal{B}_j}\mathbf{A} \, {}^{\mathcal{B}_j}\widetilde{\mathbf{a}} = {}^{\mathcal{B}_i}\widetilde{\mathbf{a}} \, {}^{\mathcal{B}_i/\mathcal{B}_j}\mathbf{A} \tag{5.43}$$

Corollary 5.1.1 (Theorem 5.1.1)

In $\mathbb{E}^3$*, frames* $\mathcal{B}_i$ *are right-handed rectangular trihedron as shown in Fig. 5.1, for* $i = 1, 2$*. In view of Eq.* (5.26)*, the position component vector may be derived analogously as*

$$\boxed{{}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{P}) = {}^{\mathcal{B}_1\mathcal{B}_2}\mathbf{A} \, {}^{\mathcal{B}_2}\boldsymbol{\pi}(\mathbf{O}_2, \mathbf{P}) + {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{O}_2)} \tag{5.44}$$

See Fig. 5.1 for the illustration of Eq, (5.44)*. This equation plays an important role in rigid-multibody kinematics and dynamics.*

Remark 5.1.2 (Eq. (5.44))

1. ***Directional Cosine Matrix:*** *Invoking Eq.* (5.15), ${}^{\mathcal{B}_1\mathcal{B}_2}\mathbf{A}$ *in Eq.* (5.44) *may be expressed in terms of* ${}^{\mathcal{B}_1}\mathbf{e}$ *and* ${}^{\mathcal{B}_2}\mathbf{e}$ *as*

$$
\begin{aligned}
{}^{\mathcal{B}_1\mathcal{B}_2}\mathbf{A} &= {}^{\mathcal{B}_1}\mathbf{e} \cdot {}^{\mathcal{B}_2}\mathbf{e}^T \\
&= \begin{bmatrix} {}^{\mathcal{B}_1}\vec{\mathbf{e}}_1 \cdot {}^{\mathcal{B}_2}\vec{\mathbf{e}}_1 & {}^{\mathcal{B}_1}\vec{\mathbf{e}}_1 \cdot {}^{\mathcal{B}_2}\vec{\mathbf{e}}_2 & {}^{\mathcal{B}_1}\vec{\mathbf{e}}_1 \cdot {}^{\mathcal{B}_2}\vec{\mathbf{e}}_3 \\ {}^{\mathcal{B}_1}\vec{\mathbf{e}}_2 \cdot {}^{\mathcal{B}_2}\vec{\mathbf{e}}_1 & {}^{\mathcal{B}_1}\vec{\mathbf{e}}_2 \cdot {}^{\mathcal{B}_2}\vec{\mathbf{e}}_2 & {}^{\mathcal{B}_1}\vec{\mathbf{e}}_2 \cdot {}^{\mathcal{B}_2}\vec{\mathbf{e}}_3 \\ {}^{\mathcal{B}_1}\vec{\mathbf{e}}_3 \cdot {}^{\mathcal{B}_2}\vec{\mathbf{e}}_1 & {}^{\mathcal{B}_1}\vec{\mathbf{e}}_3 \cdot {}^{\mathcal{B}_2}\vec{\mathbf{e}}_2 & {}^{\mathcal{B}_1}\vec{\mathbf{e}}_3 \cdot {}^{\mathcal{B}_2}\vec{\mathbf{e}}_3 \end{bmatrix}
\end{aligned}
\tag{5.45}
$$

That is, the components yields

$$
{}^{\mathcal{B}_1\mathcal{B}_2}A_{ij} = {}^{\mathcal{B}_1}\vec{\mathbf{e}}_i \cdot {}^{\mathcal{B}_2}\vec{\mathbf{e}}_j = \cos\sphericalangle({}^{\mathcal{B}_1}\vec{\mathbf{e}}_i, {}^{\mathcal{B}_2}\vec{\mathbf{e}}_j) \tag{5.46}
$$

2. *The determinant of* ${}^{\mathcal{B}_1\mathcal{B}_2}\mathbf{A}$ *is given as*

$$
\det({}^{\mathcal{B}_1\mathcal{B}_2}\mathbf{A}) = +1 \tag{5.47}
$$

as long as the right-handedness condition, i.e., Eq. (5.31), *holds. In other words, the orthogonal matrix* ${}^{\mathcal{B}_1\mathcal{B}_2}\mathbf{A}$ *belongs to the* ***special orthogonal group*** $SO(3)$[7] *if we assume Eq.* (5.31) *holds:*

$$
{}^{\mathcal{B}_1\mathcal{B}_2}\mathbf{A} \in SO(3) \tag{5.48}
$$

[7] *See Definition A.2.4*

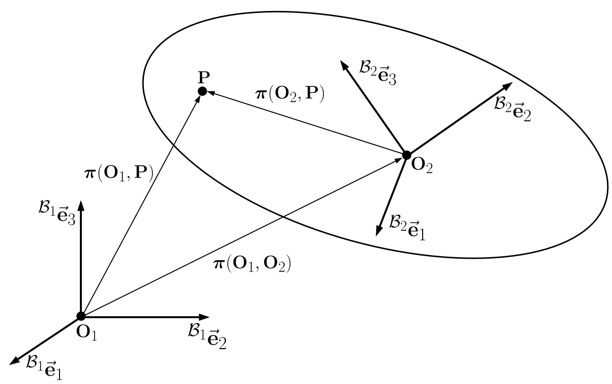


Figure 5.1: Three-dimensional Euclidean Space

5.2 Angular Orientations

In this section, we show two approaches to express the angular orientation of a rigid body in $\mathbb{E}^3$ as a function of the generalized coordinates; namely, the ***Euler angles*** (ϕ, θ, ψ) and ***Euler parameters***. Without loss of generality, let us assume the origins of the frames $\mathcal{B}_i$ used coincides with each other, i.e., $\vec{\boldsymbol{\pi}}(\mathbf{O}_i, \mathbf{O}_j) = \vec{\mathbf{0}}$.

5.2.1 Euler Angles

In order to completely describe the orientation of a rigid body in $\mathbb{E}^3$, let us introduce three independent parameters (ϕ, θ, ψ) called the ***Euler angles***. The orientation of the rigid body is determined as a result of the following three successive rotational steps.

Step 1: Let $\mathcal{B}_0 : (\mathbf{O}; \{{}^{\mathcal{B}_0}\vec{\mathbf{e}}_i\}_{i=1}^n)$ be the reference frame in $\mathbb{E}^3$. Suppose $\mathcal{B}_1 : (\mathbf{O}; \{{}^{\mathcal{B}_1}\vec{\mathbf{e}}_i\}_{i=1}^n)$ is rigidly attached to the rigid body in $\mathbb{E}^3$, and the frame $\mathcal{B}_1$ initially coincides with the frame $\mathcal{B}_0$. Then, the first rotation by angle ϕ in the counterclockwise direction about the ${}^{\mathcal{B}_0}\vec{\mathbf{e}}_3$-axis as yields

$$ {}^{\mathcal{B}_1}\mathbf{e} = {}^{\mathcal{B}_1\mathcal{B}_0}\mathbf{A}\,{}^{\mathcal{B}_0}\mathbf{e} \tag{5.49}$$

(see Eq. (5.8)) where ${}^{\mathcal{B}_1\mathcal{B}_0}\mathbf{A} \in SO(3)$ is given by

$$ {}^{\mathcal{B}_1\mathcal{B}_0}\mathbf{A} = \mathbf{A}_{\mathrm{z}}(\phi) = \begin{bmatrix} \cos(\phi) & \sin(\phi) & 0 \\ -\sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{5.50}$$

Step 2: Suppose $\mathcal{B}_2 : (\mathbf{O}; \{{}^{\mathcal{B}_2}\vec{\mathbf{e}}_i\}_{i=1}^n)$ is rigidly attached to the rigid body in $\mathbb{E}^3$, and the frame $\mathcal{B}_2$ initially coincides with the frame $\mathcal{B}_1$. Then, the second rotation by angle θ in the counterclockwise direction about the ${}^{\mathcal{B}_1}\vec{\mathbf{e}}_1$-axis as yields

$$ {}^{\mathcal{B}_2}\mathbf{e} = {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A}\,{}^{\mathcal{B}_1}\mathbf{e} \tag{5.51}$$

where ${}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A} \in SO(3)$ is given by

$$ {}^{\mathcal{B}_2\mathcal{B}_1}\mathbf{A} = \mathbf{A}_{\mathrm{x}}(\theta) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta) & \sin(\theta) \\ 0 & -\sin(\theta) & \cos(\theta) \end{bmatrix} \tag{5.52}$$

Step 3: Suppose $\mathcal{B}_3 : (\mathbf{O}; \{{}^{\mathcal{B}_3}\vec{\mathbf{e}}_i\}_{i=1}^n)$ is rigidly attached to the rigid body in $\mathbb{E}^3$, and the frame $\mathcal{B}_3$ initially coincides with the frame $\mathcal{B}_2$. It is this frame $\mathcal{B}_3$ that we use to express the coordinates of any point in the rigid body; however, the objective here is to determine the coordinates with respect to the initial frame $\mathcal{B}_0$. Then, the third (last) rotation by angle ψ in the counterclockwise direction about the ${}^{\mathcal{B}_2}\vec{\mathbf{e}}_3$-axis yields

$$ {}^{\mathcal{B}_3}\mathbf{e} = {}^{\mathcal{B}_3\mathcal{B}_2}\mathbf{A}\,{}^{\mathcal{B}_2}\mathbf{e} \tag{5.53}$$

where ${}^{\mathcal{B}_3\mathcal{B}_2}\mathbf{A} \in SO(3)$ is given by

$$
{}^{\mathcal{B}_3\mathcal{B}_2}\mathbf{A} = \mathbf{A}_{\mathrm{z}}(\psi) = \begin{bmatrix} \cos(\psi) & \sin(\psi) & 0 \\ -\sin(\psi) & \cos(\psi) & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{5.54}
$$

From Eqns. (5.49)-(5.53), we can relate ${}^{\mathcal{B}_3}\mathbf{e}$ to the original ${}^{\mathcal{B}_0}\mathbf{e}$ as

$$
{}^{\mathcal{B}_3}\mathbf{e} = \mathbf{A}_{(313)}\, {}^{\mathcal{B}_0}\mathbf{e} \tag{5.55}
$$

where

$$
\begin{aligned}
\mathbf{A}_{(313)} &:= \mathbf{A}_{\mathrm{z}}(\psi)\mathbf{A}_{\mathrm{x}}(\theta)\mathbf{A}_{\mathrm{z}}(\phi) \\
&= \begin{bmatrix} \cos(\psi)\cos(\phi) - \sin(\psi)\cos(\theta)\sin(\phi) & \sin(\psi)\cos(\phi) + \cos(\psi)\cos(\theta)\sin(\phi) & \sin(\theta)\sin(\phi) \\ -\cos(\psi)\sin(\phi) - \sin(\psi)\cos(\theta)\cos(\phi) & -\sin(\psi)\sin(\phi) + \cos(\psi)\cos(\theta)\cos(\phi) & \sin(\theta)\cos(\phi) \\ \sin(\psi)\sin(\theta) & -\cos(\psi)\sin(\theta) & \cos(\theta) \end{bmatrix}
\end{aligned} \tag{5.56}
$$

Remark 5.2.1 (Euler Angles)

1. $\mathbf{A}_{(313)}$ *belongs to the special orthogonal group* $SO(3)$ *for* $\mathbf{A}_{\mathrm{z}}(\phi), \mathbf{A}_{\mathrm{x}}(\theta), \mathbf{A}_{\mathrm{z}}(\psi) \in SO(3)$*:*

$$
\mathbf{A}_{(313)}\,(\mathbf{A}_{(313)})^T = (\mathbf{A}_{\mathrm{z}}(\psi)\mathbf{A}_{\mathrm{x}}(\theta)\mathbf{A}_{\mathrm{z}}(\phi))(\mathbf{A}_{\mathrm{z}}(\psi)\mathbf{A}_{\mathrm{x}}(\theta)\mathbf{A}_{\mathrm{z}}(\phi))^T = \mathbf{I}_3 \;\; \textit{and} \;\; \det(\mathbf{A}_{(313)}) = +1 \tag{5.57}
$$

2. *The Euler angles*

$$
\phi \in [0, 2\pi), \quad \theta \in [0, 2\pi], \quad \psi \in [0, 2\pi) \tag{5.58}
$$

However, a serious ***singularity*** *issue occurs whenever the* ${}^{\mathcal{B}_1}\vec{\mathbf{e}}_1$*-axis in* ***step 1*** *and the* ${}^{\mathcal{B}_2}\vec{\mathbf{e}}_3$*-axis in* ***step 3*** *are aligned. This situation happens if* $\theta = 0$ *or* $\theta = \pi$*.*

3. *When a numerical value of* $\mathbf{A}_{(313)}$ *is available as* $\hat{\mathbf{A}} = [\hat{A}_{ij}] \simeq \mathbf{A}_{(313)}$, *we can calculate the* ***Euler angles*** (ϕ, θ, ψ) *from*

$$\begin{aligned} \sin(\phi) &= \hat{A}_{13}/\hat{A}, \quad \cos(\phi) = \hat{A}_{23}/\hat{A} \\ \sin(\theta) &= \hat{A}, \quad \cos(\theta) = \hat{A}_{33} \\ \sin(\psi) &= \hat{A}_{31}/\hat{A}, \quad \cos(\psi) = -\hat{A}_{32} \end{aligned} \tag{5.59}$$

where $\hat{A} := \sqrt{1 - \hat{A}_{33}^2}$.

4. *If we change the order of the successive rotations, the resulting transformation matrices may become different from the one in Eq.* (5.56) *which are obtained by rotating axes* 3, 1, *and* 3 *sequentially [3→1→3]. For example, rotation [3→2→1] leads to*

$$^{\mathcal{B}_3}\mathbf{e} = \mathbf{A}_{(321)}\ {}^{\mathcal{B}_0}\mathbf{e} \tag{5.60}$$

where $\mathbf{A}_{(321)}$ *is given in Eq.* (5.62) *overleaf. In this case, the angles* $(\varphi_{c_1}, \varphi_{c_2}, \varphi_{c_3})$ *are called the* ***Cardan angles***. *On the other hand, rotation [1→2→3] leads to*

$$^{\mathcal{B}_3}\mathbf{e} = \mathbf{A}_{(123)}\ {}^{\mathcal{B}_0}\mathbf{e} \tag{5.61}$$

where $\mathbf{A}_{(123)}$ *is given in Eq.* (5.63). *In this case, the angles* $(\varphi_{b_1}, \varphi_{b_2}, \varphi_{b_3})$ *are called the* ***Bryant angles***. *Notice that the initial and final frames, i.e.,* $\mathcal{B}_0$ *and* $\mathcal{B}_3$, *respectively, in Eqns.* (5.55), (5.60), *and* (5.64) *are the same. Similar to the case of the Euler angles, the singularity issues may occur at the critical points during the numerical simulation using the Cardan or Bryant angles*[8] *; however, we can dispense with this problem if we use the so-called* ***Euler parameters***, *which will be introduced in the next subsection, instead.*

[8] *The critical points are:* $\varphi_{c_2} = \pi/2$ *for the case of Cardan angles.*

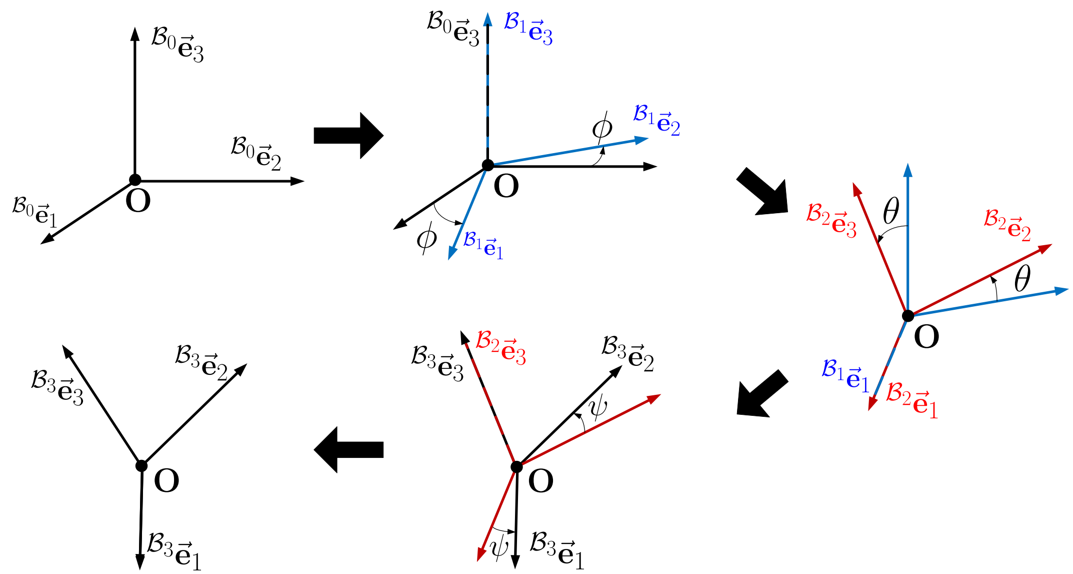


Figure 5.2: Euler Angles

$$\mathbf{A}_{(321)} := \mathbf{A}_{\mathrm{x}}(\varphi_{\mathrm{c}_3})\mathbf{A}_{\mathrm{y}}(\varphi_{\mathrm{c}_2})\mathbf{A}_{\mathrm{z}}(\varphi_{\mathrm{c}_1})$$

$$= \begin{bmatrix} \cos(\varphi_{\mathrm{c}_1})\cos(\varphi_{\mathrm{c}_2}) & \sin(\varphi_{\mathrm{c}_1})\cos(\varphi_{\mathrm{c}_2}) & -\sin(\varphi_{\mathrm{c}_2}) \\ -\sin(\varphi_{\mathrm{c}_1})\cos(\varphi_{\mathrm{c}_3}) + \cos(\varphi_{\mathrm{c}_1})\sin(\varphi_{\mathrm{c}_2})\sin(\varphi_{\mathrm{c}_3}) & \cos(\varphi_{\mathrm{c}_1})\cos(\varphi_{\mathrm{c}_3}) + \sin(\varphi_{\mathrm{c}_1})\sin(\varphi_{\mathrm{c}_2})\sin(\varphi_{\mathrm{c}_3}) & \cos(\varphi_{\mathrm{c}_2})\sin(\varphi_{\mathrm{c}_3}) \\ \sin(\varphi_{\mathrm{c}_1})\sin(\varphi_{\mathrm{c}_3}) + \sin(\varphi_{\mathrm{c}_2})\cos(\varphi_{\mathrm{c}_1})\cos(\varphi_{\mathrm{c}_3}) & -\cos(\varphi_{\mathrm{c}_1})\sin(\varphi_{\mathrm{c}_3}) + \cos(\varphi_{\mathrm{c}_3})\sin(\varphi_{\mathrm{c}_1})\sin(\varphi_{\mathrm{c}_2}) & \cos(\varphi_{\mathrm{c}_2})\cos(\varphi_{\mathrm{c}_3}) \end{bmatrix} \tag{5.62}$$

$$\mathbf{A}_{(123)} := \mathbf{A}_{\mathrm{z}}(\varphi_{\mathrm{b}_3})\mathbf{A}_{\mathrm{y}}(\varphi_{\mathrm{b}_2})\mathbf{A}_{\mathrm{x}}(\varphi_{\mathrm{b}_1})$$

$$= \begin{bmatrix} \cos(\varphi_{\mathrm{b}_2})\cos(\varphi_{\mathrm{c}_3}) & \cos(\varphi_{\mathrm{b}_1})\sin(\varphi_{\mathrm{c}_3}) + \cos(\varphi_{\mathrm{c}_3})\sin(\varphi_{\mathrm{b}_1})\sin(\varphi_{\mathrm{b}_2}) & \sin(\varphi_{\mathrm{b}_1})\sin(\varphi_{\mathrm{c}_3}) - \sin(\varphi_{\mathrm{b}_2})\cos(\varphi_{\mathrm{b}_1})\cos(\varphi_{\mathrm{c}_3}) \\ -\cos(\varphi_{\mathrm{b}_2})\sin(\varphi_{\mathrm{c}_3}) & \cos(\varphi_{\mathrm{b}_1})\cos(\varphi_{\mathrm{c}_3}) - \sin(\varphi_{\mathrm{b}_1})\sin(\varphi_{\mathrm{b}_2})\sin(\varphi_{\mathrm{c}_3}) & \cos(\varphi_{\mathrm{c}_3})\sin(\varphi_{\mathrm{b}_1}) + \cos(\varphi_{\mathrm{b}_1})\sin(\varphi_{\mathrm{b}_2})\sin(\varphi_{\mathrm{c}_3}) \\ \sin(\varphi_{\mathrm{b}_2}) & -\cos(\varphi_{\mathrm{b}_2})\sin(\varphi_{\mathrm{b}_1}) & \cos(\varphi_{\mathrm{b}_1})\cos(\varphi_{\mathrm{b}_2}) \end{bmatrix} \tag{5.63}$$

5.2.2 Rotation about an Arbitrary Axis

Consider the reference Cartesian frame $\mathcal{B}_0 : (\mathbf{O}; \{^{\mathcal{B}_0}\vec{\mathbf{e}}_i\}_{i=1}^n)$ in $\mathbb{E}^3$ again. Suppose Cartesian frame $\mathcal{B}_3 : (\mathbf{O}; \{^{\mathcal{B}_3}\vec{\mathbf{e}}_i\}_{i=1}^n)$, which is rigidly fixed to a rigid body in $\mathbb{E}^3$, is *directly* obtained by the rotation of $\mathcal{B}_0$ about an arbitrary axis $\vec{\mathbf{n}}$ by φ (in the counter-clock wise positive direction) as shown in Fig. 5.3:

$$^{\mathcal{B}_3}\mathbf{e} = {}^{\mathcal{B}_3\mathcal{B}_0}\mathbf{A}\ {}^{\mathcal{B}_0}\mathbf{e}, \quad {}^{\mathcal{B}_3\mathcal{B}_0}\mathbf{A} = \mathbf{A}_{\mathrm{n}}(\varphi) \in SO(3) \tag{5.64}$$

Notice that the origins of the frames are assumed to coincide, and assume $\|\vec{\mathbf{n}}\| = 1$. This rotation about $\vec{\mathbf{n}}$ implies $^{\mathcal{B}_1}\mathbf{n} = {}^{\mathcal{B}_3}\mathbf{n} =: \mathbf{n} = [n_1, n_2, n_3]^T \in \mathbb{R}^3$; that is,

$$\mathbf{n} = {}^{\mathcal{B}_0}\mathbf{e} \cdot \vec{\mathbf{n}} = {}^{\mathcal{B}_3}\mathbf{e} \cdot \vec{\mathbf{n}} \quad \text{or} \quad \vec{\mathbf{n}} = n_i\, {}^{\mathcal{B}_0}\vec{\mathbf{e}}_i = n_i\, {}^{\mathcal{B}_3}\vec{\mathbf{e}}_i \tag{5.65}$$

Suppose this rotation maps point $\mathbf{P} \in \mathbb{E}^3$ to $\mathbf{Q} \in \mathbb{E}^3$ in the body [9] , and let the position vectors be

$$\vec{\pi}(\mathbf{O}, \mathbf{P}) \ := \ \vec{\mathbf{p}} = {}^{\mathcal{B}_0}\mathbf{p}^T\, {}^{\mathcal{B}_0}\mathbf{e} = {}^{\mathcal{B}_3}\mathbf{p}^T\, {}^{\mathcal{B}_3}\mathbf{e} \tag{5.66}$$

$$\vec{\pi}(\mathbf{O}, \mathbf{Q}) \ := \ \vec{\mathbf{q}} = {}^{\mathcal{B}_0}\mathbf{q}^T\, {}^{\mathcal{B}_0}\mathbf{e} = {}^{\mathcal{B}_3}\mathbf{q}^T\, {}^{\mathcal{B}_3}\mathbf{e} \tag{5.67}$$

respectively. Note that the components of $\vec{\mathbf{p}}$ with respect to the frame $\mathcal{B}_0$ must be same as the components of $\vec{\mathbf{q}}$ with respect to the frame $\mathcal{B}_3$ for the rotation for the rigid body, i.e., we have

$$^{\mathcal{B}_0}\mathbf{p} = {}^{\mathcal{B}_3}\mathbf{q} \quad \text{or} \quad {}^{\mathcal{B}_0}p_i = {}^{\mathcal{B}_3}q_i \ \text{ for } \ i = 1, 2, 3 \tag{5.68}$$

From the geometry, we see that the position vector, $\vec{\mathbf{p}}$, yields

$$\vec{\mathbf{p}} = \vec{\pi}(\mathbf{O}, \mathbf{S}) + \vec{\pi}(\mathbf{S}, \mathbf{P}) \tag{5.69}$$

[9] Point **P** lies in the rigid body before the rotation, and point **Q** lies in the same location in the body *after* the rotation.

where vector $\vec{\pi}(\mathbf{O},\mathbf{S})$ is the projection of $\vec{\mathbf{p}}$ to the unit vector $\vec{\mathbf{n}}$ given by

$$\vec{\pi}(\mathbf{O},\mathbf{S}) = \mathrm{Proj}(\vec{\mathbf{p}},\vec{\mathbf{n}}) = (\vec{\mathbf{p}}\cdot\vec{\mathbf{n}})\vec{\mathbf{n}} \tag{5.70}$$

Hence, $\vec{\pi}(\mathbf{S},\mathbf{P})$, which is the projection of $\vec{\mathbf{p}}$ perpendicular to $\vec{\mathbf{n}}$ is obtained as

$$\vec{\pi}(\mathbf{S},\mathbf{P}) = \vec{\mathbf{p}} - (\vec{\mathbf{p}}\cdot\vec{\mathbf{n}})\vec{\mathbf{n}} \tag{5.71}$$

On the other hand, the position vector $\vec{\mathbf{q}}$ yields

$$\vec{\mathbf{q}} = \vec{\pi}(\mathbf{O},\mathbf{S}) + \vec{\pi}(\mathbf{S},\mathbf{U}) + \vec{\pi}(\mathbf{U},\mathbf{Q}) \tag{5.72}$$

where $\vec{\pi}(\mathbf{O},\mathbf{S})$ is given in Eq. (5.70); and $\vec{\pi}(\mathbf{S},\mathbf{U})$ and $\vec{\pi}(\mathbf{U},\mathbf{Q})$ are obtained as follows: From the geometry,

$$\|\vec{\pi}(\mathbf{S},\mathbf{P})\| = \|\vec{\pi}(\mathbf{S},\mathbf{Q})\| = \|\vec{\pi}(\mathbf{S},\mathbf{T})\| \tag{5.73}$$

Therefore,

$$\begin{aligned}\vec{\pi}(\mathbf{S},\mathbf{U}) &= \|\vec{\pi}(\mathbf{S},\mathbf{Q})\|\cos(\varphi)\frac{\vec{\pi}(\mathbf{S},\mathbf{P})}{\|\vec{\pi}(\mathbf{S},\mathbf{P})\|} = \vec{\pi}(\mathbf{S},\mathbf{P})\cos(\varphi)\\ &= [\vec{\mathbf{p}} - (\vec{\mathbf{p}}\cdot\vec{\mathbf{n}})\vec{\mathbf{n}}]\cos(\varphi)\end{aligned} \tag{5.74}$$

From the relation

$$\vec{\mathbf{n}}\times\vec{\pi}(\mathbf{S},\mathbf{P}) = \underbrace{\|\vec{\mathbf{n}}\|}_{=1}\,\|\vec{\pi}(\mathbf{S},\mathbf{P})\|\sin(\varphi)\frac{\vec{\pi}(\mathbf{S},\mathbf{T})}{\|\vec{\pi}(\mathbf{S},\mathbf{T})\|} = \vec{\pi}(\mathbf{S},\mathbf{T})\sin(\varphi) \tag{5.75}$$

we obtain

$$\begin{aligned}\vec{\pi}(\mathbf{U},\mathbf{Q}) &= \|\vec{\pi}(\mathbf{S},\mathbf{Q})\|\sin(\varphi)\frac{\vec{\pi}(\mathbf{S},\mathbf{T})}{\|\vec{\pi}(\mathbf{S},\mathbf{T})\|} = \vec{\pi}(\mathbf{S},\mathbf{T})\sin(\varphi)\\ &= [\vec{\mathbf{n}}\times\vec{\pi}(\mathbf{S},\mathbf{P})]\sin(\varphi) = [\vec{\mathbf{n}}\times\vec{\mathbf{p}} - (\vec{\mathbf{p}}\cdot\vec{\mathbf{n}})\underbrace{\vec{\mathbf{n}}\times\vec{\mathbf{n}}}_{\mathbf{0}}]\sin(\varphi)\\ &= \vec{\mathbf{n}}\times\vec{\mathbf{p}}\sin(\varphi)\end{aligned} \tag{5.76}$$

Hence, Eq. (5.72) can be written as

$$\begin{aligned}\vec{\mathbf{q}} &= (\vec{\mathbf{p}}\cdot\vec{\mathbf{n}})\vec{\mathbf{n}} + [\vec{\mathbf{p}} - (\vec{\mathbf{p}}\cdot\vec{\mathbf{n}})\vec{\mathbf{n}}]\cos(\varphi) + \vec{\mathbf{n}}\times\vec{\mathbf{p}}\sin(\varphi)\\ &= \cos(\varphi)\vec{\mathbf{p}} + [1-\cos(\varphi)]\,(\vec{\mathbf{p}}\cdot\vec{\mathbf{n}})\vec{\mathbf{n}} + \sin(\varphi)\vec{\mathbf{n}}\times\vec{\mathbf{p}} \qquad (5.77)\end{aligned}$$

With respect to the frame $\mathcal{B}_0$, the position vector $\vec{\mathbf{q}}$ yields

$$^{\mathcal{B}_0}\mathbf{q}^T\,{}^{\mathcal{B}_0}\mathbf{e} = \left[\cos(\varphi)\,{}^{\mathcal{B}_0}\mathbf{p}^T + [1-\cos(\varphi)]\,({}^{\mathcal{B}_0}\mathbf{p}^T\mathbf{n})\mathbf{n}^T + \sin(\varphi)\,(\widetilde{\mathbf{n}}\,{}^{\mathcal{B}_0}\mathbf{p})^T\right]{}^{\mathcal{B}_0}\mathbf{e} \qquad (5.78)$$

where $\widetilde{\mathbf{n}} \in \mathbb{R}^{3\times3}$ is the tilde matrix of $\mathbf{n}$ defined as

$$\widetilde{\mathbf{n}} = \begin{bmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{bmatrix} \in \mathbb{R}^{3\times3} \qquad (5.79)$$

Therefore,

$$^{\mathcal{B}_0}\mathbf{q} = \cos(\varphi)\,{}^{\mathcal{B}_0}\mathbf{p} + [1-\cos(\varphi)]\,({}^{\mathcal{B}_0}\mathbf{p}^T\mathbf{n})\mathbf{n} + \sin(\varphi)\,\widetilde{\mathbf{n}}\,{}^{\mathcal{B}_0}\mathbf{p} \qquad (5.80)$$

Due to the relation

$$[({}^{\mathcal{B}_0}\mathbf{p}^T\mathbf{n})\mathbf{n}]_i = {}^{\mathcal{B}_0}p_j n_j n_i = (n_i n_j)^{\mathcal{B}_0}p_j \quad \text{i.e.,} \quad ({}^{\mathcal{B}_0}\mathbf{p}^T\mathbf{n})\mathbf{n} = (\mathbf{n}\mathbf{n}^T)\,{}^{\mathcal{B}_0}\mathbf{p} \qquad (5.81)$$

Eq. (5.80) becomes

$$\begin{aligned}{}^{\mathcal{B}_0}\mathbf{q} &= \left[\cos(\varphi)\mathbf{I}_3 + [1-\cos(\varphi)]\,\mathbf{n}\mathbf{n}^T + \sin(\varphi)\,\widetilde{\mathbf{n}}\right]{}^{\mathcal{B}_0}\mathbf{p} \qquad (5.82)\\ &= \underbrace{\left[\cos(\varphi)\mathbf{I}_3 + [1-\cos(\varphi)]\,\mathbf{n}\mathbf{n}^T + \sin(\varphi)\,\widetilde{\mathbf{n}}\right]}_{{}^{\mathcal{B}_0\mathcal{B}_3}\mathbf{A}}{}^{\mathcal{B}_3}\mathbf{q} \qquad (5.83)\end{aligned}$$

where we have used Eq. (5.68). That is, the orthogonal transformation matrix ${}^{\mathcal{B}_0\mathcal{B}_3}\mathbf{A}$ is

$$^{\mathcal{B}_0\mathcal{B}_3}\mathbf{A} = \cos(\varphi)\mathbf{I}_3 + [1-\cos(\varphi)]\,\mathbf{n}\mathbf{n}^T + \sin(\varphi)\,\widetilde{\mathbf{n}} \qquad (5.84)$$

Recognizing ${}^{\mathcal{B}_3\mathcal{B}_0}\mathbf{A} = {}^{\mathcal{B}_0\mathcal{B}_3}\mathbf{A}^{T}$[10] , ${}^{\mathcal{B}_3\mathcal{B}_0}\mathbf{A}$ is finally obtained as:

$$\boxed{\mathbf{A}_{\mathrm{n}}(\varphi) = {}^{\mathcal{B}_3\mathcal{B}_0}\mathbf{A} = \cos(\varphi)\mathbf{I}_3 + [1-\cos(\varphi)]\,\mathbf{n}\mathbf{n}^T - \sin(\varphi)\,\widetilde{\mathbf{n}} \in SO(3)} \tag{5.87}$$

where the property of the skew-symmetry, $\widetilde{\mathbf{n}}^T = -\widetilde{\mathbf{n}}$ has been used.

Remark 5.2.2 (Eq. (5.87))

1. *For the rotation about* ${}^{\mathcal{B}_0}\vec{\mathbf{e}}_1$ *by* φ, *i.e.,* $\mathbf{n} = [1,0,0]^T$, *Eq.* (5.87) *reduces to*

$$\mathbf{A}_{\mathrm{n}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\varphi) & \sin(\varphi) \\ 0 & -\sin(\varphi) & \cos(\varphi) \end{bmatrix} =: \mathbf{A}_{\mathrm{n}_1} \tag{5.88}$$

The angle φ *in Eq.* (5.88) *is the rotation angle about* ${}^{\mathcal{B}_0}\vec{\mathbf{e}}_1$ *on the hyperplane spanned by* ${}^{\mathcal{B}_0}\vec{\mathbf{e}}_2$ *and* ${}^{\mathcal{B}_0}\vec{\mathbf{e}}_3$. *Similarly,*

$$\mathbf{A}_{\mathrm{n}} = \begin{bmatrix} \cos(\varphi) & 0 & -\sin(\varphi) \\ 0 & 1 & 0 \\ \sin(\varphi) & 0 & \cos(\varphi) \end{bmatrix} \quad \textit{for}\ \ \mathbf{n} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} =: \mathbf{A}_{\mathrm{n}_2} \tag{5.89}$$

$$\mathbf{A}_{\mathrm{n}} = \begin{bmatrix} \cos(\varphi) & \sin(\varphi) & 0 \\ -\sin(\varphi) & \cos(\varphi) & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \textit{for}\ \ \mathbf{n} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} =: \mathbf{A}_{\mathrm{n}_3} \tag{5.90}$$

The angles φ *in Eq.* (5.89) *and Eq.* (5.90) *are the rotation angles about* ${}^{\mathcal{B}_0}\vec{\mathbf{e}}_1$ *on the hyperplane spanned by* ${}^{\mathcal{B}_0}\vec{\mathbf{e}}_1$ *and* ${}^{\mathcal{B}_0}\vec{\mathbf{e}}_3$, *and on the hyperplane spanned by* ${}^{\mathcal{B}_0}\vec{\mathbf{e}}_1$

[10] This relation can be proved as follows: From ${}^{\mathcal{B}_0}\mathbf{e} = {}^{\mathcal{B}_0\mathcal{B}_3}\mathbf{A}^{\mathcal{B}_3}\mathbf{e}$ and ${}^{\mathcal{B}_3}\mathbf{e} = {}^{\mathcal{B}_3\mathcal{B}_0}\mathbf{A}^{\mathcal{B}_0}\mathbf{e}$, we readily have

$${}^{\mathcal{B}_0}\mathbf{e} = {}^{\mathcal{B}_0\mathcal{B}_3}\mathbf{A}^{\mathcal{B}_3}\mathbf{e} = {}^{\mathcal{B}_0\mathcal{B}_3}\mathbf{A}^{\mathcal{B}_3\mathcal{B}_0}\mathbf{A}^{\mathcal{B}_0}\mathbf{e} \tag{5.85}$$

Hence, ${}^{\mathcal{B}_0\mathcal{B}_3}\mathbf{A}^{\mathcal{B}_3\mathcal{B}_0}\mathbf{A} = \mathbf{I}_3$ or

$${}^{\mathcal{B}_3\mathcal{B}_0}\mathbf{A} = {}^{\mathcal{B}_0\mathcal{B}_3}\mathbf{A}^{-1} = {}^{\mathcal{B}_0\mathcal{B}_3}\mathbf{A}^{T} \tag{5.86}$$

must hold.

and ${}^{\mathcal{B}_0}\vec{\mathbf{e}}_2$*, respectively. Eqns.* (5.88)-(5.90) *can be expressed as*

$$\mathbf{A}_{\mathrm{n_i}} = \exp\left(\mathbf{J}_i\,\varphi\right) = \sum_{i=0}^{\infty}\frac{(\mathbf{J}_i\,\varphi)^{2i}}{(2i)!} + \sum_{i=0}^{\infty}\frac{(\mathbf{J}_i\,\varphi)^{2i+1}}{(2i+1)!} \tag{5.91}$$

where $\mathbf{J}_i \in SO(3)$ *(for* $i = 1, 2, 3$*) are defined as*

$$\mathbf{J}_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}, \quad \mathbf{J}_2 = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad \mathbf{J}_3 = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{5.92}$$

For $i = 3$, [11]

$$\begin{aligned} \exp\left(\mathbf{J}_1\,\varphi\right) &= \sum_{i=0}^{\infty}\frac{(\mathbf{J}_3\,\varphi)^{2i}}{(2i)!} + \sum_{i=0}^{\infty}\frac{(\mathbf{J}_3\,\varphi)^{2i+1}}{(2i+1)!} \\ &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}\underbrace{\sum_{i=0}^{\infty}\frac{(-1)^i\varphi^{2i}}{(2i)!}}_{\cos(\varphi)} + \underbrace{\begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{\mathbf{J}_3}\underbrace{\sum_{i=0}^{\infty}\frac{(-1)^i\varphi^{2i+1}}{(2i+1)!}}_{\sin(\varphi)} \\ &= \begin{bmatrix} \cos(\varphi) & \sin(\varphi) & 0 \\ -\sin(\varphi) & \cos(\varphi) & 0 \\ 0 & 0 & 1 \end{bmatrix} = \mathbf{A}_{\mathrm{n_3}} \end{aligned} \tag{5.93}$$

We can show the proofs for $i = 1, 2$ *in a similar manner.*

[11] *The Taylor series expansion about* $\varphi = 0$ *(i.e., the Maclaurin expansion) for* $\sin(\varphi)$ *and* $\cos(\varphi)$ *are:*

$$\begin{aligned} \sin(\varphi) &= \varphi - \frac{\varphi^3}{3!} + \frac{\varphi^5}{5!} - \frac{\varphi^7}{7!} + \cdots = \sum_{i=0}^{\infty}\frac{(-1)^i\varphi^{2i+1}}{(2i+1)!} \\ \cos(\varphi) &= 1 - \frac{\varphi^2}{2!} + \frac{\varphi^4}{4!} - \frac{\varphi^6}{6!} + \cdots = \sum_{i=0}^{\infty}\frac{(-1)^i\varphi^{2i}}{(2i)!} \end{aligned}$$

2. ***Infinitesimally Small Rotations:*** *The Taylor series expansion of* $\mathbf{A}_\mathrm{n}$ *about a fixed* φ_0 *yields:*

$$\mathbf{A}_\mathrm{n} = \mathbf{A}_\mathrm{n}(\varphi_0) + \Delta\varphi D\mathbf{A}_\mathrm{n}(\varphi_0) + \frac{\Delta\varphi^2}{2}D^2\mathbf{A}_\mathrm{n}(\varphi_0) + \frac{\Delta\varphi^3}{3!}D^3\mathbf{A}_\mathrm{n}(\varphi_0) + \cdots \tag{5.94}$$

where $\Delta\varphi := \varphi - \varphi_0$, *and* $D^k\mathbf{A}_\mathrm{n}$ *denotes the* k^{th} *derivative of* $\mathbf{A}_\mathrm{n}$ *with respect to* φ. *Without loss of generality, taking* $\varphi_0 = 0$ *in Eq.* (5.94) *yields*

$$\mathbf{A}_\mathrm{n} = \mathbf{I}_3 - \Delta\phi\,\widetilde{\mathbf{n}} + \frac{\Delta\varphi^2}{2}[\mathbf{n}\mathbf{n}^T - \mathbf{I}_3] - \frac{\Delta\varphi^3}{6}[\mathbf{n}\mathbf{n}^T + \sin(\varphi)\,\widetilde{\mathbf{n}}] + \cdots \tag{5.95}$$

Since the first-order linear approximation of $\mathbf{A}_\mathrm{n}$ *is given as*

$$\mathbf{A}_\mathrm{n} = {}^{\mathcal{B}_3\mathcal{B}_0}\mathbf{A} \approx \mathbf{I}_3 - \Delta\phi\,\widetilde{\mathbf{n}} \tag{5.96}$$

we get ${}^{\mathcal{B}_0\mathcal{B}_3}\mathbf{A} = {}^{\mathcal{B}_3\mathcal{B}_0}\mathbf{A}^T \approx \mathbf{I}_3 + \Delta\phi\,\widetilde{\mathbf{n}}$ *and*

$${}^{\mathcal{B}_0}\mathbf{q} = {}^{\mathcal{B}_0\mathcal{B}_3}\mathbf{A}\,{}^{\mathcal{B}_3}\mathbf{q} = {}^{\mathcal{B}_0\mathcal{B}_3}\mathbf{A}\,{}^{\mathcal{B}_0}\mathbf{p} \approx {}^{\mathcal{B}_0}\mathbf{p} + \Delta\phi\,\widetilde{\mathbf{n}}\,{}^{\mathcal{B}_0}\mathbf{p} \tag{5.97}$$

Hence,

$$\boxed{\vec{\mathbf{q}} \approx \vec{\mathbf{p}} + \Delta\phi\,\vec{\mathbf{n}} \times \vec{\mathbf{p}} \quad \textit{i.e,} \quad \vec{\pi}(\mathbf{O},\mathbf{Q}) \approx \vec{\pi}(\mathbf{O},\mathbf{P}) + \Delta\phi\,\vec{\mathbf{n}} \times \vec{\pi}(\mathbf{O},\mathbf{P})} \tag{5.98}$$

Notice that the linearized $\mathbf{A}_\mathrm{n}$ *shown in Eq.* (5.96) *can be expressed with* $\mathbf{J}_i$ *defined in Eq.* (5.92) *as*

$$\begin{aligned}\mathbf{A}_\mathrm{n} \approx \mathbf{I}_3 - \Delta\phi\,\widetilde{\mathbf{n}} &= \begin{bmatrix} 1 & \Delta\varphi\,n_3 & -\Delta\varphi\,n_2 \\ -\Delta\varphi\,n_3 & 1 & \Delta\varphi\,n_1 \\ \Delta\varphi\,n_2 & -\Delta\varphi\,n_1 & 1 \end{bmatrix} \\ &= \mathbf{I}_3 + \mathbf{J}_i\,\Delta\varphi\,n_i = \mathbf{I}_3 + \mathbf{J}_1\,\Delta\varphi\,n_1 + \mathbf{J}_2\,\Delta\varphi\,n_2 + \mathbf{J}_3\,\Delta\varphi\,n_3\end{aligned} \tag{5.99}$$

for $|\Delta\varphi| \ll 1$.

3. Consider the eigenvalue problem, $\mathbf{A}_\mathrm{n}\mathbf{v} = \lambda\mathbf{v}$ *where* $\mathbf{A}_\mathrm{n}$ *is given in Eq.* (5.87)*. In order to find* λ *such that this equation has a nonzero solution* $\mathbf{v}$*, the linear operator* $(\mathbf{A}_\mathrm{n} - \lambda\mathbf{I}_3)$ *for* $(\mathbf{A}_\mathrm{n} - \lambda\mathbf{I}_3)\mathbf{v} = \mathbf{0}$ *must be invertible, i.e., the roots* λ *of the characteristic equation*

$$\det(\mathbf{A}_\mathrm{n} - \lambda\mathbf{I}_3) = 0 \tag{5.100}$$

are the eigenvalues, and the corresponding $\mathbf{v}$ *are the eigenvectors. By solving Eq.* (5.100)*, three eigenvalues are obtained as*

$$\lambda_1 = 1, \quad \lambda_{2,3} = \frac{\mathrm{tr}(\mathbf{A}_\mathrm{n}) - 1}{2} \pm \mathtt{i}\sqrt{1 - \left(\frac{\mathrm{tr}(\mathbf{A}_\mathrm{n}) - 1}{2}\right)^2} \tag{5.101}$$

where $\mathtt{i} \equiv \sqrt{-1}$*. Since the trace of* $\mathbf{A}_\mathrm{n}$ *is given as*

$$\mathrm{tr}(\mathbf{A}_\mathrm{n}) = A_{\mathrm{n}\,11} + A_{\mathrm{n}\,22} + A_{\mathrm{n}\,33} = [1 - \cos(\varphi)]\underbrace{(n_1^2 + n_2^2 + n_3^2)}_{=1} + 2\cos(\varphi) = 1 + 2\cos(\varphi) \tag{5.102}$$

the eigenvalues $\lambda_{2,3}$ *can be written as*

$$\lambda_{2,3} = \cos(\varphi) \pm \mathtt{i}\sin(\varphi) = \exp(\pm\mathtt{i}\varphi) \tag{5.103}$$

The eigenvector $\mathbf{v}_1$ *associated with the eigenvalue* $\lambda_1 = 1$ *is given as* $\mathbf{v}_1 = \mathbf{n}$*, i.e.,*

$$\mathbf{A}_\mathrm{n}\mathbf{n} = \mathbf{n} \tag{5.104}$$

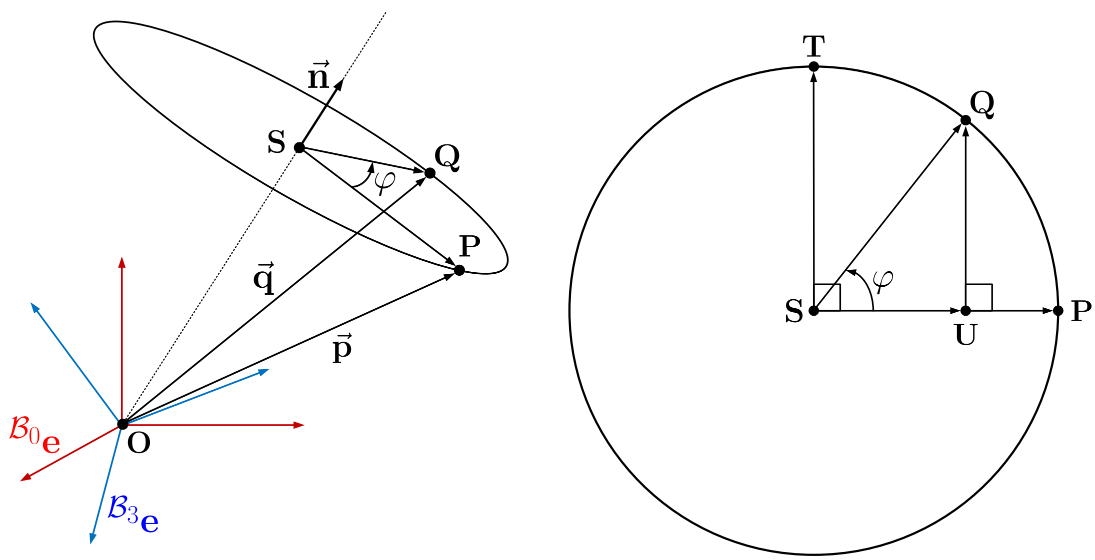


Figure 5.3: Three-dimensional Euclidean Space

5.2.3 Euler Parameters

Here, we define the so-called ***Euler parameters***: ε_i for $i = 1, 2, 3, 4$. In the matrix form,

$$\boldsymbol{\varepsilon} = [\varepsilon_0, \varepsilon_1, \varepsilon_2, \varepsilon_3]^T = [\varepsilon_0, \boldsymbol{\eta}^T]^T \tag{5.105}$$

where

$$\varepsilon_0 := \cos(\frac{\varphi}{2}) \quad \text{and} \quad \boldsymbol{\eta} = [\varepsilon_1, \varepsilon_2, \varepsilon_3]^T := \mathbf{n}\sin(\frac{\varphi}{2}) \tag{5.106}$$

Invoking the relation, $||\mathbf{n}||^2 = \mathbf{n}^T\mathbf{n} = 1$, we have

$$||\boldsymbol{\varepsilon}||^2 = \boldsymbol{\varepsilon}^T\boldsymbol{\varepsilon} = \varepsilon_i\varepsilon_i = \varepsilon_0^2 + \boldsymbol{\eta}^T\boldsymbol{\eta} = \cos^2(\frac{\varphi}{2}) + \mathbf{n}^T\mathbf{n}\sin^2(\frac{\varphi}{2}) = 1 \tag{5.107}$$

We now express $\mathbf{A}_\mathrm{n}$ given in Eq. (5.87) using the Euler parameters. Using the Prosthaphaeresis formulas[12] , the following identities are obtained:

$$\begin{aligned} 1-\cos(\varphi) &= 1-\cos(\frac{\varphi}{2}+\frac{\varphi}{2}) = [1-\cos^2(\frac{\varphi}{2})]+\sin^2(\frac{\varphi}{2}) = 2\sin^2(\frac{\varphi}{2}) && (5.108)\\ \sin(\varphi) &= \sin(\frac{\varphi}{2}+\frac{\varphi}{2}) = \sin(\frac{\varphi}{2})\cos(\frac{\varphi}{2})+\cos(\frac{\varphi}{2})\sin(\frac{\varphi}{2}) = 2\sin(\frac{\varphi}{2})\cos(\frac{\varphi}{2}) && (5.109)\end{aligned}$$

and from Eq. (5.108),

$$\cos(\varphi) = 1-2\sin^2(\frac{\varphi}{2}) = 1-[1-2\cos^2(\frac{\varphi}{2})] = 2\cos^2(\frac{\varphi}{2})-1 \tag{5.110}$$

Therefore, making use of Eqns. (5.108)-(5.110), $\mathbf{A}_\mathrm{n}$ can be written in terms of the Euler parameters as

$$\begin{aligned} \mathbf{A}_\mathrm{n}(\varphi) &= {}^{\mathcal{B}_3\mathcal{B}_0}\mathbf{A} = \cos(\varphi)\mathbf{I}_3 + [1-\cos(\varphi)]\,\mathbf{n}\mathbf{n}^T - \sin(\varphi)\,\widetilde{\mathbf{n}} \\ &= [\underbrace{2\cos^2(\frac{\varphi}{2})}_{\varepsilon_0^2}-1]\mathbf{I}_3 + 2\,\underbrace{(\mathbf{n}\sin(\frac{\varphi}{2}))(\mathbf{n}\sin(\frac{\varphi}{2}))^T}_{\boldsymbol{\eta}\boldsymbol{\eta}^T} - 2\,\underbrace{\cos(\frac{\varphi}{2})}_{\varepsilon_0}\,\underbrace{\widetilde{\mathbf{n}}\sin(\frac{\varphi}{2})}_{\widetilde{\boldsymbol{\eta}}} \\ &= (2\varepsilon_0^2-1)\mathbf{I}_3 + 2(\boldsymbol{\eta}\boldsymbol{\eta}^T - \varepsilon_0\widetilde{\boldsymbol{\eta}}) \\ &= \begin{bmatrix} 2(\varepsilon_0^2+\varepsilon_1^2)-1 & 2(\varepsilon_1\varepsilon_2+\varepsilon_0\varepsilon_3) & 2(\varepsilon_1\varepsilon_3-\varepsilon_0\varepsilon_2) \\ 2(\varepsilon_1\varepsilon_2-\varepsilon_0\varepsilon_3) & 2(\varepsilon_0^2+\varepsilon_2^2)-1 & 2(\varepsilon_2\varepsilon_3+\varepsilon_0\varepsilon_1) \\ 2(\varepsilon_1\varepsilon_3+\varepsilon_0\varepsilon_2) & 2(\varepsilon_2\varepsilon_3-\varepsilon_0\varepsilon_1) & 2(\varepsilon_0^2+\varepsilon_3^2)-1 \end{bmatrix} =: \mathbf{A}_\mathrm{n}^\varepsilon(\boldsymbol{\varepsilon}) && (5.111)\end{aligned}$$

Hence,

$$\boxed{\begin{aligned} &\mathbf{A}_\mathrm{n}(\varphi) = {}^{\mathcal{B}_3\mathcal{B}_0}\mathbf{A} = \mathbf{A}_\mathrm{n}^\varepsilon(\boldsymbol{\varepsilon}) = (2\varepsilon_0^2-1)\mathbf{I}_3 + 2(\boldsymbol{\eta}\boldsymbol{\eta}^T - \varepsilon_0\widetilde{\boldsymbol{\eta}}) \\ &\text{with } \ \|\boldsymbol{\varepsilon}\|^2 = \boldsymbol{\varepsilon}^T\boldsymbol{\varepsilon} = 1 \end{aligned}} \tag{5.112}$$

---

[12] The Prosthaphaeresis formulas are the following trigonometry formulas:

$$\begin{aligned} \sin(\alpha\pm\beta) &= \sin(\alpha)\cos(\beta)\pm\cos(\alpha)\sin(\beta) \\ \cos(\alpha\pm\beta) &= \cos(\alpha)\cos(\beta)\mp\sin(\alpha)\sin(\beta) \end{aligned}$$

Using the relations, $(\boldsymbol{\eta}\boldsymbol{\eta}^T)^T = \boldsymbol{\eta}\boldsymbol{\eta}^T$ and $\widetilde{\boldsymbol{\eta}}^T = -\widetilde{\boldsymbol{\eta}}$, ${}^{\mathcal{B}_0\mathcal{B}_3}\mathbf{A}$ can be readily expressed in terms of the Euler parameters as

$$\boxed{\begin{aligned} {}^{\mathcal{B}_0\mathcal{B}_3}\mathbf{A} &= {}^{\mathcal{B}_3\mathcal{B}_0}\mathbf{A}^T = (\mathbf{A}_{\mathrm{n}}^{\varepsilon}(\boldsymbol{\varepsilon}))^T = (2\varepsilon_0^2 - 1)\mathbf{I}_3 + 2(\boldsymbol{\eta}\boldsymbol{\eta}^T + \varepsilon_0\widetilde{\boldsymbol{\eta}}) \\ &= \begin{bmatrix} 2(\varepsilon_0^2 + \varepsilon_1^2) - 1 & 2(\varepsilon_1\varepsilon_2 - \varepsilon_0\varepsilon_3) & 2(\varepsilon_1\varepsilon_3 + \varepsilon_0\varepsilon_2) \\ 2(\varepsilon_1\varepsilon_2 + \varepsilon_0\varepsilon_3) & 2(\varepsilon_0^2 + \varepsilon_2^2) - 1 & 2(\varepsilon_2\varepsilon_3 - \varepsilon_0\varepsilon_1) \\ 2(\varepsilon_1\varepsilon_3 - \varepsilon_0\varepsilon_2) & 2(\varepsilon_2\varepsilon_3 + \varepsilon_0\varepsilon_1) & 2(\varepsilon_0^2 + \varepsilon_3^2) - 1 \end{bmatrix} \\ &\text{with } \|\boldsymbol{\varepsilon}\|^2 = \boldsymbol{\varepsilon}^T\boldsymbol{\varepsilon} = 1 \end{aligned}} \tag{5.113}$$

Remark 5.2.3 (Euler Parameters)

1. *When a numerical value of* ${}^{\mathcal{B}_0\mathcal{B}_3}\mathbf{A} = \mathbf{A}_{(313)}^T$ *is available as* $\hat{\mathbf{A}} = [\hat{A}_{ij}] \simeq {}^{\mathcal{B}_0\mathcal{B}_3}\mathbf{A}$*, the Euler parameters can be determined as follows: Find* ε_0 *from*

$$\varepsilon_0 = \pm\frac{1}{2}\sqrt{\mathrm{tr}\left(\hat{\mathbf{A}}\right) + 1} \tag{5.114}$$

where $\mathrm{tr}(\hat{\mathbf{A}}) = \hat{A}_{ii} = \hat{A}_{11} + \hat{A}_{22} + \hat{A}_{33}$*. If* $\varepsilon_0 \neq 0$*, find* ε_i *(for* $i = 1, 2, 3$*) from*

$$\varepsilon_1 = \frac{\hat{A}_{32} - \hat{A}_{23}}{4\varepsilon_0}, \quad \varepsilon_2 = \frac{\hat{A}_{13} - \hat{A}_{31}}{4\varepsilon_0}, \quad \varepsilon_3 = \frac{\hat{A}_{21} - \hat{A}_{12}}{4\varepsilon_0} \tag{5.115}$$

If $\varepsilon_0 = 0$ *from Eq.* (5.114)*, find* ε_i *(for* $i = 1, 2, 3$*) from one of the following options:*

(Option 1)

$$\begin{aligned} \varepsilon_1 &= \pm\frac{1}{2}\sqrt{2\hat{A}_{11} - \mathrm{tr}\left(\hat{\mathbf{A}}\right) + 1} \\ \varepsilon_2 &= \frac{\hat{A}_{12} + \hat{A}_{21}}{4\varepsilon_1}, \quad \varepsilon_3 = \frac{\hat{A}_{13} + \hat{A}_{31}}{4\varepsilon_1} \end{aligned} \tag{5.116}$$

(Option 2)

$$\begin{aligned} \varepsilon_2 &= \pm\frac{1}{2}\sqrt{2\hat{A}_{22} - \mathrm{tr}\left(\hat{\mathbf{A}}\right) + 1} \\ \varepsilon_1 &= \frac{\hat{A}_{12} + \hat{A}_{21}}{4\varepsilon_2}, \quad \varepsilon_3 = \frac{\hat{A}_{23} + \hat{A}_{32}}{4\varepsilon_2} \end{aligned} \tag{5.117}$$

(Option 3)

$$
\begin{aligned}
\varepsilon_3 &= \pm\frac{1}{2}\sqrt{2\hat{A}_{33} - \mathrm{tr}\left(\hat{\mathbf{A}}\right) + 1} \\
\varepsilon_1 &= \frac{\hat{A}_{13} + \hat{A}_{31}}{4\varepsilon_3}, \quad \varepsilon_2 = \frac{\hat{A}_{23} + \hat{A}_{32}}{4\varepsilon_3}
\end{aligned}
\tag{5.118}
$$

Theorem 5.2.1

The transformation matrix defined with the Euler parameters as in Eq. (5.113) *can be decomposed into*

$$
\left(\mathbf{A}_{\mathrm{n}}^{\varepsilon}(\boldsymbol{\varepsilon})\right)^T = \mathbf{A}_{\mathrm{E}_1}(\boldsymbol{\varepsilon})\ \mathbf{A}_{\mathrm{E}_2}^T(\boldsymbol{\varepsilon}) \tag{5.119}
$$

where $\mathbf{A}_{\mathrm{E}_\ell}(\boldsymbol{\varepsilon}) \in \mathbb{R}^{3\times 4}$ *for* $\ell = 1$ *and* $\ell = 2$ *are defined as*

$$
\mathbf{A}_{\mathrm{E}_1}(\boldsymbol{\varepsilon}) = \begin{bmatrix} -\boldsymbol{\eta} & \varepsilon_0\mathbf{I}_3 + \widetilde{\boldsymbol{\eta}} \end{bmatrix} \tag{5.120}
$$

$$
\mathbf{A}_{\mathrm{E}_2}(\boldsymbol{\varepsilon}) = \begin{bmatrix} -\boldsymbol{\eta} & \varepsilon_0\mathbf{I}_3 - \widetilde{\boldsymbol{\eta}} \end{bmatrix} \tag{5.121}
$$

respectively.

Proof. Substituting the following relation,

$$
\begin{aligned}
2\varepsilon_0^2 - 1 &= 2\cos^2(\frac{\varphi}{2}) - 1 = \cos^2(\frac{\varphi}{2}) - \sin^2(\frac{\varphi}{2}) \\
&= \cos^2(\frac{\varphi}{2}) - \underbrace{\mathbf{n}^T\mathbf{n}}_{\mathbf{I}_3}\sin^2(\frac{\varphi}{2}) \\
&= \varepsilon_0^2 - \boldsymbol{\eta}^T\boldsymbol{\eta}
\end{aligned}
\tag{5.122}
$$

into Eq. (5.113) yields:

$$
\begin{aligned}
\left(\mathbf{A}_{\mathrm{n}}^{\varepsilon}(\boldsymbol{\varepsilon})\right)^T &= (2\varepsilon_0^2 - 1)\mathbf{I}_3 + 2(\boldsymbol{\eta}\boldsymbol{\eta}^T + \varepsilon_0\widetilde{\boldsymbol{\eta}}) \\
&= (\varepsilon_0^2 - \boldsymbol{\eta}^T\boldsymbol{\eta})\mathbf{I}_3 + 2\boldsymbol{\eta}\boldsymbol{\eta}^T + 2\varepsilon_0\widetilde{\boldsymbol{\eta}} \\
&= \varepsilon_0^2\mathbf{I}_3 + \underbrace{\left(\boldsymbol{\eta}\boldsymbol{\eta}^T - \boldsymbol{\eta}^T\boldsymbol{\eta}\mathbf{I}_3\right)}_{\widetilde{\boldsymbol{\eta}}\widetilde{\boldsymbol{\eta}}} + \boldsymbol{\eta}\boldsymbol{\eta}^T + 2\varepsilon_0\widetilde{\boldsymbol{\eta}} \\
&= \boldsymbol{\eta}\boldsymbol{\eta}^T + \varepsilon_0^2\mathbf{I}_3 + \widetilde{\boldsymbol{\eta}}\widetilde{\boldsymbol{\eta}} + 2\varepsilon_0\widetilde{\boldsymbol{\eta}} \\
&= \boldsymbol{\eta}\boldsymbol{\eta}^T + (\varepsilon_0\mathbf{I}_3 + \widetilde{\boldsymbol{\eta}})\,(\varepsilon_0\mathbf{I}_3 + \widetilde{\boldsymbol{\eta}}) \\
&= \begin{bmatrix} -\boldsymbol{\eta} & \varepsilon_0\mathbf{I}_3 + \widetilde{\boldsymbol{\eta}} \end{bmatrix} \begin{bmatrix} -\boldsymbol{\eta}^T \\ \varepsilon_0\mathbf{I}_3 + \widetilde{\boldsymbol{\eta}} \end{bmatrix} = \underbrace{\begin{bmatrix} -\boldsymbol{\eta} & \varepsilon_0\mathbf{I}_3 + \widetilde{\boldsymbol{\eta}} \end{bmatrix}}_{\mathbf{A}_{\mathrm{E}_1}} \underbrace{\begin{bmatrix} -\boldsymbol{\eta}^T \\ (\varepsilon_0\mathbf{I}_3 - \widetilde{\boldsymbol{\eta}})^T \end{bmatrix}}_{\mathbf{A}_{\mathrm{E}_2}^T} \\
&= \mathbf{A}_{\mathrm{E}_1}(\boldsymbol{\varepsilon})\,\mathbf{A}_{\mathrm{E}_2}^T(\boldsymbol{\varepsilon})
\end{aligned} \tag{5.123}
$$

Note that $\mathbf{A}_{\mathrm{n}}^{\varepsilon}(\boldsymbol{\varepsilon})$ can be also readily obtained as $\mathbf{A}_{\mathrm{n}}^{\varepsilon}(\boldsymbol{\varepsilon}) = \mathbf{A}_{\mathrm{E}_2}\mathbf{A}_{\mathrm{E}_1}^T$. ∎

5.3 Velocity Vectors

5.3.1 Angular Velocity Vectors

Definition 5.3.1 (Angular Velocity)

Suppose a Cartesian frame $\mathcal{B}_1 : (\mathbf{O}; \{{}^{\mathcal{B}_1}\vec{\mathbf{e}}_i\}_{i=1}^n)$ is rotating at an angular velocity, ${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\omega}}$, with respect to an initial Cartesian frame $\mathcal{B}_0 : (\mathbf{O}; \{{}^{\mathcal{B}_0}\vec{\mathbf{e}}_i\}_{i=1}^n)$. The angular velocity vector of frame $\mathcal{B}_1$ with respect to frame $\mathcal{B}_0$, i.e., the relative angular velocity vector of $\mathcal{B}_1$ with respect to $\mathcal{B}_0$, is defined as:

$$\boxed{{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\omega}} := \lim_{\Delta t \to 0} \frac{\Delta\vec{\boldsymbol{\phi}}}{\Delta t}} \tag{5.124}$$

where $\vec{\Delta\boldsymbol{\phi}}$ is the rotation vector between the frames, $\mathcal{B}_0$ and $\mathcal{B}_1$. Note that the right-hand side of Eq. (5.124) *is the time derivative with respect to frame $\mathcal{B}_0$; hence, we write it as*

$$ {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} = \frac{{}^{\mathcal{B}_0}d\vec{\boldsymbol{\phi}}}{dt} \tag{5.125}$$

Theorem 5.3.1

Consider a vector, $\vec{\mathbf{s}}$, which is fixed in a rigid body Ω; and assume that frame $\mathcal{B}_1$ is currently fixed to Ω whilst frame $\mathcal{B}_0$ was fixed to Ω initially. Vector $\vec{\mathbf{s}}$ can be regarded as any vector which connects any fixed two points $\mathbf{P}_1$ and $\mathbf{P}_2$ in Ω: $\vec{\mathbf{s}} \equiv \vec{\pi}(\mathbf{P}_1, \mathbf{P}_2)$. The time derivative of vector $\vec{\mathbf{s}}$ with respect to the initial frame, $\mathcal{B}_0$, is denoted by ${}^{\mathcal{B}_0}\mathfrak{D}_t\,\vec{\mathbf{s}}$; and it is always perpendicular to both ${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}$ and $\vec{\mathbf{s}}$, and the following relation holds:

$$\boxed{{}^{\mathcal{B}_0}\mathfrak{D}_t\,\vec{\mathbf{s}} = {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \vec{\mathbf{s}}} \tag{5.126}$$

Remark 5.3.1

1. *Recall Eq.* (5.98) *for the case of an infinitesimally small rotation about $\vec{\mathbf{n}}$ by $\Delta\phi$:*

$$\vec{\pi}(\mathbf{O}, \mathbf{Q}) \approx \vec{\pi}(\mathbf{O}, \mathbf{P}) + \Delta\phi\,\vec{\mathbf{n}} \times \vec{\pi}(\mathbf{O}, \mathbf{P}) \tag{5.127}$$

   In this special case, the rotation vector is given as

$$\vec{\Delta\boldsymbol{\phi}} = \Delta\phi\,\vec{\mathbf{n}} \tag{5.128}$$

   Therefore,

$${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} = \lim_{\Delta t \to 0} \frac{\vec{\Delta\boldsymbol{\phi}}}{\Delta t} = \lim_{\Delta t \to 0} \frac{\Delta\phi}{\Delta t}\vec{\mathbf{n}} = \frac{d\phi}{dt}\vec{\mathbf{n}} = \dot{\phi}\vec{\mathbf{n}} \tag{5.129}$$

2. *The angular velocity vector, ${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}$, can be decomposed in terms of $\mathcal{B}_\ell$ (for $\ell = 0, 1$) as:*

$${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} = {}^{\mathcal{B}_\ell}\mathbf{e}^T\;{}^{\mathcal{B}_\ell}_{\mathcal{B}_1|\mathcal{B}_0}\omega = {}^{\mathcal{B}_\ell}_{\mathcal{B}_1|\mathcal{B}_0}\omega^T\;{}^{\mathcal{B}_\ell}\mathbf{e} \tag{5.130}$$

   where ${}^{\mathcal{B}_\ell}_{\mathcal{B}_1|\mathcal{B}_0}\omega \in \mathbb{R}^3$ is the component vector of ${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}$ in terms of $\mathcal{B}_\ell$.

3. *Considering the case,* $\vec{\mathbf{s}} = {}^{\mathcal{B}_1}\vec{\mathbf{e}}_i$ *(for* $i = 1, 2, 3$*), we can derive the following useful relations after a straightforward work:*

$$ {}^{\mathcal{B}_0}\mathfrak{D}_t\, {}^{\mathcal{B}_1}\mathbf{e} \;=\; -{}^{\mathcal{B}_1}\mathbf{e} \times {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\omega}} = -{}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\; {}^{\mathcal{B}_1}\mathbf{e} \tag{5.131}$$

$$ {}^{\mathcal{B}_0}\mathfrak{D}_t\, {}^{\mathcal{B}_1}\mathbf{e}^T \;=\; {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\omega}} \times {}^{\mathcal{B}_1}\mathbf{e}^T = {}^{\mathcal{B}_1}\mathbf{e}^T\; {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}} \tag{5.132}$$

4. *The angular velocity vector possesses the following properties (Proof omitted):*

$$\boxed{\begin{array}{l} {}_{\mathcal{B}_i|\mathcal{B}_j}\vec{\boldsymbol{\omega}} = -{}_{\mathcal{B}_j|\mathcal{B}_i}\vec{\boldsymbol{\omega}} \\ {}^{\mathcal{B}_\ell}_{\mathcal{B}_i|\mathcal{B}_j}\boldsymbol{\omega} = -{}^{\mathcal{B}_\ell}_{\mathcal{B}_j|\mathcal{B}_i}\boldsymbol{\omega}, \quad {}^{\mathcal{B}_\ell}_{\mathcal{B}_i|\mathcal{B}_j}\widetilde{\boldsymbol{\omega}} = -{}^{\mathcal{B}_\ell}_{\mathcal{B}_j|\mathcal{B}_i}\widetilde{\boldsymbol{\omega}} \\ {}_{\mathcal{B}_i|\mathcal{B}_j}\vec{\boldsymbol{\omega}} = {}_{\mathcal{B}_i|\mathcal{B}_k}\vec{\boldsymbol{\omega}} + {}_{\mathcal{B}_k|\mathcal{B}_j}\vec{\boldsymbol{\omega}} \end{array}} \tag{5.133}$$

Theorem 5.3.2 (Poisson's Equations)

Time derivative of the transformation matrix from $\mathcal{B}_1$ *to* $\mathcal{B}_0$ *is given as:*

$$\boxed{ {}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}} = \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right) = \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)} \tag{5.134}$$

where ${}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}} := {}^{\mathcal{B}_0}\mathfrak{D}_t\, {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A} = {}^{\mathcal{B}_1}\mathfrak{D}_t\, {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}$[13] *. Or equivalently,*

$$ {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}} \;=\; \left({}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}}\right)\, {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T = \left({}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}}\right)\, {}^{\mathcal{B}_1/\mathcal{B}_0}\mathbf{A} \tag{5.135}$$

$$ {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}} \;=\; {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T\, \left({}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}}\right) = {}^{\mathcal{B}_1/\mathcal{B}_0}\mathbf{A}\, \left({}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}}\right) \tag{5.136}$$

Proof. Recall that ${}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}$ can be written as ${}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A} = {}^{\mathcal{B}_0}\mathbf{e} \cdot {}^{\mathcal{B}_1}\mathbf{e}^T$; see Eq. (5.45). The

[13] *Note that the time derivative of any real component matrix* $[\mathbf{A}]_{ij} \in \mathbb{R}$ *or vector* $[\mathbf{v}]_i \in \mathbb{R}$ *is regardless of the frame the time derivative refers to; in other word, the time derivative of a real number is independent from the frame which we refer to.*

time derivative of ${}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}$ in terms of $\mathcal{B}_0$ yields:

$$\begin{aligned}
{}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}} &= {}^{\mathcal{B}_0}\mathfrak{D}_t\, {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A} = {}^{\mathcal{B}_0}\mathfrak{D}_t \left({}^{\mathcal{B}_0}\mathbf{e} \cdot {}^{\mathcal{B}_1}\mathbf{e}^T\right) \\
&= \underbrace{\left({}^{\mathcal{B}_0}\mathfrak{D}_t\, {}^{\mathcal{B}_0}\mathbf{e}\right)}_{\mathbf{0}} \cdot {}^{\mathcal{B}_1}\mathbf{e}^T + {}^{\mathcal{B}_0}\mathbf{e} \cdot \underbrace{\left({}^{\mathcal{B}_0}\mathfrak{D}_t\, {}^{\mathcal{B}_1}\mathbf{e}^T\right)}_{\text{Use Eq.(5.132)}} \\
&= \underbrace{\left({}^{\mathcal{B}_0}\mathbf{e} \cdot {}^{\mathcal{B}_1}\mathbf{e}^T\right)}_{{}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}}\ {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}} \\
&= \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right) \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)
\end{aligned} \tag{5.137}$$

Similarly, the time derivative of ${}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}$ in terms of $\mathcal{B}_1$ yields:

$$\begin{aligned}
{}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}} &= {}^{\mathcal{B}_1}\mathfrak{D}_t\, {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A} = {}^{\mathcal{B}_1}\mathfrak{D}_t \left({}^{\mathcal{B}_0}\mathbf{e} \cdot {}^{\mathcal{B}_1}\mathbf{e}^T\right) \\
&= \underbrace{\left({}^{\mathcal{B}_1}\mathfrak{D}_t\, {}^{\mathcal{B}_0}\mathbf{e}\right)}_{\text{Use Eq.(5.131)}} \cdot {}^{\mathcal{B}_1}\mathbf{e}^T + {}^{\mathcal{B}_0}\mathbf{e} \cdot \underbrace{\left({}^{\mathcal{B}_1}\mathfrak{D}_t\, {}^{\mathcal{B}_1}\mathbf{e}^T\right)}_{\mathbf{0}} \\
&= \underbrace{\left(-{}^{\mathcal{B}_0}_{\mathcal{B}_0|\mathcal{B}_1}\widetilde{\boldsymbol{\omega}}\right)}_{{}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}} \underbrace{\left({}^{\mathcal{B}_0}\mathbf{e} \cdot {}^{\mathcal{B}_1}\mathbf{e}^T\right)}_{{}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}} \\
&= \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right) \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)
\end{aligned} \tag{5.138}$$

Remark 5.3.2

1. *From Eq.* (5.138), *we readily have*

$$ {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}} = \left({}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}}\right)\ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T \tag{5.139}$$

   Substituting Eq. (5.137) *yields*

$$ {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}} = \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T \tag{5.140}$$

Since we have ${}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}} = {}^{\mathcal{B}_1}\widetilde{\mathbf{e}} \cdot {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\omega}}$ *from* ${}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega} = {}^{\mathcal{B}_1}\mathbf{e} \cdot {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\omega}}$, [14] *we get*

$$
\begin{aligned}
{}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}} &= {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ {}^{\mathcal{B}_1}\widetilde{\mathbf{e}} \cdot {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\omega}}\ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T \\
&= \left(\underbrace{{}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ {}^{\mathcal{B}_1}\widetilde{\mathbf{e}}\ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T}_{\textit{Use Eq. } (5.40)} \right) \cdot {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\omega}} \\
&= \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (5.141)
\end{aligned}
$$

$$
\boxed{{}^{\mathcal{B}_0}_{\mathcal{B}_0|\mathcal{B}_1}\boldsymbol{\omega} = \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right) \left({}^{\mathcal{B}_1}_{\mathcal{B}_0|\mathcal{B}_1}\boldsymbol{\omega}\right)} \qquad (5.142)
$$

5.3.2 Velocity Vectors

Theorem 5.3.3 (Velocity Vector)

Consider a point, $\mathbf{P} \in \mathbb{E}^3$, *as shown in Fig. 5.1. Suppose frame* $\mathcal{B}_1$ *in the figure is rotating at* ${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\omega}}$ *with respect to frame* $\mathcal{B}_0$ [15] *. The time derivative of* $\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P})$ *in terms of* $\mathcal{B}_0$ *leads to the velocity vector of point* $\mathbf{P}$ *with respect to* $\mathcal{B}_0$, *and it is given as:*

$$
\boxed{{}^{\mathcal{B}_0}\mathfrak{D}_t\ \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P}) = {}^{\mathcal{B}_0}\mathfrak{D}_t\ \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{O}_1) + {}^{\mathcal{B}_1}\mathfrak{D}_t\ \vec{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{P}) + {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\omega}} \times \vec{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{P})} \qquad (5.143)
$$

The first term in the right-hand side of Eq. (5.143) *is the velocity vector of point* $\mathbf{O}_1$ *with respect to* $\mathcal{B}_0$, *i.e., the velocity of point* $\mathbf{O}_1$ *observed from point* $\mathbf{O}$. *Similarly, the second term in the right-hand side of Eq.* (5.143) *is the velocity vector of point* $\mathbf{P}$ *with respect to* $\mathcal{B}_1$, *i.e., the velocity of point* $\mathbf{P}$ *observed from point* $\mathbf{O}_1$. *This term vanishes if point* $\mathbf{P}$ *is fixed to the rigid body,* Ω*: Eq.* (5.143) *can be reduced to*

$$
\boxed{{}^{\mathcal{B}_0}\mathfrak{D}_t\ \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P}) = {}^{\mathcal{B}_0}\mathfrak{D}_t\ \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{O}_1) + {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\omega}} \times \vec{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{P})} \qquad (5.144)
$$

---

[14] *See Eq.* (5.38)

[15] ${}_{\mathcal{B}_j|\mathcal{B}_i}\vec{\boldsymbol{\omega}}$ *denotes the angular velocity of frame* $\mathcal{B}_j$ *with respect to frame* $\mathcal{B}_i$. *If* $j = i$, *we have* ${}_{\mathcal{B}_j|\mathcal{B}_i}\vec{\boldsymbol{\omega}} = \vec{\mathbf{0}}$.

Proof. From the geometry (Fig. 5.1), we have

$$\vec{\pi}(\mathbf{O},\mathbf{P}) = \vec{\pi}(\mathbf{O},\mathbf{O}_1) + \vec{\pi}(\mathbf{O}_1,\mathbf{P}) \tag{5.145}$$

Taking the time derivative with respect to $\mathcal{B}_0$ yields

$$\begin{aligned} {}^{\mathcal{B}_0}\mathfrak{D}_t\, \vec{\pi}(\mathbf{O},\mathbf{P}) &= {}^{\mathcal{B}_0}\mathfrak{D}_t\, \vec{\pi}(\mathbf{O},\mathbf{O}_1) + {}^{\mathcal{B}_0}\mathfrak{D}_t\, \vec{\pi}(\mathbf{O}_1,\mathbf{P}) \\ &= {}^{\mathcal{B}_0}\mathfrak{D}_t\, \vec{\pi}(\mathbf{O},\mathbf{O}_1) + {}^{\mathcal{B}_0}\mathfrak{D}_t\, \vec{\pi}(\mathbf{O}_1,\mathbf{P}) + {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \vec{\pi}(\mathbf{O}_1,\mathbf{P}) \end{aligned} \tag{5.146}$$

where Eq. (5.126) has been used.

Theorem 5.3.4 (Velocity Component Vector)

The component form of the velocity vector given in Eq. (5.143) *in terms of frame* $\mathcal{B}_0$ *yields:*

$$\boxed{{}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}) = {}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{O}_1) + {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\left[{}^{\mathcal{B}_1}\dot{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P}) + \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right)\, {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P})\right]} \tag{5.147}$$

where ${}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P})$ *and* ${}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{O}_1)$ *denote the velocity component vectors of the velocities of points* $\mathbf{P}$ *and* $\mathbf{O}$ *with respect to frame* $\mathcal{B}_0$*, respectively; and* ${}^{\mathcal{B}_1}\dot{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P})$ *denotes the velocity component vector of the velocity of point* $\mathbf{P}$ *with respect to frame* $\mathcal{B}_1$*.*

Proof. The left-hand side and the first term of the right-hand side of Eq. (5.143) can be decomposed in terms of $\mathcal{B}_0$ as

$${}^{\mathcal{B}_0}\mathfrak{D}_t\, \vec{\pi}(\mathbf{O},\mathbf{P}) = {}^{\mathcal{B}_0}\mathbf{e}^T\, {}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}) \tag{5.148}$$

$${}^{\mathcal{B}_0}\mathfrak{D}_t\, \vec{\pi}(\mathbf{O},\mathbf{O}_1) = {}^{\mathcal{B}_0}\mathbf{e}^T\, {}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{O}_1) \tag{5.149}$$

Notice that the time derivative of a real component vector is independent of frames we refer to; that is,

$${}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}) = {}^{\mathcal{B}_0}\mathfrak{D}_t\, {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{P}) = {}^{\mathcal{B}_1}\mathfrak{D}_t\, {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{P}) \tag{5.150}$$

$${}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{O}_1) = {}^{\mathcal{B}_0}\mathfrak{D}_t\, {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{O}_1) = {}^{\mathcal{B}_1}\mathfrak{D}_t\, {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{O}_1) \tag{5.151}$$

As to the second term of the right-hand side of Eq. (5.143), we have

$$\begin{aligned} {}^{\mathcal{B}_1}\mathfrak{D}_t\, \vec{\pi}(\mathbf{O}_1, \mathbf{P}) &= {}^{\mathcal{B}_1}\mathbf{e}^T\ {}^{\mathcal{B}_1}\dot{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{P}) = \left({}^{\mathcal{B}_0}\mathbf{e}^T\ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\ {}^{\mathcal{B}_1}\dot{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{P}) \\ &= {}^{\mathcal{B}_0}\mathbf{e}^T\ \left[{}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ {}^{\mathcal{B}_1}\dot{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{P})\right] \end{aligned} \tag{5.152}$$

The last term of the right-hand side of Eq. (5.143) can be also written in terms of $\mathcal{B}_0$ as

$$\begin{aligned} {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \vec{\pi}(\mathbf{O}_1, \mathbf{P}) &= {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \left({}^{\mathcal{B}_0}\mathbf{e}^T\ {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{P})\right) \\ &= \underbrace{\left({}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times {}^{\mathcal{B}_0}\mathbf{e}^T\right)}_{{}^{\mathcal{B}_0}\mathbf{e}^T\ {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}}\ \underbrace{{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{P})}_{{}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{P})} \\ &= {}^{\mathcal{B}_0}\mathbf{e}^T\ \underbrace{\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)}_{\text{Use Eq. (5.134)}}\ {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{P}) \\ &= {}^{\mathcal{B}_0}\mathbf{e}^T\ \left[{}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\ {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{P})\right] \end{aligned} \tag{5.153}$$

Substituting Eq. (5.148) - Eq. (5.153) into Eq. (5.143) yields

$${}^{\mathcal{B}_0}\mathbf{e}^T\ {}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P}) = {}^{\mathcal{B}_0}\mathbf{e}^T\ \left[{}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{O}_1) + {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ {}^{\mathcal{B}_1}\dot{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{P}) + {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\ {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{P})\right] \tag{5.154}$$

Hence, the velocity component form of Eq. (5.143) in terms of $\mathcal{B}_0$ is obtained as

$${}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P}) = {}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{O}_1) + {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\left[{}^{\mathcal{B}_1}\dot{\boldsymbol{\pi}}(\mathbf{O}_1, \mathbf{P}) + {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\ {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1, \mathbf{P})\right] \tag{5.155}$$

5.4 Acceleration Vectors

5.4.1 Angular Acceleration Vectors

Definition 5.4.1 (Angular Acceleration)

Suppose a Cartesian frame $\mathcal{B}_1$ is rotating at an angular velocity, ${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\alpha}$, with respect to an initial Cartesian frame $\mathcal{B}_0$. The angular acceleration vector of frame $\mathcal{B}_1$ with respect *to frame* $\mathcal{B}_0$ *is defined as the time derivative of the angular velocity* ${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}$*. That is, if the time derivative is performed with respect to an arbitrary frame,* $\mathcal{B}_i$*,*

$$\boxed{{}^{(\mathcal{B}_i)}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\alpha} := {}^{\mathcal{B}_i}\mathfrak{D}_t\ {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}} \tag{5.156}$$

Remark 5.4.1

1. *If we take the time derivative of* ${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}$ *with respect to frame* $\mathcal{B}_0$*, i.e.,* $\mathcal{B}_i = \mathcal{B}_0$*, we have*

$$\begin{aligned}
{}^{(\mathcal{B}_0)}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\alpha} &:= {}^{\mathcal{B}_0}\mathfrak{D}_t\ {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \\
&= {}^{\mathcal{B}_1}\mathfrak{D}_t\ {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} + \underbrace{{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}}_{=\mathbf{0}} \\
&= {}^{\mathcal{B}_1}\mathfrak{D}_t\ {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} =: {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\alpha}
\end{aligned} \tag{5.157}$$

   Hence,

$${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\alpha} := {}^{\mathcal{B}_0}\mathfrak{D}_t\ {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} = {}^{\mathcal{B}_1}\mathfrak{D}_t\ {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \tag{5.158}$$

5.4.2 Acceleration Vectors

Theorem 5.4.1 (Acceleration Vector)

Consider a point, $\mathbf{P} \in \mathbb{E}^3$*, as shown in Fig. 5.1. Suppose frame* $\mathcal{B}_1$ *in the figure is rotating at* ${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}$ *with respect to frame* $\mathcal{B}_0$*; see Theorem 5.3.3. The time derivative of* ${}^{\mathcal{B}_0}\mathfrak{D}_t\ \vec{\pi}(\mathbf{O},\mathbf{P})$ *in Eq.* (5.143) *in terms of* $\mathcal{B}_0$ *leads to the acceleration vector of point* $\mathbf{P}$ *with respect to* $\mathcal{B}_0$ *at time* t *as:* [16]

$$\boxed{\begin{aligned}
{}^{\mathcal{B}_0}\mathfrak{D}_t^2\ \vec{\pi}(\mathbf{O},\mathbf{P}) = {}&{}^{\mathcal{B}_0}\mathfrak{D}_t^2\ \vec{\pi}(\mathbf{O},\mathbf{O}_1) \\
&+ {}^{\mathcal{B}_1}\mathfrak{D}_t^2\ \vec{\pi}(\mathbf{O}_1,\mathbf{P}) + {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\alpha} \times \vec{\pi}(\mathbf{O}_1,\mathbf{P}) \\
&+ 2\ {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times {}^{\mathcal{B}_1}\mathfrak{D}_t\ \vec{\pi}(\mathbf{O}_1,\mathbf{P}) \\
&+ {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \left[{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \vec{\pi}(\mathbf{O}_1,\mathbf{P})\right]
\end{aligned}} \tag{5.159}$$

[16] ${}^{\mathcal{B}_0}\mathfrak{D}_t^2 = {}^{\mathcal{B}_0}\mathfrak{D}_t{}^{\mathcal{B}_0}\mathfrak{D}_t$ *denotes the second time derivative with respect to frame* $\mathcal{B}_0$*.*

where the first term on the right-hand side denotes the acceleration vector of point $\mathbf{O}_1$ *with respect to frame* $\mathcal{B}_0$*; the second term denotes the acceleration vector of point* $\mathbf{P}$ *with respect to frame* $\mathcal{B}_1$*; the third term is the acceleration due to the angular acceleration of frame* $\mathcal{B}_1$ *with respect to frame* $\mathcal{B}_0$*; the fourth term is known as the* ***Coriolis acceleration vector****; and the last term is called as the* ***centripetal acceleration vector****. If point* $\mathbf{P}$ *is fixed to the rigid body,* Ω*, Eq.* (5.159) *can be readily reduced to*

$$\boxed{\begin{aligned} {}^{\mathcal{B}_0}\mathfrak{D}_t^2\, \vec{\pi}(\mathbf{O},\mathbf{P}) = {}& {}^{\mathcal{B}_0}\mathfrak{D}_t^2\, \vec{\pi}(\mathbf{O},\mathbf{O}_1) \\ & + {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\alpha} \times \vec{\pi}(\mathbf{O}_1,\mathbf{P}) \\ & + {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \left[{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \vec{\pi}(\mathbf{O}_1,\mathbf{P})\right] \end{aligned}} \tag{5.160}$$

Proof. The time derivative of ${}^{\mathcal{B}_0}\mathfrak{D}_t\, \vec{\pi}(\mathbf{O},\mathbf{P})$ in Eq. (5.143) in terms of $\mathcal{B}_0$ yields:

$${}^{\mathcal{B}_0}\mathfrak{D}_t^2\, \vec{\pi}(\mathbf{O},\mathbf{P}) = {}^{\mathcal{B}_0}\mathfrak{D}_t^2\, \vec{\pi}(\mathbf{O},\mathbf{O}_1) + {}^{\mathcal{B}_0}\mathfrak{D}_t\, \left[{}^{\mathcal{B}_1}\mathfrak{D}_t\, \vec{\pi}(\mathbf{O}_1,\mathbf{P})\right] + {}^{\mathcal{B}_0}\mathfrak{D}_t\, \left[{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \vec{\pi}(\mathbf{O}_1,\mathbf{P})\right] \tag{5.161}$$

The second and last terms in the right-hand side in the equation above can be written as

$${}^{\mathcal{B}_0}\mathfrak{D}_t\, \left[{}^{\mathcal{B}_1}\mathfrak{D}_t\, \vec{\pi}(\mathbf{O}_1,\mathbf{P})\right] = {}^{\mathcal{B}_1}\mathfrak{D}_t^2\, \vec{\pi}(\mathbf{O}_1,\mathbf{P}) + {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times {}^{\mathcal{B}_1}\mathfrak{D}_t\, \vec{\pi}(\mathbf{O}_1,\mathbf{P}) \tag{5.162}$$

and

$$\begin{aligned} {}^{\mathcal{B}_0}\mathfrak{D}_t\, \left[{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \vec{\pi}(\mathbf{O}_1,\mathbf{P})\right] &= {}^{\mathcal{B}_1}\mathfrak{D}_t\, \left[{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \vec{\pi}(\mathbf{O}_1,\mathbf{P})\right] + {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \left[{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \vec{\pi}(\mathbf{O}_1,\mathbf{P})\right] \\ &= \underbrace{\left({}^{\mathcal{B}_1}\mathfrak{D}_t\, {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}\right)}_{{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\alpha}} \times \vec{\pi}(\mathbf{O}_1,\mathbf{P}) + {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \left({}^{\mathcal{B}_1}\mathfrak{D}_t\, \vec{\pi}(\mathbf{O}_1,\mathbf{P})\right) \\ &\quad + {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \left[{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \vec{\pi}(\mathbf{O}_1,\mathbf{P})\right] \end{aligned} \tag{5.163}$$

respectively. Hence, Eq. (5.159) is readily obtained by substituting Eq. (5.162) and Eq. (5.163) into Eq. (5.161).

Theorem 5.4.2 (Acceleration Component Vector)

The component form of the acceleration vector given in Eq. (5.159) *in terms of frame* $\mathcal{B}_0$ *yields:*

$$\boxed{\begin{aligned}{}^{\mathcal{B}_0}\ddot{\pi}(\mathbf{O},\mathbf{P}) ={}& {}^{\mathcal{B}_0}\ddot{\pi}(\mathbf{O},\mathbf{O}_1)\\ &+ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ {}^{\mathcal{B}_1}\ddot{\pi}(\mathbf{O}_1,\mathbf{P}) + {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\alpha}\right){}^{\mathcal{B}_1}\pi(\mathbf{O}_1,\mathbf{P})\\ &+ 2\ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right){}^{\mathcal{B}_1}\dot{\pi}(\mathbf{O}_1,\mathbf{P})\\ &+ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right){}^{\mathcal{B}_1}\pi(\mathbf{O}_1,\mathbf{P})\end{aligned}} \tag{5.164}$$

where ${}^{\mathcal{B}_0}\ddot{\pi}(\mathbf{O},\mathbf{P})$ *and* ${}^{\mathcal{B}_0}\ddot{\pi}(\mathbf{O},\mathbf{O}_1)$ *are the acceleration component vectors of points* $\mathbf{P}$ *and* $\mathbf{O}_1$*, respectively, with respect to* $\mathcal{B}_0$*. If* $\mathbf{P}$ *is a fixed point in* Ω*, Eq.* (5.164) *can be readily reduced to*

$$\boxed{\begin{aligned}{}^{\mathcal{B}_0}\ddot{\pi}(\mathbf{O},\mathbf{P}) ={}& {}^{\mathcal{B}_0}\ddot{\pi}(\mathbf{O},\mathbf{O}_1)\\ &+ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\alpha}\right){}^{\mathcal{B}_1}\pi(\mathbf{O}_1,\mathbf{P})\\ &+ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right){}^{\mathcal{B}_1}\pi(\mathbf{O}_1,\mathbf{P})\end{aligned}} \tag{5.165}$$

Proof. The left-hand side and the first term of the right-hand side of Eq. (5.159) can be written as

$$\begin{aligned}{}^{\mathcal{B}_0}\mathfrak{D}_t^2\ \vec{\pi}(\mathbf{O},\mathbf{P}) &= {}^{\mathcal{B}_0}\mathbf{e}^T\ {}^{\mathcal{B}_0}\ddot{\pi}(\mathbf{O},\mathbf{P}) &(5.166)\\ {}^{\mathcal{B}_0}\mathfrak{D}_t^2\ \vec{\pi}(\mathbf{O},\mathbf{O}_1) &= {}^{\mathcal{B}_0}\mathbf{e}^T\ {}^{\mathcal{B}_0}\dot{\pi}(\mathbf{O},\mathbf{O}_1) &(5.167)\end{aligned}$$

where the acceleration component vectors are given as the second time derivative of the position component vectors:

$$\begin{aligned}{}^{\mathcal{B}_0}\ddot{\pi}(\mathbf{O},\mathbf{P}) &= {}^{\mathcal{B}_0}\mathfrak{D}_t^2\ {}^{\mathcal{B}_0}\pi(\mathbf{O},\mathbf{P}) = {}^{\mathcal{B}_1}\mathfrak{D}_t^2\ {}^{\mathcal{B}_0}\pi(\mathbf{O},\mathbf{P}) &(5.168)\\ {}^{\mathcal{B}_0}\ddot{\pi}(\mathbf{O},\mathbf{O}_1) &= {}^{\mathcal{B}_0}\mathfrak{D}_t^2\ {}^{\mathcal{B}_0}\pi(\mathbf{O},\mathbf{O}_1) = {}^{\mathcal{B}_1}\mathfrak{D}_t^2\ {}^{\mathcal{B}_0}\pi(\mathbf{O},\mathbf{O}_1) &(5.169)\end{aligned}$$

The second term on the right-hand side of Eq. (5.159) denotes the acceleration of point **P** with respect to $\mathcal{B}_1$, and it can be written as

$$^{\mathcal{B}_1}\mathfrak{D}_t^2\ \vec{\pi}(\mathbf{O}_1,\mathbf{P}) = {}^{\mathcal{B}_1}\mathbf{e}^T\ {}^{\mathcal{B}_1}\dot{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P}) = {}^{\mathcal{B}_0}\mathbf{e}^T\ \left[{}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ {}^{\mathcal{B}_1}\dot{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P})\right] \tag{5.170}$$

The third term on the right-hand side of Eq. (5.159) is given as

$$\begin{aligned} {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\alpha}\times\vec{\pi}(\mathbf{O}_1,\mathbf{P}) &= \underbrace{{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\alpha}\times[{}^{\mathcal{B}_1}\mathbf{e}^T}_{{}^{\mathcal{B}_1}\mathbf{e}^T\ {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\alpha}}\ {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P})] \\ &= {}^{\mathcal{B}_1}\mathbf{e}^T\ \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\alpha}\right)\ {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) \\ &= {}^{\mathcal{B}_0}\mathbf{e}^T\ \left[{}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\alpha}\right)\ {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P})\right] \end{aligned} \tag{5.171}$$

The fourth and last terms on the right-hand side of Eq. (5.159) yields:

$$\begin{aligned} 2\ {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}\times{}^{\mathcal{B}_1}\mathfrak{D}_t\ \vec{\pi}(\mathbf{O}_1,\mathbf{P}) &= 2\ {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}\times\left[{}^{\mathcal{B}_1}\mathbf{e}^T\ {}^{\mathcal{B}_1}\dot{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P})\right] \\ &= 2\ \underbrace{{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}\times[{}^{\mathcal{B}_0}\mathbf{e}^T}_{{}^{\mathcal{B}_0}\mathbf{e}^T\ {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}}\ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ {}^{\mathcal{B}_1}\dot{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P})] \\ &= 2\ {}^{\mathcal{B}_0}\mathbf{e}^T\ \underbrace{\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right)\ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}}_{\text{Use Eq. (5.134)}}\ {}^{\mathcal{B}_1}\dot{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P}) \\ &= {}^{\mathcal{B}_0}\mathbf{e}^T\ \left[2\ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right)\ {}^{\mathcal{B}_1}\dot{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P})\right] \end{aligned} \tag{5.172}$$

and

$$\begin{aligned} {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}\times\left[{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}\times\vec{\pi}(\mathbf{O}_1,\mathbf{P})\right] &= {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}\times[\underbrace{{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}\times{}^{\mathcal{B}_1}\mathbf{e}^T}_{{}^{\mathcal{B}_1}\mathbf{e}^T\ {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}}\ {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P})] \\ &= \underbrace{\left({}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}\times{}^{\mathcal{B}_1}\mathbf{e}^T\right)}_{{}^{\mathcal{B}_1}\mathbf{e}^T\ {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}}\ \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right)\ {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) \\ &= {}^{\mathcal{B}_1}\mathbf{e}^T\ {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\ \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right)\ {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) \\ &= {}^{\mathcal{B}_0}\mathbf{e}^T\ \left[{}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\ \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right)\ \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right)\ {}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P})\right] \end{aligned} \tag{5.173}$$

respectively. Substituting Eq. (5.166), Eq. (5.167), Eq. (5.170), Eq. (5.171), Eq. (5.172), and Eq. (5.173) into Eq. (5.159) leads to Eq. (5.164).

5.5 Variations

5.5.1 Virtual Displacement and Rotation Vectors

Definition 5.5.1 (Virtual Displacement Vector)

Suppose the position vector, $\vec{\pi}(\mathbf{O},\mathbf{P})$, can be expressed as a function of time $t \in \mathbb{I} \subset \mathbb{R}$ and the generalized coordinates $\mathbf{q}(t) = (q_1, q_2, \cdots, q_{n_g})^T : \mathbb{I} \to Q$ as $\vec{\mathbf{r}}(\mathbf{q},t) := \vec{\pi}(\mathbf{O},\mathbf{P})$. The virtual displacement of the position vector $\vec{\mathbf{r}}(\mathbf{q},t) = \vec{\pi}(\mathbf{O},\mathbf{P})$, or variation of $\vec{\mathbf{r}}(\mathbf{q},t) = \vec{\pi}(\mathbf{O},\mathbf{P})$, is defined as the differential of $\vec{\mathbf{r}}(\mathbf{q},t)$ with the fixed time t; that is, time t is treated as the independent variable, and therefore its variation is defined to be zero: $\delta t = 0$. Hence,

$$\delta\vec{\mathbf{r}}(\mathbf{q},t) = \sum_{k=1}^{n_g} \frac{\partial \vec{\mathbf{r}}(\mathbf{q},t)}{\partial q_i}\delta q_i + \frac{\partial \vec{\mathbf{r}}(\mathbf{q},t)}{\partial t}\underbrace{\delta t}_{0} = \frac{\partial \vec{\mathbf{r}}(\mathbf{q},t)}{\partial q_i}\delta q_i \tag{5.174}$$

For convention, δ is used for variations to distinct from differentials, d.

Remark 5.5.1

1. *In $\mathbb{E}^n$, the component form of the position vector with respect to a Cartesian frame $\mathcal{B}_\ell$ is simply given by*

$$\delta\vec{\mathbf{r}} = \delta\vec{\pi}(\mathbf{O},\mathbf{P}) = {}^{\mathcal{B}_\ell}\mathbf{e}^T \left(\delta^{\mathcal{B}_\ell}\boldsymbol{\pi}(\mathbf{O},\mathbf{P})\right) = \left(\delta^{\mathcal{B}_\ell}\boldsymbol{\pi}(\mathbf{O},\mathbf{P})\right)^T \ {}^{\mathcal{B}_\ell}\mathbf{e} \tag{5.175}$$

where the virtual displacement component vector is defined as

$$\delta^{\mathcal{B}_\ell}\mathbf{r} = \delta^{\mathcal{B}_\ell}\boldsymbol{\pi}(\mathbf{O},\mathbf{P}) := \left[\delta^{\mathcal{B}_\ell}\pi_1(\mathbf{O},\mathbf{P}), \delta^{\mathcal{B}_\ell}\pi_2(\mathbf{O},\mathbf{P}), \cdots, \delta^{\mathcal{B}_\ell}\pi_n(\mathbf{O},\mathbf{P})\right]^T \in \mathbb{R}^n \tag{5.176}$$

When $n = 3$, it reduces to the case of $\mathbb{E}^3$.

2. *This definition can be extended with the help of so-called* ***geometric constraint equations*** *to be discussed later; see Definition 6.1.3.*

Theorem 5.5.1 (Virtual Displacement Vector)

From the velocity vector given in Eq. (5.143), *the virtual displacement vector of* ${}^{\mathcal{B}_\ell}\boldsymbol{\pi}(\mathbf{O},\mathbf{P})$ *is obtained as*

$$\boxed{{}^{\mathcal{B}_0}\delta\,\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}) = {}^{\mathcal{B}_0}\delta\,\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{O}_1) + \underbrace{{}^{\mathcal{B}_1}\delta\,\vec{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P}) + {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\varpi}} \times \vec{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P})}_{{}^{\mathcal{B}_0}\delta\,\vec{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P})}} \tag{5.177}$$

where ${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\varpi}} := {}^{\mathcal{B}_0}\delta\vec{\boldsymbol{\phi}}$ *is the* ***virtual rotation vector*** *of frame* $\mathcal{B}_1$ *with respect to frame* $\mathcal{B}_0$*. If point* $\mathbf{P}$ *is fixed to the rigid body,* Ω*, it reduces to*

$$\boxed{{}^{\mathcal{B}_0}\delta\,\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}) = {}^{\mathcal{B}_0}\delta\,\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{O}_1) + \underbrace{{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\varpi}} \times \vec{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P})}_{{}^{\mathcal{B}_0}\delta\,\vec{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P})}} \tag{5.178}$$

Proof. From the velocity vector given in Eq. (5.143), we can derive the virtual displacement vector of ${}^{\mathcal{B}_\ell}\boldsymbol{\pi}(\mathbf{O},\mathbf{P})$ by following the steps: (1) multiply by dt, (2) change the notation from d to δ, and then (3) set $\delta t = 0$. That is, From Eq. (5.143), we have

$$\frac{{}^{\mathcal{B}_0}d}{dt}\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}) = \frac{{}^{\mathcal{B}_0}d}{dt}\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{O}_1) + \frac{{}^{\mathcal{B}_1}d}{dt}\vec{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P}) + \underbrace{\frac{{}^{\mathcal{B}_0}d\vec{\boldsymbol{\phi}}}{dt}}_{{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}} \times \vec{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P})$$

Multiplying by dt, we get

$${}^{\mathcal{B}_0}d\,\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}) = {}^{\mathcal{B}_0}d\,\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{O}_1) + {}^{\mathcal{B}_1}d\,\vec{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P}) + {}^{\mathcal{B}_0}d\vec{\boldsymbol{\phi}} \times \vec{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P}) \tag{5.179}$$

Changing the differential notation to variational notation yields

$${}^{\mathcal{B}_0}\delta\,\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}) = {}^{\mathcal{B}_0}\delta\,\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{O}_1) + {}^{\mathcal{B}_1}\delta\,\vec{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P}) + {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\varpi}} \times \vec{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P}) \tag{5.180}$$

where ${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\varpi}} := {}^{\mathcal{B}_0}\delta\vec{\boldsymbol{\phi}}$ denotes the virtual rotation vector of $\mathcal{B}_1$ with respect to $\mathcal{B}_0$. Since frame $\mathcal{B}_1$ is the body-fixed frame, if $\mathbf{P}$ is fixed to the rigid body, Ω, the thrid term of the right-hand side vanishes; therefore, Eq. (5.178) is readily obtained.

Definition 5.5.2 (Virtual Rotation Component Vector)

The component form of the virtual rotation, ${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\varpi}}$, is defined ${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\varpi}}$ satisfies the variational form of Poisson's equation given in Theorem 5.3.2. That is,

$$\delta\ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A} = \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\ \left({}^{\mathcal{B}_1}_{\mathcal{B}_0|\mathcal{B}_1}\widetilde{\boldsymbol{\varpi}}\right) = \left({}^{\mathcal{B}_0}_{\mathcal{B}_0|\mathcal{B}_1}\widetilde{\boldsymbol{\varpi}}\right)\ \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right) \tag{5.181}$$

Or equivalently,

$$\begin{aligned} {}^{\mathcal{B}_0}_{\mathcal{B}_0|\mathcal{B}_1}\widetilde{\boldsymbol{\varpi}} &= \left(\delta\ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T = \left(\delta\ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\ {}^{\mathcal{B}_1/\mathcal{B}_0}\mathbf{A} && (5.182)\\ {}^{\mathcal{B}_1}_{\mathcal{B}_0|\mathcal{B}_1}\widetilde{\boldsymbol{\varpi}} &= {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T\ \left(\delta\ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right) = {}^{\mathcal{B}_1/\mathcal{B}_0}\mathbf{A}\ \left(\delta\ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right) && (5.183) \end{aligned}$$

where ${}^{\mathcal{B}_\ell}_{\mathcal{B}_0|\mathcal{B}_1}\widetilde{\boldsymbol{\varpi}} \in SO(3)$ denotes the tilde matrix of the virtual rotation component vector, in terms of frame $\mathcal{B}_\ell$, of frame $\mathcal{B}_1$ with respect to frame $\mathcal{B}_0$ (for $\ell = 1, 2$).

Remark 5.5.2

1. *With this definition, we have the following corresponding relations between the differential and variational quantities:*

$$\begin{aligned} {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\omega}} &\Leftrightarrow {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\varpi}}\\ {}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}} &\Leftrightarrow \delta\ {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A} \end{aligned} \tag{5.184}$$

Theorem 5.5.2 (Virtual Displacement Component Vector)

In view of Eq. (5.147) *in Theorem 5.3.4, the virtual displacement component vector in terms of frame $\mathcal{B}_0$ is obtained as*

$$\boxed{\begin{aligned} \delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{P}) &= \delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{O}_1) + {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\left[\delta^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) + \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\varpi}}\right){}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P})\right]\\ &= \delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{O}_1) + \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\delta^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) + \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\varpi}}\right){}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P})\\ &= \delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{O}_1) + \underbrace{\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\delta^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P})}_{\delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P})} - \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right){}^{\mathcal{B}_1}\widetilde{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P})\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\varpi}\right) \end{aligned}} \tag{5.185}$$

Proof. Multiplying Eq. (5.147) by dt, we get

$$d\,{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{P}) = d\,{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{O}_1) + {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\left[d\,{}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) + \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}dt\right){}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P})\right] \quad (5.186)$$

Changing d to δ (with $\delta t = 0$), we readily obtain

$$\delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{P}) = \delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{O}_1) + {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\left[\delta^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) + \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\varpi}}\right){}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P})\right] \quad (5.187)$$

which is identical to the first line of Eq. (5.185). Note that, likewise the differentials, the variation of a scalar quantity is independent of the frames we refer to.

In order to obtain the expressions in the second and last lines in Eq. (5.185), Eq. (5.187) may be modified as follows:

$$\begin{aligned}
\delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{P}) &= \delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{O}_1) + \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\delta^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) + \underbrace{{}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\varpi}}\right)}_{\text{Use Eq. (5.181)}}{}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) \\
&= \delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{O}_1) + \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\delta^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) + \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\varpi}}\right)\underbrace{\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right){}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P})}_{{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P})} \\
&= \delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{O}_1) + \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\delta^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) + \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\varpi}}\right){}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) \quad (5.188)
\end{aligned}$$

and

$$\begin{aligned}
\delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{P}) &= \delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{O}_1) + \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\delta^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) + {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\underbrace{\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\varpi}}\right){}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P})}_{-{}^{\mathcal{B}_1}\widetilde{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P})\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\varpi}\right)} \\
&= \delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{O}_1) + \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\delta^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O}_1,\mathbf{P}) - \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right){}^{\mathcal{B}_1}\widetilde{\boldsymbol{\pi}}(\mathbf{O}_1,\mathbf{P})\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\varpi}\right) \quad (5.189)
\end{aligned}$$

respectively.

5.5.2 Virtual Velocity Vector and Variation of Angular Velocity Vector

Definition 5.5.3 (Virtual Velocity Vector)

In accordance with the notations in Definition 5.5.1, the variation of the time derivative of $\vec{\mathbf{r}}(\mathbf{q},t) := \vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P})$ *is defined as the virtual velocity of* $\vec{\mathbf{r}}(\mathbf{q},t) : Q \times \mathbb{I} \to \mathbb{V}^n$*:*

For $\vec{\mathbf{v}}(\mathbf{q},\dot{\mathbf{q}},t) := d\vec{\mathbf{r}}/dt$*,*

$$\begin{aligned} \delta\vec{\mathbf{v}}(\mathbf{q},\dot{\mathbf{q}},t) &= \frac{\partial\vec{\mathbf{v}}(\mathbf{q},\dot{\mathbf{q}},t)}{\partial q_i}\underbrace{\delta q_i}_{0} + \frac{\partial\vec{\mathbf{v}}(\mathbf{q},\dot{\mathbf{q}},t)}{\partial \dot{q}_i}\delta\dot{q}_i + \frac{\partial\vec{\mathbf{v}}(\mathbf{q},\dot{\mathbf{q}},t)}{\partial t}\underbrace{\delta t}_{0} \\ &= \frac{\partial\vec{\mathbf{v}}(\mathbf{q},\dot{\mathbf{q}},t)}{\partial \dot{q}_i}\delta\dot{q}_i \end{aligned} \tag{5.190}$$

Notice that the generalized coordinates, $\mathbf{q}(t) : \mathbb{I} \to Q$*, as well as time* $t \in \mathbb{I} \subset \mathbb{R}$*, are treated as the independent variables for the derivation of the virtual velocity:* $\delta\mathbf{q} = \mathbf{0}$ *and* $\delta t = 0$*.*

Remark 5.5.3

1. *In* $\mathbb{E}^n$*, the component form of the position vector with respect to a Cartesian frame* $\mathcal{B}_\ell$ *is simply given by*

$$\delta\vec{\mathbf{v}} = {}^{\mathcal{B}_\ell}\mathbf{e}^T\ \left(\delta^{\mathcal{B}_\ell}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P})\right) = \left(\delta^{\mathcal{B}_\ell}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P})\right)^T\ {}^{\mathcal{B}_\ell}\mathbf{e} \tag{5.191}$$

where $\delta^{\mathcal{B}_\ell}\mathbf{v} = \delta^{\mathcal{B}_\ell}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}) = [\delta^{\mathcal{B}_\ell}\dot{\pi}_i(\mathbf{O},\mathbf{P})] \in \mathbb{R}^n$ *(for* $i = 1,2,\cdots,n$*) denotes the virtual velocity component vector. When* $n = 3$*, it reduces to the case of* $\mathbb{E}^3$*.*

2. *Since the time derivative of* $\vec{\mathbf{r}}(\mathbf{q},t) := \vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P})$ *gives the velocity vector as*

$$\vec{\mathbf{v}} = \frac{\partial\vec{\mathbf{r}}(\mathbf{q},t)}{\partial q_i}\underbrace{\frac{dq_i}{dt}}_{\dot{q}_i} + \frac{\partial\vec{\mathbf{r}}(\mathbf{q},t)}{\partial t}dt \tag{5.192}$$

we have

$$\frac{\partial\vec{\mathbf{v}}(\mathbf{q},\dot{\mathbf{q}},t)}{\partial \dot{q}_i} = \frac{\partial\vec{\mathbf{r}}(\mathbf{q},t)}{\partial q_i} \tag{5.193}$$

Hence, Eq. (5.190) *can be also written as*

$$\delta\vec{\mathbf{v}}(\mathbf{q},\dot{\mathbf{q}},t) = \frac{\partial\vec{\mathbf{v}}(\mathbf{q},\dot{\mathbf{q}},t)}{\partial\dot{q}_i}\delta\dot{q}_i = \frac{\partial\vec{\mathbf{r}}(\mathbf{q},t)}{\partial q_i}\delta\dot{q}_i \tag{5.194}$$

Definition 5.5.4 (Variation of Angular Velocity Component Vector)

Consider the angular velocity of $\mathcal{B}_1$ *with respect to* $\mathcal{B}_0$*:* ${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}$*. The variation of the component vector of* ${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}$ *in terms of frame* $\mathcal{B}_0$ *is given as*

$$\boxed{\delta\,{}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega} = {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\varpi}} - \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\varpi}\right)} \tag{5.195}$$

Similarly, the variation of the component vector of ${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}$ *in terms of frame* $\mathcal{B}_1$ *is given as*

$$\boxed{\delta\,{}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega} = {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\varpi}} + \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\varpi}\right)} \tag{5.196}$$

Proof. The variation of the tilde matrix of the component vector of the angular velocity of $\mathcal{B}_1$ with respect to $\mathcal{B}_0$ in terms of $\mathcal{B}_0$ is obtained from Eq. (5.135) in Theorem 5.3.2 as

$$\begin{aligned}
\delta\,{}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}} &= \delta\left[\left({}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}}\right)\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T\right)\right] \\
&= \left(\delta\,{}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}}\right)\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T\right) + \left({}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}}\right)\left(\delta\,{}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T\right)
\end{aligned} \tag{5.197}$$

Taking the time derivative of Eq. (5.182) in Definition 5.5.2, we get

$$\begin{aligned}
{}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\widetilde{\boldsymbol{\varpi}}} &= \mathfrak{D}_t\,{}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\varpi}} = \mathfrak{D}_t\left[\left(\delta\,{}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T\right)\right] \\
&= \left(\delta\,{}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}}\right)\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T\right) + \left(\delta\,{}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\left({}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}}^T\right)
\end{aligned} \tag{5.198}$$

That is,

$$\left(\delta\,{}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}}\right)\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T\right) = {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\widetilde{\boldsymbol{\varpi}}} - \left(\delta\,{}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\left({}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}}^T\right) \tag{5.199}$$

Substituting Eq. (5.199) into Eq. (5.197) yields:

$$\delta\,{}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}} = {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\widetilde{\boldsymbol{\varpi}}} - \left(\delta\,{}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\left({}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}}^T\right) + \left({}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}}\right)\left(\delta\,{}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T\right) \tag{5.200}$$

Using Poisson's equation, ${}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}} = ({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}})({}^{\mathcal{B}_1/\mathcal{B}_0}\mathbf{A})$ (see Theorem 5.3.2), we obtain

$$\begin{aligned}
\delta\, {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}} &= {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\widetilde{\boldsymbol{\varpi}}} - \left(\delta\, {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\left[\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\left({}^{\mathcal{B}_1/\mathcal{B}_0}\mathbf{A}\right)\right]^T + \left[\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\left({}^{\mathcal{B}_1/\mathcal{B}_0}\mathbf{A}\right)\right]\left(\delta\, {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T\right) \\
&= {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\widetilde{\boldsymbol{\varpi}}} - \underbrace{\left(\delta\, {}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\left({}^{\mathcal{B}_1/\mathcal{B}_0}\mathbf{A}^T\right)}_{{}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\varpi}}}\ \underbrace{{}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}^T}_{-{}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}} + {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\ \underbrace{\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\left(\delta\, {}^{\mathcal{B}_1/\mathcal{B}_0}\mathbf{A}^T\right)}_{{}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\varpi}}^T} \\
&= {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\widetilde{\boldsymbol{\varpi}}} + \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\varpi}}\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right) - \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\varpi}}\right) \\
&= {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\widetilde{\boldsymbol{\varpi}}} + \left[\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\varpi}^T\right) - \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\varpi}^T\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right)\mathbf{I}_3\right] \\
&\quad - \left[\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\varpi}\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}^T\right) - \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}^T\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\varpi}\right)\mathbf{I}_3\right] \\
&= {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\widetilde{\boldsymbol{\varpi}}} + \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\varpi}^T\right) - \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\varpi}\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}^T\right) \\
&\quad + \underbrace{\left[\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}^T\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\varpi}\right) - \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\varpi}^T\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right)\right]}_{\mathbf{0}}\mathbf{I}_3 \\
&= {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\widetilde{\boldsymbol{\varpi}}} + \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\varpi}^T\right) - \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\varpi}\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}^T\right) \\
&= {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\widetilde{\boldsymbol{\varpi}}} + \mathrm{Skew}\left(\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\varpi}}\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right)\right) \\
&= {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\widetilde{\boldsymbol{\varpi}}} - \mathrm{Skew}\left(\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\varpi}\right)\right) \qquad (5.201)
\end{aligned}$$

where $\mathbf{I}_3 = [\delta_{ij}] \in \mathbb{R}^{3\times 3}$ denotes the identity matrix. Hence, we have

$$\delta\, {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega} = {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\varpi}} - \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\varpi}\right) \qquad (5.202)$$

Eq. (5.196) can be derived in a similar manner. ∎

Chapter 6

RIGID-BODY KINEMATICS: Constraint Equations

6.1 Constraint Equations and Virtual Displacements

In a system of multi-bodies, constraints are imposed among the bodies with the object of generating a desired motion to achieve a design purpose of the mechanism. The relative motion between the bodies are restricted by way of constraints; and the constraints are usually expressed in analytical form using the generalized coordinates, $\mathbf{q}(t) = (q_1, q_2, \cdots, q_{n_g})$. The virtual displacements, which were introduced in Definition 5.5.1, may be formally defined, based on the constraint equations.

6.1.1 Generalized Coordinates

Suppose point $\mathbf{P} \in \mathbb{E}^3$ is an arbitrary point in rigid body Ω_ℓ for $\ell = 1, 2, \cdots, n_b$ where n_b denotes the number of rigid bodies in a system. Let $\vec{\mathbf{r}} \equiv \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P})$ where $\mathbf{O} \in \mathbb{E}^3$

is the origin point of the inertia reference frame, $\mathcal{B}_0$. Vector $\vec{\mathbf{r}}$ in the Cartesian frame, in general, could be expressed as a function of n_{g} numbers of parameters and time $t \in \mathbb{I} \subset \mathbb{R}_{+}$,

$$\vec{\mathbf{r}} = \vec{\mathbf{r}}(\mathbf{q}, t) = \vec{\mathbf{r}}(q_1, q_2, \cdots, q_{n_{\mathrm{g}}}) \tag{6.1}$$

The n_{g} numbers of parameters, $\mathbf{q}(t)$, are called ***generalized coordinates***. We assume the Jacobian defined by $\partial\vec{\mathbf{r}}/\partial\mathbf{q}$ is regular (or nonsingular), i.e., the determinant of the Jacobian is non-zero: $\det(\partial\vec{\mathbf{r}}/\partial\mathbf{q}) \neq \mathbf{0}\ \forall\mathbf{q}$. This assumption implies that mapping between $\vec{\mathbf{r}}$ and $\mathbf{q}$ is one-to-one. The choice of $\mathbf{q}$ is left for analyst.

6.1.2 Classification of Constraint Equations

There are two kinds of constraint equations, i.e., ***holonomic*** and ***nonholonomic*** constraints as defined below.

Definition 6.1.1 (Holonomic Constraints)

If constraint equations are given as implicit functions of the generalized coordinates, $\mathbf{q}(t)$, *only, the constraint equations are classified as* ***holonomic-scleronomic****. On the other hand, if constraint equations are given as implicit functions of time* $t \in \mathbb{I}$ *as well as the generalized coordinates,* $\mathbf{q}(t)$, *the constraint equations are classified as* ***holonomic-rhenomic****.*

$$\boxed{\begin{array}{rcl} \mathbf{\Phi}(\mathbf{q}) = \mathbf{0} & \Leftrightarrow & \textit{Holonomic-Scleronomic} \\ \mathbf{\Phi}(\mathbf{q}, t) = \mathbf{0} & \Leftrightarrow & \textit{Holonomic-Rheoomic} \end{array}} \tag{6.2}$$

Remark 6.1.1 (Holonomic Constraint Equations)

1. $\mathbf{\Phi} \in \mathbb{R}^{n_{\mathrm{c}}}$ *where* n_{c} *denotes the number of constraint equations is a smooth constraint function. We assume the Jacobian,* $\mathbf{G} = [G_{ij}] \in \mathbb{R}^{n_{\mathrm{c}} \times n_{\mathrm{g}}}$, *possesses the full*

rank for each $\mathbf{q}$,

$$\operatorname{rank}(\mathbf{G}) = n_{\mathrm{c}} \tag{6.3}$$

where $\mathbf{G}$ *is defined as*

$$\mathbf{G} := \nabla\boldsymbol{\Phi} = \frac{\partial\boldsymbol{\Phi}}{\partial\mathbf{q}} \quad \text{or} \quad G_{ij} := \partial_j\Phi_i = \frac{\partial\Phi_i}{\partial q_j} \tag{6.4}$$

(for $i = 1, 2, \cdots, n_{\mathrm{c}}$ *and* $j = 1, 2, \cdots, n_{\mathrm{g}}$*) such that constraint equations are independent. If the constraint equations are not independent, i.e.,* $\operatorname{rank}(\mathbf{G}) \neq n_{\mathrm{c}}$*, actual number of constraint equations becomes less than* n_{c}*.*

2. *By imposing the constraints to a system of multibodies, the* ***configuration manifold****, denoted as set* Q*, can be defined for the system as*

$$Q := \left\{\mathbf{q} \in \mathbb{R}^{n_{\mathrm{g}}} \mid \boldsymbol{\Phi} = \mathbf{0}\right\} \tag{6.5}$$

It is noteworthy to mention that the trajectories of all bodies in the system can be defined by a single curve in Q *by introducing the generalized coordinates. The generalized velocity,* $\dot{\mathbf{q}}(t)$*, is defined on the tangent space at* $\mathbf{q} \in Q$*:* $\dot{\mathbf{q}}(t) : \mathbb{I} \to T_{\mathbf{q}}Q$ *where*

$$T_{\mathbf{q}}Q := \left\{\dot{\mathbf{q}} \in \mathbb{R}^{n_{\mathrm{g}}} \mid \dot{\boldsymbol{\Phi}} = \mathbf{G}\dot{\mathbf{q}} = \mathbf{0}\right\} \tag{6.6}$$

which spans the kernel of $\mathbf{G}$*, i.e.,* $\ker(\mathbf{G}) = T_{\mathbf{q}}Q$*. Note that both* Q *and* $T_{\mathbf{q}}Q$ *have the same size of* n_{dof}*, the* ***number of degrees of freedom*** *of the system; in other words, they are* n_{dof}*-dimensional manifolds. If* $\mathbf{G}$ *has full rank* n_{c}*, i.e., if Eq. (6.3) is satiesfied, the number of degrees of freedom is given by*

$$n_{\mathrm{dof}} = n_{\mathrm{g}} - n_{\mathrm{c}} \tag{6.7}$$

*The **tangent bundle** (also called as **velocity phase space** or **state space**) is defined as*

$$TQ := \left\{(\mathbf{q}, \dot{\mathbf{q}}) \in \mathbb{R}^{n_{\mathrm{g}}} \times \mathbb{R}^{n_{\mathrm{g}}} \mid \ \mathbf{\Phi} = \mathbf{0} \ \ \textit{and} \ \ \dot{\mathbf{\Phi}} = \mathbf{G}\dot{\mathbf{q}} = \mathbf{0}\right\} \tag{6.8}$$

We assume the set, TQ, is a $2n_{\mathrm{dof}}$-dimensional manifold.

3. *If $n_{\mathrm{g}} = n_{\mathrm{dof}}$, the generalized coordinates, $\mathbf{q}(t) : \mathbb{I} \to Q$, of the system are called as **minimal generalized coordinates**. We employ $\mathbf{q}(t) = \mathbf{s}(t) = (s_1, s_2, \cdots, s_{n_{\mathrm{dof}}})^T(t) : \mathbb{I} \to Q = \mathbb{R}^{n_{\mathrm{dof}}}$ for the minimal generalized coordinates when $n_{\mathrm{g}} = n_{\mathrm{dof}}$ whenever it is necessary.*

Definition 6.1.2 (Nonholonomic Constraints)

*If constraint equations are given as implicit functions of not only the generalized coordinates, $\mathbf{q}(t)$, (and time $t \in \mathbb{I}$), but also the generalized velocities, $\dot{\mathbf{q}}(t)$, the constraint equations are classified as **nonholonomic-bilateral**:*

$$\boxed{\mathbf{\Phi}(\mathbf{q}, \dot{\mathbf{q}}, t) = \mathbf{0} \quad \Leftrightarrow \quad \textit{Nonholonomic-Bilateral}} \tag{6.9}$$

*If an inequality is involved, the constraint equations are classified as **nonholonomic-unilateral**:*

$$\boxed{\mathbf{\Phi}(\mathbf{q}, \dot{\mathbf{q}}, t) \geq \mathbf{0} \quad \Leftrightarrow \quad \textit{Nonholonomic-Unilateral}} \tag{6.10}$$

Remark 6.1.2 (Nonholonomic Constraint Equations)

1. *Nonholonomic bilateral constraint equations may often have the following form*

$$\mathbf{\Phi}(\mathbf{q}, \dot{\mathbf{q}}, t) = \mathbf{B}^{\mathrm{c}}(\mathbf{q}, t)\dot{\mathbf{q}} + \mathbf{b}^{\mathrm{c}}(\mathbf{q}, t) = \mathbf{0} \tag{6.11}$$

with $\mathbf{B}^{\mathrm{c}} \in \mathbb{R}^{n_{\mathrm{c}} \times n_{\mathrm{g}}}$ and $\mathbf{b}^{\mathrm{c}} \in \mathbb{R}^{n_{\mathrm{c}}}$. From Eq. (6.11), *we have*

$$\mathbf{B}^{\mathrm{c}}(\mathbf{q}, t)\delta\mathbf{q} = \mathbf{0} \tag{6.12}$$

6.1.3 Virtual Displacement Vector

Definition 6.1.3 (Virtual Displacement Vector)

Consider holonomic constraint equations. The virtual displacement vector must be chosen in such a way that the first variation of $\mathbf{\Phi} \in \mathbb{R}^{n_c}$ *is zero:*

$$\boxed{\delta\mathbf{\Phi} = \mathbf{G}\delta\mathbf{q} = \mathbf{0}} \tag{6.13}$$

where $\mathbf{G}$ *is as defined in Eq.* (6.4).

Remark 6.1.3

1. *For holonomic-rheonomic constraint equations, for example, virtual displacements,* $\delta\mathbf{q}(t)$*, at a fixed time* t*, must satisfy*

$$\mathbf{\Phi}(\mathbf{q}, t) = \mathbf{\Phi}(\mathbf{q}', t) = \mathbf{0} \tag{6.14}$$

where $\mathbf{q}'(t) = \mathbf{q}(t) + \delta\mathbf{q}(t)$.

6.2 Constraint Forces and Virtual Work due to Constraint Forces

Definition 6.2.1 (Virtual Work due to Constraint Forces and Generalized Constraint Forces)

Let us denote constraint forces (or forces of constraints) acting on body Ω_ℓ *by* $\vec{\mathbf{f}}^{c}_{\ell}$*. If each body is subject to infinitesimally small virtual displacement,* $\delta\vec{\mathbf{r}}_\ell$ *for* $\ell = 1, 2, \cdots n_b$*, the virtual work due to the constraint forces is defined as*

$$\delta W^c := \vec{\mathbf{f}}^c_1 \cdot \delta\vec{\mathbf{r}}_1 + \vec{\mathbf{f}}^c_2 \cdot \delta\vec{\mathbf{r}}_2 + \cdots + \vec{\mathbf{f}}^c_{n_b} \cdot \delta\vec{\mathbf{r}}_{n_b} = \vec{\mathbf{f}}^c_\ell \cdot \delta\vec{\mathbf{r}}_\ell \tag{6.15}$$

Assuming $\vec{\mathbf{r}}_\ell = \vec{\mathbf{r}}_\ell(\mathbf{q}, t)$*, we have*

$$\delta W^c = \vec{\mathbf{f}}^c_\ell \cdot \delta\vec{\mathbf{r}}_\ell(\mathbf{q}, t) = \underbrace{\vec{\mathbf{f}}^c_\ell \cdot \frac{\partial\vec{\mathbf{r}}_\ell}{\partial q_i}}_{Q^c_i} \delta q_i = Q^c_i \delta q_i \tag{6.16}$$

for $i = 1, 2, \cdots, n_{\mathrm{g}}$, *or*

$$\delta W^{\mathrm{c}} = (\mathbf{Q}^{\mathrm{c}})^T \delta \mathbf{q} = \delta \mathbf{q}^T \mathbf{Q}^{\mathrm{c}} \tag{6.17}$$

where $\mathbf{Q}^{\mathrm{c}} := \vec{\mathbf{f}}_\ell^{\mathrm{c}} \cdot \partial_i \vec{\mathbf{r}}_\ell \in \mathbb{R}^{n_{\mathrm{g}}}$ *is called the* ***generalized constraint forces****.*

Remark 6.2.1

1. *The generalized constraint forces and constraint forces are related one another via*

$$\vec{\mathbf{f}}_\ell^{\mathrm{c}} = Q_i^{\mathrm{c}} \frac{\partial q_i(\vec{\mathbf{r}}_1, \vec{\mathbf{r}}_2, \cdots, \vec{\mathbf{r}}_{n_{\mathrm{b}}}, t)}{\partial \vec{\mathbf{r}}_\ell} \quad \text{and} \quad Q_i^{\mathrm{c}} = \vec{\mathbf{f}}_\ell^{\mathrm{c}} \cdot \frac{\partial \vec{\mathbf{r}}_\ell(\mathbf{q}, t)}{\partial q_i} \tag{6.18}$$

2. δW^{c} *denotes simply the total virtual work due to the constraint forces; and we cannot usually find some state function,* W^{c}*, since* δW^{c} *does not, in general, denote the first variation of* W^{c}*.*

Theorem 6.2.1 (Constraint Force Vector with the Lagrange Multipliers)

Consider holonomic constraint equations; see Definition 6.1.1. Constraint forces do no virtual work, i.e.,

$$\boxed{\delta W^{\mathrm{c}} = 0} \tag{6.19}$$

for all allowed virtual displacements if and only if there exists n_{c} *numbers of parameters,* $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \cdots, \lambda_{n_{\mathrm{c}}})^T \in \mathbb{R}^{n_{\mathrm{c}}}$*, called the* ***Lagrange multipliers****, in such a way that the generalized constraint forces can be written as*

$$\boxed{Q_i^{\mathrm{c}} = \boldsymbol{\lambda}^T \frac{\partial \boldsymbol{\Phi}(\mathbf{q}, t)}{\partial q_i} = \lambda_k \frac{\partial \Phi_k(\mathbf{q}, t)}{\partial q_i} = \lambda_k G_{ki}} \tag{6.20}$$

for $k = 1, 2, \cdots, n_{\mathrm{c}}$ *and* $i = 1, 2, \cdots, n_{\mathrm{g}}$, *or*

$$\boxed{\mathbf{Q}^{\mathrm{c}} = (Q_1^{\mathrm{c}}, Q_2^{\mathrm{c}} \cdots, Q_{n_{\mathrm{g}}}^{\mathrm{c}})^T = \boldsymbol{\lambda}^T \mathbf{G} = \mathbf{G}^T \boldsymbol{\lambda}} \tag{6.21}$$

Proof. See [59, p. 50].

Remark 6.2.2

1. *Virtual work due to constraint forces is not equivalent with the physical work done by the constraint forces. If the constraint equations are independent from time, i.e., in the case of holonomic-scleronomic constraints, the constraint forces do not do both physical work and virtual work; while, in the case of holonomic-rheonomic constraints, the constraint forces do not do virtual work, but may still do physical work.*

2. *Substituting Eq.* (6.20) *into Eq.* $(6.18)_1$, *we can obtain the constraint force as*

$$\vec{\mathbf{f}}_\ell^{\mathrm{c}} = \lambda^T \frac{\partial \mathbf{\Phi}(\mathbf{q}, t)}{\partial q_i} \frac{\partial q_i}{\partial \vec{\mathbf{r}}_\ell} = \lambda^T \frac{\partial \bar{\mathbf{\Phi}}(\vec{\mathbf{r}}_1, \vec{\mathbf{r}}_2, \cdots, \vec{\mathbf{r}}_{n_\mathrm{b}})}{\partial \vec{\mathbf{r}}_\ell} \tag{6.22}$$

where $\bar{\mathbf{\Phi}}(\vec{\mathbf{r}}_1, \vec{\mathbf{r}}_2, \cdots, \vec{\mathbf{r}}_{n_\mathrm{b}}) = \mathbf{\Phi}(\mathbf{q}, t)$ *is the constraint equation in the Cartesian frame.*

6.3 Modeling and Formulations of Kinematic Pairs

Two neighboring rigid bodies are coupled by means of geometric constraints, which prevent relative translational or/and rotational motion of those rigid bodies. The kinematic pairs are classified into two categories: (1) ***Lower pairs*** and (2) ***Higher pairs***.

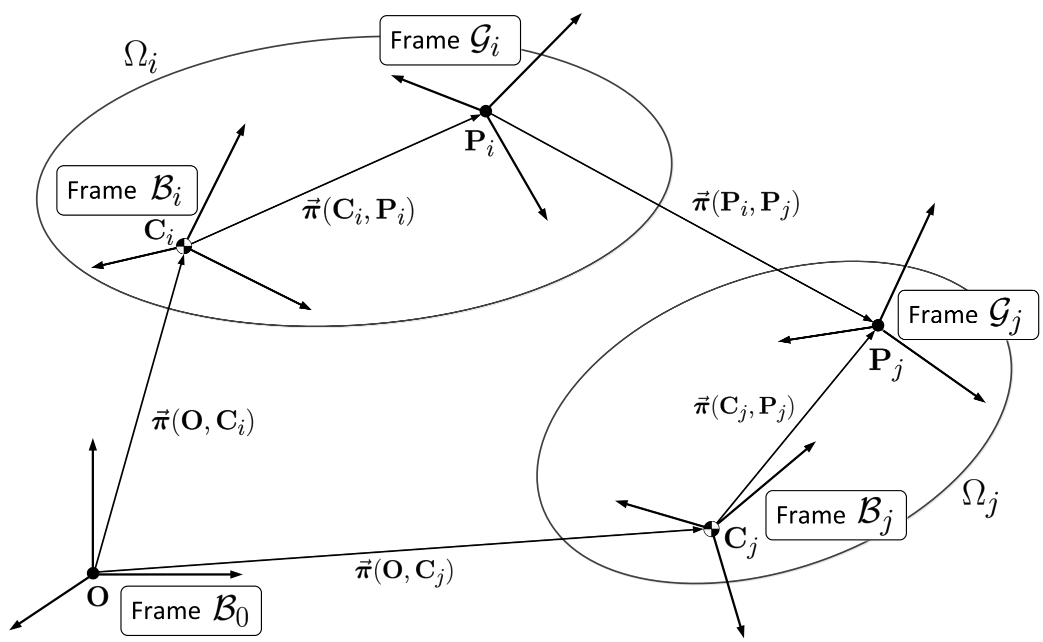


Figure 6.1: Two Bodies in $\mathbb{E}^3$

In Fig. 6.1, the Cartesian frame, $\mathcal{B}_0 : (\mathbf{O}; \{{}^{\mathcal{B}_0}\vec{\mathbf{e}}_\ell\}_{\ell=1}^{n_{\dim}})$, is the inertial reference frame; and $\mathcal{B}_i : (\mathbf{C}_i; \{{}^{\mathcal{B}_i}\vec{\mathbf{e}}_\ell\}_{\ell=1}^{n_{\dim}})$ and $\mathcal{B}_j : (\mathbf{C}_j; \{{}^{\mathcal{B}_j}\vec{\mathbf{e}}_\ell\}_{\ell=1}^{n_{\dim}})$ are the Cartesian frames fixed to the rigid bodies, Ω_i and Ω_j, respectively, at the centroid points. In addition, Cartesian frames, $\mathcal{G}_i : (\mathbf{P}_i; \{{}^{\mathcal{G}_i}\vec{\mathbf{e}}_\ell\}_{\ell=1}^{n_{\dim}})$ and $\mathcal{G}_j : (\mathbf{P}_j; \{{}^{\mathcal{G}_j}\vec{\mathbf{e}}_\ell\}_{\ell=1}^{n_{\dim}})$ are also fixed to the rigid bodies, Ω_i and Ω_j, at points $\mathbf{P}_i$ and $\mathbf{P}_j$, respectively. $n_{\dim}$ denotes the numbers of dimension, and we assume $n_{\dim} = 3$ throughout this chapter. For the sake of convenience, we introduce the vectors

$$\vec{\mathbf{s}}_i^\ell \equiv {}^{\mathcal{G}_i}\vec{\mathbf{e}}_\ell \quad \text{and} \quad \vec{\mathbf{s}}_j^\ell \equiv {}^{\mathcal{G}_j}\vec{\mathbf{e}}_\ell \tag{6.23}$$

for $\ell = 1, 2, 3$. That is, the component vectors of $\vec{\mathbf{s}}_i^\ell$ with respect to frame $\mathcal{G}_i$ and the component vectors of $\vec{\mathbf{s}}_j^\ell$ with respect to frame $\mathcal{G}_j$ yield:

$$\begin{aligned}
{}^{\mathcal{G}_i}\mathbf{s}_i^1 &= {}^{\mathcal{G}_j}\mathbf{s}_j^1 = [1,0,0]^T \\
{}^{\mathcal{G}_i}\mathbf{s}_i^2 &= {}^{\mathcal{G}_j}\mathbf{s}_j^2 = [0,1,0]^T \\
{}^{\mathcal{G}_i}\mathbf{s}_i^3 &= {}^{\mathcal{G}_j}\mathbf{s}_j^3 = [0,0,1]^T
\end{aligned} \tag{6.24}$$

6.3.1 Lower Pairs

Spherical Pair

The simplest joint to formulate may be the spherical pair (joint). Two points, $\mathbf{P}_i \in \Omega_i \subset \mathbb{E}^3$ and $\mathbf{P}_j \in \Omega_j \subset \mathbb{E}^3$, coincide, i.e., $\vec{\boldsymbol{\pi}}(\mathbf{P}_i, \mathbf{P}_j) = \mathbf{0}$; and the pair (joint) prevents all relative translational motion between bodies Ω_i and Ω_j. From the geometry, we have

$$\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_i) + \vec{\boldsymbol{\pi}}(\mathbf{C}_i, \mathbf{P}) = \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_j) + \vec{\boldsymbol{\pi}}(\mathbf{C}_j, \mathbf{P}) \tag{6.25}$$

with $\mathbf{P} := \mathbf{P}_i = \mathbf{P}_j$. Hence, the constraint equation is obtained from the component form of Eq. (6.25) with respect to the inertial reference frame, $\mathcal{B}_0$, as

$$\boxed{\mathbf{\Phi}^{(\mathrm{S})}(\mathbf{q}) = {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{C}_i) - {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{C}_j) + \underbrace{{}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\,{}^{\mathcal{B}_i}\boldsymbol{\pi}(\mathbf{C}_i, \mathbf{P})}_{{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{C}_i,\mathbf{P})} - \underbrace{{}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\,{}^{\mathcal{B}_j}\boldsymbol{\pi}(\mathbf{C}_j, \mathbf{P})}_{{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{C}_j,\mathbf{P})} = \mathbf{0} \in \mathbb{R}^3} \tag{6.26}$$

where $\mathbf{\Phi}^{(\mathrm{S})} = \mathbf{0}$ denotes the constraint equations for the spherical (S) pair. The variation of Eq. (6.26) is therefore given as

$$\begin{aligned}
\mathbf{0} &= \delta\mathbf{\Phi}^{(\mathrm{S})} \\
&= \delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{C}_i) - \delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{C}_j) + \left(\delta^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right){}^{\mathcal{B}_i}\boldsymbol{\pi}(\mathbf{C}_i, \mathbf{P}) - \left(\delta^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right){}^{\mathcal{B}_j}\boldsymbol{\pi}(\mathbf{C}_j, \mathbf{P}) \\
&= \delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{C}_i) - \delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{C}_j) \\
&\quad - \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_i, \mathbf{P})\right)\left({}^{\mathcal{B}_i}_{\mathcal{B}_i|\mathcal{B}_0}\boldsymbol{\varpi}\right) + \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_j, \mathbf{P})\right)\left({}^{\mathcal{B}_j}_{\mathcal{B}_j|\mathcal{B}_0}\boldsymbol{\varpi}\right)
\end{aligned} \tag{6.27}$$

Hence,

$$\boxed{\mathbf{G}^{(\mathrm{S})}(\mathbf{q}) = \left[\mathbf{I}_3 \quad -\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_i,\mathbf{P})\right) \quad -\mathbf{I}_3 \quad \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_j,\mathbf{P})\right)\right] \in \mathbb{R}^{3\times 12}} \tag{6.28}$$

Note that there is no constraint imposed to prevent the relative rotational motion between the bodies.

Hinge (Revolve) Pair

The hinge pair, also called the revolve pair, prevents not only all relative translational motion between bodies Ω_i and Ω_j, i.e.,

$$\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_i) + \vec{\boldsymbol{\pi}}(\mathbf{C}_i,\mathbf{P}) = \vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_j) + \vec{\boldsymbol{\pi}}(\mathbf{C}_j,\mathbf{P}) \tag{6.29}$$

with $\mathbf{P} := \mathbf{P}_i = \mathbf{P}_j$, but also two relative rotational motions by

$$
\begin{aligned}
{}^{\mathcal{G}_i}\vec{\mathbf{e}}_1 \cdot {}^{\mathcal{G}_j}\vec{\mathbf{e}}_3 &= 0 \quad \Leftrightarrow \quad \vec{\mathbf{s}}_i^{\,1} \cdot \vec{\mathbf{s}}_j^{\,3} = 0 && (6.30)\\
{}^{\mathcal{G}_i}\vec{\mathbf{e}}_2 \cdot {}^{\mathcal{G}_j}\vec{\mathbf{e}}_3 &= 0 \quad \Leftrightarrow \quad \vec{\mathbf{s}}_i^{\,2} \cdot \vec{\mathbf{s}}_j^{\,3} = 0 && (6.31)
\end{aligned}
$$

Hence, Eq. (6.30) and Eq. (6.31) can be expressed as

$$
\begin{aligned}
0 &= \vec{\mathbf{s}}_i^{\,1} \cdot \vec{\mathbf{s}}_j^{\,3}\\
&= \underbrace{\left[{}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\ \left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)\right]}_{{}^{\mathcal{B}_0}\mathbf{s}_i^1}{}^T\ \underbrace{\left[{}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\ \left({}^{\mathcal{B}_j}\mathbf{s}_j^3\right)\right]}_{{}^{\mathcal{B}_0}\mathbf{s}_j^3}\\
&= \left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)^T\ \underbrace{\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)^T\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)}_{{}^{\mathcal{B}_i/\mathcal{B}_j}\mathbf{A}}\left({}^{\mathcal{B}_j}\mathbf{s}_j^3\right) =: \Phi_1^{(\mathrm{H})_\mathrm{r}} && (6.32a)
\end{aligned}
$$

and

$$
\begin{aligned}
0 &= \vec{\mathbf{s}}_i^{\,2} \cdot \vec{\mathbf{s}}_j^{\,3}\\
&= \left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)^T\ \underbrace{\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)^T\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)}_{{}^{\mathcal{B}_i/\mathcal{B}_j}\mathbf{A}}\left({}^{\mathcal{B}_j}\mathbf{s}_j^3\right) =: \Phi_2^{(\mathrm{H})_\mathrm{r}} && (6.32b)
\end{aligned}
$$

respectively, where $\Phi_{\ell}^{(\mathrm{H})_{\mathrm{r}}}$ (for $\ell = 1, 2$) denotes the constraint equations for the hinge (H) pair in the rotational motion. Therefore, the constraint equations for the hinge pair are given as

$$\boxed{\mathbf{\Phi}^{(\mathrm{H})}(\mathbf{q}) = \begin{bmatrix} \mathbf{\Phi}^{(\mathrm{H})_{\mathrm{t}}}(\mathbf{q}) \\ \mathbf{\Phi}^{(\mathrm{H})_{\mathrm{r}}}(\mathbf{q}) \end{bmatrix} = \mathbf{0} \in \mathbb{R}^5} \tag{6.33}$$

The variation of $\mathbf{\Phi}^{(\mathrm{H})_{\mathrm{t}}}(\mathbf{q}) = \mathbf{0}$ is given in Eq. (6.27). On the other hand, the variation of $\Phi_1^{(\mathrm{H})_{\mathrm{r}}} = 0$ is obtained as

$$\begin{aligned} 0 &= \delta\Phi_1^{(\mathrm{H})_{\mathrm{r}}} = \delta\left[\vec{\mathbf{s}}_i^1 \cdot \vec{\mathbf{s}}_j^3\right] \\ &= \underbrace{\left[{}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\,{}^{\mathcal{B}_i}\mathbf{s}_i^1\right]^T}_{{}^{\mathcal{B}_0}\mathbf{s}_i^1} \underbrace{\left[(\delta\,{}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A})\,{}^{\mathcal{B}_j}\mathbf{s}_j^3\right]}_{\delta{}^{\mathcal{B}_0}\mathbf{s}_j^3} + \underbrace{\left[{}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\,{}^{\mathcal{B}_j}\mathbf{s}_j^3\right]^T}_{{}^{\mathcal{B}_0}\mathbf{s}_j^3} \underbrace{\left[(\delta\,{}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A})\,{}^{\mathcal{B}_i}\mathbf{s}_i^1\right]}_{\delta{}^{\mathcal{B}_0}\mathbf{s}_i^1} \\ &= -\left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\widetilde{\mathbf{s}}_j^3\right)\left({}^{\mathcal{B}_j}_{\mathcal{B}_j|\mathcal{B}_0}\boldsymbol{\varpi}\right) \\ &\quad -\left({}^{\mathcal{B}_j}\mathbf{s}_j^3\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^1\right)\left({}^{\mathcal{B}_i}_{\mathcal{B}_i|\mathcal{B}_0}\boldsymbol{\varpi}\right) \end{aligned} \tag{6.34}$$

Similarly,

$$\begin{aligned} 0 &= \delta\Phi_2^{(\mathrm{H})_{\mathrm{r}}} = \delta\left[\vec{\mathbf{s}}_i^2 \cdot \vec{\mathbf{s}}_j^3\right] \\ &= -\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\widetilde{\mathbf{s}}_j^3\right)\left({}^{\mathcal{B}_j}_{\mathcal{B}_j|\mathcal{B}_0}\boldsymbol{\varpi}\right) \\ &\quad -\left({}^{\mathcal{B}_j}\mathbf{s}_j^3\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^2\right)\left({}^{\mathcal{B}_i}_{\mathcal{B}_i|\mathcal{B}_0}\boldsymbol{\varpi}\right) \end{aligned} \tag{6.35}$$

Hence, from Eq. (6.28), Eq. (6.34), and Eq. (6.35), matrix $\mathbf{G}^{(\mathrm{H})}(\mathbf{q}) \in \mathbb{R}^{5\times 12}$ is obtained as follows:

$$
\boxed{
\begin{aligned}
\mathbf{G}_{11}^{(\mathrm{H})} &= \mathbf{I}_3 \\
\mathbf{G}_{12}^{(\mathrm{H})} &= -\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_i, \mathbf{P})\right) \\
\mathbf{G}_{13}^{(\mathrm{H})} &= -\mathbf{I}_3 \\
\mathbf{G}_{14}^{(\mathrm{H})} &= \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_j, \mathbf{P})\right) \\
\mathbf{G}_{21}^{(\mathrm{H})} &= \mathbf{G}_{23}^{(\mathrm{H})} = [0, 0, 0] \\
\mathbf{G}_{22}^{(\mathrm{H})} &= -\left({}^{\mathcal{B}_j}\mathbf{s}_j^3\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^1\right) \\
\mathbf{G}_{24}^{(\mathrm{H})} &= -\left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\widetilde{\mathbf{s}}_j^3\right) \\
\mathbf{G}_{31}^{(\mathrm{H})} &= \mathbf{G}_{33}^{(\mathrm{H})} = [0, 0, 0] \\
\mathbf{G}_{32}^{(\mathrm{H})} &= -\left({}^{\mathcal{B}_j}\mathbf{s}_j^3\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^2\right) \\
\mathbf{G}_{34}^{(\mathrm{H})} &= -\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right) \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\widetilde{\mathbf{s}}_j^3\right)
\end{aligned}
}
\tag{6.36}
$$

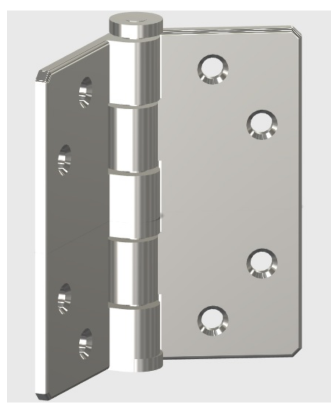


Figure 6.2: Hinge Pair

Hinge rotation angle: As discussed in [49, p. 154], the ***hinge rotation angle***, α, sometimes explicitly appears. In these cases, we simply add the following rotational constraint equation:

$$0 = \Phi_3^{(\mathrm{H})_\mathrm{r}} = \sin(\theta - \alpha) \tag{6.37}$$

where θ denotes the rotation angle, and we assume $|\theta - \alpha|$ remains small. From Fig. 6.3,

$$^{\mathcal{G}_i}\vec{\mathbf{e}}_2 \cdot {}^{\mathcal{G}_j}\vec{\mathbf{e}}_1 = \cos(90^\circ - \theta) = \sin(\theta) \quad \Leftrightarrow \quad \vec{\mathbf{s}}_i^2 \cdot \vec{\mathbf{s}}_j^1 = \sin(\theta) \tag{6.38}$$

$$^{\mathcal{G}_i}\vec{\mathbf{e}}_1 \cdot {}^{\mathcal{G}_j}\vec{\mathbf{e}}_1 = \cos(\theta) \quad \Leftrightarrow \quad \vec{\mathbf{s}}_i^1 \cdot \vec{\mathbf{s}}_j^1 = \cos(\theta) \tag{6.39}$$

Hence, Eq. (6.37) follows that

$$\begin{aligned}
0 &= \Phi_3^{(\mathrm{H})_\mathrm{r}} = \sin(\theta)\cos(\alpha) - \cos(\theta)\sin(\alpha) \\
&= (\vec{\mathbf{s}}_i^2 \cdot \vec{\mathbf{s}}_j^1)\cos(\alpha) - (\vec{\mathbf{s}}_i^1 \cdot \vec{\mathbf{s}}_j^1)\sin(\alpha) \\
&= \vec{\mathbf{s}}_j^1 \cdot \left[\vec{\mathbf{s}}_i^2 \cos(\alpha) - \vec{\mathbf{s}}_i^1 \sin(\alpha)\right] \\
&= ({}^{\mathcal{B}_0}\mathbf{s}_j^1)^T \left[{}^{\mathcal{B}_0}\mathbf{s}_i^2 \cos(\alpha) - {}^{\mathcal{B}_0}\mathbf{s}_i^1 \sin(\alpha)\right] \quad (\because {}^{\mathcal{B}_0}\mathbf{e}^T \cdot {}^{\mathcal{B}_0}\mathbf{e} = \mathbf{I}_3) \\
&= ({}^{\mathcal{B}_j}\mathbf{s}_j^1)^T ({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A})^T \left[({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}){}^{\mathcal{B}_i}\mathbf{s}_i^2 \cos(\alpha) - ({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}){}^{\mathcal{B}_i}\mathbf{s}_i^1 \sin(\alpha)\right]
\end{aligned} \tag{6.40}$$

Since $({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A})^T({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}) = ({}^{\mathcal{B}_j/\mathcal{B}_0}\mathbf{A})({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}) = {}^{\mathcal{B}_j/\mathcal{B}_i}\mathbf{A}$, we get

$$\boxed{0 = \Phi_3^{(\mathrm{H})_\mathrm{r}} = \left({}^{\mathcal{B}_j}\mathbf{s}_j^1\right)^T \left({}^{\mathcal{B}_j/\mathcal{B}_i}\mathbf{A}\right)\left[\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)\cos(\alpha) - \left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)\sin(\alpha)\right]} \tag{6.41}$$

The variation of $\Phi_3^{(\mathrm{H})_\mathrm{r}}$ is obtained by taking the variation of Eq. (6.40) as

$$\begin{aligned}
0 =& \delta\Phi_3^{(\mathrm{H})_\mathrm{r}} \\
=& \left[\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\mathbf{s}_j^1\right)\right]^T \delta\left[\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right){}^{\mathcal{B}_i}\mathbf{s}_i^2 \cos(\alpha) - \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right){}^{\mathcal{B}_i}\mathbf{s}_i^1 \sin(\alpha)\right] \\
&+ \left[\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right){}^{\mathcal{B}_i}\mathbf{s}_i^2 \cos(\alpha) - \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right){}^{\mathcal{B}_i}\mathbf{s}_i^1 \sin(\alpha)\right]^T \delta\left[\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\mathbf{s}_j^1\right)\right]
\end{aligned} \tag{6.42}$$

From

$$\delta\left[\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\mathbf{s}_j^1\right)\right] = \left(\delta^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\mathbf{s}_j^1\right) = -\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\widetilde{\mathbf{s}}_j^1\right)\left({}^{\mathcal{B}_j}_{\mathcal{B}_j|\mathcal{B}_0}\boldsymbol{\varpi}\right) \tag{6.43}$$

and

$$
\begin{aligned}
& \delta\left[\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right){}^{\mathcal{B}_i}\mathbf{s}_i^2\cos(\alpha)-\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right){}^{\mathcal{B}_i}\mathbf{s}_i^1\sin(\alpha)\right] \\
= & \left(\delta^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)\cos(\alpha)-\left(\delta^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)\sin(\alpha)\delta\alpha \\
& -\left(\delta^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)\sin(\alpha)-\left(\delta^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)\cos(\alpha)\delta\alpha \\
= & -\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left[\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^2\right)\cos(\alpha)-\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^1\right)\sin(\alpha)\right]\left({}^{\mathcal{B}_i}_{\mathcal{B}_i|\mathcal{B}_0}\boldsymbol{\varpi}\right) \\
& -\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left[\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)\sin(\alpha)+\left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)\cos(\alpha)\right]\delta\alpha
\end{aligned}
\tag{6.44}
$$

Eq. (6.42) follows that

$$
0 = \delta\Phi_3^{(\mathrm{H})_\mathrm{r}} \tag{6.45}
$$

$$
\begin{aligned}
= & -\left[\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\mathbf{s}_j^1\right)\right]^T\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left[\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^2\right)\cos(\alpha)-\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^1\right)\sin(\alpha)\right]\left({}^{\mathcal{B}_i}_{\mathcal{B}_i|\mathcal{B}_0}\boldsymbol{\varpi}\right) \\
& -\left[\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\mathbf{s}_j^1\right)\right]^T\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left[\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)\sin(\alpha)+\left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)\cos(\alpha)\right]\delta\alpha \\
& -\left[\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right){}^{\mathcal{B}_i}\mathbf{s}_i^2\cos(\alpha)-\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right){}^{\mathcal{B}_i}\mathbf{s}_i^1\sin(\alpha)\right]^T\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\widetilde{\mathbf{s}}_j^1\right)\left({}^{\mathcal{B}_j}_{\mathcal{B}_j|\mathcal{B}_0}\boldsymbol{\varpi}\right) \\
= & -\left({}^{\mathcal{B}_i}\mathbf{s}_j^1\right)^T\left[\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^2\right)\cos(\alpha)-\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^1\right)\sin(\alpha)\right]\left({}^{\mathcal{B}_i}_{\mathcal{B}_i|\mathcal{B}_0}\boldsymbol{\varpi}\right) \\
& -\left({}^{\mathcal{B}_i}\mathbf{s}_j^1\right)^T\left[\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)\sin(\alpha)+\left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)\cos(\alpha)\right]\delta\alpha \\
& -\left[\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)\cos(\alpha)-\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)\sin(\alpha)\right]^T\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\widetilde{\mathbf{s}}_j^1\right)\left({}^{\mathcal{B}_j}_{\mathcal{B}_j|\mathcal{B}_0}\boldsymbol{\varpi}\right)
\end{aligned}
\tag{6.46}
$$

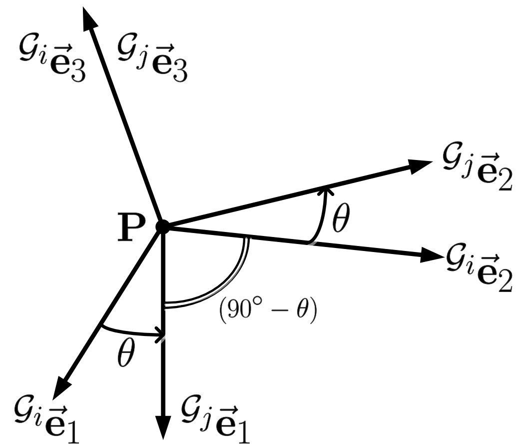


Figure 6.3: Rotation Angle θ

From the geometry,

$$-{}^{\mathcal{G}_i}\vec{\mathbf{e}}_2 = {}^{\mathcal{G}_i}\vec{\mathbf{e}}_1 \cdot {}^{\mathcal{G}_i}\vec{\mathbf{e}}_3 = {}^{\mathcal{G}_i}\vec{\mathbf{e}}_1 \cdot {}^{\mathcal{G}_j}\vec{\mathbf{e}}_3 \tag{6.47}$$

$${}^{\mathcal{G}_i}\vec{\mathbf{e}}_1 = {}^{\mathcal{G}_i}\vec{\mathbf{e}}_2 \cdot {}^{\mathcal{G}_i}\vec{\mathbf{e}}_3 = {}^{\mathcal{G}_i}\vec{\mathbf{e}}_2 \cdot {}^{\mathcal{G}_j}\vec{\mathbf{e}}_3 \tag{6.48}$$

The component form of Eq. (6.47) with respect to $\mathcal{B}_i$ takes the form

$$-{}^{\mathcal{B}_i}\mathbf{s}_i^2 = \left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^1\right)\left({}^{\mathcal{B}_i}\mathbf{s}_j^3\right) \tag{6.49}$$

since

$$-\left({}^{\mathcal{B}_i}\mathbf{e}\right)^T\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right) = \underbrace{\left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)^T\left({}^{\mathcal{B}_i}\mathbf{e}\right) \times \left({}^{\mathcal{B}_i}\mathbf{e}\right)^T}_{\left({}^{\mathcal{B}_i}\mathbf{e}\right)^T\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^1\right)}\left({}^{\mathcal{B}_i}\mathbf{s}_j^3\right) \tag{6.50}$$

Similarly, the component form of Eq. (6.48) with respect to $\mathcal{B}_i$ takes the form

$${}^{\mathcal{B}_i}\mathbf{s}_i^1 = \left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^2\right)\left({}^{\mathcal{B}_i}\mathbf{s}_j^3\right) \tag{6.51}$$

Substituting Eq. (6.47)/Eq. (6.48) into Eq. (6.38)/Eq. (6.39), respectively, we have

$$\sin(\theta) = -\left(\vec{\mathbf{s}}_i^1 \times \vec{\mathbf{s}}_j^3\right) \cdot \left(\vec{\mathbf{s}}_j^1\right) \tag{6.52}$$

$$\cos(\theta) = \left(\vec{\mathbf{s}}_i^2 \times \vec{\mathbf{s}}_j^3\right) \cdot \left(\vec{\mathbf{s}}_j^1\right) \tag{6.53}$$

or in the component forms with respect to $\mathcal{B}_i$,

$$\sin(\theta) = -\left({}^{\mathcal{B}_i}\mathbf{s}_j^1\right)^T \left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^1\right)\left({}^{\mathcal{B}_i}\mathbf{s}_j^3\right) \tag{6.54}$$

$$\cos(\theta) = \left({}^{\mathcal{B}_i}\mathbf{s}_j^1\right)^T \left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^2\right)\left({}^{\mathcal{B}_i}\mathbf{s}_j^3\right) \tag{6.55}$$

Therefore, substituting Eq. (6.49) and Eq. (6.51), the second term in the right-hand side of Eq. (6.46) becomes

$$\begin{aligned}
& -\left({}^{\mathcal{B}_i}\mathbf{s}_j^1\right)^T \left[\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)\sin(\alpha) + \left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)\cos(\alpha)\right]\delta\alpha \\
= & -\left[-\left({}^{\mathcal{B}_i}\mathbf{s}_j^1\right)^T \left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^1\right)\left({}^{\mathcal{B}_i}\mathbf{s}_j^3\right)\sin(\alpha) + \left({}^{\mathcal{B}_i}\mathbf{s}_j^1\right)^T \left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^2\right)\left({}^{\mathcal{B}_i}\mathbf{s}_j^3\right)\cos(\alpha)\right]\delta\alpha \\
= & -\left[-\sin(\theta)\sin(\alpha) + \cos(\theta)\cos(\alpha)\right]\delta\alpha = -\cos(\theta-\alpha)\delta\alpha \\
\approx & -\delta\alpha
\end{aligned} \tag{6.56}$$

since $\cos(\theta - \alpha) \approx 1$ for a sufficiently small $|\theta - \alpha|$. The third term in the right-hand side of Eq. (6.46) becomes

$$\begin{aligned}
& -\left[\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)\cos(\alpha) - \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)\sin(\alpha)\right]^T \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\widetilde{\mathbf{s}}_j^1\right)\left({}^{\mathcal{B}_j}_{\mathcal{B}_j|\mathcal{B}_0}\boldsymbol{\varpi}\right) \\
= & -\left[\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\widetilde{\mathbf{s}}_j^1\right)\left({}^{\mathcal{B}_j}_{\mathcal{B}_j|\mathcal{B}_0}\boldsymbol{\varpi}\right)\right]^T \left[\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)\cos(\alpha) - \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)\sin(\alpha)\right] \\
= & -\left({}^{\mathcal{B}_j}_{\mathcal{B}_j|\mathcal{B}_0}\boldsymbol{\varpi}\right)^T \underbrace{\left({}^{\mathcal{B}_j}\widetilde{\mathbf{s}}_j^1\right)^T}_{-\left({}^{\mathcal{B}_j}\widetilde{\mathbf{s}}_j^1\right)} \left({}^{\mathcal{B}_j/\mathcal{B}_i}\mathbf{A}\right)\left[\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)\cos(\alpha) - \left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)\sin(\alpha)\right] \\
= & \left({}^{\mathcal{B}_j}_{\mathcal{B}_j|\mathcal{B}_0}\boldsymbol{\varpi}\right)^T \left({}^{\mathcal{B}_j/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_j^1\right)\left[\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)\cos(\alpha) - \left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)\sin(\alpha)\right] \\
= & \left({}^{\mathcal{B}_j}_{\mathcal{B}_j|\mathcal{B}_0}\boldsymbol{\varpi}\right)^T \left({}^{\mathcal{B}_j/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^3\right)\underbrace{\left[\sin(90^\circ - \theta)\cos(\alpha) + \sin(\theta)\sin(\alpha)\right]}_{=\cos(\theta-\alpha)\approx 1} \\
\approx & \left[\left({}^{\mathcal{B}_j/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^3\right)\right]^T \left({}^{\mathcal{B}_j}_{\mathcal{B}_j|\mathcal{B}_0}\boldsymbol{\varpi}\right)
\end{aligned} \tag{6.57}$$

Remark 6.3.1

The external torque applied to the hinge pair, $\mathcal{T}_{\mathrm{H}}$, can be found from the virtual work,

$$\delta W_{\mathrm{H}} = \mathcal{T}_{\mathrm{H}}\delta\alpha \tag{6.58}$$

Prismatic Pair

From the geometry, one gets

$$\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_i) + \vec{\boldsymbol{\pi}}(\mathbf{C}_i, \mathbf{P}_i) + \vec{\boldsymbol{\pi}}(\mathbf{P}_i, \mathbf{P}_j) = \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_j) + \vec{\boldsymbol{\pi}}(\mathbf{C}_j, \mathbf{P}_j) \tag{6.59}$$

That is,

$$\vec{\boldsymbol{\pi}}(\mathbf{P}_i, \mathbf{P}_j) = \left[\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_j) + \vec{\boldsymbol{\pi}}(\mathbf{C}_j, \mathbf{P}_j)\right] - \left[\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_i) + \vec{\boldsymbol{\pi}}(\mathbf{C}_i, \mathbf{P}_i)\right] \tag{6.60}$$

or

$${}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{P}_i, \mathbf{P}_j) = {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{C}_j) + {}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\,{}^{\mathcal{B}_j}\boldsymbol{\pi}(\mathbf{C}_j, \mathbf{P}_j) - {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{C}_i) - {}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\,{}^{\mathcal{B}_i}\boldsymbol{\pi}(\mathbf{C}_i, \mathbf{P}_i) \tag{6.61}$$

The prismatic pair is defined by the following two translational constraints,

$$\begin{aligned} {}^{\mathcal{G}_i}\vec{\mathbf{e}}_1 \cdot \vec{\boldsymbol{\pi}}(\mathbf{P}_i, \mathbf{P}_j) &= 0 \\ {}^{\mathcal{G}_i}\vec{\mathbf{e}}_2 \cdot \vec{\boldsymbol{\pi}}(\mathbf{P}_i, \mathbf{P}_j) &= 0 \end{aligned} \tag{6.62}$$

and the rotational constraints due to the equality of the orientations of the two body-fixed frames,

$$\begin{aligned} {}^{\mathcal{G}_i}\vec{\mathbf{e}}_1 \cdot {}^{\mathcal{G}_j}\vec{\mathbf{e}}_2 &= 0 \\ {}^{\mathcal{G}_i}\vec{\mathbf{e}}_2 \cdot {}^{\mathcal{G}_j}\vec{\mathbf{e}}_3 &= 0 \\ {}^{\mathcal{G}_i}\vec{\mathbf{e}}_3 \cdot {}^{\mathcal{G}_j}\vec{\mathbf{e}}_1 &= 0 \end{aligned} \tag{6.63}$$

We can define the constraint equations for the prismatic (P) pair in the translational motion, i.e., $\mathbf{\Phi}^{(\mathrm{P})_\mathrm{t}} = \mathbf{0} \in \mathbb{R}^2$, from Eq. (6.62) as

$$\begin{aligned} 0 &= \vec{\mathbf{s}}_i^1 \cdot \vec{\boldsymbol{\pi}}(\mathbf{P}_i, \mathbf{P}_j) \\ &= \left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right) {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{P}_i, \mathbf{P}_j) =: \Phi_1^{(\mathrm{P})_\mathrm{t}} \end{aligned} \tag{6.64a}$$

and

$$
\begin{aligned}
0 &= \vec{\mathbf{s}}_i^2 \cdot \vec{\boldsymbol{\pi}}(\mathbf{P}_i, \mathbf{P}_j) \\
&= \left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right) {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{P}_i, \mathbf{P}_j) =: \Phi_2^{(\mathrm{P})_\mathrm{t}} \qquad (6.64\mathrm{b})
\end{aligned}
$$

respectively, where ${}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{P}_i, \mathbf{P}_j)$ is given in Eq. (6.61). Similarly, the constraint equations for the prismatic (P) pair in the rotational motion, i.e., $\boldsymbol{\Phi}^{(\mathrm{P})_\mathrm{r}} = \mathbf{0} \in \mathbb{R}^3$, are defined from Eq. (6.63) as

$$
0 = \left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right) \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right) \left({}^{\mathcal{B}_j}\mathbf{s}_j^2\right) =: \Phi_1^{(\mathrm{P})_\mathrm{r}} \qquad (6.65)
$$

$$
0 = \left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right) \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right) \left({}^{\mathcal{B}_j}\mathbf{s}_j^3\right) =: \Phi_2^{(\mathrm{P})_\mathrm{r}} \qquad (6.66)
$$

$$
0 = \left({}^{\mathcal{B}_i}\mathbf{s}_i^3\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right) \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right) \left({}^{\mathcal{B}_j}\mathbf{s}_j^1\right) =: \Phi_3^{(\mathrm{P})_\mathrm{r}} \qquad (6.67)
$$

respectively. Hence, the constraint equations for the prismatic pair is given as

$$
\boxed{\boldsymbol{\Phi}^{(\mathrm{P})}(\mathbf{q}) := \begin{bmatrix} \boldsymbol{\Phi}^{(\mathrm{P})_\mathrm{t}}(\mathbf{q}) \\ \boldsymbol{\Phi}^{(\mathrm{P})_\mathrm{r}}(\mathbf{q}) \end{bmatrix} = \mathbf{0} \in \mathbb{R}^5} \qquad (6.68)
$$

The variation of $\boldsymbol{\Phi}^{(\mathrm{P})}(\mathbf{q})$ is obtained as follows:

$$
\begin{aligned}
0 = \delta\Phi_1^{(\mathrm{P})_\mathrm{t}} &= \left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\left(\delta\, {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{P}_i, \mathbf{P}_j)\right) \\
&\quad - {}^{\mathcal{B}_0}\boldsymbol{\pi}^T(\mathbf{P}_i, \mathbf{P}_j) \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^1\right) \left({}^{\mathcal{B}_i}_{\mathcal{B}_i|\mathcal{B}_0}\boldsymbol{\varpi}\right) \qquad (6.69) \\
0 = \delta\Phi_2^{(\mathrm{P})_\mathrm{t}} &= \left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\left(\delta\, {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{P}_i, \mathbf{P}_j)\right) \\
&\quad - {}^{\mathcal{B}_0}\boldsymbol{\pi}^T(\mathbf{P}_i, \mathbf{P}_j) \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^2\right) \left({}^{\mathcal{B}_i}_{\mathcal{B}_i|\mathcal{B}_0}\boldsymbol{\varpi}\right) \qquad (6.70)
\end{aligned}
$$

and

$$
\begin{aligned}
0 = \delta\Phi_1^{(\mathrm{P})_\mathrm{r}} \quad &= \quad -\left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\widetilde{\mathbf{s}}_j^2\right)\left({}^{\mathcal{B}_j}_{\mathcal{B}_j|\mathcal{B}_0}\boldsymbol{\varpi}\right) \\
&\quad\; -\left({}^{\mathcal{B}_j}\mathbf{s}_j^2\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^1\right)\left({}^{\mathcal{B}_i}_{\mathcal{B}_i|\mathcal{B}_0}\boldsymbol{\varpi}\right) \qquad (6.71) \\
0 = \delta\Phi_2^{(\mathrm{P})_\mathrm{r}} \quad &= \quad -\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\widetilde{\mathbf{s}}_j^3\right)\left({}^{\mathcal{B}_j}_{\mathcal{B}_j|\mathcal{B}_0}\boldsymbol{\varpi}\right) \\
&\quad\; -\left({}^{\mathcal{B}_j}\mathbf{s}_j^3\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^2\right)\left({}^{\mathcal{B}_i}_{\mathcal{B}_i|\mathcal{B}_0}\boldsymbol{\varpi}\right) \qquad (6.72) \\
0 = \delta\Phi_3^{(\mathrm{P})_\mathrm{r}} \quad &= \quad -\left({}^{\mathcal{B}_i}\mathbf{s}_i^3\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\widetilde{\mathbf{s}}_j^1\right)\left({}^{\mathcal{B}_j}_{\mathcal{B}_j|\mathcal{B}_0}\boldsymbol{\varpi}\right) \\
&\quad\; -\left({}^{\mathcal{B}_j}\mathbf{s}_j^1\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^3\right)\left({}^{\mathcal{B}_i}_{\mathcal{B}_i|\mathcal{B}_0}\boldsymbol{\varpi}\right) \qquad (6.73)
\end{aligned}
$$

where $\delta\,{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{P}_i, \mathbf{P}_j)$ is obtained from Eq. (6.61) as

$$
\begin{aligned}
\delta\,{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{P}_i, \mathbf{P}_j) =& \delta\,{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{C}_j) - \delta\,{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{C}_i) \\
&+ \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right){}^{\mathcal{B}_i}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_i, \mathbf{P}_i)\left({}^{\mathcal{B}_i}_{\mathcal{B}_i|\mathcal{B}_0}\boldsymbol{\varpi}\right) - \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right){}^{\mathcal{B}_j}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_j, \mathbf{P}_j)\left({}^{\mathcal{B}_j}_{\mathcal{B}_j|\mathcal{B}_0}\boldsymbol{\varpi}\right)
\end{aligned}
\qquad (6.74)
$$

Hence, matrix $\mathbf{G}^{(\mathrm{P})}(\mathbf{q}) \in \mathbb{R}^{5\times 12}$ is obtained as:

$$
\boxed{
\begin{aligned}
\mathbf{G}^{(\mathrm{P})}_{11} &= -\left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\\
\mathbf{G}^{(\mathrm{P})}_{12} &= \left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right){}^{\mathcal{B}_i}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_i, \mathbf{P}_i)\\
&\quad - {}^{\mathcal{B}_0}\boldsymbol{\pi}^T(\mathbf{P}_i, \mathbf{P}_j) \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^1\right)\\
\mathbf{G}^{(\mathrm{P})}_{13} &= \left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\\
\mathbf{G}^{(\mathrm{P})}_{14} &= -\left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right){}^{\mathcal{B}_j}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_j, \mathbf{P}_j)\\
\mathbf{G}^{(\mathrm{P})}_{21} &= -\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\\
\mathbf{G}^{(\mathrm{P})}_{22} &= \left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right){}^{\mathcal{B}_i}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_i, \mathbf{P}_i)\\
&\quad - {}^{\mathcal{B}_0}\boldsymbol{\pi}^T(\mathbf{P}_i, \mathbf{P}_j) \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^2\right)\\
\mathbf{G}^{(\mathrm{P})}_{23} &= \left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\\
\mathbf{G}^{(\mathrm{P})}_{24} &= -\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right){}^{\mathcal{B}_j}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_j, \mathbf{P}_j)\\
\mathbf{G}^{(\mathrm{P})}_{31} &= \mathbf{G}^{(\mathrm{P})}_{33} = [0, 0, 0]\\
\mathbf{G}^{(\mathrm{P})}_{32} &= -\left({}^{\mathcal{B}_j}\mathbf{s}_j^2\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^1\right)\\
\mathbf{G}^{(\mathrm{P})}_{34} &= -\left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\widetilde{\mathbf{s}}_j^2\right)\\
\mathbf{G}^{(\mathrm{P})}_{41} &= \mathbf{G}^{(\mathrm{P})}_{43} = [0, 0, 0]\\
\mathbf{G}^{(\mathrm{P})}_{42} &= -\left({}^{\mathcal{B}_j}\mathbf{s}_j^3\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^2\right)\\
\mathbf{G}^{(\mathrm{P})}_{44} &= -\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\widetilde{\mathbf{s}}_j^3\right)\\
\mathbf{G}^{(\mathrm{P})}_{51} &= \mathbf{G}^{(\mathrm{P})}_{53} = [0, 0, 0]\\
\mathbf{G}^{(\mathrm{P})}_{52} &= -\left({}^{\mathcal{B}_j}\mathbf{s}_j^1\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^3\right)\\
\mathbf{G}^{(\mathrm{P})}_{54} &= -\left({}^{\mathcal{B}_i}\mathbf{s}_i^3\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right)\left({}^{\mathcal{B}_j}\widetilde{\mathbf{s}}_j^1\right)
\end{aligned}
}
\tag{6.75}
$$

Prismatic pair displacement: As discussed in [49, p. 157], an additional constraint is required when the ***prismatic pair displacement***, u, explicitly appears. That is,

$$\boxed{\begin{aligned} 0 &= \Phi_1^{(\mathrm{P})_t} \\ &:= {}^{\mathcal{G}_i}\vec{\mathbf{e}}_1 \cdot \vec{\boldsymbol{\pi}}(\mathbf{P}_i, \mathbf{P}_j) - u \equiv \vec{\mathbf{s}}_i^1 \cdot \vec{\boldsymbol{\pi}}(\mathbf{P}_i, \mathbf{P}_j) - u \\ &= \left[\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)\right]^T \, {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{P}_i, \mathbf{P}_j) - u \end{aligned}} \tag{6.76}$$

The variation of $\Phi_1^{(\mathrm{P})_t}$ given in Eq. (6.76) is obtained as

$$\begin{aligned} 0 &= \delta\Phi_1^{(\mathrm{P})_t} \\ &= \left[\left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)\right]^T \delta\, {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{P}_i, \mathbf{P}_j) \\ &\quad - \left({}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{P}_i, \mathbf{P}_j)\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\right)\left({}^{\mathcal{B}_i}\widetilde{\mathbf{s}}_i^1\right)\left({}^{\mathcal{B}_i}_{\mathcal{B}_i|\mathcal{B}_0}\boldsymbol{\varpi}\right) \\ &\quad -\delta u \end{aligned} \tag{6.77}$$

where $\delta\, {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{P}_i, \mathbf{P}_j)$ is given in Eq. (6.74).

Remark 6.3.2

The external force applied to the prismatic pair, f_P, can be found from the virtual work,

$$\delta W_\mathrm{P} = f_\mathrm{P}\delta u \tag{6.78}$$

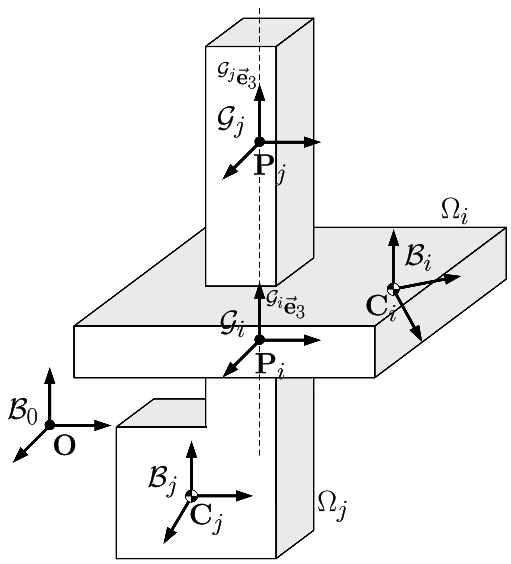


Figure 6.4: Prismatic Pair

Cylindrical Pair

The cylindrical pair is defined by the translational constraints, which are identical for the prismatic pair, i.e.,

$$
\begin{aligned}
{}^{\mathcal{G}_i}\vec{\mathbf{e}}_1 \cdot \vec{\boldsymbol{\pi}}(\mathbf{P}_i, \mathbf{P}_j) &= 0 \\
{}^{\mathcal{G}_i}\vec{\mathbf{e}}_2 \cdot \vec{\boldsymbol{\pi}}(\mathbf{P}_i, \mathbf{P}_j) &= 0
\end{aligned}
\tag{6.79}
$$

and the following two rotational constraints,

$$
\begin{aligned}
{}^{\mathcal{G}_i}\vec{\mathbf{e}}_1 \cdot {}^{\mathcal{G}_j}\vec{\mathbf{e}}_3 &= 0 \\
{}^{\mathcal{G}_i}\vec{\mathbf{e}}_2 \cdot {}^{\mathcal{G}_j}\vec{\mathbf{e}}_3 &= 0
\end{aligned}
\tag{6.80}
$$

which are actually the same as the ones for the hinge pair. Hence, the constraint equations for the cylindrical (C) pair are given as

$$\boxed{\mathbf{\Phi}^{(\mathrm{C})}(\mathbf{q}) = \begin{bmatrix} \mathbf{\Phi}^{(\mathrm{C})_\mathrm{t}}(\mathbf{q}) \\ \mathbf{\Phi}^{(\mathrm{C})_\mathrm{r}}(\mathbf{q}) \end{bmatrix} = \begin{bmatrix} \mathbf{\Phi}^{(\mathrm{P})_\mathrm{t}}(\mathbf{q}) \\ \mathbf{\Phi}^{(\mathrm{H})_\mathrm{r}}(\mathbf{q}) \end{bmatrix} = \mathbf{0} \in \mathbb{R}^4} \tag{6.81}$$

where the constraint equations for the cylindrical pair in the translational motion and rotational motion, i.e., $\mathbf{\Phi}^{(\mathrm{C})_\mathrm{t}} = \mathbf{\Phi}^{(\mathrm{P})_\mathrm{t}} = \mathbf{0} \in \mathbb{R}^2$ and $\mathbf{\Phi}^{(\mathrm{C})_\mathrm{r}}(\mathbf{q}) = \mathbf{\Phi}^{(\mathrm{H})_\mathrm{r}}(\mathbf{q}) = \mathbf{0} \in \mathbb{R}^2$, are given in Eq. (6.64) and Eq. (6.32), respectively. The corresponding $\mathbf{G}(\mathbf{q}) \in \mathbb{R}^{4\times 12}$ is therefore readily obtained.

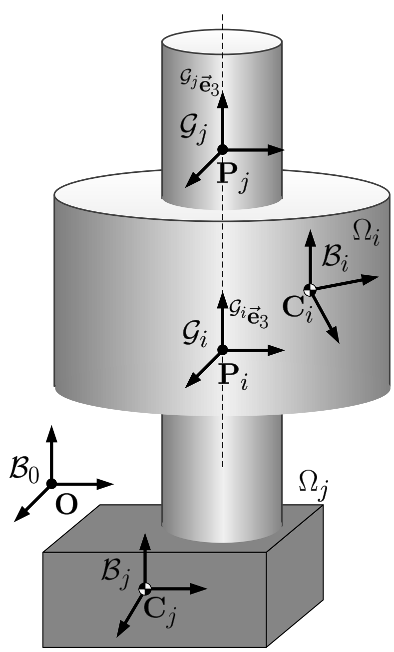


Figure 6.5: Cylindrical Pair

Screw Pair

By adding two more constraints to $\mathbf{\Phi}^{(C)}(\mathbf{q}) = \mathbf{0}$, given in Eq. (6.81), the constraint equations for the screw pair are obtained. Let

$$\Phi_\ell^{(Sc)_t}(\mathbf{q}) = \Phi_\ell^{(C)_t}(\mathbf{q}) = 0 \tag{6.82}$$

$$\Phi_\ell^{(Sc)_r}(\mathbf{q}) = \Phi_\ell^{(C)_r}(\mathbf{q}) = 0 \tag{6.83}$$

for $\ell = 1, 2$. Suppose points $\mathbf{P}_i$ and $\mathbf{P}_j$ initially coincides together, i.e., $\mathbf{P}_i(t_0) = \mathbf{P}_i(t_0)$. At time t, the distance between $\mathbf{P}_i(t)$ and $\mathbf{P}_j(t)$ can be expressed with the ***screw pitch***, p, and the ***screw rotation angle***, α, as

$$\left\|\vec{\boldsymbol{\pi}}(\mathbf{P}_i, \mathbf{P}_j)\right\| = p\alpha \tag{6.84}$$

That is, an additional translational constraint equation is

$$\Phi_3^{(C)_t} = {}^{\mathcal{G}_i}\vec{\mathbf{e}}_3 \cdot \vec{\boldsymbol{\pi}}(\mathbf{P}_i, \mathbf{P}_j) = 0 \tag{6.85}$$

The ***screw rotation angle***, α^p, is taken into consideration by adding

$$0 = \Phi_3^{(C)_r} = \left({}^{\mathcal{B}_j}\mathbf{s}_j^1\right)^T \left({}^{\mathcal{B}_j/\mathcal{B}_i}\mathbf{A}\right)\left[\left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)\cos(\alpha^p) - \left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)\sin(\alpha^p)\right] \tag{6.86}$$

which is similar to the constraint equation for the hinge pair; see Eq. (6.41). The corresponding $\mathbf{G}(\mathbf{q}) \in \mathbb{R}^{6\times 12}$ is readily obtained.

Planar Pair

The planar pair (see Fig. 6.6) is defined by the following translational and rotational conditions:

$$\Phi^{(F)_t} = {}^{\mathcal{G}_i}\vec{\mathbf{e}}_3 \cdot \vec{\boldsymbol{\pi}}(\mathbf{P}_i, \mathbf{P}_j) = 0 \tag{6.87}$$

$$\Phi_1^{(F)_r} = {}^{\mathcal{G}_i}\vec{\mathbf{e}}_1 \cdot {}^{\mathcal{G}_j}\vec{\mathbf{e}}_3 = 0 \tag{6.88}$$

$$\Phi_2^{(F)_r} = {}^{\mathcal{G}_i}\vec{\mathbf{e}}_2 \cdot {}^{\mathcal{G}_j}\vec{\mathbf{e}}_3 = 0 \tag{6.89}$$

Hence, the constraint equations for the planar (F) pair are given as

$$\boxed{\mathbf{\Phi}^{(\mathrm{F})}(\mathbf{q}) = \begin{bmatrix} \Phi^{(\mathrm{F})_\mathrm{t}}(\mathbf{q}) \\ \mathbf{\Phi}^{(\mathrm{F})_\mathrm{r}}(\mathbf{q}) \end{bmatrix} = \mathbf{0} \in \mathbb{R}^3} \tag{6.90}$$

where

$$0 = \Phi^{(\mathrm{F})_\mathrm{t}} = \left({}^{\mathcal{B}_i}\mathbf{s}_i^3\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right) {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{P}_i, \mathbf{P}_j) \tag{6.91}$$

and

$$0 = \Phi_1^{(\mathrm{F})_\mathrm{r}} = \left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right) \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right) \left({}^{\mathcal{B}_j}\mathbf{s}_j^3\right) \tag{6.92}$$

$$0 = \Phi_2^{(\mathrm{F})_\mathrm{r}} = \left({}^{\mathcal{B}_i}\mathbf{s}_i^2\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right) \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right) \left({}^{\mathcal{B}_j}\mathbf{s}_j^3\right) \tag{6.93}$$

The corresponding $\mathbf{G}(\mathbf{q}) \in \mathbb{R}^{3\times 12}$ is readily obtained.

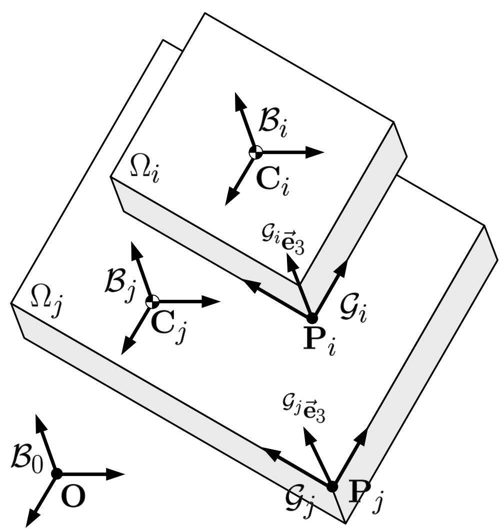


Figure 6.6: Planar Pair

6.3.2 Higher Pairs

Universal Pair

We define the body-fixed frames, $\mathcal{G}_i : (\mathbf{P}_i; \{^{\mathcal{G}_i}\vec{\mathbf{e}}_\ell\}_{\ell=1}^3)$ and $\mathcal{G}_j : (\mathbf{P}_j; \{^{\mathcal{G}_j}\vec{\mathbf{e}}_\ell\}_{\ell=1}^3)$, such that (1) the origins coincide each other, i.e., $\mathbf{P} := \mathbf{P}_i = \mathbf{P}_j$, i.e.,

$$\vec{\pi}(\mathbf{O}, \mathbf{C}_i) + \vec{\pi}(\mathbf{C}_i, \mathbf{P}) = \vec{\pi}(\mathbf{O}, \mathbf{C}_j) + \vec{\pi}(\mathbf{C}_j, \mathbf{P}) \tag{6.94}$$

and (2) the base vectors, $^{\mathcal{G}_i}\vec{\mathbf{e}}_1$ and $^{\mathcal{G}_j}\vec{\mathbf{e}}_2$, are orthogonal each other, i.e.,

$$^{\mathcal{G}_i}\vec{\mathbf{e}}_1 \cdot {}^{\mathcal{G}_j}\vec{\mathbf{e}}_2 = 0 \tag{6.95}$$

Hence, the constraint equations for the universal (U) pair are given as

$$\boxed{\mathbf{\Phi}^{(\mathrm{U})}(\mathbf{q}) = \begin{bmatrix} \mathbf{\Phi}^{(\mathrm{U})_\mathrm{t}}(\mathbf{q}) \\ \Phi^{(\mathrm{U})_\mathrm{r}}(\mathbf{q}) \end{bmatrix} = \mathbf{0} \in \mathbb{R}^4} \tag{6.96}$$

where

$$\mathbf{\Phi}^{(\mathrm{U})}(\mathbf{q}) = {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{C}_i) - {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{C}_j) + {}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}\,{}^{\mathcal{B}_i}\boldsymbol{\pi}(\mathbf{C}_i, \mathbf{P}) - {}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\,{}^{\mathcal{B}_j}\boldsymbol{\pi}(\mathbf{C}_j, \mathbf{P}) \tag{6.97}$$

which is identical to Eq. (6.26), and

$$\Phi^{(\mathrm{U})_\mathrm{r}}(\mathbf{q}) = \left({}^{\mathcal{B}_i}\mathbf{s}_i^1\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right) \left({}^{\mathcal{B}_0/\mathcal{B}_j}\mathbf{A}\right) \left({}^{\mathcal{B}_j}\mathbf{s}_j^2\right) \tag{6.98}$$

The variation of $\mathbf{\Phi}^{(\mathrm{U})}$ and its corresponding $\mathbf{G}(\mathbf{q}) \in \mathbb{R}^{4\times 12}$ may be obtained following the similar procedures for the lower pairs.

Point-to-plane Pair

$$^{\mathcal{G}_i}\vec{\mathbf{e}}_3 \cdot \vec{\pi}(\mathbf{P}_i, \mathbf{P}_j) = 0 \tag{6.99}$$

The only constraint equation for the point-to-plane pair is

$$\boxed{\Phi^{(\mathrm{PP})}(\mathbf{q}) := \left({}^{\mathcal{B}_i}\mathbf{s}_i^3\right)^T \left({}^{\mathcal{B}_0/\mathcal{B}_i}\mathbf{A}^T\right) {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{P}_i, \mathbf{P}_j) = 0 \in \mathbb{R}^1} \tag{6.100}$$

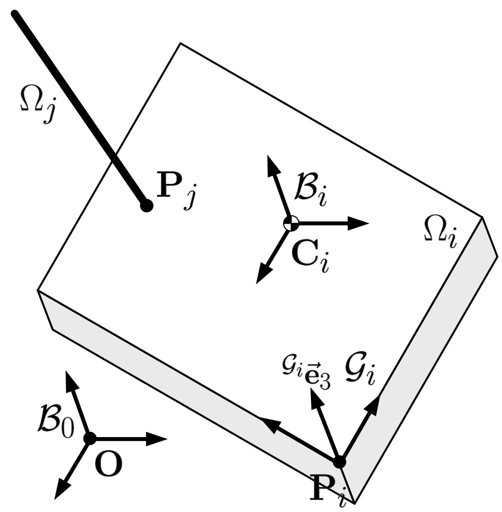


Figure 6.7: Point-to-plane Pair

Chapter 7

RIGID-BODY DYNAMICS: Equations of Motion

7.1 Introduction: Newton's Equation of Motion for a System of N Particles

The equation of motion for rigid-body dynamics is gained by way of the direct extension of the equation of motion for a dynamical system of N particles; therefore, in the first place, consider a dynamical system of N number of particles in $\mathbb{E}^3$ as shown in Fig. Suppose a Cartesian frame $\mathcal{B}_0$ is fixed in space, and not accelerated in both translational and rotational senses: such frame is called the ***inertial reference frame***.

From the Newton's second law, the equation of motion of particle i of a constant mass, $m_i > 0$, is given as

$$m_i \vec{\mathbf{a}}_i = \vec{\mathbf{f}}_i \tag{7.1}$$

where $\vec{\mathbf{a}}_i := {}^{\mathcal{B}_0}\mathfrak{D}_t^2\, \vec{\mathbf{r}}_i$, in which $\vec{\mathbf{r}}_i := \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P}_i)$, denotes the acceleration vector of particle

i with respect to $\mathcal{B}_0$, and $\vec{\mathbf{f}}_i$ denotes the total force, or the sum of all forces, acting on particle i. the total force on particle i may be constituted of the external and internal forces acting on particle i as

$$\vec{\mathbf{f}}_i = \vec{\mathbf{f}}_i^{\text{ext}} + \vec{\mathbf{f}}_i^{\text{int}} = \vec{\mathbf{f}}_i^{\text{ext}} + \sum_{j=1}^{N} \vec{\mathbf{f}}_{ij}^{\text{int}} \tag{7.2}$$

The internal forces among the particles in the system satisfy:

$$\vec{\mathbf{f}}_{ij}^{\text{int}} + \vec{\mathbf{f}}_{ji}^{\text{int}} = \vec{\mathbf{0}} \;\text{ and }\; \vec{\mathbf{f}}_{ii}^{\text{int}} = \vec{\mathbf{0}} \tag{7.3}$$

for $i, j = 1, 2, \cdots, N$. The external force, $\vec{\mathbf{f}}_i^{\text{ext}}$, can be decomposed into two parts, i.e., the applied forces and the constraint forces:

$$\vec{\mathbf{f}}_i^{\text{ext}} = \vec{\mathbf{f}}_i^{\text{appl}} + \vec{\mathbf{f}}_i^{\text{const}} \tag{7.4}$$

For a system of N particles, the equation of motion may yield

$$\begin{aligned}\sum_{i=1}^{N} m_i \vec{\mathbf{a}}_i = \sum_{i=1}^{N} \vec{\mathbf{f}}_i &= \sum_{i=1}^{N} \vec{\mathbf{f}}_i^{\text{ext}} + \underbrace{\sum_{i=1}^{N}\sum_{j=1}^{N} \vec{\mathbf{f}}_{ij}^{\text{int}}}_{\vec{\mathbf{0}}} \\ &= \sum_{i=1}^{N} \vec{\mathbf{f}}_i^{\text{appl}} + \sum_{i=1}^{N} \vec{\mathbf{f}}_i^{\text{const}}\end{aligned} \tag{7.5}$$

We define the center of mass of the system as

$$\frac{1}{m}\sum_{i=1}^{N} m_i \vec{\mathbf{r}}_i = \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}) \tag{7.6}$$

where $\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C})$ denotes the radius vector of point $\mathbf{C} \in \mathbb{E}^3$, the point of the center of mass of the system or the centroid point, about the origin point, $\mathbf{O}$; and m denotes the total mass of the system defined by

$$m := \sum_{i=1}^{N} m_i \tag{7.7}$$

Therefore, Eq. (7.5) can be written in terms of the center of mass as

$$\boxed{m\ {}^{\mathcal{B}_0}\mathfrak{D}_t^2\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}) = \vec{\mathbf{f}}^{\text{ext}} = \sum_{i=1}^{N}\vec{\mathbf{f}}_i^{\text{ext}}} \tag{7.8}$$

where ${}^{\mathcal{B}_0}\mathfrak{D}_t^2\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C})$ is the acceleration at the center of mass in terms of $\mathcal{B}_0$. Note that the summation of the external forced applied at every particle in the system, as given in the right-hand side of Eq. (7.8), can be viewed as the resultant external force applied at point $\mathbf{C}$.

7.2 Newton-Euler System of Equations for a Rigid Body

7.2.1 Linear and Angular Momenta of a Rigid Body

Definition 7.2.1 (Linear Momentum of a Rigid Body)

Consider a rigid body, Ω, in a system in $\mathbb{E}^3$. Suppose $\mathcal{B}_0$ is an inertial reference frame fixed in space. The linear momentum of Ω about point $\mathbf{O} \in \mathbb{E}^3$ is defined as

$$_{\mathbf{O}}\vec{\mathbf{L}} := \int_{\Omega} {}^{\mathcal{B}_0}\mathfrak{D}_t\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P})dm \tag{7.9}$$

where $\mathbf{P} \in \Omega \subset \mathbb{E}^3$ is an arbitrary point in the rigid body.

Theorem 7.2.1

The linear momentum for a rigid body, Ω, defined in Definition 7.2.1, can be written as

$$_{\mathbf{O}}\vec{\mathbf{L}} = m\ {}^{\mathcal{B}_0}\mathfrak{D}_t\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}) \tag{7.10}$$

where $m := \int_\Omega dm = \int_\Omega \rho dV > 0$, in which $\rho > 0$ is the density function of Ω, denotes the mass of the rigid body Ω; and $\mathbf{C} \in \Omega \subset \mathbb{E}^3$ denotes the point of the center of mass of the rigid body. Point $\mathbf{C}$ is defined by

$$\int_\Omega \vec{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})dm = \mathbf{0} \tag{7.11}$$

where $\mathbf{P} \in \Omega \subset \mathbb{E}^3$ *is an arbitrary point in the rigid body.*

Proof. From the definition, we have

$$_{\mathbf{O}}\vec{\mathbf{L}} := \int_{\Omega} {}^{\mathcal{B}_0}\mathfrak{D}_t \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P}) dm \tag{7.12}$$

Substituting $\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P}) = \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}) + \vec{\boldsymbol{\pi}}(\mathbf{C}, \mathbf{P})$ yields

$$\begin{aligned} _{\mathbf{O}}\vec{\mathbf{L}} &= \int_{\Omega} {}^{\mathcal{B}_0}\mathfrak{D}_t \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}) dm + \int_{\Omega} {}^{\mathcal{B}_0}\mathfrak{D}_t \vec{\boldsymbol{\pi}}(\mathbf{C}, \mathbf{P}) dm \\ &= \underbrace{\int_{\Omega} dm}_{m} \, {}^{\mathcal{B}_0}\mathfrak{D}_t \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}) + {}^{\mathcal{B}_0}\mathfrak{D}_t \underbrace{\int_{\Omega} \vec{\boldsymbol{\pi}}(\mathbf{C}, \mathbf{P}) dm}_{\mathbf{0}} \\ &= m \, {}^{\mathcal{B}_0}\mathfrak{D}_t \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}) \end{aligned} \tag{7.13}$$

Therefore, Eq. (7.10) has been proven. Note that Eq. (7.10) can be viewed as the direct extension of Eq. (7.8) to a rigid body. ∎

Theorem 7.2.2 (Linear Momentum Component Vector)

The component form of the linear momentum of Ω *about point* $\mathbf{O}$ *with respect to* $\mathcal{B}_0$ *is readily obtained as*

$${}^{\mathcal{B}_0}_{\mathbf{O}}\mathbf{L} = m {}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}) \in \mathbb{R}^3 \tag{7.14}$$

Proof. Proof is omitted.

Definition 7.2.2 (Angular Momentum of a Rigid Body)

Consider a rigid body, Ω*, in a system in* $\mathbb{E}^3$*. Suppose an inertial reference frame* $\mathcal{B}_0$ *is fixed in space, and frame* $\mathcal{B}_1$ *is fixed at the point of the center of mass of* Ω*. The angular momentum of* Ω *about point* $\mathbf{O} \in \mathbb{E}^3$ *is defined as*

$$_{\mathbf{O}}\vec{\mathbf{J}} := \int_{\Omega} \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P}) \times {}^{\mathcal{B}_0}\mathfrak{D}_t \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P}) dm \tag{7.15}$$

where $\mathbf{P} \in \Omega \subset \mathbb{E}^3$ *is an arbitrary point in the rigid body. Similarly, the angular momentum of* Ω *about point* $\mathbf{C} \in \Omega \subset \mathbb{E}^3$ *is defined as*

$$ {}_{\mathbf{C}}\vec{\mathbf{J}} := \int_{\Omega} \vec{\pi}(\mathbf{C},\mathbf{P}) \times {}^{\mathcal{B}_0}\mathfrak{D}_t \vec{\pi}(\mathbf{O},\mathbf{P}) dm \tag{7.16} $$

Theorem 7.2.3

The angular momentum of Ω *about point* $\mathbf{C}$ *can be written as*

$$ {}_{\mathbf{C}}\vec{\mathbf{J}} = \int_{\Omega} \vec{\pi}(\mathbf{C},\mathbf{P}) \times {}^{\mathcal{B}_0}\mathfrak{D}_t \vec{\pi}(\mathbf{C},\mathbf{P}) dm \tag{7.17} $$

Proof. From Eq. (7.16), we get

$$ {}_{\mathbf{C}}\vec{\mathbf{J}} = \int_{\Omega} \vec{\pi}(\mathbf{C},\mathbf{P}) \times {}^{\mathcal{B}_0}\mathfrak{D}_t \vec{\pi}(\mathbf{O},\mathbf{C}) dm + \int_{\Omega} \vec{\pi}(\mathbf{C},\mathbf{P}) \times {}^{\mathcal{B}_0}\mathfrak{D}_t \vec{\pi}(\mathbf{C},\mathbf{P}) dm \tag{7.18} $$

Since the first term of Eq. (7.18) vanishes as

$$ \int_{\Omega} \vec{\pi}(\mathbf{C},\mathbf{P}) \times {}^{\mathcal{B}_0}\mathfrak{D}_t \vec{\pi}(\mathbf{O},\mathbf{C}) dm = \underbrace{\int_{\Omega} \vec{\pi}(\mathbf{C},\mathbf{P}) dm}_{\mathbf{0}} \times {}^{\mathcal{B}_0}\mathfrak{D}_t \vec{\pi}(\mathbf{O},\mathbf{C}) = \mathbf{0} \tag{7.19} $$

Eq. (7.18) yields Eq. (7.17). ∎

Theorem 7.2.4 (Time Derivative of the Angular Momentum of a Rigid Body)

The time derivative of Eq. (7.17) *with respect to* $\mathcal{B}_0$ *is obtained as*

$$ \begin{aligned} {}^{\mathcal{B}_0}\mathfrak{D}_t \, {}_{\mathbf{C}}\vec{\mathbf{J}} = & \int_{\Omega} \vec{\pi}(\mathbf{C},\mathbf{P}) \times \left[{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\alpha} \times \vec{\pi}(\mathbf{C},\mathbf{P}) \right] dm \\ & + \int_{\Omega} \vec{\pi}(\mathbf{C},\mathbf{P}) \times ({}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times [{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \vec{\pi}(\mathbf{C},\mathbf{P})]) dm \end{aligned} \tag{7.20} $$

where ${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\alpha}$ *and* ${}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}$ *are the angular acceleration and angular velocity vectors of the body-fixed frame of* Ω, $\mathcal{B}_1$, *with respect to the inertia reference frame,* $\mathcal{B}_0$, *respectively.*

Proof. Taking the time derivative of Eq. (7.17) yields

$$\begin{aligned}
{}^{\mathcal{B}_0}\mathfrak{D}_t\ {}_{\mathbf{C}}\vec{\mathbf{J}} &= {}^{\mathcal{B}_0}\mathfrak{D}_t \int_\Omega \vec{\pi}(\mathbf{C},\mathbf{P}) \times {}^{\mathcal{B}_0}\mathfrak{D}_t\vec{\pi}(\mathbf{C},\mathbf{P})dm \\
&= \int_\Omega \underbrace{{}^{\mathcal{B}_0}\mathfrak{D}_t\vec{\pi}(\mathbf{C},\mathbf{P}) \times {}^{\mathcal{B}_0}\mathfrak{D}_t\vec{\pi}(\mathbf{C},\mathbf{P})}_{\mathbf{0}}\, dm + \int_\Omega \vec{\pi}(\mathbf{C},\mathbf{P}) \times {}^{\mathcal{B}_0}\mathfrak{D}_t^2\vec{\pi}(\mathbf{C},\mathbf{P})dm \\
&= \int_\Omega \vec{\pi}(\mathbf{C},\mathbf{P}) \times {}^{\mathcal{B}_0}\mathfrak{D}_t^2\vec{\pi}(\mathbf{C},\mathbf{P})dm
\end{aligned} \tag{7.21}$$

In view of Eq. (5.159) in Theorem 5.4.1, the acceleration vector, ${}^{\mathcal{B}_0}\mathfrak{D}_t^2\vec{\pi}(\mathbf{C},\mathbf{P})$, can be expressed as

$$\begin{aligned}
{}^{\mathcal{B}_0}\mathfrak{D}_t^2\vec{\pi}(\mathbf{C},\mathbf{P}) =& {}^{\mathcal{B}_1}\mathfrak{D}_t^2\ \vec{\pi}(\mathbf{C},\mathbf{P}) + {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\alpha} \times \vec{\pi}(\mathbf{C},\mathbf{P}) \\
&+ 2\ {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times {}^{\mathcal{B}_1}\mathfrak{D}_t\ \vec{\pi}(\mathbf{C},\mathbf{P}) + {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times [{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \vec{\pi}(\mathbf{C},\mathbf{P})]
\end{aligned} \tag{7.22}$$

Since point $\mathbf{P}$ is an arbitrary point fixed in Ω, the first term of Eq. (7.22) vanishes; therefore, we get

$$\begin{aligned}
{}^{\mathcal{B}_0}\mathfrak{D}_t\ {}_{\mathbf{C}}\vec{\mathbf{J}} =& \int_\Omega \vec{\pi}(\mathbf{C},\mathbf{P}) \times ({}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\alpha} \times \vec{\pi}(\mathbf{C},\mathbf{P}) + {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times [{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \vec{\pi}(\mathbf{C},\mathbf{P})])\, dm \\
&+ 2{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times {}^{\mathcal{B}_1}\mathfrak{D}_t \underbrace{\int_\Omega \vec{\pi}(\mathbf{C},\mathbf{P})dm}_{\mathbf{0}}
\end{aligned} \tag{7.23}$$

Hence, Eq. (7.20) has been proven. ∎

Theorem 7.2.5

(Component Form of the Time Derivative of the Angular Momentum of a Rigid Body)

The component form of ${}^{\mathcal{B}_0}\mathfrak{D}_t\ {}_{\mathbf{C}}\vec{\mathbf{J}}$ *with respect to the body-fixed frame,* $\mathcal{B}_1$*, is given as*

$${}^{\mathcal{B}_1}_{\mathbf{C}}\dot{\mathbf{J}} = \left({}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\alpha\right) + \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right)\left({}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\omega\right) \in \mathbb{R}^3 \tag{7.24}$$

where

$${}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I} := -\int_\Omega \left({}^{\mathcal{B}_1}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\right)\left({}^{\mathcal{B}_1}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\right) dm \in \mathbb{R}^{3\times 3} \tag{7.25}$$

is the moment of inertia tensor of Ω about point $\mathbf{C}$ with respect to frame $\mathcal{B}_1$. Similarly, the component form of ${}^{\mathcal{B}_0}\mathfrak{D}_t\ {}_{\mathbf{C}}\vec{\mathbf{J}}$ with respect to the inertia reference frame, $\mathcal{B}_0$, is obtained as

$$ {}^{\mathcal{B}_0}_{\mathbf{C}}\dot{\mathbf{J}} = \left({}^{\mathcal{B}_0}_{\mathbf{C}}\mathfrak{I}\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\alpha}\right) + \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\ \left({}^{\mathcal{B}_0}_{\mathbf{C}}\mathfrak{I}\right)\ \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right) \in \mathbb{R}^3 \tag{7.26} $$

where

$$ {}^{\mathcal{B}_0}_{\mathbf{C}}\mathfrak{I} := -\int_{\Omega}\left({}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\right)\ \left({}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\right) dm \in \mathbb{R}^{3\times 3} \tag{7.27} $$

is the moment of inertia tensor of Ω about point $\mathbf{C}$ with respect to frame $\mathcal{B}_1$.

Proof. The first term of Eq. (7.20) may be written

$$ \begin{aligned} & \int_{\Omega}\vec{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P}) \times \left[{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\alpha}} \times \vec{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\right] dm \\ = \ & -\int_{\Omega}\vec{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P}) \times \left[\vec{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P}) \times {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\alpha}}\right] dm \\ = \ & -\int_{\Omega}\vec{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P}) \times [\underbrace{\vec{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P}) \times ({}^{\mathcal{B}_1}\mathbf{e}^T}_{{}^{\mathcal{B}_1}\mathbf{e}^T\ {}^{\mathcal{B}_1}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})}\ {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\alpha})]dm \\ = \ & -\int_{\Omega}\underbrace{\vec{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P}) \times {}^{\mathcal{B}_1}\mathbf{e}}_{{}^{\mathcal{B}_1}\mathbf{e}^T\ \vec{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})}\ {}^{\mathcal{B}_1}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\ {}^{\mathcal{B}_1}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\alpha}\right) dm \\ = \ & {}^{\mathcal{B}_1}\mathbf{e}^T\left({}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\alpha}\right) \end{aligned} \tag{7.28} $$

where ${}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I}$ is the moment of inertia tensor of Ω about point $\mathbf{C}$ with respect to frame $\mathcal{B}_1$

as defined in Eq. (7.25). On the other hand, the second term of Eq. (7.20) yields

$$\begin{aligned}
&\int_\Omega \vec{\pi}(\mathbf{C},\mathbf{P}) \times ({}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times [{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \vec{\pi}(\mathbf{C},\mathbf{P})])dm \\
= \; & -\int_\Omega \vec{\pi}(\mathbf{C},\mathbf{P}) \times ({}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times [\vec{\pi}(\mathbf{C},\mathbf{P}) \times {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega}])dm \\
= \; & -\int_\Omega \vec{\pi}(\mathbf{C},\mathbf{P}) \times ({}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times [\underbrace{\vec{\pi}(\mathbf{C},\mathbf{P}) \times ({}^{\mathcal{B}_1}\mathbf{e}^T}_{{}^{\mathcal{B}_1}\mathbf{e}^T\, {}^{\mathcal{B}_1}\widetilde{\pi}(\mathbf{C},\mathbf{P})} \; {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\omega)])dm \\
= \; & -\int_\Omega \vec{\pi}(\mathbf{C},\mathbf{P}) \times (\underbrace{{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times [{}^{\mathcal{B}_1}\mathbf{e}^T}_{{}^{\mathcal{B}_1}\mathbf{e}^T\, {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}} \; {}^{\mathcal{B}_1}\widetilde{\pi}\mathbf{C},\mathbf{P}) \; {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\omega])dm \\
= \; & -\int_\Omega \underbrace{\vec{\pi}(\mathbf{C},\mathbf{P}) \times {}^{\mathcal{B}_1}\mathbf{e}^T}_{{}^{\mathcal{B}_1}\mathbf{e}^T\, {}^{\mathcal{B}_1}\widetilde{\pi}(\mathbf{C},\mathbf{P})} \; {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega} \; {}^{\mathcal{B}_1}\widetilde{\pi}(\mathbf{C},\mathbf{P}) \; {}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\omega])dm \\
= \; & -{}^{\mathcal{B}_1}\mathbf{e}^T \int_\Omega {}^{\mathcal{B}_1}\widetilde{\pi}(\mathbf{C},\mathbf{P}) \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right) {}^{\mathcal{B}_1}\widetilde{\pi}(\mathbf{C},\mathbf{P}) \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\omega\right) dm
\end{aligned} \tag{7.29}$$

Substituting the relation,

$$ {}^{\mathcal{B}_1}\widetilde{\pi}(\mathbf{C},\mathbf{P}) \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right) = \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right) {}^{\mathcal{B}_1}\widetilde{\pi}(\mathbf{C},\mathbf{P}) + \operatorname{spin}\left({}^{\mathcal{B}_1}\widetilde{\pi}(\mathbf{C},\mathbf{P}) \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\omega\right)\right) \tag{7.30}$$

the second term of Eq. (7.20) can be finally written as

$$\begin{aligned}
&\int_\Omega \vec{\pi}(\mathbf{C},\mathbf{P}) \times ({}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times [{}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\omega} \times \vec{\pi}(\mathbf{C},\mathbf{P})])dm \\
= \; & {}^{\mathcal{B}_1}\mathbf{e}^T \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right) \left({}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I}\right) \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\omega\right)
\end{aligned} \tag{7.31}$$

where we have used Eq. (7.25) and

$$ \operatorname{spin}\left({}^{\mathcal{B}_1}\widetilde{\pi}(\mathbf{C},\mathbf{P}) \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\omega\right)\right) {}^{\mathcal{B}_1}\widetilde{\pi}(\mathbf{C},\mathbf{P}) \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\omega\right) = \mathbf{0} \tag{7.32}$$

Hence,

$$ {}^{\mathcal{B}_0}\mathfrak{D}_t \; {}_{\mathbf{C}}\vec{\mathbf{J}} = {}^{\mathcal{B}_1}\mathbf{e}^T \underbrace{\left[\left({}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\alpha\right) + \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right) \left({}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I}\right) \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\omega\right)\right]}_{{}^{\mathcal{B}_1}_{\mathbf{C}}\dot{\mathbf{J}}} \tag{7.33}$$

Therefore, the component vector of ${}^{\mathcal{B}_0}\mathfrak{D}_t\ {}_{\mathbf{C}}\vec{\mathbf{J}}$ with respect to frame $\mathcal{B}_1$ is obtained as in Eq. (7.24). In a similar manner, the component vector of ${}^{\mathcal{B}_0}\mathfrak{D}_t\ {}_{\mathbf{C}}\vec{\mathbf{J}}$ with respect to the inertia reference frame, $\mathcal{B}_0$, is obtained as in Eq. (7.26). ∎

7.2.2 Newton-Euler Equations of Motion for a Rigid Body

Theorem 7.2.6 (Equations of Motion for a Rigid Body)

Consider a rigid body, Ω, in a system in $\mathbb{E}^3$. Suppose an inertial reference frame $\mathcal{B}_0$ is fixed in space, and frame $\mathcal{B}_1$ is fixed at the point of the center of mass of Ω. Then, the equation of motion for Ω in the translational sense is given as

$$\boxed{{}^{\mathcal{B}_0}\mathfrak{D}_t\ {}_{\mathbf{O}}\vec{\mathbf{L}} = m\ {}^{\mathcal{B}_0}\mathfrak{D}_t^2\vec{\pi}(\mathbf{O},\mathbf{C}) = \vec{\mathbf{f}}^{\text{ext}}} \tag{7.34}$$

where $\vec{\mathbf{f}}^{\text{ext}}$ denotes the resultant external force applied to Ω defined as

$$\vec{\mathbf{f}}^{\text{ext}} := \int_\Omega d\vec{\mathbf{f}}^{\text{ext}} \tag{7.35}$$

and point $\mathbf{C} \in \mathbb{E}^3$ is the centroid point of Ω. And, the equation of motion for Ω in the rotational sense about point $\mathbf{O} \in \mathbb{E}^3$ is given as

$$\boxed{{}^{\mathcal{B}_0}\mathfrak{D}_t\ {}_{\mathbf{O}}\vec{\mathbf{J}} = \int_\Omega \vec{\pi}(\mathbf{O},\mathbf{P}) \times \underbrace{{}^{\mathcal{B}_0}\mathfrak{D}_t^2\ \vec{\pi}(\mathbf{O},\mathbf{P})dm}_{d\vec{\mathbf{f}}^{\text{ext}}} = {}_{\mathbf{O}}\vec{\mathcal{T}}} \tag{7.36}$$

where ${}_{\mathbf{O}}\vec{\mathcal{T}}$ denotes the total torque (or moment) vector of Ω in terms of point $\mathbf{O}$, i.e., the origin of $\mathcal{B}_0$.

Theorem 7.2.7 (Equations of Motion for a Rigid Body: In the Component Forms)

The component forms of the equation of motion with respect to the inertial reference frame $\mathcal{B}_0$ and the body-fixed frame, $\mathcal{B}_1$, in the translational sense are given as

$$\boxed{\begin{aligned} {}^{\mathcal{B}_0}_{\mathbf{O}}\dot{\mathbf{L}} &= m\ {}^{\mathcal{B}_0}\ddot{\pi}(\mathbf{O},\mathbf{C}) = {}^{\mathcal{B}_0}\mathbf{f}^{\text{ext}} \\ {}^{\mathcal{B}_1}_{\mathbf{O}}\dot{\mathbf{L}} &= m\ {}^{\mathcal{B}_1}\ddot{\pi}(\mathbf{O},\mathbf{C}) = {}^{\mathcal{B}_1}\mathbf{f}^{\text{ext}} \end{aligned}} \tag{7.37}$$

respectively. In the rotational sense, the component forms of the equation of motion with respect to $\mathcal{B}_0$ *and* $\mathcal{B}_1$ *are given as*

$$\boxed{\begin{aligned} {}^{\mathcal{B}_0}_{\mathbf{O}}\dot{\mathbf{J}} &= \left({}^{\mathcal{B}_0}_{\mathbf{C}}\Im\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\omega}\right) + \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right)\left({}^{\mathcal{B}_0}_{\mathbf{C}}\Im\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\omega\right) = {}^{\mathcal{B}_0}_{\mathbf{C}}\mathcal{T} \\ {}^{\mathcal{B}_1}_{\mathbf{O}}\dot{\mathbf{J}} &= \left({}^{\mathcal{B}_1}_{\mathbf{C}}\Im\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\omega}\right) + \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\omega}\right)\left({}^{\mathcal{B}_1}_{\mathbf{C}}\Im\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\omega\right) = {}^{\mathcal{B}_1}_{\mathbf{C}}\mathcal{T} \end{aligned}} \tag{7.38}$$

respectively, where ${}^{\mathcal{B}_\ell}_{\mathbf{C}}\Im \in \mathbb{R}^{3\times 3}$ *denotes the moment of inertia tensor with respect to base* $\mathcal{B}_\ell$ *(for* $\ell = 0, 1$*).*

Eq. (7.37) *is known as* ***Newton's equation of motion*** *whilst Eq.* (7.38) *is known as* ***Euler's equation of motion*** *in the component forms. The set of Eq.* (7.37) *and Eq.* (7.38) *is sometimes called as the* ***Newton-Euler system of equations of motion*** *in the component form.*

Proof. The proofs of the Newton's and Euler's equations of motion of Ω with respect to frames $\mathcal{B}_0$ and $\mathcal{B}_1$ are shown below.

Newton's Equation of Motion - (1) With respect to $\mathcal{B}_0$: With $\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}) = {}^{\mathcal{B}_0}\mathbf{e}^T\,{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{C})$ and $\vec{\mathbf{f}}^{\text{ext}} = {}^{\mathcal{B}_0}\mathbf{e}^T\,{}^{\mathcal{B}_0}\mathbf{f}^{\text{ext}}$, we can readily obtain Eq. $(7.37)_1$ from Eq. (7.34).

Newton's Equation of Motion - (2) With respect to $\mathcal{B}_1$: Likewise, with $\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}) = {}^{\mathcal{B}_1}\mathbf{e}^T\,{}^{\mathcal{B}_1}\boldsymbol{\pi}(\mathbf{O},\mathbf{C})$ and $\vec{\mathbf{f}}^{\text{ext}} = {}^{\mathcal{B}_1}\mathbf{e}^T\,{}^{\mathcal{B}_1}\mathbf{f}^{\text{ext}}$, we can readily obtain Eq. $(7.37)_2$ from Eq. (7.34).

Euler's Equation of Motion - (1) With respect to $\mathcal{B}_0$: From Eq. (7.36), we have

$$\begin{aligned} {}_{\mathbf{O}}\vec{\mathcal{T}} = {}^{\mathcal{B}_0}\mathbf{e}^T\,{}^{\mathcal{B}_0}_{\mathbf{O}}\mathcal{T} &= \int_\Omega [\underbrace{{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{P})^T\,{}^{\mathcal{B}_0}\mathbf{e}] \times [{}^{\mathcal{B}_0}\mathbf{e}^T}_{{}^{\mathcal{B}_0}\mathbf{e}^T\,{}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P})}\,{}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P})]dm \\ &= {}^{\mathcal{B}_0}\mathbf{e}^T \int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P})\,{}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P})dm \end{aligned} \tag{7.39}$$

Therefore, the torque (or moment) component vector of Ω in terms of $\mathbf{O}$ with respect to $\mathcal{B}_0$ is given as

$$ {}^{\mathcal{B}_0}_{\mathbf{O}}\mathcal{T} = \int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P})\,{}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P})dm \tag{7.40}$$

Eq. (7.40) can be modified as follows:

$$
\begin{aligned}
{}^{\mathcal{B}_0}_{\mathbf{O}}\mathcal{T} &= \int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P})\ {}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P})dm \\
&= \int_\Omega \left[{}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}) + {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\right]\ \left[{}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}) + {}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\right] dm \\
&= \int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C})\ {}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C})dm + \int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\ {}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})dm \\
&\quad + \int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\ {}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C})dm + \int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C})\ {}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})dm \\
&= {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C})\ {}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}) \underbrace{\int_\Omega dm}_{m} + \int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\ {}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})dm \\
&\quad + \underbrace{\int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})dm}_{\mathbf{0}}\ {}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}) + {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C})\ \underbrace{\int_\Omega {}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})dm}_{\mathbf{0}} \\
&= m\ {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C})\ {}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}) + \int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\ {}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})dm
\end{aligned}
\tag{7.41}
$$

By setting $\vec{\mathbf{s}} = \vec{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})$ in Theorem 5.3.1, we get

$$
\begin{aligned}
{}^{\mathcal{B}_0}\mathfrak{D}_t\vec{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P}) = {}^{\mathcal{B}_0}\mathbf{e}^T\ {}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P}) &= {}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\omega}} \times \vec{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P}) \\
&= \underbrace{[{}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}^T\ {}^{\mathcal{B}_0}\mathbf{e}] \times [{}^{\mathcal{B}_0}\mathbf{e}^T}_{{}^{\mathcal{B}_0}\mathbf{e}^T\ {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}}\ {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{C},\mathbf{P})] \\
&= {}^{\mathcal{B}_0}\mathbf{e}^T\ {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\ {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{C},\mathbf{P})
\end{aligned}
\tag{7.42}
$$

That is,

$$
{}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P}) = {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\ {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{C},\mathbf{P}) = -{}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\ {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega} \tag{7.43}
$$

Substituting Eq. (7.43) into Eq. (7.41) yields:

$$\begin{aligned}
{}^{\mathcal{B}_0}_{\mathbf{O}}\mathcal{T} &= m\,{}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C})\,{}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}) \\
&\quad + \int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\,\frac{d}{dt}\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\,{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{C},\mathbf{P})\right)dm \\
&= m\,{}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C})\,{}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}) \\
&\quad + \int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\,\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\widetilde{\boldsymbol{\omega}}}\right)\,{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{C},\mathbf{P})dm \\
&\quad + \int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\,\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\,\underbrace{{}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})}_{-{}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\,{}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}}\;dm \\
&= m\,{}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C})\,{}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}) \\
&\quad + \int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\,\underbrace{\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\widetilde{\boldsymbol{\omega}}}\right)\,{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{C},\mathbf{P})}_{-{}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\,{}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\omega}}}dm \\
&\quad - \int_\Omega \left[{}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\,\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\right]\,{}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\,\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right)dm \\
&= m\,{}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C})\,{}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}) \\
&\quad - \int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\,{}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})dm\,\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\omega}}\right) \\
&\quad - \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\,\int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\,{}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})dm\,\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right) \\
&\quad - \int_\Omega \underbrace{\mathrm{spin}\left({}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\,\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right)\right)\,{}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\,\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right)}_{\mathbf{0}}dm \\
&= m\,{}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C})\,{}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}) \\
&\quad - \int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\,{}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})dm\,\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\omega}}\right) \\
&\quad - \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\,\int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\,{}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})dm\,\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right) \qquad (7.44)
\end{aligned}$$

where the following relation has been used from the third to the fourth equations,

$$ {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\,\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right) = \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\,{}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P}) + \mathrm{spin}\left({}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\,\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right)\right) \qquad (7.45)$$

Using the ***moment of inertia tensor*** of Ω about point $\mathbf{C}$ with respect to the inertial reference frame, $\mathcal{B}_0$, as defined in Eq. (7.27), Eq. (7.44) can be written as

$$ {}^{\mathcal{B}_0}_{\mathbf{O}}\mathcal{T} = m\ {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C})\ {}^{\mathcal{B}_0}\ddot{\vec{\pi}}(\mathbf{O},\mathbf{C}) + {}^{\mathcal{B}_0}_{\mathbf{C}}\mathfrak{I}\ \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\omega}}\right) + \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\ {}^{\mathcal{B}_0}_{\mathbf{C}}\mathfrak{I}\ \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right) \tag{7.46} $$

The torque (or moment) vector in terms of point $\mathbf{C}$, i.e., ${}_{\mathbf{C}}\vec{\mathcal{T}} = {}^{\mathcal{B}_0}\mathbf{e}^T\ {}^{\mathcal{B}_0}_{\mathbf{C}}\vec{\mathcal{T}}$, may be given as

$$ \begin{aligned} {}_{\mathbf{C}}\vec{\mathcal{T}} &= \int_\Omega \vec{\pi}(\mathbf{C},\mathbf{P}) \times d\vec{\mathbf{f}}^{\text{ext}} \\ &= \int_\Omega \vec{\pi}(\mathbf{O},\mathbf{P}) \times d\vec{\mathbf{f}}^{\text{ext}} - \int_\Omega \vec{\pi}(\mathbf{O},\mathbf{C}) \times d\vec{\mathbf{f}}^{\text{ext}} \\ &= {}_{\mathbf{O}}\vec{\mathcal{T}} - \vec{\pi}(\mathbf{O},\mathbf{C}) \times \vec{\mathbf{f}}^{\text{ext}} \\ &= {}^{\mathcal{B}_0}\mathbf{e}^T\ \left[{}^{\mathcal{B}_0}_{\mathbf{O}}\mathcal{T} - {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}\ {}^{\mathcal{B}_0}\mathbf{f}^{\text{ext}}\right] \end{aligned} \tag{7.47} $$

Therefore, the component form of ${}_{\mathbf{C}}\vec{\mathcal{T}}$ with respect to $\mathcal{B}_0$ takes the form

$$ \begin{aligned} {}^{\mathcal{B}_0}_{\mathbf{C}}\mathcal{T} &= {}^{\mathcal{B}_0}_{\mathbf{O}}\mathcal{T} - {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}\ \left({}^{\mathcal{B}_0}\mathbf{f}^{\text{ext}}\right) \\ &= {}^{\mathcal{B}_0}_{\mathbf{O}}\mathcal{T} - {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}\ \left(m\ {}^{\mathcal{B}_0}\ddot{\vec{\pi}}(\mathbf{O},\mathbf{C})\right) \end{aligned} \tag{7.48} $$

With the help of Eq. (7.48), the component form of the Euler equation of motion of Ω with respect to the inertial reference frame, $\mathcal{B}_0$, is finally obtained as

$$ {}^{\mathcal{B}_0}_{\mathbf{C}}\mathcal{T} = \left({}^{\mathcal{B}_0}_{\mathbf{C}}\mathfrak{I}\right)\ \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\omega}}\right) + \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\ \left({}^{\mathcal{B}_0}_{\mathbf{C}}\mathfrak{I}\right)\ \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right) \tag{7.49} $$

Euler's Equation of Motion - (2) With respect to $\mathcal{B}_1$: The moment of inertia tensor defined in Eq. (7.27) can be expressed in terms of $\mathcal{B}_1$ as

$$ \begin{aligned} {}^{\mathcal{B}_0}_{\mathbf{C}}\mathfrak{I} &= -\int_\Omega {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\ {}^{\mathcal{B}_0}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})dm \\ &= -\int_\Omega \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\ \left({}^{\mathcal{B}_1}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\right)\ \underbrace{\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T\right)\ \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)}_{\mathbf{I}_3}\ \left({}^{\mathcal{B}_1}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\right)\ \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T\right)dm \\ &= \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\ \underbrace{\left[-\int_\Omega \left({}^{\mathcal{B}_1}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\right)\ \left({}^{\mathcal{B}_1}\widetilde{\boldsymbol{\pi}}(\mathbf{C},\mathbf{P})\right)dm\right]}_{{}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I}}\ \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T\right) \\ &= \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\ \left({}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I}\right)\ \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T\right) \end{aligned} \tag{7.50} $$

where ${}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I}$ is the moment of inertia tensor of Ω about point $\mathbf{C}$ with respect to frame $\mathcal{B}_1$, defined in Eq. (7.25). Notice that the moment of inertia tensor follows the rule given in Eq. (5.41). Similarly, we have

$$ {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}} = \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T\right) \tag{7.51} $$

For ${}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\omega}}$,

$$ \begin{aligned} {}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\omega}} &= \frac{d}{dt}\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right) = \frac{d}{dt}\left(\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right)\right) \\ &= \underbrace{\left({}^{\mathcal{B}_0/\mathcal{B}_1}\dot{\mathbf{A}}\right)}_{\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)}\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right) + \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\omega}}\right) \\ &= \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\underbrace{\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right)}_{\mathbf{0}} + \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\omega}}\right) \\ &= \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\omega}}\right) \end{aligned} \tag{7.52} $$

where we have used Poisson's equations in Theorem 5.3.2.

Hence, the component form of Euler's equation of motion of Ω with respect to $\mathcal{B}_1$ may be readily obtained from Eq. (7.53) as

$$ \begin{aligned} \underbrace{{}^{\mathcal{B}_0}_{\mathbf{C}}\mathcal{T}}_{\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\left({}^{\mathcal{B}_1}_{\mathbf{C}}\mathcal{T}\right)} &= \left({}^{\mathcal{B}_0}_{\mathbf{C}}\mathfrak{I}\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\omega}}\right) + \left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\left({}^{\mathcal{B}_0}_{\mathbf{C}}\mathfrak{I}\right)\left({}^{\mathcal{B}_0}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right) \\ &= \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\left({}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I}\right)\underbrace{\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)}_{\mathbf{I}}\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\omega}}\right) \\ &\quad + \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\underbrace{\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)}_{\mathbf{I}}\left({}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I}\right) \\ &\quad \underbrace{\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)}_{\mathbf{I}}\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right) \\ &= \left({}^{\mathcal{B}_0/\mathcal{B}_1}\mathbf{A}\right)\left[\left({}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\omega}}\right) + \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\left({}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right)\right] \end{aligned} \tag{7.53} $$

Therefore,

$$ {}^{\mathcal{B}_1}_{\mathbf{C}}\mathcal{T} = \left({}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\omega}}\right) + \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\left({}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right) \tag{7.54} $$

This equation is very useful to describe the rotational motion of Ω. ∎

Remark 7.2.1

1. *From a practical point of view, the Newton-Euler equations of motion of Ω in $\mathbb{E}^3$ can be summarized as*

$$\boxed{\begin{aligned} &{}^{\mathcal{B}_0}_{\mathbf{O}}\dot{\mathbf{L}} = m\ {}^{\mathcal{B}_0}\ddot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}) = {}^{\mathcal{B}_0}\mathbf{f}^{\mathrm{ext}} \in \mathbb{R}^3 \\ &{}^{\mathcal{B}_1}_{\mathbf{O}}\dot{\mathbf{J}} = \left({}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\dot{\boldsymbol{\omega}}\right) + \left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right)\left({}^{\mathcal{B}_1}_{\mathbf{C}}\mathfrak{I}\right)\left({}^{\mathcal{B}_1}_{\mathcal{B}_1|\mathcal{B}_0}\boldsymbol{\omega}\right) = {}^{\mathcal{B}_1}_{\mathbf{C}}\mathcal{T} \in \mathbb{R}^3 \end{aligned}} \tag{7.55}$$

7.3 Dynamics of Rigid Bodies

In this section, we first show the derivation of the Newton-Euler system of equations of motion for a system of rigid bodies subject to kinematic constraints from the ***principle of virtual work***. For one rigid body case, this principle naturally leads to the Newton-Euler system of equations discussed in the previous section.

7.3.1 Principle of Virtual Work

Suppose there exists n_{b} numbers of rigid bodies in a system subject to kinematic constraints; then, in view of Eq. (7.34), we can write Newton's equation of motion for a rigid body, Ω_ℓ for $\ell = 1, 2, \cdots, n_{\mathrm{b}}$, as

$${}^{\mathcal{B}_0}\mathfrak{D}_t\ {}_{\mathbf{O}}\vec{\mathbf{L}}_\ell = \vec{\mathbf{f}}^{\mathrm{ext}}_\ell \tag{7.56}$$

where ${}_{\mathbf{O}}\vec{\mathbf{L}}_\ell$ is the linear momentum vector of Ω_ℓ about $\mathbf{O} \in \mathbb{E}^3$ defined as

$${}_{\mathbf{O}}\vec{\mathbf{L}}_\ell := \int_{\Omega_\ell} {}^{\mathcal{B}_0}\mathfrak{D}_t\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}_\ell)dm = m_\ell\ {}^{\mathcal{B}_0}\mathfrak{D}_t\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_\ell) \tag{7.57}$$

in which $m_\ell := \int_{\Omega_\ell} dm$ denotes the mass of Ω_ℓ, and $\mathbf{C}_\ell \in \mathbb{E}^3$ and $\mathbf{P}_\ell \in \mathbb{E}^3$ denote the point of center of mass in Ω_ℓ and an arbitrary point in Ω_ℓ. Because of the constraints imposed to the system, the constraint force applied to Ω_ℓ, $\vec{\mathbf{f}}_\ell^{\mathrm{c}}$, must be taken into account; hence, the external force vector applied to Ω_ℓ, $\vec{\mathbf{f}}_\ell^{\mathrm{ext}}$, may be divided into the applied force vector and the constraint force vector as

$$\vec{\mathbf{f}}_\ell^{\mathrm{ext}} = \vec{\mathbf{f}}_\ell^{\mathrm{appl}} + \vec{\mathbf{f}}_\ell^{\mathrm{c}} \tag{7.58}$$

Theorem 7.3.1 (d'Alembert's Principle for Dynamical Systems)

d'Alembert's Principle states:

$$\boxed{\vec{\mathbf{f}}_\ell^{\mathrm{ext}} + \vec{\mathbf{f}}_\ell^{\mathrm{iner}} = \mathbf{0}} \tag{7.59}$$

for $\ell = 1, 2, \cdots, n_{\mathrm{b}}$ *where* $\vec{\mathbf{f}}_\ell^{\mathrm{iner}}$ *is the inertia force vector of* Ω_ℓ *defined as*

$$\vec{\mathbf{f}}_\ell^{\mathrm{iner}} := -{}^{\mathcal{B}_0}\mathfrak{D}_t\ {}_{\mathbf{O}}\vec{\mathbf{L}}_\ell \tag{7.60}$$

Remark 7.3.1

1. *Mathematically, Eq.* (7.59) *is readily obtained from Newton's equation of motion, Eq.* (7.56). *Eq.* (7.59) *can be written as*

$$\vec{\mathbf{f}}_\ell^{\mathrm{appl}} + \vec{\mathbf{f}}_\ell^{\mathrm{c}} + \left(-\int_{\Omega_\ell} {}^{\mathcal{B}_0}\mathfrak{D}_t^2 \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P}_\ell)dm\right) = \mathbf{0} \tag{7.61}$$

Theorem 7.3.2 (Principle of Virtual Work for Rigid Bodies: First Expression)

Let $\mathcal{B}_0 : (\mathbf{O}; \{{}^{\mathcal{B}_0}\vec{\mathbf{e}}_i\}_{i=1}^3)$ *and* $\mathcal{B}_\ell : (\mathbf{C}_\ell; \{{}^{\mathcal{B}_\ell}\vec{\mathbf{e}}_i\}_{i=1}^3)$ *be the inertial reference frame and the body-fixed frame of* Ω_ℓ *of the centroid,* $\mathbf{C}_\ell$*, respectively.* ***The principle of virtual work states: The sum of the virtual work due to every force applied to a system in any arbitrary virtual displacement is zero****; which leads to the first expression of the principle of virtual work for a system of rigid bodies,* Ω_ℓ *(for* $\ell = 1, 2, \cdots, n_{\mathrm{b}}$*):*

$$\boxed{\begin{aligned} 0 = &\left[\vec{\mathbf{f}}_1^{\mathrm{appl}} - {}^{\mathcal{B}_0}\mathfrak{D}_t\ {}_{\mathbf{O}}\vec{\mathbf{L}}_1\right]\cdot\delta\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_1) + \cdots + \left[\vec{\mathbf{f}}_{n_{\mathrm{b}}}^{\mathrm{appl}} - {}^{\mathcal{B}_0}\mathfrak{D}_t\ {}_{\mathbf{O}}\vec{\mathbf{L}}_{n_{\mathrm{b}}}\right]\cdot\delta\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_{n_{\mathrm{b}}}) \\ &+ \left[{}_{\mathbf{C}_1}\vec{\mathcal{T}}_1^{\mathrm{appl}} - {}^{\mathcal{B}_0}\mathfrak{D}_t\ {}_{\mathbf{C}_1}\vec{\mathbf{J}}_1\right]\cdot\left({}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\varpi}}\right) + \cdots + \left[{}_{\mathbf{C}_{n_{\mathrm{b}}}}\vec{\mathcal{T}}_{n_{\mathrm{b}}}^{\mathrm{appl}} - {}^{\mathcal{B}_0}\mathfrak{D}_t\ {}_{\mathbf{C}_{n_{\mathrm{b}}}}\vec{\mathbf{J}}_{n_{\mathrm{b}}}\right]\cdot\left({}_{\mathcal{B}_{n_{\mathrm{b}}}|\mathcal{B}_0}\vec{\boldsymbol{\varpi}}\right)\end{aligned}} \tag{7.62}$$

where ${}_{\mathbf{C}_\ell}\vec{\mathcal{T}}_\ell^{\text{appl}}$ denotes the torque (or moment) vector applied to body Ω_ℓ about point $\mathbf{C}_\ell$ due to the applied force, $\vec{\mathbf{f}}_\ell^{\text{appl}}$.

Proof. Multiplying Eq. (7.59) by the variation of vector $\vec{\pi}(\mathbf{O}, \mathbf{P}_\ell)$, we obtain

$$\sum_{\ell=1}^{n_b} \vec{\mathbf{f}}_\ell^{\text{ext}} \cdot \delta\vec{\mathbf{r}}_\ell + \left(- \sum_{\ell=1}^{n_b} \int_{\Omega_\ell} \vec{\mathbf{a}}_\ell^{\mathbf{p}} \cdot \delta\vec{\mathbf{r}}_\ell dm \right) = 0 \tag{7.63}$$

where we defined $\vec{\mathbf{a}}_\ell^{\mathbf{p}} := {}^{\mathcal{B}_0}\mathfrak{D}_t^2 \vec{\pi}(\mathbf{O}, \mathbf{P}_\ell)$ and $\delta\vec{\mathbf{r}}_\ell := \delta\vec{\pi}(\mathbf{O}, \mathbf{P}_\ell)$ for the sake of simplicity. Eq. (7.63) readily yields

$$\sum_{\ell=1}^{n_b} \vec{\mathbf{f}}_\ell^{\text{appl}} \cdot \delta\vec{\mathbf{r}}_\ell + \sum_{\ell=1}^{n_b} \vec{\mathbf{f}}_\ell^{\text{c}} \cdot \delta\vec{\mathbf{r}}_\ell + \left(- \sum_{\ell=1}^{n_b} \int_{\Omega_\ell} \vec{\mathbf{a}}_\ell^{\mathbf{p}} \cdot \delta\vec{\mathbf{r}}_\ell dm \right) = 0 \tag{7.64}$$

where $\vec{\mathbf{f}}_\ell^{\text{appl}} = \int_{\Omega_\ell} d\vec{\mathbf{f}}_\ell^{\text{appl}}$. Defining the virtual work functions due to the applied force, constraint force, and inertia force as

$$\delta W^{\text{appl}} := \sum_{\ell=1}^{n_b} \int_{\Omega_\ell} d\vec{\mathbf{f}}_\ell^{\text{appl}} \cdot \delta\vec{\mathbf{r}}_\ell \equiv \int_{\Omega_\ell} d\vec{\mathbf{f}}_\ell^{\text{appl}} \cdot \delta\vec{\mathbf{r}}_\ell \tag{7.65}$$

$$\delta W^{\text{c}} := \sum_{\ell=1}^{n_b} \vec{\mathbf{f}}_\ell^{\text{c}} \cdot \delta\vec{\mathbf{r}}_\ell \equiv \vec{\mathbf{f}}_\ell^{\text{c}} \cdot \delta\vec{\mathbf{r}}_\ell \tag{7.66}$$

$$\delta W^{\text{iner}} := -\sum_{\ell=1}^{n_b} \int_{\Omega_\ell} \vec{\mathbf{a}}_\ell^{\mathbf{p}} \cdot \delta\vec{\mathbf{r}}_\ell dm \equiv -\int_{\Omega_\ell} \vec{\mathbf{a}}_\ell^{\mathbf{p}} \cdot \delta\vec{\mathbf{r}}_\ell dm \tag{7.67}$$

Eq. (7.64) can be written as

$$\delta W^{\text{appl}} + \delta W^{\text{c}} + \delta W^{\text{iner}} = 0 \tag{7.68}$$

It is immensely important to notice that the virtual work due to the constraint force is zero, i.e., $\delta W^{\text{c}} = 0$; see Theorem 6.2.1. Therefore,

$$\delta W^{\text{appl}} + \delta W^{\text{iner}} = 0 \tag{7.69}$$

Similar to δW^{c} as discussed in Remark 6.2.1-(2), state functions, W^{appl} and W^{iner} do not exist in general.

Since point $\mathbf{P}_\ell$ is fixed in Ω_ℓ for $\ell = 1, 2, \cdots, n_\mathrm{b}$, $\delta\vec{\mathbf{r}}_\ell$ may be written, in view of Eq. (5.178) in Theorem 5.5.1, as

$$\delta\vec{\mathbf{r}}_\ell := \delta\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P}_\ell) = \delta\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_\ell) + ({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\boldsymbol{\varpi}}) \times \vec{\boldsymbol{\pi}}(\mathbf{C}_\ell, \mathbf{P}_\ell) \tag{7.70}$$

where ${}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\boldsymbol{\varpi}}$ is the virtual rotation vector of frame $\mathcal{B}_\ell$ with respect to the inertial reference frame, $\mathcal{B}_0$. Frame $\mathcal{B}_\ell : (\mathbf{C}_\ell; \{{}^{\mathcal{B}_\ell}\vec{\mathbf{e}}_i\}_{i=1}^3)$ is the body-fixed frame of Ω_ℓ.

Substituting Eq. (7.70) into Eq. (7.67), the virtual work due to the applied force yields:

$$\begin{aligned}
\delta W^{\mathrm{appl}} &= \vec{\mathbf{f}}_\ell^{\mathrm{appl}} \cdot \delta\vec{\mathbf{r}}_\ell = \vec{\mathbf{f}}_\ell^{\mathrm{appl}} \cdot [\delta\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_\ell) + ({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\boldsymbol{\varpi}}) \times \vec{\boldsymbol{\pi}}(\mathbf{C}_\ell, \mathbf{P}_\ell)] \\
&= \underbrace{\int_{\Omega_1} d\vec{\mathbf{f}}_1^{\mathrm{appl}} \cdot \delta\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_1) + \cdots + \int_{\Omega_{n_\mathrm{b}}} d\vec{\mathbf{f}}_{n_\mathrm{b}}^{\mathrm{appl}} \cdot \delta\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_{n_\mathrm{b}})}_{=: \sum_{\ell=1}^{\prime n_\mathrm{b}} \int_{\Omega_\ell} d\vec{\mathbf{f}}_\ell^{\mathrm{appl}} \cdot \delta\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_\ell)} \\
&\quad + \underbrace{\int_{\Omega_1} d\vec{\mathbf{f}}_1^{\mathrm{appl}} \cdot ({}_{\mathcal{B}_1|\mathcal{B}_0}\vec{\boldsymbol{\varpi}}) \times \vec{\boldsymbol{\pi}}(\mathbf{C}_1, \mathbf{P}_1) + \cdots + \int_{\Omega_{n_\mathrm{b}}} d\vec{\mathbf{f}}_{n_\mathrm{b}}^{\mathrm{appl}} \cdot \left({}_{\mathcal{B}_{n_\mathrm{b}}|\mathcal{B}_0}\vec{\boldsymbol{\varpi}}\right) \times \vec{\boldsymbol{\pi}}(\mathbf{C}_{n_\mathrm{b}}, \mathbf{P}_{n_\mathrm{b}})}_{=: \sum_{\ell=1}^{\prime n_\mathrm{b}} \int_{\Omega_\ell} d\vec{\mathbf{f}}_\ell^{\mathrm{appl}} \cdot ({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\boldsymbol{\varpi}}) \times \vec{\boldsymbol{\pi}}(\mathbf{C}_\ell, \mathbf{P}_\ell)} \\
&= \sum_{\ell=1}^{n_\mathrm{b}}{}' \int_{\Omega_\ell} d\vec{\mathbf{f}}_\ell^{\mathrm{appl}} \cdot \delta\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_\ell) + \sum_{\ell=1}^{n_\mathrm{b}}{}' \int_{\Omega_\ell} d\vec{\mathbf{f}}_\ell^{\mathrm{appl}} \cdot ({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\boldsymbol{\varpi}}) \times \vec{\boldsymbol{\pi}}(\mathbf{C}_\ell, \mathbf{P}_\ell) \\
&= \sum_{\ell=1}^{n_\mathrm{b}}{}' \vec{\mathbf{f}}_\ell^{\mathrm{appl}} \cdot \delta\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_\ell) + \sum_{\ell=1}^{n_\mathrm{b}}{}' \underbrace{\int_{\Omega_\ell} \vec{\boldsymbol{\pi}}(\mathbf{C}_\ell, \mathbf{P}_\ell) \times d\vec{\mathbf{f}}_\ell^{\mathrm{appl}}}_{{}_{\mathbf{C}_\ell}\vec{\mathcal{T}}_\ell^{\mathrm{appl}}} \cdot ({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\boldsymbol{\varpi}})
\end{aligned} \tag{7.71}$$

where ${}_{\mathbf{C}}\vec{\mathcal{T}}_\ell$ denotes the applied torque (or moment) vector of Ω_ℓ in terms of point $\mathbf{C}_\ell$.

Invoking Eq. (5.160) in Theorem 5.4.1, i.e., the acceleration vector, $\vec{\mathbf{a}}_\ell^{\mathbf{p}} := {}^{\mathcal{B}_0}\mathfrak{D}_t^2\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P}_\ell)$, can be written as

$$\begin{aligned}
\vec{\mathbf{a}}_\ell^{\mathbf{p}} := {}^{\mathcal{B}_0}\mathfrak{D}_t^2\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P}_\ell) = {}^{\mathcal{B}_0}\mathfrak{D}_t^2\, \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_\ell) + {}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\alpha} \times \vec{\boldsymbol{\pi}}(\mathbf{C}_\ell, \mathbf{P}_\ell) \\
+ {}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\omega} \times [{}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\omega} \times \vec{\boldsymbol{\pi}}(\mathbf{C}_\ell, \mathbf{P}_\ell)]
\end{aligned} \tag{7.72}$$

the virtual work due to the applied force yields:

$$
\begin{aligned}
\delta W^{\text{iner}} &= -\sum_{\ell=1}^{n_\mathrm{b}} \int_{\Omega_\ell} \vec{\mathbf{a}}_\ell^{\mathbf{p}} \cdot \delta\vec{\mathbf{r}}_\ell dm \\
&= \left(-\int_{\Omega_1} {}^{\mathcal{B}_0}\mathfrak{D}_t^2 \vec{\pi}(\mathbf{O},\mathbf{P}_1)\cdot\delta\vec{\pi}(\mathbf{O},\mathbf{P}_1)dm\right) + \cdots + \left(-\int_{\Omega_{n_\mathrm{b}}} {}^{\mathcal{B}_0}\mathfrak{D}_t^2 \vec{\pi}(\mathbf{O},\mathbf{P}_{n_\mathrm{b}})\cdot\delta\vec{\pi}(\mathbf{O},\mathbf{P}_{n_\mathrm{b}})dm\right) \\
&=: -\sum_{\ell=1}^{n_\mathrm{b}}{}' \int_{\Omega_\ell} \underbrace{{}^{\mathcal{B}_0}\mathfrak{D}_t^2 \vec{\pi}(\mathbf{O},\mathbf{P}_\ell)}_{\text{Eq. (7.72)}} \cdot \delta\vec{\pi}(\mathbf{O},\mathbf{P}_\ell)dm \\
&= -\underbrace{\sum_{\ell=1}^{n_\mathrm{b}}{}' \int_{\Omega_\ell} {}^{\mathcal{B}_0}\mathfrak{D}_t^2\, \vec{\pi}(\mathbf{O},\mathbf{C}_\ell)\cdot\delta\vec{\pi}(\mathbf{O},\mathbf{P}_\ell)dm}_{\text{Term 1}} \\
&\quad -\underbrace{\sum_{\ell=1}^{n_\mathrm{b}}{}' \int_{\Omega_\ell} {}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\alpha}\times\vec{\pi}(\mathbf{C}_\ell,\mathbf{P}_\ell)\cdot\delta\vec{\pi}(\mathbf{O},\mathbf{P}_\ell)dm}_{\text{Term 2}} \\
&\quad -\underbrace{\sum_{\ell=1}^{n_\mathrm{b}}{}' \int_{\Omega_\ell} {}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\omega}\times\left[{}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\omega}\times\vec{\pi}(\mathbf{C}_\ell,\mathbf{P}_\ell)\right]\cdot\delta\vec{\pi}(\mathbf{O},\mathbf{P}_\ell)dm}_{\text{Term 3}}
\end{aligned}
\tag{7.73}
$$

where terms 1,2, and 3 in Eq. (7.77) are given as

$$
\begin{aligned}
\text{Term 1} &= \sum_{\ell=1}^{n_\mathrm{b}}{}' \int_{\Omega_\ell} dm\ {}^{\mathcal{B}_0}\mathfrak{D}_t^2\, \vec{\pi}(\mathbf{O},\mathbf{C}_\ell)\cdot\delta\vec{\pi}(\mathbf{O},\mathbf{C}_\ell) \\
&\quad + \sum_{\ell=1}^{n_\mathrm{b}}{}' \int_{\Omega_\ell} {}^{\mathcal{B}_0}\mathfrak{D}_t^2\, \vec{\pi}(\mathbf{O},\mathbf{C}_\ell)\cdot\left({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\varpi}\right)\times\vec{\pi}(\mathbf{C}_\ell,\mathbf{P}_\ell) \\
&= \sum_{\ell=1}^{n_\mathrm{b}}{}' m_\ell\ {}^{\mathcal{B}_0}\mathfrak{D}_t^2\, \vec{\pi}(\mathbf{O},\mathbf{C}_\ell)\cdot\delta\vec{\pi}(\mathbf{O},\mathbf{C}_\ell) \\
&\quad + \sum_{\ell=1}^{n_\mathrm{b}}{}' \underbrace{\int_{\Omega_\ell} \vec{\pi}(\mathbf{C}_\ell,\mathbf{P}_\ell)dm}_{\mathbf{0}} \times {}^{\mathcal{B}_0}\mathfrak{D}_t^2\, \vec{\pi}(\mathbf{O},\mathbf{C}_\ell)\cdot\left({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\varpi}\right) \\
&= \sum_{\ell=1}^{n_\mathrm{b}}{}' m_\ell\ {}^{\mathcal{B}_0}\mathfrak{D}_t^2\, \vec{\pi}(\mathbf{O},\mathbf{C}_\ell)\cdot\delta\vec{\pi}(\mathbf{O},\mathbf{C}_\ell)
\end{aligned}
\tag{7.74}
$$

$$
\begin{aligned}
\text{Term 2} &= \sum_{\ell=1}^{n_\text{b}}{}' \, {}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\alpha} \times \underbrace{\int_{\Omega_\ell} \vec{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell) dm}_{\mathbf{0}} \cdot \delta\vec{\pi}(\mathbf{O}, \mathbf{C}_\ell) \\
&\quad + \sum_{\ell=1}^{n_\text{b}}{}' \int_{\Omega_\ell} [{}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\alpha} \times \vec{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell)] \cdot [({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\varpi}) \times \vec{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell)] dm \\
&= \sum_{\ell=1}^{n_\text{b}}{}' \int_{\Omega_\ell} \vec{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell) \times [({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\alpha}) \times \vec{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell)] \, dm \cdot ({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\varpi})
\end{aligned}
\tag{7.75}
$$

$$
\begin{aligned}
\text{Term 3} &= \sum_{\ell=1}^{n_\text{b}}{}' \, {}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\omega} \times [{}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\omega} \times \underbrace{\int_{\Omega_\ell} \vec{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell) dm}_{\mathbf{0}}] \cdot \delta\vec{\pi}(\mathbf{O}, \mathbf{C}_\ell) \\
&\quad + \sum_{\ell=1}^{n_\text{b}}{}' \int_{\Omega_\ell} {}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\omega} \times [{}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\omega} \times \vec{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell)] \cdot [({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\varpi}) \times \vec{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell)] \, dm \\
&= \sum_{\ell=1}^{n_\text{b}}{}' \int_{\Omega_\ell} \vec{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell) \times [{}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\omega} \times [{}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\omega} \times \vec{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell)]] \, dm \cdot ({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\varpi})
\end{aligned}
\tag{7.76}
$$

respectively. Substituting Eq. (7.74)-Eq. (7.76) into Eq. (7.77), we finally obtain

$$
\delta W^{\text{iner}} = -\sum_{\ell=1}^{n_\text{b}}{}' \left({}^{\mathcal{B}_0}\mathfrak{D}_t \; {}_{\mathbf{O}}\vec{\mathbf{L}}_\ell\right) \cdot \delta\vec{\pi}(\mathbf{O}, \mathbf{C}_\ell) - \sum_{\ell=1}^{n_\text{b}}{}' \int_{\Omega_\ell} \left({}^{\mathcal{B}_0}\mathfrak{D}_t \; {}_{\mathbf{C}_\ell}\vec{\mathbf{J}}_\ell\right) dm \cdot ({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\varpi}) \tag{7.77}
$$

where the time derivative of the linear momentum vector (see Eq. (7.10) in Theorem 7.2.1) of Ω_ℓ in terms of $\mathcal{B}_0$ is given as

$$
{}^{\mathcal{B}_0}\mathfrak{D}_t \; {}_{\mathbf{O}}\vec{\mathbf{L}}_\ell = m_\ell \; {}^{\mathcal{B}_0}\mathfrak{D}_t^2 \vec{\pi}(\mathbf{O}, \mathbf{C}_\ell) \tag{7.78}
$$

and, invoking Eq. (7.20) in Theorem 7.2.4, the time derivative of the angular momentum vector of Ω_ℓ about point $\mathbf{C}_\ell$ is given as

$$
\begin{aligned}
{}^{\mathcal{B}_0}\mathfrak{D}_t \; {}_{\mathbf{C}_\ell}\vec{\mathbf{J}}_\ell =& \vec{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell) \times [({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\alpha}) \times \vec{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell)] \\
&+ \vec{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell) \times [{}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\omega} \times [{}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\omega} \times \vec{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell)]]
\end{aligned}
\tag{7.79}
$$

Substituting Eq. (7.71) and Eq. (7.77) into Eq. (7.80) yields

$$\begin{aligned} 0 &= \delta W^{\text{appl}} + \delta W^{\text{iner}} \\ &= \sum_{\ell=1}^{n_b}{}' \left[\vec{\mathbf{f}}_\ell^{\text{appl}} - {}^{\mathcal{B}_0}\mathfrak{D}_t \; {}_{\mathbf{O}}\vec{\mathbf{L}}_\ell \right] \cdot \delta\vec{\pi}(\mathbf{O}, \mathbf{C}_\ell) + \sum_{\ell=1}^{n_b}{}' \left[{}_{\mathbf{C}_\ell}\vec{\mathcal{T}}_\ell^{\text{appl}} - {}^{\mathcal{B}_0}\mathfrak{D}_t \; {}_{\mathbf{C}_\ell}\vec{\mathbf{J}}_\ell \right] \cdot \left({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\varpi} \right) \end{aligned} \tag{7.80}$$

Hence, Eq. (7.62) has been proven. ∎

Theorem 7.3.3 (Principle of Virtual Work for Rigid Bodies: Second Expression) *The second expression of the principle of virtual work reads:*

$$\boxed{\int_{t_0}^{t_L} \delta\mathscr{K}\, dt + \int_{t_0}^{t_L} \delta W^{\text{appl}} dt = 0} \tag{7.81}$$

with the conditions that the variation of $\vec{\mathbf{r}}_\ell^*(t)$ *and the virtual rotation,* ${}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\varpi}$*, vanish at all points of* Ω_ℓ *at* $t = t_0$ *and* $t = t_L$*:*

$$\delta\vec{\mathbf{r}}_\ell^*(t_0) = \delta\vec{\mathbf{r}}_\ell^*(t_L) = \mathbf{0} \tag{7.82}$$

$$\delta_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\varpi}(t_0) = \delta_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\varpi}(t_L) = \mathbf{0} \tag{7.83}$$

where $\delta\mathscr{K}$ *is the first variation of kinetic energy function of a system of rigid bodies; see Theorem 7.3.5.*

Proof. Let $\vec{\mathbf{r}}_\ell^*(t) = \vec{\pi}(\mathbf{O}, \mathbf{C}_\ell)$. Integrating Eq. (7.80) in time from time $t = t_0$ to $t = t_L$ yields

$$\begin{aligned} 0 = &\int_{t_0}^{t_L} \sum_{\ell=1}^{n_b} \left[\vec{\mathbf{f}}_\ell^{\text{appl}} - {}^{\mathcal{B}_0}\mathfrak{D}_t \; {}_{\mathbf{O}}\vec{\mathbf{L}}_\ell \right] \cdot \delta\vec{\mathbf{r}}_\ell^* dt \\ &+ \int_{t_0}^{t_L} \sum_{\ell=1}^{n_b} \left[{}_{\mathbf{C}_\ell}\vec{\mathcal{T}}_\ell^{\text{appl}} - {}^{\mathcal{B}_0}\mathfrak{D}_t \; {}_{\mathbf{C}_\ell}\vec{\mathbf{J}}_\ell \right] \cdot \left({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\varpi} \right) dt \end{aligned} \tag{7.84}$$

By integration by parts, we have

$$\begin{aligned}
-\int_{t_0}^{t_L}\sum_{\ell=1}^{n_b} {}^{\mathcal{B}_0}\mathfrak{D}_t\, {}_{\mathbf{O}}\vec{\mathbf{L}}_\ell \cdot \delta\vec{\mathbf{r}}^*_\ell dt &= -\int_{t_0}^{t_L}\sum_{\ell=1}^{n_b} m_\ell\, {}^{\mathcal{B}_0}\mathfrak{D}_t^2 \vec{\mathbf{r}}^*_\ell \cdot \delta\vec{\mathbf{r}}^*_\ell dt \\
&= \underbrace{-\sum_{\ell=1}^{n_b}\left[m_\ell\, {}^{\mathcal{B}_0}\mathfrak{D}_t\, \vec{\mathbf{r}}^*_\ell \cdot \delta\vec{\mathbf{r}}^*_\ell\right]_{t_0}^{t_L}}_{\mathbf{0}\ \because\ \text{Eq. (7.82)}} + \int_{t_0}^{t_L}\sum_{\ell=1}^{n_b} m_\ell\, {}^{\mathcal{B}_0}\mathfrak{D}_t\, \vec{\mathbf{r}}^*_\ell \cdot {}^{\mathcal{B}_0}\mathfrak{D}_t\, \delta\vec{\mathbf{r}}^*_\ell dt \\
&= \int_{t_0}^{t_L}\sum_{\ell=1}^{n_b}{}' \left(\delta\, {}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_\ell)\right)^T \left[m_\ell\, {}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_\ell)\right] dt \qquad (7.85)
\end{aligned}$$

and

$$\begin{aligned}
&-\int_{t_0}^{t_L}\sum_{\ell=1}^{n_b}\left({}^{\mathcal{B}_0}\mathfrak{D}_t\ {}_{\mathbf{C}_\ell}\vec{\mathbf{J}}_\ell\right)\cdot\left({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\boldsymbol{\varpi}}\right) dt \\
&= \underbrace{-\sum_{\ell=1}^{n_b}\left[\left({}_{\mathbf{C}_\ell}\vec{\mathbf{J}}_\ell\right)\cdot\left({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\boldsymbol{\varpi}}\right)\right]_{t_0}^{t_L}}_{\mathbf{0}\ \because\ \text{Eq. (7.83)}} + \int_{t_0}^{t_L}\sum_{\ell=1}^{n_b}\left({}_{\mathbf{C}_\ell}\vec{\mathbf{J}}_\ell\right)\cdot\left({}^{\mathcal{B}_0}\mathfrak{D}_t\ {}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\boldsymbol{\varpi}}\right) dt \\
&= \sum_{\ell=1}^{n_b}\left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\boldsymbol{\varpi}\right)^T \left[\left({}^{\mathcal{B}_\ell}_{\mathbf{C}_\ell}\mathfrak{I}\right)\left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\boldsymbol{\omega}\right)\right] \qquad (7.86)
\end{aligned}$$

Hence, Eq. (7.84) can be written as

$$\int_{t_0}^{t_L}\delta\mathscr{K}\, dt + \int_{t_0}^{t_L}\underbrace{\sum_{\ell=1}^{n_b}\left[\vec{\mathbf{f}}^{\text{appl}}_\ell\cdot\delta\vec{\mathbf{r}}^*_\ell + {}_{\mathbf{C}_\ell}\vec{\mathcal{T}}^{\text{appl}}_\ell\cdot\left({}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\boldsymbol{\varpi}}\right)\right]}_{\delta W^{\text{appl}}} dt = 0 \qquad (7.87)$$

where $\delta\mathscr{K}$ denotes the first variation of the kinetic energy of the system of n_b rigid bodies as given in Eq. (7.100) in Theorem 7.3.5. ∎

Kinetic Energy and Potential Energy functions of a System of Rigid Bodies

Definition 7.3.1 (Kinetic Energy Function of a System of Rigid Bodies)

The kinetic energy of a system of rigid bodies, $\mathscr{K}$, is defined as the summation of the kinetic energy functions of all bodies in the system, $\mathscr{K}_\ell$ for $\ell = 1, 2, \cdots, n_\text{b}$:

$$\boxed{\mathscr{K} := \sum_{\ell=1}^{n_b}\mathscr{K}_\ell \quad \text{where} \quad \mathscr{K}_\ell := \frac{1}{2}\int_{\Omega_\ell}\left[{}^{\mathcal{B}_0}\mathfrak{D}_t\, \vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}_\ell)\right]\cdot\left[{}^{\mathcal{B}_0}\mathfrak{D}_t\, \vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}_\ell)\right] dm} \qquad (7.88)$$

where $\mathbf{P}$ *denotes an arbitrary point in body* ω_ℓ*.*

Theorem 7.3.4

(Kinetic Energy of a System of Rigid Bodies: Translation and Rotation Kinetic Energy Functions)

The kinetic energy function of body Ω_ℓ*, i.e.,* $\mathscr{K}_\ell$*, can be written as*

$$\boxed{\begin{aligned}\mathscr{K}_\ell =& \frac{1}{2} m_\ell \left({}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_\ell)\right)^T \left({}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_\ell)\right) \\ &+ \frac{1}{2}\left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\boldsymbol{\omega}\right)^T \left({}^{\mathcal{B}_\ell}_{\mathbf{C}_\ell}\mathfrak{I}\right)\left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\boldsymbol{\omega}\right)\end{aligned}} \tag{7.89}$$

where $m_\ell = \int_{\Omega_\ell} dm = \int_{\Omega_\ell} \rho_\ell dV$*, with the density function* ρ_ℓ*, denotes the mass of* Ω_ℓ*, and* ${}^{\mathcal{B}_\ell}_{\mathbf{C}_\ell}\mathfrak{I}$ *denotes the moment of inertia tensor of* Ω_ℓ *about point* $\mathbf{C}_\ell$ *with respect to frame* $\mathcal{B}_\ell$*, as similarly defined in Eq. (7.25), i.e.,*

$${}^{\mathcal{B}_\ell}_{\mathbf{C}_\ell}\mathfrak{I} := \int_{\Omega_\ell} {}^{\mathcal{B}_\ell}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_\ell,\mathbf{P}_\ell)^T \, {}^{\mathcal{B}_\ell}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_\ell,\mathbf{P}_\ell) dm \tag{7.90}$$

Proof. Substituting

$${}^{\mathcal{B}_0}\mathfrak{D}_t\, \vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}_\ell) = {}^{\mathcal{B}_0}\mathfrak{D}_t\, \vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_\ell) + {}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\boldsymbol{\omega}} \times \vec{\boldsymbol{\pi}}(\mathbf{C}_\ell,\mathbf{P}_\ell) \tag{7.91}$$

(see Eq. (5.144) in Theorem 5.3.3) into the definition of $\mathscr{K}_\ell$ in Eq. (7.88), we get

$$\begin{aligned}\mathscr{K}_\ell =& \underbrace{\frac{1}{2}\int_{\Omega_\ell}\left[{}^{\mathcal{B}_0}\mathfrak{D}_t\, \vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_\ell)\right]\cdot\left[{}^{\mathcal{B}_0}\mathfrak{D}_t\, \vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_\ell)\right] dm}_{\mathscr{K}_\ell^{(1)}} \\ &+ \underbrace{\frac{1}{2}\int_{\Omega_\ell}\left[{}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\boldsymbol{\omega}} \times \vec{\boldsymbol{\pi}}(\mathbf{C}_\ell,\mathbf{P}_\ell)\right]\cdot\left[{}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\boldsymbol{\omega}} \times \vec{\boldsymbol{\pi}}(\mathbf{C}_\ell,\mathbf{P}_\ell)\right] dm}_{\mathscr{K}_\ell^{(2)}} \\ &+ \underbrace{\int_{\Omega_\ell} {}^{\mathcal{B}_0}\mathfrak{D}_t\, \vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_\ell)\cdot {}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\boldsymbol{\omega}} \times \vec{\boldsymbol{\pi}}(\mathbf{C}_\ell,\mathbf{P}_\ell) dm}_{\mathscr{K}_\ell^{(3)}}\end{aligned} \tag{7.92}$$

where $\mathscr{K}_\ell^{(1)}$, $\mathscr{K}_\ell^{(2)}$, and $\mathscr{K}_\ell^{(3)}$ are the ***translation kinetic energy function*** of rigid body Ω_ℓ, the ***rotation kinetic energy function*** of rigid body Ω_ℓ, and the ***translation-rotation coupling kinetic energy function*** of rigid body Ω_ℓ, respectively.

$\mathscr{K}_\ell^{(1)}$ can be readily written as

$$\begin{aligned}\mathscr{K}_\ell^{(1)} &= \frac{1}{2}\int_{\Omega_\ell} {}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_\ell)^T \underbrace{({}^{\mathcal{B}_0}\mathbf{e}\cdot{}^{\mathcal{B}_0}\mathbf{e}^T)}_{\mathbf{0}} {}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_\ell)dm \\ &= \underbrace{\frac{1}{2}\int_{\Omega_\ell} dm}_{m_\ell}\left[{}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_\ell)\right]^T\left[{}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_\ell)\right]\end{aligned} \tag{7.93}$$

where m_ℓ denotes the mass of Ω_ℓ.

Substituting

$$_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\boldsymbol{\omega}}\times\vec{\boldsymbol{\pi}}(\mathbf{C}_\ell,\mathbf{P}_\ell) = {}^{\mathcal{B}_\ell}\mathbf{e}^T\left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right){}^{\mathcal{B}_\ell}\boldsymbol{\pi}(\mathbf{C}_\ell,\mathbf{P}_\ell) \tag{7.94}$$

into the expression of the rotation kinetic energy, $\mathscr{K}_\ell^{(2)}$, in Eq. (7.92), we get

$$\mathscr{K}_\ell^{(2)} = \frac{1}{2}\int_{\Omega_\ell}\left[\left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right){}^{\mathcal{B}_\ell}\boldsymbol{\pi}(\mathbf{C}_\ell,\mathbf{P}_\ell)\right]^T \underbrace{{}^{\mathcal{B}_\ell}\mathbf{e}\cdot{}^{\mathcal{B}_\ell}\mathbf{e}^T}_{\mathbf{I}}\left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right){}^{\mathcal{B}_\ell}\boldsymbol{\pi}(\mathbf{C}_\ell,\mathbf{P}_\ell) \tag{7.95}$$

Since

$$\left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\widetilde{\boldsymbol{\omega}}\right){}^{\mathcal{B}_\ell}\boldsymbol{\pi}(\mathbf{C}_\ell,\mathbf{P}_\ell) = -{}^{\mathcal{B}_\ell}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_\ell,\mathbf{P}_\ell)\left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\boldsymbol{\omega}\right) \tag{7.96}$$

Eq. (7.95) becomes

$$\mathscr{K}_\ell^{(2)} = \frac{1}{2}\left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\boldsymbol{\omega}\right)^T\left({}^{\mathcal{B}_\ell}_{\mathbf{C}_\ell}\mathfrak{I}\right)\left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\boldsymbol{\omega}\right) \tag{7.97}$$

where ${}^{\mathcal{B}_\ell}_{\mathbf{C}_\ell}\mathfrak{I}$ is the moment of inertia tensor of Ω_ℓ about point $\mathbf{C}_\ell$ with respect to frame $\mathcal{B}_\ell$, as defined in Eq. (7.90).

$\mathscr{K}_\ell^{(3)}$ vanishes as can be seen from

$$\begin{aligned}
\mathscr{K}_\ell^{(3)} &= \int_{\Omega_\ell} [{}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_\ell)^T\ {}^{\mathcal{B}_0}\mathbf{e}] \cdot [\underbrace{{}_{\mathcal{B}_\ell|\mathcal{B}_0}\vec{\boldsymbol{\omega}} \times {}^{\mathcal{B}_\ell}\mathbf{e}^T}_{{}^{\mathcal{B}_\ell}\mathbf{e}^T\ {}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\widetilde{\omega}}\ {}^{\mathcal{B}_\ell}\boldsymbol{\pi}(\mathbf{C}_\ell,\mathbf{P}_\ell)]dm \\
&= {}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_\ell)^T\ \underbrace{{}^{\mathcal{B}_0}\mathbf{e}\cdot{}^{\mathcal{B}_\ell}\mathbf{e}^T}_{{}^{\mathcal{B}_0/\mathcal{B}_\ell}\mathbf{A}} \left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\widetilde{\omega}\right) \underbrace{\int_{\Omega_\ell} {}^{\mathcal{B}_\ell}\boldsymbol{\pi}(\mathbf{C}_\ell,\mathbf{P}_\ell)dm}_{\mathbf{0}} \\
&= 0
\end{aligned} \tag{7.98}$$

From Eq. (7.93), Eq. (7.97), and Eq. (7.98), the kinetic energy function for Ω_ℓ is obtained as given in Eq. (7.89). ∎

Theorem 7.3.5 (First Variation of the Kinetic Energy Function of Rigid Bodies)

The first variation of the kinetic energy of a system of n_b rigid bodies is given by

$$\boxed{\delta\mathscr{K} = \sum_{\ell=1}^{n_\text{b}} \delta\mathscr{K}_\ell = \sum_{\ell=1}^{n_\text{b}}{}' \int_{\Omega_\ell} \left[{}^{\mathcal{B}_0}\mathfrak{D}_t\ \vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}_\ell)\right] \cdot \left[{}^{\mathcal{B}_0}\mathfrak{D}_t\ \delta\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}_\ell)\right] dm} \tag{7.99}$$

Or equivalently,

$$\boxed{\begin{aligned}
\delta\mathscr{K} &= \sum_{\ell=1}^{n_\text{b}} \delta\mathscr{K}_\ell \\
&= \sum_{\ell=1}^{n_\text{b}}{}' \left(\delta\,{}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_\ell)\right)^T \left[m_\ell\ {}^{\mathcal{B}_0}\dot{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_\ell)\right] \\
&\quad + \sum_{\ell=1}^{n_\text{b}}{}' \left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\boldsymbol{\varpi}\right)^T \left[\left({}^{\mathcal{B}_\ell}_{\mathbf{C}_\ell}\mathfrak{I}\right)\left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\boldsymbol{\omega}\right)\right]
\end{aligned}} \tag{7.100}$$

Proof. Taking the variation of $\mathscr{K}_\ell$ in Eq. (7.88) directly, we get

$$\begin{aligned}
\delta\mathscr{K}_\ell &= \sum_{\ell=1}^{n_\text{b}} \int_{\Omega_\ell} \left[{}^{\mathcal{B}_0}\mathfrak{D}_t\ \vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}_\ell)\right] \cdot \delta\left[{}^{\mathcal{B}_0}\mathfrak{D}_t\ \vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}_\ell)\right] dm \\
&= \sum_{\ell=1}^{n_\text{b}} \int_{\Omega_\ell} \left[{}^{\mathcal{B}_0}\mathfrak{D}_t\ \vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}_\ell)\right] \cdot \left[{}^{\mathcal{B}_0}\mathfrak{D}_t\ \delta\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{P}_\ell)\right] dm
\end{aligned} \tag{7.101}$$

Note that δ and ${}^{\mathcal{B}_0}\mathfrak{D}_t$ commute. Similarly, Eq. (7.100) can be derived by taking the variation of $\mathscr{K}_\ell$ in Eq. (7.89). ∎

Definition 7.3.2 (Potential Energy Function of a System of Rigid Bodies)

*Suppose n_{b} numbers of **rigid** bodies undergo body forces, $\vec{\mathbf{b}}_\ell$ in Ω_ℓ, and surface trasctions, $\vec{\mathbf{t}}_\ell$ on $\partial\Omega_\ell^t$. The total potential energy function of a system of the rigid bodies due to $\vec{\mathbf{b}}_\ell$ and $\vec{\mathbf{t}}_\ell$ is defined as*

$$\boxed{\mathscr{U} := \sum_{\ell=1}^{n_{\mathrm{b}}} \mathscr{U}_\ell = \sum_{\ell=1}^{n_{\mathrm{b}}} \mathscr{U}_\ell^{\mathrm{ext}} + \sum_{\ell=1}^{n_{\mathrm{b}}} \underbrace{\mathscr{U}_\ell^{\mathrm{int}}}_{0} = \sum_{\ell=1}^{n_{\mathrm{b}}} \mathscr{U}_\ell^{\mathrm{ext}} = \sum_{\ell=1}^{n_{\mathrm{b}}} \mathscr{U}_\ell^{\mathrm{b}} + \sum_{\ell=1}^{n_{\mathrm{b}}} \mathscr{U}_\ell^{\mathrm{t}}} \tag{7.102}$$

where $\sum_{\ell=1}^{n_{\mathrm{b}}} \mathscr{U}_\ell^{\mathrm{ext}} = \mathscr{U}_\ell^{\mathrm{b}} + \mathscr{U}_\ell^{\mathrm{t}}$ denotes the external potential energy of Ω_ℓ; and $\mathscr{U}_\ell^{\mathrm{b}}$ and $\mathscr{U}_\ell^{\mathrm{t}}$ are the potential energy functions of Ω_ℓ due to the body force and surface traction vectors, defined as

$$\mathscr{U}_\ell^{\mathrm{b}} = -\int_{\Omega_\ell} \vec{\mathbf{b}}_\ell \cdot \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P}_\ell) dV \tag{7.103}$$

$$\mathscr{U}_\ell^{\mathrm{t}} = -\int_{\partial\Omega_\ell^t} \vec{\mathbf{t}}_\ell \cdot \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P}_\ell) dA \tag{7.104}$$

respectively, for $\ell = 1, 2, \cdots, n_{\mathrm{b}}$. Note that $\mathscr{U}_\ell^{\mathrm{int}}$ denotes the internal potential energy function (or the strain energy function) of Ω_ℓ, and it is zero for a rigid body; therefore, the total potential energy of a system of rigid bodies is equivalent to the external potential energy of the system.

Theorem 7.3.6

(Potential Energy of a System of Rigid Bodies: Translation and Rotation Potential Energy Functions)

*The total potential energy of a system of **rigid** bodies can be written as*

$$\boxed{\begin{aligned}\mathscr{U} &= \sum_{\ell=1}^{n_b} \mathscr{U}_\ell^{\text{ext}} \\ &= -\sum_{\ell=1}^{n_b}{}' \, {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{C}_\ell)^T \left({}^{\mathcal{B}_0}\mathbf{f}_\ell^{\text{con}}\right) \\ &\quad - \sum_{\ell=1}^{n_b}{}' \int_{\Omega_\ell} \left[\left({}^{\mathcal{B}_0/\mathcal{B}_\ell}\mathbf{A}\right)\left({}^{\mathcal{B}_\ell}\boldsymbol{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell)\right)\right]^T \left({}^{\mathcal{B}_0}\mathbf{b}_\ell\right) dV \\ &\quad - \sum_{\ell=1}^{n_b}{}' \int_{\partial\Omega_\ell^t} \left[\left({}^{\mathcal{B}_0/\mathcal{B}_\ell}\mathbf{A}\right)\left({}^{\mathcal{B}_\ell}\boldsymbol{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell)\right)\right]^T \left({}^{\mathcal{B}_0}\mathbf{t}_\ell\right) dA\end{aligned}} \tag{7.105}$$

where the component form of the (external) conservative force vector with respect to $\mathcal{B}_0$ is given by

$${}^{\mathcal{B}_0}\mathbf{f}_\ell^{\text{con}} = \int_{\Omega_\ell} {}^{\mathcal{B}_0}\mathbf{b}_\ell \, dV + \int_{\partial\Omega_\ell^t} {}^{\mathcal{B}_0}\mathbf{t}_\ell \, dA \tag{7.106}$$

Proof. Substituting

$$\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P}_\ell) = \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_\ell) + \vec{\boldsymbol{\pi}}(\mathbf{C}_\ell, \mathbf{P}_\ell) \tag{7.107}$$

into Eq. (7.102) yields

$$\mathscr{U} = \sum_{\ell=1}^{n_b} \mathscr{U}_\ell^{(1)} + \sum_{\ell=1}^{n_b} \mathscr{U}_\ell^{(2)} \tag{7.108}$$

where $\mathscr{U}_\ell^{(1)}$ denotes the ***translation potential energy function*** of Ω_ℓ, i.e., the potential associated with the translational motion of Ω_ℓ, and $\mathscr{U}_\ell^{(2)}$ denotes the ***rotational potential energy function*** of Ω_ℓ, i.e., the potential associated with the rotational motion of Ω_ℓ:

$$\mathscr{U}_\ell^{(1)} := -\int_{\Omega_\ell} \vec{\mathbf{b}}_\ell \cdot \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_\ell) dV - \int_{\partial\Omega_\ell^t} \vec{\mathbf{t}}_\ell \cdot \vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_\ell) dA \tag{7.109}$$

$$\mathscr{U}_\ell^{(2)} := -\int_{\Omega_\ell} \vec{\mathbf{b}}_\ell \cdot \vec{\boldsymbol{\pi}}(\mathbf{C}_\ell, \mathbf{P}_\ell) dV - \int_{\partial\Omega_\ell^t} \vec{\mathbf{t}}_\ell \cdot \vec{\boldsymbol{\pi}}(\mathbf{C}_\ell, \mathbf{P}_\ell) dA \tag{7.110}$$

From Eq. (7.109),

$$\mathscr{U}_\ell^{(1)} = -\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{C}_\ell) \cdot \vec{\mathbf{f}}_\ell^{\text{con}} = -{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{C}_\ell)^T \left({}^{\mathcal{B}_0}\mathbf{f}_\ell^{\text{con}}\right) \tag{7.111}$$

where the ***conservative force vector***, $\mathbf{f}_\ell^{\text{con}} = {}^{\mathcal{B}_0}\mathbf{e}^T \; {}^{\mathcal{B}_0}\mathbf{f}_\ell^{\text{con}}$, is given as

$$\vec{\mathbf{f}}_\ell^{\text{con}} = \int_{\Omega_\ell} \vec{\mathbf{b}}_\ell \, dV + \int_{\partial\Omega_\ell^t} \vec{\mathbf{t}}_\ell \, dA \tag{7.112}$$

Note that the conservative force is equivalent to the external conservative force for a rigid body. In the case of a flexible body, the conservative force may consist of not only the external conservative force as defined in Eq. (7.112), but also the internal conservative force which can be defined as $\nabla\mathscr{U}_\ell^{\text{int}}$.

From Eq. (7.110),

$$\begin{aligned}
\mathscr{U}_\ell^{(2)} &= -\int_{\Omega_\ell} {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell)^T \; {}^{\mathcal{B}_0}\mathbf{b}_\ell \, dV - \int_{\partial\Omega_\ell^t} {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell)^T \; {}^{\mathcal{B}_0}\mathbf{t}_\ell \, dA \\
&= -\int_{\Omega_\ell} \left[\left({}^{\mathcal{B}_0/\mathcal{B}_\ell}\mathbf{A}\right)\left({}^{\mathcal{B}_\ell}\boldsymbol{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell)\right)\right]^T \left({}^{\mathcal{B}_0}\mathbf{b}_\ell\right) dV \\
&\quad -\int_{\partial\Omega_\ell^t} \left[\left({}^{\mathcal{B}_0/\mathcal{B}_\ell}\mathbf{A}\right)\left({}^{\mathcal{B}_\ell}\boldsymbol{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell)\right)\right]^T \left({}^{\mathcal{B}_0}\mathbf{t}_\ell\right) dA
\end{aligned} \tag{7.113}$$

Hence, from Eq. (7.111) and Eq. (7.113), the total potential energy function is obtained as in Eq. (7.105). ∎

Theorem 7.3.7 (First Variation of the Total Potential Energy Function of Rigid Bodies) *The first variation of the total potential energy of a system of n_b* ***rigid*** *bodies is given by*

$$\boxed{\delta\mathscr{U} = -\sum_{\ell=1}^{n_\text{b}}{}' \left(\delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{C}_\ell)^T\right) \left({}^{\mathcal{B}_0}\mathbf{f}_\ell^{\text{con}}\right) - \sum_{\ell=1}^{n_\text{b}}{}' \left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\boldsymbol{\varpi}^T\right) \left({}^{\mathcal{B}_\ell}_{\mathbf{C}_\ell}\mathcal{T}_\ell\right)} \tag{7.114}$$

where ${}^{\mathcal{B}_\ell}_{\mathbf{C}_\ell}\mathcal{T}_\ell$ denotes the torque component vector about point $\mathbf{C}_\ell$ of Ω_ℓ in terms of frame $\mathcal{B}_\ell$.

Proof. The first variation of the total potential energy of a system of n_b rigid bodies can be written as

$$\delta\mathscr{U} = \sum_{\ell=1}^{n_\text{b}} \delta\mathscr{U}_\ell^{(1)} + \sum_{\ell=1}^{n_\text{b}} \delta\mathscr{U}_\ell^{(2)} \tag{7.115}$$

where $\delta\mathscr{U}_\ell^{(1)}$ is obtained by taking the variation of Eq. (7.111), i.e.,

$$\delta\mathscr{U}_\ell^{(1)} = -\delta\vec{\boldsymbol{\pi}}(\mathbf{O},\mathbf{C}_\ell)\cdot\vec{\mathbf{f}}_\ell^{\text{con}} = -\delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O},\mathbf{C}_\ell)^T\ \left({}^{\mathcal{B}_0}\mathbf{f}_\ell^{\text{con}}\right) \tag{7.116}$$

and $\delta\mathscr{U}_\ell^{(2)}$ is , on the other hand, obtained by taking the variation of Eq. (7.110), i.e.,

$$\delta\mathscr{U}_\ell^{(2)} = -\int_{\Omega_\ell}\vec{\mathbf{b}}_\ell\cdot\delta\vec{\boldsymbol{\pi}}(\mathbf{C}_\ell,\mathbf{P}_\ell)dV - \int_{\partial\Omega_\ell^t}\vec{\mathbf{t}}_\ell\cdot\delta\vec{\boldsymbol{\pi}}(\mathbf{C}_\ell,\mathbf{P}_\ell)dA \tag{7.117}$$

In view of Eq. (5.185)-(3) in Theorem 5.5.2, we have

$$\delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{C}_\ell,\mathbf{P}_\ell) = -\left({}^{\mathcal{B}_0/\mathcal{B}_\ell}\mathbf{A}\right){}^{\mathcal{B}_\ell}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_\ell,\mathbf{P}_\ell)\left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\boldsymbol{\varpi}\right) \tag{7.118}$$

Hence, the first term in the right-hand side of Eq. (7.121) yields

$$\begin{aligned}
& -\int_{\Omega_\ell}\vec{\mathbf{b}}_\ell\cdot\delta\vec{\boldsymbol{\pi}}(\mathbf{C}_\ell,\mathbf{P}_\ell)\,dV \\
= & -\int_{\Omega_\ell}\left({}^{\mathcal{B}_0}\mathbf{b}_\ell^T\right)\delta^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{C}_\ell,\mathbf{P}_\ell)\,dV \\
= & \int_{\Omega_\ell}\left({}^{\mathcal{B}_0}\mathbf{b}_\ell^T\right)\left({}^{\mathcal{B}_0/\mathcal{B}_\ell}\mathbf{A}\right){}^{\mathcal{B}_\ell}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_\ell,\mathbf{P}_\ell)\left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\boldsymbol{\varpi}\right)dV \\
= & \int_{\Omega_\ell}\left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\boldsymbol{\varpi}^T\right)\underbrace{{}^{\mathcal{B}_\ell}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_\ell,\mathbf{P}_\ell)^T}_{-{}^{\mathcal{B}_\ell}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_\ell,\mathbf{P}_\ell)}\left({}^{\mathcal{B}_0/\mathcal{B}_\ell}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0}\mathbf{b}_\ell\right)dV \\
= & -\left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\boldsymbol{\varpi}^T\right)\int_{\Omega_\ell}{}^{\mathcal{B}_\ell}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_\ell,\mathbf{P}_\ell)\left({}^{\mathcal{B}_0/\mathcal{B}_\ell}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0}\mathbf{b}_\ell\right)dV
\end{aligned} \tag{7.119}$$

Following a similar manner, the second term in the right-hand side of Eq. (7.121) may yield

$$\begin{aligned}
& -\int_{\partial\Omega_\ell^t}\vec{\mathbf{t}}_\ell\cdot\delta\vec{\boldsymbol{\pi}}(\mathbf{C}_\ell,\mathbf{P}_\ell)dA \\
& = -\left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\boldsymbol{\varpi}^T\right)\int_{\partial\Omega_\ell^t}{}^{\mathcal{B}_\ell}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_\ell,\mathbf{P}_\ell)\left({}^{\mathcal{B}_0/\mathcal{B}_\ell}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0}\mathbf{t}_\ell\right)dA
\end{aligned} \tag{7.120}$$

Therefore,

$$\delta\mathscr{U}_\ell^{(2)} = -\left({}^{\mathcal{B}_\ell}_{\mathcal{B}_\ell|\mathcal{B}_0}\boldsymbol{\varpi}^T\right)\left({}^{\mathcal{B}_\ell}_{\mathbf{C}_\ell}\mathcal{T}_\ell\right) \tag{7.121}$$

where ${}^{\mathcal{B}_\ell}_{\mathbf{C}_\ell}\mathcal{T}_\ell$ is the torque component vector about point $\mathbf{C}_\ell$ of Ω_ℓ in terms of frame $\mathcal{B}_\ell$,[1]

$$\begin{aligned}{}^{\mathcal{B}_\ell}_{\mathbf{C}_\ell}\mathcal{T}_\ell = &\int_{\Omega_\ell} {}^{\mathcal{B}_\ell}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_\ell, \mathbf{P}_\ell) \left({}^{\mathcal{B}_0/\mathcal{B}_\ell}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0}\mathbf{b}_\ell\right) dV \\ &+ \int_{\partial\Omega_\ell^t} {}^{\mathcal{B}_\ell}\widetilde{\boldsymbol{\pi}}(\mathbf{C}_\ell, \mathbf{P}_\ell) \left({}^{\mathcal{B}_0/\mathcal{B}_\ell}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0}\mathbf{t}_\ell\right) dA\end{aligned} \tag{7.123}$$

Hence, from Eq. (7.116) and Eq. (7.121), the first variation of the total potential energy for the system of n_b rigid bodies is given as in Eq. (7.114). ∎

7.3.2 Hamilton's Principle

Hamilton's Principle for Unconstrained Systems

Single-field form: As mentions in Subsection 6.1.1, assume the vector, $\vec{\mathbf{r}}_\ell = \vec{\pi}(\mathbf{O}, \mathbf{P}_\ell)$ can be expressed in terms of the generalized coordinates $\mathbf{q}$ and time $t \in \mathbb{I}$ as

$$\vec{\mathbf{r}}_\ell = \vec{\mathbf{r}}_\ell(\mathbf{q}, t) = \vec{\mathbf{r}}(q_1, q_2, \cdots, q_{n_\mathrm{g}}, t) \tag{7.124}$$

Then, the total time derivative of $\vec{\mathbf{r}}_\ell$ with respect to the inertial reference frame, $\mathcal{B}_0$, is given as a function of the generalized coordinates, generalized velocities, and time as

$${}^{\mathcal{B}_0}\mathfrak{D}_t\, \vec{\mathbf{r}}_\ell(\mathbf{q}, t) = \frac{\partial \vec{\mathbf{r}}_\ell(\mathbf{q}, t)}{\partial q_i}\dot{q}_i + \frac{\partial \vec{\mathbf{r}}_\ell(\mathbf{q}, t)}{\partial t} \tag{7.125}$$

---

[1] It is clear that the right-hand side of Eq. (7.123) indicates the torque ${}^{\mathcal{B}_\ell}_{\mathbf{C}_\ell}\mathcal{T}_\ell$ from

$$\begin{aligned}{}_{\mathbf{C}_\ell}\vec{\mathcal{T}}_\ell &= \int_{\Omega_\ell} \vec{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell) \times \vec{\mathbf{b}}_\ell\, dV + \int_{\partial\Omega_\ell^t} \vec{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell) \times \vec{\mathbf{t}}_\ell\, dA \\ &= \int_{\Omega_\ell} \underbrace{\vec{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell) \times [{}^{\mathcal{B}_\ell}\mathbf{e}^T}_{{}^{\mathcal{B}_\ell}\mathbf{e}^T\left({}^{\mathcal{B}_\ell}\widetilde{\boldsymbol{\pi}}\mathbf{C}_\ell, \mathbf{P}_\ell)\right)} \quad \underbrace{{}^{\mathcal{B}_\ell}\mathbf{b}_\ell}_{\left({}^{\mathcal{B}_0/\mathcal{B}_\ell}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0}\mathbf{b}_\ell\right)} \quad]\, dV \\ &\quad + \int_{\partial\Omega_\ell^t} \underbrace{\vec{\pi}(\mathbf{C}_\ell, \mathbf{P}_\ell) \times [{}^{\mathcal{B}_\ell}\mathbf{e}^T}_{{}^{\mathcal{B}_\ell}\mathbf{e}^T\left({}^{\mathcal{B}_\ell}\widetilde{\boldsymbol{\pi}}\mathbf{C}_\ell, \mathbf{P}_\ell)\right)} \quad \underbrace{{}^{\mathcal{B}_\ell}\mathbf{t}_\ell}_{\left({}^{\mathcal{B}_0/\mathcal{B}_\ell}\mathbf{A}^T\right)\left({}^{\mathcal{B}_0}\mathbf{t}_\ell\right)} \quad]\, dA \\ &= {}^{\mathcal{B}_\ell}\mathbf{e}^T \left({}^{\mathcal{B}_\ell}_{\mathbf{C}_\ell}\mathcal{T}_\ell\right)\end{aligned} \tag{7.122}$$

Therefore, in view of Eq. (7.88) in Definition 7.3.1, the kinetic energy of a system of n_b rigid bodies can be expressed as

$$\begin{aligned} \mathscr{K}(\mathbf{q},\dot{\mathbf{q}},t) &= \sum_{\ell=1}^{n_\mathrm{b}} \mathscr{K}_\ell(\mathbf{q},\dot{\mathbf{q}},t) \\ &= \underbrace{\sum_{\ell=1}^{n_\mathrm{b}} \mathscr{K}_\ell^{[1]}(\mathbf{q},\dot{\mathbf{q}},t)}_{=:\mathscr{K}^{[1]}(\mathbf{q},\dot{\mathbf{q}},t)} + \underbrace{\sum_{\ell=1}^{n_\mathrm{b}} \mathscr{K}_\ell^{[2]}(\mathbf{q},\dot{\mathbf{q}},t)}_{=:\mathscr{K}^{[2]}(\mathbf{q},\dot{\mathbf{q}},t)} + \underbrace{\sum_{\ell=1}^{n_\mathrm{b}} \mathscr{K}_\ell^{[3]}(\mathbf{q},t)}_{=:\mathscr{K}^{[3]}(\mathbf{q},t)} \end{aligned} \tag{7.126}$$

where $\mathscr{K}_\ell^{[\mathrm{k}]}$ (for $k = 1, 2, 3$) are defined as

$$\mathscr{K}_\ell^{[1]}(\mathbf{q},\dot{\mathbf{q}},t) := \frac{\dot{q}_i\dot{q}_j}{2}\underbrace{\left(\int_{\Omega_\ell} \frac{\partial\vec{\mathbf{r}}_\ell(\mathbf{q},t)}{\partial q_i}\cdot\frac{\partial\vec{\mathbf{r}}_\ell(\mathbf{q},t)}{\partial q_j}dm\right)}_{=:M^\ell_{ij}(\mathbf{q},t)} = \frac{1}{2}\dot{\mathbf{q}}^T\mathbf{M}^\ell(\mathbf{q},t)\dot{\mathbf{q}} \tag{7.127}$$

$$\mathscr{K}_\ell^{[2]}(\mathbf{q},\dot{\mathbf{q}},t) := \underbrace{\left(\int_{\Omega_\ell} \frac{\partial\vec{\mathbf{r}}_\ell(\mathbf{q},t)}{\partial q_i}\cdot\frac{\partial\vec{\mathbf{r}}_\ell(\mathbf{q},t)}{\partial t}dm\right)}_{=:m^\ell_i(\mathbf{q},t)}\dot{q}_i = \dot{\mathbf{q}}^T\mathbf{m}^\ell(\mathbf{q},t) \tag{7.128}$$

$$\mathscr{K}_\ell^{[3]}(\mathbf{q},t) := \int_{\Omega_\ell} \frac{\partial\vec{\mathbf{r}}_\ell(\mathbf{q},t)}{\partial t}\cdot\frac{\partial\vec{\mathbf{r}}_\ell(\mathbf{q},t)}{\partial t}dm \tag{7.129}$$

Notice that, if $\vec{\mathbf{r}}_\ell$ does not depend on time explicitly, Eq. (7.126) redues to

$$\mathscr{K}(\mathbf{q},\dot{\mathbf{q}},t) = \mathscr{K}^{[1]}(\mathbf{q},\dot{\mathbf{q}},t) \tag{7.130}$$

Likewise, in view of Definition 7.3.2, the potential energy function for a system of n_b rigid bodies can be expressed, with the help of Eq. (7.124), as a function of the generalized coordinates and time as

$$\mathscr{U}(\mathbf{q},t) = \sum_{\ell=1}^{n_\mathrm{b}} \mathscr{U}_\ell(\mathbf{q},t) \tag{7.131}$$

Theorem 7.3.8 (Hamilton's Principle for Unconstrained Systems)

The standard variational principle for Hamilton's principle for unconstrained systems reads:

$$\boxed{\delta\mathscr{I} + \int_{t_0}^{t_\mathrm{L}} \delta W^{\mathrm{ncon}} dt = 0} \tag{7.132}$$

*where $\mathscr{I}$ is the **action integral** defined as*

$$\mathscr{I}[\mathbf{q}] := \int_{t_0}^{t_\mathrm{L}} \mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}, t)dt \tag{7.133}$$

with the Lagrangian function of the form

$$\mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}, t) = \mathscr{T}(\mathbf{q}, \dot{\mathbf{q}}, t) - \mathscr{U}(\mathbf{q}, t) \tag{7.134}$$

and δW^{ncon} represents the virtual work done on the system by non-conservative forces, i.e., forces which are not derivable from potential energy functions. Eq. (7.134) *is equivalent to the second expression of the principle of virtual work (Theorem 7.3.3).*

Under the restrictions,

$$\delta\vec{\mathbf{r}}_\ell(t_0) = \delta\vec{\mathbf{r}}_\ell(t_\mathrm{L}) = \mathbf{0}, \tag{7.135}$$

which imply

$$\delta\mathbf{q}(t_0) = \delta\mathbf{q}(t_\mathrm{L}) = \mathbf{0}, \tag{7.136}$$

Eq. (7.132) *is equivalent to **Lagrange's equation of motion**:*

$$\boxed{\mathfrak{E}_i[\mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}, t)] \equiv \left(\frac{d}{dt}\frac{\partial}{\partial \dot{q}_i} - \frac{\partial}{\partial q_i}\right)\mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}, t) = Q_i^{\mathrm{ncon}}} \tag{7.137}$$

where Q_i^{ncon} is the generalized non-conservative force.

Proof. Suppose that the applied force can be divided into the conservative and non-conservative forces, $\vec{\mathbf{f}}_\ell^{\mathrm{con}}$ and $\vec{\mathbf{f}}_\ell^{\mathrm{ncon}}$, respectively:

$$\vec{\mathbf{f}}_\ell^{\mathrm{appl}} = \int_{\Omega_\ell} d\vec{\mathbf{f}}_\ell^{\mathrm{appl}} = \underbrace{\int_{\Omega_\ell} d\vec{\mathbf{f}}_\ell^{\mathrm{con}}}_{\vec{\mathbf{f}}_\ell^{\mathrm{con}}} + \underbrace{\int_{\Omega_\ell} d\vec{\mathbf{f}}_\ell^{\mathrm{ncon}}}_{\vec{\mathbf{f}}_\ell^{\mathrm{ncon}}} \tag{7.138}$$

Since the conservative forces are defined as the forces which are derivable from potential energy functions via

$$\vec{\mathbf{f}}_\ell^{\mathrm{con}} := -\frac{\partial \mathscr{U}}{\partial \vec{\mathbf{r}}_\ell} \tag{7.139}$$

the work due to the applied force yields

$$
\begin{aligned}
\delta W^{\text{appl}} &= \int_{\Omega_\ell} d\vec{\mathbf{f}}^{\text{appl}} \cdot \delta\vec{\mathbf{r}}_\ell = \underbrace{\int_{\Omega_\ell} d\vec{\mathbf{f}}^{\text{con}} \cdot \delta\vec{\mathbf{r}}_\ell}_{\delta W^{\text{con}}} + \underbrace{\int_{\Omega_\ell} d\vec{\mathbf{f}}^{\text{ncon}} \cdot \delta\vec{\mathbf{r}}_\ell}_{\delta W^{\text{ncon}}} \\
&= \underbrace{\int_{\Omega_\ell} d\vec{\mathbf{f}}^{\text{con}} \cdot \frac{\partial\vec{\mathbf{r}}_\ell}{\partial q_i}}_{Q_i^{\text{con}}} \delta q_i + \underbrace{\int_{\Omega_\ell} d\vec{\mathbf{f}}^{\text{ncon}} \cdot \frac{\partial\vec{\mathbf{r}}_\ell}{\partial q_i}}_{Q_i^{\text{ncon}}} \delta q_i \\
&= \left[-\frac{\partial\mathscr{U}}{\partial q_i} + Q_i^{\text{ncon}}\right]\delta q_i
\end{aligned} \tag{7.140}
$$

where δW^{con} and δW^{ncon} are the virtual work functions due to the conservative and non-conservative forces, respectively; and $\mathbf{Q}^{\text{con}} = [Q_i^{\text{con}}]$ and $\mathbf{Q}^{\text{ncon}} = [Q_i^{\text{ncon}}]$ are the generalized conservative and non-conservative force vectors, respectively. Noticing that

$$
\delta W^{\text{con}} = Q_i^{\text{con}}\delta q_i = \int_{\Omega_\ell} d\vec{\mathbf{f}}^{\text{con}} \cdot \frac{\partial\vec{\mathbf{r}}_\ell}{\partial q_i}\delta q_i = -\frac{\partial\mathscr{U}(\mathbf{q}, t)}{\partial q_i}\delta q_i = -\delta\mathscr{U}(\mathbf{q}, t) \tag{7.141}
$$

it follows that the second expression of the principle of virtual work (Eq. (7.81) in Theorem 7.3.3) leads to Eq. (7.132):

$$
\begin{aligned}
0 &= \int_{t_0}^{t_{\text{L}}} \delta\mathscr{K}\, dt + \int_{t_0}^{t_{\text{L}}} \delta W^{\text{appl}} dt \\
&= \int_{t_0}^{t_{\text{L}}} \left[\delta\mathscr{K} + \delta W^{\text{con}} + \delta W^{\text{ncon}}\right] dt \\
&= \int_{t_0}^{t_{\text{L}}} \left[\delta\left(\mathscr{K} - \mathscr{U}\right) + \delta W^{\text{ncon}}\right] dt \\
&= \delta \int_{t_0}^{t_{\text{L}}} \mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}, t) dt + \int_{t_0}^{t_{\text{L}}} \delta W^{\text{ncon}} dt
\end{aligned} \tag{7.142}
$$

where $\mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}, t)$ is the Lagrangian function defined as in Eq. (7.134).

The first term in the left-hand side of Eq. (7.81) in Theorem 7.3.3 may yield (by way of integration by parts)

$$
\begin{aligned}
&\int_{t_0}^{t_\mathrm{L}} \delta\mathscr{K}(\mathbf{q},\dot{\mathbf{q}},t)dt \\
=\;& \int_{t_0}^{t_\mathrm{L}} \left(\frac{\partial\mathscr{K}}{\partial\dot{q}_i} \underbrace{\delta\dot{q}_i}_{\mathfrak{D}_t\delta q_i} + \frac{\partial\mathscr{K}}{\partial q_i}\delta q_i + \frac{\partial\mathscr{K}}{\partial t} \underbrace{\delta t}_{\equiv 0} \right) dt \\
=\;& \left[\tfrac{\partial\mathscr{K}}{\partial\dot{q}_i}\delta q_i\right]_{t_0}^{t_\mathrm{L}} - \int_{t_0}^{t_\mathrm{L}} \frac{d}{dt}\left(\frac{\partial\mathscr{K}}{\partial\dot{q}_i}\right)\delta q_i dt + \int_{t_0}^{t_\mathrm{L}} \frac{\partial\mathscr{K}}{\partial q_i}\delta q_i\, dt
\end{aligned}
\tag{7.143}
$$

where $\mathfrak{D}_t = d/dt$ denotes the time derivative operator. Notice that the frame to which the time derivative refers does not need to be specified when we take the time derivatives of the generalized coordinates and the generalized velocities. Under the restrictions given in Eq. (7.136), Eq. (7.143) results in the from,

$$
\int_{t_0}^{t_\mathrm{L}} \delta\mathscr{K}(\mathbf{q},\dot{\mathbf{q}},t)dt = \int_{t_0}^{t_\mathrm{L}} \left[\frac{\partial\mathscr{K}}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial\mathscr{K}}{\partial\dot{q}_i}\right)\right]\delta q_i\, dt \tag{7.144}
$$

Therefore, the second expression of the principle of virtual work under Eq. (7.136) is equivalent to

$$
\begin{aligned}
0 \;=\;& \int_{t_0}^{t_\mathrm{L}} \delta\mathscr{K}\, dt + \int_{t_0}^{t_\mathrm{L}} \delta W^{\mathrm{appl}} dt \\
=\;& \int_{t_0}^{t_\mathrm{L}} \left[\frac{\partial}{\partial q_i}(\mathscr{K} - \mathscr{U}) - \frac{d}{dt}\left(\frac{\partial\mathscr{K}}{\partial\dot{q}_i}\right) + Q_i^{\mathrm{ncon}}\right]\delta q_i\, dt \\
=\;& \int_{t_0}^{t_\mathrm{L}} \left[\frac{\partial}{\partial q_i}(\mathscr{L}) - \frac{d}{dt}\left(\frac{\partial\mathscr{L}}{\partial\dot{q}_i}\right) + Q_i^{\mathrm{ncon}}\right]\delta q_i\, dt
\end{aligned}
\tag{7.145}
$$

Because δq_i (for $i = 1, 2, \cdots, n_\mathrm{g} = n_\mathrm{dof}$) are arbitrary,

$$
\frac{d}{dt}\left(\frac{\partial\mathscr{L}}{\partial\dot{q}_i}\right) - \frac{\partial}{\partial q_i}(\mathscr{L}) = Q_i^{\mathrm{ncon}} \tag{7.146}
$$

By introducing the operator, $\mathfrak{E}_i$,

$$
\mathfrak{E}_i[(\bullet)] \equiv \left(\frac{d}{dt}\frac{\partial}{\partial\dot{q}_i} - \frac{\partial}{\partial q_i}\right)(\bullet) \tag{7.147}
$$

Eq. (7.146) can be written in a compact form as

$$\mathfrak{E}_i[\mathscr{L}(\mathbf{q},\dot{\mathbf{q}},t)] = Q_i^{\mathrm{ncon}} \tag{7.148}$$

which is identical to Eq. (7.137). ∎

Remark 7.3.2

1. *Eq.* (7.137) *leads to*

$$\begin{aligned} Q_i^{\mathrm{ncon}} &= \mathfrak{E}_i[\mathscr{L}(\mathbf{q},\dot{\mathbf{q}},t)] \\ &= \underbrace{\frac{\partial^2\mathscr{L}}{\partial\dot{q}_i\partial\dot{q}_j}}_{\sum_{\ell=1}^{n_\mathrm{b}} M_{ij}^{\ell}(\mathbf{q},t)}\ddot{q}_j + \frac{\partial^2\mathscr{L}}{\partial\dot{q}_i\partial q_j}\dot{q}_j + \frac{\partial^2\mathscr{L}}{\partial\dot{q}_i\partial t} - \frac{\partial\mathscr{L}}{\partial q_i} \end{aligned} \tag{7.149}$$

*If the Lagrangian is **regular**, in other words, if the matrix,* $[\mathbf{M}]_{ij} = M_{ij}(\mathbf{q},t) := \sum_{\ell=1}^{n_\mathrm{b}} M_{ij}^{\ell}(\mathbf{q},t)$, *is invertible, i.e.,*

$$\det(M_{ij}(\mathbf{q},t)) = \det\left(\frac{\partial^2\mathscr{L}}{\partial\dot{q}_i\partial\dot{q}_j}\right) \neq 0 \tag{7.150}$$

Eq. (7.149) *can be written as*

$$\ddot{q}_j = [\mathbf{M}^{-1}(\mathbf{q},t)]_{ji}\left(Q_i^{\mathrm{ncon}} + \frac{\partial\mathscr{L}}{\partial q_i} - \frac{\partial^2\mathscr{L}}{\partial\dot{q}_i\partial t} - \frac{\partial^2\mathscr{L}}{\partial\dot{q}_i\partial q_k}\dot{q}_k\right) \tag{7.151}$$

If Lagrangian function of a system is given, and it is regular, Eq. (7.149) *gives the relationship between the generalized coordinates and the generalized velocities and acceleration.*

2. *If all applied forces are derivable from the system potential energy, i.e.,* $Q_i^{\mathrm{ncon}} = 0$, *Theorem 7.3.9 reads:*

$$\boxed{\delta\mathscr{I} = 0 \ \ \textit{with} \ \ \delta\mathbf{q}(t_0) = \delta\mathbf{q}(t_\mathrm{L}) = \mathbf{0},} \tag{7.152}$$

is equivalent to Lagrange's equation of motion of the form

$$\boxed{\mathfrak{E}_i[\mathscr{L}(\mathbf{q},\dot{\mathbf{q}},t)] = 0} \tag{7.153}$$

Two-field form: Introducing new variables, $v_i(t) = [\mathbf{v}(t)]_i : \mathbb{I} \to \mathbb{R}$ for $i = 1, 2, \cdots, n_{\mathrm{g}}$, define the ***modified kinetic energy*** as

$$\mathscr{K}^*(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t) := \mathscr{K}^{*[1]}(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t) + \mathscr{K}^{[2]}(\mathbf{q}, \dot{\mathbf{q}}, t) + \mathscr{K}^{[3]}(\mathbf{q}, t) \tag{7.154}$$

where $\mathscr{K}^{[2]}(\mathbf{q}, \dot{\mathbf{q}}, t)$ and $\mathscr{K}^{[3]}(\mathbf{q}, t)$ are given as in Eq. (7.128) and Eq. (7.129), respectively, and $\mathscr{K}^{*[1]}$ is defined as

$$\mathscr{K}^{*[1]}(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t) := \mathbf{v}^T\mathbf{M}(\mathbf{q}, t)\dot{\mathbf{q}} - \frac{1}{2}\mathbf{v}^T\mathbf{M}(\mathbf{q}, t)\mathbf{v} \tag{7.155}$$

If $\vec{\mathbf{r}}_\ell$ does not depend on time explicitly, i.e., $\vec{\mathbf{r}}_\ell = \vec{\mathbf{r}}_\ell(\mathbf{q})$, we have

$$\mathscr{K}^*(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t) = \mathscr{K}^{*[1]}(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t) \tag{7.156}$$

Employing $\mathscr{K}^*$, given in Eq. (7.154), instead of $\mathscr{K}$, defined in Eq. (7.126), the ***modified Lagrangian function*** can be written as

$$\mathscr{L}^*(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t) = \mathscr{K}^*(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t) - \mathscr{U}(\mathbf{q}, t) \tag{7.157}$$

Based on this modified Lagrangian, Theorem 7.3.9 may be written in the form of the two-field stationary principle as follows:

Theorem 7.3.9

Hamilton's Principle for Unconstrained Systems: Two-field Stationary Principle

The two-field stationary principle for unconstrained systems reads:

$$\boxed{\delta\mathscr{I}^* + \int_{t_0}^{t_{\mathrm{L}}} \delta W^{\mathrm{ncon}} dt = 0} \tag{7.158}$$

*where $\mathscr{I}^*$ is the **modified action integral** defined as*

$$\mathscr{I}^*[\mathbf{q}, \mathbf{v}] := \int_{t_0}^{t_{\mathrm{L}}} \mathscr{L}^*(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t)dt \tag{7.159}$$

with the modified Lagrangian function defined in Eq. (7.157), *and* δW^{ncon} *represents the virtual work done on the system by non-conservative forces. Under the restrictions,*

$$\delta \mathbf{q}(t_0) = \delta \mathbf{q}(t_{\mathrm{L}}) = \mathbf{0}, \tag{7.160}$$

Eq. (7.158) *is equivalent to:*

$$\boxed{\mathfrak{E}_i[\mathscr{L}^*(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t)] = Q_i^{\mathrm{ncon}} \;\; \textit{and} \;\; \dot{\mathbf{q}}(t) = \mathbf{v}(t)} \tag{7.161}$$

Proof. From Eq. (7.158), we have

$$\begin{aligned}
0 &= \delta \int_{t_0}^{t_{\mathrm{L}}} \mathscr{L}^*(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t) dt + \int_{t_0}^{t_{\mathrm{L}}} \delta W^{\mathrm{ncon}} dt \\
&= \int_{t_0}^{t_{\mathrm{L}}} \left(\frac{\partial \mathscr{L}^*}{\partial q_i} \delta q_i + \frac{\partial \mathscr{L}^*}{\partial \dot{q}_i} \delta \dot{q}_i + \frac{\partial \mathscr{L}^*}{\partial v_i} \delta v_i + \frac{\partial \mathscr{L}^*}{\partial t} \underbrace{\delta t}_{0} + Q_i^{\mathrm{ncon}} \delta q_i \right) dt \\
&= \int_{t_0}^{t_{\mathrm{L}}} \left(\frac{\partial \mathscr{L}^*}{\partial q_i} - \frac{d}{dt} \left(\frac{\partial \mathscr{L}^*}{\partial \dot{q}_i} \right) + Q_i^{\mathrm{ncon}} \right) \delta q_i dt + \underbrace{\frac{\partial \mathscr{L}^*}{\partial q_i} \delta q_i \bigg|_{t_0}^{t_{\mathrm{L}}}}_{0 \,\because\, \mathrm{Eq.}(7.160)} \\
&\quad + \int_{t_0}^{t_{\mathrm{L}}} M_{ij} \left[\dot{q}_j - v_j \right] \delta v_i dt \\
&= \int_{t_0}^{t_{\mathrm{L}}} \left(\mathfrak{E}_i[\mathscr{L}^*(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t)] - Q_i^{\mathrm{ncon}} \right) \delta q_i dt + \int_{t_0}^{t_{\mathrm{L}}} M_{ij} \left[v_j - \dot{q}_j \right] \delta v_i dt
\end{aligned} \tag{7.162}$$

Since δq_i and δv_i are independent, the stationary conditions in terms of q_i and v_i are obtained as

$$\begin{aligned}
\mathfrak{E}_i[\mathscr{L}^*(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t)] - Q_i^{\mathrm{ncon}} &= 0 \\
M_{ij} \left[v_j - \dot{q}_j \right] &= 0
\end{aligned} \tag{7.163}$$

respectively. Obviously, Eq. (7.163) leads to Eq. (7.161). ∎

Remark 7.3.3

1. *If* $\vec{\mathbf{r}}_\ell = \vec{\mathbf{r}}_\ell(\mathbf{q})$, *Eq.* (7.161) *yields:*

$$\mathfrak{E}_i[\mathscr{L}^*(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t)] = M_{ij}(\mathbf{q}) \dot{v}_j + Q_i^{\mathrm{con}}(\mathbf{q}, t) = Q_i^{\mathrm{ncon}} \tag{7.164}$$

together with $\dot{q}_i(t) = v_i(t)$.

Hamilton's Canonical Equations

Introducing new variables, $v_i = [\mathbf{v}]_i \in \mathbb{R}$ for $i = 1, 2, \cdots, n_g$, in such a way that

$$v_i = \dot{q}_i, \text{ i.e., } \phi_i := v_i - \dot{q}_i = 0 \tag{7.165}$$

define the modified Lagrangian function as

$$\mathscr{L}_H(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, \mathbf{p}, t) := \mathscr{L}(\mathbf{q}, \mathbf{v}, t) - p_i\phi_i \tag{7.166}$$

where the Lagrangian function, $\mathscr{L}(\mathbf{q}, \mathbf{v}, t)$, is defined as

$$\mathscr{L}(\mathbf{q}, \mathbf{v}, t) = \mathscr{K}(\mathbf{q}, \mathbf{v}, t) + \mathscr{U}(\mathbf{q}, t) \tag{7.167}$$

and $p_i(t) = [\mathbf{p}(t)]_i : \mathbb{I} \to \mathbb{R}$ (for $i = 1, 2, \cdots, n_g$) are the ***Lagrange multipliers***.

Theorem 7.3.10 (Hamilton's Principle for Hamilton's Canonical Equations)

The variational principle, represented by

$$\boxed{\delta\mathscr{I}_H + \int_{t_0}^{t_L} \delta W^{\text{ncon}} dt = 0} \tag{7.168}$$

with the condition,

$$\delta\mathbf{q}(t_0) = \delta\mathbf{q}(t_L) = \mathbf{0}, \tag{7.169}$$

where the action integral, $\mathscr{I}_H$, is defined as

$$\mathscr{I}_H[\mathbf{q}, \mathbf{v}, \mathbf{p}] := \int_{t_0}^{t_L} \mathscr{L}_H(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, \mathbf{p}, t)dt, \tag{7.170}$$

can be equivalently written as the variational principle, represented as

$$\boxed{\delta \int_{t_0}^{t_L} \left[p_i\dot{q}_i - \mathscr{H}(\mathbf{q}, \mathbf{p}, t)\right] dt + \int_{t_0}^{t_L} \delta W^{\text{ncon}} dt = 0} \tag{7.171}$$

with the restriction, Eq. (7.169)*. Function* $\mathscr{H}$*, known as the* ***Hamiltonian function****, is defined as*

$$\mathscr{H}(\mathbf{q}, \mathbf{p}, t) := p_i v_i(\mathbf{q}, \mathbf{p}, t) - \mathscr{L}(\mathbf{q}, \mathbf{v}(\mathbf{q}, \mathbf{p}, t), t) \tag{7.172}$$

Eq. (7.171) *with the subsidiary condition, Eq.* (7.169)*, is equivalent to*

$$\boxed{\begin{aligned} \dot{p}_i &= -\frac{\partial \mathscr{H}}{\partial q_i} + Q_i^{\text{ncon}} \\ \dot{q}_i &= \frac{\partial \mathscr{H}}{\partial p_i} \end{aligned}} \tag{7.173}$$

which are known as the ***Hamilton's canonical equations****.*

Proof. Following a similar procedure in Eq. (7.162), Eq. (7.168), under the subsidiary condition, Eq. (7.169), yields:

$$\begin{aligned} 0 &= \int_{t_0}^{t_{\mathrm{L}}} \left[\frac{\partial \mathscr{L}_{\mathrm{H}}}{\partial q_i} \delta q_i + \frac{\partial \mathscr{L}_{\mathrm{H}}}{\partial \dot{q}_i} \delta \dot{q}_i + \frac{\partial \mathscr{L}_{\mathrm{H}}}{\partial v_i} \delta v_i + \frac{\partial \mathscr{L}_{\mathrm{H}}}{\partial p_i} \delta p_i + Q_i^{\text{ncon}} \delta q_i \right] dt \\ &= \int_{t_0}^{t_{\mathrm{L}}} \left(\mathfrak{E}_i[\mathscr{L}_{\mathrm{H}}] - Q_i^{\text{ncon}} \right) \delta q_i dt - \underbrace{\left. \frac{\partial \mathscr{L}_{\mathrm{H}}}{\partial q_i} \delta q_i \right|_{t_0}^{t_{\mathrm{L}}}}_{0 \because \text{Eq.(7.169)}} \\ &\quad - \int_{t_0}^{t_{\mathrm{L}}} \frac{\partial \mathscr{L}_{\mathrm{H}}}{\partial v_i} \delta v_i dt - \int_{t_0}^{t_{\mathrm{L}}} \frac{\partial \mathscr{L}_{\mathrm{H}}}{\partial p_i} \delta p_i dt \end{aligned} \tag{7.174}$$

Since δq_i, δv_i, and δp_i are independent, we get the following stationary conditions with respect to q_i, v_i, and p_i:

$$\mathfrak{E}_i[\mathscr{L}_{\mathrm{H}}] - Q_i^{\text{ncon}} = 0 \quad \Rightarrow \quad \dot{p}_i = \frac{\partial \mathscr{L}(\mathbf{q}, \mathbf{v}, t)}{\partial q_i} + Q_i^{\text{ncon}} \tag{7.175}$$

$$\frac{\partial \mathscr{L}_{\mathrm{H}}}{\partial v_i} = 0 \quad \Rightarrow \quad p_i = \frac{\partial \mathscr{L}(\mathbf{q}, \mathbf{v}, t)}{\partial v_i} \tag{7.176}$$

$$\frac{\partial \mathscr{L}_{\mathrm{H}}}{\partial p_i} = 0 \quad \Rightarrow \quad \dot{q}_i = v_i \tag{7.177}$$

respectively. Suppose Eq. (7.176) can be solved for v_i in terms of $(\mathbf{q}, \mathbf{p}, t)$ as[2]

$$p_i = \frac{\partial \mathscr{L}(\mathbf{q}, \mathbf{v}, t)}{\partial v_i} \Longrightarrow v_i = v_i(\mathbf{q}, \mathbf{p}, t) \tag{7.180}$$

then, we can express $\mathscr{L}_{\mathrm{H}}$ in terms of $(\mathbf{q}, \mathbf{p}, t)$ as

$$\begin{aligned}
& \mathscr{L}_{\mathrm{H}}(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}(\mathbf{q}, \mathbf{p}, t), \mathbf{p}, t) \\
= \;& \mathscr{L}(\mathbf{q}, \mathbf{v}(\mathbf{q}, \mathbf{p}, t), t) - p_i[v_i(\mathbf{q}, \mathbf{p}, t) - \dot{q}_i] \\
= \;& p_i\dot{q}_i - \underbrace{[p_i v_i(\mathbf{q}, \mathbf{p}, t) - \mathscr{L}(\mathbf{q}, \mathbf{v}(\mathbf{q}, \mathbf{p}, t), t)]}_{=:\mathscr{H}(\mathbf{q}, \mathbf{p}, t)} \\
= \;& p_i\dot{q}_i - \mathscr{H}(\mathbf{q}, \mathbf{p}, t)
\end{aligned} \tag{7.181}$$

where $\mathscr{H}(\mathbf{q}, \mathbf{p}, t)$ is the Hamiltonian function of the system, defined in Eq. (7.172).

Now, we can re-write Eq. (7.168) with the Hamiltonian function as Eq. (7.171). With the restriction, Eq. (7.169), Eq. (7.171) yields

$$\begin{aligned}
0 &= \int_{t_0}^{t_{\mathrm{L}}} \left[(\delta p_i)\dot{q}_i + p_i\delta\dot{q}_i - \frac{\partial \mathscr{H}}{\partial q_i}\delta q_i - \frac{\partial \mathscr{H}}{\partial p_i}\delta p_i + Q_i^{\mathrm{ncon}}\delta q_i\right] dt \\
&= \int_{t_0}^{t_{\mathrm{L}}} \left[-\dot{p}_i - \frac{\partial \mathscr{H}}{\partial q_i} + Q_i^{\mathrm{ncon}}\right]\delta q_i + \underbrace{p_i\delta q_i|_{t_0}^{t_{\mathrm{L}}}}_{0 \,\because\, \mathrm{Eq.(7.169)}} \\
&\quad + \int_{t_0}^{t_{\mathrm{L}}} \left[\dot{q}_i - \frac{\partial \mathscr{H}}{\partial p_i}\right]\delta p_i dt
\end{aligned} \tag{7.182}$$

Since δq_i and δp_i are independent, we finally obtain the ***Hamilton's canonical equations***, given in Eq. (7.173). ∎

[2] We assume the following condition holds:

$$\det\left(\frac{\partial^2 \mathscr{L}(\mathbf{q}, \mathbf{v}, t)}{\partial v_i \partial v_j}\right) = \det\left(\frac{\partial p_i}{\partial v_j}\right) \neq 0 \tag{7.178}$$

so that the inverse transformation,

$$v_i = v_i(\mathbf{q}, \mathbf{p}, t) \Longrightarrow p_i = \frac{\partial \mathscr{L}(\mathbf{q}, \mathbf{v}, t)}{\partial v_i} \tag{7.179}$$

is also possible.

Remark 7.3.4

1. *In the Lagrange formalism, only the generalized coordinates, $q_i(t)$, are independent; whilst, in the Hamilton formalism, the canonical momenta, $p_i(t)$, as well as the generalized coordinates, $q_i(t)$, are independent. It is important to notice that te generalized velocities, $\dot{q}_i(t)$, are dependent variables.*

2. *The transition from the generalized coordinates, $\mathbf{q}(t)$, to $\mathbf{z}(t) := (\mathbf{q}^T, \mathbf{p}^T)^T(t)$, known as the the **canonical variables**, is achieved via the so-called the **Legendre transformation**: Taking the differential of the Lagrangian function, $\mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}, t)$, we have*

$$d\mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}, t) = \frac{\partial \mathscr{L}}{\partial q_i} dq_i + \frac{\partial \mathscr{L}}{\partial \dot{q}_i} d\dot{q}_i + \frac{\partial \mathscr{L}}{\partial t} dt = a_i^1 dq_i + a_i^2 d\dot{q}_i + a^3 dt \tag{7.183}$$

where $a_i^1 := \partial \mathscr{L} / \partial q_i$, $a_i^2 := \partial \mathscr{L} / \partial \dot{q}_i$, and $a^3 := \partial \mathscr{L} / \partial t$. By defining a new function, F, in the form

$$F := a_i^2 \dot{q}_i - \mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}, t) \tag{7.184}$$

we write the differential as

$$\begin{aligned} dF &= d\left(a_i^2 \dot{q}_i\right) - d\mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}, t) \\ &= \dot{q}_i da_i^2 + a_i^2 d\dot{q}_i - \underbrace{\frac{\partial \mathscr{L}}{\partial q_i}}_{a_i^1} dq_i - \underbrace{\frac{\partial \mathscr{L}}{\partial \dot{q}_i}}_{a_i^2} d\dot{q}_i - \underbrace{\frac{\partial \mathscr{L}}{\partial t}}_{a^3} dt \\ &= -a_i^1 dq_i + \dot{q}_i da_i^2 - a^3 dt \end{aligned} \tag{7.185}$$

Comparison between Eq. (7.183) and Eq. (7.185) shows that the argument of the new function, F, are q_i, a_i^2, and t while the arguments of the Lagrangian function are q_i, $\dot{q}_i$, and t. Function F is actually the Hamiltonian, $\mathscr{H}(\mathbf{q}, \mathbf{p}, t)$, defined in Eq. (7.172), which is a function of the generalized coordinates, q_i, canonical momenta, $p_i \equiv a_i^2 = \partial \mathscr{L} / \partial \dot{q}_i$, and time t.

From Eq. (7.185), *we have*

$$d\mathscr{H} = dF = -\frac{\partial \mathscr{L}}{\partial q_i} dq_i + \dot{q}_i dp_i - \frac{\partial \mathscr{L}}{\partial t} dt \tag{7.186}$$

Invoking Lagrange's equation of motion, $\mathfrak{E}_i[\mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}, t)] = Q_i^{\text{ncon}}$, *i.e.,*

$$\mathfrak{E}_i[\mathscr{L}] = \frac{d}{dt} \underbrace{\left(\frac{\partial \mathscr{L}}{\partial \dot{q}_i} \right)}_{p_i} - \frac{\partial \mathscr{L}}{\partial q_i} = Q_i^{\text{ncon}} \tag{7.187}$$

Eq. (7.186) *can be written as*

$$d\mathscr{H} = dF = \left[Q_i^{\text{ncon}} - \dot{p}_i \right] dq_i + \dot{q}_i dp_i - \frac{\partial \mathscr{L}}{\partial t} dt \tag{7.188}$$

Comparing the coefficients of dq_i, dp_i, *and* dt *in Eq.* (7.188) *with the coefficients of* dq_i, dp_i, *and* dt, *respectively, in the equation given by taking the direct differential of* $\mathscr{H}(\mathbf{q}, \mathbf{p}, t)$, *i.e.,*

$$d\mathscr{H} = \frac{\partial \mathscr{H}}{\partial q_i} dq_i + \frac{\partial \mathscr{H}}{\partial p_i} dp_i + \frac{\partial \mathscr{H}}{\partial t} dt \tag{7.189}$$

we readily obtain Hamilton's canonical equations, Eq. (7.173), *together with*

$$-\frac{\partial \mathscr{L}}{\partial t} = \frac{\partial \mathscr{H}}{\partial t} \tag{7.190}$$

3. *Hamilton's canonical equations, given in Eq.* (7.173), *can be written, with* ***Poisson's bracket*** *(see Definition 2.4.2), as:*

$$\boxed{\begin{aligned} \dot{p}_i &= [p_i, \mathscr{H}] + Q_i^{\text{ncon}} \\ \dot{q}_i &= [q_i, \mathscr{H}] \end{aligned}} \tag{7.191}$$

If $Q_i^{\text{ncon}} = 0$, *we have*

$$\boxed{\begin{aligned} \dot{p}_i &= [p_i, \mathscr{H}] \\ \dot{q}_i &= [q_i, \mathscr{H}] \end{aligned}} \tag{7.192}$$

Hamilton's Principle for Constrained Systems

Single-field form: If there exist ***holonomic*** constraints[3] in a system, we now need to modify the unconstrained problem,

$$\text{minimize } \mathscr{I}[\mathbf{q}] \tag{7.193}$$

so that holonomic constraint equations, $\mathbf{\Phi} = \mathbf{0}$, are included:

$$\text{minimize } \mathscr{I}[\mathbf{q}] \;\; s.t. \;\; \mathbf{\Phi} = \mathbf{0} \tag{7.194}$$

The problem, describe in Eq. (7.194), may be actually treated as an unconstrained problem with a modified action integral, $\widetilde{\mathscr{I}}[\mathbf{q}]$, as

$$\text{minimize } \widetilde{\mathscr{I}}[\mathbf{q}, \boldsymbol{\lambda}] \tag{7.195}$$

The most basic form of $\widetilde{\mathscr{I}}[\mathbf{q}, \boldsymbol{\lambda}]$ is achieved by the ***Lagrange multiplier method***: Making use of n_{c} numbers of the Lagrange multipliers, $\lambda_k = [\boldsymbol{\lambda}]_k$ (for $k = 1, 2, \cdots, n_{\mathrm{c}}$), define

$$\widetilde{\mathscr{I}}[\mathbf{q}, \boldsymbol{\lambda}] := \int_{t_0}^{t_{\mathrm{L}}} \widetilde{\mathscr{L}}(\mathbf{q}, \dot{\mathbf{q}}, \boldsymbol{\lambda}, t) dt \tag{7.196}$$

where the modified Lagrangian function is given as

$$\begin{aligned} \widetilde{\mathscr{L}}(\mathbf{q}, \dot{\mathbf{q}}, \boldsymbol{\lambda}, t) &:= \mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}, t) - \lambda_k \Phi_k \\ &= \mathscr{T}(\mathbf{q}, \dot{\mathbf{q}}, t) - \mathscr{U}(\mathbf{q}, t) - \lambda_k \Phi_k \end{aligned} \tag{7.197}$$

($\lambda_k \Phi_k = \boldsymbol{\lambda}^T \mathbf{\Phi} = \mathbf{\Phi}^T \boldsymbol{\lambda}$). Holonomic constraint equations can be holonomic-scleronomic or holonomic-rheonomic; however, we assume they are holonomic-rheonomic in the following discussions in this subsection, i.e., $\Phi_k(\mathbf{q}, t) = [\mathbf{\Phi}(\mathbf{q}, t)]_k$ for $k = 1, 2, \cdots, n_{\mathrm{c}}$, since holonomic-scleronomic constraints, i.e., $\Phi_k(\mathbf{q}) = [\mathbf{\Phi}(\mathbf{q})]_k$, are just special cases.

[3] See Definition 6.1.1

Theorem 7.3.11

Hamilton's Principle for Constrained Systems: Lagrange Multiplier Method

Hamilton's principle for holonomic constrained systems reads:

$$\boxed{\delta\widetilde{\mathscr{I}} + \int_{t_0}^{t_L} \delta W^{\mathrm{ncon}} dt = 0} \tag{7.198}$$

where the modified action integral is defined in Eq. (7.196)*. Eq.* (7.198) *with the subsidiary condition,*

$$\delta\mathbf{q}(t_0) = \delta\mathbf{q}(t_L) = \mathbf{0}, \tag{7.199}$$

is equivalent to Lagrange's equation of motion with the holonomic constraint equation:

$$\boxed{\begin{aligned} \mathfrak{E}_i[\mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}, t)] + \lambda_k G_{ki} &= Q_i^{\mathrm{ncon}} \\ \Phi_k(\mathbf{q}, t) &= 0 \end{aligned}} \tag{7.200}$$

(for $i = 1, 2, \cdots, n_g$ and $k = 1, 2, \cdots, n_c$) where $\mathbf{G} \in \mathbb{R}^{n_c \times n_g}$ is defined as $G_{ki} = [\mathbf{G}]_{ki} :=$ $\partial_i \Phi_k = \frac{\partial \Phi_k}{\partial q_i}$ (see Eq. (6.4)*).*

Proof. From Eq. (7.198), we have

$$\begin{aligned} 0 &= \int_{t_0}^{t_L} \delta\left[\mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}, t) - \lambda_i \Phi_i(\mathbf{q}, t)\right] dt + \int_{t_0}^{t_L} \delta W^{\mathrm{ncon}} dt \\ &= \int_{t_0}^{t_L} \left[\frac{\partial \mathscr{L}}{\partial q_i}\delta q_i + \frac{\partial \mathscr{L}}{\partial \dot{q}_i}\delta \dot{q}_i - \Phi_k \delta\lambda_k - \lambda_k \underbrace{\delta\Phi_k}_{G_{ki}\delta q_i} + Q_i^{\mathrm{ncon}}\delta q_i\right] dt \\ &= -\int_{t_0}^{t_L} \left(\mathfrak{E}_i[\mathscr{L}] + \lambda_k G_{ki} - Q_i^{\mathrm{ncon}}\right)\delta q_i dt + \underbrace{\frac{\partial \mathscr{L}}{\partial \dot{q}_i}\delta q_i\Big|_{t_0}^{t_L}}_{0 \,\because\, \mathrm{Eq.}(7.199)} \\ &\quad - \int_{t_0}^{t_L} \Phi_k \delta\lambda_k dt \end{aligned} \tag{7.201}$$

Since δq_i (for $i = 1, 2, \cdots, n_g$) and $\delta\lambda_k$ (for $k = 1, 2, \cdots, n_c$) are independent, the stationary conditions with respect to q_i and λ_k are readily obtained as given in Eq. (7.200). ∎

Theorem 7.3.12

[Hamilton's Principle for Constrained Systems: Augmented Lagrange Multiplier Method]

*Define the **augmented action integral** as*

$$\widetilde{\mathscr{I}} := \int_{t_0}^{t_L} \widetilde{\mathscr{L}}(\mathbf{q}, \dot{\mathbf{q}}, \boldsymbol{\lambda}, t)dt \tag{7.202}$$

where the augmented Lagrangian function is defined as

$$\widetilde{\mathscr{L}} := \mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}, t) - \kappa\lambda_k\Phi_k(\mathbf{q}, t) - \frac{\varsigma}{2}\Phi_k(\mathbf{q}, t)\Phi_k(\mathbf{q}, t) \tag{7.203}$$

with a scaling factor, $\kappa \in \mathbb{R}$, and the penalty coefficient, $\varsigma \in \mathbb{R}$.

Then, Hamilton's principle for holonomic constrained systems reads:

$$\boxed{\delta\widetilde{\mathscr{I}} + \int_{t_0}^{t_L} \delta W^{\mathrm{ncon}} dt = 0} \tag{7.204}$$

under the subsidiary condition,

$$\delta\mathbf{q}(t_0) = \delta\mathbf{q}(t_L) = \mathbf{0} \tag{7.205}$$

is equivalent to the system of equations,

$$\boxed{\begin{aligned} \mathfrak{E}_i[\mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}, t)] + (\kappa\,\lambda_k + \varsigma\,\Phi_k)\,G_{ki} &= Q_i^{\mathrm{ncon}} \\ \kappa\,\Phi_k(\mathbf{q}, t) &= 0 \end{aligned}} \tag{7.206}$$

Proof. Eq. (7.204) yields

$$\begin{aligned}
0 &= \int_{t_0}^{t_L} \left[\delta\mathscr{L}(\mathbf{q}, \dot{\mathbf{q}}, t) - \kappa\delta(\lambda_k\Phi_k) - \frac{\varsigma}{2}\delta(\Phi_k\Phi_k) + \delta W^{\text{ncon}} \right] dt \\
&= \int_{t_0}^{t_L} \left[\frac{\partial\mathscr{L}}{\partial q_i}\delta q_i + \frac{\partial\mathscr{L}}{\partial \dot{q}_i}\delta\dot{q}_i - \kappa\Phi_k\delta\lambda_k - \kappa\lambda_k\delta\Phi_k \right. \\
&\quad \left. -\varsigma\,\Phi_k\delta\Phi_k + Q_i^{\text{ncon}}\delta q_i \right] dt \\
&= -\int_{t_0}^{t_L} \left(\mathfrak{E}_i[\mathscr{L}] + \kappa\,\lambda_k G_{ki} + \varsigma\,\Phi_k G_{ki} - Q_i^{\text{ncon}} \right) \delta q_i dt \\
&\quad + \underbrace{\frac{\partial\mathscr{L}}{\partial \dot{q}_i}\delta q_i \Big|_{t_0}^{t_L}}_{0\,\because\,\text{Eq.(7.205)}} - \int_{t_0}^{t_L} \kappa\,\Phi_k\delta\lambda_k dt
\end{aligned} \tag{7.207}$$

Since δq_i (for $i = 1, 2, \cdots, n_g$) and $\delta\lambda_k$ (for $k = 1, 2, \cdots, n_c$) are independent, the stationary conditions with respect to q_i and λ_k are readily obtained as given in Eq. (7.206). ∎

Two-field form: Hamilton's principle for nonconstrained systems (see Theorem 7.3.9) can be extended to constrained systems by introducing $v_i(t) = [\mathbf{v}(t)]_i : \mathbb{I} \to \mathbb{R}$ (for $i = 1, 2, \cdots, n_g$).

Theorem 7.3.13 (Hamilton's Principle for Constrained Systems)

Define the modified action integral as

$$\widetilde{\mathscr{I}^*}[\mathbf{q}, \mathbf{v}, \boldsymbol{\lambda}] := \int_{t_0}^{t_L} \widetilde{\mathscr{L}^*}(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t) dt \tag{7.208}$$

with the modified Lagrangian function defined as

$$\widetilde{\mathscr{L}^*}(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, \boldsymbol{\lambda}, t) := \mathscr{L}^*(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t) - \lambda_k\Phi_k \tag{7.209}$$

for the Lagrange multiplier method, or

$$\widetilde{\mathscr{L}^*}(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, \boldsymbol{\lambda}, t) := \mathscr{L}^*(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t) - \kappa\lambda_k\Phi_k(\mathbf{q}, t) - \frac{\varsigma}{2}\Phi_k(\mathbf{q}, t)\Phi_k(\mathbf{q}, t) \tag{7.210}$$

for the augmented Lagrange multiplier method.

Then, the stationary principle for constrained systems reads:

$$\boxed{\delta\widetilde{\mathscr{I}^*} + \int_{t_0}^{t_\mathrm{L}} \delta W^{\mathrm{ncon}} dt = 0,} \tag{7.211}$$

under the subsidiary conditions,

$$\delta\mathbf{q}(t_0) = \delta\mathbf{q}(t_\mathrm{L}) = \mathbf{0}, \tag{7.212}$$

is equivalent to:

$$\boxed{\begin{aligned} \mathfrak{E}_i[\mathscr{L}^*(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t)] + \lambda_k G_{ki} &= Q_i^{\mathrm{ncon}} \\ \dot{\mathbf{q}}(t) &= \mathbf{v}(t) \\ \Phi_k(\mathbf{q}, t) &= 0 \end{aligned}} \tag{7.213}$$

for the Lagrange multiplier method, and

$$\boxed{\begin{aligned} \mathfrak{E}_i[\mathscr{L}^*(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t)] + [\kappa\, \lambda_k + \varsigma\, \Phi_k]\, G_{ki} &= Q_i^{\mathrm{ncon}} \\ \dot{\mathbf{q}}(t) &= \mathbf{v}(t) \\ \kappa\, \Phi_k(\mathbf{q}, t) &= 0 \end{aligned}} \tag{7.214}$$

for the augmented Lagrange method.

Proof. Consider the case of the augmented Lagrange multiplier method. From Eq. (7.211), we have

$$0 = \int_{t_0}^{t_\mathrm{L}} \delta\left[\mathscr{L}^*(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t) - \kappa\, \lambda_k \Phi_k - \frac{\varsigma}{2}\Phi_k\, \Phi_k\right] dt + \int_{t_0}^{t_\mathrm{L}} \delta W^{\mathrm{ncon}} dt \tag{7.215}$$

Since we have

$$\int_{t_0}^{t_\mathrm{L}} \delta\mathscr{L}^*(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t) dt = -\int_{t_0}^{t_\mathrm{L}} \mathfrak{E}_i[\mathscr{L}^*(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t)] dt + \underbrace{\left.\frac{\partial \mathscr{L}^*}{\partial q_i}\delta q_i\right|_{t_0}^{t_\mathrm{L}}}_{0\ \because\ \mathrm{Eq.(7.212)}} \tag{7.216}$$

in view of Eq. (7.162) in the proof of Theorem 7.3.9 and

$$\kappa\,\delta(\lambda_k\Phi_k) + \frac{\varsigma}{2}\delta(\Phi_k\,\Phi_k) = [\kappa\,\lambda_k + \varsigma\,\Phi_k]\,G_{ki} + \kappa\,\Phi_k\delta\lambda_k \tag{7.217}$$

in view of Eq. (7.207) in the proof of Theorem 7.3.12, Eq. (7.215) can be written in the form

$$\begin{aligned} 0 = &\int_{t_0}^{t_L} (\mathfrak{E}_i[\mathscr{L}^*(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, t)]dt + [\kappa\,\lambda_k + \varsigma\,\Phi_k]\,G_{ki} - Q_i^{\mathrm{ncon}})\,\delta q_i\,dt \\ &- \int_{t_0}^{t_L} M_{ij}\left[\dot{q}_j - v_j\right]\delta v_i dt + \int_{t_0}^{t_L} \kappa\,\Phi_k\delta\lambda_k\,dt \end{aligned} \tag{7.218}$$

Hence, the stationary conditions with respect to q_i, v_i, and λ_k are obtained as Eq. (7.214). When Eq. (7.214) is satisfied, it is obvious that Eq. (7.211) is also satisfied. For $\kappa = 1$ and $\varsigma = 0$, we readily have the proof for the case of the Lagrange multiplier method. ∎

Hamilton's Canonical Equations for Constrained Systems

Following a similar procedure in Subsection 7.3.2, the Hamilton's principle for the Hamilton's canonical equations for constrained systems are summarized as follows:

Theorem 7.3.14 (Hamilton's Principle for Hamilton's Canonical Equations)
Define the modified action integral as

$$\widetilde{\mathscr{I}_{\mathrm{H}}}[\mathbf{q}, \mathbf{v}, \mathbf{p}, \boldsymbol{\lambda}] := \int_{t_0}^{t_L} \widetilde{\mathscr{L}_{\mathrm{H}}}(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, \mathbf{p}, \boldsymbol{\lambda}, t)\,dt \tag{7.219}$$

where the modified Lagrangian function is defined as

$$\widetilde{\mathscr{L}_{\mathrm{H}}}(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, \mathbf{p}, \boldsymbol{\lambda}, t) := \mathscr{L}_{\mathrm{H}}(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, \mathbf{p}, t) - \lambda_k\,\Phi_k \tag{7.220}$$

for the Lagrange multiplier method and

$$\widetilde{\mathscr{L}_{\mathrm{H}}}(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, \mathbf{p}, \boldsymbol{\lambda}, t) := \mathscr{L}_{\mathrm{H}}(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, \mathbf{p}, t) - \kappa\,\lambda_k\,\Phi_k - \frac{\varsigma}{2}\,\Phi_k\,\Phi_k \tag{7.221}$$

for the augmented Lagrange Multiplier method, in which $\mathscr{L}_{\mathrm{H}}$ *is given as in Eq.* (7.166), *i.e.,*

$$\mathscr{L}_{\mathrm{H}}(\mathbf{q}, \dot{\mathbf{q}}, \mathbf{v}, \mathbf{p}, t) := \mathscr{L}(\mathbf{q}, \mathbf{v}, t) - p_i \left[v_i - \dot{q}_i\right] \tag{7.222}$$

Then, the variational principle, represented by

$$\boxed{\delta \widetilde{\mathscr{I}_{\mathrm{H}}} + \int_{t_0}^{t_{\mathrm{L}}} \delta W^{\mathrm{ncon}} dt = 0} \tag{7.223}$$

with the subsidiary condition,

$$\delta \mathbf{q}(t_0) = \delta \mathbf{q}(t_{\mathrm{L}}) = \mathbf{0}, \tag{7.224}$$

can be equivalently written as the variational principle,

$$\boxed{\delta \int_{t_0}^{t_{\mathrm{L}}} \left[p_i \dot{q}_i - \widetilde{\mathscr{H}}(\mathbf{q}, \mathbf{p}, \boldsymbol{\lambda}, t)\right] dt + \int_{t_0}^{t_{\mathrm{L}}} \delta W^{\mathrm{ncon}} dt = 0} \tag{7.225}$$

with the restriction, Eq. (7.224)*. The modified Hamiltonian function,* $\widetilde{\mathscr{H}}$*, is defined as*

$$\widetilde{\mathscr{H}}(\mathbf{q}, \mathbf{p}, \boldsymbol{\lambda}, t) := p_i v_i(\mathbf{q}, \mathbf{p}, t) - \widetilde{\mathscr{L}^*}(\mathbf{q}, \mathbf{v}(\mathbf{q}, \mathbf{p}, t), \boldsymbol{\lambda}, t) \tag{7.226}$$

in which

$$\widetilde{\mathscr{L}^*}(\mathbf{q}, \mathbf{v}(\mathbf{q}, \mathbf{p}, t), \boldsymbol{\lambda}, t) := \mathscr{L}(\mathbf{q}, \mathbf{v}(\mathbf{q}, \mathbf{p}, t), t) - \lambda_k \Phi_k \tag{7.227}$$

for the Lagrange multiplier method and

$$\widetilde{\mathscr{L}^*}(\mathbf{q}, \mathbf{v}(\mathbf{q}, \mathbf{p}, t), \boldsymbol{\lambda}, t) := \mathscr{L}(\mathbf{q}, \mathbf{v}(\mathbf{q}, \mathbf{p}, t), t) - \kappa \lambda_k \Phi_k - \frac{\varsigma}{2} \Phi_k \Phi_k \tag{7.228}$$

for the augmented Lagrange multiplier method.

Eq. (7.225) *with the subsidiary condition, Eq.* (7.224)*, is equivalent to Hamilton's* *canonical equations for constrained systems:*

$$\boxed{\begin{aligned} \dot{p}_i &= -\frac{\partial \mathscr{H}}{\partial q_i} - \lambda_k\, G_{ki} + Q_i^{\text{ncon}} \\ \dot{q}_i &= \frac{\partial \mathscr{H}}{\partial p_i} \\ \Phi_k(\mathbf{q}, t) &= 0 \end{aligned}} \tag{7.229}$$

for the Lagrange multiplier method, and

$$\boxed{\begin{aligned} \dot{p}_i &= -\frac{\partial \mathscr{H}}{\partial q_i} - [\kappa\, \lambda_k + \varsigma\, \Phi_k]\, G_{ki} + Q_i^{\text{ncon}} \\ \dot{q}_i &= \frac{\partial \mathscr{H}}{\partial p_i} \\ \kappa\, \Phi_k(\mathbf{q}, t) &= 0 \end{aligned}} \tag{7.230}$$

for the augmented Lagrange multiplier method.

Proof. Consider the case of the augmented Lagrange multiplier method since the proof for the Lagrange multiplier method can be readily reduced from it. Following a similar procedure shown in the proof for Theorem 7.3.10, we can obtain

$$\begin{aligned} 0 \;\; = \;\; & -\left[\frac{d}{dt}\left(\frac{\partial \mathscr{L}_{\text{H}}}{\partial \dot{q}_i}\right) - \frac{\partial \mathscr{L}_{\text{H}}}{\partial q_i} + (\kappa\, \lambda_k + \varsigma\, \Phi_k)\, G_{ki} - Q_i^{\text{ncon}}\right] \delta q_i \\ & + \kappa\, \Phi_k \delta\lambda_k - \frac{\partial \mathscr{L}_{\text{H}}}{\partial v_i}\delta v_i - \frac{\partial \mathscr{L}_{\text{H}}}{\partial p_i}\delta p_i - \underbrace{\frac{\partial \mathscr{L}^*}{\partial q_i}\delta q_i\bigg|_{t_0}^{t_{\text{L}}}}_{0\,\because\,\text{Eq.(7.224)}} \end{aligned} \tag{7.231}$$

from Eq. (7.223) with Eq. (7.224); therefore, the stationary conditions with respect to q_i, p_i, λ_k, and v_i are given as:

$$\dot{p}_i - \frac{\partial \mathscr{L}(\mathbf{q}, \mathbf{v}, t)}{\partial q_i} \;\; = \;\; Q_i^{\text{ncon}} - (\kappa\, \lambda_k + \varsigma\, \Phi_k)\, G_{ki} \tag{7.232}$$

$$\dot{q}_i \;\; = \;\; v_i \tag{7.233}$$

$$\kappa\, \Phi_k \;\; = \;\; 0 \tag{7.234}$$

$$p_i \;\; = \;\; \frac{\partial \mathscr{L}(\mathbf{q}, \mathbf{v}, t)}{\partial v_i} \tag{7.235}$$

respectively. Suppose we have

$$p_i = \frac{\partial \mathscr{L}(\mathbf{q}, \mathbf{v}, t)}{\partial v_i} \Longleftrightarrow v_i = v_i(\mathbf{q}, \mathbf{p}, t) \tag{7.236}$$

from Eq. (7.235); then,

$$\begin{aligned}
\widetilde{\mathscr{L}_{\mathrm{H}}} &= \mathscr{L}(\mathbf{q}, \mathbf{v}(\mathbf{q}, \mathbf{p}, t), t) - p_i \left[v_i(\mathbf{q}, \mathbf{p}, t) - \dot{q}_i \right] - \kappa\, \lambda_k\, \Phi_k - \frac{\varsigma}{2}\, \Phi_k\, \Phi_k \\
&= p_i \dot{q}_i - \underbrace{[\overbrace{p_i v_i(\mathbf{q}, \mathbf{p}, t) - \mathscr{L}(\mathbf{q}, \mathbf{v}(\mathbf{q}, \mathbf{p}, t), t)}^{\mathscr{H}(\mathbf{q}, \mathbf{p}, t)} + \kappa\, \lambda_k\, \Phi_k + \frac{\varsigma}{2}\, \Phi_k\, \Phi_k]}_{=: \widetilde{\mathscr{H}}(\mathbf{q}, \mathbf{p}, \boldsymbol{\lambda}, t)} \\
&= p_i \dot{q}_i - \widetilde{\mathscr{H}}(\mathbf{q}, \mathbf{p}, \boldsymbol{\lambda}, t)
\end{aligned} \tag{7.237}$$

or

$$\widetilde{\mathscr{H}}(\mathbf{q}, \mathbf{p}, \boldsymbol{\lambda}, t) := \mathscr{H}(\mathbf{q}, \mathbf{p}, t) + \kappa\, \lambda_k\, \Phi_k + \frac{\varsigma}{2}\, \Phi_k\, \Phi_k \tag{7.238}$$

Therefore,

$$\begin{aligned}
0 &= \delta \int_{t_0}^{t_{\mathrm{L}}} \left[p_i \dot{q}_i - \widetilde{\mathscr{H}}(\mathbf{q}, \mathbf{p}, \boldsymbol{\lambda}, t) \right] dt + \int_{t_0}^{t_{\mathrm{L}}} \delta W^{\mathrm{ncon}} dt \\
&= \int_{t_0}^{t_{\mathrm{L}}} \left[\dot{q}_i \delta p_i + p_i \delta \dot{q}_i - \frac{\partial \widetilde{\mathscr{H}}}{\partial q_i} \delta q_i - \frac{\partial \widetilde{\mathscr{H}}}{\partial p_i} \delta p_i - \frac{\partial \widetilde{\mathscr{H}}}{\partial \lambda_k} \delta \lambda_k + Q_i^{\mathrm{ncon}} \delta q_i \right] dt \\
&= \int_{t_0}^{t_{\mathrm{L}}} \left[\dot{q}_i - \frac{\partial \widetilde{\mathscr{H}}}{\partial p_i} \right] \delta p_i dt - \int_{t_0}^{t_{\mathrm{L}}} \frac{\partial \widetilde{\mathscr{H}}}{\partial \lambda_k} \lambda_k dt \\
&\quad + \int_{t_0}^{t_{\mathrm{L}}} \left[-\frac{\partial \widetilde{\mathscr{H}}}{\partial q_i} + Q_i^{\mathrm{ncon}} - \dot{p}_i \right] \delta q_i dt + \underbrace{p_i \delta q_i |_{t_0}^{t_{\mathrm{L}}}}_{0 \because \mathrm{Eq.}(7.224)}
\end{aligned} \tag{7.239}$$

Since we have

$$\frac{\partial \widetilde{\mathscr{H}}}{\partial q_i} = \frac{\partial \mathscr{H}(\mathbf{q}, \mathbf{p}, t)}{\partial q_i} + \kappa\, \lambda_k\, G_{ki} + \varsigma\, \Phi_k\, G_{ki} \tag{7.240}$$

$$\frac{\partial \widetilde{\mathscr{H}}}{\partial p_i} = \frac{\partial \mathscr{H}(\mathbf{q}, \mathbf{p}, t)}{\partial p_i} \tag{7.241}$$

$$\frac{\partial \widetilde{\mathscr{H}}}{\partial \lambda_k} = \kappa\, \Phi_k \tag{7.242}$$

the stationary conditions with respect to q_i, p_i, and λ_k are obtained as Hamilton's canonical equations for constrained systems, shown in Eq. (7.230), respectively. ∎

Chapter 8

Flexible Multibody Dynamics

8.1 Absolute Nodal Coordinate (ANC) Formulation

8.1.1 ANC Formation in $\mathbb{E}^2$

Suppose we have a system of n_{b} beams in $\mathbb{E}^2$, and consider the I^{th} element (Ω_I) at time $t \in (t_0, t_L] \subset \mathbb{R}$, as shown in Fig. 8.1. Let $\mathcal{B}_0 : (\mathbf{O}; \{{}^{\mathcal{B}_0}\vec{\mathbf{e}}_\ell\}_{\ell=1}^2)$ and $\mathcal{B}_I : (\mathbf{P}_1^I; \{{}^{\mathcal{B}_I}\vec{\mathbf{e}}_\ell\}_{\ell=1}^2)$ be the inertial reference Cartesian frame fixed in $\mathbb{E}^2$ and the body-fixed Cartesian frame of Ω_I, respectively. The position vectors of the end points of element I, i.e., $\mathbf{P}_1^I$ and $\mathbf{P}_2^I$, are given as

$$\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P}_1^I) = {}^{\mathcal{B}_0}\mathbf{e}^T \left[{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{P}_1^I)\right] =: {}^{\mathcal{B}_0}\mathbf{e}^T \begin{bmatrix} \Upsilon_1 \\ \Upsilon_2 \end{bmatrix} \tag{8.1}$$

$$\vec{\boldsymbol{\pi}}(\mathbf{O}, \mathbf{P}_2^I) = {}^{\mathcal{B}_0}\mathbf{e}^T \left[{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{P}_2^I)\right] =: {}^{\mathcal{B}_0}\mathbf{e}^T \begin{bmatrix} \Upsilon_5 \\ \Upsilon_6 \end{bmatrix} \tag{8.2}$$

respectively, where $\Upsilon_1(t)$, $\Upsilon_2(t)$ $\Upsilon_5(t)$, and $\Upsilon_6(t)$ are the element nodal coordinates (positions) with respect to $\mathcal{B}_0$. Using an arbitrary position vector, $\vec{\mathbf{R}} := \vec{\pi}(\mathbf{O}, \mathbf{P}^I)$ for $\mathbf{P}^I \in \Omega_I$,

$$\begin{bmatrix} {}^{\mathcal{B}_0}\mathbf{R}\big|_{X=0} \\ {}^{\mathcal{B}_0}\mathbf{R}\big|_{X=L_0} \end{bmatrix} = [\Upsilon_1, \Upsilon_2, \Upsilon_5, \Upsilon_6]^T \tag{8.3}$$

where $L_0 > 0$ denotes the natural length of the element, i.e., the length of the beam in the unreformed configuration. The element nodal coordinates (slopes) with respect to $\mathcal{B}_0$ are defined as

$$\begin{bmatrix} \frac{\partial}{\partial X}\big|_{X=0} {}^{\mathcal{B}_0}\mathbf{R} \\ \frac{\partial}{\partial X}\big|_{X=L_0} {}^{\mathcal{B}_0}\mathbf{R} \end{bmatrix} = [\Upsilon_3, \Upsilon_4, \Upsilon_7, \Upsilon_8]^T \tag{8.4}$$

Therefore, the vector of the nodal coordinates for element I is given by

$$\boldsymbol{\Upsilon} = \begin{bmatrix} \Upsilon_1 & \Upsilon_2 & \Upsilon_3 & \Upsilon_4 & \Upsilon_5 & \Upsilon_6 & \Upsilon_7 & \Upsilon_8 \end{bmatrix}^T \in \mathbb{R}^8 \tag{8.5}$$

Using $\boldsymbol{\Upsilon}$, given above, the position vector, $\vec{\pi}(\mathbf{O}, \mathbf{P}^I) =: \vec{\mathbf{R}} = {}^{\mathcal{B}_0}\mathbf{e}^{T\,\mathcal{B}_0}\mathbf{R}$, may be expressed with the global shape function, $\mathbf{S}$, as[1]

$$\boxed{{}^{\mathcal{B}_0}\mathbf{R} = \mathbf{S}\boldsymbol{\Upsilon}} \tag{8.7}$$

[1] We employ the cubic interpolation functions for the components of ${}^{\mathcal{B}_0}\mathbf{R}$. For the X-component,

$$ {}^{\mathcal{B}_0}R_1 \simeq {}^{\mathcal{B}_0}R_1^h = c_0 + c_1 X + c_2 X^2 + c_3 X^3 \tag{8.6}$$

The coefficients, c_i (for $i = 0, 1, 2, 3, 4$), can be determined with the help of the boundary conditions, given in Eq. (8.3) and Eq. (8.4). By repeating a similar procedure for the Y-component, ${}^{\mathcal{B}_0}R_2$, we can obtain Eq. (8.7).

where

$$\mathbf{S} := \begin{bmatrix} 1-3\xi^2+2\xi^3 & 0 \\ 0 & 1-3\xi^2+2\xi^3 \\ L_0(\xi-2\xi^2+\xi^3) & 0 \\ 0 & L_0(\xi-2\xi^2+\xi^3) \\ 3\xi^2-2\xi^3 & 0 \\ 0 & 3\xi^2-2\xi^3 \\ L_0(-\xi^2+\xi^3) & 0 \\ 0 & L_0(-\xi^2+\xi^3) \end{bmatrix}^T \in \mathbb{R}^{2\times 8} \tag{8.8}$$

with $\xi := X/L_0 \in [0,1] \subset \mathbb{R}$. [2]

[2] Actually, Eq. (8.7) should be written as

$$^{\mathcal{B}_0}\mathbf{R} \simeq {}^{\mathcal{B}_0}\mathbf{R}^h = \mathbf{S}\boldsymbol{\Upsilon} \tag{8.9}$$

where $^{\mathcal{B}_0}\mathbf{R}^h = [^{\mathcal{B}_0}R_1^h, {}^{\mathcal{B}_0}R_2^h]^T$ since the (cubic) interpolation functions have been employed for the approximation of $^{\mathcal{B}_0}\mathbf{R}$.

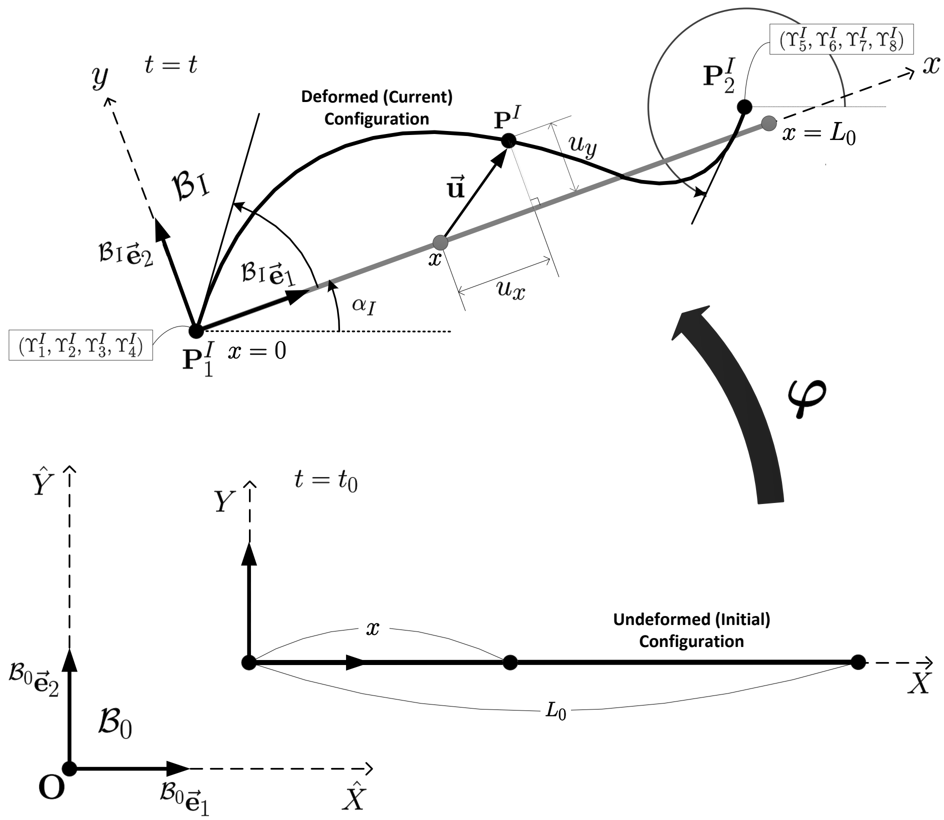


Figure 8.1: ANC Formulation - Beam Element in $\mathbb{E}^2$

Theorem 8.1.1 (Kinetic Energy Function of Ω_I)

The kinetic energy of element I, $\mathscr{T}_I(\dot{\Upsilon}) : \mathbb{R}^8 \to \mathbb{R}$, is given as

$$\boxed{\mathscr{T}_I = \frac{1}{2}\dot{\Upsilon}^T \mathbf{M}_I \dot{\Upsilon}} \tag{8.10}$$

where

$$\mathbf{M}_I := \int_{\Omega_I} \rho_I \mathbf{S}^T \mathbf{S} dV \in \mathbb{R}^{8\times 8} \tag{8.11}$$

in which ρ_I denotes the density function for Ω_I is the constant element mass matrix.

Proof. From the definition of the kinetic energy, we get

$$\begin{aligned}\mathscr{T}_I &= \frac{1}{2}\int_{\Omega_I} \rho_I({}^{\mathscr{B}_0}\mathfrak{D}_t\vec{\mathbf{R}}) \cdot ({}^{\mathscr{B}_0}\mathfrak{D}_t\vec{\mathbf{R}})dV \\ &= \frac{1}{2}\int_{\Omega_I} \rho_I({}^{\mathscr{B}_0}\dot{\mathbf{R}}^T)({}^{\mathscr{B}_0}\dot{\mathbf{R}})dV \\ &= \frac{1}{2}\dot{\boldsymbol{\Upsilon}}^T \underbrace{\int_{\Omega_I} \rho_I\mathbf{S}^T\mathbf{S}dV}_{=:\mathbf{M}_I}\dot{\boldsymbol{\Upsilon}} \end{aligned} \tag{8.12}$$

since ${}^{\mathscr{B}_0}\dot{\mathbf{R}}^h = \mathbf{S}\,\dot{\boldsymbol{\Upsilon}}$. ∎

Remark 8.1.1

The element mass matrix is constant, symmetric, and positive-definite, and it can be explicitly written as

$$\mathbf{M}_I = m_I\begin{bmatrix} \frac{13}{35} & 0 & \frac{11L_0}{210} & 0 & \frac{9}{70} & 0 & -\frac{13L_0}{420} & 0 \\ & \frac{13}{35} & 0 & \frac{11L_0}{210} & 0 & \frac{9}{70} & 0 & -\frac{13L_0}{420} \\ & & \frac{L_0^2}{105} & 0 & \frac{13L_0}{420} & 0 & -\frac{L_0^2}{140} & 0 \\ & & & \frac{L_0^2}{105} & 0 & \frac{13L_0}{420} & 0 & -\frac{L_0^2}{140} \\ & & & & \frac{13}{35} & 0 & -\frac{11L_0}{210} & 0 \\ & & & & & \frac{13}{35} & 0 & -\frac{11L_0}{210} \\ & & & & & & \frac{L_0^2}{105} & 0 \\ \text{sym.} & & & & & & & \frac{L_0^2}{105} \end{bmatrix} \tag{8.13}$$

where $m_I := \int_{\Omega_I} \rho_I dV$ is the mass of Ω_I.

Beam Deformation

From Fig. 8.1, we have

$$\vec{\pi}(\mathbf{P}_1^I, \mathbf{P}^I) = \vec{\pi}(\mathbf{O}, \mathbf{P}^I) - \vec{\pi}(\mathbf{O}, \mathbf{P}_1^I) \tag{8.14}$$

Therefore, the component vector of $\vec{\boldsymbol{\pi}}(\mathbf{P}^I_1, \mathbf{P}^I) = {}^{\mathcal{B}_0}\mathbf{e}^T\, {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{P}^I_1, \mathbf{P}^I)$ with respect to the inertial reference frame, $\mathcal{B}_0$, can be expressed as

$$\begin{aligned} {}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{P}^I_1, \mathbf{P}^I) &= \underbrace{{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{P}^I)}_{\mathbf{S}\boldsymbol{\Upsilon}} - \underbrace{{}^{\mathcal{B}_0}\boldsymbol{\pi}(\mathbf{O}, \mathbf{P}^I_1)}_{\mathbf{S}(0)\boldsymbol{\Upsilon}} \\ &= [\mathbf{S} - \mathbf{S}(0)]\,\boldsymbol{\Upsilon} = \begin{bmatrix} \mathbf{S}_1 - \mathbf{S}_1(0) \\ \mathbf{S}_2 - \mathbf{S}_2(0) \end{bmatrix} \boldsymbol{\Upsilon} \end{aligned} \tag{8.15}$$

where $\mathbf{S}_i$ (for $i = 1, 2$) are the i^{th} rows of $\mathbf{S}$, and $\mathbf{S}_i(0) = \mathbf{S}_i|_{\xi=0}$ (for $i = 1, 2$) are the i^{th} rows of $\mathbf{S}$ at $\xi = 0$, i.e.,

$$\begin{aligned} &\mathbf{S}_1 - \mathbf{S}_1(0) \\ = &\begin{bmatrix} -3\xi^2 + 2\xi^3 & 0 & L(\xi - 2\xi^2 + \xi^3) & 0 & 3\xi^2 - 2\xi^3 & 0 & L(-\xi^2 + \xi^3) & 0 \end{bmatrix} \end{aligned} \tag{8.16}$$

$$\begin{aligned} &\mathbf{S}_2 - \mathbf{S}_2(0) \\ = &\begin{bmatrix} 0 & -3\xi^2 + 2\xi^3 & 0 & L(\xi - 2\xi^2 + \xi^3) & 0 & 3\xi^2 - 2\xi^3 & 0 & L(-\xi^2 + \xi^3) \end{bmatrix} \end{aligned} \tag{8.17}$$

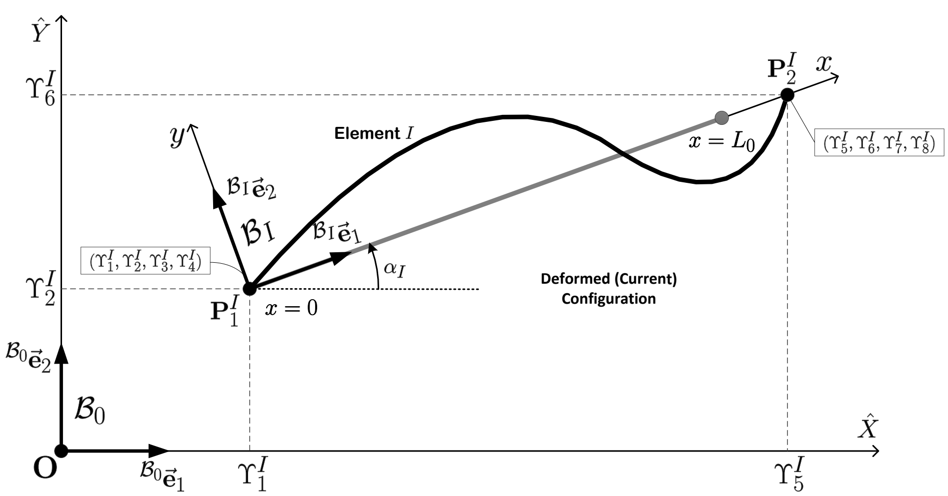


Figure 8.2: Pinned Frame

The component vector of displacement $\vec{\mathbf{u}} = {}^{\mathcal{B}_I}\mathbf{e}^T\, {}^{\mathcal{B}_I}\mathbf{u}$, shown in Fig. 8.1, with respect to frame $\mathcal{B}_I$ can be expressed as

$$ {}^{\mathcal{B}_I}\mathbf{u} = \begin{bmatrix} u_x \\ u_y \end{bmatrix} = \begin{bmatrix} \vec{\boldsymbol{\pi}}(\mathbf{P}_1^I, \mathbf{P}^I) \cdot {}^{\mathcal{B}_I}\vec{\mathbf{e}}_1 - x \\ \vec{\boldsymbol{\pi}}(\mathbf{P}_1^I, \mathbf{P}^I) \cdot {}^{\mathcal{B}_I}\vec{\mathbf{e}}_2 \end{bmatrix} \tag{8.18} $$

Let $\vec{\mathbf{s}}_I^1 \equiv {}^{\mathcal{B}_I}\vec{\mathbf{e}}_1$ and $\vec{\mathbf{s}}_I^2 \equiv {}^{\mathcal{B}_I}\vec{\mathbf{e}}_2$. The component vector of $\vec{\mathbf{s}}_I^1$ with respect to $\mathcal{B}_0$, i.e., ${}^{\mathcal{B}_0}\mathbf{s}_I^1$, can be written as

$$ {}^{\mathcal{B}_0}\mathbf{s}_I^1 = \left({}^{\mathcal{B}_0/\mathcal{B}_I}\mathbf{A}\right)\underbrace{\left({}^{\mathcal{B}_I}\mathbf{s}_I^1\right)}_{[1,0]^T} = \begin{bmatrix} [{}^{\mathcal{B}_0/\mathcal{B}_I}\mathbf{A}]_{11} \\ [{}^{\mathcal{B}_0/\mathcal{B}_I}\mathbf{A}]_{21} \end{bmatrix} = \begin{bmatrix} \bar{\eta}_1(\boldsymbol{\Upsilon}) \\ \bar{\eta}_2(\boldsymbol{\Upsilon}) \end{bmatrix} =: \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \mathbf{a} \in \mathbb{R}^2 \tag{8.19} $$

where functions $\bar{\eta}_i(\boldsymbol{\Upsilon}) =: a_i$ (for $i = 1, 2$) are given by [3]

$$ \begin{aligned} \bar{\eta}_1(\boldsymbol{\Upsilon}) = \cos(\alpha) = \frac{\Upsilon_5 - \Upsilon_1}{\sqrt{(\Upsilon_5 - \Upsilon_1)^2 + (\Upsilon_6 - \Upsilon_2)^2}} \\ \bar{\eta}_2(\boldsymbol{\Upsilon}) = \sin(\alpha) = \frac{\Upsilon_6 - \Upsilon_2}{\sqrt{(\Upsilon_5 - \Upsilon_1)^2 + (\Upsilon_6 - \Upsilon_2)^2}} \end{aligned} \tag{8.21} $$

for the *pinned-frame* case, i.e., point $\mathbf{P}_2^I$ is on the x-axis; see Fig. 8.2.[4] Therefore, from the orthogonality condition, the component vector of $\vec{\mathbf{s}}_I^2$ with respect to $\mathcal{B}_0$, i.e., ${}^{\mathcal{B}_0}\mathbf{s}_I^2$, may be given by

$$ {}^{\mathcal{B}_0}\mathbf{s}_I^2 = \begin{bmatrix} -\bar{\eta}_2(\boldsymbol{\Upsilon}) \\ \bar{\eta}_1(\boldsymbol{\Upsilon}) \end{bmatrix} =: \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \mathbf{b} \in \mathbb{R}^2 \tag{8.23} $$

[3] The transformation matrix ${}^{\mathcal{B}_0/\mathcal{B}_I}\mathbf{A} \in SO(2)$ is given by

$$ {}^{\mathcal{B}_0/\mathcal{B}_I}\mathbf{A} = \begin{bmatrix} \cos(\alpha) & -\sin(\alpha) \\ \sin(\alpha) & \cos(\alpha) \end{bmatrix} \tag{8.20} $$

[4] For the *tangent-frame* case, shown in Fig. 8.3, $\bar{\eta}_i(\boldsymbol{\Upsilon})$ are given by

$$ \bar{\eta}_1(\boldsymbol{\Upsilon}) = \frac{\Upsilon_3}{\sqrt{\Upsilon_3^2 + \Upsilon_4^2}} \quad \text{and} \quad \bar{\eta}_2(\boldsymbol{\Upsilon}) = \frac{\Upsilon_4}{\sqrt{\Upsilon_3^2 + \Upsilon_4^2}} \tag{8.22} $$

Hence, the transformation matrix ${}^{\mathcal{B}_0/\mathcal{B}_I}\mathbf{A} \in SO(2)$ may be generally written as

$$ {}^{\mathcal{B}_0/\mathcal{B}_I}\mathbf{A}(\boldsymbol{\Upsilon}) = \begin{bmatrix} \bar{\eta}_1(\boldsymbol{\Upsilon}) & -\bar{\eta}_2(\boldsymbol{\Upsilon}) \\ \bar{\eta}_2(\boldsymbol{\Upsilon}) & \bar{\eta}_1(\boldsymbol{\Upsilon}) \end{bmatrix} \tag{8.24} $$

Substituting Eq. (8.15), Eq. (8.19), and Eq. (8.23) into Eq. (8.18), we obtain

$$ \boxed{ {}^{\mathcal{B}_I}\mathbf{u} = \begin{bmatrix} u_x \\ u_y \end{bmatrix} = \underbrace{\begin{bmatrix} \bar{\eta}_1(\boldsymbol{\Upsilon}) & \bar{\eta}_2(\boldsymbol{\Upsilon}) \\ -\bar{\eta}_2(\boldsymbol{\Upsilon}) & \bar{\eta}_1(\boldsymbol{\Upsilon}) \end{bmatrix}}_{{}^{\mathcal{B}_I/\mathcal{B}_0}\mathbf{A}} [\mathbf{S} - \mathbf{S}(0)]\, \boldsymbol{\Upsilon} - \begin{bmatrix} x \\ 0 \end{bmatrix} } \tag{8.25} $$

with ${}^{\mathcal{B}_I/\mathcal{B}_0}\mathbf{A} = {}^{\mathcal{B}_0/\mathcal{B}_I}\mathbf{A}^T$; that is, the displacement components, u_x and u_y, are of the forms,

$$ u_x = \bar{\eta}_1\ [\mathbf{S}_1 - \mathbf{S}_1(0)]\, \boldsymbol{\Upsilon} + \bar{\eta}_2\ [\mathbf{S}_2 - \mathbf{S}_2(0)]\, \boldsymbol{\Upsilon} - x \tag{8.26} $$

$$ u_y = -\bar{\eta}_2\ [\mathbf{S}_1 - \mathbf{S}_1(0)]\, \boldsymbol{\Upsilon} + \bar{\eta}_1\ [\mathbf{S}_2 - \mathbf{S}_2(0)]\, \boldsymbol{\Upsilon} \tag{8.27} $$

respectively.

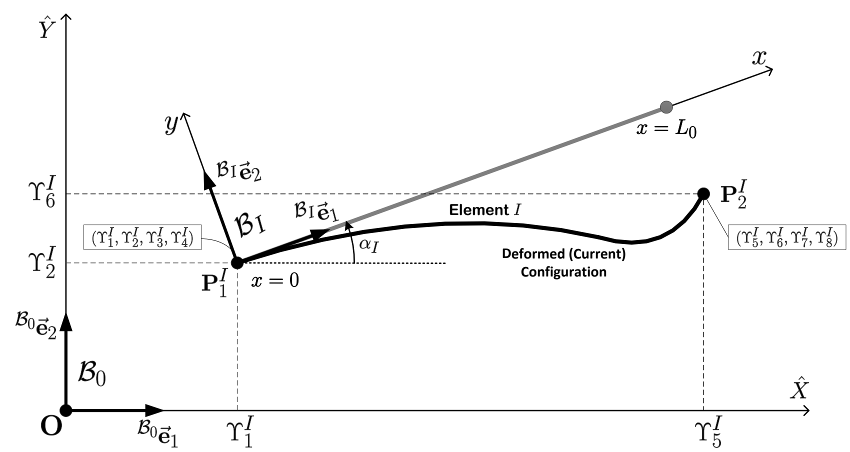


Figure 8.3: Tangent Frame

Theorem 8.1.2 (Strain Energy Function of Ω_I: Global-level formulation)

Cauchy strain case:[5] *The strain energy of Ω_I, $\mathscr{U}_I^{\text{int}}$, is obtained as*

$$\mathscr{U}_I^{\text{int}} = \underbrace{\int_0^{L_0} \frac{EA_0}{2}(\mathfrak{D}\, u_x)^2 dx}_{\mathscr{U}_I^{\text{axial}}} + \underbrace{\int_0^{L_0} \frac{EI}{2}(\mathfrak{D}^2\, u_y)^2 dx}_{\mathscr{U}_I^{\text{bend}}} \tag{8.30}$$

where u_x and u_y are given in Eq. (8.26) and Eq. (8.27), respectively. After some tedious, but straightforward work, the strain energy functions due to the axial and bending effects are expressed as

$$\begin{aligned} \mathscr{U}_I^{\text{axial}} &= -\left(Z_{pi}^{\text{a}_1}\right) a_p\, \Upsilon_i + \frac{\Upsilon_i\, \Upsilon_j}{2}\left(Z_{piqj}^{\text{a}_2}\right) a_p\, a_q & (8.31)\\ \mathscr{U}_I^{\text{bend}} &= \frac{\Upsilon_i\, \Upsilon_j}{2}\left(Z_{piqj}^{\text{b}_1}\right) b_p\, b_q & (8.32) \end{aligned}$$

respectively, for $p, q = 1, 2$ and $i, j = 1, 2, \cdots, 8$, where

$$\begin{aligned} Z_{pi}^{\text{a}_1} &:= EA_0 \int_0^1 S'_{pi}\, d\xi \\ Z_{piqj}^{\text{a}_2} &:= \frac{EA_0}{L_0}\int_0^1 S'_{pi}\, S'_{qj}\, d\xi \\ Z_{piqj}^{\text{b}_1} &:= \frac{EI}{L_0^3}\int_0^1 S''_{pi}\, S''_{qj}\, d\xi \end{aligned} \tag{8.33}$$

in which $S'_{pi} := \partial S_{pi}/\partial\xi$ and $S''_{pi} := \partial^2 S_{pi}/\partial\xi^2$. Note that $S_{pi} \equiv [\mathbf{S}]_{pi} \in \mathbb{R}$.

---

[5] *From the elementary linear elasticity theory, that the **Cauchy strain** component in the x-direction is defined as*

$$\varepsilon_x := \mathfrak{D}u_x - (\mathfrak{D}^2 u_y)y \tag{8.28}$$

*On the other hand, the **Green-Lagrange model** is based on the **Green-Lagrange strain** of component in the x-direction of the form,*

$$\varepsilon_x^{(\text{GL})} := \underbrace{\mathfrak{D}u_x - (\mathfrak{D}^2 u_y)y}_{\varepsilon_c} + \frac{1}{2}\left[\left(\mathfrak{D}u_y\right)^2 + \left(\mathfrak{D}u_x - (\mathfrak{D}^2 u_y)y\right)^2\right] \tag{8.29}$$

Green-Lagrange strain case: *Using the Green-Lagrange strain, defined in Eq.* (8.29), *in stead of the Cauchy strain, the strain energy of* Ω_I, $\mathscr{U}_I^{\text{int}}$, *is obtained as*

$$\mathscr{U}_I^{\text{int (GL)}} = \int_{\Omega_I} E \left(\varepsilon_1^{\text{(GL)}}\right)^2 dV = \mathscr{U}_I^{\text{axial (GL)}} + \mathscr{U}_I^{\text{bend (GL)}} \tag{8.34}$$

where the strain energy functions due to the axial and bending effects are given by

$$\begin{aligned} \mathscr{U}_I^{\text{axial (GL)}} &= -\frac{\Upsilon_i\,\Upsilon_j}{4}\left(Z^{\text{a}_2}_{piqj}\right)\left[a_p\,a_q + b_p\,b_q\right] \\ &\quad + \frac{\Upsilon_i\,\Upsilon_j\,\Upsilon_k\,\Upsilon_\ell}{8}\left(Z^{\text{a}_3}_{piqjrkt\ell}\right)\left[a_p\,a_q\,a_r\,a_t + b_p\,b_q\,b_r\,b_t + a_p\,a_q\,b_r\,b_t\right] \end{aligned} \tag{8.35}$$

$$\begin{aligned} \mathscr{U}_I^{\text{bend (GL)}} &= -\frac{\Upsilon_i\,\Upsilon_j}{4}\left(Z^{\text{b}_1}_{piqj}\right) b_p\,b_q \\ &\quad + \frac{\Upsilon_i\,\Upsilon_j\,\Upsilon_k\,\Upsilon_\ell}{4}\left(Z^{\text{b}_2}_{piqjrkt\ell}\right)\left[b_p\,b_q\,b_r\,b_t + 3a_p\,a_q\,b_r\,b_t\right] \\ &\quad + \frac{\Upsilon_i\,\Upsilon_j\,\Upsilon_k\,\Upsilon_\ell}{4}\left(Z^{\text{b}_3}_{piqjrkt\ell}\right) b_p\,b_q\,b_r\,b_t \end{aligned} \tag{8.36}$$

for $p, q, r, t = 1, 2$ *and* $i, j, k, \ell = 1, 2, \cdots, 8$ *in which*

$$\begin{aligned} Z^{\text{a}_3}_{piqjrkt\ell} &:= \frac{EA_0}{L_0^3}\int_0^1 S'_{pi}\,S'_{qj}\,S'_{rk}\,S'_{t\ell}\,d\xi \\ Z^{\text{b}_2}_{piqjrkt\ell} &:= \frac{EI}{L_0^5}\int_0^1 S'_{pi}\,S'_{qj}\,S''_{rk}\,S''_{t\ell}\,d\xi \\ Z^{\text{b}_3}_{piqjrkt\ell} &:= \frac{E\hat{I}}{L_0^7}\int_0^1 S''_{pi}\,S''_{qj}\,S''_{rk}\,S''_{t\ell}\,d\xi \end{aligned} \tag{8.37}$$

respectively, with $\hat{I} := \iint y^4 dydz$.

Equation of Motion for Multibody Systems By summing all element kinetic energy function and strain energy function given in Theorem 8.1.1 and Theorem 8.1.2/8.1.3 in a system, the system kinetic energy and strain energy functions are defined:

$$\mathscr{T}(\dot{\boldsymbol{\Upsilon}}) := \sum_{i=1}^{n_\text{b}} \mathscr{T}_I(\dot{\boldsymbol{\Upsilon}}^I) \;\text{ and }\; \mathscr{U}^{\text{int}}(\boldsymbol{\Upsilon}) := \sum_{i=1}^{n_\text{b}} \mathscr{U}_I^{\text{int}}(\boldsymbol{\Upsilon}^I) \tag{8.38}$$

respectively. Here, we clarify $\boldsymbol{\Upsilon}^I(t) : \mathbb{I} \to \mathbb{R}^6$ denotes the vector of the nodal variables for element Ω_I, and $\boldsymbol{\Upsilon}$ is the vector of the nodal variables for the system, i.e., $\boldsymbol{\Upsilon}(t) := (\boldsymbol{\Upsilon}^{1\,T}, \boldsymbol{\Upsilon}^{2\,T}, \cdots, \boldsymbol{\Upsilon}^{n_\mathrm{b}\,T})^T(t) : \mathbb{I} \to \bar{Q}$; that is, $\boldsymbol{\Upsilon}(t)$ is the local coordinates of a $6n_\mathrm{b}$-dimensional real differentiable configuration manifold $\bar{Q}$. Then, we can define the Lagrangian function for the system $\mathscr{L}(\boldsymbol{\Upsilon}, \dot{\boldsymbol{\Upsilon}}) : TQ \to \mathbb{R}$ as a summation over the element Lagrangian functions of each body as

$$\mathscr{L}(\boldsymbol{\Upsilon}, \dot{\boldsymbol{\Upsilon}}) = \sum_{i=1}^{n_\mathrm{b}} \mathscr{L}_I = \mathscr{T}(\dot{\boldsymbol{\Upsilon}}) - \mathscr{U}^{\,\mathrm{int}}(\boldsymbol{\Upsilon}) \tag{8.39}$$

If there exist external conservative forces in the system such as gravitational forces, we can define the total potential energy function as

$$\mathscr{U} = \mathscr{U}^{\,\mathrm{int}} + \mathscr{U}^{\,\mathrm{con}} \tag{8.40}$$

where $\mathscr{U}^{\,\mathrm{con}} := \sum_{i=1}^{n_\mathrm{b}}$ denotes the system external potential energy due to those forces; and therefore the system Lagrangian function becomes

$$\mathscr{L}(\boldsymbol{\Upsilon}, \dot{\boldsymbol{\Upsilon}}) = \mathscr{T}(\dot{\boldsymbol{\Upsilon}}) - \mathscr{U}(\boldsymbol{\Upsilon}) \tag{8.41}$$

For the Lagrangian function defined in Eq. (8.41), Lagrange's equation of motion yields

$$\begin{aligned} \mathbf{0} &= \frac{d}{dt}\left(\frac{\partial \mathscr{L}(\boldsymbol{\Upsilon}, \dot{\boldsymbol{\Upsilon}})}{\partial \dot{\boldsymbol{\Upsilon}}}\right) - \frac{\partial \mathscr{L}(\boldsymbol{\Upsilon}, \dot{\boldsymbol{\Upsilon}})}{\partial \boldsymbol{\Upsilon}} \\ &= \mathbf{M}\ddot{\boldsymbol{\Upsilon}} + \mathbf{Q}^{\mathrm{int}}(\boldsymbol{\Upsilon}) - \mathbf{Q}^{\mathrm{con}}(\boldsymbol{\Upsilon}) \end{aligned} \tag{8.42}$$

with given initial conditions $(\boldsymbol{\Upsilon}, \dot{\boldsymbol{\Upsilon}})(t_0)$, where $\mathbf{M}$ is the system mass matrix obtained by assembling $\mathbf{M}_I$ over the system; and $\mathbf{Q}^{\mathrm{int}}(\boldsymbol{\Upsilon}) := \mathfrak{D}\,\mathscr{U}^{\,\mathrm{int}}(\boldsymbol{\Upsilon})$ and $\mathbf{Q}^{\mathrm{con}}(\boldsymbol{\Upsilon}) := -\mathfrak{D}\,\mathscr{U}^{\,\mathrm{con}}(\boldsymbol{\Upsilon})$ denote the total internal force vector and the total conservative force vector applied in the system, respectively.

The Legendre transformation defines the canonical momentum $\Upsilon_{\mathcal{P}} \in T^*_{\Upsilon}\bar{Q}$ that is conjugate to $\Upsilon \in \bar{Q}$ as

$$\Upsilon_{\mathcal{P}} := \frac{\partial \mathscr{L}(\Upsilon, \dot{\Upsilon})}{\partial \dot{\Upsilon}} \tag{8.43}$$

via the fibre derivative[6] of $\mathscr{L}(\Upsilon, \dot{\Upsilon}) : TQ \to \mathbb{R}$, and the corresponding Hamiltonian function $\mathscr{H}(\Upsilon, \Upsilon_{\mathcal{P}}) : T^*Q \to \mathbb{R}$ is defined as

$$\mathscr{H}(\Upsilon, \Upsilon_{\mathcal{P}}) = \Upsilon_{\mathcal{P}}^T \dot{\Upsilon} - \mathscr{L}(\Upsilon, \dot{\Upsilon}) = \mathscr{T}(\Upsilon_{\mathcal{P}}) + \mathscr{U}(\Upsilon) \tag{8.44}$$

Hence, the Hamilton's canonical equations, which are equivalent to Eq. (8.42), is obtained as

$$\begin{aligned} \dot{\Upsilon} &= [\Upsilon, \mathscr{H}] = \frac{\partial \mathscr{H}(\Upsilon, \Upsilon_{\mathcal{P}})}{\partial \Upsilon_{\mathcal{P}}} = \mathbf{M}\dot{\Upsilon} \\ \dot{\Upsilon}_{\mathcal{P}} &= [\Upsilon_{\mathcal{P}}, \mathscr{H}] = -\frac{\partial \mathscr{H}(\Upsilon, \Upsilon_{\mathcal{P}})}{\partial \Upsilon} = -\mathbf{Q}^{\text{int}}(\Upsilon) + \mathbf{Q}^{\text{con}}(\Upsilon) \end{aligned} \tag{8.45}$$

with given initial conditions $(\Upsilon, \Upsilon_{\mathcal{P}})(t_0)$.

A remarkable feature of the ANC formulation is that the symmetric and positive-definite $\mathbf{M}$ is constant; however, due to the the internal force $\mathbf{Q}^{\text{int}}(\Upsilon)$ becomes extremely highly nonlinear due to the potential energy functions given in Theorem 8.1.2, which causes serious numerical instabilities; see [60] for more detailed discussion. In order to avoid this problem, a simplified version of the ANC formulation is available as shown below.

8.1.2 Simplified ANC Formulation: Simplifications of the Strain Energy Functions

As we can see, the strain energy in the ANC formulation tends to be highly nonlinear, which causes that the internal force, derived from the strain energy function, involves

[6] See Proposition 2.4.1

highly nonlinear terms as functions of the nodal coordinates. From the pragmatic point of view, this may be the main inadequacy of the ANC formulation; and it often leads to instability issues during the iterative process, such as the Newton-type iterative method. Perhaps, the most common way to simplify the strain energy is based on the following two assumptions: (1) The difference between L_0 and L is sufficiently small, and (2) The deformation of the beam element in the axial direction is sufficiently small, and the curvature, $\kappa = \mathfrak{D}^2 u_y$, appearing in the strain energy due to the bending effect, is given in X. Assumptions (1) and (2) dramatically reduce the internal forces due to the axial and bending effects, respectively.

- From Assumption (1), we assume the axial strain, ε_1, is approximately given as

$$\varepsilon_1 = \mathfrak{D}\, u_x \approx \frac{L - L_0}{L_0} \tag{8.46}$$

where L_0 and L are the length of the beam element in the undeformed and deformed configurations, respectively. Using $\boldsymbol{\Upsilon}$, L may be written as

$$L = \sqrt{(\Upsilon_5 - \Upsilon_1)^2 + (\Upsilon_6 - \Upsilon_2)^2} \tag{8.47}$$

Substituting Eq. (8.46) into the definition of the strain energy function due to the axial effect, we get

$$\mathscr{U}_I^{\text{axial}} \approx \int_0^{L_0} \frac{EA_0}{2} \left(\frac{L - L_0}{L_0}\right)^2 dx = \frac{EA_0}{2L_0}\, (L - L_0)^2 \tag{8.48}$$

From Eq. (8.48), the (generalized) internal force vector due to the axial effect for element I may be given as

$$\mathbf{Q}_I^{\text{axial}} = \frac{\partial \mathscr{U}_I^{\text{axial}}}{\partial \boldsymbol{\Upsilon}} \approx \left(\mathbf{K}_I^{\text{axial}}\right) \boldsymbol{\Upsilon} \tag{8.49}$$

where $\mathbf{\Upsilon} \in \mathbb{R}^8$ is the nodal coordinates of element I, and the stiffness, $\mathbf{K}_I^{\text{axial}} \in \mathbb{R}^{8\times 8}$, is defined as

$$\mathbf{K}_I^{\text{axial}} := \frac{EA}{L}\left(\frac{L-L_0}{L}\right)\begin{bmatrix} 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ & 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ & & 0 & 0 & 0 & 0 & 0 & 0 \\ & & & 0 & 0 & 0 & 0 & 0 \\ & & & & 1 & 0 & 0 & 0 \\ & & & & & 1 & 0 & 0 \\ & & & & & & 0 & 0 \\ \text{sym.} & & & & & & & 0 \end{bmatrix} \tag{8.50}$$

- From Assumption (2), we have

$$\lim_{\Delta\xi\to 0}\frac{\mathbf{S}(\xi+\Delta\xi)-\mathbf{S}(\xi)}{\Delta\xi}\mathbf{\Upsilon} = \mathbf{S}'(\xi)\mathbf{\Upsilon} \approx \begin{bmatrix}\cos(\varphi) \\ \sin(\varphi)\end{bmatrix} \tag{8.51}$$

Therefore,

$$\mathbf{S}''(\xi)\mathbf{\Upsilon} \approx \begin{bmatrix}-\sin(\varphi) \\ \cos(\varphi)\end{bmatrix}\frac{d\varphi}{d\xi} \approx \begin{bmatrix}-\sin(\varphi) \\ \cos(\varphi)\end{bmatrix}\kappa \tag{8.52}$$

where κ denotes the *curvature* at point $\mathbf{P}^I$, defined as[7]

$$\kappa := \frac{1}{\hat{\rho}} = \frac{d\varphi}{dx} \approx \frac{d\varphi}{dX} = \frac{d\varphi}{d\xi} \tag{8.56}$$

[7] More accurately, the curvature, κ, is defined through

$$\hat{\rho} := \frac{1}{|\kappa|} \tag{8.53}$$

If the component form of $\vec{\boldsymbol{\pi}}(\mathbf{P}_1^I, \mathbf{P}^I)$ in terms of the Cartesian frame, $\mathcal{B}_I$, is ${}^{\mathcal{B}}(\boldsymbol{\pi}\mathbf{P}_1^I, \mathbf{P}^I) = [x, y]^T$, the radius of curvature is given in the form

$$\hat{\rho} = \frac{(\dot{x}^2+\dot{y}^2)^(3/2)}{|\dot{x}\ddot{y}-\dot{y}\ddot{x}|} \tag{8.54}$$

in which $\hat{\rho}$ is the *radius of curvature* (or also called *the radius of the osculating circle*) at point $\mathbf{P}^I$ in element I; see Fig. 8.4. Therefore, the strain energy function due to the bending effect may be approximated as

$$
\begin{aligned}
\mathscr{U}_I^{\text{bend}} &= \int_0^{L_0} \frac{EI}{2}(\mathfrak{D}^2\, u_y)^2 dx = \int_0^{L_0} \frac{EI}{2}\kappa^2 dx \\
&\approx \int_0^1 \frac{EI}{2}\left[\mathbf{S}''\boldsymbol{\Upsilon}\right]^T \left[\mathbf{S}''\boldsymbol{\Upsilon}\right] d\xi \\
&= \frac{1}{2}\boldsymbol{\Upsilon}^T \underbrace{\left[\int_0^1 EI\,(\mathbf{S}'')^T(\mathbf{S}'')d\xi\right]}_{=:\mathbf{K}_I^{\text{bend}}} \boldsymbol{\Upsilon}
\end{aligned}
\tag{8.57}
$$

Hence, the (generalized) internal force due to the bending effect is obtained as

$$
\mathbf{Q}_I^{\text{bend}} = \frac{\partial \mathscr{U}_I^{\text{bend}}}{\partial \boldsymbol{\Upsilon}} \approx \left(\mathbf{K}_I^{\text{bend}}\right)\boldsymbol{\Upsilon} \tag{8.58}
$$

where $\boldsymbol{\Upsilon} \in \mathbb{R}^8$ is the nodal coordinates of element I, and the stiffness, $\mathbf{K}_I^{\text{bend}} \in \mathbb{R}^{8\times 8}$, is defined as

$$
\mathbf{K}_I^{\text{bend}} := \frac{EI}{L_0^3}
\begin{bmatrix}
12 & 0 & 6L_0 & 0 & -12 & 0 & 6L_0 & 0 \\
 & 12 & 0 & 6L_0 & 0 & -12 & 0 & 6L_0 \\
 & & 4L_0^2 & 0 & -6L_0 & 0 & 2L_0^2 & 0 \\
 & & & 4L_0^2 & 0 & -6L_0 & 0 & 2L_0^2 \\
 & & & & 12 & 0 & -6L_0 & 0 \\
 & & & & & 12 & 0 & -6L_0 \\
 & & & & & & 4L_0^2 & 0 \\
\text{sym.} & & & & & & & 4L_0^2
\end{bmatrix}
\tag{8.59}
$$

in the exact sense. If the curve of element I is given in the form, $y = f(x)$, $\hat{\rho}$ can be written as

$$
\hat{\rho} = \frac{\left[1 + \left(\frac{dy}{dx}\right)^2\right]^{3/2}}{\left|\frac{d^2y}{dx^2}\right|} \tag{8.55}
$$

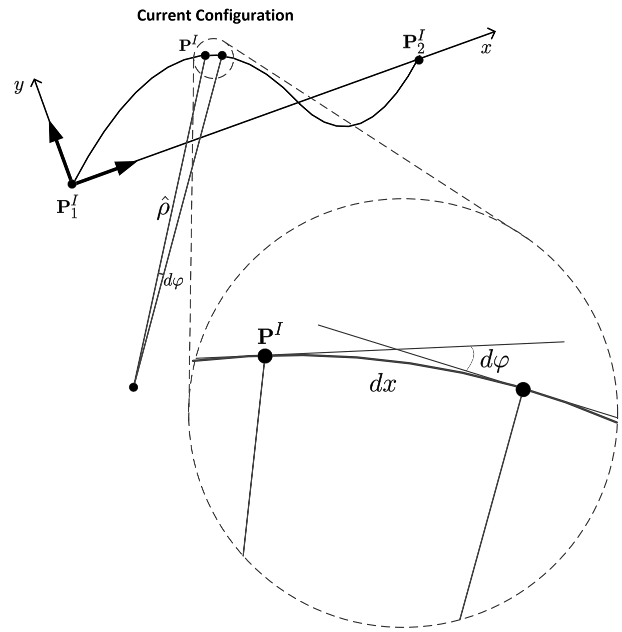


Figure 8.4: Curvature at $\mathbf{P}^I$

Remark 8.1.2

The (generalized) internal force acting on element I is approximately given as

$$\mathbf{Q}_I^{\text{int}} = \mathbf{Q}_I^{\text{axial}} + \mathbf{Q}_I^{\text{bend}} \approx \left(\mathbf{K}_I^{\text{axial}} + \mathbf{K}_I^{\text{bend}}\right)\boldsymbol{\Upsilon} \tag{8.60}$$

Notice that $\mathbf{K}_I^{\text{axial}}$ needs to be updated every iteration due to L, appearing in Eq. (8.50)*; while $\mathbf{K}_I^{\text{bend}}$ remains constant during simulation.*

8.1.3 An Alternative Formulation based on Dirac's Canonical Theory of Constraints

Element-level formulation: Description in terms of $\mathcal{B}_I$

It is important to note that Eq. (8.7) is based on the inertial reference frame, $\mathcal{B}_0$, i.e., Eq. (8.7) is in the global-level formulation; however, we can also formulate the position vector, referring to element frame $\mathcal{B}_I$ instead. Consider the position vector, $\vec{\boldsymbol{\pi}}(\mathbf{P}_1^I, \mathbf{P}^I) =: \vec{\mathbf{r}} = {}^{\mathcal{B}_I}\mathbf{e}^{T\,\mathcal{B}_I}\mathbf{r}$. Defining the vector of nodal coordinates for element I in the body-fixed frame, $\mathcal{B}_I$, as

$$\boldsymbol{\upsilon} = \begin{bmatrix} \upsilon_1 & \upsilon_2 & \upsilon_3 & \upsilon_4 & \upsilon_5 \end{bmatrix}^T \tag{8.61}$$

where the coordinates of points $\mathbf{P}_1^I$ and $\mathbf{P}_2^I$ are given by (υ_1, υ_2) and $(\upsilon_3, \upsilon_4, \upsilon_5)$ in which

$$\begin{bmatrix} \left.\frac{\partial}{\partial x}\right|_{x=0} {}^{\mathcal{B}_I}\mathbf{r} \\ \left.\frac{\partial}{\partial x}\right|_{x=L_0} {}^{\mathcal{B}_I}\mathbf{r} \end{bmatrix} = [\upsilon_1, \upsilon_2, \upsilon_4, \upsilon_5]^T \tag{8.62}$$

and

$$\left.{}^{\mathcal{B}_I}\mathbf{r}\right|_{x=L_0} = \upsilon_3 \tag{8.63}$$

Following a similar procedure for the derivation of Eq. (8.7), the component form of vector $\vec{\boldsymbol{\pi}}(\mathbf{P}_1^I, \mathbf{P}^I)$ with respect to $\mathcal{B}_I$ may be written as

$$\boxed{{}^{\mathcal{B}_I}\mathbf{r} = \mathbf{s}\boldsymbol{\upsilon}} \tag{8.64}$$

where the element shape function, $\mathbf{s}$, is given as

$$\mathbf{s} := \begin{bmatrix} L_0(\eta - 2\eta^2 + \eta^3) & 0 \\ 0 & L_0(\eta - 2\eta^2 + \eta^3) \\ 3\eta^2 - 2\eta^3 & 0 \\ L_0(-\eta^2 + \eta^3) & 0 \\ 0 & L_0(-\eta^2 + \eta^3) \end{bmatrix}^T \in \mathbb{R}^{2\times 5} \tag{8.65}$$

with $\eta := x/L_0 \in [0,1] \subset \mathbb{R}$. The displacement component vector, ${}^{\mathcal{B}_I}\mathbf{u}$, which was written in the global sense as in Eq. (8.25), can be expressed as

$$\boxed{{}^{\mathcal{B}_I}\mathbf{u} = \begin{bmatrix} u_x \\ u_y \end{bmatrix} = \begin{bmatrix} r_x - x \\ r_y \end{bmatrix}} \tag{8.66}$$

in the element sense, where r_x and r_y are defined as

$$r_x := \vec{\mathbf{r}} \cdot {}^{\mathcal{B}_I}\vec{\mathbf{e}}_1 = {}^{\mathcal{B}_I}\mathbf{r}^T \underbrace{{}^{\mathcal{B}_I}\mathbf{s}_I^1}_{[1,0]^T} = \boldsymbol{\upsilon}^T \mathbf{s}^T \begin{bmatrix} 1 \\ 0 \end{bmatrix} = s_{1i}\,\upsilon_i \tag{8.67}$$

$$r_y := \vec{\mathbf{r}} \cdot {}^{\mathcal{B}_I}\vec{\mathbf{e}}_2 = {}^{\mathcal{B}_I}\mathbf{r}^T \underbrace{{}^{\mathcal{B}_I}\mathbf{s}_I^2}_{[0,1]^T} = \boldsymbol{\upsilon}^T \mathbf{s}^T \begin{bmatrix} 0 \\ 1 \end{bmatrix} = s_{2i}\,\upsilon_i \tag{8.68}$$

for $i = 1, 2, \cdots, 5$.

Remark 8.1.3

Let $\upsilon_i = [\boldsymbol{\upsilon}]_i$ and $\Upsilon_j = [\boldsymbol{\Upsilon}]_j$ (for $i = 1, 2, \cdots, 5$ and $j = 1, 2, \cdots, 8$) be the nodal variables for Ω_I . The relations between υ_i and Υ_j can be expressed with functions a_p and b_p (for $p = 1, 2$) for Ω_I, given in Eq. (8.19) and Eq. (8.23), from the geometry as:

$$\begin{aligned} \upsilon_1 &= a_1\,\Upsilon_3 + a_2\,\Upsilon_4 \\ \upsilon_2 &= b_1\,\Upsilon_3 + b_2\,\Upsilon_4 \\ \upsilon_3 &= a_1\,(\Upsilon_5 - \Upsilon_1) + a_2\,(\Upsilon_6 - \Upsilon_2) \\ \upsilon_4 &= a_1\,\Upsilon_7 + a_2\,\Upsilon_8 \\ \upsilon_5 &= b_1\,\Upsilon_7 + b_2\,\Upsilon_8 \end{aligned} \tag{8.69}$$

or simply

$$\boldsymbol{\upsilon} = \bar{\mathbf{T}}\,\boldsymbol{\Upsilon} \tag{8.70}$$

where

$$\bar{\mathbf{T}} := \begin{bmatrix} 0 & 0 & a_1 & a_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & b_1 & b_1 & 0 & 0 & 0 & 0 \\ -a_1 & -a_2 & 0 & 0 & a_1 & a_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & a_1 & a_2 \\ 0 & 0 & 0 & 0 & 0 & 0 & b_1 & b_2 \end{bmatrix} \in \mathbb{R}^{5\times 8} \tag{8.71}$$

Theorem 8.1.3 (Strain Energy Function of Ω_I: Element-level formulation)

Cauchy strain case: *Employing the displacements, u_x andu_y, given in Eq.* (8.66), *instead of the ones given in Eq.* (8.25), *the strain energy function for Ω_I in terms of $\boldsymbol{\upsilon}$ is given as*[8]

$$\mathscr{V}_I^{\text{int}} = \mathscr{V}_I^{\text{axial}} + \mathscr{V}_I^{\text{bend}} \tag{8.73}$$

where

$$\mathscr{V}_I^{\text{axial}} = -\left(H_i^{\text{a}_1}\right)\upsilon_i + \frac{\upsilon_i\,\upsilon_j}{2}H_{1i1j}^{\text{a}_2} \tag{8.74}$$

$$\mathscr{V}_I^{\text{bend}} = \frac{\upsilon_i\,\upsilon_j}{2}H_{2i2j}^{\text{b}_1} \tag{8.75}$$

in which

$$\begin{aligned} H_i^{\text{a}_1} &:= EA_0\int_0^1 s'_{1i}\,d\eta \\ H_{piqj}^{\text{a}_2} &:= \frac{EA_0}{L_0}\int_0^1 s'_{pi}\,s'_{qj}\,d\eta \\ H_{piqj}^{\text{b}_1} &:= \frac{EI}{L_0^3}\int_0^1 s''_{pi}\,s''_{qj}\,d\eta \end{aligned} \tag{8.76}$$

[8] *The potential energy functions in terms of $\boldsymbol{\upsilon}$ and $\boldsymbol{\upsilon}$ have the same value (but different forms):*

$$\mathscr{U}(\boldsymbol{\Upsilon}) = \mathscr{V}(\boldsymbol{\upsilon}) \tag{8.72}$$

for $p, q = 1, 2$ and $i, j = 1, 2, \cdots, 5$, with $s'_{pi} := \partial s_{pi}/\partial\eta$ and $s''_{pi} := \partial^2 s_{pi}/\partial\eta^2$. Note that $s_{pi} \equiv [\mathbf{s}]_{pi} \in \mathbb{R}$.

Green-Lagrange strain case: *Using the Green-Lagrange strain, the strain energy of Ω_I, $\mathscr{V}_I^{\text{int}}$, is given as*

$$\mathscr{V}_I^{\text{int (GL)}} = \int_{\Omega_I} E\left(\varepsilon_1^{\text{(GL)}}\right)^2 dV = \mathscr{V}_I^{\text{axial (GL)}} + \mathscr{V}_I^{\text{bend (GL)}} \tag{8.77}$$

where

$$\begin{aligned}
\mathscr{V}_I^{\text{axial (GL)}} &= -\frac{\upsilon_i\,\upsilon_j}{4}\left[\left(H^{\text{a}_2}_{1i1j}\right) + \left(H^{\text{a}_2}_{2i2j}\right)\right] \\
&\quad + \frac{\upsilon_i\,\upsilon_j\,\upsilon_k\,\upsilon_\ell}{8}\left[\left(H^{\text{a}_3}_{1i1j1k1\ell}\right) + \left(H^{\text{a}_3}_{2i2j2k2\ell}\right) + \left(H^{\text{a}_3}_{1i1j2k2\ell}\right)\right] \qquad (8.78)\\
\mathscr{V}_I^{\text{bend (GL)}} &= -\frac{\upsilon_i\,\upsilon_j}{4}\left(H^{\text{b}_1}_{2i2j}\right) \\
&\quad + \frac{\upsilon_i\,\upsilon_j\,\upsilon_k\,\upsilon_\ell}{4}\left[\left(H^{\text{b}_2}_{2i2j2k2\ell}\right) + 3\left(H^{\text{b}_2}_{1i1j2k2\ell}\right)\right] \\
&\quad + \frac{\upsilon_i\,\upsilon_j\,\upsilon_k\,\upsilon_\ell}{8}\left(H^{\text{b}_3}_{2i2j2k2\ell}\right) \qquad (8.79)
\end{aligned}$$

in which

$$\begin{aligned}
H^{\text{a}_3}_{piqjrkt\ell} &:= \frac{EA_0}{L_0^3}\int_0^1 s'_{pi}\, s'_{qj}\, s'_{rk}\, s'_{t\ell}\, d\eta \\
H^{\text{b}_2}_{piqjrkt\ell} &:= \frac{EI}{L_0^5}\int_0^1 s'_{pi}\, s'_{qj}\, s''_{rk}\, s''_{t\ell}\, d\eta \\
H^{\text{b}_3}_{piqjrkt\ell} &:= \frac{E\hat{I}}{L_0^7}\int_0^1 s''_{pi}\, s''_{qj}\, s''_{rk}\, s''_{t\ell}\, d\eta
\end{aligned} \tag{8.80}$$

for $p, q, r, t = 1, 2$ and $i, j, k, \ell = 1, 2, \cdots, 5$.

Eq. (8.64) is usually used for so-called the floating reference formulation. The idea of the alternative ANC formulation is that we employ the strain energy in the element level with respect to $\mathscr{B}_I$, instead of the traditional way based on the global-level formulation, and remedy the high nonlinearity problem in the internal force term in Eq. (8.42) or Eq. (8.45), as originally suggested in [61]. This original approach is based on Dirac's canonical theory of constraints [46, 62].

Define an augmented Lagrangian function $\widetilde{\mathcal{L}} : T(Q \times \mathbb{Q} \times \mathbb{R}^2 \times \mathbb{R}^2 \times \mathbb{R}^{n_c}) \to \mathbb{R}$ as

$$\begin{aligned}&\widetilde{\mathcal{L}}(\boldsymbol{\Upsilon}, \dot{\boldsymbol{\Upsilon}}, \boldsymbol{\upsilon}, \dot{\boldsymbol{\upsilon}}, \mathbf{a}, \dot{\mathbf{a}}, \mathbf{b}, \dot{\mathbf{b}}, \boldsymbol{\lambda}, \dot{\boldsymbol{\lambda}}) \\ &= \mathscr{T}(\dot{\boldsymbol{\Upsilon}}) - \mathscr{V}(\boldsymbol{\upsilon}) - \boldsymbol{\lambda}^T \boldsymbol{\Phi}(\boldsymbol{\Upsilon}, \boldsymbol{\upsilon}, \mathbf{a}, \mathbf{b})\end{aligned} \tag{8.81}$$

where Q denotes a 8-dimensional differentiable configuration manifold for $\boldsymbol{\Upsilon}$ for Ω_I, $\mathbb{Q}$ denotes a 5-dimensional differentiable configuration manifold for $\boldsymbol{\upsilon}$ for Ω_I, $\boldsymbol{\Phi} \in \mathbb{R}^{n_c}$ denotes the constraint function of the system, and $\boldsymbol{\lambda}(t) : \mathbb{I} \to \mathbb{R}^{n_c}$ is the Lagrange multiplier vector. The key idea is that the potential energy $\mathscr{V}(\boldsymbol{\upsilon})$ in Eq. (8.81) has the same value with $\mathscr{U}(\boldsymbol{\Upsilon})$, i.e.,

$$\mathscr{U}(\boldsymbol{\Upsilon}) = \mathscr{V}(\boldsymbol{\upsilon}) \tag{8.82}$$

Vectors $\mathbf{a} \in \mathbb{R}^2$ and $\mathbf{b} \in \mathbb{R}^2$ are as defined in Eq. (8.19) and Eq. (8.23), respectively. The constraint equation defined from Eq. (8.21), Eq. (8.23), and Eq. (8.70) as

$$\mathbf{0} = \boldsymbol{\Phi} := \begin{bmatrix} a_1 - \bar{\eta}_1(\boldsymbol{\Upsilon}) \\ a_2 - \bar{\eta}_2(\boldsymbol{\Upsilon}) \\ b_1 + \bar{\eta}_2(\boldsymbol{\Upsilon}) \\ b_2 - \bar{\eta}_1(\boldsymbol{\Upsilon}) \\ \boldsymbol{\upsilon} - \bar{\mathbf{T}}(\mathbf{a}, \mathbf{b})\,\boldsymbol{\Upsilon} \end{bmatrix} \in \mathbb{R}^{n_c} \tag{8.83}$$

By the Legendre transformation, we can define the canonical momentum that is conjugate to $\boldsymbol{\Upsilon} \in Q$ as

$$\boldsymbol{\Upsilon}_{\mathcal{P}} := \frac{\partial \widetilde{\mathcal{L}}}{\partial \dot{\boldsymbol{\Upsilon}}} = \frac{\partial \mathscr{T}}{\partial \dot{\boldsymbol{\Upsilon}}} = \mathbf{M}\dot{\boldsymbol{\Upsilon}} \tag{8.84}$$

However, this augmented Lagrangian function $\widetilde{\mathscr{L}}$ is ***degenerate*** in $\boldsymbol{\upsilon}$, $\mathbf{a}$, $\mathbf{b}$, and $\boldsymbol{\lambda}$ since

$$\begin{aligned}
\boldsymbol{\upsilon}_{\mathcal{P}} &:= \frac{\partial \widetilde{\mathcal{L}}}{\partial \dot{\boldsymbol{\upsilon}}} = \mathbf{0} \\
\mathbf{a}_{\mathcal{P}} &:= \frac{\partial \widetilde{\mathcal{L}}}{\partial \dot{\mathbf{a}}} = \mathbf{0} \\
\mathbf{b}_{\mathcal{P}} &:= \frac{\partial \widetilde{\mathcal{L}}}{\partial \dot{\mathbf{b}}} = \mathbf{0} \\
\boldsymbol{\lambda}_{\mathcal{P}} &:= \frac{\partial \widetilde{\mathcal{L}}}{\partial \dot{\boldsymbol{\lambda}}} = \mathbf{0}
\end{aligned} \tag{8.85}$$

where $\boldsymbol{\upsilon}_{\mathcal{P}}$, $\mathbf{a}_{\mathcal{P}}$, $\mathbf{b}_{\mathcal{P}}$, and $\boldsymbol{\lambda}_{\mathcal{P}}$ are the canonical momentum vectors that are conjugate to $\boldsymbol{\upsilon}$, $\mathbf{a}$, $\mathbf{b}$, and $\boldsymbol{\lambda}$, respectively. Therefore, viewing Eq. (8.85) as invariants of the system, define Hamiltonian function $\widetilde{\mathscr{H}}'$ as

$$\widetilde{\mathcal{H}}' := \widetilde{\mathcal{H}} + \boldsymbol{\eta}_{\upsilon}^T \boldsymbol{\upsilon}_{\mathcal{P}} + \boldsymbol{\eta}_{\mathrm{a}}^T \mathbf{a}_{\mathcal{P}} + \boldsymbol{\eta}_{\mathrm{b}}^T \mathbf{b}_{\mathcal{P}} + \boldsymbol{\eta}_{\lambda}^T \boldsymbol{\lambda}_{\mathcal{P}} \tag{8.86}$$

where $\widetilde{\mathcal{H}} = \mathscr{T}(\boldsymbol{\Upsilon}_{\mathcal{P}}) + \mathscr{V}(\boldsymbol{\upsilon}) + \boldsymbol{\lambda}^T \boldsymbol{\Phi}(\boldsymbol{\Upsilon}, \boldsymbol{\upsilon}, \mathbf{a}, \mathbf{b}) : T^*(Q \times \mathbb{Q} \times \mathbb{R}^2 \times \mathbb{R}^2 \times \mathbb{R}^9) \to \mathbb{R}$ is the augmented Hamiltonian function that corresponds to $\widetilde{\mathcal{L}}$ in Eq. (8.81), and $\boldsymbol{\eta}_{\upsilon} \in \mathbb{R}^{5n_{\mathrm{b}}}$, $\boldsymbol{\eta}_{\mathrm{a}} \in \mathbb{R}^2$, $\boldsymbol{\eta}_{\mathrm{b}} \in \mathbb{R}^2$, and $\boldsymbol{\eta}_{\lambda} \in \mathbb{R}^{n_{\mathrm{c}}}$ are the additional Lagrange multipliers introduced so as to enforce Eq. (8.85).

Employing Poisson's bracket defined in Proposition 8.1.1 for the autonomous $\widetilde{\mathcal{H}}'$, the canonical equations for the system are obtained as follows:

$$
\begin{aligned}
\dot{\boldsymbol{\Upsilon}} &= [\boldsymbol{\Upsilon}, \widetilde{\mathcal{H}}']_* = \frac{\partial \widetilde{\mathcal{H}}'}{\partial \boldsymbol{\Upsilon}_{\mathcal{P}}} = \frac{\partial \mathcal{T}}{\partial \boldsymbol{\Upsilon}_{\mathcal{P}}} = \mathbf{M}^{-1}\boldsymbol{\Upsilon}_{\mathcal{P}} \\
\dot{\boldsymbol{\Upsilon}}_{\mathcal{P}} &= [\boldsymbol{\Upsilon}_{\mathcal{P}}, \widetilde{\mathcal{H}}']_* = -\frac{\partial \widetilde{\mathcal{H}}'}{\partial \boldsymbol{\Upsilon}} = -\left(\frac{\partial \boldsymbol{\Phi}}{\partial \boldsymbol{\Upsilon}}\right)^T \boldsymbol{\lambda} \\
\dot{\boldsymbol{\upsilon}} &= [\boldsymbol{\upsilon}, \widetilde{\mathcal{H}}']_* = \frac{\partial \widetilde{\mathcal{H}}'}{\partial \boldsymbol{\upsilon}_{\mathcal{P}}} = \boldsymbol{\eta}_{\upsilon} \\
\dot{\boldsymbol{\upsilon}}_{\mathcal{P}} &= [\boldsymbol{\upsilon}_{\mathcal{P}}, \widetilde{\mathcal{H}}']_* = -\frac{\partial \widetilde{\mathcal{H}}'}{\partial \boldsymbol{\upsilon}} = -\frac{\partial \mathcal{V}}{\partial \boldsymbol{\upsilon}} - \left(\frac{\partial \boldsymbol{\Phi}}{\partial \boldsymbol{\upsilon}}\right)^T \boldsymbol{\lambda} \\
\dot{\mathbf{a}} &= [\mathbf{a}, \widetilde{\mathcal{H}}']_* = \frac{\partial \widetilde{\mathcal{H}}'}{\partial \mathbf{a}_{\mathcal{P}}} = \boldsymbol{\eta}_{\mathrm{a}} \\
\dot{\mathbf{a}}_{\mathcal{P}} &= [\mathbf{a}_{\mathcal{P}}, \widetilde{\mathcal{H}}']_* = -\frac{\partial \widetilde{\mathcal{H}}'}{\partial \mathbf{a}} = -\left(\frac{\partial \boldsymbol{\Phi}}{\partial \mathbf{a}}\right)^T \boldsymbol{\lambda} \\
\dot{\mathbf{b}} &= [\mathbf{b}, \widetilde{\mathcal{H}}']_* = \frac{\partial \widetilde{\mathcal{H}}'}{\partial \mathbf{b}_{\mathcal{P}}} = \boldsymbol{\eta}_{\mathrm{b}} \\
\dot{\mathbf{b}}_{\mathcal{P}} &= [\mathbf{b}_{\mathcal{P}}, \widetilde{\mathcal{H}}']_* = -\frac{\partial \widetilde{\mathcal{H}}'}{\partial \mathbf{b}} = -\left(\frac{\partial \boldsymbol{\Phi}}{\partial \mathbf{b}}\right)^T \boldsymbol{\lambda} \\
\dot{\boldsymbol{\lambda}} &= [\boldsymbol{\lambda}, \widetilde{\mathcal{H}}']_* = \frac{\partial \widetilde{\mathcal{H}}'}{\partial \boldsymbol{\lambda}_{\mathcal{P}}} = \boldsymbol{\eta}_{\lambda} \\
\dot{\boldsymbol{\lambda}}_{\mathcal{P}} &= [\boldsymbol{\lambda}_{\mathcal{P}}, \widetilde{\mathcal{H}}']_* = -\frac{\partial \widetilde{\mathcal{H}}'}{\partial \boldsymbol{\lambda}} = -\boldsymbol{\Phi}
\end{aligned}
\tag{8.87}
$$

Proposition 8.1.1 (Poisson's Bracket on $\mathbb{P}$)

Define Poisson's bracket on the extended cotangent bundle $\mathbb{P}$ as

$$
\boxed{
\begin{aligned}
[A, B]_* := {} & \frac{\partial A}{\partial \boldsymbol{\Upsilon}}\frac{\partial B}{\partial \boldsymbol{\Upsilon}_{\mathcal{P}}} - \frac{\partial A}{\partial \boldsymbol{\Upsilon}_{\mathcal{P}}}\frac{\partial B}{\partial \boldsymbol{\Upsilon}} + \frac{\partial A}{\partial \boldsymbol{\upsilon}}\frac{\partial B}{\partial \boldsymbol{\upsilon}_{\mathcal{P}}} - \frac{\partial A}{\partial \boldsymbol{\upsilon}_{\mathcal{P}}}\frac{\partial B}{\partial \boldsymbol{\upsilon}} \\
& + \frac{\partial A}{\partial \mathbf{a}}\frac{\partial B}{\partial \mathbf{a}_{\mathcal{P}}} - \frac{\partial A}{\partial \mathbf{a}_{\mathcal{P}}}\frac{\partial B}{\partial \mathbf{a}} + \frac{\partial A}{\partial \mathbf{b}}\frac{\partial B}{\partial \mathbf{b}_{\mathcal{P}}} - \frac{\partial A}{\partial \mathbf{b}_{\mathcal{P}}}\frac{\partial B}{\partial \mathbf{b}} \\
& + \frac{\partial A}{\partial \boldsymbol{\lambda}}\frac{\partial B}{\partial \boldsymbol{\lambda}_{\mathcal{P}}} - \frac{\partial A}{\partial \boldsymbol{\lambda}_{\mathcal{P}}}\frac{\partial B}{\partial \boldsymbol{\lambda}}
\end{aligned}
}
\tag{8.88}
$$

(for $i = 1, 2, \cdots, n_{\mathrm{g}}$ and $k = 1, 2, \cdots, n_{\mathrm{c}}$) for arbitrary functions, $A(\mathbf{q}, \mathbf{p}, \boldsymbol{\lambda}, \boldsymbol{\zeta}, t)$ and

$B(\mathbf{q}, \mathbf{p}, \boldsymbol{\lambda}, \boldsymbol{\zeta}, t)$.

It is important to note that Eq. (8.85) is valid only on the cotangent bundle defined by $\boldsymbol{\zeta} = \mathbf{0}$. To emphasize this point, employ the ***weak equation*** [46]. That is, $\boldsymbol{\upsilon}_{\mathcal{P}} \approx \mathbf{0}$, $\mathbf{a}_{\mathcal{P}} \approx \mathbf{0}$, $\mathbf{b}_{\mathcal{P}} \approx \mathbf{0}$, and $\boldsymbol{\lambda}_{\mathcal{P}} \approx \mathbf{0}$, and therefore,

$$\begin{aligned}
\mathbf{0} &\approx \dot{\boldsymbol{\upsilon}}_{\mathcal{P}} = -\frac{\partial \mathscr{V}}{\partial \boldsymbol{\upsilon}} - \mathbf{G}_{\upsilon}^T \boldsymbol{\lambda} \\
\mathbf{0} &\approx \dot{\mathbf{a}}_{\mathcal{P}} = -\mathbf{G}_{\mathbf{a}}^T(\boldsymbol{\Upsilon})\boldsymbol{\lambda} \\
\mathbf{0} &\approx \dot{\mathbf{b}}_{\mathcal{P}} = -\mathbf{G}_{\mathbf{b}}^T(\boldsymbol{\Upsilon})\boldsymbol{\lambda} \\
\mathbf{0} &\approx \dot{\boldsymbol{\lambda}}_{\mathcal{P}} = -\boldsymbol{\Phi}
\end{aligned} \tag{8.89}$$

where

$$\mathbf{G}_{\upsilon} := \frac{\partial \boldsymbol{\Phi}}{\partial \boldsymbol{\upsilon}}, \quad \mathbf{G}_{\mathbf{a}}(\boldsymbol{\Upsilon}) := \frac{\partial \boldsymbol{\Phi}}{\partial \mathbf{a}}, \quad \mathbf{G}_{\mathbf{b}}(\boldsymbol{\Upsilon}) := \frac{\partial \boldsymbol{\Phi}}{\partial \mathbf{b}} \tag{8.90}$$

Note that $\mathbf{G}_{\upsilon}$ is constant, and $\mathbf{G}_{\mathbf{a}}$ and $\mathbf{G}_{\mathbf{b}}$ depend only on $\boldsymbol{\Upsilon}$. Therefore, we can obtain

$$\boldsymbol{\lambda}(t) \approx \boldsymbol{\Lambda}(\boldsymbol{\Upsilon}, \mathbf{a}, \mathbf{b}) \tag{8.91}$$

from

$$\begin{aligned}
&\mathbf{0} \approx \left.\frac{\partial}{\partial \boldsymbol{\upsilon}}\right|_{\boldsymbol{\upsilon}=\bar{\mathbf{T}}\boldsymbol{\Upsilon}} \mathscr{V}(\boldsymbol{\upsilon}) + \mathbf{G}_{\upsilon}^T \boldsymbol{\lambda} \\
&\mathbf{0} \approx \mathbf{G}_{\mathbf{a}}^T(\boldsymbol{\Upsilon})\boldsymbol{\lambda}, \quad \mathbf{0} \approx \mathbf{G}_{\mathbf{b}}^T(\boldsymbol{\Upsilon})\boldsymbol{\lambda}
\end{aligned} \tag{8.92}$$

Hence, the governing equation is finally obtained as

$$\boxed{\begin{aligned}
\dot{\boldsymbol{\Upsilon}} &= \mathbf{M}^{-1}\boldsymbol{\Upsilon}_{\mathcal{P}} \\
\dot{\boldsymbol{\Upsilon}}_{\mathcal{P}} &= -\left(\frac{\partial \boldsymbol{\Phi}}{\partial \boldsymbol{\Upsilon}}\right)^T \boldsymbol{\Lambda}(\boldsymbol{\Upsilon}, \mathbf{a}, \mathbf{b})
\end{aligned} \quad \forall t \in \mathbb{I}} \tag{8.93}$$

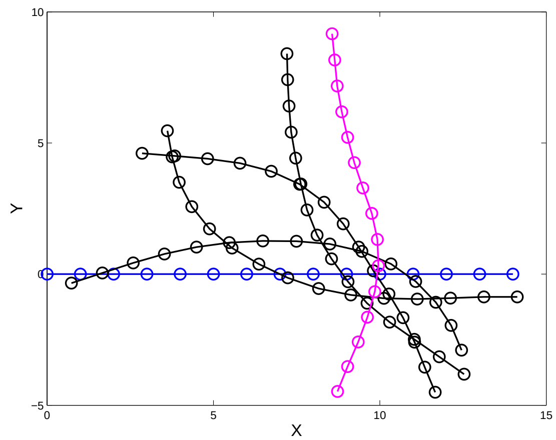
together with given initial conditions $(\boldsymbol{\Upsilon}, \boldsymbol{\Upsilon}_{\mathcal{P}})(t_0)$ as a system of first-order ODEs. Equivalently, it can be written in a system of second-order ODEs as

$$\boxed{\mathbf{M}\ddot{\boldsymbol{\Upsilon}} = -\left(\frac{\partial \boldsymbol{\Phi}}{\partial \boldsymbol{\Upsilon}}\right)^T \boldsymbol{\Lambda}(\boldsymbol{\Upsilon}, \mathbf{a}, \mathbf{b}) \quad \forall t \in \mathbb{I}} \tag{8.94}$$

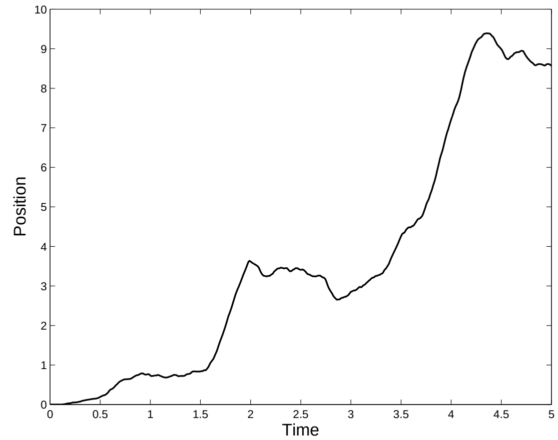
together with given initial conditions $(\boldsymbol{\Upsilon}, \dot{\boldsymbol{\Upsilon}})(t_0)$.

Example 8.1.1 (Flying flexible Rod)

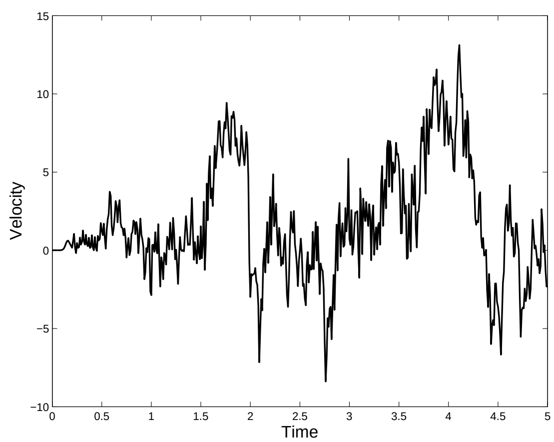
Consider a flying flexible rod of length $L = 14$ *m. Suppose external torque* $T = 90$ *Nm (in the counter-clock wise direction) and force* $f_X = 5$ *N and* $f_y = 5$ *N are applied at the most right node of the rod for* $[0, 1]$ *sec. Let the cross-sectional area, density, Young's modulus, and moment of inertia be:* $A = 0.01 \times 0.01$ m^2, $\rho = 7,000$ kg/m^3, $E = 1 \times 10^8$ N/m^2, *and* $I = 5 \times 10^6$ *, respectively. Employ time step size* $\Delta t = 0.01$ *sec and tolerance* 10^{-8} *for the Newton-type iteration. Let* $t \in \mathbb{I} = [0, 5]$ *sec. Fig. 8.5 and Fig. 8.7 shows the numerical results obtained by the MPR-MPA method and MPR-EPA method, respectively, with* 14 *elements for Eq.* (8.94). *Similarly, Fig. 8.5 and Fig. 8.7 shows the numerical results obtained by the MPR-MPA method and MPR-EPA method, respectively, with* 7 *elements. In the configuration plots, the configurations in blue color denote the initial configurations; in pink, the final configuration at time* $t = 5$ *sec. As expected, the configurations with more elements (14 elemets) are more smooth than the ones for only* 7 *elements. Note that the discrete total energy is bounded for every case since both algorithms are symplectic.*



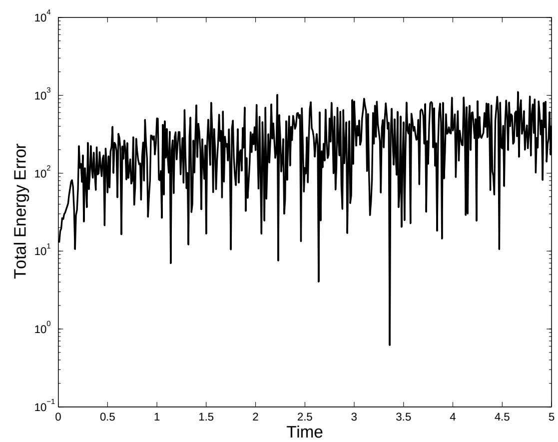
(a) Configuration



(b) Position Υ_1^n

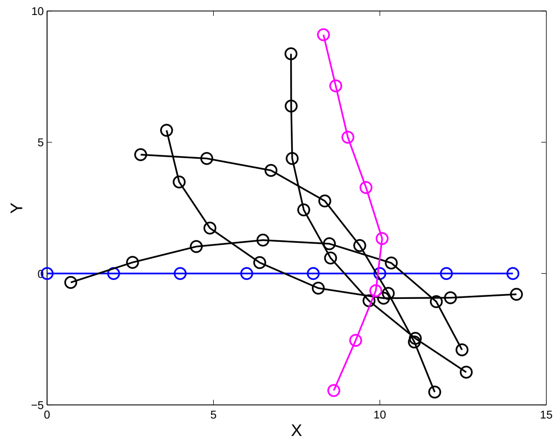


(c) Velocity $\dot{\Upsilon}_1^n$

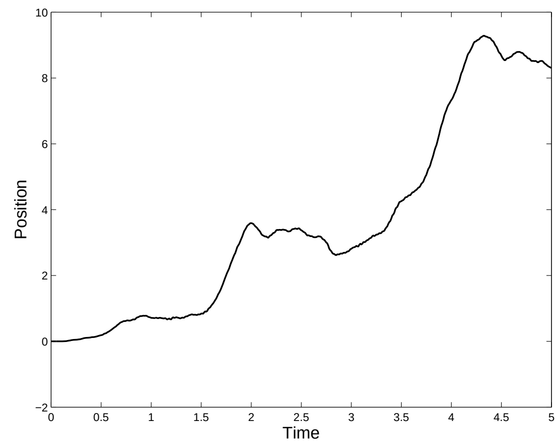


(d) Total Energy Error

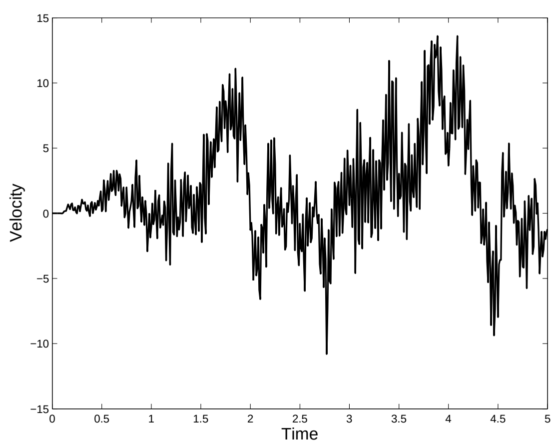
Figure 8.5: Numerical Results for Example 8.1.1: MPR-EPA Method with 14 Elements



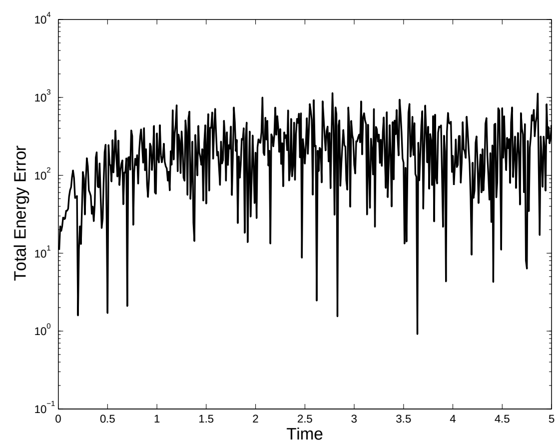
(a) Configuration



(b) Position Υ_1^n

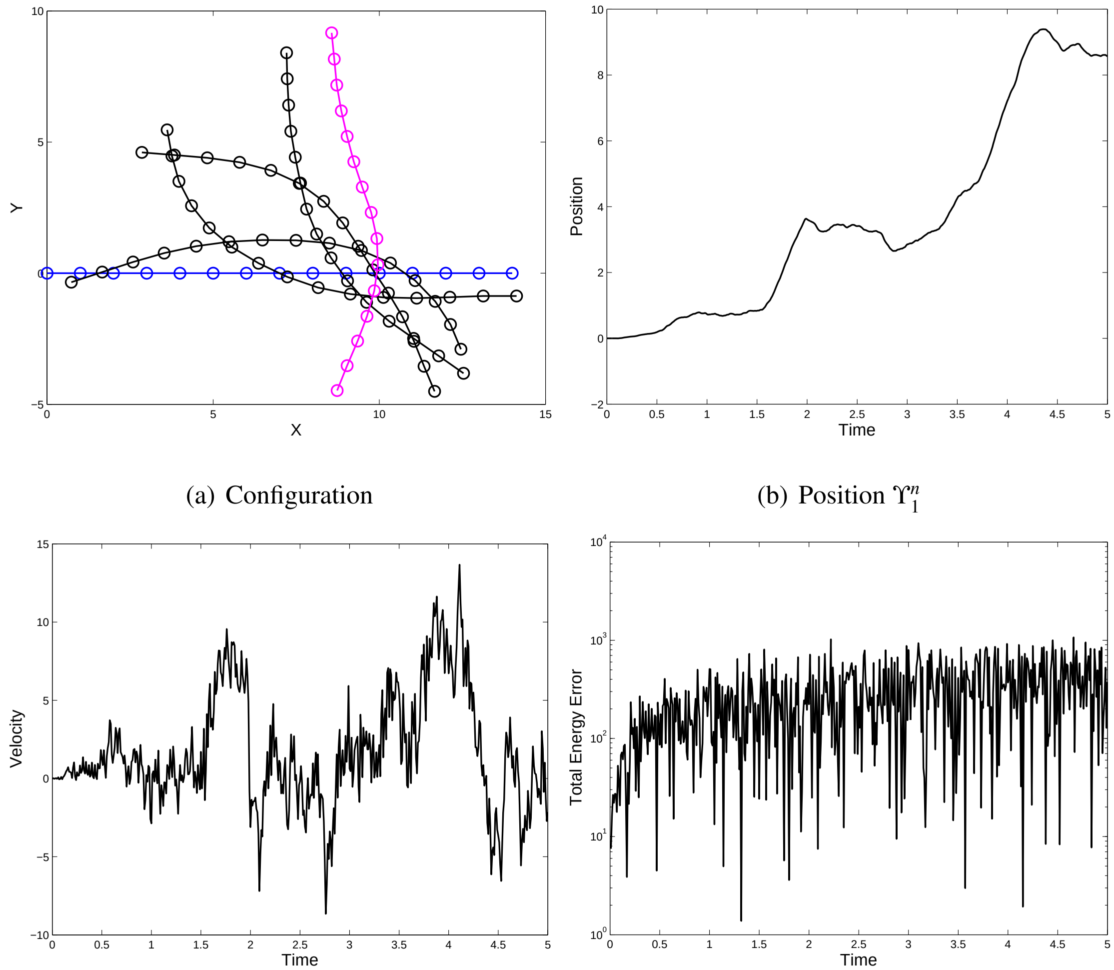


(c) Velocity $\dot{\Upsilon}_1^n$



(d) Total Energy Error

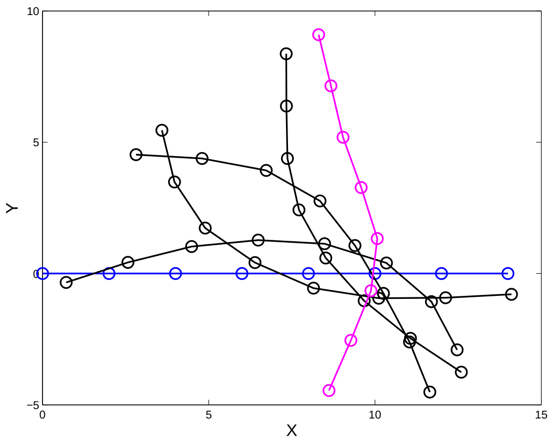
Figure 8.6: Numerical Results for Example 8.1.1: MPR-EPA Method with 7 Elements



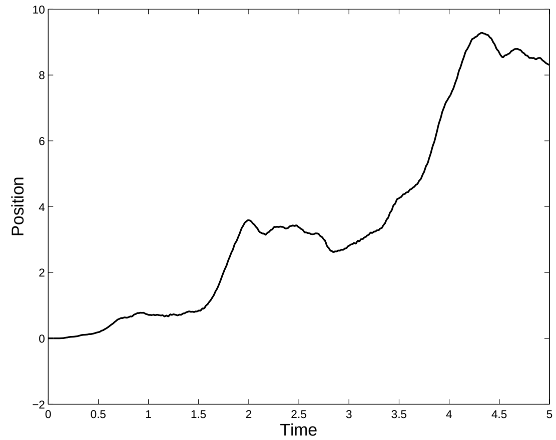
(a) Configuration (b) Position Υ_1^n

(c) Velocity $\dot{\Upsilon}_1^n$ (d) Total Energy Error

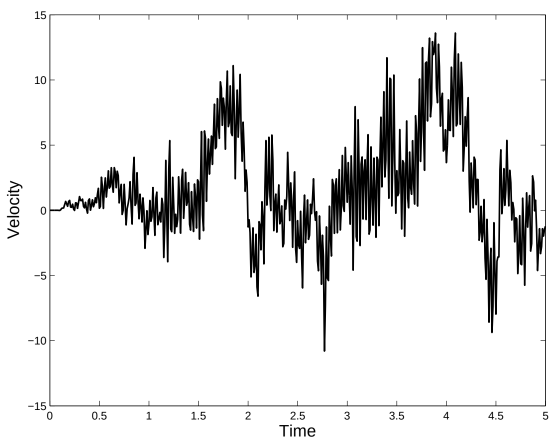
Figure 8.7: Numerical Results for Example 8.1.1: MPR-MPA Method with 14 Elements



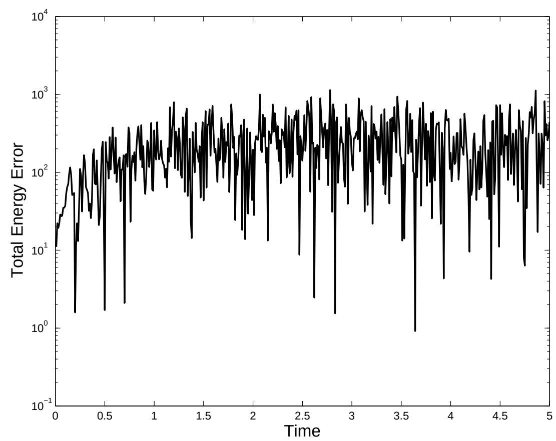
(a) Configuration



(b) Position Υ_1^n



(c) Velocity $\dot{\Upsilon}_1^n$



(d) Total Energy Error

Figure 8.8: Numerical Results for Example 8.1.1: MPR-MPA Method with 7 Elements

Chapter 9

Conclusions

The various designs and developments of the isochronous time integration architectures for ODE and DAE systems, the ODE-*i*Integrators and DAE-*i*Integrators, have been proposed. The main ideas and concepts presented in this thesis may be summarized as follows: These algorithmic architectures and frameworks allow us to numerically solve a host of science and engineering problems both in second- and first-order systems with robustness and with various numerical advantages such as second-order time accuracy and numerically dissipative and non-dissipative features, only with a single simulation toolkit.

This unified algorithmic architecture includes the generalized single step single solve families of algorithms designed for second- and first-order systems, and the simple adaptation processes, proposed in chapters 2 and 3 for ODEs and DAEs, respectively, relate the generalized algorithmic framework for second-order systems to the one for first-order systems.

Most time integration techniques presented in the literature so far need to be programmed in an independent manner. In contrast, the *i*Integrators dispense with these tedious tasks completely, as explained in this thesis extensively, and those commonly-used time integration schemes are actually the constituents of the *i*Integrators. Besides, the *i*Integrators naturally include numerous other methods and can suggest a host of hitherto unknown optimal schemes, depending on the problems that analysts want to solve. In the light of these basic intrinsic features of the *i*Integrators, the superiority of the *i*Integrators over the most time integration schemes, especially in the sense of the linear multi-step methods, are evident.

It should be noted that the DAE-*i*Integrators are based on the structure of the ODE-*i*Integrators, and the adaptation process for DAE cases conforms to the one for ODE cases. There exist various types of formulations in DAEs as summarized at the beginning of Chapter 3; and the DAE-*i*Integrators have been designed in such a way that they can be directly applied to all cases presented without losing the numerical advantages that the original ODE-*i*Integrators possess. In addition, as investigated in Chapter 4, the DAE-*i*Integrators can be applied even for the subdomain problems formulated in DAEs, and provide new attractive features that the other approaches in the literature currently available do not possess, especially with regard to the time accuracy of the algorithms. As mentioned already throughout this thesis, a wide variety of science and engineering problems can be cast into an ODE or DAE system, and perhaps one of the most typical examples is the multibody dynamics. Chapters 5-8 provided the theoretical investigations on the various basic and advanced topics in the area with a new in-depth look to support the theoretical understanding of the computational DAE problems.

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Appendix A

Definitions

A.1 Euclidean Spaces

Let $\mathbb{E}^n$ denote a ***n-dimensional Euclidean space***. The elements of an n-dimensional Euclidean space $\mathbb{E}^n$ are called ***points***. In $\mathbb{E}^n$, one defines a ***Cartesian frame*** $\mathcal{B}$ (see Definition A.1.1); and every point $\mathbf{P}$ in $\mathbb{E}^n$ has coordinates $(p_1, p_2, \cdots, p_n) \in \mathbb{R}^n$ with respect to $\mathcal{B}$, where $\mathbb{R}^n$ is the ***n-dimensional real arithmetic space*** defined as

$$\mathbb{R}^n = \underbrace{\mathbb{R} \times \mathbb{R} \times \cdots \times \mathbb{R}}_{n \text{ times; } \times\text{: Cartesian set product}} = \{(p_1, p_2, \cdots, p_n) | \; p_i \in \mathbb{R} \;\text{ for }\; i = 1, 2, \cdots, n\} \tag{A.1}$$

$\mathbb{R}$ is the field of real numbers; and the elements of $\mathbb{R}$ are called ***scalars***. The ***distance*** between two points, $\mathbf{P} \in \mathbb{E}^n$ and $\mathbf{Q} \in \mathbb{E}^n$, is defined by a map $\mathrm{dis} : \mathbb{E}^n \times \mathbb{E}^n \to \mathbb{R}$

$$\mathrm{dis}(\mathbf{P}, \mathbf{Q}) = \sqrt{\sum_{i=1}^{n} (p_i - q_i)} \geq 0 \tag{A.2}$$

where $p_i \in \mathbb{R}$ and $q_i \in \mathbb{R}$ are the coordinates of points $\mathbf{P}$ and $\mathbf{Q}$, respectively. Note that $\mathrm{dis}(\mathbf{P}, \mathbf{Q}) = 0$ if and only if $\mathbf{P} = \mathbf{Q}$; and $\mathrm{dis}(\mathbf{P}, \mathbf{Q}) = \mathrm{dis}(\mathbf{Q}, \mathbf{P})$. Furthermore, the

triangle inequality (or ***Pythagoras' theorem***) essentially holds in $\mathbb{E}^n$:

$$\boxed{\operatorname{dis}(\mathbf{P},\mathbf{Q}) + \operatorname{dis}(\mathbf{Q},\mathbf{S}) \geq \operatorname{dis}(\mathbf{P},\mathbf{S}) \quad \forall \mathbf{P},\mathbf{Q},\mathbf{S} \in \mathbb{E}^n} \tag{A.3}$$

Vectors are defined as the difference between two points; and the elements of $\mathbb{V}^n$ are called ***vectors***. Define a map $\boldsymbol{\pi} : \mathbb{E}^n \times \mathbb{E}^n \rightarrow \mathbb{V}^n$ as

$$\boldsymbol{\pi}(\mathbf{Q},\mathbf{P}) = \mathbf{P} - \mathbf{Q} = (p_i - q_i)\vec{\mathbf{e}}_i \quad \forall \mathbf{P},\mathbf{Q} \in \mathbb{E}^n \tag{A.4}$$

See Theorem A.1.2 for the properties of the mapping $\boldsymbol{\pi}$. $(p_i - q_i)$ for $i = 1, 2, \cdots, n$ are the coordinates of the vector $\boldsymbol{\pi}(\mathbf{Q},\mathbf{P}) \in \mathbb{V}^n$, and they can be expressed as

$$p_i - q_i = \boldsymbol{\pi}(\mathbf{Q},\mathbf{P}) \cdot \vec{\mathbf{e}}_i \tag{A.5}$$

Two vectors $\boldsymbol{\pi}(\mathbf{Q},\mathbf{P}) \in \mathbb{V}^n$ and $\boldsymbol{\pi}(\mathbf{Q}',\mathbf{P}') \in \mathbb{V}^n$ are ***equivalent*** if they have the same ***length*** (see Eq. (A.9b) in Definition A.1.3), i.e., $\|\boldsymbol{\pi}(\mathbf{Q},\mathbf{P})\| = \|\boldsymbol{\pi}(\mathbf{Q}',\mathbf{P}')\|$, and are parallel. If $\mathbf{Q} = \mathbf{O} \in \mathbb{E}^n$ (***origin***) in Eq. (A.4), i.e.,

$$\boldsymbol{\pi}(\mathbf{O},\mathbf{P}) = \mathbf{P} - \mathbf{O} = p_i\vec{\mathbf{e}}_i \tag{A.6}$$

$\boldsymbol{\pi}(\mathbf{O},\mathbf{P}) \in \mathbb{V}^n$ is called the ***radius vector*** (or ***position vector***) of $\mathbf{P} \in \mathbb{E}^n$ with respect to $\mathcal{B}$.

Definition A.1.1 (Cartesian Frame $\mathcal{B}$ for $\mathbb{E}^n$)

*A Cartesian frame $\mathcal{B}$ for $\mathbb{E}^n$ is defined by an origin $\mathbf{O} \in \mathbb{E}^n$ and orthonormal base vectors $\vec{\mathbf{e}}_i$ for $i = 1, 2, \cdots, n$ defined in the associated **vector space** $\mathbb{V}^n$ (see Definition A.1.2). The orthonormal base vectors $\vec{\mathbf{e}}_i$ satisfy*

$$\vec{\mathbf{e}}_i \cdot \vec{\mathbf{e}}_j = \delta_{ij} \tag{A.7a}$$

where "·" denotes the ***scalar product*** *(see Definition A.1.3), and δ_{ij} is the* ***Kronecker delta*** *symbol defined as*

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \tag{A.7b}$$

for $i, j = 1, 2, \cdots, n$.

Definition A.1.2 (Vector Space or Linear Space)

$\mathbb{V}^n$ is called a ***vector space*** *(or* ***linear space****) over the real scalar fields $\mathbb{R}$ if*

$$\begin{aligned} &\vec{\mathbf{x}} + \vec{\mathbf{y}} \in \mathbb{V}^n \\ &c\vec{\mathbf{x}} \in \mathbb{V}^n \end{aligned} \quad \forall \vec{\mathbf{x}}, \vec{\mathbf{y}} \in \mathbb{V}^n \text{ and } c \in \mathbb{R} \tag{A.8}$$

One refers to elements of $\mathbb{V}^n$ as ***vectors****. An* ***scalar product*** *(see Definition A.1.3) on $\mathbb{V}^n$ holds for each ordered pair of vectors $\vec{\mathbf{x}} \in \mathbb{V}^n$ and $\vec{\mathbf{y}} \in \mathbb{V}^n$.*

Definition A.1.3 (Scalar Product or dot Product)

Scalar product *(or* ***dot product****) of two real vectors $\vec{\mathbf{x}}, \vec{\mathbf{y}} \in \mathbb{V}^n$ is defined as*

$$\begin{aligned} \vec{\mathbf{x}} \cdot \vec{\mathbf{y}} &= (x_i\vec{\mathbf{e}}_i) \cdot (y_i\vec{\mathbf{e}}_i) = x_i y_j \vec{\mathbf{e}}_i \cdot \vec{\mathbf{e}}_j = x_i y_j \delta_{ij} \\ &= x_i y_i = \mathbf{x}^T\mathbf{y} = (\mathbf{x}, \mathbf{y}) \end{aligned} \tag{A.9a}$$

The ***length*** *or* ***norm*** *of $\vec{\mathbf{x}} \in \mathbb{V}^n$ is defined as*

$$||\vec{\mathbf{x}}||_2 := ||\vec{\mathbf{x}}|| = \sqrt{\vec{\mathbf{x}} \cdot \vec{\mathbf{x}}} = (x_i x_i)^{1/2} = \sqrt{\mathbf{x}^T\mathbf{x}} = \sqrt{(\mathbf{x}, \mathbf{x})} \tag{A.9b}$$

and an (acute) ***angle*** *between two vectors $\vec{\mathbf{x}}, \vec{\mathbf{y}} \in \mathbb{V}^n$ is defined as*

$$\theta = \arccos\left(\frac{\vec{\mathbf{x}} \cdot \vec{\mathbf{y}}}{||\vec{\mathbf{x}}||||\vec{\mathbf{y}}||}\right) \in [0, \pi] \tag{A.9c}$$

Theorem A.1.1 (Properties of the Scalar Product)

The scalar product possesses the following properties:

$$\begin{aligned} \textbf{\textit{Symmmetry:}}\quad & \vec{\mathbf{x}} \cdot \vec{\mathbf{y}} = \vec{\mathbf{y}} \cdot \vec{\mathbf{x}} \\ \textbf{\textit{Linearity:}}\quad & (\vec{\mathbf{x}} + \vec{\mathbf{y}}) \cdot \vec{\mathbf{z}} = \vec{\mathbf{x}} \cdot \vec{\mathbf{z}} + \vec{\mathbf{y}} \cdot \vec{\mathbf{z}} \\ & (c\vec{\mathbf{x}}) \cdot \vec{\mathbf{y}} = \vec{\mathbf{x}} \cdot (c\vec{\mathbf{y}}) = c\vec{\mathbf{x}} \cdot \vec{\mathbf{y}} \\ \textbf{\textit{Positive-definiteness:}}\quad & \vec{\mathbf{x}} \cdot \vec{\mathbf{x}} > 0 \ \ \textit{if}\ \vec{\mathbf{x}} \neq \vec{\mathbf{0}}, \quad \vec{\mathbf{x}} \cdot \vec{\mathbf{x}} = 0 \ \ \textit{if and only if}\ \ \vec{\mathbf{x}} = \vec{\mathbf{0}} \end{aligned} \tag{A.10}$$

for all $\vec{\mathbf{x}}, \vec{\mathbf{y}}, \vec{\mathbf{z}} \in \mathbb{V}^n$ *and* $c \in \mathbb{R}$.

Theorem A.1.2 (Properties of $\boldsymbol{\pi} : \mathbb{E}^n \times \mathbb{E}^n \to \mathbb{V}^n$)

The mapping $\boldsymbol{\pi} : \mathbb{E}^n \times \mathbb{E}^n \to \mathbb{V}^n$ *possesses the following properties:*

$$\left.\begin{aligned} & \boldsymbol{\pi}(\mathbf{Q}, \mathbf{P}) + \boldsymbol{\pi}(\mathbf{P}, \mathbf{S}) = \boldsymbol{\pi}(\mathbf{Q}, \mathbf{S}) \\ & \boldsymbol{\pi} : \mathbb{R}^0 \times \mathbb{E}^n \ \textit{is a bijection.} \end{aligned}\right. \quad \forall \mathbf{P}, \mathbf{Q}, \mathbf{S} \in \mathbb{E}^n \tag{A.11}$$

where $\mathbb{R}^0 \equiv \{0\}$.

A.2 Rotation Groups

A.2.1 Orthogonal Groups

Consider ***rotations*** of a vector $\vec{\mathbf{x}} = x_i \vec{\mathbf{e}}_i = \mathbf{x}^T \mathbf{e} \in \mathbb{V}^n$, described by a ***linear transformation*** (see Definition A.2.1) as

$$\mathbf{x}' = \mathcal{F}(\mathbf{x}) = \mathbf{A}\mathbf{x} \tag{A.12}$$

If the length of the vector $\vec{\mathbf{x}} = x_i \vec{\mathbf{e}}_i = \mathbf{x}^T \mathbf{e} \in \mathbb{V}^n$ does not change under the transformation, i.e., $||\vec{\mathbf{x}}'||^2 = ||\vec{\mathbf{x}}||^2$ holds where

$$||\vec{\mathbf{x}}'||^2 = \vec{\mathbf{x}}' \cdot \vec{\mathbf{x}}' = (\mathbf{x}', \mathbf{x}') = (\mathcal{F}(\mathbf{x}), \mathcal{F}(\mathbf{x})) = (\mathbf{A}\mathbf{x})^T (\mathbf{A}\mathbf{x}) = \mathbf{x}^T (\mathbf{A}^T \mathbf{A})\mathbf{x} = (\mathbf{x}, \mathbf{A}^T \mathbf{A}\mathbf{x}) \tag{A.13}$$

it is evident that $\mathbf{A}$ is ***orthogonal***. That is, $(\mathbf{x}', \mathbf{x}') = (\mathbf{x}, \mathbf{x})$ if and only if $\mathbf{A} \in O(n)$. In other words, $\mathbf{A}$ belongs to the ***orthogonal group*** (see Definition A.2.3) if the linear transformation preserves the scalar product of any two vectors in $\mathbb{V}^n$. Such a linear transformation is called the ***orthogonal transformation***; see Definition A.2.2.

Definition A.2.1 (Linear Transformation)

*A mapping $\mathcal{F} : \mathbb{R}^n \to \mathbb{R}^n$ is a **linear transformation** if*

$$\mathcal{F}(c_1\mathbf{x} + c_2\mathbf{y}) = c_1\mathcal{F}(\mathbf{x}) + c_2\mathcal{F}(\mathbf{y}) \quad \forall\ \mathbf{x}, \mathbf{y} \in \mathbb{R}^n \text{ and } c_1, c_2 \in \mathbb{R} \tag{A.14}$$

Definition A.2.2 (Orthogonal Transformation)

*A linear transformation $\mathcal{F} : \mathbb{R}^n \to \mathbb{R}^n$ is a **orthogonal transformation** if the length is invariant under the transformation:*

$$(\mathcal{F}(\mathbf{x}), \mathcal{F}(\mathbf{y})) = (\mathbf{x}, \mathbf{y}) \quad \forall\ \mathbf{x}, \mathbf{y} \in \mathbb{R}^n \tag{A.15}$$

Definition A.2.3 (Orthogonal Group $O(n)$)

The orthogonal group $O(n)$ consists of the real orthogonal matrices $\mathbf{A} = [A_{ij}] \in \mathbb{R}^{n\times n}$ which satisfy

$$\mathbf{A}^T\mathbf{A} = \mathbf{A}\mathbf{A}^T = \mathbf{I}_n \ \text{ or } \ \mathbf{A}^{-1} = \mathbf{A}^T$$

Note that the above orthogonality condition readily leads to

$$\det(\mathbf{A}^T\mathbf{A}) = \det(\mathbf{A}^T)\det(\mathbf{A}) = (\det(\mathbf{A}))^2 = 1, \quad \textit{i.e.}, \ \det(\mathbf{A}) = \pm 1$$

The orthogonal group $O(n)$ may be written as:

$$O(n) := \{\mathbf{A} |\ \mathbf{A}^T\mathbf{A} = \mathbf{A}\mathbf{A}^T = \mathbf{I}_n\} \tag{A.16a}$$

Definition A.2.4 (Special Orthogonal Group $SO(n)$)

The special orthogonal group $SO(n)$ is defined as the set of the real orthogonal matrices with $\det(\mathbf{A}) = +1$*:*

$$SO(n) := \{\mathbf{A} |\ \mathbf{A}^T\mathbf{A} = \mathbf{A}\mathbf{A}^T = \mathbf{I}_n \ \& \ \det(\mathbf{A}) = +1\} \tag{A.17a}$$

Appendix B

A Brief Review of Matrix Decompositions

B.1 Eigendecomposition

Let $\mathcal{V}$ be the set of all vectors, and assume $\mathcal{V}$ possesses the structure of a real vector space,

$$\begin{aligned} &\mathbf{x} + \mathbf{y} \in \mathcal{V} \ \ \forall \mathbf{x},\ \mathbf{y} \in \mathcal{V} \\ &\alpha \mathbf{x} \in \mathcal{V} \ \ \forall \mathbf{x} \in \mathcal{V} \text{ and } \alpha \in \mathbb{R} \end{aligned} \tag{B.1}$$

where $\mathbb{R}$ denotes the field of real numbers. Consider a basis for $\mathcal{V}$, $\{\mathbf{e}_i\}_{i=1}^n \equiv \{\mathbf{e}_1, \mathbf{e}_2, \cdots, \mathbf{e}_n\}$. Suppose any vector $\mathbf{x} \in \mathcal{V}$ can be uniquely decomposed as

$$\mathbf{x} = x_1 \mathbf{e}_1 + x_2 \mathbf{e}_2 + \cdots + x_n \mathbf{e}_n = x_i \mathbf{e}_i \tag{B.2}$$

where $x_i = \mathbf{x} \cdot \mathbf{e}_i \in \mathbb{R}$ are the components of $\mathbf{x}$ in the basis $\{\mathbf{e}_i\}_{i=1}^n$. The matrix representation of $\mathbf{x}$ in the given basis reads

$$\{\mathbf{x}\} = (x_1, x_2, \cdots, x_n)^T \in \mathbb{R}^n \tag{B.3}$$

Notice that a given vector $\mathbf{x}$ can be written in different matrix representations depending on the choice of basis. A second-order tensor on $\mathcal{V}$, $\mathbf{A} \in \mathcal{V}^2$, is the mapping, $\mathbf{A} : \mathcal{V} \to \mathcal{V}$, and it is linear if

$$\begin{aligned} &\mathbf{A}(\mathbf{x}+\mathbf{y}) = \mathbf{A}\mathbf{x} + \mathbf{A}\mathbf{y} \;\; \forall \mathbf{x},\; \mathbf{v} \in \mathcal{V} \\ &\mathbf{A}(\alpha\mathbf{x}) = \alpha\mathbf{A}\mathbf{x} \;\; \forall \mathbf{x} \in \mathcal{V} \text{ and } \alpha \in \mathbb{R} \end{aligned} \tag{B.4}$$

Note that $\mathcal{V}^2$ denotes the set of second-order tensors, and assume it possesses the structure of a real vector space,

$$\begin{aligned} &\mathbf{A}+\mathbf{B} \in \mathcal{V}^2 \;\; \forall \mathbf{A},\; \mathbf{B} \in \mathcal{V}^2 \\ &\alpha\mathbf{A} \in \mathcal{V}^2 \;\; \forall \mathbf{A} \in \mathcal{V}^2 \text{ and } \alpha \in \mathbb{R} \end{aligned} \tag{B.5}$$

The matrix representation of $\mathbf{A}$ in a given coordinate frame is $[\mathbf{A}] \in \mathbb{R}^{n\times n}$, and its components is $A_{ij} \in \mathbb{R}$.

Eigenvalues and Eigenvectors: Consider a second-order real tensor, $\mathbf{A} \in \mathcal{V}^2$, which maps a vector, $\mathbf{y} \in \mathcal{V}$, to another vector, $\mathbf{x} \in \mathcal{V}$,

$$\mathbf{y} = \mathbf{A}(\mathbf{x}) = \mathbf{A}\mathbf{x} \tag{B.6}$$

or in the index notation,

$$y_i = A_{ij}x_j \tag{B.7}$$

in which $A_{ij} \in \mathbb{R}$ for $i, j = 1, 2, \cdots, n$. We call $\mathbf{A}(\mathbf{x}) = \mathbf{A}\mathbf{x} : \mathcal{V} \to \mathcal{V}$ a ***linear transformation***. When $y_i \in \mathbb{R}$ is collinear with $x_i \in \mathbb{R}$, i.e., $y_i = \zeta x_i$ for $\zeta \in \mathbb{R}$, we have

$$y_i = \zeta x_i = A_{ij}x_j \tag{B.8}$$

or

$$\left(A_{ij} - \zeta\delta_{ij}\right)x_j = 0 \tag{B.9}$$

which has non-trivial solutions for $x_i \neq 0$ only if $A_{ij} - \zeta\delta_{ij}$ is singular, i.e.,

$$f(\zeta) \equiv \det(A_{ij} - \zeta\delta_{ij}) = 0 \tag{B.10}$$

where det represents the determinant function on second-order tensors. Note that "non-trivial solutions" mean non-zero vectors x_i which satisfy Eq. (B.9). $f(\zeta)$ is called the characteristic polynomial, and the roots of the characteristic equation for A_{ij}, Eq. (B.10), are called the ***eigenvalues*** (or principal values) of A_{ij}. The corresponding x_i are the ***eigenvectors*** (or principal directions) of A_{ij}.

Remarks (*Eigenvalues and Eigenvectors*):

- There exists at least one eigenvector associated with each distinct eigenvalue.
- If an eigenvalue is real, $\zeta \in \mathbb{R}$, then the components of the associated eigenvector may be also real, $\{\mathbf{x}\} \in \mathbb{R}^n$.
- Let $(\zeta_i, \mathbf{x}_i)$ for $i = 1, 2, \cdots, m$, where m is the number of *distinct* eigenvalues, be ***eigenpairs***. $(\zeta_1, \zeta_2, \cdots, \zeta_m)$ denotes a set of m eigenvalues of $\mathbf{A}$, and $(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_m)$ denotes a set of m eigenvectors of $\mathbf{A}$. ζ_i is a eigenvalue which is associated with $\mathbf{x}_i$. The set of the eigenvectors is ***linearly independent***.
- When $A_{ij} = A_{ji}$ (***symmetric***), all eigenvalues are real. Therefore, the associated eigenvectors are also real. Also, any two eigenvectors associated with distinct eigenvalues of the symmetric $\mathbf{A}$ are ***orthogonal***, i.e., $(\mathbf{x}_i, \mathbf{x}_j) = 0$ for $i \neq j$ where $(\cdot, \cdot)$ denotes an inner product defined in the vector space; hence, a set of the eigenvectors is said to be orthogonal. If the non-zero eigenvectors in a set are normalized, the set of the eigenvectors is said to be ***orthonormal***. Note that if a

set of vectors $(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_m)$ is orthogonal and $\mathbf{x}_i \neq \mathbf{0}$, it is linearly independent; hence, an orthonormal set of vectors is always linearly independent.

- The eigenvalues of a symmetric, positive-definite A_{ij} are strictly positive. That is, for an eigenpair $(\zeta, \mathbf{x})$,

$$0 < x_i A_{ij} x_j = x_i x_i \zeta = \zeta \tag{B.11}$$

  where we have used $A_{ij} x_j = \zeta x_i$. Similarly, for a symmetric, positive semi-definite A_{ij}, we have $0 \leq \zeta$.

- From Eq. (B.10), the characteristic equation for $[\mathbf{A}] \in \mathbb{R}^{3\times 3}$ may be written in the form

$$f(\zeta) = \zeta^3 - I_1 \zeta^2 - I_2 \zeta - I_3 = 0 \tag{B.12}$$

  where the first, second, and third invariants are given by

$$I_1 = A_{ii} \tag{B.13}$$

$$I_2 = \frac{1}{2}(A_{ij}A_{ji} - A_{ii}A_{jj}) \tag{B.14}$$

$$\begin{aligned} I_3 &= \tfrac{1}{6}(\epsilon_{ijk}\epsilon_{pqr}A_{ip}A_{jq}A_{kr}) \\ &= \tfrac{1}{6}(2A_{ij}A_{jk}A_{ki} - 3A_{ij}A_{ji}A_{kk} + A_{ii}A_{jj}A_{kk}) \end{aligned} \tag{B.15}$$

  respectively. I_i (for $i = 1, 2, 3$) are independent from the coordinate system in which they are expressed.

Eigendecomposition: For each eigenpair $(\zeta_i, \mathbf{x}_i)$, we can write $\mathbf{A}\mathbf{x}_i = \zeta_i \mathbf{x}_i$ (no sum on i); therefore,

$$\mathbf{AP} = \mathbf{PW} \tag{B.16}$$

where $\mathbf{W} = \mathrm{diag}(\zeta_1, \zeta_2, \cdots, \zeta_n) \in \mathcal{V}^2$ and $\mathbf{P} = [\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n] \in \mathcal{V}^2$. Because a set of the eigenvectors of $\mathbf{A}$, $(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n)$, is linearly independent, $\mathbf{P}$ is non-singular (invertible), i.e., $\mathbf{P}^{-1} \in \mathcal{V}^2$ exists such that $\mathbf{P}\mathbf{P}^{-1} = \mathbf{P}^{-1}\mathbf{P} = \mathbf{I}$, where $\mathbf{I} \in \mathcal{V}^2$ denotes the identity tensor with $[\mathbf{I}]_{ij} = \delta_{ij}$. Hence,

$$\mathbf{A} = \mathbf{P}\mathbf{W}\mathbf{P}^{-1} \quad \text{or} \quad A_{ij} = P_{i\ell} W_{\ell k} P^{-1}_{kj} \tag{B.17}$$

or

$$\mathbf{W} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P} \quad \text{or} \quad W_{ij} = P^{-1}_{i\ell} A_{\ell k} P_{kj} \tag{B.18}$$

where $[\mathbf{P}^{-1}]_{ij} = P^{-1}_{ij}$. Eq. (B.17) is called the ***eigendecomposition*** of $\mathbf{A}$.

Remarks (*Eigendecomposition*):

- We showed the eigendecomposition in the linear vector space $\mathcal{V}$ over the real scalar field $\mathbb{R}$, but it can be also discussed in the same manner in $\mathcal{V}$ over the complex field $\mathbb{C}$.

- If $A_{ij} = A_{ji}$ (symmetric) and the eigenvectors are normalized, then the normalized eigenvectors span an orthonormal basis, and we have

$$\mathbf{P}^{-1} = \mathbf{P}^T \quad \text{or} \quad P^{-1}_{ij} = P_{ji} \tag{B.19}$$

  That is,

$$\mathbf{P}\mathbf{P}^T = \mathbf{P}^T\mathbf{P} = \mathbf{I} \quad \text{or} \quad P_{ik}P_{jk} = P_{ki}P_{kj} = \delta_{ij} \tag{B.20}$$

  Therefore, in this particular case, Eq. (B.17) and Eq. (B.18) can be written as

$$\begin{aligned} \mathbf{A} &= \mathbf{P}\mathbf{W}\mathbf{P}^T \quad \text{or} \quad A_{ij} = P_{i\ell} W_{\ell k} P_{jk} && \text{(B.21)} \\ \mathbf{W} &= \mathbf{P}^T\mathbf{A}\mathbf{P} \quad \text{or} \quad W_{ij} = P_{\ell i} A_{\ell k} P_{kj} && \text{(B.22)} \end{aligned}$$

  respectively.

Similarity Transformation: Suppose that Z_{ij} maps a vector x'_i to another vector x_i via $x_i = Z_{ij}x'_j$. Assuming Z_{ij} is non-singular, we can write $x'_i = P^{-1}_{ij}x_j$. In view of Eq. (B.7), the coordinate transformation $y_i = Z_{ij}y'_j$ yields

$$y'_i = Z^{-1}_{ij}y_j = Z^{-1}_{ij}A_{jk}x_k = Z^{-1}_{ij}A_{jk}Z_{k\ell}x'_\ell = W_{i\ell}x'_\ell \tag{B.23}$$

We can see that x'_i is mapped to y'_i via $W_{ij} = Z^{-1}_{i\ell}A_{\ell k}Z_{kj}$. A second-order tensor $\mathbf{B} \in \mathcal{V}^2$ is said to be ***similar*** to $\mathbf{A} \in \mathcal{V}^2$ if there exists a non-singular $\mathbf{Z} \in \mathcal{V}^2$ such that

$$\mathbf{B} = \mathbf{Z}^{-1}\mathbf{A}\mathbf{Z} \quad \text{or} \quad B_{ij} = Z^{-1}_{i\ell}A_{\ell k}Z_{kj} \tag{B.24}$$

Note that $\mathbf{A}$ is also similar to $\mathbf{B}$ since $\mathbf{A} = \mathbf{Q}^{-1}\mathbf{B}\mathbf{Q}$ where $\mathbf{Q} = \mathbf{Z}^{-1}$. Eq. (B.24) is known as the similarity transformation from $\mathbf{A}$ to $\mathbf{B}$. A set of vectors $(\mathbf{z}_1, \mathbf{z}_2, \cdots, \mathbf{z}_n)$ for $\mathbf{Z} = [\mathbf{z}_1, \mathbf{z}_2, \cdots, \mathbf{z}_n] \in \mathcal{V}^2$ in Eq. (B.24) does not need to be orthogonal (or orthonormal). When $\mathbf{Z} = \mathbf{P}$, we have $\mathbf{B} = \mathbf{W}$; see Eq. (B.18).

Remarks (*Similarity Transformation*):

- The trace is invariant under the similarity transformation;

$$\mathrm{tr}(B_{ij}) = \mathrm{tr}(Z^{-1}_{ik}A_{k\ell}Z_{\ell j}) = \mathrm{tr}(Z^{-1}_{i\ell}Z_{\ell k}A_{kj}) = \mathrm{tr}(A_{ij}) \tag{B.25}$$

  where tr represents the trace function on second-order tensors.

- The determinant is also invariant under the similarity transformation, and $\mathbf{A}$ and $\mathbf{B}$ in Eq. (B.24) have the same eigenvalues;

$$\begin{aligned} \det(B_{ij} - \zeta\delta_{ij}) &= \det(Z^{-1}_{ik}A_{k\ell}Z_{\ell j} - \zeta\delta_{ij}) = \det(Z^{-1}_{ik}[A_{k\ell} - \zeta\delta_{k\ell}]Z_{\ell j}) \\ &= \frac{\det(Z_{k\ell})}{\det(Z_{pq})}\det(A_{ij} - \zeta\delta_{ij}) = \det(A_{ij} - \zeta\delta_{ij}) \end{aligned} \tag{B.26}$$

- If $\mathbf{A}$ in Eq. (B.24) has an eigenvector $\mathbf{x} \neq \mathbf{0}$, we have the following relation from $\mathbf{A}\mathbf{x} = \zeta\mathbf{x}$, using Eq. (B.24):

$$B_{ij}(Z^{-1}_{jk} x_k) = \zeta(Z^{-1}_{ij} x_j) \tag{B.27}$$

  That is, $\mathbf{Z}^{-1}\mathbf{x}$ is the eigenvector of $\mathbf{B}$ associated with ζ.

B.2 Schur Decomposition

If components of a square tensor, say $\mathbf{P}$, are complex, i.e., $P_{ij} \in \mathbb{C}$ for $i, j = 1, 2, \cdots, n$, $\mathbf{P}$ is called a complex tensor. If every components of $\mathbf{P}$ are imaginary or zero, $\mathbf{P}$ is called an imaginary tensor. $\mathbf{P}$ is called a ***unitary tensor*** if it satisfies

$$\mathbf{P}^{-1} = \mathbf{P}^{\dagger} \quad \text{or} \quad P^{-1}_{ij} = \overline{P}_{ji} \tag{B.28}$$

or

$$\mathbf{P}\mathbf{P}^{\dagger} = \mathbf{P}^{\dagger}\mathbf{P} = \mathbf{I} \quad \text{or} \quad P_{ik}\overline{P}_{jk} = \overline{P}_{ki}P_{kj} = \delta_{ij} \tag{B.29}$$

where † denotes the conjugate transpose (or Hermitian transpose) and the overbar denotes a scalar complex conjugate. The definition of the conjugate transpose follows $\mathbf{P}^{\dagger} = \overline{\mathbf{P}}^{T} = \overline{\mathbf{P}^{T}}$, and $\mathbf{P}^{\dagger}$ is called the adjoint of $\mathbf{P}$. Note that we can see, from Eq. (B.29), the column and row vectors which construct the unitary tensor $\mathbf{P}$ respectively span an orthonormal basis.

Unitary Transformation: Consider a linear transformation $\mathbf{A}(\mathbf{x}) = \mathbf{A}\mathbf{x} : \mathbb{C}^n \to \mathbb{C}^n$ on $\mathcal{V}$ over complex numbers with inner product $(\cdot, \cdot)$, and let $\mathbf{y} = \mathbf{A}(\mathbf{x}) = \mathbf{A}\mathbf{x}$. Suppose $\mathbf{P} = [\mathbf{p}_1, \mathbf{p}_2, \cdots, \mathbf{p}_n] \in \mathcal{V}^2$, where a set $(\mathbf{p}_1, \mathbf{p}_2, \cdots, \mathbf{p}_n)$ is orthonormal, i.e., $(\mathbf{p}_i, \mathbf{p}_j) =$

δ_{ij}, exists such that

$$\begin{aligned}\mathbf{y}' &= \mathbf{P}^{-1}\mathbf{y} = \mathbf{P}^{\dagger}\mathbf{y} \quad \text{or} \quad y_i' = P_{ij}^{-1} y_j = \overline{P}_{ji} y_j \\ \mathbf{x}' &= \mathbf{P}^{-1}\mathbf{x} = \mathbf{P}^{\dagger}\mathbf{x} \quad \text{or} \quad x_i' = P_{ij}^{-1} x_j = \overline{P}_{ji} x_j\end{aligned} \tag{B.30}$$

Then, we get

$$\mathbf{y}' = \mathbf{P}^{\dagger}\mathbf{A}\mathbf{P}\mathbf{x}' = \mathbf{B}\mathbf{x}' \tag{B.31}$$

Note that a set $(\mathbf{p}_1, \mathbf{p}_2, \cdots, \mathbf{p}_n)$ is orthonormal implies $\mathbf{P}$ is unitary. If there exists a unitary tensor $\mathbf{P}$ such that

$$\mathbf{B} = \mathbf{P}^{\dagger}\mathbf{A}\mathbf{P} \quad \text{or} \quad B_{ij} = \overline{P}_{\ell i} A_{\ell k} P_{kj} \tag{B.32}$$

then $\mathbf{B}$ is said to be unitarily equivalent to $\mathbf{A}$, and Eq. (B.32) is known as the ***unitary transformation*** (or unitary similarity transformation) from $\mathbf{A}$ to $\mathbf{B}$. From Eq. (B.32), we have

$$\mathbf{A} = \mathbf{P}\mathbf{B}\mathbf{P}^{\dagger} \quad \text{or} \quad A_{ij} = P_{i\ell} B_{\ell k} \overline{P}_{jk} \tag{B.33}$$

Schur Decomposition: There exists a unitary tensor $\mathbf{P} \in \mathcal{V}^2$ such that a square tensor $\mathbf{A} \in \mathcal{V}^2$ with $A_{ij} \in \mathbb{C}$ for $i, j = 1, 2, \cdots, n$ is decomposed as

$$\mathbf{A} = \mathbf{P}\mathbf{T}\mathbf{P}^{\dagger} \tag{B.34}$$

where $\mathbf{T} \in \mathcal{V}^2$ is a upper triangular tensor given by

$$\mathbf{T} = \mathbf{W} + \mathbf{N} = \mathbf{P}^{\dagger}\mathbf{A}\mathbf{P} \tag{B.35}$$

in which $\mathbf{W} = \mathrm{diag}(\zeta_1, \zeta_2, \cdots, \zeta_n) \in \mathcal{V}^2$, where ζ_i is the eigenvalues of $\mathbf{A}$, and $\mathbf{N} \in \mathcal{V}^2$ is a strictly upper triangular tensor, i.e., $N_{ij} = 0$ for $1 < i < n$ and $1 < j < i$. Eq. (B.34) is called the ***Schur decomposition*** of $\mathbf{A}$, and $\mathbf{T}$ is called a ***Schur canonical form*** of $\mathbf{A}$.

Proof (*Schur Decomposition*): Consider an eigenpair $(\zeta_1, \mathbf{x}_1)$ of $\mathbf{A}$, where $\mathbf{x}_1$ is a normalized eigenvector, i.e., $(\mathbf{x}_1, \mathbf{x}_1) = 1$. Choose a set of vectors, $(\mathbf{w}_2, \mathbf{w}_3, \cdots, \mathbf{w}_n)$, such that $(\mathbf{x}_1, \mathbf{w}_2, \mathbf{w}_3, \cdots, \mathbf{w}_n)$ becomes orthonormal, using the ***Gram-Schmidt orthgonalization*** technique, and define

$$\mathbf{Q} = [\mathbf{x}_1, \mathbf{w}_2, \mathbf{w}_3, \cdots, \mathbf{w}_n] = [\mathbf{x}_1, \mathbf{W}] \tag{B.36}$$

Since a set of the vectors, $(\mathbf{x}_1, \mathbf{w}_2, \mathbf{w}_3, \cdots, \mathbf{w}_n)$, is orthonormal, i.e., $(\mathbf{x}_1, \mathbf{w}_i) = 0$ for $i = 2, 3, \cdots, n$ and $\mathbf{Q}$ is unitary, we have

$$\begin{aligned} \mathbf{Q}^\dagger\mathbf{A}\mathbf{Q} &= \mathbf{Q}^\dagger\mathbf{A}\,[\mathbf{x}_1, \mathbf{W}] = \mathbf{Q}^\dagger\,[\mathbf{A}\mathbf{x}_1, \mathbf{A}\mathbf{W}] \\ &= \begin{bmatrix} \mathbf{x}_1^\dagger \\ \mathbf{W}^\dagger \end{bmatrix} [\zeta_1\mathbf{x}_1, \mathbf{A}\mathbf{W}] = \begin{bmatrix} \zeta_1 & \mathbf{b}^\dagger \\ \mathbf{0} & \mathbf{C} \end{bmatrix} \end{aligned} \tag{B.37}$$

where $\mathbf{b}^\dagger := \mathbf{x}_1^\dagger\mathbf{A}\mathbf{W}$ and $\mathbf{C} := \mathbf{W}_1^\dagger\mathbf{A}\mathbf{W}$. There exists a unitary $[\mathbf{V}] \in \mathbb{C}^{(n-1)\times(n-1)}$ such that $\mathbf{V}^\dagger\mathbf{C}\mathbf{V}$ becomes upper triangular; therefore, defining a unitary $\mathbf{U} := \mathrm{diag}(\zeta_1, \mathbf{V})$, we obtain

$$\mathbf{P}^\dagger\mathbf{A}\mathbf{P} = \begin{bmatrix} \zeta_1 & \mathbf{b}^\dagger\mathbf{V} \\ \mathbf{0} & \mathbf{V}^\dagger\mathbf{C}\mathbf{V} \end{bmatrix} \tag{B.38}$$

where $\mathbf{P} = \mathbf{Q}\mathbf{U}$ is also unitary. Notice that the right-hand side of Eq. (B.38) is upper triangular. Since unitary equivalent tensors possess the same eigenvalues, we can write

$$\mathbf{T} = \begin{bmatrix} \zeta_1 & \mathbf{b}^\dagger\mathbf{V} \\ \mathbf{0} & \mathbf{V}^\dagger\mathbf{C}\mathbf{V} \end{bmatrix} \tag{B.39}$$

in Eq. (B.38). ■

Remarks (*Schur Decomposition*):

- $\mathbf{A}$ is a ***normal*** tensor which satisfies the relation

$$\mathbf{A}\mathbf{A}^\dagger = \mathbf{A}^\dagger\mathbf{A} \ \text{ or } \ A_{ik}\overline{A}_{jk} = \overline{A}_{ki}A_{kj} \tag{B.40}$$

  if and only if $\mathbf{T} = \mathbf{W} = \mathbf{P}^\dagger\mathbf{A}\mathbf{P}$, where where $\mathbf{P}$ is unitary, is given in a ***diagonal Schur canonical form***. Some examples of normal tensors are: Hermitian tensors ($\mathbf{A}^\dagger = \mathbf{A}$), skew-hermitian tensors ($\mathbf{A}^\dagger = -\mathbf{A}$), and unitary tensors. From $\mathbf{W} = \mathbf{P}^\dagger\mathbf{A}\mathbf{P}$, we have $\mathbf{P}\mathbf{W} = \mathbf{A}\mathbf{P}$; that is, $\mathbf{A}\mathbf{p}_i = \zeta_i\mathbf{p}_i$ (no sum on i) for $i = 1, 2, \cdots, n$. Therefore, we can take the orthonormal vector, $\mathbf{p}_i$ as an normalized eigenvector of $\mathbf{A}$, i.e., $\mathbf{p}_i = \mathbf{x}_i$. Hence, $\mathbf{A}$ is normal if and only if $\mathbf{A}$ possesses linearly independent eigenvectors $\mathbf{x}_i$ for $i = 1, 2, \cdots, n$.

- If $\mathbf{A}$ is a real tensor and its eigenvalues are real, i.e., $A_{ij} \in \mathbb{R}$ and $\zeta_i \in \mathbb{R}$, respectively, then $\mathbf{P}$ is also real.

B.3 QR Decomposition

Again, consider a linear transformation $\mathbf{A}(\mathbf{x}) = \mathbf{A}\mathbf{x}$ on $\mathcal{V}$ over complex numbers with inner product $(\cdot, \cdot)$, and let $\mathbf{y} = \mathbf{A}(\mathbf{x}) = \mathbf{A}\mathbf{x}$; however, suppose $\mathbf{A}(\mathbf{x}) : \mathbb{C}^n \to \mathbb{C}^m$, i.e., $y_i = A_{ij}x_j$ for $i = 1, 2, \cdots, m$ and $j = 1, 2, \cdots, n$. Suppose that the standard orthonormal set of vectors $(\mathbf{e}_1, \mathbf{e}_2, \cdots, \mathbf{e}_n)$ is used as a basis for the domain space, i.e., $\mathbf{x} = x_j\mathbf{e}_j$ for $j = 1, 2, \cdots, n$, while an arbitrary orthonormal set of vectors $(\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_m)$ is used as a basis for the range space, i.e., $\mathbf{y} = y_i\mathbf{q}_i$ for $i = 1, 2, \cdots, m$. That is, $\mathbf{A} = A_{ij}\mathbf{q}_i \otimes \mathbf{e}_j$ is a two-point tensor. Defining a unitary tensor $\mathbf{Q} = [\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_m]$ ($[\mathbf{Q}] \in \mathbb{C}^{m\times m}$), the new coordinates $\mathbf{y}' = y'_i\mathbf{q}_i$ can be given by

$$\mathbf{y}' = \mathbf{Q}^{-1}\mathbf{y} = \mathbf{Q}^\dagger\mathbf{y} \ \text{ or } \ y'_i = Q^{-1}_{ij}y_j = \overline{Q}_{ji}y_j \tag{B.41}$$

Therefore, we obtain $\mathbf{y}' = \mathbf{A}'\mathbf{x}$ where

$$\mathbf{A}' := \mathbf{Q}^{\dagger}\mathbf{A} \tag{B.42}$$

That is,

$$\mathbf{A} = \mathbf{Q}\mathbf{A}' \tag{B.43}$$

QR Decomposition: There exists a unitary $\mathbf{Q} = [\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_m] \in \mathcal{V}^2$ ($[\mathbf{Q}] \in \mathbb{C}^{m\times m}$) such that $[\mathbf{A}] \in \mathbb{C}^{m\times n}$ ($m \geq n$) is decomposed as

$$\mathbf{A} = \mathbf{Q}\mathbf{R} \tag{B.44}$$

where $[\mathbf{R}] \in \mathbb{C}^{m\times n}$ denotes a right triangular tensor. This decomposition is called the ***QR decomposition*** of $\mathbf{A}$.

Proof (*QR Decomposition*): Proof for the QR decomposition is omitted. However, we can see the decomposition, $\mathbf{A} = \mathbf{Q}\mathbf{R}$, is possible via the Gram-Schmidt orthogonalization technique; see below.

Remarks (*QR Decomposition*):

- By introducing an arbitrary orthonormal basis $\{\mathbf{q}_i\}_{i=1}^{n}$ only for the range space in the linear transformation, $[\mathbf{A}] \in \mathbb{C}^{m\times n}$ ($m \geq n$) could be reduced by means of the QR decomposition.

- We can express the QR decomposition in a more compact form as follows. $\mathbf{A} = \mathbf{Q}\mathbf{R}$ if and only if $\mathbf{A} = \mathbf{Q}_0\mathbf{R}_0$ where $\mathbf{Q}_0 := [\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_n] \in \mathcal{V}^2$ ($[\mathbf{Q}_0] \in \mathbb{C}^{m\times n}$) and $[\mathbf{R}_0] \in \mathbb{C}^{n\times n}$ is given as a reduced form of the right triangular tensor $[\mathbf{R}] \in \mathbb{C}^{m\times n}$.

Gram-Schmidt Orthgonalization

Suppose that we have a *linearly independent* set of vectors $(\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_n)$ in $\mathcal{V}$ with inner product $(\cdot, \cdot)$. That is, there exists a_i (for $i = 1, 2, \cdots n$) which is not all zero such that $a_i \mathbf{a}_i = \mathbf{0}$. From the *linearly independent* set of vectors $(\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_s)$, we can gradually construct an *orthonormal* set of vectors $(\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_s)$ (for $1 \leq s \leq n$) by following the Gram-Schmidt orthogonalization process. A basis $\{\mathbf{q}_i\}_{i=1}^{s}$ spans the same vector subspace as does $\{\mathbf{a}_i\}_{i=1}^{s}$.

Standard Process:

Step 1: Set $\mathbf{q}_1 = \mathbf{a}_1 / R_{11}$ where $R_{11} := a_1 = \|\mathbf{a}_1\| = \sqrt{(\mathbf{a}_1, \mathbf{a}_1)} = (\mathbf{a}_1^\dagger \mathbf{a}_1)^{1/2}$ [1] .

Step 2: Set

$$\mathbf{q}_2 = \frac{\mathbf{a}_2 - R_{12}\mathbf{q}_1}{R_{22}} \tag{B.45}$$

where $R_{22} := \|\mathbf{a}_2 - R_{12}\mathbf{q}_1\|$, and R_{12} is determined from $(\mathbf{q}_1, \mathbf{q}_2) = 0$ and $(\mathbf{q}_1, \mathbf{q}_1) = 1$, i.e., $R_{12} := (\mathbf{q}_1, \mathbf{a}_2)$. Hence, Eq. (B.45) yields

$$\mathbf{q}_2 = \frac{\mathbf{a}_2 - (\mathbf{q}_1, \mathbf{a}_2)\mathbf{q}_1}{\|\mathbf{a}_2 - (\mathbf{q}_1, \mathbf{a}_2)\mathbf{q}_1\|} \tag{B.46}$$

Notice that $\{\mathbf{q}\}_{i=1}^{2}$ is orthonormal and spans the same vector subspace as does $\{\mathbf{a}\}_{i=1}^{2}$.

Step 3: Set

$$\mathbf{q}_3 = \frac{\mathbf{a}_3 - R_{13}\mathbf{q}_1 - R_{23}\mathbf{q}_2}{R_{33}} \tag{B.47}$$

[1] **Vector Norms:** Here, we employ $\|\cdot\| \equiv \|\cdot\|_2$. For a vector $\mathbf{a} = a_i \mathbf{a}_i$ for $i = 1, 2, \cdots, n$, we can define the following three kinds of the vector norms: $\|\mathbf{a}\|_1 := \sum_{i=1}^{n} |a_i|$, $\|\mathbf{a}\|_2 \equiv \|\mathbf{a}\| := \left(\sum_{i=1}^{n} |a_i|^2\right)^{1/2}$, and $\|\mathbf{a}\|_\infty := \max_i |a_i|$.

where $R_{33} := \|\mathbf{a}_3 - R_{13}\mathbf{q}_1 - R_{23}\mathbf{q}_2\|$, and R_{13} and R_{23} are determined from $(\mathbf{q}_1, \mathbf{q}_3) = 0$, $(\mathbf{q}_2, \mathbf{q}_3) = 0$, $(\mathbf{q}_1, \mathbf{q}_1) = (\mathbf{q}_2, \mathbf{q}_2) = 1$, and $(\mathbf{q}_1, \mathbf{q}_2) = 0$, i.e., $R_{13} := (\mathbf{q}_1, \mathbf{a}_3)$ and $R_{23} := (\mathbf{q}_2, \mathbf{a}_3)$. Hence, Eq. (B.47) yields

$$\mathbf{q}_3 = \frac{\mathbf{a}_3 - (\mathbf{q}_1, \mathbf{a}_3)\mathbf{q}_1 - (\mathbf{q}_2, \mathbf{a}_3)\mathbf{q}_2}{\|\mathbf{a}_3 - (\mathbf{q}_1, \mathbf{a}_3)\mathbf{q}_1 - (\mathbf{q}_2, \mathbf{a}_3)\mathbf{q}_2\|} \tag{B.48}$$

Notice that $\{\mathbf{q}\}_{i=1}^{3}$ is orthonormal and spans the same vector subspace as does $\{\mathbf{a}\}_{i=1}^{3}$.

$\vdots$

Step *s*: $(s \leq n)$ Set

$$\mathbf{q}_s = \frac{\mathbf{a}_s - \sum_{k=1}^{s-1} R_{ks}\mathbf{q}_k}{R_{ss}} \tag{B.49}$$

where $R_{ss} := \left\|\mathbf{a}_s - \sum_{k=1}^{s-1} R_{ks}\mathbf{q}_k\right\|$ and $R_{ks} := (\mathbf{q}_k, \mathbf{a}_s)$.

Remarks (*Gram-Schmidt Orthgonalization*):

- Since we can show $\mathbf{a}_s$ as $\mathbf{a}_s = R_{is}\mathbf{q}_i$ for $i = 1, 2, \cdots, s$, we are able to express $\mathbf{A} = [\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_s]$ in the form of the QR decomposition as

  $$\mathbf{A} = \mathbf{QR} \tag{B.50}$$

  where $\mathbf{Q} = [\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_s]$ and $\mathbf{R}$ is upper triangular with $[\mathbf{R}]_{ij} = R_{ij}$.

- This standard process of the Gram-Schmidt orthgonalization is really sensitive to round-off errors. Therefore, modified Gram-Schmidt orthgonalization process (shown below) is strongly suggested to be programmed. The modified process returns more accurate results than the standard process does; however, Eq. (B.50) remains the same.

Modified Process:

Step 1: Set $\mathbf{a}_1^{(1)} = \mathbf{a}_1$, then normalize it as $\mathbf{q}_1 = \mathbf{a}_1^{(1)}/R_{11}$ where $R_{11} := \|\mathbf{a}_1^{(1)}\|$. Then, modify $\mathbf{a}_j$ (for $j = 2, 3, \cdots, s$) as

$$\mathbf{a}_j^{(1)} = \mathbf{a}_j - R_{1j}\mathbf{q}_1 \tag{B.51}$$

where $R_{1j} := (\mathbf{q}_1, \mathbf{a}_j)$.

Step 2: Normalize $\mathbf{a}_2^{(1)}$ and get $\mathbf{q}_2 = \mathbf{a}_2^{(1)}/R_{22}$ where $R_{22} := \|\mathbf{a}_2^{(1)}\|$. Then, modify $\mathbf{a}_\ell^{(1)}$ (for $\ell = 3, 4, \cdots, s$) as

$$\mathbf{a}_\ell^{(2)} = \mathbf{a}_\ell^{(1)} - R_{2\ell}\mathbf{q}_2 \tag{B.52}$$

where $R_{2\ell} := (\mathbf{q}_2, \mathbf{a}_\ell^{(1)})$.

Step 3: Normalize $\mathbf{a}_3^{(2)}$ and get $\mathbf{q}_3 = \mathbf{a}_3^{(2)}/R_{33}$ where $R_{33} := \|\mathbf{a}_3^{(2)}\|$. Then, modify $\mathbf{a}_p^{(2)}$ (for $p = 4, 5, \cdots, s$) as

$$\mathbf{a}_p^{(3)} = \mathbf{a}_p^{(2)} - R_{3p}\mathbf{q}_3 \tag{B.53}$$

where $R_{3p} := (\mathbf{q}_3, \mathbf{a}_p^{(2)})$.

$\vdots$

Step s: ($s \leq n$) Normalize $\mathbf{a}_s^{(s-1)}$ and get $\mathbf{q}_s = \mathbf{a}_s^{(s-1)}/R_{ss}$ where $R_{ss} := \|\mathbf{a}_s^{(s-1)}\|$. Notice that $\mathbf{q}_s$ obtained from this process is identical to the one shown in Eq. (B.49).

B.4 Singular Value Decomposition (SVD)

Generalized Unitary Transformation: Again, consider a linear transformation $\mathbf{A}(\mathbf{x}) = \mathbf{A}\mathbf{x}$ on $\mathcal{V}$ over complex numbers with inner product $(\cdot, \cdot)$, and let $\mathbf{y} = \mathbf{A}(\mathbf{x}) = \mathbf{A}\mathbf{x}$. Let $\mathbf{A}(\mathbf{x}) : \mathbb{C}^n \to \mathbb{C}^m$, i.e., $y_i = A_{ij}x_j$ for $i = 1, 2, \cdots, m$ and $j = 1, 2, \cdots, n$. Unlike the case of the QR decomposition, we introduce two different arbitrary orthonormal sets of vectors, $(\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_n)$ and $(\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_m)$, for the bases for the domain space and the range space, respectively. Defining the unitary matrices, $\mathbf{V} := [\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_n] \in \mathcal{V}^2$ ($[\mathbf{V}] \in \mathbb{C}^{n\times n}$) and $\mathbf{U} := [\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_m] \in \mathcal{V}^2$ ($[\mathbf{U}] \in \mathbb{C}^{m\times m}$), the new coordinates $\mathbf{x}' = x'_i\mathbf{v}_i$ and $\mathbf{y}' = y'_i\mathbf{u}_i$ can be given respectively by

$$\mathbf{x}' = \mathbf{V}^{-1}\mathbf{x} = \mathbf{V}^{\dagger}\mathbf{x} \quad \text{or} \quad x'_i = V^{-1}_{ij}x_j = \overline{V}_{ji}x_j \tag{B.54}$$

$$\mathbf{y}' = \mathbf{U}^{-1}\mathbf{y} = \mathbf{U}^{\dagger}\mathbf{y} \quad \text{or} \quad y'_i = U^{-1}_{ij}y_j = \overline{U}_{ji}y_j \tag{B.55}$$

Hence, from $\mathbf{y} = \mathbf{A}\mathbf{x}$, we obtain $\mathbf{y}' = \mathbf{A}'\mathbf{x}'$ where

$$\mathbf{A}' = \mathbf{U}^{\dagger}\mathbf{A}\mathbf{V} \tag{B.56}$$

Eq. (B.56) is known as the ***generalized unitary transformation*** (or generalized unitary similarity transformation) from $\mathbf{A}$ to $\mathbf{A}'$. From Eq. (B.56), we can readily get

$$\mathbf{A} = \mathbf{U}\mathbf{A}'\mathbf{V}^{\dagger} \tag{B.57}$$

SVD: There *exist* unitary $\mathbf{U} = [\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_m] \in \mathcal{V}^2$ ($[\mathbf{U}] \in \mathbb{C}^{m\times m}$) and unitary $\mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_n] \in \mathcal{V}^2$ ($[\mathbf{V}] \in \mathbb{C}^{n\times n}$) such that $\mathbf{A} \in \mathcal{V}^2$ ($[\mathbf{A}] \in \mathbb{C}^{m\times n}$) with $\text{rank}(\mathbf{A}) = \text{rank}(\mathbf{A}^{\dagger}) = d$ is decomposed as

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^{\dagger} \tag{B.58}$$

where $\mathbf{\Sigma} \in \mathcal{V}^2$ denotes a diagonal form of $\mathbf{A}'$ with $[\mathbf{\Sigma}] \in \mathbb{C}^{m \times n}$, and it is given by

$$\mathbf{\Sigma} = \begin{bmatrix} \mathbf{D} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \tag{B.59}$$

in which $\mathbf{D} = \text{diag}(\sigma_1, \sigma_2, \cdots, \sigma_d)$ ($[\mathbf{D}] \in \mathbb{C}^{d \times d}$) with

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_d > 0 \tag{B.60}$$

Here, σ_i (for $i = 1, 2, \cdots, d$) are called the ***singular values*** of $\mathbf{A}$. The columns of $\mathbf{U}$ and $\mathbf{V}$, i.e., $\mathbf{u}_i$ (for $i = 1, 2, \cdots, m$) and $\mathbf{v}_j$ (for $j = 1, 2, \cdots, n$), are called the ***left singular vectors*** and ***right singular vectors*** of $\mathbf{A}$, respectively.

Proof (*SVD*): Suppose that an orthonormal set of eigenvectors $(\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_d)$ associated respectively with a set of eigenvalues $(\sigma_1^2, \sigma_2^2, \cdots, \sigma_d^2)$ of $\mathbf{A}^\dagger \mathbf{A}$ is given. Hence, we have

$$(\mathbf{A}^\dagger \mathbf{A})\mathbf{v}_i = \sigma_i^2 \mathbf{v}_i \ \ \text{(no sum on } i\text{)} \tag{B.61}$$

for an eigenpair $(\sigma_i^2, \mathbf{v}_i)$ of $\mathbf{A}^\dagger \mathbf{A}$. Define $\mathbf{u}_i \in \mathcal{V}$ (for $i = 1, 2, \cdots, d$) as

$$\mathbf{u}_i := \sigma_i^{-1} \mathbf{A} \mathbf{v}_i \ \ \text{(no sum on } i\text{)} \tag{B.62}$$

so that

$$\mathbf{A}\mathbf{v}_i = \sigma_i \mathbf{u}_i \ \ \text{(no sum on } i\text{)} \tag{B.63}$$

We can see that a set of the vectors $(\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_d)$ is orthonormal such that $\mathbf{u}_i$ (for $i = 1, 2, \cdots, d$) are the eigenvectors of $\mathbf{A}\mathbf{A}^\dagger$, associated respectively with the eigenvalues

σ_i^2 (for $i = 1, 2, \cdots, d$) of $\mathbf{AA}^\dagger$ from

$$\begin{aligned}
(\mathbf{AA}^\dagger)\mathbf{u}_i &= (\mathbf{AA}^\dagger)(\sigma_i^{-1}\mathbf{Av}_i) \\
&= \sigma_i^{-1}\mathbf{A}(\mathbf{A}^\dagger\mathbf{Av}_i) \\
&= \sigma_i^{-1}\mathbf{A}(\sigma_i^2\mathbf{v}_i) \\
&= \sigma_i^2(\sigma_i^{-1}\mathbf{Av}_i) \\
&= \sigma_i^2\mathbf{u}_i
\end{aligned} \tag{B.64}$$

(no sum on i). The orthonormality of $(\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_d)$ can be seen from

$$\begin{aligned}
(\mathbf{u}_i, \mathbf{u}_j) &= (\sigma_i^{-1}\mathbf{Av}_i, \sigma_j^{-1}\mathbf{Av}_j) \\
&= \sigma_i^{-1}\sigma_j^{-1}(\mathbf{Av}_i, \mathbf{Av}_j) = \sigma_i^{-1}\sigma_j^{-1}(\mathbf{Av}_i)^\dagger(\mathbf{Av}_j) \\
&= \sigma_i^{-1}\sigma_j^{-1}\mathbf{v}_i^\dagger\mathbf{A}^\dagger(\mathbf{Av}_j) = \sigma_i^{-1}\sigma_j^{-1}\mathbf{v}_i^\dagger(\mathbf{A}^\dagger\mathbf{Av}_j) \\
&= \sigma_i^{-1}\sigma_j^{-1}(\mathbf{v}_i, \mathbf{A}^\dagger\mathbf{Av}_j) = \sigma_i^{-1}\sigma_j^{-1}(\mathbf{v}_i, \sigma_j^2\mathbf{v}_j) \\
&= \sigma_i^{-1}\sigma_j(\mathbf{v}_i, \mathbf{v}_j)
\end{aligned} \tag{B.65}$$

(no sum on i and j)[2] ; that is, $(\mathbf{u}_i, \mathbf{u}_j) = \delta_{ij}$. From Eq. (B.63), we can readily get

$$\mathbf{v}_i = \sigma_i\mathbf{A}^\dagger\mathbf{u}_i \quad \text{(no sum on } i\text{)} \tag{B.66}$$

For $i = 1, 2, \cdots, d$, $\mathbf{v}_i$ and $\mathbf{u}_i$ are the eigenvectors of $\mathbf{A}^\dagger\mathbf{A}$ and $\mathbf{AA}^\dagger$ respectively, and both are associated with the same eigenvalues σ_i^2. Notice that both $\mathbf{A}^\dagger\mathbf{A} \in \mathcal{V}^2$ and

[2] Alternatively, we can show the orthogonality of $(\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_d)$ from

$$\begin{aligned}
(\mathbf{u}_i, \mathbf{u}_j) &= (\sigma_i^{-1}\mathbf{Av}_i, \sigma_j^{-1}\mathbf{Av}_j) = \sigma_i^{-1}\sigma_j^{-1}(\mathbf{Av}_i, \mathbf{Av}_j) = \sigma_i^{-1}\sigma_j^{-1}(\mathbf{Av}_i)^\dagger(\mathbf{Av}_j) \\
&= \sigma_i^{-1}\sigma_j^{-1}\left(\mathbf{A}^\dagger(\mathbf{Av}_i)\right)^\dagger\mathbf{v}_j = \sigma_i^{-1}\sigma_j^{-1}(\mathbf{A}^\dagger\mathbf{Av}_i, \mathbf{v}_j) \\
&= \sigma_i^{-1}\sigma_j^{-1}(\sigma_i^2\mathbf{v}_i, \mathbf{v}_j) = \sigma_i\sigma_j^{-1}(\mathbf{v}_i, \mathbf{v}_j) \quad \text{(no sum on } i \text{ and } j\text{)}
\end{aligned}$$

$\mathbf{AA}^\dagger \in \mathcal{V}^2$ are hermitian since they satisfy the relations $(\mathbf{A}^\dagger\mathbf{A})^\dagger = \mathbf{A}^\dagger\mathbf{A}$ and $(\mathbf{AA}^\dagger)^\dagger = \mathbf{AA}^\dagger$, respectively.

The null space $\mathcal{V}_0$ of $\mathbf{A} \in \mathcal{V}^2$ with $[\mathbf{A}] \in \mathbb{C}^{m\times n}$ is defined by the linear subspace of $\mathcal{V}$, consisting of the set of all solutions $\boldsymbol{\mu}_\ell \in \mathcal{V}_0 \subset \mathcal{V}$ which satisfy the homogeneous equation $\mathbf{A}\boldsymbol{\mu}_\ell = \mathbf{0}$. If $\mathrm{rank}(\mathbf{A}) = d$, the null space of $\mathbf{A}$ has the dimension of $n - d$.

Consider the square harmitian $\mathbf{A}^\dagger\mathbf{A}$, i.e., $[\mathbf{A}^\dagger\mathbf{A}] \in \mathbb{C}^{n\times n}$. Since $(\mathbf{A}^\dagger\mathbf{A})\boldsymbol{\mu}_\ell = \mathbf{0}$ if and only if $\mathbf{A}\boldsymbol{\mu}_\ell = \mathbf{0}$, the solutions to $(\mathbf{A}^\dagger\mathbf{A})\boldsymbol{\mu}_\ell = \mathbf{0}$, i.e., $\boldsymbol{\mu}_\ell$, are in the null space of $\mathbf{A}$. Because of $\mathrm{rank}(\mathbf{A}) = d$, we know the null space of $\mathbf{A}$ has the dimension of $n - d$; therefore, in view of $(\mathbf{A}^\dagger\mathbf{A})\boldsymbol{\mu}_\ell = \mathbf{0}$ and Eq. (B.61), we conclude that there exists $n - d$ eigenvectors $\mathbf{v}_\ell$ which are associated with the eigenvalues $\sigma_\ell^2 = 0$. That is, there exists the eigenpairs $(\sigma_\ell^2, \mathbf{v}_\ell)$ with $\sigma_\ell^2 = 0$ (for $\ell = d+1, d+2, \cdots, n$) in addition to the eigenpairs $(\sigma_i^2, \mathbf{v}_i)$ (for $i = 1, 2, \cdots, d$). Note that $\sigma_i^2 > 0$ (for $i = 1, 2, \cdots, d$) is guaranteed from

$$\begin{aligned}
\sigma_i^2 \|\mathbf{v}_i\|^2 &= \sigma_i^2(\mathbf{v}_i, \mathbf{v}_i) = (\mathbf{v}_i, \sigma_i^2\mathbf{v}_i) = (\mathbf{v}_i, \mathbf{A}^\dagger\mathbf{A}\mathbf{v}_i) \\
&= \mathbf{v}_i^\dagger(\mathbf{A}^\dagger\mathbf{A}\mathbf{v}_i) = (\mathbf{A}\mathbf{v}_i)^\dagger(\mathbf{A}\mathbf{v}_i) = (\mathbf{A}\mathbf{v}_i, \mathbf{A}\mathbf{v}_i) \\
&= \|\mathbf{A}\mathbf{v}_i\|^2 > 0
\end{aligned} \tag{B.67}$$

(no sum on i) for $\mathbf{v}_i \neq \mathbf{0}$ and $\mathbf{A}\mathbf{v}_i \neq \mathbf{0}$, where we used Eq. (B.61). Hence, we always have strictly positive singular values of $\mathbf{A}$ for $i = 1, 2, \cdots, d$, i.e., $\sigma_i > 0$. Summarizing, $\mathbf{A}^\dagger\mathbf{A}$ possesses the set of n eigenvalues

$$(\sigma_1^2, \sigma_2^2, \cdots, \sigma_d^2, \underbrace{0, 0, \cdots, 0}_{n-d}) \tag{B.68}$$

and they are associated with the set of n eigenvectors of $\mathbf{A}^\dagger\mathbf{A}$,

$$(\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_d, \underbrace{\mathbf{v}_{d+1}, \mathbf{v}_{d+2}, \cdots, \mathbf{v}_n}_{n-d}) \tag{B.69}$$

with the following relation

$$\begin{aligned} \mathbf{A}^{\dagger}\mathbf{A}\mathbf{v}_i &= \sigma_i^2 \mathbf{v}_i \ \text{ for } i = 1, 2, \cdots, d \\ \mathbf{A}\mathbf{v}_i &= \mathbf{0} \ \text{ for } i = d+1, d+2, \cdots, n \end{aligned} \tag{B.70}$$

(no sum on i).

Following a similar discussion, we can obtain the following result for the square harmitian $\mathbf{A}\mathbf{A}^{\dagger}$, i.e., $[\mathbf{A}\mathbf{A}^{\dagger}] \in \mathbb{C}^{m\times m}$: $\mathbf{A}\mathbf{A}^{\dagger}$ possesses the set of m eigenvalues

$$(\sigma_1^2, \sigma_2^2, \cdots, \sigma_d^2, \underbrace{0, 0, \cdots, 0}_{m-d}) \tag{B.71}$$

and they are associated with the set of m eigenvectors of $\mathbf{A}\mathbf{A}^{\dagger}$,

$$(\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_d, \underbrace{\mathbf{u}_{d+1}, \mathbf{u}_{d+2}, \cdots, \mathbf{u}_m}_{m-d}) \tag{B.72}$$

with the following relation

$$\begin{aligned} \mathbf{A}\mathbf{A}^{\dagger}\mathbf{u}_i &= \sigma_i^2 \mathbf{u}_i \ \text{ for } i = 1, 2, \cdots, d \\ \mathbf{A}\mathbf{u}_i &= \mathbf{0} \ \text{ for } i = d+1, d+2, \cdots, m \end{aligned} \tag{B.73}$$

(no sum on i).

Employing $\mathbf{v}_i$ (for $i = 1, 2, \cdots, n$) and $\mathbf{u}_j$ (for $j = 1, 2, \cdots, m$) for $\mathbf{V}$ and $\mathbf{U}$, respectively, we can finally obtain $\mathbf{U}^{\dagger}\mathbf{A}\mathbf{V} = \mathbf{\Sigma}$; therefore, $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^{\dagger}$. ■

Remarks (*SVD*):

- It is well-known that SVD is closely related to the ***proper orthogonal decomposition*** (POD), which is also known as the ***Karhunen-Loeve decomposition***, the ***principle component analysis*** (PCA), etc. We will emphasize the connection between SVD and POD and how POD is used for model reduction in transient systems in the following sections carefully.

- Since $\mathbf{U}$ and $\mathbf{V}$ are unitary, we have

$$\mathbf{A}^\dagger\mathbf{A} = (\mathbf{U\Sigma V}^\dagger)^\dagger(\mathbf{U\Sigma V}^\dagger) = \mathbf{V\Sigma}^\dagger\mathbf{U}^\dagger\mathbf{U\Sigma V}^\dagger = \mathbf{V\Sigma}^\dagger\mathbf{\Sigma V}^\dagger \tag{B.74}$$

$$\mathbf{AA}^\dagger = (\mathbf{U\Sigma V}^\dagger)(\mathbf{U\Sigma V}^\dagger)^\dagger = \mathbf{U\Sigma V}^\dagger\mathbf{V\Sigma}^\dagger\mathbf{U}^\dagger = \mathbf{U\Sigma\Sigma}^\dagger\mathbf{U}^\dagger \tag{B.75}$$

where

$$\mathbf{\Sigma}^\dagger\mathbf{\Sigma} = \mathrm{diag}(\sigma_1^2, \sigma_2^2, \cdots, \sigma_d^2, \underbrace{0, 0, \cdots, 0}_{n-d}) \tag{B.76}$$

$$\mathbf{\Sigma\Sigma}^\dagger = \mathrm{diag}(\sigma_1^2, \sigma_2^2, \cdots, \sigma_d^2, \underbrace{0, 0, \cdots, 0}_{m-d}) \tag{B.77}$$

From Eq. (B.74) and Eq. (B.76), it is clear that the right singular vectors, $\mathbf{v}_j$ (for $j = 1, 2, \cdots, n$), are the eigenvectors of $\mathbf{A}^\dagger\mathbf{A}$ and σ_k^2 (for $k = 1, 2, \cdots, d$) and zeros are the eigenvalues of $\mathbf{A}^\dagger\mathbf{A}$. Similarly, From Eq. (B.75) and Eq. (B.77), it is clear that the left singular vectors, $\mathbf{u}_i$ (for $j = 1, 2, \cdots, m$), are the eigenvectors of $\mathbf{AA}^\dagger$ and σ_k^2 (for $k = 1, 2, \cdots, d$) and zeros are the eigenvalues of $\mathbf{AA}^\dagger$.

- Both $\mathbf{A}^\dagger\mathbf{A}$ and $\mathbf{AA}^\dagger$ are positive semi-definite; see,

$$(\boldsymbol{\nu}, \mathbf{A}^\dagger\mathbf{A}\boldsymbol{\nu}) = \boldsymbol{\nu}^\dagger\mathbf{A}^\dagger\mathbf{A}\boldsymbol{\nu} = (\mathbf{A}\boldsymbol{\nu}, \mathbf{A}\boldsymbol{\nu}) = ||\mathbf{A}\boldsymbol{\nu}||^2 \geq 0 \tag{B.78}$$

$$(\boldsymbol{\eta}, \mathbf{AA}^\dagger\boldsymbol{\eta}) = \boldsymbol{\eta}^\dagger\mathbf{AA}^\dagger\boldsymbol{\eta} = (\mathbf{A}^\dagger\boldsymbol{\eta}, \mathbf{A}^\dagger\boldsymbol{\eta}) = ||\mathbf{A}^\dagger\boldsymbol{\eta}||^2 \geq 0 \tag{B.79}$$

for arbitrary vectors, $\{\boldsymbol{\nu}\} \in \mathbb{C}^n$ and $\{\boldsymbol{\eta}\} \in \mathbb{C}^m$

- From $\mathbf{A} = \mathbf{U\Sigma V}^\dagger$ with rank($\mathbf{A}$) = d, we can write $\mathbf{A}$ as

$$\mathbf{A} = \sum_{i=1}^{d} \sigma_i \mathbf{u}_i \mathbf{v}_i^\dagger \tag{B.80}$$

- If rank($\mathbf{A}$) = d, we can write $\mathbf{A} = \mathbf{U\Sigma V}^\dagger$ in a compact form as

$$\mathbf{A} = \mathbf{U}^0\mathbf{\Sigma}^0(\mathbf{V}^0)^\dagger = \mathbf{U}^0\mathbf{D}(\mathbf{V}^0)^\dagger \tag{B.81}$$

with $\mathbf{\Sigma}^0 \equiv \mathbf{D} = \mathrm{diag}(\sigma_1, \sigma_2 \cdots, \sigma_d)$, $\mathbf{V}^0 = [\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_d] \in \mathcal{V}^2$ ($[\mathbf{V}^0] \in \mathbb{C}^{n\times d}$), and $\mathbf{U}^0 = [\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_d] \in \mathcal{V}^2$ ($[\mathbf{U}^0] \in \mathbb{C}^{m\times d}$).

- From Eq. (B.63), we have

$$\mathbf{U\Sigma V}^\dagger \mathbf{v}_i = \sigma_i \mathbf{u}_i \quad \text{(no sum on } i\text{)} \tag{B.82}$$

This equation implies that a vector obtained from $\mathbf{v}_i$, via (1) rotation due to $\mathbf{V}^\dagger$, (2) stretch due to $\mathbf{\Sigma}$, and then (3) rotation due to $\mathbf{U}$, is collinear with $\mathbf{u}_i$. The largest singular value of $\mathbf{A}$, i.e., σ_1, which is also the square root of the largest eigenvalue of $\mathbf{A}^\dagger\mathbf{A}$, is the magnitude [3] of $\mathbf{A}$ in the sense of

$$\sigma_1 = \|\mathbf{A}\|_2 = \max_{\mathbf{x}\neq\mathbf{0}}\{\frac{\|\mathbf{Ax}\|_2}{\|\mathbf{x}\|_2}\} = \max_{\mathbf{x}\neq\mathbf{0}}\{\frac{(\mathbf{Ax},\mathbf{Ax})}{(\mathbf{x},\mathbf{x})}\} = \max_{\mathbf{x}\neq\mathbf{0}}\{\frac{(\mathbf{x},\mathbf{A}^\dagger\mathbf{Ax})}{(\mathbf{x},\mathbf{x})}\} \tag{B.83}$$

- If $\mathbf{A}$ is a real tensor, then, both $\mathbf{V}$ and $\mathbf{U}$ become orthogonal real tensors. Apparently, $\mathbf{A}^T\mathbf{A}$ and $\mathbf{AA}^T$ are symmetric. In this case, Eq. (B.81) can be written as

$$\mathbf{A} = \mathbf{U}^0\mathbf{B}^0 \tag{B.84}$$

[3] **Second-order Tensor Norms:** For a linear transformation $\mathbf{A}(\mathbf{x}) = \mathbf{Ax} : \mathbb{C}^n \to \mathbb{C}^m$ with $[\mathbf{A}] \in \mathbb{C}^{m\times n}$, we can define the following three kinds of the second-order tensor norms:

$$\begin{aligned}
\|\mathbf{A}\|_1 &:= \max_{\mathbf{x}\neq\mathbf{0}}\{\frac{\|\mathbf{Ax}\|_1}{\|\mathbf{x}\|_1}\} = \max_j \sum_{i=1}^m |A_{ij}| \\
\|\mathbf{A}\|_2 &:= \max_{\mathbf{x}\neq\mathbf{0}}\{\frac{\|\mathbf{Ax}\|_2}{\|\mathbf{x}\|_2}\} = \sigma_1 \\
\|\mathbf{A}\|_\infty &:= \max_{\mathbf{x}\neq\mathbf{0}}\{\frac{\|\mathbf{Ax}\|_\infty}{\|\mathbf{x}\|_\infty}\} = \max_i \sum_{j=1}^m |A_{ij}|
\end{aligned}$$

where $\mathbf{B}^0 := \mathbf{D}(\mathbf{V}^0)^T$. Therefore, the column vectors of $\mathbf{A}$ yield

$$\begin{aligned}\mathbf{a}_i &= B^0_{ji}\mathbf{u}_j = D_{jp}V^0_{ip}\mathbf{u}_j = D_{jp}V^0_{ip}\mathbf{u}_r\delta_{rj} \\ &= U^0_{kr}(U^0_{kj}D_{jp}V^0_{ip})\mathbf{u}_r = U^0_{kr}A_{ki}\mathbf{u}_r \\ &= (\mathbf{a}_i, \mathbf{u}_r)\mathbf{u}_r = \sum_{r=1}^{d}(\mathbf{a}_i, \mathbf{u}_r)\mathbf{u}_r \end{aligned} \tag{B.85}$$

for $r = 1, 2, \cdots, d$. $(\mathbf{a}_i, \mathbf{u}_r)$ are called the Fourier coefficients of $\mathbf{a}_i$ in the basis $\{\mathbf{u}_r\}_{r=1}^d$.

Least Squares Approximation: Suppose N points $(x_i, y_i) \in \mathbb{R}^2$ (for $i = 1, 2, \cdots, N$) are given. Our objective is to find the best linear function which approximates (x_i, y_i). If the predicted value of y_i measured at x_i is given by

$$\hat{y}_i = \alpha_1 x_i + \alpha_2 \tag{B.86}$$

with $\alpha_1, \alpha_2 \in \mathbb{R}$, we can define the residual as

$$r_i := \hat{y}_i - y_i = \alpha_1 x_i + \alpha_2 - y_i \tag{B.87}$$

The residual is not zero unless otherwise $\hat{y}_i = y_i$. Note that we can write Eq. (B.86) in the form

$$\mathbf{y} = \mathbf{A}\mathbf{x} \quad \text{or} \quad \{\mathbf{y}\} = [\mathbf{A}]\{\mathbf{x}\} \tag{B.88}$$

where $\{\mathbf{y}\} = (y_1, y_2, \cdots, y_N)^T \in \mathbb{R}^N$, $\{\mathbf{x}\} = (\alpha_1, \alpha_2)^T \in \mathbb{R}^2$, and

$$[\mathbf{A}] = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_N & 1 \end{bmatrix} \in \mathbb{R}^{N\times 2} \tag{B.89}$$

Therefore, Eq. (B.87) can be written as

$$\mathbf{r} := \mathbf{A}\mathbf{x} - \mathbf{y} \tag{B.90}$$

where $\{\mathbf{r}\} = (r_1, r_2, \cdots, r_N)^T \in \mathbb{R}^N$. In order to find the unknowns α_1 and α_2 such that the linear function becomes the *best*, we minimize the sum of the squared residual, S. That is,

$$\min S = \min \ ||\mathbf{r}||^2 \tag{B.91}$$

where

$$\begin{aligned} ||\mathbf{r}||^2 &= (\mathbf{r}, \mathbf{r}) = \mathbf{r}^T\mathbf{r} = r_i r_i \\ &= (A_{ij}x_j - y_i)(A_{ik}x_k - y_i) \\ &= A_{ij}x_j A_{ik}x_k - A_{ik}x_k y_i - y_i A_{ik}x_k + y_i y_i \\ &= x_j A_{ij} A_{ik} x_k - 2x_j A_{ij} y_i + y_i y_i \\ &= (\mathbf{x}, \mathbf{A}^T\mathbf{A}\mathbf{x}) - 2(\mathbf{x}, \mathbf{A}^T\mathbf{y}) + (\mathbf{y}, \mathbf{y}) \end{aligned} \tag{B.92}$$

The necessary condition for Eq. (B.91) is given by

$$\mathbf{0} = \frac{\partial S}{\partial \mathbf{x}} = 2\mathbf{A}^T\mathbf{A}\mathbf{x} - 2\mathbf{A}^T\mathbf{y} \tag{B.93}$$

That is,

$$\mathbf{A}^T\mathbf{A}\mathbf{x} = \mathbf{A}^T\mathbf{y} \tag{B.94}$$

Eq. (B.94) is known as the ***normal equation***. If the real symmetric square tensor $\mathbf{A}^T\mathbf{A}$ is non-singular, i.e., rank($\mathbf{A}$) = 2, we have a *unique* solution for Eq. (B.94), and it is

$$\mathbf{x} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{y} \tag{B.95}$$

Substituting Eq. (B.95) into Eq. (B.90), we get

$$\mathbf{r} = \mathbf{A}(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{y} - \mathbf{y} \tag{B.96}$$

which is not zero in general. Notice that premultiplying Eq. (B.96) by $\mathbf{A}^T$ yields $\mathbf{A}^T\mathbf{r} = (\mathbf{A}, \mathbf{r}) = \mathbf{0}$; that is, the residual vector $\mathbf{r}$ is perpendicular to the vector space spanned by the column vectors which construct $\mathbf{A}$. Hence, we can see that vector $\mathbf{A}(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{y}$ in Eq. (B.96) is given as the projection of $\mathbf{y}$ onto the column space of $\mathbf{A}$. By enforcing $\mathbf{r} \cong \mathbf{0}$ in Eq. (B.96), we finally get the linear function which minimizes S.

Remarks (*Least Squares Approximation*):

- Suppose a real rectangular tensor $[\mathbf{A}] \in \mathbb{R}^{m\times n}$ is given, and suppose it satisfies the normal equation, $\mathbf{A}^T\mathbf{A}\mathbf{x} = \mathbf{A}^T\mathbf{y}$. By decomposing the real tensor $\mathbf{A}$ by SVD, we get $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$. Then, we have $\mathbf{A}^T\mathbf{A} = \mathbf{V}\mathbf{\Sigma}^T\mathbf{\Sigma}\mathbf{V}^T$; see Eq. (B.74).

  $\mathbf{\Sigma}^T\mathbf{\Sigma}$ is non-singular if and only if $\mathrm{rank}(\mathbf{A}) = n$. It is clear that $\mathbf{A}^T\mathbf{A}$ becomes non-singular when $\mathbf{\Sigma}^T\mathbf{\Sigma}$ is non-singular. Hence, the normal equation possesses a *unique* solution, $\mathbf{x} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{y}$, if and only if $\mathrm{rank}(\mathbf{A}) = n$.

  Actually, the normal equation has a solution even if $\mathbf{A}^T\mathbf{A} = \mathbf{V}\mathbf{\Sigma}^T\mathbf{\Sigma}\mathbf{V}^T$ is singular. The normal equation is *solvable* (but it does not have a unique solution) if and only if $(\mathbf{v}_i, \mathbf{A}^T\mathbf{y}) = 0$ (for $i = d+1, d+2, \cdots, n$) which is always true; see

  $$(\mathbf{v}_i, \mathbf{A}^T\mathbf{y}) = (\mathbf{v}_i, \mathbf{V}\mathbf{\Sigma}^T\mathbf{U}^T\mathbf{y}) = \mathbf{v}_i^T\,[\sigma_1\mathbf{v}_1, \sigma_2\mathbf{v}_2, \cdots, \sigma_d\mathbf{v}_d]\,\mathbf{U}^T\mathbf{y} = 0 \qquad \text{(B.97)}$$

  (for $i = d+1, d+2, \cdots, n$) where $d = \mathrm{rank}(\mathbf{A})$ and we used the relation $(\mathbf{v}_i, \mathbf{v}_j) = 0$ for $i \neq j$.

- Suppose a real rectangular tensor $[\mathbf{A}] \in \mathbb{R}^{m\times n}$ is given. Defining $\mathbf{z} := \mathbf{V}^T\mathbf{x} \in \mathcal{V}$, we may write

$$\begin{aligned}
||\mathbf{r}||^2 &= ||\mathbf{A}\mathbf{x}-\mathbf{y}||^2 = \left\|\mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T\mathbf{x}-\mathbf{y}\right\|^2 = ||\mathbf{U}\boldsymbol{\Sigma}\mathbf{z}-\mathbf{y}||^2 \\
&= (U_{ij}\Sigma_{jk}z_k - y_i)(U_{i\ell}\Sigma_{\ell p}z_p - y_i) \\
&= U_{ij}U_{i\ell}\Sigma_{jk}\Sigma_{\ell p}z_k z_p - 2U_{ij}\Sigma_{jk}z_k y_i + y_i y_j \delta_{ij} \\
&= \Sigma_{jk}z_k\Sigma_{jp}z_p - 2\Sigma_{jk}z_k U_{ij}y_i + U_{ik}y_i U_{jk}y_j \\
&= (\Sigma_{jk}z_k - U_{\ell j}y_\ell)(\Sigma_{jp}z_p - U_{ij}y_i) \\
&= \left\|\boldsymbol{\Sigma}\mathbf{z}-\mathbf{U}^T\mathbf{y}\right\|^2 = ||\boldsymbol{\Sigma}\mathbf{z}-\mathbf{w}||^2 \qquad \text{(B.98)}
\end{aligned}$$

where $\mathbf{w} := \mathbf{U}^T\mathbf{y} \in \mathcal{V}$, and we used the relation, $U_{ki}U_{kj} = U_{ik}U_{jk} = \delta_{ij}$. Recalling that $\boldsymbol{\Sigma} = \text{diag}(\sigma_1, \sigma_2, \cdots, \sigma_m)$ where $\sigma_i = 0$ for $i = d+1, d+2, \cdots, m$ with $\text{rank}(\mathbf{A}) = d$, Eq. (B.98) yields

$$\begin{aligned}
||\mathbf{r}||^2 &= ||\boldsymbol{\Sigma}\mathbf{z}-\mathbf{w}||^2 = \sum_{i=1}^{m}(\sigma_i z_i - w_i)^2 \\
&= \sum_{i=1}^{d}(\sigma_i z_i - w_i)^2 + \sum_{i=d+1}^{m} w_i^2 \qquad \text{(B.99)}
\end{aligned}$$

When $z_i = w_i/\sigma_i$ (no sum on i) (for $i = 1, 2, \cdots, d$) and arbitrary z_i (for $i = d+1, d+2, \cdots, m$), $||\mathbf{r}||^2 = ||\boldsymbol{\Sigma}\mathbf{z}-\mathbf{w}||^2$ in Eq. (B.99) is minimized. Hence, the solution $\mathbf{x}$ which minimizes $||\mathbf{r}||^2 = ||\mathbf{A}\mathbf{x}-\mathbf{y}||^2$ can be expressed via $\mathbf{x} = \mathbf{V}\mathbf{z}$ ($\because \mathbf{V}^T = \mathbf{V}^{-1}$) with $z_i = w_i/\sigma_i$ (no sum on i) (for $i = 1, 2, \cdots, d$) and arbitrary z_i (for $i = d+1, d+2, \cdots, m$). From the following relation,

$$||\mathbf{x}||^2 = ||\mathbf{V}\mathbf{z}||^2 = (V_{ij}z_j)(V_{ik}z_k) = \delta_{jk}z_j z_k = z_j z_j = ||\mathbf{z}||^2 \qquad \text{(B.100)}$$

we see that $||\mathbf{x}||^2$ is minimized when $||\mathbf{z}||^2$ is minimized, and $||\mathbf{z}||^2$ is minimized by setting $z_i = 0$ (for $i = d+1, d+2, \cdots, m$).

From $\mathbf{w} = \mathbf{\Sigma z}$, define $[\mathbf{\Sigma}^{+}] \in \mathbb{R}^{n \times m}$ such that $\mathbf{z} = \mathbf{\Sigma}^{+}\mathbf{w}$ as

$$\mathbf{\Sigma}^{+} := \begin{bmatrix} \mathbf{D}' & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \tag{B.101}$$

where $\mathbf{D}' := \mathrm{diag}(\sigma_1^{-1}, \sigma_2^{-1}, \cdots, \sigma_d^{-1})$. Then, we can relate $\mathbf{x}$ and $\mathbf{y}$ directly as follows:

$$\mathbf{x} = \mathbf{Vz} = \mathbf{V\Sigma}^{+}\mathbf{w} = \mathbf{V\Sigma}^{+}\mathbf{U}^{T}\mathbf{y} = \mathbf{A}^{+}\mathbf{y} \tag{B.102}$$

where $\mathbf{A}^{+} := \mathbf{V\Sigma}^{+}\mathbf{U}^{T}$ ($[\mathbf{A}^{+}] \in \mathbb{R}^{n \times m}$) is known as a ***generalized inverse*** (or ***pseudo-inverse***) of $\mathbf{A}$.

Appendix C

Model Reduction by Proper Orthogonal Decomposition (POD) in Dynamical Systems and the Application of Algorithm 2.2.1

C.1 Proper Orthogonal Decomposition (POD)

The development of a model reduction technique like POD is of great interest due to its tremendous ability to decrease the computational cost of a large-scale simulation. There exists various types of model order reduction techniques; but, the method based on POD has been widely used in science and engineering fields. The original idea of POD emanates from the Principal Components Analysis (PCA) method; refer to [63]. PCA is named differently in different areas of applications, such as Karhunen-Loeve transform (KLT) in signal processing and singular value decomposition (SVD) in linear algebra. In engineering applications PCA is often called POD, which was introduced in [64] for an application of coherent structures of turbulent flow.

A large amount of research on POD has been motivated by applications in turbulence and coherent structure in fluid dynamics [65, 66], structural dynamics, image processing [67], optimal control of partial differential equations [68, 69] and so on.

In this section, the proper orthogonal decomposition (POD) using the method of snapshots for finite dimensional systems is summarized, mainly following [70].

Snapshot Data Set: Suppose n_{snap} ***snapshots*** $\mathbf{q}_i$ at time $t = t_i$ (for $i = 1, 2, \cdots, n_{\text{snap}}$) are obtained ($\{\mathbf{q}_i\} \in \mathbb{R}^N$ where N denotes the number of degree of freedom of the original system). The snapshot data sets are usually obtained from solving the original large-dimensional discrete system of equations of interest, such as $\mathbf{F}(\mathbf{q}, \dot{\mathbf{q}}, t) = \mathbf{0}$ and $\mathbf{F}(\mathbf{q}, \dot{\mathbf{q}}, \ddot{\mathbf{q}}, t) = \mathbf{0}$. Since the snapshots do not necessarily possess a zero mean, center $\mathbf{q}_i$ by

$$\hat{\mathbf{q}}_i = \mathbf{q}_i - E[\mathbf{q}_i] \tag{C.1}$$

where $E[\mathbf{q}_i]$ denotes the expectation of $\mathbf{q}_i$. $E[\mathbf{q}_i]$ gives the mean of $\mathbf{q}_i$, assuming all probabilities of $\mathbf{q}_i$ (for $i = 1, 2, \cdots, n_{\text{snap}}$) are the same,

$$E[\mathbf{q}_i] = \langle \mathbf{q}_i \rangle = \frac{1}{n_{\text{snap}}} \sum_{i=1}^{n_{\text{snap}}} \mathbf{q}_i \tag{C.2}$$

where $\langle \cdot \rangle$ denotes the averaging operator. Then, construct the snapshot tensor, $[\mathbf{A}] \in \mathbb{R}^{N \times n_{\text{snap}}}$, as

$$\mathbf{A} = [\hat{\mathbf{q}}_1, \hat{\mathbf{q}}_2, \cdots, \hat{\mathbf{q}}_{n_{\text{snap}}}] \tag{C.3}$$

Applying SVD, $\mathbf{A}$ can be decomposed as

$$\mathbf{A} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T \tag{C.4}$$

Recalling Eq. (B.85), we can express the column vectors of $\mathbf{A}$, i.e., $\mathbf{q}_i$, using the column vectors of $\mathbf{U}$ as

$$\hat{\mathbf{q}}_i = (\hat{\mathbf{q}}_i, \mathbf{u}_j)\mathbf{u}_j = \sum_{j=1}^{d}(\hat{\mathbf{q}}_i, \mathbf{u}_j)\mathbf{u}_j \tag{C.5}$$

Note that $(\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_d)$ is orthonormal.

POD Basis: Orthonormal base vectors $\boldsymbol{\varphi}_i$ (for $i = 1, 2, \cdots, s$) which maximize the projection of the column vectors of $\mathbf{A}$ onto $\boldsymbol{\varphi}_i$ in the average sense are called the ***POD base vectors***, and $\{\boldsymbol{\varphi}_i\}_{i=1}^{s}$ is called the ***POD basis*** of rank s. Such $\boldsymbol{\varphi}_i$ can be found from the following recursive constrained optimization problem, and they are given by the left singular vectors $\mathbf{u}_i$, i.e., the column vectors of $\mathbf{U}$.

$$\max_{\{\boldsymbol{\varphi}_i\}\in\mathbb{R}^N} \sum_{i=1}^{s}\sum_{j=1}^{n_{\text{snap}}} \left|(\hat{\mathbf{q}}_j, \boldsymbol{\varphi}_i)\right|^2 \quad \text{s.t.} \quad (\boldsymbol{\varphi}_i, \boldsymbol{\varphi}_j) = \delta_{ij} \tag{C.6}$$

for $s \in (1, 2, \cdots, d) \subset \mathbb{N}^+$ with $d \leq \min(N, n_{\text{snap}})$.

Proof (*POD Basis*): Define the Lagrangian function $\mathcal{L} \in \mathbb{R}$ associated with the recursive constrained optimization problem shown above as

$$\mathcal{L} := \sum_{i=1}^{s}\sum_{j=1}^{n_{\text{snap}}} \left|(\hat{\mathbf{q}}_j, \boldsymbol{\varphi}_i)\right|^2 + \lambda_{ij}\left[\delta_{ij} - (\boldsymbol{\varphi}_i, \boldsymbol{\varphi}_j)\right] \tag{C.7}$$

where λ_{ij} denotes the Lagrange multiplier. Using the relation

$$(\hat{\mathbf{q}}_j, \boldsymbol{\varphi}_i) = \{\hat{\mathbf{q}}_j\}_k\{\boldsymbol{\varphi}_i\}_k = A_{kj}\{\boldsymbol{\varphi}_i\}_k = (\mathbf{A}, \boldsymbol{\varphi}_i) \tag{C.8}$$

we have

$$\begin{aligned}
\sum_{i=1}^{s}\sum_{j=1}^{n_{\text{snap}}}\left|(\hat{\mathbf{q}}_j,\boldsymbol{\varphi}_i)\right|^2 &= (\hat{\mathbf{q}}_j,\boldsymbol{\varphi}_i)(\hat{\mathbf{q}}_j,\boldsymbol{\varphi}_i) = (A_{kj}\{\boldsymbol{\varphi}_i\}_k)(A_{\ell j}\{\boldsymbol{\varphi}_i\}_\ell) \\
&= A_{kj}A_{\ell j}\{\boldsymbol{\varphi}_i\}_\ell\{\boldsymbol{\varphi}_i\}_k \\
&= (\mathbf{A}\mathbf{A}^T\boldsymbol{\varphi}_i,\boldsymbol{\varphi}_i) \quad \text{(sum on } i) \\
&= \sum_{i=1}^{s}(\mathbf{A}\mathbf{A}^T\boldsymbol{\varphi}_i,\boldsymbol{\varphi}_i)
\end{aligned} \tag{C.9}$$

Therefore, Eq. (C.7) yields

$$\mathcal{L} = \sum_{i=1}^{s}(\mathbf{A}\mathbf{A}^T\boldsymbol{\varphi}_i,\boldsymbol{\varphi}_i) + \lambda_{ij}\left[\delta_{ij} - (\boldsymbol{\varphi}_i,\boldsymbol{\varphi}_j)\right] \tag{C.10}$$

First-order necessary optimality conditions for $\boldsymbol{\varphi}_i$ being an extremum of Eq. (C.10) is given from $\delta\mathcal{L} = 0$ as

$$\begin{aligned}
\mathbf{0} = \frac{\partial\mathcal{L}}{\partial\boldsymbol{\varphi}_\ell} &= 2\mathbf{A}\mathbf{A}^T\boldsymbol{\varphi}_i\delta_{i\ell} - \lambda_{ij}\boldsymbol{\varphi}_i\delta_{j\ell} - \lambda_{ij}\boldsymbol{\varphi}_j\delta_{i\ell} \\
&= 2\mathbf{A}\mathbf{A}^T\boldsymbol{\varphi}_\ell - (\lambda_{i\ell} + \lambda_{\ell i})\boldsymbol{\varphi}_i
\end{aligned} \tag{C.11}$$

and

$$0 = \frac{\partial\mathcal{L}}{\partial\lambda_{ij}} = \delta_{ij} - (\boldsymbol{\varphi}_i,\boldsymbol{\varphi}_j) \tag{C.12}$$

Hence,

$$\begin{aligned}
\mathbf{A}\mathbf{A}^T\boldsymbol{\varphi}_\ell &= \frac{1}{2}(\lambda_{i\ell} + \lambda_{\ell i})\boldsymbol{\varphi}_i \quad (\text{for } i = 1, 2, \cdots, s) \\
&= \frac{1}{2}\sum_{i=1}^{s}(\lambda_{i\ell} + \lambda_{\ell i})\boldsymbol{\varphi}_i
\end{aligned} \tag{C.13}$$

for all $\ell \in (1, 2, \cdots, s)$, and the orthonormal relation

$$(\boldsymbol{\varphi}_i,\boldsymbol{\varphi}_j) = \delta_{ij} \tag{C.14}$$

Now, our objective is to prove that Eq. (C.13) and Eq. (C.14), i.e., the first-order necessary optimality conditions for the recursive constrained optimization problem, shown in Eq. (C.6), is equivalent to the eigenvalue problem

$$\mathbf{A}\mathbf{A}^T\boldsymbol{\varphi}_\ell = \lambda_\ell\boldsymbol{\varphi}_\ell \quad \forall\ \ell \in (1, 2, \cdots, s) \tag{C.15}$$

(no sum on ℓ). Proof by means of the method of mathematical induction is shown below:

1. **Base case:** When $s = 1$, we have $k = 1$ and Eq. (C.13) yields

$$\mathbf{A}\mathbf{A}^T\boldsymbol{\varphi}_1 = \lambda_1\boldsymbol{\varphi}_1 \tag{C.16}$$

where $\lambda_1 \equiv \lambda_{11}$. We can readily see that Eq. (C.15) holds for this base case.

2. **Induction step:** *Suppose* that

$$\mathbf{A}\mathbf{A}^T\boldsymbol{\varphi}_\ell = \frac{1}{2}\sum_{i=1}^{s-1}(\lambda_{i\ell} + \lambda_{\ell i})\boldsymbol{\varphi}_i = \lambda_\ell\boldsymbol{\varphi}_\ell \quad \forall\ \ell \in (1, 2, \cdots, s-1) \tag{C.17}$$

(no sum on ℓ) holds (*inductive hypothesis*). Then, show that

$$\mathbf{A}\mathbf{A}^T\boldsymbol{\varphi}_\ell = \lambda_\ell\boldsymbol{\varphi}_\ell \quad \forall\ \ell \in (1, 2, \cdots, s) \tag{C.18}$$

(no sum on ℓ) also holds.

Due to the inductive hypothesis, Eq. (C.17), we must prove

$$\mathbf{A}\mathbf{A}^T\boldsymbol{\varphi}_s = \lambda_s\boldsymbol{\varphi}_s \tag{C.19}$$

(no sum on s) in order to prove Eq. (C.18). From Eq. (C.13), we have

$$\mathbf{A}\mathbf{A}^T\boldsymbol{\varphi}_s = \frac{1}{2}\sum_{i=1}^{s}(\lambda_{is} + \lambda_{si})\boldsymbol{\varphi}_i \tag{C.20}$$

when $\ell = s$. Since $(\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2, \cdots, \boldsymbol{\varphi}_s)$ is orthonormal,

$$\begin{aligned}
0 &= (\boldsymbol{\varphi}_s, \boldsymbol{\varphi}_\ell) \ \ \forall\ \ell \in (1, 2, \cdots, s-1) \\
&= \lambda_\ell(\boldsymbol{\varphi}_s, \boldsymbol{\varphi}_\ell) = (\boldsymbol{\varphi}_s, \lambda_\ell \boldsymbol{\varphi}_\ell) \ \ \text{(no sum on } \ell) \\
&= (\boldsymbol{\varphi}_s, \mathbf{A}\mathbf{A}^T \boldsymbol{\varphi}_\ell) \quad \because \text{Eq. (C.17)} \\
&= \boldsymbol{\varphi}_s^T \mathbf{A}\mathbf{A}^T \boldsymbol{\varphi}_\ell \\
&= \{\boldsymbol{\varphi}_s\}_i A_{ij} A_{kj} \{\boldsymbol{\varphi}_\ell\}_k = A_{kj} A_{ij} \{\boldsymbol{\varphi}_s\}_i \{\boldsymbol{\varphi}_\ell\}_k \\
&= (\mathbf{A}\mathbf{A}^T \boldsymbol{\varphi}_s, \boldsymbol{\varphi}_\ell) \\
&= (\frac{1}{2} \sum_{i=1}^{s} (\lambda_{is} + \lambda_{si}) \boldsymbol{\varphi}_i, \boldsymbol{\varphi}_\ell) \quad \because \text{Eq. (C.20)} \\
&= \frac{1}{2} \sum_{i=1}^{s} (\lambda_{is} + \lambda_{si}) (\boldsymbol{\varphi}_i, \boldsymbol{\varphi}_\ell) = \frac{1}{2} \sum_{i=1}^{s} (\lambda_{is} + \lambda_{si}) \delta_{i\ell} \\
&= \frac{1}{2} (\lambda_{\ell s} + \lambda_{s\ell})
\end{aligned} \tag{C.21}$$

Therefore,

$$\lambda_{\ell s} + \lambda_{s\ell} = 0 \tag{C.22}$$

Hence, Eq. (C.20) yields

$$\begin{aligned}
\mathbf{A}\mathbf{A}^T \boldsymbol{\varphi}_s &= \frac{1}{2} \sum_{i=1}^{s} (\lambda_{is} + \lambda_{si}) \boldsymbol{\varphi}_i \\
&= \frac{1}{2} \sum_{i=1}^{s-1} (\lambda_{is} + \lambda_{si}) \boldsymbol{\varphi}_i + \frac{1}{2} (\lambda_{ss} + \lambda_{ss}) \boldsymbol{\varphi}_s \ \ \text{(no sum on } s) \\
&= \lambda_s \boldsymbol{\varphi}_s
\end{aligned} \tag{C.23}$$

where $\lambda_s \equiv \lambda_{ss}$. Therefore, the first-order necessary optimality conditions for the recursive constrained optimization problem has been proven to be given as Eq. (C.15). Comparison between Eq. (C.15) and Eq. (B.64), i.e.,

$$\mathbf{A}\mathbf{A}^T \boldsymbol{\varphi}_\ell = \lambda_\ell \boldsymbol{\varphi}_\ell \ \ \text{and} \ \ \mathbf{A}\mathbf{A}^T \mathbf{u}_i = \sigma_i^2 \mathbf{u}_i \tag{C.24}$$

implies that the left singular vectors, i.e., the column vectors of $\mathbf{U}$, can be actually used as the ***POD base vectors***, and the associated eigenvalues yield $\lambda_\ell \equiv \sigma_\ell^2$. $\{\boldsymbol{\varphi}_\ell\}_{\ell=1}^s \equiv \{\mathbf{u}_\ell\}_{\ell=1}^s$ are called the ***POD basis*** of rank $s \in (1, 2, \cdots, d)$. ■

Remarks (*POD Basis*):

- Consider an arbitrary vector $\mathbf{w}$ with $\|\mathbf{w}\| = 1$. By expressing $\mathbf{w}$ in terms of the orthonormal basis $\{\mathbf{u}_\ell\}_{\ell=1}^s$, we have

$$\mathbf{w} = \sum_{i=1}^{s} (\mathbf{w}, \mathbf{u}_i)\mathbf{u}_i = (\mathbf{w}, \mathbf{u}_i)\mathbf{u}_i \tag{C.25}$$

Then, we can show

$$\begin{aligned}
\sum_{j=1}^{n_{\text{snap}}} \left|(\hat{\mathbf{q}}_j, \mathbf{w})\right|^2 &= (\hat{\mathbf{q}}_j, \mathbf{w})(\hat{\mathbf{q}}_j, \mathbf{w}) \\
&= (\hat{\mathbf{q}}_j, (\mathbf{w}, \mathbf{u}_i)\mathbf{u}_i)(\hat{\mathbf{q}}_j, (\mathbf{w}, \mathbf{u}_k)\mathbf{u}_k) \\
&= ((\hat{\mathbf{q}}_j, \mathbf{u}_i)\hat{\mathbf{q}}_j, \mathbf{u}_k)(\mathbf{w}, \mathbf{u}_i)(\mathbf{w}, \mathbf{u}_k) \\
&= (A_{sj}A_{rj}\{\mathbf{u}_i\}_r, \{\mathbf{u}_k\}_s)(\mathbf{w}, \mathbf{u}_i)(\mathbf{w}, \mathbf{u}_k) \\
&= (\mathbf{A}\mathbf{A}^T\mathbf{u}_i, \mathbf{u}_k)(\mathbf{w}, \mathbf{u}_i)(\mathbf{w}, \mathbf{u}_k) \\
&= \sigma_i^2 \left|(\mathbf{w}, \mathbf{u}_i)\right|^2 = \sum_{i=1}^{s} \sigma_i^2 \left|(\mathbf{w}, \mathbf{u}_i)\right|^2
\end{aligned} \tag{C.26}$$

where we used $\mathbf{A}\mathbf{A}^T\mathbf{u}_i = \sigma_i^2\mathbf{u}_i$ (no sum on i). Notice that

$$\begin{aligned}
\sum_{i=1}^{s} \sigma_i^2 \left|(\mathbf{w}, \mathbf{u}_i)\right|^2 \leq \sum_{i=1}^{s} \sigma_i^2 \sum_{i=1}^{s} \left|(\mathbf{w}, \mathbf{u}_i)\right|^2 &= \sum_{i=1}^{s} \sigma_i^2 \\
&= \sum_{i=1}^{s} \sum_{j=1}^{n_{\text{snap}}} \left|(\hat{\mathbf{q}}_j, \mathbf{u}_i)\right|^2
\end{aligned} \tag{C.27}$$

due to the relation

$$\sum_{i=1}^{s} \left|(\mathbf{w}, \mathbf{u}_i)\right|^2 = (\mathbf{w}, \mathbf{u}_i)(\mathbf{w}, \mathbf{u}_i) = (\mathbf{w}, (\mathbf{w}, \mathbf{u}_i)\mathbf{u}_i) = (\mathbf{w}, \mathbf{w}) = 1 \tag{C.28}$$

and the fact that $\mathbf{u}_i$ satisfies

$$\begin{aligned}
\sum_{i=1}^{s}\sum_{j=1}^{n_{\text{snap}}}\left|(\hat{\mathbf{q}}_j,\mathbf{u}_i)\right|^2 &= (\hat{\mathbf{q}}_j,\mathbf{u}_i)(\hat{\mathbf{q}}_j,\mathbf{u}_i)\\
&= A_{rj}\{\mathbf{u}_i\}_r A_{pj}\{\mathbf{u}_i\}_p\\
&= A_{pj}A_{rj}\{\mathbf{u}_i\}_r\{\mathbf{u}_i\}_p \ \ \text{(also sum on } i\text{)}\\
&= \sum_{i=1}^{s}(\mathbf{A}\mathbf{A}^T\mathbf{u}_i,\mathbf{u}_i)\\
&= \sum_{i=1}^{s}\sigma_i^2 = \sum_{i=1}^{s}\lambda_i > 0
\end{aligned} \tag{C.29}$$

- The POD basis of rank s, $\boldsymbol{\varphi}_i = \mathbf{u}_i$, can be equivalently found from the following recursive constrained optimization problem

$$\min_{\{\boldsymbol{\varphi}_i\}\in\mathbb{R}^N}\sum_{j=1}^{n_{\text{snap}}}\|\hat{\mathbf{q}}_j-\sum_{i=1}^{s}(\hat{\mathbf{q}}_j,\boldsymbol{\varphi}_i)\boldsymbol{\varphi}_i\|^2 \quad \text{s.t.} \quad (\boldsymbol{\varphi}_i,\boldsymbol{\varphi}_j)=\delta_{ij} \tag{C.30}$$

for $s \in (1, 2, \cdots, d) \subset \mathbb{N}^+$ with $d \le \min(N, n_{\text{snap}})$. The Lagrangian defined from Eq. (C.30) is

$$\mathcal{L} := \sum_{j=1}^{n_{\text{snap}}}\|\hat{\mathbf{q}}_j-\sum_{i=1}^{s}(\hat{\mathbf{q}}_j,\boldsymbol{\varphi}_i)\boldsymbol{\varphi}_i\|^2+\lambda_{ij}\left[\delta_{ij}-(\boldsymbol{\varphi}_i,\boldsymbol{\varphi}_j)\right] \tag{C.31}$$

The necessary optimality conditions are given by the eigenvalue problem shown in Eq. (C.15).

- **Computation Process of a POD basis of rank** s

(i) ***Method of Snapshots:*** If $n_{\text{snap}} < N$, compute $\mathbf{u}_i$ from the following steps:

Step 1: Compute $\{\mathbf{v}_i\} \in \mathbb{R}^{n_{\text{snap}}}$ (for $j = 1, 2, \cdots, s$) from Eq. (B.61)

$$(\mathbf{A}^T\mathbf{A})\mathbf{v}_i = \sigma_i^2\mathbf{v}_i \ \ \text{(no sum on } i\text{)}$$

Step 2: Compute $\{\mathbf{u}_i\} \in \mathbb{R}^N$ (for $i = 1, 2, \cdots, s$) from Eq. (B.62)

$$\mathbf{u}_i := \sigma_i^{-1}\mathbf{A}\mathbf{v}_i \quad \text{(no sum on } i\text{)}$$

where $\sigma_i = \sqrt{\lambda_i}$.

(ii) If $n_{\text{snap}} > N$, compute $\{\mathbf{u}_i\} \in \mathbb{R}^N$ (for $i = 1, 2, \cdots, s$) from Eq. (B.64), i.e.,

$$(\mathbf{A}\mathbf{A}^T)\mathbf{u}_i = \sigma_i^2\mathbf{u}_i$$

- There is no theoretical criterion to determine the value of the truncation degree of the PDO basis, $s \in (1, 2, \cdots, d)$ with $d \leq \min(N, n_{\text{snap}})$. The choice of $s \in (1, 2, \cdots, d)$ is commonly determined from the relative error [1]

$$\varepsilon_{\text{rel}} := \frac{\varepsilon}{\|\mathbf{A}\|_{\text{F}}^2} < \text{TOL} \tag{C.32}$$

where TOL is an error tolerance, and ε denotes the absolute error of $\mathbf{A}$ of rank d defined by

$$\varepsilon := \left\|\mathbf{A} - \boldsymbol{\Phi}\boldsymbol{\Phi}^T\mathbf{A}\right\|_{\text{F}}^2 \tag{C.33}$$

with the POD base tensor

$$\boldsymbol{\Phi} = [\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2, \cdots, \boldsymbol{\varphi}_s] = [\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_s] \tag{C.34}$$

[1] **Frobenius Norm:** The Frobenius norm of a second-order tensor $[\mathbf{A}] \in \mathbb{R}^{m\times n}$ or $\mathbb{C}^{m\times n}$ is defined as the square root of the sum of the absolute squares of its elements,

$$\|\mathbf{A}\|_{\text{F}} := \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n}\left|A_{ij}\right|^2} = \sqrt{\text{tr}(\mathbf{A}^\dagger\mathbf{A})}$$

The Frobenius norm is a norm in the sense that it satisfies the following relations:

$$\begin{aligned}
&\|\mathbf{A}\|_{\text{F}} > 0 \;\; \forall\, \mathbf{A} \neq \mathbf{0}, \quad \|\mathbf{A}\|_{\text{F}} = 0 \;\text{ iff } \mathbf{A} = \mathbf{0}\\
&\|\alpha\mathbf{A}\|_{\text{F}} = |\alpha|\,\|\mathbf{A}\|_{\text{F}} \quad \forall\, \alpha \in \mathbb{R} \text{ or } \mathbb{C},\; \mathbf{A} \in \mathcal{V}^2\\
&\|\mathbf{A}\mathbf{B}\|_{\text{F}} \leq \|\mathbf{A}\|_{\text{F}} + \|\mathbf{B}\|_{\text{F}} \quad \forall\, \mathbf{A}, \mathbf{B} \in \mathcal{V}^2
\end{aligned}$$

In above equation, $\mathbf{\Phi\Phi}^T$ can be recognized as the orthonormal projection since it projects $\mathbf{A}$ onto the s-dimensional subspace spanned by $\mathbf{\Phi}$ as can be seen from

$$\Phi_{ik}\Phi_{\ell k}A_{\ell j} = \{\mathbf{u}_k\}_i\{\mathbf{u}_k\}_\ell A_{\ell j} = \mathbf{u}_k\mathbf{u}_k^T A_{\ell j} \tag{C.35}$$

By using SVD, $\mathbf{A} = \mathbf{U\Sigma V}^T = \sum_{i=1}^d \sigma_i \mathbf{u}_i \mathbf{v}_i^T$; hence, eq. (C.33) yields

$$\varepsilon = \left\| \sum_{i=1}^{d} \sigma_i \mathbf{u}_i \mathbf{v}_i^T - \sum_{i=1}^{s} \sigma_i \mathbf{u}_i \mathbf{v}_i^T \right\|_{\mathrm{F}}^2 = \left\| \sum_{i=s+1}^{d} \sigma_i \mathbf{u}_i \mathbf{v}_i^T \right\|_{\mathrm{F}}^2 \tag{C.36}$$

After some straightforward works, we can show that Eq. (C.32) yields

$$\varepsilon_{\mathrm{rel}} = \frac{\sum_{i=s+1}^{d} \sigma_i^2}{\sum_{j=1}^{d} \sigma_j^2} < \mathrm{TOL} \tag{C.37}$$

The number of the POD basis vectors, s, should be the smallest integer which satisfies the above optimal criterion given in Eq. (C.37), or equivalently,

$$\bar{\varepsilon}_s := \frac{\sum_{i=1}^{s} \sigma_i^2}{\sum_{j=1}^{d} \sigma_j^2} > 1 - \mathrm{TOL} \tag{C.38}$$

We commonly take $1 - \mathrm{TOL} = 0.99$ (Ad-hoc criterion). Notice that

$$0 < \bar{\varepsilon}_1 \le \bar{\varepsilon}_2 \le \cdots \le \bar{\varepsilon}_d = 1 \tag{C.39}$$

C.2 Model Order Reductions by the POD method for Second- and First-order ODEs

In this section, we show the model reductions of linear and nonlinear time-invariant ordinary differential equations (ODEs) in both second- and first-order system by using the POD basis.

C.2.1 Second-order ODEs

Linear Dynamical Systems: Consider the following initial-value problem consists of the second-order ODE and the initial conditions in linear systems:

$$\begin{aligned} &\mathbf{M}\ddot{\mathbf{q}} + \mathbf{C}\dot{\mathbf{q}} + \mathbf{K}\mathbf{q} = \mathbf{f}(t) \quad \forall t \in \mathbb{I} = [t_0, T] \subset \mathbb{R} \\ &\text{with} \quad \mathbf{q}(t_0) = \mathbf{q}^0 \quad \text{and} \quad \dot{\mathbf{q}}(t_0) = \mathbf{v}^0 \end{aligned} \tag{C.40}$$

where $[\mathbf{M}] \in \mathbb{R}^{N\times N}$, $[\mathbf{C}] \in \mathbb{R}^{N\times N}$, and $[\mathbf{K}] \in \mathbb{R}^{N\times N}$ denote the mass, damping, and stiffness matrices, respectively; $\{\mathbf{f}(t)\} : \mathbb{I} \to \mathbb{R}^N$ denotes the time-dependent externally applied force vector; and $\{\ddot{\mathbf{q}}(t)\} : \mathbb{I} \to \mathbb{R}^N$, $\{\dot{\mathbf{q}}(t)\} : \mathbb{I} \to \mathbb{R}^N$, and $\{\mathbf{q}(t)\} : \mathbb{I} \to \mathbb{R}^N$ denote the acceleration, velocity, and configuration vectors.

$$\mathbf{q}(t) \approx \mathbf{\Phi}\boldsymbol{\xi}(t) = \boldsymbol{\varphi}_i \xi_i(t) \tag{C.41}$$

for $i = 1, 2, \cdots, n_\mathrm{r} < N$. The orthonormal set of vectors $(\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2, \cdots, \boldsymbol{\varphi}_{n_\mathrm{r}})$ spans a subspace $\mathcal{V}_\Phi \subset \mathcal{V}$. The subspace $\mathcal{V}_\Phi$ is known as the ***ansatz space*** for POD. From Eq. (C.41), we have

$$\dot{\mathbf{q}}(t) \approx \mathbf{\Phi}\dot{\boldsymbol{\xi}}(t) \quad = \quad \boldsymbol{\varphi}_i \dot{\xi}_i(t) \tag{C.42}$$

$$\ddot{\mathbf{q}}(t) \approx \mathbf{\Phi}\dot{\boldsymbol{\xi}}(t) \quad = \quad \boldsymbol{\varphi}_i \ddot{\xi}_i(t) \tag{C.43}$$

Substitute Eq. (C.41) - Eq. (C.43) into the balance equation in Eq. (C.40), and then define the residual vector $\{\mathbf{r}\} \in \mathbb{R}^N$ as

$$\mathbf{r} := \mathbf{M}\mathbf{\Phi}\ddot{\boldsymbol{\xi}} + \mathbf{C}\mathbf{\Phi}\dot{\boldsymbol{\xi}} + \mathbf{K}\mathbf{\Phi}\boldsymbol{\xi} - \mathbf{f} \tag{C.44}$$

Note that $\mathbf{r} \neq \mathbf{0}$ in general. Now, premultiply Eq. (C.44) by $\mathbf{\Phi}^T$ and set $(\mathbf{\Phi}, \mathbf{r})$ to be zero, assuming the residual vector $\mathbf{r}$ is perpendicular to the ansatz space spanned by $\boldsymbol{\varphi}_i$.

Hence, we obtain

$$(\boldsymbol{\Phi}, \mathbf{r}) = \hat{\mathbf{M}}\ddot{\boldsymbol{\xi}} + \hat{\mathbf{C}}\dot{\boldsymbol{\xi}} + \hat{\mathbf{K}}\boldsymbol{\xi} - \hat{\mathbf{f}} = \mathbf{0} \tag{C.45}$$

where

$$\hat{\mathbf{M}} := (\boldsymbol{\Phi}, \mathbf{M}\boldsymbol{\Phi}) = \boldsymbol{\Phi}^T \mathbf{M}\boldsymbol{\Phi}, \quad [\hat{\mathbf{M}}] \in \mathbb{R}^{n_\mathrm{r} \times n_\mathrm{r}} \tag{C.46}$$

$$\hat{\mathbf{C}} := (\boldsymbol{\Phi}, \mathbf{C}\boldsymbol{\Phi}) = \boldsymbol{\Phi}^T \mathbf{C}\boldsymbol{\Phi}, \quad [\hat{\mathbf{C}}] \in \mathbb{R}^{n_\mathrm{r} \times n_\mathrm{r}} \tag{C.47}$$

$$\hat{\mathbf{K}} := (\boldsymbol{\Phi}, \mathbf{K}\boldsymbol{\Phi}) = \boldsymbol{\Phi}^T \mathbf{K}\boldsymbol{\Phi}, \quad [\hat{\mathbf{K}}] \in \mathbb{R}^{n_\mathrm{r} \times n_\mathrm{r}} \tag{C.48}$$

$$\hat{\mathbf{f}} := (\boldsymbol{\Phi}, \mathbf{f}) = \boldsymbol{\Phi}^T \mathbf{f}, \quad \{\hat{\mathbf{f}}\} \in \mathbb{R}^{n_\mathrm{r}} \tag{C.49}$$

Note that Eq. (C.45) is exactly in the form of the normal equation obtained in the least squares approximation. Next, we need to project the initial conditions, following a similar procedure. From eq. (C.41), we can define the residual vectors for the initial conditions also as

$$\mathbf{r}_{\mathrm{q}_0} := \boldsymbol{\Phi}\boldsymbol{\xi}(t_0) - \mathbf{q}^0 \tag{C.50}$$

$$\mathbf{r}_{\mathrm{v}_0} := \boldsymbol{\Phi}\dot{\boldsymbol{\xi}}(t_0) - \mathbf{v}^0 \tag{C.51}$$

which are not equal to zero in general. Project $\mathbf{r}_{\mathrm{q}_0}$ and $\mathbf{r}_{\mathrm{v}_0}$ onto the ansatz space spanned by $\boldsymbol{\varphi}_i$ by premultiplying by $\boldsymbol{\Phi}^T$ and set $(\boldsymbol{\Phi}, \mathbf{r}_{\mathrm{q}_0})$ and $(\boldsymbol{\Phi}, \mathbf{r}_{\mathrm{v}_0})$ to be zero:

$$(\boldsymbol{\Phi}, \mathbf{r}_{\mathrm{q}_0}) = \boldsymbol{\Phi}^T \boldsymbol{\Phi}\boldsymbol{\xi}(t_0) - \boldsymbol{\Phi}^T \mathbf{q}^0 = \mathbf{0} \tag{C.52}$$

$$(\boldsymbol{\Phi}, \mathbf{r}_{\mathrm{v}_0}) = \boldsymbol{\Phi}^T \boldsymbol{\Phi}\dot{\boldsymbol{\xi}}(t_0) - \boldsymbol{\Phi}^T \mathbf{v}^0 = \mathbf{0} \tag{C.53}$$

Hence, we obtain

$$\boldsymbol{\xi}(t_0) = (\boldsymbol{\Phi}^T \boldsymbol{\Phi})^{-1} \boldsymbol{\Phi}^T \mathbf{q}^0 \tag{C.54}$$

$$\dot{\boldsymbol{\xi}}(t_0) = (\boldsymbol{\Phi}^T \boldsymbol{\Phi})^{-1} \boldsymbol{\Phi}^T \mathbf{v}^0 \tag{C.55}$$

Summarizing, the original system, shown in Eq. (C.40), has been reduced to

$$\begin{aligned}&\hat{\mathbf{M}}\ddot{\boldsymbol{\xi}} + \hat{\mathbf{C}}\dot{\boldsymbol{\xi}} + \hat{\mathbf{K}}\boldsymbol{\xi} = \hat{\mathbf{f}} \quad \forall t \in \mathbb{I} = [t_0, T] \subset \mathbb{R}\\ &\text{with}\\ &\boldsymbol{\xi}(t_0) = (\boldsymbol{\Phi}^T\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^T\mathbf{q}^0\\ &\dot{\boldsymbol{\xi}}(t_0) = (\boldsymbol{\Phi}^T\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^T\mathbf{v}^0\end{aligned} \tag{C.56}$$

Nonlinear Dynamical Systems: The similar approach can be applied for nonlinear systems. Consider the following initial-value problem consists of the second-order ODE and the initial conditions in nonlinear systems:

$$\begin{aligned}&\mathbf{F}(\mathbf{q}, \dot{\mathbf{q}}, \ddot{\mathbf{q}}, t) = \mathbf{0} \quad \forall t \in \mathbb{I} = [t_0, T] \subset \mathbb{R}\\ &\text{with} \quad \mathbf{q}(t_0) = \mathbf{q}^0 \quad \text{and} \quad \dot{\mathbf{q}}(t_0) = \mathbf{v}^0\end{aligned} \tag{C.57}$$

with $\{\mathbf{F}\} \in \mathbb{R}^N$ and $\{\mathbf{q}\} \in \mathbb{R}^N$. Employing the ansatz given in Eq. (C.41) for the balance equation, define the residual vector $\{\mathbf{r}\} \in \mathbb{R}^N$ as

$$\mathbf{r} := \mathbf{F}(\boldsymbol{\Phi}\boldsymbol{\xi}, \boldsymbol{\Phi}\dot{\boldsymbol{\xi}}, \boldsymbol{\Phi}\ddot{\boldsymbol{\xi}}, t) \tag{C.58}$$

Hence, $(\boldsymbol{\Phi}, \mathbf{r}) = \mathbf{0}$ yields

$$\boldsymbol{\Phi}^T\mathbf{F}(\boldsymbol{\Phi}\boldsymbol{\xi}, \boldsymbol{\Phi}\dot{\boldsymbol{\xi}}, \boldsymbol{\Phi}\ddot{\boldsymbol{\xi}}, t) = \mathbf{0} \tag{C.59}$$

Summarizing, the original system, shown in Eq. (C.57), has been reduced to

$$\begin{aligned}&\boldsymbol{\Phi}^T\mathbf{F}(\boldsymbol{\Phi}\boldsymbol{\xi}, \boldsymbol{\Phi}\dot{\boldsymbol{\xi}}, \boldsymbol{\Phi}\ddot{\boldsymbol{\xi}}, t) = \mathbf{0} \quad \forall t \in \mathbb{I} = [t_0, T] \subset \mathbb{R}\\ &\text{with}\\ &\boldsymbol{\xi}(t_0) = (\boldsymbol{\Phi}^T\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^T\mathbf{q}^0\\ &\dot{\boldsymbol{\xi}}(t_0) = (\boldsymbol{\Phi}^T\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^T\mathbf{v}^0\end{aligned} \tag{C.60}$$

C.2.2 First-order ODEs

Following the same procedures, we can readily derive the reduced form of the linear and nonlinear dynamical systems.

Linear Dynamical Systems: Consider the following initial-value problem consists of the first-order ODE and the initial condition in linear systems:

$$\begin{aligned} &\mathbf{M}\dot{\mathbf{q}} + \mathbf{K}\mathbf{q} = \mathbf{f}(t) \quad \forall t \in \mathbb{I} = [t_0, T] \subset \mathbb{R} \\ &\text{with} \quad \mathbf{q}(t_0) = \mathbf{q}^0 \end{aligned} \tag{C.61}$$

This original system can be reduced to the following reduced model:

$$\begin{aligned} &\hat{\mathbf{M}}\dot{\boldsymbol{\xi}} + \hat{\mathbf{K}}\boldsymbol{\xi} = \hat{\mathbf{f}} \quad \forall t \in \mathbb{I} = [t_0, T] \subset \mathbb{R} \\ &\text{with} \\ &\boldsymbol{\xi}(t_0) = (\boldsymbol{\Phi}^T\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^T\mathbf{q}^0 \end{aligned} \tag{C.62}$$

Nonlinear Dynamical Systems: Consider the following initial-value problem consists of the second-order ODE and the initial conditions in nonlinear systems:

$$\begin{aligned} &\mathbf{F}(\mathbf{q}, \dot{\mathbf{q}}, t) = \mathbf{0} \quad \forall t \in \mathbb{I} = [t_0, T] \subset \mathbb{R} \\ &\text{with} \quad \mathbf{q}(t_0) = \mathbf{q}^0 \end{aligned} \tag{C.63}$$

with $\{\mathbf{F}\} \in \mathbb{R}^N$ and $\{\mathbf{q}\} \in \mathbb{R}^N$. This original system can be reduced to the following reduced model:

$$\begin{aligned} &\boldsymbol{\Phi}^T\mathbf{F}(\boldsymbol{\Phi}\boldsymbol{\xi}, \boldsymbol{\Phi}\dot{\boldsymbol{\xi}}, t) = \mathbf{0} \quad \forall t \in \mathbb{I} = [t_0, T] \subset \mathbb{R} \\ &\text{with} \\ &\boldsymbol{\xi}(t_0) = (\boldsymbol{\Phi}^T\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^T\mathbf{q}^0 \end{aligned} \tag{C.64}$$

C.3 Application of Algorithm 2.2.1

Numerically non-dissipative and dissipative schemes: The numerically non-dissipative schemes within Algorithm 2.2.1 are obtained by $\rho_\infty^{\min} = \rho_\infty^{\max} = 1$ and free parameter $\rho_\infty^{s} \in [0, 1]$. These methods, U0V0(1,1,ρ_∞^{s}) and V0U0(1,1,ρ_∞^{s}), [2] are symplectic and conserve the discrete total energy and momenta within the time step $[t_n, t_{n+1}]$ for linear transient systems. The most common and basic non-dissipative members (within the GS4-2 family) are the MPR-EPA method, i.e., U0V0/V0U0$(1, 1, 1)$, implicit Newmark method, i.e., U0V0$(1, 1, 0)$, and MPR-MPA method, i.e., V0U0$(1, 1, 0)$.

Although it is usually preferred to use non-dissipative schemes, it is well-known that such schemes are prone to numerical instabilities due to high frequencies produced by the finite element discretization in structural dynamic problems. In such a case, we need a so-called numerically dissipative scheme instead. The GSSSS family of algorithms also encompasses numerous new numerically dissipative schemes as well as commonly-used ones such as the WBZ method, HHT-α method, and three parameter optimal schemes (which is identical to the Generalized-α method). It is immensely important to note that those commonly-used numerically dissipative algorithms belong to only U0V1 family; therefore, the U0V0/V0U0 optimal family of numerically dissipative schemes, which can be obtained from $\rho_\infty^{\min} = \rho_\infty^{s} \in [0, 1)$ in addition to $\rho_\infty^{\max} = 1$ (notice that the resulting algorithms from the U0 and V0 families are identical), possesses a superiority (over either U0V1 or V0U1 dissipative schemes) from a numeric point of view.

Construction of Φ: First of all, we need to solve the original system of equation,

[2] Algorithms within the U0 family and V0 family are expressed as U0($\rho_\infty^{\min}$,$\rho_\infty^{\max}$,ρ_∞^{s}) and V0($\rho_\infty^{\min}$,$\rho_\infty^{\max}$,ρ_∞^{s}), respectively.

$\mathbf{M}\ddot{\mathbf{q}} = \mathbf{f}(\mathbf{q}, \dot{\mathbf{q}}, t)$ where the state vector is $\mathbf{q} \in \mathbb{R}^N$, for n_{snap} time steps, with a time integration technique since the POD basis is constructed based on solutions of the original system. Suppose the original system suffers from high frequency issues, and we have no choice but to employ a numerically dissipative scheme, such as U0V0/V0U0($\rho_\infty, 1, \rho_\infty$) optimal algorithm with $\rho_\infty \in [0, 1)$, instead of a numerically non-dissipative scheme. Then, $\rho_\infty \in [0, 1)$ as close to unity as possible is preferable to minimize a numerical error.

Model reduction: Once we obtain the POD basis, we can reduce the original system to the system given in Eq. (C.56) with $\boldsymbol{\xi} \in \mathbb{R}^{n_\text{r}}$ ($n_\text{r} < N$). By reducing the system size via the POD model reduction, we may be able to dispense with the high frequency issue; herein, let us apply a numerically non-dissipative scheme to solve the reduced system as

$$\hat{\mathbf{M}}\tilde{\ddot{\boldsymbol{\xi}}}^n = \hat{\mathbf{f}}(\boldsymbol{\Phi}\tilde{\boldsymbol{\xi}}^n, \boldsymbol{\Phi}\tilde{\dot{\boldsymbol{\xi}}}^n, t_{n+W_1}) \tag{C.65}$$

for $n \in \{0, 1, 2, \cdots, n^{\text{r}}_{\text{steps}} - 1\}$, where the algorithmic vectors, $\tilde{\boldsymbol{\xi}}^n$, $\tilde{\dot{\boldsymbol{\xi}}}^n$, and $\tilde{\ddot{\boldsymbol{\xi}}}^n$, and the associated updates are defined in the same manner as given in Eq. (2.5b)-Eq. (2.5d) and Eq. (2.5e)-Eq. (2.5g), respectively. Once we complete the simulation in the reduced system, we can recover the approximated displacement, velocity, and acceleration in the original system as

$$^*\mathbf{q}^n = \boldsymbol{\Phi}\boldsymbol{\xi}^n, \quad ^*\mathbf{v}^n = \boldsymbol{\Phi}\dot{\boldsymbol{\xi}}^n, \quad \text{and} \quad ^*\mathbf{a}^n = \boldsymbol{\Phi}\ddot{\boldsymbol{\xi}}^n \tag{C.66}$$

The strategy described here is summarized in Fig.C.1.

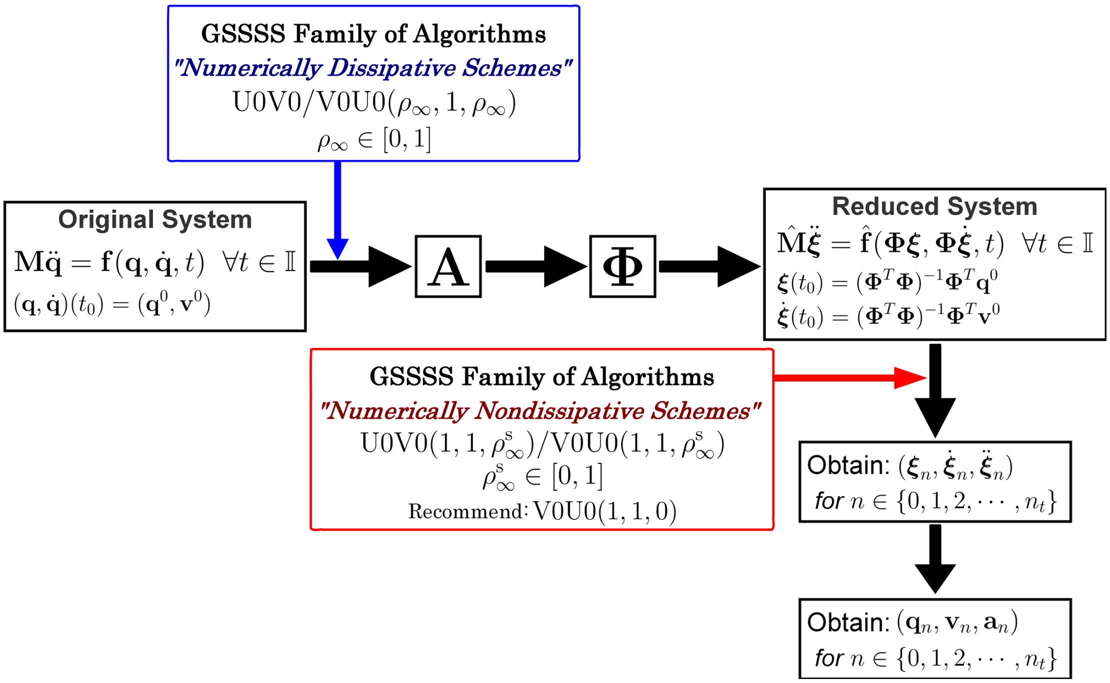
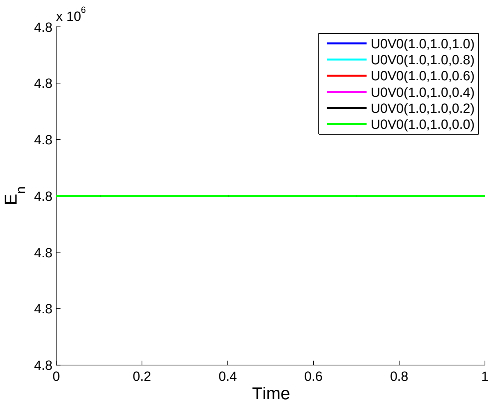


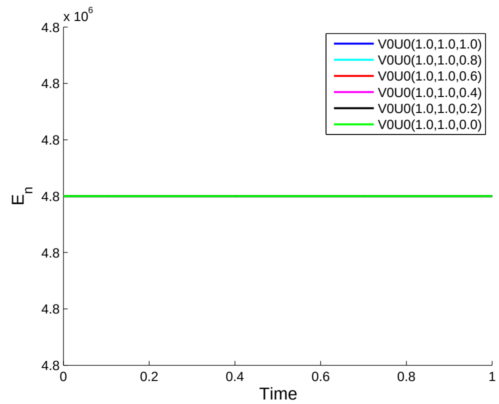
Figure C.1: Application of Algorithm 2.2.1

Remark C.3.1 (Discrete Energy Conservation)

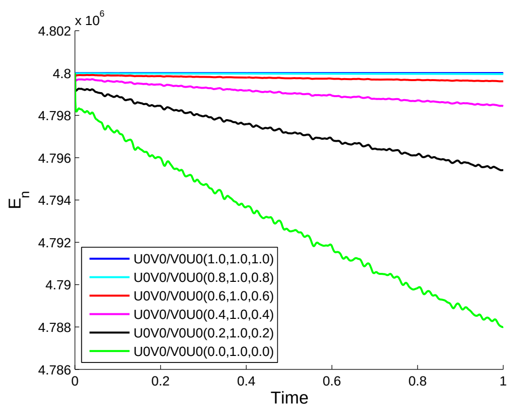
Consider a linear dynamical system and suppose the mechanical energy of the system is defined as $\mathscr{E}^h(\mathbf{q}, \mathbf{v}) = \frac{1}{2}\mathbf{v}^T\mathbf{M}\mathbf{v} + \frac{1}{2}\mathbf{q}^T\mathbf{K}\mathbf{q} - \mathbf{q}^T\mathbf{g}(t)$ *for all* $t \in \mathbb{I}$*. If we solve the original system without model reduction by the exact energy-momentum conserving schemes, i.e., either U0V0(1,1,*ρ_∞^{s}*) or V0U0(1,1,*ρ_∞^{s}*) in the linear system, we have* $\mathscr{E}^h(\mathbf{q}^n, \mathbf{v}^n) = \mathscr{E}^h(\mathbf{q}^{n+1}, \mathbf{v}^{n+1})$*; see Fig. C.2(a)(b). On the other hand, if we use the U0V0/V0U0(*$\rho_\infty, 1, \rho_\infty$*) algorithm with* $\rho_\infty \in [0, 1)$*, the exact energy conservation feature within a time step is usually lost, and the system energy tends to dissipate more severely as* $\rho_\infty \to 0$*; see Fig. C.2(c).*



(a) U0V0($1.0, 1.0, \rho_\infty^s$)



(b) V0U0($1.0, 1.0, \rho_\infty^s$)



(c) U0V0/V0U0($\rho_\infty, 1.0, \rho_\infty$)

Figure C.2: Total Energy History for the Linear System

C.4 Numerical Examples

In this section, we provide two numerical examples to demonstrate the proposed approach (see Fig. C.1). The results are compared with benchmark solutions, which are obtained by solving the original systems with a reasonably small time step size. The approach begins with solving for POD snapshots. A relatively large time step size is used as cheaper computation is desired. Displacement-, velocity- and acceleration-based snapshots are obtained and used to generate reduced systems. The reduced systems are solved using non-dissipative schemes with the same time step size as the one used in the benchmark solution. The results of different output field based POD methods are compared with the benchmark solution in terms of errors and energy conservation.

Example C.4.1 (Clamped Bar)

Our first example is a clamped bar system with prescribed load/boundary conditions as shown in Fig. C.3. The length and cross-sectional area of the bar are 90 *m and* 1 *m*^{2}*, respectively. The material of the bar is assumed to be homogeneous and isotropic; and the density and Young's modulus are selected as* $\rho = 8000$ *kg/m*^{3} *and* $E = 30 \times 10^6$ *N/m*^{2}*, respectively. The total number of elements used for the analysis is* 30*; and constant external force* $f = 10$ *N is applied at node* 5 *with given initial velocity* $\dot{q}_5(0) =$ 10 *m/sec at the same node. The numerical solutions at node* 5 *and system energy responses for* $\mathbb{I} = [0, 1\,\text{sec}]$ *with the POD rank of only* 7 *are shown below. Fig. C.4-Fig. C.6 compare the numerical results based on the displacement-, velocity-, and acceleration-based POD for the same* ρ_∞ *values; and Fig. C.7-Fig. C.9 compare the numerical results for different* ρ_∞ *values for the same POD approaches.*

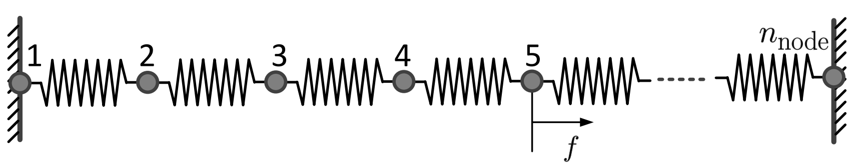
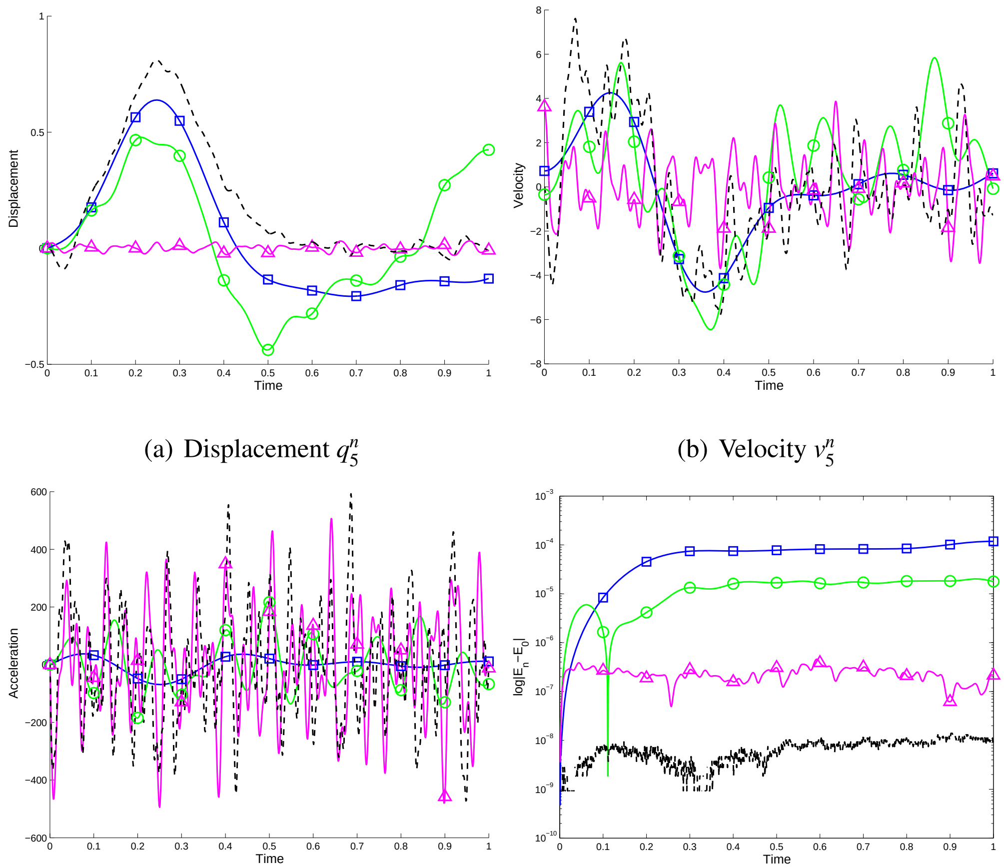


Figure C.3: Problem Illustration of Example C.4.1



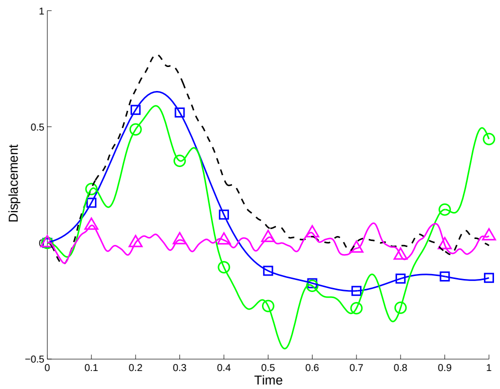
(a) Displacement q_5^n

(b) Velocity v_5^n

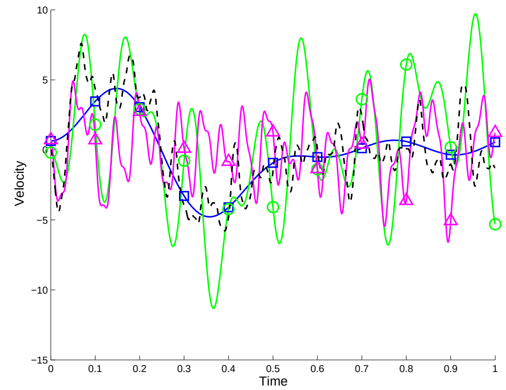
(c) Acceleration a_5^n

(d) Total Energy

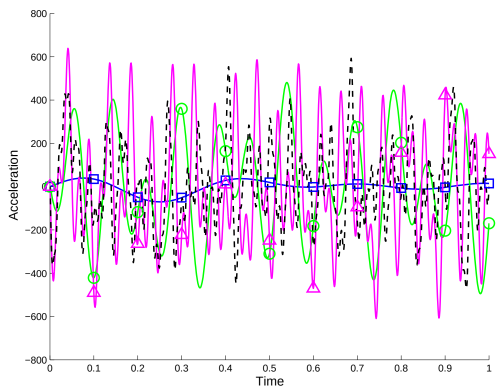
Figure C.4: Comparisons of the Displacement-based (□), Velocity-based (◯), and Acceleration-based (△) POD Methods: U0/V0(0.9,1,0.9) → V0(1,1,0)



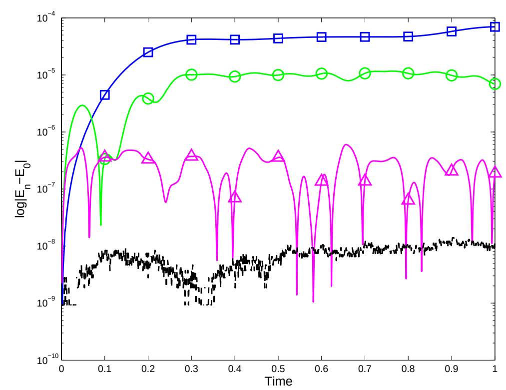
(a) Displacement q_5^n



(b) Velocity v_5^n

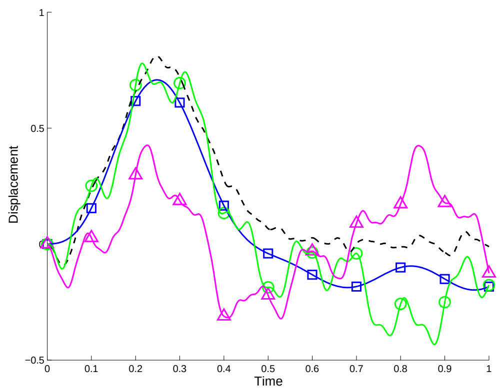


(c) Acceleration a_5^n

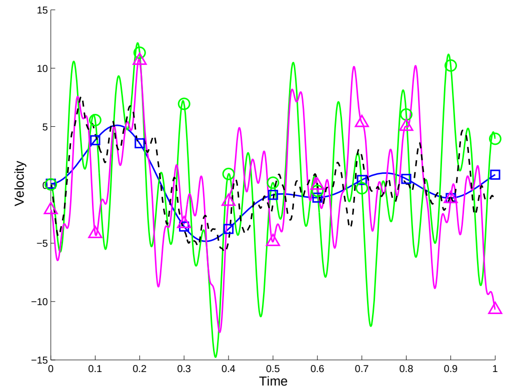


(d) Total Energy

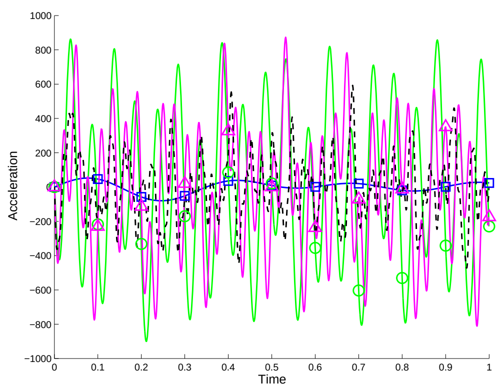
Figure C.5: Comparisons of the Displacement-based (□), Velocity-based (◯), and Acceleration-based (△) POD Methods: U0/V0(0.5,1,0.5) → V0(1,1,0)



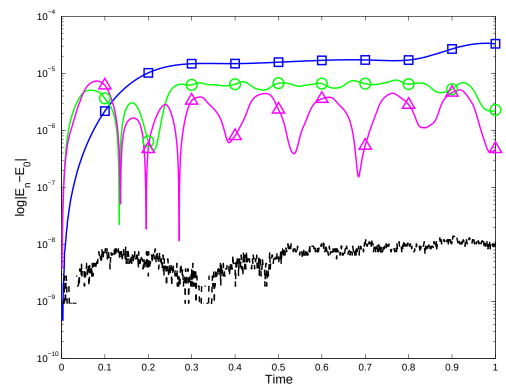
(a) Displacement q_5^n



(b) Velocity v_5^n

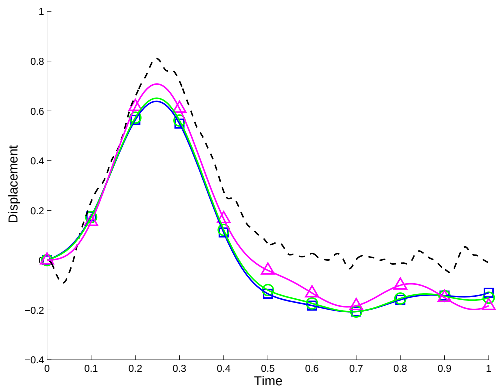


(c) Acceleration a_5^n

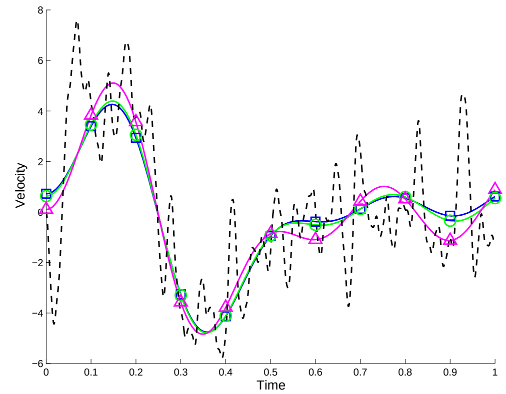


(d) Total Energy

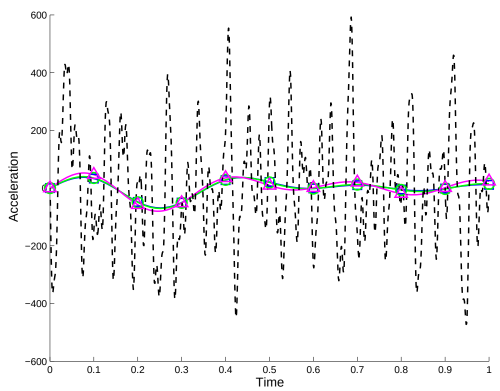
Figure C.6: Comparisons of the Displacement-based (□), Velocity-based (◯), and Acceleration-based (△) POD Methods: U0/V0(0.0,1.0,0.0) → V0(1,1,0)



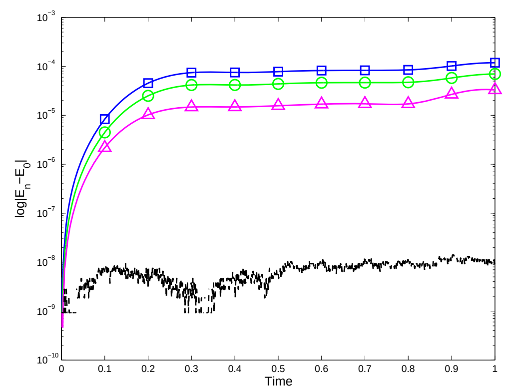
(a) Displacement q_5^n



(b) Velocity v_5^n

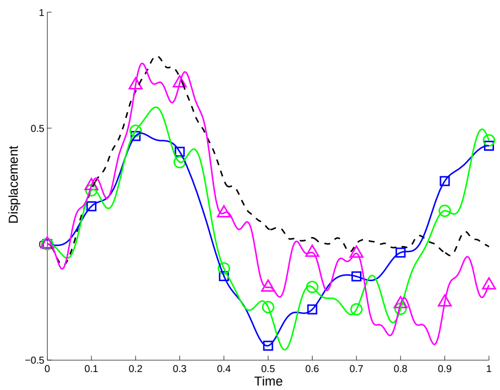


(c) Acceleration a_5^n

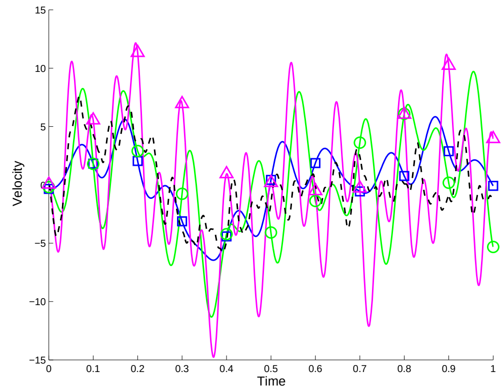


(d) Total Energy

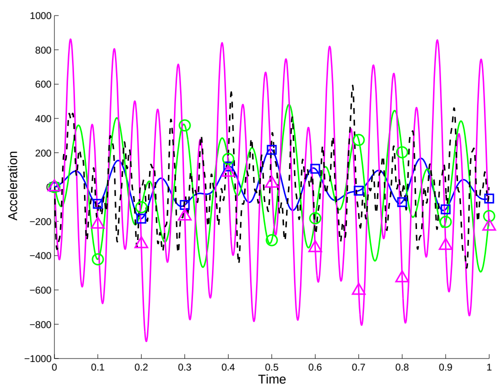
Figure C.7: Comparisons of Various ρ_∞ with the Displacement-based POD method: U0/V0(ρ_∞,1,ρ_∞) with $\rho_\infty = 0.9$ (□), $\rho_\infty = 0.5$ (◯), and $\rho_\infty = 0.0$ (△) → V0(1,1,0)



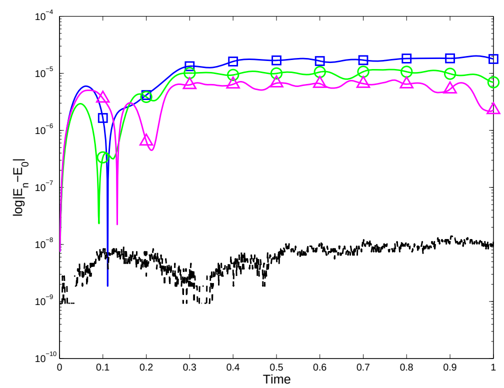
(a) Displacement q_5^n



(b) Velocity v_5^n

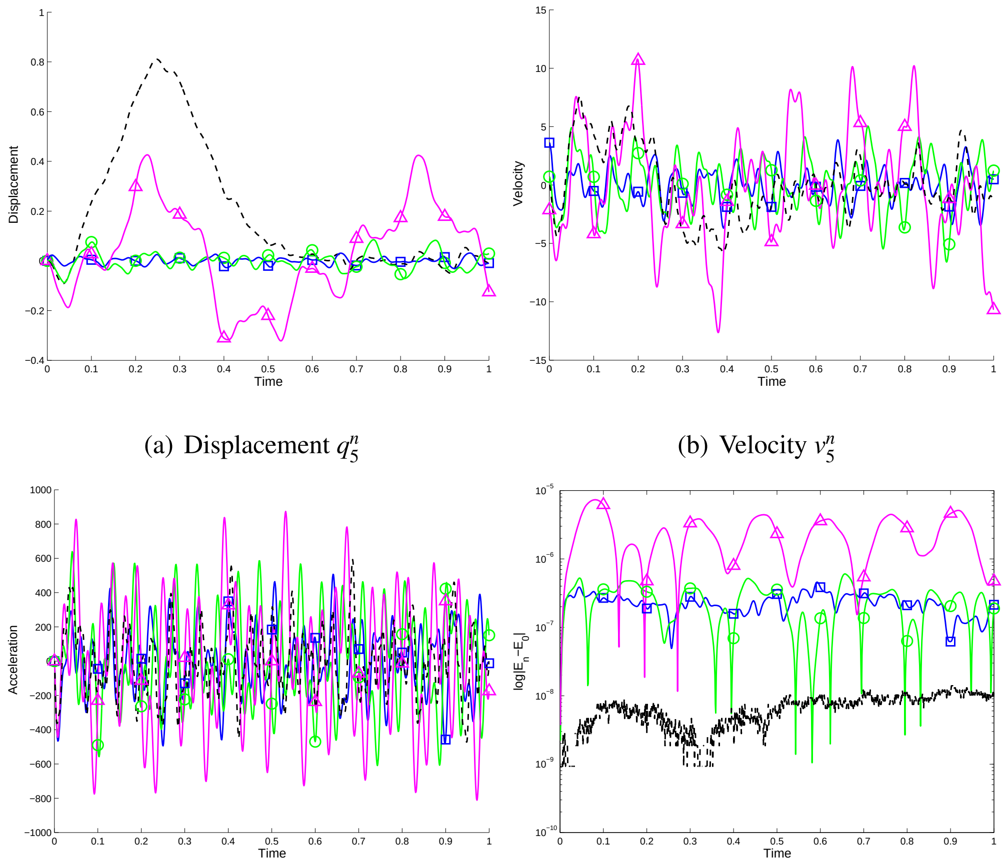


(c) Acceleration a_5^n



(d) Total Energy

Figure C.8: Comparisons of Various ρ_∞ with the Velocity-based POD Method: U0/V0(ρ_∞,1,ρ_∞) with $\rho_\infty = 0.9$ (□), $\rho_\infty = 0.5$ (◯), and $\rho_\infty = 0.0$ (△) → V0(1,1,0)



(a) Displacement q_5^n (b) Velocity v_5^n

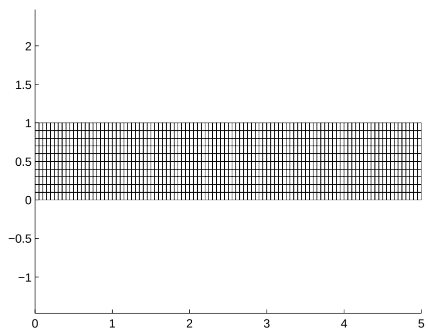
(c) Acceleration a_5^n (d) Total Energy

Figure C.9: Comparisons of Various ρ_∞ with the Acceleration-based POD Method: U0/V0(ρ_∞,1,ρ_∞) with $\rho_\infty = 0.9$ (□), $\rho_\infty = 0.5$ (◯), and $\rho_\infty = 0.0$ (△) → V0(1,1,0)

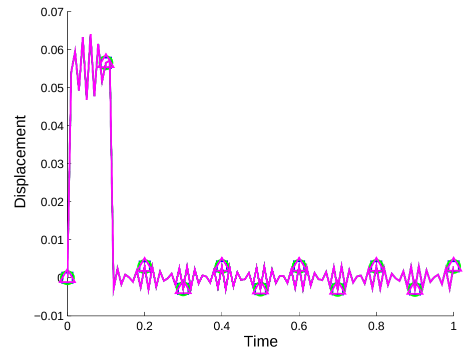
Example C.4.2 (Plate under Tangential Load)

The second example is a thin plate under a tangential load. The plate is 5 *m in length and* 1 *m in width. Tangential load* 1×10^6 N/m^2 *is applied at one end in the tangential direction, while the other end is fully constrained. A quadrilateral element with* 4 *nodes is used to mesh the geometry. The generated mesh has* 1,000 *elements, i.e., 1,111 nodes in total; see Fig. C.10-(a) for the initial undeformed configuration. Young's modulus, Poisson's ratio, and density used are* $E = 1 \times 10^8$ *psi,* $\nu = 0.3$*, and* $\rho = 1$

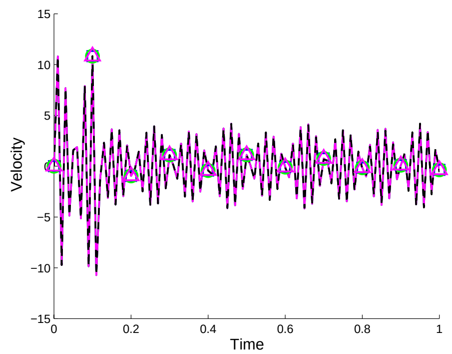
kg/m^3, respectively; and the plane stress assumption is employed. The simulation time is 1 sec: $\mathbb{I} = [0, 1 \text{ sec}]$. The time step size used for the original simulation *without* the POD reduction is $(\Delta t)_\mathrm{b} = (\Delta t_n)_\mathrm{b} = 0.01$ sec. For the simulation *with* the POD reduction, $(\Delta t)_\mathrm{s} = (\Delta t_n)_\mathrm{s} = 0.05$ sec and $(\Delta t)_\mathrm{r} = (\Delta t_n)_\mathrm{r} = 0.01$ sec have been used for the snapshot generation with three different optimal schemes, i.e., U0V0/V0U0(1,1,1), U0V0/V0U0(0.5,1,0.5), and U0V0/V0U0(0,1,0) algorithms, and for the updating the reduced-order model with the V0(1,1,0) algorithm, respectively. Fig. C.10 shows the numerical results for this problem with POD basis of rank 3. Fig. C.10-(b), (c), and (d) show the time histories of the displacement, velocity, and acceleration of node 50. Fig. C.10-(d) and (e) show the total energy difference of the system. As can be seen from the figures, the numerical solutions with and without the POD reduction with POD of only rank 3 show very small differences for any ρ_∞ for this example problem. And the error in the system energy remains in the same order regardless of ρ_∞.



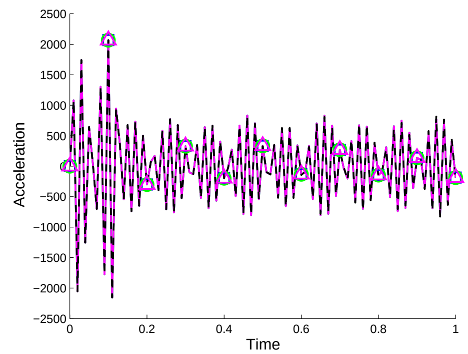
(a) Description



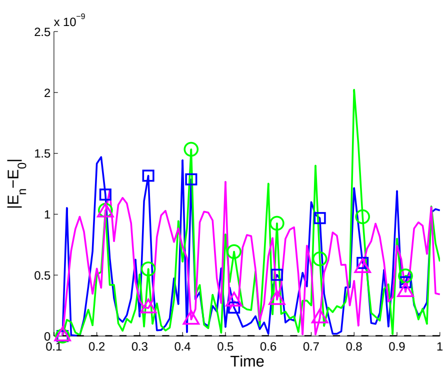
(b) Displacement



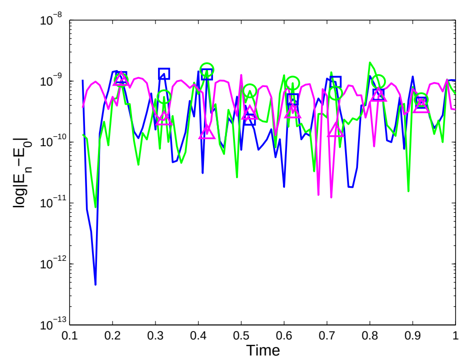
(c) Velocity



(d) Acceleration



(e) Energy Difference



(f) Energy Difference (LOG)

Figure C.10: Comparisons of Various ρ_∞ with the Displacement-based POD Method: U0V0/V0U0(ρ_∞,1.0,ρ_∞) with ρ_∞ = 1.0 (□), ρ_∞ = 0.5 (◯), and ρ_∞ = 0.0 (△) → V0(1,1,0)