A High-Order Perturbation Approach to Profile Reconstruction. I: Perfectly Conducting Gratings

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Abstract

A new method for the reconstruction of two-dimensional periodic structures from scattered far-field data is presented. The approach is based on the recently developed “Methods of Variation of Boundaries” (MVB) for the solution of forward scattering problems. Here, the inverse problem is formulated as that of minimization of an appropriate nonlinear least-squares cost functional. The analytic continuation ideas inherent to MVB are then advanced to enable a *global* line search at each step of a proposed conjugate gradients algorithm. Through a number of numerical examples it is demonstrated that such globalization may be necessary to overcome the nonconvexity of the cost which, in turn, is shown to persist even when the global minimizer is known to be unique.

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1 Introduction

The *forward problem* of calculating the electromagnetic or acoustic scattering produced by obstacles and interfaces is one of central importance in science and engineering. As such, a substantial amount of effort has been devoted in the last century to treating a variety of instances of this challenging mathematical problem. A great deal of the motivating applications (in areas ranging from optical design to radar and tomography) however, are associated with the solution of *inverse problems* and, particularly, with that of determining the nature of a body or interface (shape, location, constitutive characteristics, etc) from knowledge of its scattered field.

A number of numerical methods have been developed to deal with the difficulties associated with the nonlinear and ill-posed character of the inverse scattering problem, see e.g. [9] and the references cited there. Interestingly, all of these methods use integral equations and/or Green's formulas, and almost all involve the iterative minimization of a cost functional. In this paper we present a new method for the solution of such inverse problems, which is based on the recent development of stable, efficient and accurate high order perturbation methods, the “Methods of Variation of Boundaries” (MVB), for finding the scattering produced in bounded or unbounded configurations [5, 6, 7]. In particular, the very nature of this approach allows us to avoid the use of integral equations and, therefore, that of inexact quadrature rules. Moreover, although we shall restrict our attention here to the simplest case of two-dimensional perfectly conducting gratings, the extension of the algorithms to the cases of finite conductivity, bounded obstacles and, more importantly, fully three-dimensional geometries has been demonstrated to yield results of a quality comparable to that achieved in the case under consideration [7, 8].

Besides constituting a good starting point for the testing of our inverse solvers, the problem of reconstruction and synthesis of periodically modulated interfaces (crystal lattices, diffraction gratings, etc), is indeed one of the highest interest in modern optics. We refer the reader to the works [4, 15, 16, 17, 19] for examples of application, and to [1, 10, 11, 13, 20, 21, 22, 23, 24, 25, 26], for alternative numerical solutions to inverse problems within this context. Uniqueness for the problem of reconstruction of periodic structures from far-field data corresponding to a *finite* number of incident plane waves at distinct wavelengths was recently established in [12].

As we said, our approach will be based on MVB which, together with some issues relating to their numerical implementations, we briefly review in §2. In §3 we show how the analytic continuation ideas inherent to MVB can be used to perform *global* searches on *any* line in the space of admissible profiles. Indeed, we present an algorithm whereby the evaluation

of the field scattered by points on such a line is obtained through an appropriate analytic extension of the fields corresponding to dilations (in function space) of the *whole line*. As in the case of the original MVB, these dilations allow us to resort to the *Rayleigh hypothesis* to calculate the Taylor series of the diffracted amplitudes. Existing results on the analytic dependence of the fields on the dilation and line parameters then guarantee the possibility of continuation via Padé approximation.

As our numerical examples clearly show (see §5), the “cost landscape” of the (nonlinear) least-squares functional associated with the inverse problem presents rather pronounced non-convexities. Interestingly, we find that this remains true even when the global minimizer is known to be unique [12]. Moreover, the ill-posedness of the problem also manifests itself in the form of large flat zones in the cost surface. These characteristics then suggest that a “global” search procedure may be needed to effectively find a true minimizer. In this regard, the results in §3 open the possibility of globalization through inspection along lines and towards this end we introduce, in §4, a *conjugate gradients* algorithm based on analytic continuation. The choice of the conjugate gradients as search directions, while not the only possible one, is certainly appropriate if the flat zones contain unique minima. Moreover, the explicit dependence of the continuation formulas upon the interface profiles makes them amenable to exact gradient computations via the “multiplier technique” (see §4). Finally, in §5 we present some numerical examples which have been chosen simply to demonstrate the advantages of the extended line search. The development of a truly global algorithm where observed nonconvexity along lines is used to guide the minimization will be left for future work.

2 The Method of Variation of Boundaries

In [5] a new method was introduced for the solution of scattering problems. Based on variations of the boundaries of the scatterers and analytic continuation, this new perturbative approach led to algorithms which are applicable to a wide variety of scattering configurations. In [6] the method, which will be referred to as the “Method of Variation of Boundaries” (MVB), was applied to the study of diffraction gratings, where it was observed to yield predictions of substantially better quality than those given by classical approaches.

To introduce the MVB, let us denote by L a differential operator corresponding to the Helmholtz’ or Maxwell’s equations and let us consider a scattering problem of the form

$$\begin{aligned} L(u)(\vec{x}) &= f(\vec{x}) \quad \text{outside } \Omega_1 \\ u(\vec{x}) &= g(\vec{x}) \quad x \in \partial\Omega_1, \end{aligned}$$

where Ω_1 is the region occupied by either an obstacle or an infinite grating. The MVB is a method of solution of problems of this type, which is based on viewing Ω_1 as a perturbation of a simpler domain Ω_0 , *for which explicit solutions of the scattering problem are available*. More precisely, we begin by considering domains Ω_δ , $0 \leq \delta \leq 1$, which coincide with Ω_0 and Ω_1 for $\delta = 0$ and $\delta = 1$ respectively, and which depend analytically on the parameter δ . We know [5] that the solution $u(\vec{x}; \delta)$ corresponding to Ω_δ as well as its boundary values depend analytically on the parameter δ . By differentiation of the equations and boundary conditions with respect to δ at $\delta = 0$, we then obtain a sequence of diffraction problems for the δ -derivatives of the field u in the domain Ω_0 . Since the problem with obstacle Ω_0 admits explicit solutions, closed form expressions for *all* these δ -derivatives can be calculated recursively and, therefore, the complete Taylor series of the fields can be found. The fields u themselves are then obtained by means of appropriate *analytic continuation* mechanisms in the variable δ , which allow for the summation of the series beyond its radius of convergence [6]. In short, the MVB reduces the full problem for the given scatterer Ω_1 to a sequence of scattering problems with obstacle Ω_0 , for which solutions can be obtained in closed form.

In the case of a two-dimensional perfectly conducting grating described by a profile function $z = f(x)$ of period d , in TE (Transverse Electric) polarization, the domain Ω_1 is the region $z < f(x)$ and Ω_δ can be taken to be

$$\{(x, y, z) : z < \delta f(x)\}$$

so that, Ω_0 coincides with the half space $\{z \leq 0\}$. It is easy to see that the periodicity of the structure implies that, for a monochromatic incident wave

$$u^{in}(x, z) = e^{i\alpha x - i\beta z}, \quad (k^2 = \alpha^2 + \beta^2)$$

the scattered field $u(\cdot; \delta)$ corresponding to the domain Ω_δ admits the Rayleigh expansion

$$u(x, z; \delta) = \sum_{r=-\infty}^{\infty} B_r(\delta) e^{i\alpha_r x + i\beta_r z}, \quad (\alpha_r = \alpha + \frac{2\pi r}{d}, \quad k^2 = \beta_r^2 + \alpha_r^2). \quad (1)$$

As it follows from the work in [5], the Rayleigh amplitudes $B_r(\delta)$ possess convergent Taylor expansions

$$B_r(\delta) = \sum_{n=0}^{\infty} d_{n,r} \delta^n. \quad (2)$$

Moreover, using (1) and (2) we may rewrite the boundary condition

$$u(x, \delta f(x); \delta) = -u^{in}(x, \delta f(x)) = -e^{i\alpha x - i\beta \delta f(x)}$$

in the form

$$\sum_{r=-\infty}^{\infty} \left(\sum_{n=0}^{\infty} d_{n,r} \delta^n \right) e^{i\alpha_r x + i\beta_r \delta f(x)} = e^{i\alpha x - i\beta \delta f(x)} \quad (3)$$

According to the theory developed in [5] equation (3) holds for small values of δ (*Rayleigh hypothesis*) and is, in fact, *analytic* in δ at $\delta = 0$. Therefore, (3) may be used to solve for the coefficients $d_{n,r}$, by expanding in powers of δ (i.e. by successive differentiation at $\delta = 0$). In the case of Fourier gratings,

$$f(x) = \sum_{r=-F}^F C_{1,r} e^{i2\pi r x/d}, \quad (4)$$

and letting $C_{n,r}$ denote the r -th Fourier coefficient of the n -th power of f

$$\frac{1}{n!} f(x)^n = \sum_{r=-nF}^{nF} C_{n,r} e^{i2\pi r x/d}, \quad (5)$$

it follows that

$$d_{n,r} = -(-i\beta)^n C_{n,r} - \sum_{k=0}^{n-1} \sum_{q=\max(-kF, r-(n-k)F)}^{\min(kF, r+(n-k)F)} C_{n-k, r-q} (i\beta_q)^{n-k} d_{k,q}, \quad -nF \leq r \leq nF, \quad (\text{see [6]}). \quad (6)$$

A number of implementations of this method can be given, and a variety of numerical issues need to be considered. One of the most important of these issues is involved in the last step of the procedure: the approximation (analytic continuation) of the scattered fields from its Taylor series at a point. Among the methods of approximation that have been considered, Padé approximation (i.e. approximation based on rational functions [2]) appears to be the best suited for the problems under consideration [6]. Thus, we shall view Padé approximation as an integral part of our algorithms.

3 Global line evaluations

As we stated in the Introduction, to solve the reconstruction problem we shall ultimately resort to a gradient method for the minimization of an appropriate cost functional. In this section we show how analytic continuation can be used to find the scattering produced by a *whole line*

$$f(x) + tg(x), \quad t \in \mathbb{R},$$

of Fourier gratings. Within the context of a gradient-based algorithm, the roles of f and g will, of course, be taken by the current iterate and the search direction, respectively.

Let $B_r(t)$ denote the Rayleigh amplitudes corresponding to the profile $f(x) + tg(x)$, i.e.

$$u(x, z; t) = \sum_{r=-\infty}^{\infty} B_r(t) e^{i\alpha_r x + i\beta_r z}$$

where $u(\cdot; t)$ is the field scattered by that grating. Again here, it follows from [5] that $B_r(t)$ can be represented by a power series

$$B_r(t) = \sum_{j=0}^{\infty} a_r^j t^j \quad (7)$$

which converges near $t = 0$ and, moreover, the functions $B_r(t)$ are complex analytic in a neighborhood of the real line in the complex t -plane. However, the boundary condition

$$u(x, f(x) + tg(x); t) = -u^{in}(x, f(x) + tg(x)) = -e^{i\alpha x - i\beta(f(x) + tg(x))}$$

cannot, in general, be used directly to evaluate the coefficients a_r^j , as the Rayleigh hypothesis (cf. (3)) *will not* hold unless f is sufficiently shallow [18]. The properties of analyticity of the fields [5], on the other hand, allow for the evaluation of the amplitudes $B_r(t)$ by analytic continuation. Indeed, the condition at the surface of the conductor *can* be used to evaluate the entire Taylor series, in δ at $\delta = 0$, of the Rayleigh coefficients $B_r(t, \delta)$ corresponding to the family of gratings

$$\delta(f(x) + tg(x)), \quad t, \delta \in \mathbb{R}.$$

If we let

$$B_r(t, \delta) = \sum_{n=0}^{\infty} d_{n,r}(t) \delta^n \quad (8)$$

then, from (6), we have

$$d_{n,r}(t) = -(-i\beta)^n C_{n,r}(t) - \sum_{k=0}^{n-1} \sum_{q=\max(-kF, r-(n-k)F)}^{\min(kF, r+(n-k)F)} C_{n-k, r-q}(t) (i\beta_q)^{n-k} d_{k,q}(t), \quad -nF \leq r \leq nF, \quad (9)$$

where $C_{n,r}(t)$ is the r -th Fourier coefficient of the n -th power of $f(x) + tg(x)$. Equating like powers of t in (9) we arrive at the *recursive relations*

$$\begin{aligned} d_{n,r}^j &= -(-i\beta)^n C_{n,r}^j \\ &- \sum_{k=0}^{n-1} \sum_{q=\max(-kF, r-(n-k)F)}^{\min(kF, r+(n-k)F)} \sum_{m=0}^j C_{n-k, r-q}^{j-m} (i\beta_q)^{n-k} d_{k,q}^m, \quad -nF \leq r \leq nF, \quad 0 \leq j \leq n \end{aligned} \quad (10)$$

where

$$d_{n,r}(t) = \sum_{j=0}^n d_{n,r}^j t^j \quad (11)$$

and

$$C_{n,r}(t) = \sum_{j=0}^n C_{n,r}^j t^j.$$

Combining (7), (8) and (11) we get

$$a_r^j = \left(\sum_{n=0}^{\infty} d_{n,r}^j \delta^n \right) \Big|_{\delta=1}$$

which can then be evaluated by appropriate analytic continuation in δ , via, for instance, Padé approximation. Finally, continuation in t permits us to *globally* evaluate the functions $B_r(t)$ in (7). The whole problem is therefore reduced to that of evaluating the recursion (10). For the purpose of its numerical implementation, we note here that the equations (10) can be written in the form

$$d_{n,r}^j = -(-i\beta)^n C_{n,r}^j - \sum_{k=0}^{n-1} \left(C_{n-k} * D_k^{(n)} \right)_r^j \quad (12)$$

where $*$ denotes a two-dimensional (discrete) convolution operator, that is,

$$(A * B)_r^j = \sum_q \sum_m A_{j-m, r-q} B_{m,q}$$

and the matrices C_{n-k} and $D_k^{(n)}$ are defined by

$$(C_{n-k})_{m,q} = C_{n-k,q}^m \quad \text{and} \quad \left(D_k^{(n)} \right)_{m,q} = (i\beta_q)^{n-k} d_{k,q}^m.$$

4 The inverse problem

We consider the inverse problem of reconstructing a two-dimensional perfectly conducting grating f from knowledge of multiple-wavelength scattered data. We assume that, for each incident wave, we can measure the diffracted *efficiencies*

$$e_r^0 = \frac{\beta_r}{\beta} |B_r^0|^2 \quad (r \in U) \quad (13)$$

where U denotes the (finite) set of orders corresponding to non-evanescent (propagating) modes, i.e. $U = \{r : \beta_r \geq 0\}$ [6]. For the sake of clarity, we shall present the formulation and algorithm for the case of a single incident frequency; the generalization to any finite number of incident waves follows by straightforward superposition of the corresponding costs.

4.1 Formulation

We formulate the inverse problem as a nonlinear least-squares one in which we seek to estimate a profile f that minimizes a Tikhonov functional of the form

$$J(d(f), f) = \sum_{r \in U} w_r |e_r(d(f)) - e_r^0|^2 + \gamma \|f\|^2 \quad (w_r > 0, \gamma \geq 0) \quad (14)$$

where $d = d(f) = (d_{n,s}(f))_{0 \leq n \leq N, -NF \leq s \leq NF}$ and e_r is the r -th order efficiency (cf. (13)) corresponding to a given grating profile f . In order to minimize J , we first write the recursive formulae (6) in the form of a matrix equation

$$A(C)d = b(C) \quad (15)$$

where $C = (C_{n,r})_{0 \leq n \leq N, -NF \leq r \leq NF}$ is related to the profile f through (4) and (5), and the matrices $A(C)$ and $b(C)$ (which depend on the incidence and wavelength of radiation) are given by

$$A(C)_{nr,kq} = (i\beta_q)^{n-k} C_{n-k,q-r} \quad \text{and} \quad b(C)_{nr} = -(-ik)^{n-k} C_{n,r}.$$

As discussed in §2, once (15) has been solved, analytic continuation to the actual height of the profile can be achieved via Padé approximation, that is

$$B_r(d(C)) = \mathcal{P}_N(d_r)$$

where $d_r = (d_{n,r}(C))_{0 \leq n \leq N}$ and the operator $\mathcal{P}_N$ can be taken, for instance, as the $[\frac{N-1}{2}/\frac{N-1}{2}]$ Padé approximant to $\sum d_{n,r} \delta^n$ evaluated at $\delta = 1$

$$\mathcal{P}_N(d_r) = \frac{p_0^r + p_1^r + \cdots + p_L^r}{1 + q_1^r + \cdots + q_L^r} \equiv \frac{\langle 1, p^r \rangle}{\langle 1, q^r \rangle}, \quad \text{with } L = \frac{N-1}{2}.$$

From the general theory of Padé approximants [2] we know that the coefficients of the numerator $p^r = p^r(d(C)) = [p_0^r, p_1^r, \cdots, p_L^r]^T$ and denominator $q^r = q^r(d(C)) = [q_1^r, q_2^r, \cdots, q_L^r]^T$ satisfy equations of the form

$$\begin{aligned} \mathcal{D}(d_r) q^r &= \mathcal{R}(d_r) \\ p^r &= \mathcal{N}(d_r) \begin{bmatrix} 1 \\ q^r \end{bmatrix} \end{aligned}$$

for matrices $\mathcal{D}(d_r)$, $\mathcal{N}(d_r)$ and $\mathcal{R}(d_r)$ defined by

$$\mathcal{D}(d_r) = \begin{bmatrix} d_{L,r} & d_{L-1,r} & \cdots & d_{1,r} \\ d_{L+1,r} & d_{L,r} & \cdots & d_{2,r} \\ \vdots & \vdots & \ddots & \vdots \\ d_{2L-1,r} & d_{2L-2,r} & \cdots & d_{L,r} \end{bmatrix}, \quad \mathcal{R}(d_r) = - \begin{bmatrix} d_{L+1,r} \\ d_{L+2,r} \\ \vdots \\ d_{2L,r} \end{bmatrix}$$

and

$$\mathcal{N}(d_r) = \begin{bmatrix} d_{0,r} & 0 & \cdots & 0 \\ d_{1,r} & d_{0,r} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ d_{L,r} & d_{L-1,r} & \cdots & d_{0,r} \end{bmatrix};$$

see [6]. Our formulation of the inverse problem can then be recast as that of finding

$$\min \left\{ J(q, p, C) = \sum_{r \in U} w_r \left| \frac{\beta_r}{\beta} \left| \frac{\langle 1, p^r \rangle}{\langle 1, q^r \rangle} \right|^2 - e_r^0 \right|^2 + \gamma \sum_{r=-F}^F (r |C_{1,r}|)^2 : \right. \\ \left. q^r \in \mathbb{C}^L, p^r \in \mathbb{C}^{L+1}, C \in \mathbb{C}^{N \times NF} \right\} \quad (16)$$

subject to the constraints

$$0 = \mathcal{B}(d, q, p, C) = \begin{bmatrix} A(C)d - b(C) \\ (\mathcal{D}(d_r)q^r - \mathcal{R}(d_r))_{r \in U} \\ (p^r - \mathcal{N}(d_r) \begin{bmatrix} 1 \\ q^r \end{bmatrix})_{r \in U} \end{bmatrix} \in \mathbb{C}^{P+KL+K(L+1)} \quad (17)$$

where $P = N \times NF$, $2L + 1 = N$ and $K = \#U$, with an additional summation over frequencies in the case of multi-wavelength data.

4.2 A conjugate gradients algorithm with global line search

Our approach to the reconstruction problem takes advantage of the above formulation, (16)–(17), and it utilizes a conjugate gradients method [3] for the constrained minimization of the functional $J(q, p, C)$. In order to avoid unnecessary uses of the direct solver, the gradient computations will be performed using the *adjoint method*, see [3, 14] and the references therein. To this end, we introduce the multipliers

$$\lambda \in \mathbb{C}^P \ (P = N \times NF), \ \mu = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_K \end{bmatrix} \in \mathbb{C}^{KL} \text{ and } \eta = \begin{bmatrix} \eta_1 \\ \eta_2 \\ \vdots \\ \eta_K \end{bmatrix} \in \mathbb{C}^{K(L+1)} \ (2L + 1 = N),$$

and we define the *Lagrangian* $\mathcal{L} = \mathcal{L}(d, q, p, \lambda, \mu, \eta, C)$ by

$$\mathcal{L} = J(q, p, C) - \Lambda^T \mathcal{B}(d, q, p, C)$$

where

$$\Lambda = \begin{bmatrix} \lambda \\ \mu \\ \eta \end{bmatrix} \in \mathbb{C}^{P+KL+K(L+1)}.$$

Then, a simple calculation [3] shows that,

$$\text{if } \mathcal{B}(d(C), q(C), p(C), C) = 0 \text{ and } \mathcal{B}(d(C^0), q(C^0), p(C^0), C^0) \equiv \mathcal{B}(d^0, q^0, p^0, C^0) = 0$$

and Λ^0 solves

$$\begin{bmatrix} \nabla_d \mathcal{B} \\ \nabla_q \mathcal{B} \\ \nabla_p \mathcal{B} \end{bmatrix}_{(d^0, q^0, p^0, C^0)} \Lambda^0 = \begin{bmatrix} 0 \\ \nabla_q J \\ \nabla_p J \end{bmatrix}_{(d^0, q^0, p^0, C^0)} \quad (\text{“adjoint equations”}), \quad (18)$$

then the gradient of J along the constraint manifold satisfies

$$\begin{aligned} \frac{d}{dC} J(d(C), q(C), p(C), C) \Big|_{C=C^0} &= \nabla_C \mathcal{L}(d^0, q^0, p^0, \Lambda^0, C) \Big|_{C=C^0} \\ &= \nabla_C J(q^0, p^0, C) \Big|_{C=C^0} - (\Lambda^0)^T \nabla_C \mathcal{B}(d^0, q^0, p^0, C) \Big|_{C=C^0}. \end{aligned} \quad (19)$$

Thus, the gradient computations can be performed by solving the adjoint equations (18) to evaluate (19). Note that (18) can be written as

$$\begin{bmatrix} A(C) & (\nabla_{d_r} \mathcal{D}(d_r) q^r - \nabla_{d_r} \mathcal{R}(d_r))_{r \in U} & (\nabla_{d_r} \mathcal{N}(d_r) \begin{bmatrix} 1 \\ q^r \end{bmatrix})_{r \in U} \\ 0 & (\mathcal{D}(d_r))_{r \in U} & (\mathcal{N}(d_r))_{r \in U} \\ 0 & 0 & I \end{bmatrix}_{(d^0, q^0, p^0, C^0)} \begin{bmatrix} \lambda^0 \\ \mu^0 \\ \eta^0 \end{bmatrix} = \begin{bmatrix} 0 \\ \nabla_q J \\ \nabla_p J \end{bmatrix}_{(d^0, q^0, p^0, C^0)}$$

which can be solved by “back-substitution” [3].

5 Numerical examples

For our numerical experiments we implemented a conjugate gradients method with (local) quadratic approximations for the line search [3] to compare with the proposed global search through Padé approximation. In the examples that follow we sought to reconstruct the profile

$$f^{\text{target}}(x) = 0.045\pi (\cos(x) + \cos(2x) + \cos(3x))$$

(see Figure 1) in a variety of circumstances of multi-frequency scattered far-field (i.e. efficiency) data. The set of admissible profiles was taken to coincide with the six-dimensional family of Fourier gratings with 3 modes (i.e. $F = 3$ in (4)) and vanishing mean value.

First, we considered the minimization of the cost functional associated with data for 7 frequencies corresponding to wavelength-to-period ratios of

$$0.44, 0.49, 0.54, 0.59, 0.64, 0.69, \text{ and } 0.74. \quad (20)$$

Figure 1: Target profile for the reconstruction from scattered far-field data.

For this case we have successively plotted, in Figure 2, the iterates corresponding to the algorithm with quadratic model for the line search when the initial profile is taken to be

$$f^{\text{initial}}(x) = 0.01 \cos(x) + 0.10 \cos(3x). \quad (21)$$

As is clear from the Figure, this “initial guess” produces a series of iterates that converge to a *local minimum* of the cost functional located at

$$f^{\text{min}}(x) = -0.114 \cos(x) - 0.120 \cos(2x) + 0.634 \cos(3x). \quad (22)$$

Figure 3, on the other hand, shows that if the line search is performed with a $[5/5]$ Padé model, the presence of the global minimizer can be detected from the initial function (21). In this regard, it is interesting to observe the shape of the cost functional along the iterated directions, as shown in Figure 4. Note the overall non-convexity and, in particular, the “bistable” character clearly displayed in the first frame.

A cross-section of the graph of the cost functional in parameter space is included in Figure 5, left. The graph on the right corresponds to the cost associated with the 15 frequencies with

$$\begin{aligned} \text{wavelength-to-period ratios} = & 0.44, 0.46, 0.49, 0.51, 0.54, 0.56, 0.59, 0.62, 0.64, \\ & 0.67, 0.69, 0.71, 0.74, 0.77 \text{ and } 0.79. \end{aligned} \quad (23)$$

In both cases we have plotted the cost, normalized by the number of frequencies, corresponding to functions of the form

$$A_1 \cos(x) + A_1 \cos(2x) + A_2 \cos(3x). \quad (24)$$

This particular choice was simply taken so as to include, in a three-dimensional graph, both the target and local minimum (22) which is approximately of this form. As a result, these graphs present pronounced non-convexities. Moreover, the shape of the graph remains virtually unchanged with the additional data even when, as in this case, the reconstruction problem is known to possess a unique solution and, hence, the cost functional presents a unique global minimizer [12].

In the final set of experiments we tested the effect of the addition of *high* frequency data to the first example above. For this, the cost functional was considered for the case of 15 frequencies corresponding to wavelength-to-period ratios of

$$0.15, 0.18, 0.21, 0.24, 0.28, 0.32, 0.36, 0.40, 0.44, 0.49, 0.54, 0.59, 0.64, 0.69 \text{ and } 0.74. \quad (25)$$

Results for the quadratic and Padé models for an initial profile

$$f^{\text{initial}}(x) = -0.10 \cos(x) - 0.10 \cos(2x)$$

are contained in Figures 6–8. In this case, the quadratic model converges to a local minimum at

$$f^{\min} = -0.160 \cos(x) - 0.120 \cos(2x) - 0.132 \cos(3x).$$

Our experiments also show that an additional minimum occurs at

$$f^{\min} = -0.129 \cos(x) - 0.137 \cos(2x) + 0.274.$$

Indeed, this is reflected in the graph of Figure 9 where we have plotted the cost associated with the profiles in (24) for the present case.

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Figure 2: Successive iterates for a conjugate gradients algorithm with *quadratic* model for the line search. In each graph, the solid line corresponds to the current iterate. The dot-dashed and dashed lines represent the initial and target profiles, respectively.

Figure 3: Iterates 1 through 5 of the algorithm with Padé approximation. Dot-dashed: initial; Solid: current; Dashed: target.

Figure 4: Cost along the conjugate directions corresponding to the iterates of Figure 3.

Figure 5: Cross section, along the surface (24), of the graphs of the cost functionals, normalized by the number of frequencies. Left: 7-frequency data, cf. (20); Right: 15-frequency data, cf. (23).

Figure 6: Successive iterates for a conjugate gradients algorithm with *quadratic* model for the line search. Dot-dashed: initial; Solid: current; Dashed: target.

Figure 7: Iterates 1 through 5 of the algorithm with Padé approximation. Dot-dashed: initial; Solid: current; Dashed: target.

Figure 8: Cost along the conjugate directions corresponding to the iterates of Figure 7.

Figure 9: Cross section, along the surface (24), of the graph of the cost functional normalized by the number of frequencies for the case (25).