THE COMBINED USE OF A NONLINEAR CHERNOFF FORMULA WITH A REGULARIZATION PROCEDURE FOR TWO-PHASE STEFAN PROBLEMS

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257	H. Folmer, S. Orey	Large Deviations for the Empirical Field of a Gibbs Measure	258	A. Leizarowitz	Characterization of Optimal Trajectories on an Infinite Horizon
259	Y. Giga, T. Miyakawa, H. Osada	Two Dimensional Navier Stokes Flow with Measures as Initial Vorticity	260	M. Chipot, V. Oliker	Sur une propriete Des Fonctions Propres De l'operateur De Laplace Beltrami
261	V. Perez-Abreu	Decompositions of Semimartingales on Duals of Countably Nuclear Spaces	262	J. M. Ball	Does Rank-One Convexity Imply Quasiconvexity?
263	B. Cockburn	The Quasi-Monotone Schemes for Scalar Conservation Laws. Part 1	264	K. A. Pericak-Spector	On Radially Symmetric Simple Waves in Elasticity
265	P. N. Shivakumar, Chi-Sing Man Simon W. Rabkin	Modelling of the Heart and Pericardium at End-Diastole	266	Jose-Luis Menaldi	Probabilistic View of Estimates for Finite Difference Methods
267	Robert Hardt, Harold Rosenberg	Open Book Structures and Unicity of Minimal Submanifolds	268	Bernardo Cockburn	The Quasi-Monotone Schemes for Scalar Conservation Laws
269	H. R. Jauslin, W. Zimmermann, Jr.	Dynamics of a Model for an Ac Josephson Effect in Superfluid 4He	270	A. K. Kapila	Introductory Lecture on Reacting Flows
271	J. C. Taylor	Do Minimal Solutions of Heat Equations Characterize Diffusions?	272	J. C. Taylor	The Minimal Eigenfunctions Characterize the Ornstein-Uhlenbeck Process
273	Chi-Sing Man, Quan-Xin Sun	On the Significance of Normal Stress Effects in the Flow of Glaciers	274	Omar Hijab	On Partially Observed Control of Markov Processes
275	Lawrence Gray	The Behavior of Processes with Statistical Mechanical Properties	276	R. Hardt, D. Kinderlehrer, M. Luskin	Remarks about the Mathematical Theory
277	Cockburn, B.	The Quasi-Monotone Schemes for Scalar Conservation Laws Part III	278	M. Chipot, T. Sideris	On the Abelian Higgs Model
279	C. Foias, B. Nicolaenko, G.R.Sell, R. Temam	Inertial Manifolds for the Kuramoto-Sivashinsky Equation and an Estimate of their Lowest Dimension	280	R. Duran	On the Approximation of Miscible Displacement in Porous Media by a Method of Characteristics Combined with a Mixed Method
281	H. Aixiang, Zhang Bo	The Convergence for Nodal Expansion Method	282	V. Twersky	Dispersive Bulk Parameters for Coherent Propagation in Correlated Random Distributions
283	W.Th.F. den Hollander	Mixing Properties for Random Walk in Random Scenery	284	H.R. Jauslin	Nondifferentiable Potentials for Nonequilibrium Steady States
285	K. Meyer, G.R.Sell	Homoclinic Orbits and Bernoulli Bundles in Almost Periodic Systems	286	J. Douglas,Jr., Y. Yuan	Finite Difference Methods for the Transient Behavior of a Semiconductor Device
287	Li Kaitai, Yan Ningning	The Extrapolation for Boundary Finite Elements	288	R. Durrett, R.H. Schonmann	Stochastic Growth Models
289	David Kinderlehrer	Remarks about Equilibrium Configurations of Crystals	290	D.G. Aronson, J.L. Vazquez	Eventual C^{∞}-Regularity and Concavity for Flows in One-Dimensional Porous Media
291	L.R. Scott, J.M. Boyle, B. Bagheri	Distributed Data Structures for Scientific Computation	292	J. Douglas,Jr., P.J.Paes Leme, T. Arbogast, T. Schmitt	Simulation of Flow in Naturally Fractured Petroleum Reservoirs
293	D.G. Aronson, L.A. Caffarelli	Optimal Regularity for One-Dimensional Porous Medium Flow	294	Haïm Brezis	Liquid Crystals and Energy Estimates for S^2-Valued Maps
295	Todd Arbogast	Analysis of the Simulation of Single Phase Flow Through a Naturally Fractured Reservoir	296	He Yinnian, Li Kaitai	The Coupling Method of Finite Elements and Boundary Elements for Radiation Problems
297	T. Cazenave, A. Haraux, L. Vazquez, F.B. Weissler	Nonlinear Effects in the Wave Equation with a Cubic Restoring Force	298	M. Chipot, F.B. Weissler	Some Blow Up Results for a Nonlinear Parabolic Parabolic Equation with a Gradient Term
299	Li Kaitai	Perturbation Solutions of Simple and Double Parabolic Equation with a Gradient Term	300	Chen Zhangxin, Li Kaitai	The Convergence on the Multigrid Algorithm for Navier-Stokes Equations
301	A. Gerardi, G. Nappo	Martingale Approach for Modeling DNA Synthesis	302	D.N. Arnold, L. Ridgway Scott, Michael Vogelius	Regular Inversion of the Divergence Operator with Dirichlet Boundary Conditions on a Polygon
303	Duran, Ricardo G.	Error Analysis in L^p, $1 \leq p \leq \infty$, for Mixed Definite Element Methods for Linear and Quasi-Linear Elliptic Problems	304	Nochetto, Ricardo H., Verdi, Claudio	An Efficient Linear Scheme to Approximate Parabolic Free Boundary Problems: Error Estimates and Implementation

THE COMBINED USE OF A NONLINEAR CHERNOFF FORMULA WITH A REGULARIZATION PROCEDURE FOR TWO-PHASE STEFAN PROBLEMS

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ABSTRACT

The approximation of two-phase Stefan problems in 2-D by a nonlinear Chernoff formula combined with a regularization procedure is analyzed. The first technique allows the associated strongly nonlinear parabolic P.D.E. to be approximated by a sequence of linear elliptic problems. In addition, non-degeneracy properties can be properly exploited through the use of a smoothing process. A fully discrete scheme involving piecewise linear and constant finite elements is proposed. Energy error estimates are proven for both physical variables, namely enthalpy and temperature. These rates of convergence improve previous results.

1 - INTRODUCTION

The simplest heat transfer phenomenon involving phase change can be modelled by the following strongly nonlinear parabolic P.D.E.

$$\begin{cases} \dfrac{\partial u}{\partial t} - \Delta\,\beta(u) = 0 & \text{in } Q := \Omega \times \,]0,T[\\ \beta(u) = 0 & \text{on } \partial\Omega \times \,]0,T[\\ u = u_0 & \text{at } t = 0\,. \end{cases} \tag{1.1}$$

Here β is a nondecreasing Lipschitz continuous function, whose graph has a flat part; u denotes enthalpy and $\theta := \beta(u)$ stands for temperature. We refer to Magenes [7] for mathematical details and references. We only would like to emphasize that our present results easily extend to more general situations including a nonlinear source term, nonhomogeneous Dirichlet and/or (linear) Neumann boundary conditions, as well as different functions β (e.g., porous medium equation).

Our main concern is the efficient numerical approximation of (1.1). To this end, we combine a nonlinear Chernoff formula with a smoothing technique. The latter consists of replacing β by a strictly increasing Lipschitz continuous function β_ϵ; $\epsilon > 0$ is the regularization parameter. Perturbing β changes the nature of the problem in that there is no longer free boundary. This is not only a computational trick but also allows non-degeneracy properties to be exploited in improving the final rates of convergence, as shown in Nochetto [10, 12]. In order to use the regularity property $\| \frac{\partial u_\epsilon}{\partial t} \|_{L^2(Q)} \leqslant C\, \epsilon^{-1/2}$, special care is required in defining the initial regularized enthalpy. This issue is fully discussed here and a general recipe in 2-D is presented whenever initial non-degeneracy holds (see section 3.1); this is actually the only 2-D argument in the paper.

Once the problem has been regularized, it can be discretized in time by the following nonlinear Chernoff formula

$$\begin{cases} U^0 := u_0; \quad \text{for } n = 1, \ldots, T/\tau \\ \Theta^n - \frac{\tau}{\mu} \Delta \Theta^n = \beta_\epsilon(U^{n-1}) \\ U^n = U^{n-1} + \mu \left[\Theta^n - \beta_\epsilon(U^{n-1}) \right]; \end{cases} \tag{1.2}$$

here μ stands for a relaxation parameter satisfying $0 < \mu \leqslant L_\beta^{-1}$ ($L_\beta > 0$: Lipschitz constant of β). Nonlinear Chernoff formulae were introduced as approximations to nonlinear semigroups of contractions [2], and first used in numerical analysis in [1, 17]; no error estimates were proven there. The accuracy of such schemes (without regularization) was recently investigated by Magenes, Nochetto & Verdi [9], Magenes [8] and Nochetto & Verdi [15]. A further discretization in space is achieved by making use of continuous piecewise linear finite elements for Θ^n and piecewise constants for U^n, as in [15, 19]. At this stage, the resulting scheme can be easily implemented on a computer. Numerical experiments show that, for two-phase Stefan problems, location of the true free boundary as well as approximation of solutions nearby are more accurate when using a smoothing process as an intermediate step. In other words, the nonlinear Chernoff formula without regularization seems to produce a stronger artificial diffusion [15]. We refer to Paolini, Sacchi & Verdi [16] where performances of various linear and nonlinear algorithms are compared. This computational evidence motivates the present analysis.

In this paper we improve previous rates of convergence proved by Nochetto & Verdi [15] (see Corollary 1). Our new results coincide with those ones obtained for the standard nonlinear scheme by Jerome & Rose [6] and Nochetto [10, 12], who did not consider the effect of numerical integration. The topic was later on analyzed by Elliott [4], Nochetto & Verdi [14] and Verdi [18], but the final rates are worse than the present ones. In addition, whenever non-degeneracy holds, we can further improve the rates of convergence; however the final orders are still sublinear and, therefore, not sharp according to the approximation theory. Moreover, we can obtain an L^2-error estimate for enthalpy (see Corollary 2). A similar but optimal result was proven in [12] for the standard nonlinear scheme.

This paper is organized as follows. In section 2 we state assumptions and notation and formulate continuous and discrete problems. In section 3 we first analyze the choice of the regularized and discrete initial enthalpies and then show a strong stability of the discrete scheme. Finally, in section 4 we demonstrate the main results of this paper, namely, energy error estimates for both enthalpy u and temperature θ.

2 - FORMULATION OF THE PROBLEM

In this section we shall establish the hypotheses concerning the data and formulate precisely the continuous and the regularized problems as well as the nonlinear Chernoff formula.

2.1 - Basic assumptions and notation

Along the work we shall always assume the following hypotheses.

(H_Ω) $\Omega \subset R^2$ is a convex polygon.

Set $Q := \Omega \times]0, T[$, where $0 < T < +\infty$ is fixed.

(H_β) $\beta : R \to R$ is a nondecreasing and Lipschitz continuous function such that

$$\beta(s) := 0 \quad \text{for } 0 \leqslant s \leqslant 1 ,$$

$$0 < l_\beta \leqslant \beta'(s) \leqslant L_\beta < +\infty \qquad \text{for a.e. } s \notin [0,1] .$$

$(\mathbf{H}_{u_0})$ $\theta_0 := \beta(u_0) \in W_0^{1,\infty}(\Omega)$;
$F_0 := \{ x \in \Omega : \theta_0 = 0 \}$ is a Hölder continuous curve;
$\text{meas}(\{ x \in \Omega : 0 \leqslant \theta_0(x) \leqslant \epsilon \}) = O(\epsilon)$ (non-degeneracy property).

Now we introduce some notation concerning the time discretization. Let $\tau := T/N$ be the time step (N positive integer) and set $t^n := n\,\tau$, $I^n :=]t^{n-1}, t^n]$ for $1 \leqslant n \leqslant N$. We also set

$$z^n := z(\cdot, t^n), \quad \overline{z}^n := \frac{1}{\tau} \int_{I^n} z(\cdot, t)\, dt$$

for any function $z : Q \to \boldsymbol{R}$ which is continuous (resp. integrable) in time, and

$$\partial z^n := \frac{z^n - z^{n-1}}{\tau}, \quad 1 \leqslant n \leqslant N$$

for any given family $\{ z^n \}_{n=0}^{N}$. In addition, we introduce some notation concerning the triangulations. Let $\{ \mathbf{T}_h \}_h$ be a family of decompositions of Ω into closed triangles; as usual, h stands for the mesh size. We assume that

$(\mathbf{H}_{\mathbf{T}_h})$ the family $\{ \mathbf{T}_h \}_h$ is regular [3, p. 132].

Since quasi-uniformity [3, p. 140] is not required, local refinements are allowed.

Let us now define the discrete spaces we shall work with

$$V_h^1 := \{ \chi \in C^0(\overline{\Omega}) : \chi_{|T} \text{ is linear } \forall\, T \in \mathbf{T}_h,\ \chi = 0 \text{ on } \partial\Omega \},$$

$$V_h^0 := \{ \psi : \psi_{|T} \text{ is constant } \forall\, T \in \mathbf{T}_h \},$$

and denote by I_h the linear interpolant operator in V_h^1. We shall also need a pair of operators associated with those spaces. The first one, denoted by P_h^1, is the discrete H_0^1-projection operator. So, for any $z \in H_0^1(\Omega)$, $P_h^1 z \in V_h^1$ is defined by

$$<\nabla P_h^1 z, \nabla \chi> = <\nabla z, \nabla \chi>, \quad \forall \chi \in V_h^1. \tag{2.1}$$

Hereafter, $<\cdot,\cdot>$ denotes either the inner product in $L^2(\Omega)$ or the pairing between $H^{-1}(\Omega)$ and $H_0^1(\Omega)$. Moreover we have

$$\|z - P_h^1 z\|_{H^r(\Omega)} \leqslant C\, h^{2-[r+s]} \|z\|_{H^{2-s}(\Omega)} \quad 0 \leqslant s, r \leqslant 1, \tag{2.2}$$

for any $z \in H_0^1(\Omega) \bigcap H^{2-s}(\Omega)$. Finally, the second operator is the L^2-projection operator P_h^0 onto V_h^0, which, for any $z \in L^2(\Omega)$, is defined by

$$<P_h^0 z, \psi> = <z, \psi>, \quad \forall \psi \in V_h^0. \tag{2.3}$$

and satisfy

$$\|z - P_h^0 z\|_{H^{-r}(\Omega)} \leqslant C\, h^{r+s} \|z\|_{H^s(\Omega)} \qquad 0 \leqslant s, r \leqslant 1, \tag{2.4}$$

for all $z \in H^s(\Omega)$.

2.2 - The continuous problem

Let us now state the suitable variational formulation of the differential problem (1.1).

Problem (P): *find* $\{u, \theta\}$ *such that*

$$u \in L^\infty(0,T; L^2(\Omega)) \cap H^1(0,T; H^{-1}(\Omega)), \quad \theta \in L^2(0,T; H_0^1(\Omega)), \tag{2.5}$$

$$\theta(x,t) = \beta(u(x,t)) \quad \text{for a.e. } (x,t) \in Q, \tag{2.6}$$

$$u(\cdot, 0) = u_0, \tag{2.7}$$

$$< \frac{\partial u}{\partial t}, \phi > + < \nabla \theta, \nabla \phi > = 0, \quad \forall \phi \in H_0^1(\Omega), \text{ a.e. } t \in]0,T[. \tag{2.8}$$

Existence and uniqueness are well known for (P) (see, e.g., [7] and the references given therein). Moreover, assuming that the hypotheses ($\mathbf{H}_\beta$) and ($\mathbf{H}_{u_0}$) hold, we have that:

$$\frac{\partial u}{\partial t} \in L^\infty(0,T; H^{-1}(\Omega)), \quad \theta \in L^\infty(0,T; H_0^1(\Omega)) \cap H^1(0,T; L^2(\Omega)). \tag{2.9}$$

2.3 - The regularized problem

Let us denote by ϵ the *regularization parameter* and introduce the following approximation of β

$$\beta_\epsilon(s) := \begin{cases} \beta(s) & \text{if } s < 0 \text{ or } s > s_\epsilon \\ \epsilon s & \text{if } 0 \leqslant s \leqslant s_\epsilon \end{cases}, \tag{2.10}$$

where s_ϵ is the maximal solution of the equation $\beta(s) = \epsilon s$; thus, $s_\epsilon = 1 + C\epsilon$.

Then the regularized problem reads as follows

Problem (P_ϵ): *find* $\{u_\epsilon, \theta_\epsilon\}$ *such that*

$$u_\epsilon \in L^\infty(0,T; L^2(\Omega)) \cap H^1(0,T; H^{-1}(\Omega)), \quad \theta_\epsilon \in L^2(0,T; H_0^1(\Omega)), \tag{2.11}$$

$$\theta_\epsilon(x,t) = \beta_\epsilon(u_\epsilon(x,t)) \quad \text{for a.e. } (x,t) \in Q, \tag{2.12}$$

$$u_\epsilon(\cdot, 0) = \beta_\epsilon^{-1}(\theta_0) . \tag{2.13}$$

$$< \frac{\partial u_\epsilon}{\partial t}, \phi> + <\nabla \theta_\epsilon, \nabla \phi> = 0 , \quad \forall \phi \in H_0^1(\Omega) , \text{ a.e. } t \in]0, T[. \tag{2.14}$$

We stress that the choice (2.13) of the initial regularized enthalpy guarantees that the regularity properties (2.11) and (2.9) hold uniformly in ϵ. Moreover, in view of ($\mathbf{H}_\beta$) and ($\mathbf{H}_{u_0}$), we have

$$\|u_\epsilon\|_{L^2(0,T;H^1(\Omega))} + \|u_\epsilon\|_{H^1(0,T;L^2(\Omega))} + \|\theta_\epsilon\|_{L^2(0,T;H^2(\Omega))} \leqslant C\, \epsilon^{-1/2} . \tag{2.15}$$

2.4 - The nonlinear Chernoff formula

Finally we state the precise meaning of our fully discrete scheme associated with the nonlinear Chernoff formula (1.2). Let $0 < \mu \leqslant L_\beta^{-1}$ be a fixed number (the so-called *relaxation parameter*).

Problem ($\mathrm{P}_{\epsilon,h,\tau}$): *for any* $1 \leqslant n \leqslant N$, *find* $U^n \in V_h^0$ *and* $\Theta^n \in V_h^1$ *such that, given* $U^0 \in V_h^0$, *we have*

$$<P_h^0\Theta^n, \chi> + \frac{\tau}{\mu} <\nabla \Theta^n, \nabla \chi> = <\beta_\epsilon(U^{n-1}), \chi> , \quad \forall \chi \in V_h^1 . \tag{2.16}$$

and

$$U^n = U^{n-1} + \mu\, [\, P_h^0\Theta^n - \beta_\epsilon(U^{n-1})\,] . \tag{2.17}$$

In section 3.1 we shall analyze the choice of the discrete initial enthalpy U^0. Since the matrix of linear system (2.16) is symmetric and positive definite, the solution of ($\mathrm{P}_{\epsilon,h,\tau}$) exists and is unique. Moreover, due to the fact that $P_h^0\Theta^n$ is the value of Θ^n at the barycenter of each triangle, the equation (2.17) may be regarded as an inexpensive element-by-element algebraic correction. The fully discrete scheme is, therefore, a linearized approximation to the original strongly nonlinear P.D.E. (1.1).

3 - PRELIMINARY RESULTS

This section is devoted to prove some auxiliary results. In fact, we first deal with the choice of the initial enthalpies and then show that the discrete scheme is strongly stable.

3.1 - Error estimates for initial enthalpies

Let us start by estimating the error for the initial regularized enthalpy. Before doing that let us set $\gamma_\epsilon := \beta_\epsilon^{-1}$.

Lemma 1. *Under the assumptions* $(\mathbf{H}_\beta)$ *and* $(\mathbf{H}_{u_0})$ *there exists a positive constant C independent of* ϵ *such that*

$$\|u_0 - \gamma_\epsilon(\theta_0)\|_{L^p(\Omega)} \leqslant C\, \epsilon^{1/p} \ , \quad \text{for all } 1 \leqslant p \leqslant 2 \ . \tag{3.1}$$

Proof. By definition of $\gamma_\epsilon := \beta_\epsilon^{-1}$ it follows that

$$(u_0 - \gamma_\epsilon(\theta_0))(x) \neq 0 \quad \text{only if} \quad 0 < u_0(x) < s_\epsilon \ .$$

The assertion is then a consequence of the initial non-degeneracy property //.

Lemma 2. *Under the assumptions* $(\mathbf{H}_\Omega)$ $(\mathbf{H}_\beta)$ *and* $(\mathbf{H}_{u_0})$ *there exists a positive constant C independent of* ϵ *such that*

$$\|u_0 - \gamma_\epsilon(\theta_0)\|_{H^{-1}(\Omega)} \leqslant C\, \epsilon \ |\log \epsilon\,|^{1/2} \ . \tag{3.2}$$

Proof. Let $\phi \in H_0^1(\Omega)$ be given and set $q := p/(p-1)$ for $1 < p \leqslant 2$ to be determined. Then

$$< u_0 - \gamma_\epsilon(\theta_0), \phi > \ \leqslant \|u_0 - \gamma_\epsilon(\theta_0)\|_{L^p(\Omega)} \|\phi\|_{L^q(\Omega)} \leqslant C \ \frac{\epsilon^{1/p}}{(p-1)^{1/2}} \ \|\phi\|_{H_0^1(\Omega)} \, .$$

where we have used the 2-D Poincaré-Sobolev inequality [5, p. 158]

$$\|\phi\|_{L^q(\Omega)} \leqslant C\ q^{1/2}\, \|\phi\|_{H_0^1(\Omega)} \quad (\ C > 0 \text{ independent of } q\ )\ .$$

Therefore, taking $p = 1 + |\log \epsilon\,|^{-1}$ yields the desired result //.

Let us now analyze the choice of the discrete initial enthalpy. We first define the initial temperature Θ^0 by

$$\Theta^0 := I_h\, \theta_0 \, ; \tag{3.3}$$

thus $\Theta^0 \in W_0^{1,\infty}(\Omega) \subset H_0^1(\Omega)$, as a consequence of $(\mathbf{H}_{u_0})$. The discrete initial enthalpy is then defined by

$$U^0 := \gamma_\epsilon(P_h^0 \Theta^0) \ . \tag{3.4}$$

or equivalently

$$\beta_\epsilon(U^0) := P_h^0 \Theta^0 \ . \tag{3.5}$$

Consequently, U^0 can be easily computed element-by-element.

Lemma 3. *Under the assumptions* $(\mathbf{H}_\Omega)$, $(\mathbf{H}_\beta)$, $(\mathbf{H}_{u_0})$ *and* $(\mathbf{H}_{\mathbf{T}_h})$ *there exists a positive constant C independent of* ϵ *and h such that*

$$\|\gamma_\epsilon(P_h^0\Theta^0) - \gamma_\epsilon(\theta_0)\|_{H^{-1}(\Omega)} \leqslant C\ [\epsilon + h]\ |\log(\epsilon+h)|^{1/2}. \tag{3.6}$$

Proof. Let $\mathbf{T}_h^0$ be defined by

$$\mathbf{T}_h^0 := \{\ T \in \mathbf{T}_h : T \cap F_0 \neq \varnothing\ \}.$$

Let $T \in \mathbf{T}_h$ be given. If $T \notin \mathbf{T}_h^0$ and $\theta_0 < 0$ in T, then $P_h^0\Theta^0 < 0$. Thus

$$\|\gamma_\epsilon(P_h^0\Theta^0) - \gamma_\epsilon(\theta_0)\|_{L^\infty(T)} \leqslant C\ \|P_h^0\Theta^0 - \theta_0\|_{L^\infty(T)} \leqslant C\ h\ .$$

Suppose now that $T \notin \mathbf{T}_h^0$ and $\theta_0 > \epsilon s_\epsilon$ in T. This implies $P_h^0\Theta^0 > \epsilon s_\epsilon$ and so

$$\|\gamma_\epsilon(P_h^0\Theta^0) - \gamma_\epsilon(\theta_0)\|_{L^\infty(T)} \leqslant C\ \|P_h^0\Theta^0 - \theta_0\|_{L^\infty(T)} \leqslant C\ h\ .$$

It only remains to analyze the case: $T \in \mathbf{T}_h^0$ or $0 < \theta_0 \leqslant \epsilon s_\epsilon$ in T. Using $(\mathbf{H}_{u_0})$, it easily follows that

$$\text{meas}(\{\ x \in \Omega : x \in T \in \mathbf{T}_h^0 \ \text{ or }\ 0 < \theta_0(x) \leqslant \epsilon s_\epsilon\ \}) \leqslant C\ [h+\epsilon]\ .$$

Collecting previous estimates results in

$$\|\gamma_\epsilon(P_h^0\Theta^0) - \gamma_\epsilon(\theta_0)\|_{L^p(\Omega)} \leqslant C\ [h + \epsilon]^{1/p}, \quad \text{for all } 1 \leqslant p \leqslant 2\ .$$

This coupled with the $2-D$ Poincaré-Sobolev inequality already used in Lemma 2 gives the desired estimate //.

3.2 - Strong stability of the discrete scheme

In order to show the stability of the discrete solutions, we combine the equations (2.16) and (2.17) of the nonlinear Chernoff formula and rewrite (2.16) as follows

$$<\partial U^n, \chi> + <\nabla\Theta^n, \nabla\chi> = 0\ , \quad \forall \chi \in V_h^1\ . \tag{3.7}$$

The relaxation parameter constraints $0 < \mu \leqslant L_\beta^{-1}$ and $(\mathbf{H}_\beta)$ imply that the function

$$\alpha_\epsilon := I - \mu\,\beta_\epsilon \quad \text{satisfies} \quad 0 \leqslant \alpha_\epsilon'(s) \leqslant 1\ , \quad \text{for a.e. } s \in R\ . \tag{3.8}$$

Lemma 4. *Under the assumptions* $(\mathbf{H}_\beta)$ *and* $(\mathbf{H}_{u_0})$ *there exists a positive constant C independent of* ϵ, *h and* τ *such that*

$$\sum_{n=1}^{N} \tau <\partial U^n, \partial\beta_\epsilon(U^n)> + \max_{1\leqslant n\leqslant N} \|\nabla\Theta^n\|_{L^2(\Omega)} \leqslant C\ . \tag{3.9}$$

Proof. The proof proceeds along the same lines as those in [9. Lemma 2]. Namely, we take $\chi := \tau\,\partial\Theta^n \in V_h^1$ as a test function in (3.7), sum over n for $n = 1,\dots,m \leqslant N$, and observe that

$$P_h^0\Theta^n = \frac{1}{2}\,\beta_\epsilon(U^n) + \frac{1}{2\mu}\,U^n + \frac{1}{2\mu}\,\alpha_\epsilon(U^n) - \frac{1}{\mu}\,\alpha_\epsilon(U^{n-1})\,,$$

for $0 \leqslant n \leqslant N$, where $U^{-1} := U^0$. This equality is a consequence of the second equation (2.17) of the nonlinear Chernoff formula for $1 \leqslant n \leqslant N$ whereas the case $n = 0$ results from the definition (3.5) of U^0. Now, since

$$<\partial U^n, \chi> = <\partial U^n, P_h^0\chi>\,, \quad \forall \chi \in L^2(\Omega)\,,$$

the first term in (3.7) can be split as follows. By (3.8) we get

$$\sum_{n=1}^{m} \tau <\partial U^n, \frac{1}{2\mu}\,\partial U^n + \frac{1}{2\mu}\,\partial\alpha_\epsilon(U^n)> \geqslant$$
$$\geqslant \sum_{n=1}^{m} \tau\,[\,\frac{1}{2\mu}\,\|\partial U^n\|^2_{L^2(\Omega)} + \frac{1}{2\mu}\,\|\partial\alpha_\epsilon(U^n)\|^2_{L^2(\Omega)}\,]\,.$$

On the other hand, recalling that $U^{-1} := U^0$, the remaining contribution becomes

$$\Big|\sum_{n=2}^{m} \tau <\partial U^n, \frac{1}{\mu}\,\partial\alpha_\epsilon(U^{n-1})>\Big| \leqslant \frac{1}{2\mu}\sum_{n=1}^{m} \tau\,[\,\|\partial U^n\|^2_{L^2(\Omega)} + \|\partial\alpha_\epsilon(U^n)\|^2_{L^2(\Omega)}\,]\,.$$

Collecting these two estimates yields

$$\sum_{n=1}^{m} \tau <\partial U^n, \partial\Theta^n> \geqslant \frac{1}{2}\sum_{n=1}^{m} \tau <\partial U^n, \partial\beta_\epsilon(U^n)>\,.$$

The second term in (3.7) is easily bounded as follows

$$\sum_{n=1}^{m} \tau <\nabla\Theta^n, \partial\nabla\Theta^n> \geqslant \frac{1}{2}\,\|\nabla\Theta^m\|^2_{L^2(\Omega)} - \frac{1}{2}\,\|\nabla\Theta^0\|^2_{L^2(\Omega)}\,.$$

Then, (3.3) and $(\mathbf{H}_{u_0})$ lead to the asserted estimate //.

Remark 1. Note that $(\mathbf{H}_\beta)$ and the definition of β_ϵ imply

$$\sum_{n=1}^{N} \tau\,\|\partial\beta_\epsilon(U^n)\|^2_{L^2(\Omega)} \leqslant C \quad \text{and} \quad \sum_{n=1}^{N} \tau\,\|\partial U^n\|^2_{L^2(\Omega)} \leqslant C\,\epsilon^{-1}\,. \tag{3.10}$$

The last bound may be regarded as a discrete analogue of the middle estimate in (2.15). Moreover, based on the first bound, we can easily derive

$$\max_{1\leqslant n\leqslant N} \|U^n\|_{L^2(\Omega)} \leqslant C\,. \tag{3.11}$$

4 - THE MAIN RESULTS

We are now in a position to prove the energy error estimates for both enthalpy and temperature. We start with the effect of the regularization procedure and then conclude with the fully discrete scheme.

4.1 - Error estimates for the regularized problem

The following error estimate was proven in [12] for a rather general P.D.E. (e.g., including convection) via a parabolic duality argument. However, due to the simple structure of (1.1), we can provide a different and simplified proof as follows. Let us first introduce the notation

$$e_\theta^\epsilon := \theta - \theta_\epsilon \quad \text{and} \quad e_u^\epsilon := u - u_\epsilon .$$

Theorem 1. *Under the assumptions* $(\mathbf{H}_\Omega)$, $(\mathbf{H}_\beta)$ *and* $(\mathbf{H}_{u_0})$ *there exists a positive constant C independent of ϵ such that*

$$\begin{aligned} &\|e_\theta^\epsilon\|_{L^2(Q)} + \epsilon^{1/2}\|e_u^\epsilon\|_{L^2(Q)} + \|\int_0^t e_\theta^\epsilon\|_{L^\infty(0,T;H^1(\Omega))} + \\ &+ \|e_u^\epsilon\|_{L^\infty(0,T;H^{-1}(\Omega))} \leqslant C\ [\ \epsilon^{1/2}\,\mathrm{meas}(A_\epsilon)^{1/2} + \epsilon\,|\log\epsilon|^{1/2}]\,. \end{aligned} \tag{4.1}$$

where $A_\epsilon := \{ (x,t) \in Q : 0 \leqslant u(x,t) \leqslant s_\epsilon \}$.

Proof. Taking the difference between (2.8) and (2.14) and integrating the resulting expression on $]0,t[$, we get

$$< e_u^\epsilon(t) - e_u^\epsilon(0), \phi > + < \nabla \int_0^t e_\theta^\epsilon(s)\,ds, \nabla\phi > = 0\,, \quad \forall \phi \in H_0^1(\Omega)\,. \tag{4.2}$$

We then take $\phi = e_\theta^\epsilon(t) \in H_0^1(\Omega)$ as a test function and integrate on $]0,t_0[$, for any $0 < t_0 \leqslant T$, to obtain

$$\int_0^{t_0} < e_u^\epsilon(t), e_\theta^\epsilon(t) > dt + \frac{1}{2}\|\int_0^{t_0} \nabla e_\theta^\epsilon(t)dt\|^2_{L^2(\Omega)} = < e_u^\epsilon(0), \int_0^{t_0} e_\theta^\epsilon(t)dt > . \tag{4.3}$$

Now, observe that for a.e. $(x,t) \in Q$ we can write

$$\begin{aligned} e_u^\epsilon\, e_\theta^\epsilon &= [u - u_\epsilon][\beta_\epsilon(u) - \beta_\epsilon(u_\epsilon)] + [u - u_\epsilon][\beta(u) - \beta_\epsilon(u)] \geqslant \\ &\geqslant \frac{\epsilon}{2}\,|u - u_\epsilon|^2 + \frac{1}{2L_\beta}\,|\beta_\epsilon(u) - \beta_\epsilon(u_\epsilon)|^2 + [u - u_\epsilon][\beta(u) - \beta_\epsilon(u)] \geqslant \\ &\geqslant \frac{\epsilon}{4}\,|u - u_\epsilon|^2 + \frac{1}{4L_\beta}\,|\theta - \theta_\epsilon|^2 - [\frac{1}{2L_\beta} + \frac{1}{\epsilon}]\,|\beta(u) - \beta_\epsilon(u)|^2 . \end{aligned}$$

Moreover, definition (2.10) of β_ϵ clearly implies

$$\beta_\epsilon(u) - \beta(u) = 0 \quad \text{in } Q \setminus A_\epsilon \qquad \text{and} \qquad 0 \leqslant \beta_\epsilon(u) - \beta(u) \leqslant \epsilon u \ .$$

Consequently, we get

$$\int_0^{t_0} < e_u^\epsilon(t), e_\theta^\epsilon(t) > dt \geqslant \frac{\epsilon}{4} \|e_u^\epsilon\|^2_{L^2(0,t_0; L^2(\Omega))} + $$
$$+ \frac{1}{4L_\beta} \|e_\theta^\epsilon\|^2_{L^2(0,t_0; L^2(\Omega))} - C\,\epsilon\, \mathrm{meas}(A_\epsilon) \ .$$

To bound the right hand side of (4.3), we make use of Lemma 2; namely

$$\left| < e_u^\epsilon(0), \int_0^{t_0} e_\theta^\epsilon(t)\, dt > \right| \leqslant C\,\epsilon^2\, |\log\epsilon| + \frac{1}{4} \left\| \int_0^{t_0} \nabla e_\theta^\epsilon(t)\, dt \right\|^2_{L^2(\Omega)} .$$

Collecting the previous estimates and inserting them into (4.3), we obtain the desired error bounds. In fact, it would only remain to estimate $\|e_u^\epsilon\|_{L^\infty(0,T;H^{-1}(\Omega))}$ which is an easy consequence of (4.2). This concludes the proof //.

4.2 - Error estimates for the fully discrete scheme

In this subsection we analyze the accuracy of the nonlinear Chernoff formula $(P_{\epsilon,h,\tau})$ in approximating solutions u_ϵ and θ_ϵ of the regularized problem. So, our aim is to derive bounds in energy norms for the errors $e_\theta^{h,\tau}$ and $e_u^{h,\tau}$, which are defined by

$$e_\theta^{h,\tau}(t) := \theta_\epsilon(t) - \Theta^n, \quad e_u^{h,\tau}(t) := u_\epsilon(t) - U^n \quad \text{for } t \in I^n, \ 1 \leqslant n \leqslant N.$$

Theorem 2. *Under the assumptions* (H_Ω), (H_β), (H_{u_0}) *and* (H_{T_h}) *there exists a positive constant* C *independent of* ϵ, h *and* τ *such that*

$$\|e_\theta^{h,\tau}\|_{L^2(Q)} + \epsilon^{1/2}\|e_u^{h,\tau}\|_{L^2(Q)} + \left\|\int_0^t e_\theta^{h,\tau}\right\|_{L^\infty(0,T;H^1(\Omega))} +$$
$$+ \|e_u^{h,\tau}\|_{L^\infty(0,T;H^{-1}(\Omega))} \leqslant C\left[\frac{h^2}{\epsilon} + \frac{h}{\epsilon^{1/4}} + \frac{\tau}{\epsilon} + (\epsilon+h)\,|\log(\epsilon+h)|^{1/2}\right]. \tag{4.4}$$

Proof. Since no confusion is possible, we omit the subscripts ϵ, h and τ in all functions occurring in the discrete and continuous formulations. Let us start by writing the set of discrete equations satisfied by the continuous solution; namely

$$< \partial u^n, \phi > + < \nabla\overline{\theta}^n, \nabla\phi > = 0, \quad \forall \phi \in H_0^1(\Omega), \quad 1 \leqslant n \leqslant N \ , \tag{4.5}$$

which is obtained after integrating (2.14) on I^n. We now take the difference between (4.5) and (3.7), sum over n from 1 to $i \leqslant N$ and multiply the resulting expression by τ. Hence we obtain the following *error equation*

$$<e_u^i . \chi> + <\nabla \sum_{n=1}^{i} \tau \, \overline{e}_\theta^n . \nabla \chi> = <e_u^0 . \chi> , \quad \forall \chi \in V_h^1 . \tag{4.6}$$

The next step is to choose suitable test functions χ. Let us start by estimating the first three terms in (4.4). To do so, we take $\chi = \tau \, [P_h^1 \overline{\theta}^i - \Theta^i] = \tau \, P_h^1 \overline{e}_\theta^i \in V_h^1$ and sum over i from 1 to $m \leqslant N$. After reordering we get

$$\sum_{i=1}^{m} \int_{I^i} <e_u(t) . \theta(t) - P_h^0 \Theta^i> dt +$$
$$+ \sum_{i=1}^{m} \tau^2 <\nabla \sum_{n=1}^{i} \overline{e}_\theta^n . \nabla P_h^1 \overline{e}_\theta^i> =: I + II =$$
$$= \sum_{i=1}^{m} \int_{I^i} <u(t) - u^i . P_h^1 e_\theta(t)> dt + \tag{4.7}$$
$$+ \sum_{i=1}^{m} \int_{I^i} <e_u(t) . [I - P_h^1]\theta(t) + [I - P_h^0]\Theta^i> dt +$$
$$+ <e_u^0 . \sum_{i=1}^{m} \tau \, P_h^1 \overline{e}_\theta^i> =: III + IV + V .$$

The rest of the proof consists of estimating separately each term in the previous expression. To begin with, notice that (2.12) and (2.17) combined with (3.8) yield

$$u - \mu \, \theta = \alpha(u) \quad \text{and} \quad U^n - \mu \, P_h^0 \Theta^n = \alpha(U^{n-1}) . \tag{4.8}$$

whence

$$e_u(t) = \mu \, [\theta(t) - P_h^0 \Theta^n] + [\alpha(u(t)) - \alpha(U^{n-1})] . \tag{4.9}$$

and

$$\theta(t) - P_h^0 \Theta^n = [\beta(u(t)) - \beta(U^{n-1})] - \frac{1}{\mu} [U^n - U^{n-1}] . \tag{4.10}$$

for $t \in I^n$. The first task is to rewrite term I. In view of expressions (4.9) and (4.10), I can be split as follows

$$I = \mu \sum_{i=1}^{m} \int_{I^i} \|\theta(t) - P_h^0 \Theta^i\|_{L^2(\Omega)}^2 dt +$$
$$+ \sum_{i=1}^{m} \int_{I^i} <\alpha(u(t)) - \alpha(U^{i-1}) . \beta(u(t)) - \beta(U^{i-1})> dt -$$
$$- \frac{1}{\mu} \sum_{i=1}^{m} \int_{I^i} <\alpha(u(t)) - \alpha(U^{i-1}) . U^i - U^{i-1}> dt =: I_1 + I_2 + I_3 .$$

The fact that $\beta'(s) \geqslant \epsilon > 0$ and $0 \leqslant \alpha'(s) \leqslant 1$ for a.e. $s \in \mathbb{R}$ results in

$$I_2 \geqslant \epsilon \sum_{i=1}^{m} \int_{I^i} \|\alpha(u(t)) - \alpha(U^{i-1})\|_{L^2(\Omega)}^2 dt =: I_2^m .$$

By virtue of the stability estimate (3.10), the remaining term I_3 can be bounded as follows

$$|I_3| \leqslant \frac{1}{2} I_2^m + C \frac{\tau^2}{\epsilon} \sum_{i=1}^{m} \tau \|\partial U^i\|^2_{L^2(\Omega)} \leqslant \frac{1}{2} I_2^m + C \frac{\tau^2}{\epsilon^2} .$$

It is easily seen now that

$$I_1 + I_2 \geqslant C \epsilon \|e_u\|^2_{L^2(0,t^m;L^2(\Omega))}$$

and

$$I_1 \geqslant \frac{\mu}{2} \|e_\theta\|^2_{L^2(0,t^m;L^2(\Omega))} - C h^2 .$$

These estimates together with the previous ones provide the following bound for term I

$$I \geqslant C [\|e_\theta\|^2_{L^2(0,t^m;L^2(\Omega))} + \epsilon \|e_u\|^2_{L^2(0,t^m;L^2(\Omega))}] - C [h^2 + \frac{\tau^2}{\epsilon^2}] =$$
$$=: A + B - C [h^2 + \frac{\tau^2}{\epsilon^2}] .$$

Let us now analyze term II. To do so, we need the elementary identity

$$2 \sum_{i=1}^{m} a_i [\sum_{n=1}^{i} a_n] = [\sum_{i=1}^{m} a_i]^2 + \sum_{i=1}^{m} a_i^2 , \quad \text{for } a_i \in R^2 , \quad 1 \leqslant i \leqslant N .$$

Using approximation property (2.2) of the Ritz projection P_h^1 in conjunction with the regularity estimate $\|\int_0^t \theta\|_{L^\infty(0,T;H^2(\Omega))} \leqslant C$ yields

$$II = \frac{1}{2} \|\nabla \int_0^{t^m} P_h^1 e_\theta(t)\, dt\|^2_{L^2(\Omega)} + \frac{1}{2} \tau^2 \sum_{i=1}^{m} \|\nabla P_h^1 \bar{e}_\theta^i\|^2_{L^2(\Omega)} \geqslant$$
$$\geqslant \frac{1}{2} \|\nabla \int_0^{t^m} e_\theta(t)\, dt\|^2_{L^2(\Omega)} - C h^2 .$$

The a priori estimate $\|\frac{\partial u}{\partial t}\|_{L^2(Q)} \leqslant C \epsilon^{-1/2}$ leads to the following bound for term III

$$|III| = |\sum_{i=1}^{m} \int_{I^i} < -\int_t^{t^i} \frac{\partial u}{\partial s} ds , P_h^1 e_\theta(t) > dt | \leqslant$$
$$\leqslant \tau \|\frac{\partial u}{\partial t}\|_{L^2(0,t^m;L^2(\Omega))} \|e_\theta\|_{L^2(0,t^m;L^2(\Omega))} \leqslant \frac{1}{2} A + C \frac{\tau^2}{\epsilon} .$$

The analysis of term IV requires the following splitting

$$IV = \sum_{i=1}^{m} \int_{I^i} < e_u(t) , [I - P_h^1] \theta(t) > dt +$$
$$+ \sum_{i=1}^{m} \int_{I^i} < [I - P_h^0] u(t) , [I - P_h^0] \Theta^i > dt =: IV_1 + IV_2 .$$

where we have used the orthogonality property of P_h^0 to get rid of U^i in the second integral. We now make use of the a priori bound $\|\theta\|_{L^2(0,T:H^2(\Omega))} \leqslant C\,\epsilon^{-1/2}$ to write

$$|IV_1| \leqslant \frac{1}{2} B + C\,\frac{h^4}{\epsilon^2}.$$

For IV_2 instead, we recall the estimate $\|u\|_{L^2(0,T:H^1(\Omega))} \leqslant C\,\epsilon^{-1/2}$ and (3.9) which imply

$$|IV_2| \leqslant C\,\frac{h^2}{\epsilon^{1/2}}.$$

The bound for the remaining term V is a trivial consequence of Lemma 3, namely

$$|V| \leqslant \|e_u^0\|_{H^{-1}(\Omega)} \, \| \int_0^{t^m} \nabla e_\theta \|_{L^2(\Omega)} \leqslant$$

$$\leqslant \frac{1}{4} \| \nabla \int_0^{t^m} e_\theta \|_{L^2(\Omega)}^2 + C\,[\epsilon^2 + h^2]\,|\log(\epsilon+h)|.$$

Finally, the fact that $\int_0^t \theta \in W^{1,\infty}(0,T;H^1(\Omega))$ provides the desired estimates

$$\begin{aligned} &\|e_\theta\|_{L^2(Q)} + \epsilon^{1/2}\|e_u\|_{L^2(Q)} + \|\int_0^t e_\theta\|_{L^\infty(0,T:H^1(\Omega))} \leqslant \\ &\leqslant C\,\Big[\frac{h^2}{\epsilon} + \frac{h}{\epsilon^{1/4}} + \frac{\tau}{\epsilon} + (\epsilon+h)\,|\log(\epsilon+h)|^{1/2}\Big] =: \sigma(\epsilon,h,\tau). \end{aligned} \tag{4.11}$$

The remaining estimate $\|e_u\|_{L^\infty(0,T\cdot H^{-1}(\Omega))} \leqslant \sigma(\epsilon,h,\tau)$ follows from equation (4.6). Indeed, let $\phi \in H_0^1(\Omega)$ be given and let $\chi \in V_h^1$ be such that $\|\phi - \chi\|_{H^s(\Omega)} \leqslant C\,h^{1-s}\|\phi\|_{H_0^1(\Omega)}$, $s = 0, 1$; then

$$<e_u^i, \phi> = <e_u^i, \phi - \chi> + <e_u^0, \chi> - <\nabla \sum_{n=1}^{i} \tau\,\bar{e}_\theta^n, \nabla\chi>.$$

Finally, in view of (2.11), (3.11) and (4.11), we easily get the assertion //.

4.3 - The final error estimates

The first immediate consequence of Theorems 1 and 2 is the following estimate in energy norms for temperature and enthalpy errors which are defined by

$$e_\theta(t) := \theta(t) - \Theta^n, \quad e_u(t) := u(t) - U^n \quad \text{for } t \in I^n,\ 1 \leqslant n \leqslant N.$$

Corollary 1. *Let the assumptions* (H_Ω), (H_β), (H_{u_0}) *and* (H_{T_h}) *hold. Then choosing* $\epsilon = C_1 h^{4/3}$ *and* $\tau = C_2 h^2$ *for* C_1 *and* C_2 *being arbitrary positive* *constants, we have*

$$\|e_\theta\|_{L^2(Q)} + \|\int_0^t e_\theta\|_{L^\infty(0,T;H^1(\Omega))} + \|e_u\|_{L^\infty(0,T;H^{-1}(\Omega))} = O(h^{2/3}) . \quad (4.12)$$

In Nochetto [13] the following non-degeneracy property is shown under some *qualitative assumptions* concerning the data

$$\text{meas}(A_\epsilon) = O(\epsilon) . \quad (4.13)$$

where A_ϵ is defined in Theorem 1. As a result, we obtain the following improvement of the estimates (4.12), together with an L^2-error estimate for enthalpy.

Corollary 2. *Let the non-degeneracy property* (4.13) *and the assumptions* ($\mathbf{H}_\Omega$), ($\mathbf{H}_\beta$), ($\mathbf{H}_{u_0}$) *and* ($\mathbf{H}_{T_h}$) *hold. Then choosing* $\epsilon = C_1 h^{4/5}$ *and* $\tau = C_2 h^{8/5}$ *for* C_1 *and* C_2 *being arbitrary positive constants, we have*

$$\|e_\theta\|_{L^2(Q)} + \|\int_0^t e_\theta\|_{L^\infty(0,T;H^1(\Omega))} + \|e_u\|_{L^\infty(0,T;H^{-1}(\Omega))} = O(h^{4/5}) . \quad (4.14)$$

$$\|e_u\|_{L^2(Q)} = O(h^{2/5}) . \quad (4.15)$$

Remark 2. The non-degeneracy property (4.13) is also the basic ingredient for interfaces to be approximated, as shown in Nochetto [11]. Therefore, combining (4.13) and (4.14), error estimates in measure for free boundaries can be derived.

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