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Institutions: University of Pavia

Published on: 01 Jan 1988 - Numerical Functional Analysis and Optimization (Taylor & Francis)

Topics: Stefan problem, Nonlinear system, Piecewise linear function, Smoothing and Regularization (mathematics)

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

By

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IMA Preprint Series # 350

October 1987

INSTITUTE FOR MATHEMATICS AND ITS APPLICATIONS

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**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.

$$\left\{ \begin{array}{ll} \frac{\partial u}{\partial t} - \Delta \beta(u) = 0 & \text{in } Q := \Omega \times]0, T [\\ \beta(u) = 0 & \text{on } \partial\Omega \times]0, T [\\ u = u_0 & \text{at } t = 0 . \end{array} \right. \quad (1.1)$$

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 $\| \frac{\partial u_\epsilon}{\partial t} \|_{L^2(Q)} \leq C \epsilon^{-1/2}$, 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

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

here μ stands for a relaxation parameter satisfying $0 < \mu \leq L_\beta^{-1}$ ($L_\beta > 0$: 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 $_{\Omega}$) $\Omega \subset \mathbb{R}^2$ is a convex polygon.

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

(H $_{\beta}$) $\beta : \mathbb{R} \rightarrow \mathbb{R}$ is a nondecreasing and Lipschitz continuous function such that

$$\beta(s) := 0 \quad \text{for } 0 \leq s \leq 1 .$$

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

(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:
 $\text{meas}(\{x \in \Omega : 0 \leq \theta_0(x) \leq \epsilon\}) = O(\epsilon)$ (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 $1 \leq n \leq N$. We also set

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

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

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

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

($H_{\mathbf{T}_h}$) 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

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

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

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

$$\langle \nabla P_h^1 z, \nabla \chi \rangle = \langle \nabla z, \nabla \chi \rangle, \quad \forall \chi \in V_h^1. \quad (2.1)$$

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

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

for any $z \in H_0^1(\Omega) \cap H^{2-s}(\Omega)$. 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

$$\langle P_h^0 z, \psi \rangle = \langle z, \psi \rangle, \quad \forall \psi \in V_h^0. \quad (2.3)$$

and satisfy

$$\|z - P_h^0 z\|_{H^{-r}(\Omega)} \leq C h^{r+s} \|z\|_{H^s(\Omega)} \quad 0 \leq s, r \leq 1. \quad (2.4)$$

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

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

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

$$u(\cdot, 0) = u_0. \quad (2.7)$$

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

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

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

2.3 - The regularized problem

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

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

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

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

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

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

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

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 (H_β) and (H_{u_0}) , we have

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

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 $0 < \mu \leq L_\beta^{-1}$ be a fixed number (the so-called *relaxation parameter*).

Problem $(P_{\epsilon,h,\tau})$: for any $1 \leq n \leq N$, 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

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

and

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

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 $(P_{\epsilon,h,\tau})$ 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 (H_β) and (H_{u_0}) there exists a positive constant C independent of ϵ such that*

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

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

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

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

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

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

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

$$\langle u_0 - \gamma_\epsilon(\theta_0), \phi \rangle \leq \|u_0 - \gamma_\epsilon(\theta_0)\|_{L^p(\Omega)} \|\phi\|_{L^q(\Omega)} \leq C \frac{\epsilon^{1/p}}{(p-1)^{1/2}} \|\phi\|_{H_0^1(\Omega)},$$

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

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

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

$$\Theta^0 := J_h \theta_0 : \quad (3.3)$$

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

$$U^0 := \gamma_\epsilon(P_h^0 \Theta^0), \quad (3.4)$$

or equivalently

$$\beta_\epsilon(U^0) := P_h^0 \Theta^0. \quad (3.5)$$

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

Lemma 3. *Under the assumptions (H_Ω) , (H_β) , (H_{u_0}) and (H_{T_h}) there exists a positive constant C independent of ϵ and h such that*

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

Proof. Let T_h^0 be defined by

$$T_h^0 := \{ T \in T_h : T \cap F_0 \neq \emptyset \}.$$

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

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

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

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

It only remains to analyze the case: $T \in T_h^0$ or $0 < \theta_0 \leq \epsilon s_\epsilon$ in T . Using (H_{u_0}) , it easily follows that

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

Collecting previous estimates results in

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

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

$$\langle \partial U'', \chi \rangle + \langle \nabla \Theta'', \nabla \chi \rangle = 0, \quad \forall \chi \in V_h^1. \quad (3.7)$$

The relaxation parameter constraints $0 < \mu \leq L_\beta^{-1}$ and (H_β) imply that the function

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

Lemma 4. *Under the assumptions (H_β) and (H_{u_0}) there exists a positive constant C independent of ϵ , h and τ such that*

$$\sum_{n=1}^N \tau \langle \partial U'', \partial \beta_\epsilon(U'') \rangle + \max_{1 \leq n \leq N} \|\nabla \Theta''\|_{L^2(\Omega)} \leq C. \quad (3.9)$$

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

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

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

$$\begin{aligned} & \sum_{n=1}^m \tau \langle \partial U^n, \frac{1}{2\mu} \partial U^n + \frac{1}{2\mu} \partial \alpha_\epsilon(U^n) \rangle \geq \\ & \geq \sum_{n=1}^m \tau \left[\frac{1}{2\mu} \|\partial U^n\|_{L^2(\Omega)}^2 + \frac{1}{2\mu} \|\partial \alpha_\epsilon(U^n)\|_{L^2(\Omega)}^2 \right]. \end{aligned}$$

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

$$\left| \sum_{n=2}^m \tau \langle \partial U^n, \frac{1}{\mu} \partial \alpha_\epsilon(U^{n-1}) \rangle \right| \leq \frac{1}{2\mu} \sum_{n=1}^m \tau \left[\|\partial U^n\|_{L^2(\Omega)}^2 + \|\partial \alpha_\epsilon(U^n)\|_{L^2(\Omega)}^2 \right].$$

Collecting these two estimates yields

$$\sum_{n=1}^m \tau \langle \partial U^n, \partial \Theta^n \rangle \geq \frac{1}{2} \sum_{n=1}^m \tau \langle \partial U^n, \partial \beta_\epsilon(U^n) \rangle.$$

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

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

Then, (3.3) and (H_{u_0}) lead to the asserted estimate //.

Remark 1. Note that (H_β) and the definition of β_ϵ imply

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

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

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

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 (H_{Ω}) , (H_{β}) and (H_{u_0}) there exists a positive constant C independent of ϵ such that*

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

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

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

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

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 $0 < t_0 \leq T$, to obtain

$$\int_0^{t_0} \langle e_u^{\epsilon}(t), e_{\theta}^{\epsilon}(t) \rangle dt + \frac{1}{2} \left\| \int_0^{t_0} \nabla e_{\theta}^{\epsilon}(t) dt \right\|_{L^2(Q)}^2 = \langle e_u^{\epsilon}(0), \int_0^{t_0} e_{\theta}^{\epsilon}(t) dt \rangle. \quad (4.3)$$

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

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

Moreover, definition (2.10) of β_{ϵ} clearly implies

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

Consequently, we get

$$\begin{aligned} \int_0^{t_0} \langle e_u^\epsilon(t), e_\theta^\epsilon(t) \rangle dt &\geq \frac{\epsilon}{4} \|e_u^\epsilon\|_{L^2(0,t_0;L^2(\Omega))}^2 + \\ &+ \frac{1}{4L_\beta} \|e_\theta^\epsilon\|_{L^2(0,t_0;L^2(\Omega))}^2 - C \epsilon \text{meas}(A_\epsilon) . \end{aligned}$$

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

$$| \langle e_u^\epsilon(0), \int_0^{t_0} e_\theta^\epsilon(t) dt \rangle | \leq C \epsilon^2 |\log \epsilon| + \frac{1}{4} \| \int_0^{t_0} \nabla e_\theta^\epsilon(t) dt \|_{L^2(\Omega)}^2 .$$

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

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

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

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

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

$$\langle \partial_t u^n, \phi \rangle + \langle \nabla \bar{\theta}^n, \nabla \phi \rangle = 0, \quad \forall \phi \in H_0^1(\Omega), \quad 1 \leq n \leq N. \quad (4.5)$$

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 $i \leq N$ and multiply the resulting expression by τ . Hence we obtain the following *error equation*

$$\langle e_u^j, \chi \rangle + \langle \nabla \sum_{n=1}^j \tau \bar{e}_\theta^n, \nabla \chi \rangle = \langle e_u^0, \chi \rangle, \quad \forall \chi \in V_h^1. \quad (4.6)$$

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 $\chi = \tau [P_h^1 \bar{\theta}^i - \theta^i] = \tau P_h^1 \bar{e}_\theta^i \in V_h^1$ and sum over i from 1 to $m \leq N$. After reordering we get

$$\begin{aligned} & \sum_{i=1}^m \int_{I'} \langle e_u(t), \theta(t) - P_h^0 \theta^i \rangle dt + \\ & + \sum_{i=1}^m \tau^2 \langle \nabla \sum_{n=1}^i \bar{e}_\theta^n, \nabla P_h^1 \bar{e}_\theta^i \rangle =: I + II = \\ & = \sum_{i=1}^m \int_{I'} \langle u(t) - u^i, P_h^1 e_\theta(t) \rangle dt + \\ & + \sum_{i=1}^m \int_{I'} \langle e_u(t), [I - P_h^1] \theta(t) + [I - P_h^0] \theta^i \rangle dt + \\ & + \langle e_u^0, \sum_{i=1}^m \tau P_h^1 \bar{e}_\theta^i \rangle =: III + IV + V. \end{aligned} \quad (4.7)$$

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

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

whence

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

and

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

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

$$\begin{aligned} I &= \mu \sum_{i=1}^m \int_{I'} \|\theta(t) - P_h^0 \theta^i\|_{L^2(\Omega)}^2 dt + \\ &+ \sum_{i=1}^m \int_{I'} \langle \alpha(u(t)) - \alpha(U^{i-1}), \beta(u(t)) - \beta(U^{i-1}) \rangle dt - \\ &- \frac{1}{\mu} \sum_{i=1}^m \int_{I'} \langle \alpha(u(t)) - \alpha(U^{i-1}), U^i - U^{i-1} \rangle dt =: I_1 + I_2 + I_3. \end{aligned}$$

The fact that $\beta'(s) \geq \epsilon > 0$ and $0 \leq \alpha'(s) \leq 1$ for a.e. $s \in R$ results in

$$I_2 \geq \epsilon \sum_{i=1}^m \int_{I'} \|\alpha(u(t)) - \alpha(U^{i-1})\|_{L^2(\Omega)}^2 dt =: I_2^m.$$

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

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

It is easily seen now that

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

and

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

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

$$\begin{aligned} I &\geq C \left[\|e_\theta\|_{L^2(0, T^m; L^2(\Omega))}^2 + \epsilon \|e_u\|_{L^2(0, T^m; L^2(\Omega))}^2 \right] - C \left[h^2 + \frac{\tau^2}{\epsilon} \right] = \\ &=: A + B - C \left[h^2 + \frac{\tau^2}{\epsilon} \right]. \end{aligned}$$

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

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

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

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

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

$$\begin{aligned} |III| &= \left| \sum_{i=1}^m \int_{t'}^t \left\langle -\int_t^s \frac{\partial u}{\partial s} ds, P_h^1 e_\theta(t) \right\rangle dt \right| \leq \\ &\leq \tau \|\frac{\partial u}{\partial t}\|_{L^2(0, T^m; L^2(\Omega))} \|e_\theta\|_{L^2(0, T^m; L^2(\Omega))} \leq \frac{1}{2} A + C \frac{\tau^2}{\epsilon}. \end{aligned}$$

The analysis of term IV requires the following splitting

$$\begin{aligned} IV &= \sum_{i=1}^m \int_{t'}^t \langle e_u(t), [I - P_h^1] \theta(t) \rangle dt + \\ &+ \sum_{i=1}^m \int_{t'}^t \langle [I - P_h^0] u(t), [I - P_h^0] \theta^i \rangle dt =: IV_1 + IV_2. \end{aligned}$$

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 $\|\theta\|_{L^2(0,T;H^2(\Omega))} \leq C \epsilon^{-1/2}$ to write

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

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

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

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

$$\begin{aligned} |V| &\leq \|e_u^0\|_{H^{-1}(\Omega)} \left\| \int_0^t \nabla e_\theta \right\|_{L^2(\Omega)} \leq \\ &\leq \frac{1}{4} \left\| \nabla \int_0^t e_\theta \right\|_{L^2(\Omega)}^2 + C [\epsilon^2 + h^2] |\log(\epsilon+h)|. \end{aligned}$$

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

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

The remaining estimate $\|e_u\|_{L^\infty(0,T;H^{-1}(\Omega))} \leq \sigma(\epsilon, h, \tau)$ 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 $\|\phi - \chi\|_{H^s(\Omega)} \leq C h^{1-s} \|\phi\|_{H_0^1(\Omega)}$, $s = 0, 1$; then

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

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

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

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

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

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 (H_Ω) , (H_β) , (H_{u_0}) and (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*

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

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

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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