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A linear extrapolation method for a general phase relaxation problem

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Analisi numerica. — *A linear extrapolation method for a general phase relaxation problem.* Nota di Xun Jiang, presentata (*) dal Socio E. Magenes.

Abstract. — This paper examines a linear extrapolation time-discretization of a 2D phase relaxation model with temperature dependent convection and reaction. The model consists of a diffusion-advection PDE for temperature and an ODE with double obstacle ± 1 for phase variable. Under a stability constraint, this scheme is shown to converge with optimal orders $\mathcal{O}(\tau|\log\tau|^{1/2})$ for temperature and enthalpy, and $\mathcal{O}(\tau^{1/2}|\log\tau|^{1/2})$ for heat flux as time-step $\tau \downarrow 0$.

Key words: Phase relaxation; Stefan problem; Error estimate; Semi-implicit; Extrapolation.

Riassunto. — *Un metodo di estrapolazione lineare per un problema di rilassamento di fase generale.* Questo lavoro esamina una discretizzazione nel tempo di tipo estrapolazione lineare di un modello di rilassamento di fase 2D con convezione e reazione dipendenti dalla temperatura. Il modello consiste in una equazione a derivate parziali di tipo avvezione-diffusione nell'incognita temperatura e in una disequazione variazionale ordinaria con doppio ostacolo ± 1 per fase variabile. Sotto condizioni di stabilità si dimostra che questo schema converge con ordini ottimali $\mathcal{O}(\tau|\log\tau|^{1/2})$ per temperatura ed entalpia, ed ordini $\mathcal{O}(\tau^{1/2}|\log\tau|^{1/2})$ per flusso di calore quando il passo τ della discretizzazione temporale tende a 0.

1. Introduction

Given a regular bounded domain $\Omega \subset \mathbb{R}^2$, occupied by liquid and solid of certain material, we consider the time discretization of the following nonlinear parabolic problem with temperature dependent convection and reaction:

$$\partial_t c(\theta) + l\partial_t \chi - \nabla \cdot (A\nabla\theta + \boldsymbol{b}(\theta)) = f(\theta), \tag{1.1}$$

$$\varepsilon\partial_t\chi + \Lambda(\chi) \ni \theta, \tag{1.2}$$

for small relaxation parameter $\varepsilon > 0$. Here θ represents the temperature with zero melting temperature (after a translation) and χ is the phase variable satisfying $\chi \in \operatorname{sign}(\theta) =: \Lambda^{-1}(\theta)$, or equivalently as

$$\theta \in \Lambda(\chi) := \begin{cases} [-\infty, 0], & \chi = -1, \\ 0, & -1 < \chi < 1, \\ [0, +\infty], & \chi = +1. \end{cases} \tag{1.3}$$

To get a well-posed problem, we impose vanishing Dirichlet boundary condition for θ along with initial data θ_0 and χ_0. Other parameters are as follows: $c(s) = c(x,t,s)$ is a $C^{1,1}$ function with $c(0) = 0$, $c'(s) \geq c_0$; $A = A(x)$ is a 2×2 matrix such that $a_0|\xi|^2 \leq$ $\leq \xi^T A\xi \leq a_1|\xi|^2$ for all $\xi \in \mathbb{R}^2$, $a_0 > 0$; $\boldsymbol{b}(s) = \boldsymbol{b}(x,t,s)$ is a vector valued Lipschitz function and finally $f(s) = f(x,t,s)$ is a scalar Lipschitz function. The sum $u := c(\theta) +$ $+ l\chi$ is called the enthalpy and l the latent heat. For simplicity, we will assume that $A = I$ is the identity and $l = 1$ and point out that all the results are still valid for the general case. As $\varepsilon \downarrow 0$, the problem is clearly the well-known Stefan problem with an interface

(*) Nella seduta del 9 marzo 1996.

that separates the liquid and solid phases, across which the enthalpy displays a jump discontinuity. When $\varepsilon > 0$, a sharp interface is diffused to a thin transition layer of size $\mathcal{O}(\sqrt{\varepsilon})$ and hence we call this nonlinear system a phase relaxation model.

This model includes the following more general case:

$$\partial_t c(\theta) + l\partial_t \chi - \nabla\cdot(k(\theta)A\nabla\theta + \boldsymbol{b}(\theta)) = f(\theta)\,, \tag{1.4}$$

where $k(s) = k(x,t,s) \geqslant k_0 > 0$ is a temperature-dependent thermal conductivity. This is immediate when one takes Kirchhoff transformation:

$$\tilde{\theta}(x,t) := K(\theta(x,t)) := \int_0^{\theta(x,t)} k(x,t,s)\,ds\,.$$

Model (1.1), (1.2) was first introduced by Visintin in [12, 13] to incooperates the superheating and undercooling phenomena. For more details about this model and its relation to the Stefan problem, we refer to [3, 10-13].

There have been a vast amount of literature on error estimates of numerical approximation of Stefan problem and its variations. Most of them consider the model problem when k is constant and $c(\theta)$ is linear. One of the most successful ones is a recent result of Rulla which confirms for the first time that a nonlinear backward Euler scheme has an optimal order $\mathcal{O}(\tau)$, τ being the (uniform) time step. This result, however, is valid only when k is independent of θ and $\boldsymbol{b} = \boldsymbol{0}, f = 0$ [9]. This last temperature dependent convection case is considered in [3], but with $c(\theta) = \theta$ and thus excludes the more general case when $k = k(\theta)$. Therefore it is left as a question whether there exists a linear scheme which preserves a linear order if k depends on θ (or c is not linear).

In this paper, we examine mainly time discretization for (1.1), (1.2). Let $F(\theta) :=$ $:= \nabla\cdot\boldsymbol{b}(\theta) + f(\theta)$. The *semi-implicit Euler scheme* reads

$$(1/\tau)(c(\Theta^n) - c(\Theta^{n-1})) + (1/\tau)(X^n - X^{n-1}) - \Delta\Theta^n = F(\Theta^{n-1})\,, \tag{1.5}$$

$$(\varepsilon/\tau)(X^n - X^{n-1}) + \Lambda(X^n) \ni \Theta^n\,. \tag{1.6}$$

Here we have treated the convection and reaction explicitly. Due to the nonlinearity of c and coupling, this system leads to a strongly nonlinear algebraic system upon space discretization, which requires an iterative solver and is thus computationally inconvenient. We intend to introduce a linear scheme. Since c is smooth, we can approximate $c(\Theta^n) - c(\Theta^{n-1})$ by $c'(\Theta^{n-1})(\Theta^n - \Theta^{n-1})$. Moreover, we adjust Θ^n in (1.6) by a small amount $\Theta^n - 2\Theta^{n-1} + \Theta^{n-2}$. Thus we introduce a new scheme as follows:

$$(1/\tau)c'(\Theta^{n-1})(\Theta^n - \Theta^{n-1}) + (1/\tau)(X^n - X^{n-1}) - \Delta\Theta^n = F(\Theta^{n-1})\,, \tag{1.7}$$

$$(\varepsilon/\tau)(X^n - X^{n-1}) + \Lambda(X^n) \ni 2\Theta^{n-1} - \Theta^{n-2}\,. \tag{1.8}$$

Subsequently, we call $U^n := c(\Theta^n) + X^n$ the discrete enthalpy. The system is clearly decoupled to a linear elliptic PDE (1.7) with a nonlinear constitutive relation (1.8). We call this scheme the *extrapolation scheme* [3]. Under some natural conditions, we will show that it gives rise to an order of $\mathcal{O}(\tau|\log\tau|^{1/2})$ for θ and u, thus extend the previous results of [3, 4, 9] in 2D. In [3] a semi-explicit scheme is also considered. But the order deteriorates by an additional unremovable factor $1/\sqrt{\varepsilon}$. We do not consider this scheme in the present context.

This paper is organized as follows. In § 2 we discuss weak formulations of the two semidiscretizations (1.5), (1.6) and (1.7), (1.8). Strong stability and pointwise stability estimates are derived in § 3. They are crucial for the error analysis in § 4, which is carried out via an estimate for the semi-implicit scheme. We finish this paper by a brief discussion on Stefan problem.

2. Basic setting

In this section we shall establish the hypotheses upon the data and state precisely the continuous problems as well as the linear extrapolation scheme.

Set $Q := \Omega \times (0, T)$ where $0 < T < +\infty$ is fixed. Hereafter, the symbol $\langle \cdot, \cdot \rangle$ will indicate the L^2 pairing or the duality pairing between $H_0^1(\Omega)$ and $H^{-1}(\Omega)$ and $\|\cdot\|_k$ the norm of the Sobolev space $H_0^k(\Omega)$ for $k \geq 0$, and $H_0^{-k}(\Omega)^*$, the dual of $H_0^{-k}(\Omega)$, for $k < 0$. The weak formulation of (1.1), (1.2) reads: *Find* $\theta \in L^2(0, T; H_0^1(\Omega)) \cap H^1(0, T; L^2(\Omega))$, $\chi \in H^1(0, T; L^2(\Omega))$ *and* $z \in \Lambda(\chi)$ *a.e. in* Q *such that for all* $\phi \in H_0^1(\Omega)$ *and* $\varphi \in L^2(\Omega)$ *the following hold*

$$\langle \partial_t c(\theta) + \partial_t \chi, \phi \rangle + \langle \nabla\theta, \nabla\phi \rangle = -\langle b(\theta), \nabla\phi \rangle + \langle f(\theta), \phi \rangle \quad \textit{a.e. in } (0, T), \tag{2.1}$$

$$\varepsilon \langle \partial_t \chi, \varphi \rangle + \langle z, \varphi \rangle = \langle \theta, \varphi \rangle \quad \textit{a.e. in } (0, T), \tag{2.2}$$

$$\theta(\cdot, 0) = \theta_0, \quad \chi(\cdot, 0) = \chi_0 \quad \textit{a.e. in } \Omega, \tag{2.3}$$

where $\theta_0 \in H_0^1(\Omega) \cap L^\infty(\Omega)$ *and* $|\chi_0| \leq 1$. The functions c', b and f are assumed to be Lipschitz continuous for all $(x, t) \in Q$:

$$|c'(\theta_1) - c'(\theta_2)| \leq c_2 |\theta_1 - \theta_2|, \qquad |b(\theta_1) - b(\theta_2)| \leq L_b |\theta_1 - \theta_2|,$$
$$|f(\theta_1) - f(\theta_2)| \leq L_f |\theta_1 - \theta_2|.$$

The relation $z \in \Lambda(\chi)$ is understood in terms of maximal monotone graph. For the initial data, we take $z_0 \in \Lambda(\chi_0)$ as

$$z_0 := \begin{cases} \theta_0 - \max(\theta_0, 0), & \text{if } \chi_0 = -1, \\ 0, & \text{if } -1 < \chi_0 < 1, \\ \theta_0 - \min(\theta_0, 0), & \text{if } \chi_0 = 1. \end{cases} \tag{2.4}$$

To this end, we further assume the *compatibility condition* between θ_0 and χ_0

$$\|\theta_0 - z_0\|_0 \leq A\sqrt{\varepsilon}, \tag{2.5}$$

for $A > 0$ given. Roughly speaking, it guarantees that the temperature in the solid (liquid) phase is not too high (low). (2.5) is assumed in [3] and is equivalent to a crucial regularity assumption in [9] when an abstract setting is applied to this model (see [3, § 3] for detail). For Stefan problem as a singular limit $\varepsilon \downarrow 0$, it holds automatically. The study of [7] confirms its validity for 1D travelling waves, which reveals a transition region $\{|\chi(\cdot, t)| < 1\}$ of thickness $\mathcal{O}(\sqrt{\varepsilon})$ where $|\theta| \leq C\varepsilon^{1/2}$ and where superheating/undercooling effects take place. Existence and uniqueness of a solution are valid by standard arguments in nonlinear PDEs (see *e.g.* [12]). It satisfies the following a priori estimate

$$\|\theta\|_{L^\infty(0,T;H^1(\Omega))} + \|\partial_t u\|_{L^\infty(0,T;H^{-1}(\Omega))} + \|\theta\|_{H^1(0,T;L^2(\Omega))} \leq C\,, \tag{2.6}$$

which illustrates the typical regularity setting associated with degenerate parabolic problems. Hereafter C denotes a positive constant which may vary at the various occurrences but will always be independent of the relevant parameters ε and τ.

We next introduce the weak form of the time discretization (1.7), (1.8). Let $\tau > 0$ be the time step, $N := T/\tau$ be a positive integer, $t^n := n\tau$, and $I^n := (t^{n-1}, t^n]$ for $1 \leq n \leq N$. For any given sequence $\{y^n\}_{n=0}^N$, we set $\partial y^n := (y^n - y^{n-1})/\tau$ and $\partial^2 y^n = (\partial y^n - \partial y^{n-1})/\tau$. The extrapolation scheme reads as follows: *For any* $1 \leq n \leq N$, *find* $\Theta^n \in H_0^1(\Omega)$, $|X^n| \leq 1$ *and* $Z^n \in \Lambda(X^n)$ *a.e. in* Ω *such that*

$$\Theta^0 = \theta_0\,, \qquad X^0 = \chi_0\,, \tag{2.7}$$

$$\langle c'(\Theta^{n-1})\partial\Theta^n, \phi\rangle + \langle \partial X^n, \phi\rangle + \langle \nabla\Theta^n, \nabla\phi\rangle = -\langle b(\Theta^{n-1}), \nabla\phi\rangle + \langle f(\Theta^{n-1}), \phi\rangle, \tag{2.8}$$

$$\varepsilon\langle \partial X^n, \varphi\rangle + \langle Z^n, \varphi\rangle = \langle 2\Theta^{n-1} - \Theta^{n-2}, \varphi\rangle, \tag{2.9}$$

for all $\phi \in H_0^1(\Omega)$ *and* $\varphi \in L^2(\Omega)$. Existence and uniqueness of solution for the extrapolation scheme is rather obvious in that (2.9) provides an explicit expression for X^n

$$X^n (I - \beta)((\tau/\varepsilon)(2\Theta^{n-1} - \Theta^{n-2}) + X^{n-1})\,, \tag{2.10}$$

where $\beta(s) := \min(s+1, 0) + \max(s-1, 0)$ and (2.7) thus becomes a coercive elliptic PDE for Θ^n. It will be convenient for our stability analysis to choose $\Theta^{-1} = \Theta^{-2} := \Theta^0$, $Z^0 = z_0$ and select X^{-1} so that

$$(\varepsilon/\tau)(X^0 - X^{-1}) + Z^0 = \Theta^0\,. \tag{2.11}$$

Then the constitutive relation $\varepsilon\partial X^n + Z^n = 2\Theta^{n-1} - \Theta^{n-2}$ holds for $n \geq 0$. By (2.5), we have:

$$\sqrt{\varepsilon}\,\|\partial X^0\|_0 = (\sqrt{\varepsilon}/\tau)\,\|X^0 - X^{-1}\|_0 \leq A\,. \tag{2.12}$$

3. Stability

We begin with a strong stability estimate in energy norms needed for the error analysis in the next section.

Lemma 3.1. *There exists a constant* $C > 0$ *depending on* $c_0, A, \|\nabla\theta_0\|_0, L_b$ *and* L_f *such that the following strong stability estimate holds for both the semi-implicit scheme and the extrapolation scheme, with a constraint* $\tau \leq c_0\varepsilon/2$ *for the later*

$$\sum_{n=1}^{N} \tau\|\partial\Theta^n\|_0^2 + \max_{1\leq n\leq N} \|\nabla\Theta^n\|_0^2 \leq C\,. \tag{3.1}$$

Proof. The proofs for both schemes are almost identical. We will prove it for the extrapolation scheme only. We take $\varphi = \Theta^n - \Theta^{n-1} \in H_0^1(\Omega)$ in (2.8) to obtain, after summation from $n = 1$ to $n = m \leqslant N$,

$$(3.2) \qquad c_0\tau \sum_{n=1}^{m} \|\partial\Theta^n\|_0^2 + \tau \sum_{n=1}^{m} \langle \partial X^n, \partial\Theta^n \rangle + \sum_{n=1}^{m} \langle \nabla\Theta^n, \nabla(\Theta^n - \Theta^{n-1}) \rangle =$$

$$= -\tau \sum_{n=1}^{m} \langle b(\Theta^{n-1}), \nabla(\partial\Theta^n) \rangle + \tau \sum_{n=1}^{m} \langle f(\Theta^{n-1}), \partial\Theta^n \rangle.$$

For the third term, we apply the elementary identity

$$(3.3) \qquad 2 \sum_{n=1}^{m} a_n(a_n - a_{n-1}) = |a_m|^2 - |a_0|^2 + \sum_{n=1}^{m} |a_n - a_{n-1}|^2,$$

to get

$$\sum_{n=1}^{m} \langle \nabla\Theta^n, \nabla(\Theta^n - \Theta^{n-1}) \rangle = \frac{1}{2} \sum_{n=1}^{m} \|\nabla(\Theta^n - \Theta^{n-1})\|_0^2 + \frac{1}{2} \|\nabla\Theta^m\|_0^2 - \frac{1}{2} \|\nabla\Theta^0\|_0^2.$$

(1.8) can be written equivalently as $\varepsilon\partial X^n + Z^n = \Theta^n - \tau^2\partial^2\Theta^n$. So the function $\Theta^n - \Theta^{n-1}$ also reads

$$\Theta^n - \Theta^{n-1} = \tau^2\partial^2\Theta^n - \tau^2\partial^2\Theta^{n-1} + \varepsilon(\partial X^n - \partial X^{n-1}) + \tau\partial Z^n.$$

Therefore we can decompose the second term in (3.2) as follows:

$$(3.4) \qquad \tau \sum_{n=1}^{m} \langle \partial X^n, \partial\Theta^n \rangle = \tau^2 \sum_{n=1}^{m} \langle \partial X^n, \partial^2\Theta^n - \partial^2\Theta^{n-1} \rangle +$$

$$+ \varepsilon \sum_{n=1}^{m} \langle \partial X^n, \partial X^n - \partial X^{n-1} \rangle + \tau \sum_{n=1}^{m} \langle \partial X^n, \partial Z^n \rangle.$$

The rightmost term is nonnegative due to the monotonicity of Λ. The first term on the right hand side of (3.4) can be handled as follows via discrete integration by parts, Young's inequality and the fact that $\partial^2\Theta^0 = 0$:

$$\tau^2 \left| \sum_{n=1}^{m} \langle \partial X^n, \partial^2\Theta^n - \partial^2\Theta^{n-1} \rangle \right| =$$

$$= \tau^2 \left| \langle \partial X^m, \partial^2\Theta^m \rangle - \langle \partial X^0, \partial^2\Theta^0 \rangle - \sum_{n=1}^{m} \langle \partial X^n - \partial X^{n-1}, \partial^2\Theta^{n-1} \rangle \right| \leqslant$$

$$\leqslant \frac{4\tau}{3c_0\varepsilon} \frac{\varepsilon}{2} \|\partial X^m\|_0^2 + \frac{3}{8} c_0\tau \sum_{n=1}^{m} \|\partial\Theta^n - \partial\Theta^{n-1}\|_0^2 + \frac{4\tau}{3c_0\varepsilon} \frac{\varepsilon}{2} \sum_{n=1}^{m} \|\partial X^n - \partial X^{n-1}\|_0^2.$$

On using (3.3) once again, we arrive at

$$\varepsilon \sum_{n=1}^{m} \langle \partial X^n, \partial X^n - \partial X^{n-1} \rangle = \frac{\varepsilon}{2} \|\partial X^m\|_0^2 - \frac{\varepsilon}{2} \|\partial X^0\|_0^2 + \frac{\varepsilon}{2} \sum_{n=1}^{m} \|\partial X^n - \partial X^{n-1}\|_0^2.$$

For the convection term, we use Young's inequality to get

$$\left| \sum_{n=1}^{m} \tau\langle b(\Theta^{n-1}), \nabla(\partial\Theta^n) \rangle \right| = \left| \sum_{n=1}^{m} \tau\langle \operatorname{div} b(\Theta^{n-1}), \partial\Theta^n \rangle \right| \leqslant$$

$$\leqslant C \sum_{n=1}^{m} \tau\|\operatorname{div} b(\Theta^{n-1})\|_0^2 + (c_0/16) \sum_{n=1}^{m} \tau\|\partial\Theta^n\|_0^2 \leqslant$$

$$\leqslant CL_b \sum_{n=1}^{m} \tau\|\nabla\Theta^{n-1}\|_0^2 + (c_0/16) \sum_{n=1}^{m} \tau\|\partial\Theta^n\|_0^2.$$

Similarly, applying Young's inequality together with Poincarè's inequality, we obtain

$$\tau \sum_{n=1}^{m} |\langle f(\Theta^{n-1}), \partial\Theta^n\rangle| \leq CL_f \sum_{n=1}^{m} \tau\|\nabla\Theta^{n-1}\|_0^2 + (c_0/16) \sum_{n=1}^{m} \tau\|\partial\Theta^n\|_0^2 .$$

Combining the above estimates, as well as (2.12), and then the discrete Gronwall's inequality, the assertion follows immediately provided $\tau \leq c_0\varepsilon/2$ since $\sum_n \|\partial(\Theta^n - \Theta^{n-1})\|_0^2 \leq 2\sum_n \|\partial\Theta^n\|_0^2$. For the semi-implicit scheme, this constraint is not needed since the missing term $\sum_n \langle \partial X^n, \partial^2\Theta^n - \partial^2\Theta^{n-1}\rangle$ is the only one responsible for it. ■

In order to deal with the nonlinearity of $c(\theta)$ in (1.1), we also need the following pointwise stability inspired by [1, 4]:

LEMMA 3.2. *For both the semi-implicit and extrapolation schemes, it holds*

$$\max_{1\leq n\leq N} \|\Theta^n\|_{L^\infty(\Omega)} + \max_{1\leq n\leq N} \|X^n\|_{L^\infty(\Omega)} \leq C .$$

PROOF. Let $C_0 := \|\Theta^0\|_{L^\infty(\Omega)}$ and $L_F := L_\beta + L_f$. According to (2.10) it is clear that $\|X^n\|_{L^\infty(\Omega)} \leq 1$. With $T^n = \Theta^n$ for the semi-implicit scheme and $2\Theta^{n-1} - \Theta^{n-2}$ for the extrapolation scheme, we now proceed to prove

$$\max_{x\in\Omega} \Theta^n \leq C_n := C_0 e^{n\tau L_F/c_0} + (|F(0)|/L_F)(e^{n\tau L_F/c_0} - 1), \qquad 1 \leq n \leq N,$$

by induction which obviously implies the conclusion of the lemma. Suppose the conclusion holds for $n-1$. By virtue of (2.10), $X^n - X^{n-1} = (\tau/\varepsilon)T^n - \beta((\tau/\varepsilon)T^n + X^n)$, and thus

$$c'(\Theta^{n-1})\Theta^n - \Delta\Theta^n = \tau F(\Theta^{n-1}) - \frac{\tau}{\varepsilon}T^n + \beta\left(\frac{\tau}{\varepsilon}T^n + X^n\right) + c'(\Theta^{n-1})\Theta^{n-1} \leq$$
$$\leq \tau F(\Theta^{n-1}) + c'(\Theta^{n-1})\Theta^{n-1} \leq \tau(F(0) + L_F C_{n-1}) + c'(\Theta^{n-1})C_{n-1} .$$

By the maximum principle,

$$\max_{x\in\Omega} \Theta^n \leq \tau|F(0)|/c_0 + (1 + \tau L_F/c_0)C_{n-1} .$$

Since $1 + \tau L_F/c_0 \leq e^{\tau L_F/c_0}$, straight forward calculations lead to

$$\tau|F(0)|/c_0 + (1 + \tau L_F/c_0)C_{n-1} \leq C_n .$$

It completes the induction argument. A similar inequality holds for $\min_{x\in\Omega}\Theta^n$. ■

4. Error analysis

Let us denote the approximation error by

$$E(\varepsilon,\tau) := \max_{1\leq n\leq N} (\|u(t^n) - U^n\|_{-1} + \sqrt{\varepsilon}\|\chi(t^m) - X^m\|_0) + \tag{4.1}$$
$$+ \left(\sum_{n=1}^{N} \int_{I^n} \tau\varepsilon\|\partial_t\chi - \partial X^n\|_0^2\,dt\right)^{1/2} + \left(\sum_{n=1}^{N} \int_{I^n} (\|\theta - \Theta^n\|_0^2 + \tau\|\theta - \Theta^n\|_1^2)\,dt\right)^{1/2} .$$

First we state an error estimate for the semi-implicit scheme without proof. The basic idea of its proof traces back to [9] using semi-groups of contraction in Hilbert spaces and is further exploited in [3]. In fact, when $F = 0$, the general result of [9] in the abstract setting applies. For the case $F \neq 0$, the proof follows lines in [3, Theorem 5.2, Theorem 6.1].

LEMMA 4.1. *For the semi-implicit scheme* (1.5), (1.6), *there exists* $C > 0$, *depending on* c_0, c_2, $\|\nabla \theta_0\|_0$, *A and T but independent of* ε, *and* τ, *such that* $E(\varepsilon, \tau) \leqslant C\tau$.

Even though the semi-implicit scheme yields an optimal order τ of convergence, it requires the solution of a nonlinear elliptic problem. We now show that the extrapolation scheme exhibits the advantages of both having a linear elliptic problem and an optimal order of $\tau|\log \tau|^{1/2}$. The extra factor $\log \tau$ is due to the nonlinearity of c as showed in Lemma 4.2 below. Numerically, it is considered as a constant. We point out that the abstract setting of [9] does not apply in the present content and therefore the proof is also different.

Let $G\colon H^{-1}(\Omega) \to H_0^1(\Omega)$ stand for the Green's operator associated with $-\Delta$ and a vanishing Dirichlet boundary condition. Hence

$$G\varphi \in H_0^1(\Omega){:}\ \langle \nabla G\varphi, \nabla \psi\rangle = \langle \varphi, \psi \rangle, \qquad \forall \psi \in H_0^1(\Omega), \qquad \varphi \in H^{-1}(\Omega),$$

and

$$\|\varphi\|_{-1}^2 = \|\nabla G\varphi\|_0^2 = \langle \varphi, G\varphi\rangle. \tag{4.2}$$

Denote $Y^n := c(\Theta^n) - c(\Theta^{n-1}) - c'(\Theta^{n-1})(\Theta^n - \Theta^{n-1})$. We first need to prove a lemma that deals with the nonlinearity of $c(\theta)$. We will need the following 2D Sobolev inequality [2, pp. 155, 158]:

$$\|\phi\|_{L^q(\Omega)} \leqslant Cq^{1/2}\|\nabla \phi\|_{L^2(\Omega)}, \qquad \forall \phi \in H_0^1(\Omega). \tag{4.3}$$

As a result, the following lemma is the only place where we have to require the space dimension $d = 2$.

LEMMA 4.2. *For both semi-implicit and extrapolation schemes, there holds*

$$\sum_{n=1}^{m} |\langle Y^n, G(u(t^n) - U^n)\rangle| \leqslant C\tau|\log \tau|^{1/2} \max_{1 \leqslant n \leqslant m} \|u(t^n) - U^n\|_{-1}.$$

PROOF. For $p > 2$ sufficiently large with $p' := p/(p-1)$, we use Hölder's inequality twice to get

$$\sum_{n=1}^{m} |\langle Y^n, G(u(t^n) - U^n)\rangle| \leqslant c_2 \sum_{n=1}^{m} \langle |\Theta^n - \Theta^{n-1}|^2, |G(u(t^n) - U^n)|\rangle \leqslant$$

$$\leqslant C \sum_{n=1}^{m} \left(\int_\Omega |\Theta^n - \Theta^{n-1}|^{2p'}\right)^{1/p'} \left(\int_\Omega |G(u(t^n) - U^n)|^p\right)^{1/p} \leqslant$$

$$\leqslant C \sum_{n=1}^{m} \left(\int_\Omega |\Theta^n - \Theta^{n-1}|^2\right)^{1/p'} (\|\Theta^n - \Theta^{n-1}\|_{L^\infty(\Omega)}^{(2p'-2)/p'})\|G(u(t^n) - U^n)\|_{L^p(\Omega)}.$$

Then by Lemmas 3.1 and 3.2, (4.2) and (4.3) we further derive

$$\sum_{n=1}^{m} |\langle Y^n, G(u(t^n) - U^n)\rangle| \leqslant C \sum_{n=1}^{m} \|\Theta^n - \Theta^{n-1}\|_0^{2/p'} \sqrt{p}\, \|\nabla G(u(t^n) - U^n)\|_0 \leqslant$$

$$\leqslant C\sqrt{p} \max_{1\leqslant n\leqslant m} \|u(t^n) - U^n\|_{-1} \sum_{n=1}^{m} \|\Theta^n - \Theta^{n-1}\|_0^{2/p'} \leqslant$$

$$\leqslant C\sqrt{p} \max_{1\leqslant n\leqslant m} \|u(t^n) - U^n\|_{-1} \left(\sum_{n=1}^{m} 1^p\right)^{1/p} \left(\sum_{n=1}^{m} \|\Theta^n - \Theta^{n-1}\|_0^2\right)^{1/p'} \leqslant$$

$$\leqslant C\sqrt{p} \max_{1\leqslant n\leqslant m} \|u(t^n) - U^n\|_{-1} \tau^{-1/p} \tau^{1/p'} \leqslant C\sqrt{p}\, \tau^{1-2/p} \max_{1\leqslant n\leqslant m} \|u(t^n) - U^n\|_{-1}.$$

Choosing $p := |\log \tau|$ we derive the desired result. ■

Now we are ready to present our main theorem. We notice that it includes the result of [3, § 7] in which $c(s) = s$, but our approach is simpler and avoids seeking an extra regularity of $3/2$ derivative in time.

THEOREM 4.1. *There exists $C > 0$, depending on $c_0, c_2, \|\nabla\theta_0\|_0, A, L_b, L_f$, and T but independent of ε and τ, such that $E(\varepsilon, \tau) \leqslant C\tau|\log\tau|^{1/2}$ provided $\tau \leqslant c_0\varepsilon/4$.*

PROOF. Suppose that $\tilde{\Theta}^n, \tilde{X}^n$ and $\tilde{U}^n := \tilde{\Theta}^n + \tilde{X}^n$ are solutions to the semi-implicit scheme. Denote by Θ^n, X^n and $U^n := X^n + \Theta^n$ the solutions to the extrapolation scheme. We proceed now to compare these functions with $\tilde{\Theta}^n, \tilde{X}^n$ and $\tilde{U}^n$ solutions to (2.8) and (1.6). We subtract the corresponding differential equations to obtain two error equations:

$$\langle(\tilde{U}^n - U^n) - (\tilde{U}^{n-1} - U^{n-1}), \phi\rangle + \tau\langle\nabla(\tilde{\Theta}^n - \Theta^n), \nabla\phi\rangle = \tag{4.4}$$
$$= -\tau\langle b(\tilde{\Theta}^{n-1}), \nabla\phi\rangle,$$

$$\varepsilon\langle\partial\tilde{X} - \partial X^n, \varphi\rangle + \langle A_\delta(\tilde{X}^n) - A_\delta(X^n), \varphi\rangle = \tag{4.5}$$
$$= \langle\tilde{\Theta}^n - \Theta^n, \varphi\rangle + \tau\langle\tau\partial^2\Theta^n - \tau\partial^2\Theta^{n-1}, \varphi\rangle$$

for all $\phi \in H_0^1(\Omega)$ and $\varphi \in L^2(\Omega)$. We first take $\phi = G(\tilde{U}^n - U^n) \in H_0^1(\Omega)$, add (4.4) over n from 1 to $m \leqslant N$, and use the identity

$$2\sum_{n=1}^{m} a_n \sum_{i=1}^{n} a_i = \left|\sum_{n=1}^{m} a_n\right|^2 + \sum_{n=1}^{m} |a_n|^2, \tag{4.6}$$

and the fact $\tilde{U}^0 = U^0$ to get

$$\|\tilde{U}^m - U^m\|_{-1}^2 + \tau^2 \sum_{n=1}^{m} \|\partial(\tilde{U}^n - U^n)\|_{-1}^2 + 2\sum_{n=1}^{m} \tau\langle\tilde{\Theta}^n - \Theta^n, \tilde{X}^n - X^n\rangle +$$
$$+2\sum_{n=1}^{m} \tau\|\tilde{\Theta}^n - \Theta^n\|_0^2 - \sum_{n=1}^{m} \tau\langle b(\tilde{\Theta}^{n-1}) - b(\Theta^{n-1}), \nabla G(\tilde{U}^n - U^n)\rangle -$$
$$- \sum_{n=1}^{m} \langle Y^n, G(\tilde{U}^n - U^n)\rangle =: \mathrm{I} + \mathrm{II}.$$

Secondly, we sum (4.4) (with n replaced by i) for $1 \leqslant i \leqslant n$, choose $\phi = 2\tau(\tilde{\Theta}^n - \Theta^n) \in H_0^1(\Omega)$ as a test function, and sum the resulting expression on n from 1 to m. On using the elementary identity (4.6), we obtain

$$2 \sum_{n=1}^{m} \tau\langle c(\tilde{\Theta}^n) - c(\Theta^n), \tilde{\Theta}^n - \Theta^n \rangle +$$

$$+2 \sum_{n=1}^{m} \tau\langle \tilde{\Theta}^n - \Theta^n, \tilde{X}^n - X^n \rangle + \tau^2 \left\| \sum_{n=1}^{m} \nabla(\tilde{\Theta}^n - \Theta^n) \right\|_0^2 +$$

$$+\tau \sum_{n=1}^{m} \tau\|\nabla(\tilde{\Theta}^n - \Theta^n)\|_0^2 = -2\tau^2 \sum_{n=1}^{m} \langle b(\tilde{\Theta}^{n-1}) - b(\Theta^{n-1}), \nabla(\tilde{\Theta}^n - \Theta^n)\rangle -$$

$$-2\tau \sum_{n=1}^{m} \langle Y^n, \tilde{\Theta}^n - \Theta^n \rangle =: \mathrm{III} + \mathrm{IV}.$$

Adding the above two equations gives

$$\text{(4.7)} \quad \|\tilde{U}^m - U^m\|_{-1}^2 + 4 \sum_{n=1}^{m} \tau\langle \tilde{\Theta}^n - \Theta^n, \tilde{X}^n - X^n \rangle +$$

$$+2(1 + c_0) \sum_{n=1}^{m} \tau\|\tilde{\Theta}^n - \Theta^n\|_0^2 + \tau \sum_{n=1}^{m} \tau\|\nabla(\tilde{\Theta}^n - \Theta^n)\|_0^2 \leqslant \mathrm{I} + \mathrm{II} + \mathrm{III} + \mathrm{IV}.$$

Selecting $\varphi := 4\tau(\tilde{X}^n - X^n) \in L^2(\Omega)$ in (4.5), summing over $1 \leqslant n \leqslant m$ and using (4.6) again along with the monotonicity of Λ, we arrive at

$$\text{(4.8)} \quad 2\varepsilon\|\tilde{X}^m - X^m\|_0^2 + 2\varepsilon\tau \sum_{n=1}^{m} \tau\|\partial\tilde{X}^n - \partial X^n\|_0^2 \leqslant 2\varepsilon\|\tilde{X}^0 - X^0\|_0^2 +$$

$$+4 \sum_{n=1}^{m} \tau\langle \tilde{\Theta}^n - \Theta^n, \tilde{X}^n - X^n \rangle + 4 \sum_{n=1}^{m} \tau^2\langle \tau\partial^2\Theta^n - \tau\partial^2\Theta^{n-1}, \tilde{X}^n - X^n \rangle.$$

Adding now (4.7) and (4.8), recalling that $\tilde{X}^0 = X^0$, leads to

$$\text{(4.9)} \quad \|\tilde{U}^m - U^m\|_{-1}^2 + 2\varepsilon\|\tilde{X}^m - X^m\|_0^2 + 2 \sum_{n=1}^{m} \tau\|\tilde{\Theta}^n - \Theta^n\|_0^2 +$$

$$+\tau \sum_{n=1}^{m} \tau\|\nabla(\tilde{\Theta}^n - \Theta^n)\|_0^2 + 2\tau\varepsilon \sum_{n=1}^{m} \tau\|\partial\tilde{X}^n - \partial X^n\|_0^2 \leqslant$$

$$\leqslant 4 \sum_{n=1}^{m} \tau^2\langle \tau\partial^2\Theta^n - \tau\partial^2\Theta^{n-1}, \tilde{X}^n - X^n \rangle + \mathrm{I} + \mathrm{II} + \mathrm{III} + \mathrm{IV}.$$

For term I, we have

$$|\mathrm{I}| \leqslant \tau L_b \sum_{n=1}^{m} \|\tilde{\Theta}^{n-1} - \Theta^{n-1}\|_0 \|\tilde{U}^n - U^n\|_{-1} \leqslant$$

$$\leqslant (1/2) \sum_{n=1}^{m} \tau\|\tilde{\Theta}^{n-1} - \Theta^{n-1}\|_0^2 + C \sum_{n=1}^{m} \tau\|\tilde{U}^n - U^n\|_{-1}^2,$$

as a result of Lipschitz continuity of b and Young's inequality. By Lemma 4.2, with $u(t^n)$ replaced by $\tilde{U}^n$,

$$|\mathrm{II}| \leqslant C\tau|\log\tau|^{1/2} \max_{1 \leqslant n \leqslant m} \|\tilde{U}^n - U^n\|_{-1} \leqslant C\tau^2|\log\tau| + (1/2) \max_{1 \leqslant n \leqslant m} \|\tilde{U}^n - U^n\|_{-1}^2.$$

Using the strong stability result of Lemma 3.1 for both $\nabla\tilde{\Theta}^n$ and $\nabla\Theta^n$ as well as the Lipschitz continuity of b, we readily see

$$|\mathrm{III}| \leqslant C\tau^2 \sum_{n=1}^{m} \|\tilde{\Theta}^{n-1} - \Theta^{n-1}\|_0 \leqslant C\tau^2 + (1/2) \sum_{n=1}^{m} \tau\|\tilde{\Theta}^{n-1} - \Theta^{n-1}\|_0^2.$$

For IV, since $|Y^n| \leqslant c_2|\Theta^n - \Theta^{n-1}|^2$, we easily get

$$|\mathrm{IV}| \leqslant C\tau \sum_{n=1}^{m} \|\Theta^n - \Theta^{n-1}\|_0^2 \leqslant C\tau^2 ,$$

where we have also used Lemma 3.1. By discrete integration by parts, Lemma 3.1 and $\partial^2 \Theta^0 = 0$, we estimate the first term on the right hand side of (4.9) as follows:

$$4 \sum_{n=1}^{m} \tau^2 \langle \tau\partial^2 \Theta^n - \tau\partial^2 \Theta^{n-1}, \widetilde{X}^n - X^n \rangle =$$

$$= 4\tau^2 \langle \tau\partial^2 \Theta^m, \widetilde{X}^m - X^m \rangle - 4\tau^2 \langle \tau\partial^2 \Theta^0, \widetilde{X}^0 - X^0 \rangle -$$

$$-4\tau^2 \sum_{n=1}^{m} \langle (\widetilde{X}^n - X^n) - (\widetilde{X}^{n-1} - X^{n-1}), \tau\partial^2 \Theta^{n-1} \rangle \leqslant$$

$$\leqslant (C\tau^4/\varepsilon) \|\partial\Theta^m - \partial\Theta^{m-1}\|_0^2 + \varepsilon\tau \|\widetilde{X}^m - X^m\|_0^2 +$$

$$+\tau\varepsilon \sum_{n=1}^{m} \|\tau\partial\widetilde{X}^n - \tau\partial X^n\|_0^2 + (C\tau^4/\varepsilon) \sum_{n=1}^{m} \|\partial\Theta^{n-1} - \partial\Theta^{n-2}\|_0^2 \leqslant$$

$$\leqslant C\tau^2 + \varepsilon\tau \|\widetilde{X}^m - X^m\|_0^2 + \tau\varepsilon \sum_{n=1}^{m} \|\tau\partial\widetilde{X}^n - \tau\partial X^n\|_0^2 .$$

Inserting this inequality to (4.9), in conjunction with Lemma 3.1, discrete Gronwall's inequality yields the result of Theorem 4.1. ■

We finish our analysis with a further discussion on the Stefan problem with temperature dependent conduction, convection and reaction, namely, the singular limit of (1.4), (1.2) as $\varepsilon \downarrow 0$ which leads to (1.1) coupled with the constitutive relation $\chi \in \mathrm{sign}(\theta)$ by Kirchhoff transformation. Since the approximation of (1.1), (1.2) to the Stefan problem is of order $\mathcal{O}(\sqrt{\varepsilon})$ [6], our result shows that the extrapolation scheme is a linear scheme for the Stefan problem with a suboptimal order $\mathcal{O}(\tau|^{1/2} \log\tau|^{1/2})$ upon equating $\tau = c_0 \varepsilon/4$. For the Stefan problem, a semi-explicit scheme (or nonlinear Chernoff formula) is simpler and achieves the same order. We refer to [3, 4, 8] for more details. To our knowledge designing a linear scheme with a linear order even for the simplest Stefan problem $\partial_t u - \Delta\beta(u) = 0$ is still an open problem.

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