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A Second Order Splitting Method for the Cahn-Hilliard Equation

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Summary. A semi-discrete finite element method requiring only continuous elements is presented for the approximation of the solution of the evolutionary, fourth order in space, Cahn-Hilliard equation. Optimal order error bounds are derived in various norms for an implementation which uses mass lumping. The continuous problem has an energy based Lyapunov functional. It is proved that this property holds for the discrete problem.

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§ 1. Introduction

We shall consider a finite element approximation of the Cahn-Hilliard equation

$$\text{(1.1a)} \qquad \frac{\partial u}{\partial t} = \Delta\phi(u) - \gamma\Delta^2 u \qquad x\in\Omega,\ t>0$$

subject to initial and boundary conditions

$$\text{(1.1b)} \qquad u(x,0) = u_0(x)\ x\in\Omega,$$

$$\text{(1.1c)} \qquad \frac{\partial u}{\partial \nu} = \frac{\partial}{\partial \nu}(\phi(u) - \gamma\Delta u) = 0 \qquad x\in\partial\Omega,\ t>0$$

where Ω is a bounded domain in $\mathbb{R}^n (n\leqq 3)$ with a sufficiently smooth boundary $\partial\Omega, \nu$ is the outward unit normal vector along $\partial\Omega, \gamma$ is a prescribed positive constant and $\phi(\cdot)$ is the cubic

$$\text{(1.1d)} \qquad \phi(u) = \psi'(u); \qquad \psi(u) = \gamma_2\frac{u^4}{4} + \gamma_1\frac{u^3}{3} + \frac{\gamma_0}{2}u^2; \qquad \gamma_2 > 0.$$

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This is a generalised diffusion problem for $u(x,t)$ the concentration of one component of a binary mixture. It is used to model the phase separation which occurs upon the quenching of such a mixture into the spinodal region; for example see Langer (1971) and Novick-Cohen and Segel (1984).

It is known Elliott and Zheng (1986) that if the initial data $u_0 \in H_E^2(\Omega) \equiv \{\eta \in H^2(\Omega)\colon \partial\eta/\partial\nu = 0 \text{ on } \partial\Omega\}$ then (1.1) has a unique solution for all time. A standard conforming Galerkin finite element method requires that the approximation space be contained in $H_E^2(\Omega)$; see Elliott and French (1987) for computations in one space dimension. Another possibility is the use of nonconforming elements, Elliott and French (1989). In contrast, we propose here a splitting method based on H^1 elements. Let us introduce w, the chemical potential, defined by

$$w = \phi(u) - \gamma \Delta u.$$

If follows that (1.1a, c) may be rewritten as

$$\frac{\partial u}{\partial t} - \Delta w = 0 \qquad x \in \Omega, \quad t > 0, \tag{1.3a}$$

$$-\gamma \Delta u + \phi(u) - w = 0 \qquad x \in \Omega, \quad t > 0, \tag{1.3b}$$

$$\frac{\partial u}{\partial \nu} = 0, \quad \frac{\partial w}{\partial \nu} = 0 \qquad x \in \partial\Omega, \ t > 0. \tag{1.3c}$$

Clearly (1.3) represent a natural splitting of (1.1) into two coupled problems which are second order in space. Integrating (1.3a, b) against test functions $\eta \in H^1(\Omega)$ and using (1.3c) we obtain

$$\left(\frac{\partial u}{\partial t}, \eta\right) + (\nabla w, \nabla \eta) = 0, \tag{1.4a}$$

$$\gamma(\nabla u, \nabla \eta) + (\phi(u) - w, \eta) = 0, \tag{1.4b}$$

where $(\cdot,\cdot)$ denotes the $L^2(\Omega)$ inner product.

Let us now consider a quasi-uniform family $\mathbf{T}^h$ of polygonal decompositions of Ω (by triangles or rectangles, with boundary elements being allowed to have one curvilinear edge) with characteristic parameter $h \in (0,1)$. Associated with $\mathbf{T}^h$ is the finite element space $V^h \subset H^1(\Omega)$,

$$V^h = \{\chi \in C^0(\bar{\Omega})\colon \chi|_\tau \in \mathbf{P}_m, \tau \in \mathbf{T}^h\} \tag{1.5}$$

where $\mathbf{P}_m$ is the set of all polynomials of degree no greater than the positive integer m. The splitting method is: find $\{u^h, w^h\}\colon [0,T] \to V^h \times V^h$ such that

$$(u_t^h, \chi) + (\nabla w^h, \nabla \chi) = 0 \qquad \forall \chi \in V^h, \tag{1.6a}$$

$$\gamma(\nabla u^h, \nabla \chi) + (\phi(u^h) - w^h, \chi) = 0 \qquad \forall \chi \in V^h, \tag{1.6b}$$

$$u^h(0) = u_0^h, \tag{1.6c}$$

where $u_0^h \in V^h$ is a suitable approximation to u_0.

If $\{\chi_i\}_{i=1}^{N^h}$ is a basis for V^h and

$$M_{ij} = (\chi_i, \chi_j) \qquad \text{"mass" matrix}$$
$$K_{ij} = (\nabla \chi_i, \nabla \chi_j) \qquad \text{"stiffness" matrix}$$

then

$$u^h(t) = \sum_{i=1}^{N^h} c_i(t)\,\chi_i; \qquad w^h(t) = \sum_{i=1}^{N^h} d_i(t)\,\chi_i$$

where $\underset{\sim}{c}$ and $\underset{\sim}{d}$ solve the initial value problem

(1.7a) $$M\frac{d\underset{\sim}{c}}{dt} + K\underset{\sim}{d} = 0,$$

(1.7b) $$\gamma K\underset{\sim}{c} + \underset{\sim}{f}(\underset{\sim}{c}) = M\underset{\sim}{d}$$

with

(1.7c) $$\{\underset{\sim}{f}(\underset{\sim}{c})\}_i = (\phi(u^h(t)), \chi_i).$$

Equations (1.7a) and (1.7b) can be combined to give

(1.8) $$M\frac{d\underset{\sim}{c}}{dt} + \gamma K M^{-1} K\underset{\sim}{c} + K M^{-1}\underset{\sim}{f}(\underset{\sim}{c}) = 0.$$

Since the matrices M and K are positive definite and $\phi(\cdot)$ is defined by (1.1d), it follows that the initial value problem for (1.8) has a unique solution on some time interval, possibly depending on h. Observe that (1.8) is, in essence, a discretization of (1.1a) of the form

(1.9) $$\frac{d\underset{\sim}{c}}{dt} + \gamma A^2\underset{\sim}{c} + A\underset{\sim}{\Phi}(\mathbf{c}) = 0$$

where $A = M^{-1}K$ and $(-A)$ is the finite element approximation of the Laplacian and $\underset{\sim}{\Phi}(\mathbf{c}) = M^{-1}\underset{\sim}{f}(\mathbf{c})$. Algorithms for the numerical solution of (1.9) should not depend on the formation of the full matrix M^{-1}. In the case of piecewise linear finite elements $V^h \equiv \mathbf{S}^h$,

(1.10) $$\mathbf{S}^h = \{\chi \in C(\bar{\Omega}):\ \chi|_\tau \in \mathbf{P}_1\ \tau \in \mathbf{T}^h\},$$

with $\mathbf{T}^h$ being a simplicial decomposition of Ω, a lumped-mass numerical integration rule for the L^2 inner product leads to a diagonal mass matrix viz:

(1.11a) $$(\chi, \eta)^h = \sum_{i=1}^{N^h} m_i\,\chi(x_i)\,\eta(x_i) \qquad \chi, \eta \in C(\bar{\Omega}),$$

(1.11b) $$M_{ii} = m_i, \qquad M_{ij} = 0 \quad i \neq j,$$

where $\{x_i\}_{i=1}^{N^h}$ is the set of simplex vertices and

$$(1.12\text{a})\quad |(\chi,\eta)^h-(\chi,\eta)|\leqq Ch^2\|\chi\|_1\,\|\eta\|_1 \qquad \forall \chi,\eta\in \mathbf{S}^h,$$

$$(1.12\text{b})\quad |(\chi,\eta)^h-(\chi,\eta)|\leqq Ch^2\|\chi\|_1\,\|\eta\|_2 \qquad \forall \chi\in \mathbf{S}^h,\quad \eta\in H^2(\Omega),$$

$$(1.12\text{c})\quad c_0|\chi|_0\leqq|\chi|_h=((\chi,\chi)^h)^{\frac{1}{2}}\leqq c_1|\chi|_0 \qquad \forall \chi\in \mathbf{S}^h,$$

$$(1.12\text{d})\quad |(\chi,\eta)^h-(\chi,\eta)|\leqq Ch[h|\eta|_2+\|\eta\|_1]\,|\chi|_0 \qquad \forall \chi\in \mathbf{S}^h,\quad \eta\in H^2(\Omega),$$

$$(1.12\text{e})\quad |\eta-\chi|_h\leqq C[h^2|\eta|_2+|\eta-\chi|_0] \qquad \forall \chi\in \mathbf{S}^h,\quad \eta\in H^2(\Omega).$$

We shall prove in § 3 that the following splitting method is $O(h^2)$ accurate: find $\{u^h, w^h\}$: $[0,T]\to \mathbf{S}^h\times \mathbf{S}^h$ such that

$$(1.13\text{a})\qquad (u_t^h,\chi)^h+(\nabla w^h,\nabla\chi)=0 \qquad \forall \chi\in \mathbf{S}^h,$$

$$(1.13\text{b})\qquad \gamma(\nabla u^h,\nabla\chi)+(\phi(u^h)-w^h,\chi)^h=0 \qquad \forall \chi\in \mathbf{S}^h,$$

$$(1.13\text{c})\qquad u^h(0)=u_0^h$$

where $u_0^h\in \mathbf{S}^h$ is a suitable approximation to u_0.

In § 2 we show that the discretization methods (1.6) and (1.13) have the desirable property of inheriting interesting features of (1.1); namely the existence of a Liapunov functional, global existence in time and, in the case of $\gamma_2<0$, finite time blow up.

The analysis of (1.13) depends upon error bounds for an H^1 projection and an L^2 projection both of which are defined with numerical integration. These bounds are proved in the Appendix, together with a justification of (1.11) and (1.12).

Finally we note here, for convenience, the inverse inequalities

$$(1.14\text{a})\qquad |\chi|_{0,\infty}\leqq C\left(\ln\left(\frac{1}{h}\right)\right)^{1/2}\|\chi\|_1, \qquad n=2,$$

$$(1.14\text{b})\qquad |\chi|_{0,\infty}\leqq Ch^{-3/2}|\chi|_0, \qquad n=3,$$

$$(1.14\text{c})\qquad \|\chi\|_1\leqq\frac{C}{h}|\chi|_0$$

which hold for all $\chi\in \mathbf{S}^h$.

§ 2. Properties of the Numerical Method

It is known that the solution of (1.1) satisfies, (cf. Elliott and Zheng 1986),

$$(2.1\text{a})\qquad \int_\Omega u(x,t)\,dx=\int_\Omega u_0(x)\,dx,$$

$$(2.1\text{b})\qquad \frac{d}{dt}\mathbf{F}(u)+|w|_1^2=0, \qquad t>0$$

where

$$\mathbf{F}(u)=\frac{\gamma}{2}|u|_1^2+(\psi(u),1).$$

(2.1c) If $\gamma_2>0$ then (1.1) has a solution for all t.
(2.1d) If $\gamma_2<0$ and $-\mathbf{F}(u_0)$ is sufficiently larger then there exists a T^* such that $\lim\limits_{t\to T^*}|u(t)|_0=\infty$.

The functional $\mathbf{F}(\cdot)$ is an energy functional based upon the free energy $\psi(u)$ and the interfacial energy $\gamma|\nabla u|^2/2$. It is of physical importance. Simulating qualitative features of nonlinear evolution equations is a desirable attribute of discretization schemes. The purpose of this section is to show that (1.6) and (1.13) possess properties similar to (2.1a, b, c, d). It is sufficient to consider explicitly only the case (1.13).

The conservation of mass property (2.1a) follows immediately by taking $\chi=1$ in (1.13a), viz.

$$\frac{d}{dt}(u^h,1)^h=0$$

implies that

$$(u^h(t),1)^h=(u_0^h,1)^h. \tag{2.2}$$

Let

$$\mathbf{F}^h(\chi)=\frac{\gamma}{2}|\chi|_1^2+(\psi(\chi),1)^h \tag{2.3}$$

so that the equation

$$\frac{d}{dt}\mathbf{F}^h(u^h)=\gamma(\nabla u^h,\nabla u_t^h)+(\phi(u^h),u_t^h)^h$$

holds and taking $\chi=u_t^h$ in (1.13b) yields

$$\frac{d}{dt}\mathbf{F}^h(u^h)=(w^h,u_t^h)^h=-|w^h|_1^2, \tag{2.4}$$

where we have used $\chi=w^h$ in (1.13a).

It remains to prove discrete equivalents of (2.1c, d). This is achieved in the following two lemmas.

Lemma 2.1. *If $\gamma_2>0$ then u^h is defined in $\Omega\times[0,T]$ for any $T>0$.*

Proof. Integrate (2.4) in time to obtain

$$\mathbf{F}^h(u^h)+\int_0^T|w^h|_1^2\,dt=\mathbf{F}^h(u_0^h). \tag{2.5}$$

Since $\gamma_2 > 0$ we have

$$\psi(s) \geqq -C_0 \qquad \text{for all } s \in \mathbb{R}$$

so that

$$\mathbf{F}^h(u^h) = \frac{\gamma}{2} |u^h|_1^2 + (\psi(u^h), 1)^h \geqq \frac{\gamma}{2} |u^h|_1^2 - C$$

where C is independent of u^h. Using this in (2.5) yields the relation

$$\frac{\gamma}{2} |u^h(T)|_1^2 + \int_0^T |w^h(t)|_1^2 \, dt \leqq C + \mathbf{F}^h(u_0^h). \tag{2.6}$$

Since for constant η the equation $(\eta, 1)^h = 0$ is equivalent to $\eta = 0$, the usual proof for the Poincare inequality yields the existence of C such that

$$\|\eta\|_1 \leqq C[|\eta|_1 + |(\eta, 1)^h|] \qquad \forall \eta \in H^1(\Omega). \tag{2.7}$$

(Indeed using (1.13a) it follows that for h sufficiently small the constant C in (2.7) may be taken to be independent of h.) It follows from (2.6) and (2.7) that $u^h(t)$ is bounded in $H^1(\Omega)$ independently of t. Since $u^h \in \mathbf{S}^h$ this implies that $|u^h(t)|_{0,\infty}$ is bounded independently of t (but possibly depending on h). From this fact we deduce the global existence of a solution to (1.8). $\square$

Lemma 2.2. *If $\gamma_2 < 0$ and $-\mathbf{F}^h(u_0^h)$ is sufficiently large then there is a time T^h such that $\lim_{t \to T^h} |u^h(t)|_0 = \infty$.*

Proof. Without loss of generality we may assume that $(u_0^h, 1)^h = 0$. (If this is not the case then we study $\bar{u}^h = u^h - (u_0^h, 1)^h / |1|_h$.) From this assumption we have

$$(u^h(t), 1)^h = 0 \qquad \forall t \in [0, T] \tag{2.8}$$

where $[0, T]$ is the interval on which there exists a solution. Let $W: [0, T] \to \mathbf{S}^h$ be the solution of

$$(\nabla W, \nabla \chi) = (u^h, \chi)^h \qquad \forall \chi \in \mathbf{S}^h \tag{2.9}$$

with $(W, 1) = 0$. From the relation above and (1.13a) we have

$$W_t = -w^h + (w^h, 1)/|\Omega|.$$

Taking $\chi = W_t$ in (2.9) yields

$$\frac{1}{2} \frac{d}{dt} |W|_1^2 = (\nabla W_t, \nabla W) = -(\nabla w^h, \nabla W) = -(u^h, w^h)^h.$$

Noting (1.13b), this becomes

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} |W|_1^2 &= -\gamma |u_h|_1^2 - (\phi(u^h), u^h)^h \\ &= -2\mathbf{F}^h(u^h(t)) + (2\psi(u^h) - \phi(u^h) u^h, 1)^h. \end{aligned} \tag{2.10}$$

Since $\gamma_2<0$ there exists $C>0$ such that

$$2\psi(s)-\phi(s)\,s=-\frac{\gamma_2}{2}\,s^4-\frac{1}{3}\,\gamma_1\,s^3\geqq-\frac{\gamma_2}{4}\,s^4-C. \tag{2.11}$$

Furthermore the Cauchy-Schwarz inequality implies that

$$((u^h)^4,1)^h\geqq|u^h|_h^4/|1|^h. \tag{2.12}$$

Since, from (2.7) and (2.9), we have that

$$|W|_1\leqq C|u^h|_h, \tag{2.13}$$

inequalities (2.10), (2.11) and (2.12) imply that

$$\frac{d}{dt}|W|_1^2\geqq K|W|_1^4-4\mathbf{F}^h(u_0^h)-C \tag{2.14}$$

where K and C are is a positive constants. Provided $(-4\mathbf{F}^h(u_0^h)-C)>0$, the differential inequality (2.14) implies finite time blow-up for $|W|_1$ and hence by (2.13) of $|u^h|_h$. □

§ 3. A Second Order Splitting Method

In this section we derive optimal order error bounds for the piece-wise linear approximation (1.13) with lumped mass integration. We will use the "projections" $\{\tilde{u}^h,\tilde{w}^h\}\colon[0,T]\to\mathbf{S}^h\times\mathbf{S}^h$ defined by:

$$(\nabla\tilde{w}^h,\nabla\chi)=(-\Delta w+\delta_1^h,\chi)^h\qquad\forall\chi\in\mathbf{S}^h, \tag{3.1a}$$

$$(\tilde{w}^h-w,1)=0,\qquad(-\Delta w+\delta_1^h,1)^h=0, \tag{3.1b}$$

and

$$\gamma(\nabla\tilde{u}^h,\nabla\chi)=(\tilde{w}^h-\phi(u)-\delta_2^h,\chi)^h\qquad\forall\chi\in\mathbf{S}^h, \tag{3.2a}$$

$$(\tilde{u}^h-u,1)=0,\qquad(\tilde{w}^h-\phi(u)-\delta_2^h,1)^h=0. \tag{3.2b}$$

Thus $\{\tilde{u}^h,\tilde{w}^h\}$ satisfy discrete Neumann problems and because of the numerical integration the real numbers $\{\delta_1^h,\delta_2^h\}$ are needed to ensure compatibility. Projections of this form were used previously for the heat equation by Johnson and Thomee (1983). It is convenient to use the error decomposition:

$$u^h-u\equiv\theta^u+\rho^u\equiv(u^h-\tilde{u}^h)+(\tilde{u}^h-u), \tag{3.3a}$$

$$w^h-w\equiv\theta^w+\rho^w=(w^h-\tilde{w}^h)+(\tilde{w}^h-w). \tag{3.3b}$$

Lemma 3.1. *If $\{u,w\}$ are sufficiently smooth then, for $t\in[0,T]$,*

$$|D_t^j\rho^u|_0+h|D_t^j\rho^u|_1\leqq Ch^2\qquad j=0,1,2,\dots, \tag{3.4}$$

$$|D_t^j\rho^w|_0+h|D_t^j\rho^w|_1\leqq Ch^2\qquad j=0,1,2,\dots, \tag{3.5}$$

and, for $n \leqq 2$,

$$|D_t^j \rho^u|_{0,\infty} \leqq C h^2 (\log 1/h)^{n-1} \qquad j=0,1,2,\ldots, \tag{3.6}$$

$$|D_t^j \rho^w|_{0,\infty} \leqq C h^2 (\log 1/h)^{n-1} \qquad j=0,1,2,\ldots, \tag{3.7}$$

where C is independent of h and t and $D_t^j = (\partial/\partial t)^j$.

Proof. The key to these error bounds in Theorem A.1 of the Appendix. First we prove the bounds for ρ^w. Note that since $(\Delta w, 1) = 0$,

$$\begin{aligned} |D_t^j \delta_1^h| &\leqq C |(D_t^j (\Delta w, 1)^h| = C |(\Delta D_t^j w, 1)^h - (\Delta D_t^j w, 1)| \\ &\leqq C h^2 \|D_t^j \Delta w\|_2, \end{aligned} \tag{3.8}$$

where we have used (1.12b). The bounds (3.5) and (3.7) are now a direct consequence of Theorem (A.1).

Noting that

$$(\phi(u) - w, 1) = \gamma(\Delta u, 1) = 0$$

and from (3.1b),

$$(D_t^j \tilde{w}^h, 1) = (D_t^j w, 1) = (D_t^j \phi(u), 1)$$

we find that

$$\begin{aligned} |D_t^j \delta_2^h| &\leqq C |D_t^j (\tilde{w}^h - \phi(u), 1)^h| \\ &= C |[(D_t^j \tilde{w}^h, 1)^h - (D_t^j \tilde{w}^h, 1)] + [(D_t^j \phi(u), 1) - (D_t^j \phi(u), 1)^h]| \\ &\leqq C h^2 [\|D_t^j \tilde{w}^h\|_1 + \|D_t^j \phi(u)\|_2]. \end{aligned} \tag{3.9}$$

It follows from (3.9), (3.5) and (3.2a) that

$$(\nabla \tilde{u}^h, \nabla \chi) = (-\Delta u, \chi)^h + (\mathscr{E}, \chi)^h,$$

where

$$\mathscr{E} = \frac{1}{\gamma} (\tilde{w}^h - w - \delta_2^h)$$

and

$$|D_t^j \mathscr{E}|_h \leqq C h^2.$$

The inequalities (3.4) and (3.6) are now a direct consequence of Theorem (A.1). □

Remark 3.1. In Lemma 3.2 we will need the bound $|\tilde{u}_t^h|_{0,\infty} \leqq C$ for h sufficiently small. For $n \leqq 2$ this follows from (3.6). For $n=3$ we have, using the inverse norm inequality (1.14b) on the subspace $\mathbf{S}^h$

$$\begin{aligned} |\tilde{u}_t^h|_{0,\infty} &\leqq |u_t - \pi^h u_t|_{0,\infty} + |\pi^h u_t - \tilde{u}_t^h|_{0,\infty} + |u_t|_{0,\infty} \\ &\leqq C h^2 + h^{-3/2} |\pi^h u_t - \tilde{u}_t^h|_0 + |u_t|_{0,\infty} \\ &\leqq C(h^2 + h^{1/2}) + |u_t|_{0,\infty} \end{aligned}$$

where $\pi^h \colon C(\bar{\Omega}) \to \mathbf{S}^h$ is the piecewise linear interpolation operator.

Lemma 3.2. *There exist constants C independent of h, u^h and w^h such that if $\|u^h(\cdot)\|_\infty$ is bounded independently of h then,* $\forall t\in[0, T]$,

$$|\theta^u|_h^2+\int_0^t |\theta^w|_h^2\,d\tau \leqq Ch^4+|\theta^u(0)|_h^2, \tag{3.10}$$

$$|\theta^u|_1^2+|\theta^w|_h^2+\int_0^t [|\theta_t^u|_h^2+|\theta^w|_1^2]\,d\tau \leqq Ch^4+\|\theta^u(0)\|_1^2+|\theta^w(0)|_h^2. \tag{3.11}$$

Proof. From (1.13a) we have for each $\chi\in S^h$

$$\begin{aligned}(\theta_t^u,\chi)^h+(\nabla\theta^w,\nabla\chi)&=-(\tilde{u}_t^h,\chi)^h-(\nabla\tilde{w}^h,\nabla\chi)\\&=(-\rho_t^u,\chi)^h-(u_t,\chi)^h+(\Delta w-\delta_1^h,\chi)^h\end{aligned}$$

and since $u_t=\Delta w$ we have

$$(\theta_t^u,\chi)^h+(\nabla\theta^w,\nabla\chi)=(-\rho_t^u-\delta_1^h,\chi)\qquad\forall\chi\in\mathbf{S}^h. \tag{3.12}$$

Subtracting (1.13b) from (3.2a) we obtain

$$(\theta^w,\chi)^h-\gamma(\nabla\theta^u,\nabla\chi)=(\phi(u^h)-\phi(u)-\delta_2^h,\chi)^h\qquad\forall\chi\in\mathbf{S}^h. \tag{3.13}$$

Taking $\chi=\theta^u$ in (3.12) and $\chi=\theta^w/\gamma$ in (3.13) and adding the resulting equations yields

$$\frac{1}{2}\frac{d}{dt}|\theta^u|_h^2+|\theta^w|_h^2=(-\rho_t^u-\delta_1^h,\theta^u)^h+(\phi(u^h)-\phi(u)-\delta_2^h,\theta^u)^h/\gamma.$$

Using the bounds for ρ_t^u, δ_1^h and δ_2^h proved in Lemma 3.1 and the Lipschitz continuity of $\phi(\cdot)$, together with the assumption on $\|u^h(\cdot)\|_\infty$, we obtain

$$\frac{d}{dt}|\theta^u|_h^2+|\theta^w|_h^2\leqq C[h^4+|\theta^u|_h^2] \tag{3.14}$$

and an application of Gronwall's lemma yields (3.10).

Next, take $\chi=\theta^w$ in (3.12), $\chi=\theta_t^u$ in (3.13) and subtract the resulting equations to yield

$$\begin{aligned}|\theta^w|_1^2+\frac{\gamma}{2}\frac{d}{dt}|\theta^u|_1^2&=(-\rho_t^u-\delta_1^h,\theta^w)^h+(\delta_2^h-\phi(u^h)+\phi(u),\theta_t^u)^h\\&\leqq C[h^2|\theta^w|_h+h^2|\theta_t^u|_h+|\theta^u|_h|\theta_t^u|_h].\end{aligned} \tag{3.15}$$

Differentiating (3.13) with respect to t we obtain

$$(\theta_t^w,\chi)^h-\gamma(\nabla\theta_t^u,\nabla\chi)=([\phi(u^h)-\phi(u)]_t-\delta_{2,t}^h,\chi)^h\qquad\forall\chi\in\mathbf{S}^h. \tag{3.16}$$

Taking $\chi=\theta^w$ in (3.16); $\chi=\gamma\theta_t^u$ in (3.12) and adding the resulting relations we obtain

$$\frac{1}{2}\frac{d}{dt}|\theta^w|_h^2+\gamma|\theta_t^u|_h^2=(-\gamma\rho_t^u-\gamma\delta_1^h,\theta_t^u)^h+([\phi(u^h)-\phi(u)]_t-\delta_{2,t}^h,\theta^w)^h.$$

Noting that

$$\frac{\partial}{\partial t}[\phi(u)-\phi(u^h)]=\phi'(u)[u_t-\tilde{u}_t^h]+(\phi'(u)-\phi'(u^h))\tilde{u}_t^h$$
$$+\phi'(u^h)(\tilde{u}^h)(\tilde{u}_t^h-u_t^h),$$

the bounds for $\tilde{u}_t^h, \rho^u, \rho_t^u, \delta_1^h$ and $\delta_{2,t}^h$ obtained in Lemma 3.1 and Remark 3.1 can be used on the right-hand side of (3.17) to obtain

$$\frac{1}{2}\frac{d}{dt}|\theta^w|_h^2+\gamma|\theta_t^u|_h^2\leqq C[h^2|\theta_t^u|_h+h^2|\theta^w|_h+|\theta^u|_h|\theta^w|_h]. \tag{3.18}$$

Adding (3.15) to (3.18) and using the inequality $2ab\leqq\mathscr{E}a^2+b^2/\mathscr{E}$ in the obvious way yields, for $t\in[0,T]$,

$$|\theta_t^u|_h^2+|\theta^w|_1^2+\frac{d}{dt}|\theta^u|_1^2+\frac{d}{dt}|\theta^w|_h^2\leqq C[h^4+|\theta^u|_h^2+|\theta^w|_h^2] \tag{3.19}$$

where C depends on T, u, γ and $\|u^h\|_\infty$ but is independent of h. The estimate (3.11) is now a direct consequence of (3.19), (3.10) and Gronwall's inequality.

Theorem 3.1. *If*

$$|u(0)-u_0^h|_0\leqq Ch^2 \tag{3.20}$$

then

$$\|u-u^h\|_{L^\infty(L^2)}+\|w-w^h\|_{L^2(L^2)}\leqq Ch^2. \tag{3.21}$$

If

$$\|\tilde{u}^h(0)-u_0^h|_1\leqq Ch^2, \qquad |\tilde{w}^h(0)-w^h(0)|_0\leqq Ch^2 \tag{3.22}$$

then

$$\|u-u^h\|_{L^\infty(L^2)}+\|w-w^h\|_{L^\infty(L^2)}+\|u_t-u_t^h\|_{L^2(L^2)}\leqq Ch^2 \tag{3.23}$$

$$\|u-u^h\|_{L^\infty(H^1)}+\|w-w^h\|_{L^2(H^1)}\leqq Ch \tag{3.24}$$

and if $n\leqq 2$,

$$\|u-u^h\|_{L^\infty(L^\infty)}+\|w-w^h\|_{L^2(L^\infty)}\leqq Ch^2(\ln 1/h)^{n-1}. \tag{3.25}$$

Proof. The theorem is a direct consequence of Lemmas 3.1 and 3.2. Initially we assume $\|u^h(\cdot)\|_\infty$ is bounded independently of h on $\Omega\times[0,T]$; however, by a standard argument, we may use (3.21) and (3.23), *a posteriori*, to show this assumption holds. (See Thomee 1984, pp. 154–155.) $\square$

Corollary 3.1. *If* $u_0^h=\tilde{u}^h(0)$ *then the error estimates* (3.23)–(3.25) *of Theorem* 3.1 *hold.*

Proof. Since $\tilde{u}^h(0)-u_0^h=0$, we need only derive the second estimate of (3.22). Taking $\chi=\theta^w(0)$ in (3.13) we have

$$|\tilde{w}^h(0)-w^h(0)|_h^2=|\theta^w(0)|_h^2=(\phi(\tilde{u}^h(0))-\phi(u_0)-\delta_2^h,\theta^w(0))^h$$

or

$$|\tilde{w}^h(0)-w^h(0)|_0\leqq C(|\rho^u(0)|_0+|\delta_0^h(0)|\leqq Ch^2$$

by the estimates of Lemma 3.1. $\square$

A more practical approximation of the initial data is obtained by the H^1-projection. Define $P_1^h\colon H^1(\Omega)\to\mathbf{S}^h$ by

(3.26a) $$(\nabla(P_1^h v-v),\nabla\chi)=0\qquad\forall\chi\in\mathbf{S}^h,$$

(3.26b) $$(P_1^h v,1)=(v,1).$$

Recall that

(3.27) $$|v-P_1^h v|_0+h|v-P_1^h v|_1\leqq Ch^2\|v\|_2.$$

Corollary 3.2. *If* $u_0^h=P_1^h u_0$ *then the error estimates* (3.23)–(3.25) *of Theorem* 3.1 *hold.*

In order to prove this Corollary we need the following lemma.

Lemma 3.3. *If* $v\in H_E^2(\Omega)$ *then*

(3.28) $$|(v,\chi)-(v,\chi)^h|\leqq Ch^2\|v\|_2|\chi|_0\qquad\forall\chi\in\mathbf{S}^h.$$

Proof. Setting

$$\tilde{\chi}=\chi-M,\qquad M=(\chi,1)/|\Omega|$$

so that

$$(\tilde{\chi},1)=0\quad\text{and}\quad|M|\leqq|\chi|_0/|\Omega|^{1/2}$$

we obtain

$$\begin{aligned}|(v,\chi)-(v,\chi)^h|&\leqq|(v,\tilde{\chi})-(v,\tilde{\chi})^h|+|M|\,|(v,1)-(v,1)^h|\\&\leqq|(P_1^h v,\tilde{\chi})-(P_1^h v,\tilde{\chi})^h|\\&\quad+|(v-P_1^h v,\tilde{\chi})-(v-P_1^h v,\tilde{\chi})^h|\\&\quad+Ch^2\|v\|_2|\chi|_0.\end{aligned}$$

Applying (1.12a), an inverse norm inequality and (3.27) to the second term of the above inequality we obtain

(3.29) $$|(v,\chi)-(v,\chi)^h|\leqq|(P_1^h v,\tilde{\chi})-(P_1^h v,\tilde{\chi})^h|+Ch^2\|v\|_2|\chi|_0.$$

Defining $p^h, \bar{p}^h \in \mathbf{S}^h$ by

$$(3.30\text{a}) \qquad (\nabla p^h, \nabla \lambda) = (\tilde{\chi}, \lambda) \quad \forall \lambda \in \mathbf{S}^h, \ (p^h, 1) = 0,$$

$$(3.30\text{b}) \qquad (\nabla \bar{p}^h, \nabla \lambda) = (\tilde{\chi}, \lambda)^h \quad \forall \lambda \in \mathbf{S}, \ (\bar{p}^h, 1) = 0,$$

it follows from Theorem A.1 of the Appendix that

$$(3.31) \qquad |p - \bar{p}^h|_0 \leqq C h^2 |\tilde{\chi}|_0.$$

Furthermore

$$|(P_1^h v, \tilde{\chi}) - (P_1^h v, \tilde{\chi})^h| = |(\nabla P_1^h v, \nabla(p^h - \bar{p}^h))| = |(\nabla v, \nabla(p^h - \bar{p}^h))|,$$

and an integration by parts, using the fact that $v \in H_E^2(\Omega)$, yields

$$|(P_1^h v, \tilde{\chi}) - (P_1^h v, \tilde{\chi})^h| = |(\Delta v, p^h - \bar{p}^h)| \leqq C h^2 |\Delta v|_0 \, |\tilde{\chi}|_0.$$

This last inequality, together with (3.29), proves the lemma. $\square$

Proof of Corollary 3.2. Rewriting (3.2a) at $t=0$ we obtain

$$(3.32) \qquad (\nabla \tilde{u}^h(0), \nabla \chi) = (-\Delta u_0, \chi)^h + + \frac{(\rho^w - \delta_2^h, \chi)^h}{\gamma} \quad \forall \chi \in \mathbf{S}^h$$

and rewriting (3.26a) at $t=0$ using the fact that $u_0 \in H_E^2(\Omega)$ we obtain

$$(3.33) \qquad (\nabla P_1^h u_0, \nabla \chi) = (-\Delta u_0, \chi) \quad \forall \chi \in \mathbf{S}^h.$$

Thus referring to the proof of Theorem A.1 and taking $v = u_0$, $v^h = \tilde{u}^h(0)$, $z^h = P_1^h u_0$, $f = -\Delta u_0$ and $\mathscr{E} = (\rho^w - \delta_2^h)/\gamma$ we obtain the first inequality of (3.22) using the known bounds on ρ^w and δ_2^h. To finish the proof it is sufficient to prove

$$(3.34) \qquad |w(0) - w^h(0)|_0 \leqq C h^2$$

since

$$\tilde{w}^h(0) - w^h(0) = \rho^w + w(0) - w^h(0).$$

Introducing $P_0^h\colon H^2(\Omega) \to \mathbf{S}^h$ defined by

$$(3.35\text{a}) \qquad (P_0^h \eta - \eta, \chi)^h = 0 \quad \forall \chi \in \mathbf{S}^h$$

which satisfies, (see Appendix)

$$(3.35\text{b}) \qquad |P_0^h \eta - \eta|_h + |P_0^h \eta - \eta|_0 \leqq C h^2 |\eta|_2$$

we set

$$(3.36) \qquad \xi = w(0) - \phi(u_0), \qquad \xi^h = w^h(0) - P_0^h \phi(P_1^h u_0).$$

Note that

$$\begin{aligned}|\phi(u_0)-P_0^h\,\phi(P_1^h\,u_0)|_0 &\leqq |\phi(u_0)-P_0^h\,\phi(u_0)|_0+|P_0^h\,\phi(u_0)-P_0^h\,\phi(P_1^h\,u_0)|_0\\ &\leqq C h^2|\phi(u_0)|_2+C|P_0^h(\phi(u_0)-\phi(P_1^h\,u_0))|_h\\ &\leqq C h^2|\phi(u_0)|_2+C|\phi(u_0)-\phi(P_1^h\,u_0)|_h\\ &\leqq C h^2|\phi(u_0)|_2+C|u_0-P_1^h\,u_0|_h\\ &\leqq C h^2\end{aligned}$$

where we have used the approximation properties of P_0^h and P_1^h and the inequalities (1.12c, e). Hence (3.34) is a consequence of the estimate

$$|\xi-\xi^h|_0\leqq C h^2. \tag{3.37}$$

By definition the following equation holds:

$$\begin{aligned}(\xi^h,\chi)^h&=(w^h(0)-P_0^h\,\phi(P_1^h\,u_0),\chi)^h=(w^h(0)-\phi(P_1^h\,u_0),\chi)^h\\ &=\gamma(\nabla P_1^h\,u_0,\nabla\chi)=\gamma(\nabla u_0,\nabla\chi)=(\xi,\chi).\end{aligned}$$

Setting $E^h=\xi^h-P_0^h\,\xi$ it follows from the equation above that

$$\begin{aligned}|E^h|_0^2\leqq C|E^h|_h^2&=(\xi^h,E^h)^h-(P_0^h\,\xi,E^h)^h=(\xi,E^h)-(\xi,E^h)^h\\ &\leqq C h^2|E^h|_0\end{aligned}$$

because $\xi=-\gamma\Delta u_0\in H_E^2(\Omega)$ and Lemma 3.3 holds. Since

$$|\xi-\xi^h|_0\leqq|\xi-P_0^h\,\xi|_0+|E^h|_0$$

we finally obtain (3.37). □

Appendix

Lumped Mass Integration

We wish to define a numerical integration scheme which satisfies (1.11a, b) and (1.12a, b, c, d, e) in the cases of Ω being an open interval in $\mathbb{R}$, a rectangle in $\mathbb{R}^2$ and a convex domain in $\mathbb{R}^n (n=2,3)$ with a smooth boundary. The convexity of Ω is assumed for ease of exposition. There exists Ω^h being the union of simplices belonging to a quasi-uniform triangulation such that *either* $\Omega^h\equiv\Omega$ when Ω is an interval or rectangle *or* $\Omega^h\subset\Omega$ and the distance between $\partial\Omega$ and $\partial\Omega^h$ is bounded by Ch^2 when $\partial\Omega$ is smooth. Denoting by π_τ^h the linear interpolation operator on τ, the numerical integration scheme is defined by

$$(\chi,\eta)^h=\sum_{\tau\subset\Omega^h}\int_\tau\pi_\tau^h(\chi\eta)\,dx\qquad\forall\chi,\eta\in C(\bar\Omega) \tag{A.1}$$

which clearly satisfies (1.11). The inequalities (1.12a, b, c) are well-known for Ω being an interval or polygon. Otherwise we need to estimate $\int_{\Omega\setminus\Omega^h}\chi\eta\,dx$. However, for all $\eta \in H^1(\Omega)$, the following inequality holds, see Barrett and Elliott (1987a; Lemma 3.2).

$$(A.2)\qquad |\eta|_{0,\Omega\setminus\Omega^h} \leqq Ch[h|\eta|_{1,\Omega} + |\eta|_{0,\partial\Omega^h}] \leqq Ch\,\|\eta\|_{1,\Omega}$$

which implies that,

$$(A.3)\qquad \int_{\Omega\setminus\Omega^h} \chi\eta\,dx \leqq Ch^2\,\|\chi\|_1\,\|\eta\|_1 \qquad \forall \chi, \eta \in H^1(\Omega).$$

The bounds (1.12a, b) immediately follow. Inequality (1.12c) follows from (1.12a) and the inverse inequality (1.14c).

The error bound (1.12d) is a consequence of the definition (A.1) and the interpolation error bound on each triangle, viz.

$$\begin{aligned}|(\chi,\eta)-(\chi,\eta)^h| &= \sum_{\tau\subset\Omega^h}\int_\tau [\chi\eta - \pi_\tau^h(\chi\eta)]\,dx + \int_{\Omega\setminus\Omega^h}\chi\eta\,dx\\ &\leqq Ch^2\Big[\sum_{\tau\subset\Omega^h}|\chi\eta|_{2,\tau} + \|\chi\|_1\,\|\eta\|_1\Big].\end{aligned}$$

Expanding the semi-norm $|\chi\eta|_{2,\tau}$ and using the inverse inequalities (1.14a) yields (1.12d). Finally the inequality (1.12e) follows by noting that

$$|\eta-\chi|_h = |\pi^h\eta - \chi|_h \leqq C|\pi^h\eta-\chi|_0 \leqq C[|\pi^h\eta-\eta|_0 + |\eta-\chi|_0].$$

Finite Element Approximation of a Neumann Problem with Numerical Integration

We consider the approximation of the following semi-definite Neumann problem: let $v\in H^1(\Omega)$

$$(A.4)\qquad (\nabla u, \nabla\eta) = (f,\eta) \qquad \forall \eta\in H^1(\Omega),$$

where $f\in H^2(\Omega)$ is given and $(f,1)=0$. The finite element problem is to find $v^h\in \mathbf{S}^h$ such that

$$(A.5)\qquad (\nabla v^h, \nabla\chi) = (f+\mathscr{E},\chi)^h \qquad \forall\chi\in\mathbf{S}^h,$$

$$(A.6)\qquad (v^h - v, 1) = 0$$

and $\mathscr{E}$ satisfies,

$$(A.7)\qquad (\mathscr{E},1)^h = -(f,1)^h.$$

Condition (A.7) guarantees the existence of a unique v^h satisfying (A.5) and (A.6). We now present the approximation theorem. See Barrett and Elliott (1987b) for similar results.

Theorem A.1. *If*

$$(A.8)\qquad |\mathscr{E}|_h \leqq Ch^2$$

then the error bound

$$|v-v^h|_0+h|v-v^h|_1\leqq Ch^2 \tag{A.9}$$

holds. Furthermore, for $n\leqq 2$, *we have*

$$\|v-v^h\|_\infty\leqq C(\log 1/h)^{n-1}h^2. \tag{A.10}$$

Proof. By standard arguments the finite element Galerkin approximation $z^h\in\mathbf{S}^h$ such that

$$(\nabla z^h,\nabla\chi)=(f,\chi)\qquad\forall\chi\in\mathbf{S}^h,\qquad(z^h-v,1)=0 \tag{A.11}$$

satisfies

$$|v-z^h|_0+h|v-z^h|_1\leqq Ch^2|v|_2 \tag{A.12}$$

and

$$\|v-z^h\|_\infty\leqq Ch^2(\ln 1/h)^{1/2}\|v\|_2. \tag{A.13}$$

(Note that $H^2(\Omega)$ regularity for v follows from the assumptions concerning Ω). Comparing z^h and v^h we note that

$$\begin{aligned}(\nabla(z^h-v^h),\nabla\chi)&=(f,\chi)-(f,\chi)^h-(\mathscr{E},\chi)^h\\&\leqq Ch^2\|f\|_2\,\|\chi\|_1+|\mathscr{E}|_h\,|\chi|_h\\&\leqq Ch^2\|\chi\|_1,\end{aligned}$$

where the estimates (1.12b, c) have been used. Since the mean value of (z^h-v^h) is zero, we have by Poincare's inequality $\|z^h-v^h\|_1\leqq C|z^h-v^h|_1$. Taking $\chi=z^h-v^h$ in (A.14) yields

$$\|z^h-v^h\|\leqq Ch^2.$$

The error bounds (A.9) and (A.10) are now an immediate consequence of (A.12), (A.13) and the subspace Sobolev inequality (1.14a).

Discrete L^2-Projection

We shall prove the bounds (3.35b). Observe that, by the projection Eq. (3.35a),

$$|\eta-P_0^h\eta|_0\leqq|P_0^h\eta-\chi|_0+|\chi-\eta|_0.$$

Furthermore, the inequality

$$\begin{aligned}|\eta - P_0^h \eta|_0 &\leqq |P_0^h \eta - \chi|_0 + |\chi - \eta|_0 \\ &\leqq C|P_0^h \eta - \chi|_h + |\chi - \eta|_0 \\ &\leqq C[|\eta - \chi|_h + |\eta - \chi|_0] \qquad \forall \chi \in S^h\end{aligned}$$

holds. Choosing $\chi = \pi^h \eta$ yields (3.35b) upon noting (1.12e) and the interpolation error bound.

References

Barrett, J.W., Elliott, C.M.: Total flux estimates for a finite element approximation of elliptic equations. I.M.A. J. Numer. Anal. **7**, 129–148 (1987a)

Barrett, J.W., Elliott, C.M.: A practical finite element approximation of a semi-definite Neumann problem on a curved domain. Num. Math. **51**, 23–36 (1987b)

Elliott, C.M., French, D.: Numerical studies of the Cahn-Hilliard equation for phase separation. I.M.A. J. Appl. Math. **38**, 97–128 (1987)

Elliott, C.M., French, D.: A non-conforming finite element method for the two-dimensional Cahn-Hilliard equation. S.I.A.M. J. Numer. Anal 1989 (to appear)

Elliott, C.M., Zheng, S.: On the Cahn-Hilliard equation. Arch. Rat. Mech. Anal **96**, 339–357 (1986)

Johnson, C., Thomee, V.: Error estimates for some mixed finite element methods for parabolic type problems. RAIRO Anal. Numer. **15**, 41–78 (1983)

Langer, J.S.: Theory of spinodal decomposition in alloys. Annals of Physics **65**, 53–86 (1971)

Novick-Cohen, A., Segel, L.A.: Nonlinear aspects of the Cahn-Hilliard equation. Physica (D) **10**, 277–298 (1984)

Thomee, V.: Galerkin Finite Element Methods for Parabolic Problems. L.N.S.M. # 1054, Berlin Heidelberg, New York Springer 1984

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