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A Numerical Method for a Simplified Anisotropic Phase Field Model

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Abstract

We consider the phase field model consisting of the system of p.d.e' s

$$q(\theta)\phi_t = \nabla \cdot (A(\theta)\nabla\phi) + f(\phi, u),$$
$$u_t = \Delta u + [p(\phi)]_t,$$

where $\phi = \phi(x, y, t)$ is the phase indicator function,$\theta = \arctan(\phi_y/\phi_x)$, $u = u(x, y, t)$ is the temperature, q, p, and f are given scalar functions, and A is a 2×2 matrix of given functions of θ. This system describes the evolution of phase and temperature in a two phase medium, and is posed for $t \geq 0$ on a rectangle in the x, y plane with appropriate boundary and initial conditions. We solve the system numerically by a finite difference method, based on the explicit Euler scheme for the first equation and the Crank-Nicolson-ADI method for the second, and show results of relevant numerical experiments.

Keywords: anisotropic phase field model, finite difference methods

1. Introduction

The traditional method for the numerical solution of evolution equations modeling phase transition phenomena (e.g. solidification) is to discretize the partial differential equations (p.d.e's) that describe the mathematical model (e.g. the heat equation) in the, say, two domains where the material has different phase, and couple this discretization with appropriate interface conditions valid on the free boundary (interface) separating the two phases. This is quite complicated since it requires tracking the unknown interface and interpolating it on a given grid, or using space-time discretizations, for example adaptive grids that follow the interface.

As an alternative, one could use *phase-field models*, [1]. These models replace tracking and approximating the free interface with the introduction of another p.d.e.,

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which is coupled with the energy (heat) equation in the whole domain and, in addition to the original unknown (the temperature), of a new unknown (the *phase*) which is equal to a characteristic value, e.g. 0 in the solid and 1 in the liquid phase, and changes abruptly in a small neighborhood of the interface. The solution of this system of two coupled nonlinear parabolic p.d.e's evolves from suitable initial conditions and its solution should exhibit a sharp moving front in the phase variable that defines the interface of the two phases of the medium, and, when appropriate, describe the development of the complex geometrical patterns (*dendrites*, regions where one phase locally penetrates into the other) that occur in realistic solidification problems. The numerical solution of this coupled system of p.d.e's is quite time consuming, even in two space dimensions, since it requires fine spatial discretizations, small time steps and large total run times in order to describe the interface with some accuracy.

In this note we consider a specific phase field model in two space dimensions, due to McFadden, Wheeler, Sekerka, Wang et al., [2]−[5]. The model consists of a system of two p.d.e's of the form

$$\begin{aligned} q(\theta)\phi_t &= \nabla\cdot(A(\theta)\nabla\phi) + f(\phi,u), \\ u_t &= \Delta u + [p(\phi)]_t, \end{aligned} \tag{1}$$

where $\phi = \phi(x,y,t)$ is the phase indicator function, $\theta = \arctan(\phi_y/\phi_x)$, and $u = u(x,y,t)$ is the temperature, defined on a rectangle Ω in the x,y plane for $t \geq 0$. The functions q, f, p are given smooth scalar functions of their indicated arguments and A is the anisotropy matrix given by

$$A(\theta) = \begin{pmatrix} r^2(\theta) & -r(\theta)r'(\theta) \\ r(\theta)r'(\theta) & r^2(\theta) \end{pmatrix}.$$

Here, $r(\theta) = 1 + \delta_\gamma \cos(k\theta)$, where δ_γ is a constant characteristic of the anisotropy of the surface tension and $k > 1$ is an integer describing the direction of branching. We also have $q(\theta) = (1 + \delta_\gamma \cos(k\theta))/m(1 + \delta_\mu \cos(k\theta))$, where m is a constant and δ_μ a constant characteristic of the kinetic coefficient anisotropy. If $\delta_\gamma = \delta_\mu = 0$ the model is *isotropic*. If $\delta_\gamma = 0$ and $\delta_\mu \neq 0$ ($A(\theta) = I$), we will call the model *semi-anisotropic*. The model is supplemented by given initial conditions $\phi(x,y,0) = \phi_0(x,y)$, $u(x,y,0) = u_0(x,y)$, $(x,y) \in \Omega$, and boundary conditions of Neumann or Dirichlet type for ϕ and u on the boundary $\partial\Omega$ of Ω for $t \geq 0$.

The system (1) has been solved numerically by Wang, [4], and Wang and Sekerka, [5], in the general, *anisotropic* case (when both δ_γ and δ_μ are nonzero) by an 'explicit-implicit' finite difference scheme that uses the explicit Euler method for advancing the phase field over a temporal step by the first p.d.e. of (1), and then using an ADI (Alternating Direction Implicit) scheme for the second p.d.e to solve for the temperature field. These two references contain many interesting numerical computations and measurements of the efficiency of the underlying numerical technique.

In his Ph.D. Thesis, Sfyrakis, [6], has constructed and analyzed Euler-ADI type finite difference schemes for a generalization the system (1) in the anisotropic case.

The advantages of the schemes are their improved stability and accuracy and their potential for parallel implementation.

It should he noted that in a recent series of papers Rappaz and his collaborators, [7]−[9], have considered similar systems to (1), for which they have proved existence and uniqueness of weak solutions. They have also constructed and implemented fully discrete, adaptive finite element methods and used them to simulate dendritic growth in the anisotropic case.

In what follows, we develop in Section 2 an explicit Euler-ADI scheme that will be used in this paper. In Section 3 we describe the results of some numerical experiments that we performed with this scheme.

2. The explicit Euler-ADI method in the anisotropic case.

On a square $\Omega = [\alpha, \beta] \times [\alpha, \beta]$ of the x, y plane, we consider the following generalization of (1) in the anisotropic case: For $(x, y, t) \in \Omega \times [0, T]$ we consider the system

$$\begin{aligned} q\phi_t &= \partial_x(a\partial_x\phi) + \partial_y(d\partial_y\phi) + \partial_x(b\partial_y\phi) - \partial_y(b\partial_x\phi) + f, \\ u_t &= \Delta u + \partial_t p, \end{aligned} \tag{2}$$

where $q := q(x, y, t, \phi, \partial_x\phi, \partial_y\phi)$, $a := a(x, y, t, \phi, \partial_x\phi, \partial_y\phi)$, $d := d(x, y, t, \phi, \partial_x\phi, \partial_y\phi)$, $b := b(x, y, t, \phi, \partial_x\phi, \partial_y\phi)$, $f := f(x, y, t, \phi, u)$, $p := p(x, y, t, \phi)$ are given functions of their indicated arguments. The system (2) is supplemented with initial conditions

$$\phi(x, y, 0) = \phi_0(x, y), \;\; u(x, y, 0) = u_0(x, y), \;\; (x, y) \in \Omega \tag{3}$$

and, for example, with homogeneous Dirichlet boundary conditions on the boundary of Ω:

$$\phi(x, y, t) = 0, \;\; u(x, y, t) = 0, \;\; (x, y, t) \in \partial\Omega \times [0, T]. \tag{4}$$

We discretize (2)-(4) as follows. Let $h = (\beta - \alpha)/(J + 1)$, $J \in \mathbb{N}$ and $x_i = \alpha + ih$, $y_j = \alpha + jh$, $0 \le i, j \le J + 1$. We define $\Omega_h := \{(x_i, y_j), i, j = 1, \dots, J\}$ and $\partial\Omega_h := \{(x_i, y_j), i = 0 \text{ or } i = J + 1 \text{ or } j = 0 \text{ or } j = J + 1\}$. We let $t^n = n\Delta t$, $n = 0, \dots, N$, where $\Delta t = T/N$, and define $t^{n+\frac{1}{2}} = t^n + \Delta t/2$, $x_{i\pm\frac{1}{2}} = x_i \pm h/2$, $y_{j\pm\frac{1}{2}} = y_j \pm h/2$, and

$$S_h := \left\{ U = (U_{00}, \dots, U_{J+1,J+1})^T \in \mathbb{R}^{(J+2)\times(J+2)} : U_{ij} = 0 \text{ on } \partial\Omega_h \right\}.$$

We approximate the solution of (2)-(4) by mesh functions $U^n, \Phi^n \in S_h$ using the explicit Euler-ADI scheme defined as follows:

$$
\begin{array}{lll}
& \Phi^0_{ij} = \phi_0(x_i,y_j),\ U^0_{ij} = u_0(x_i,y_j), & (x_i,y_j) \in \Omega_h \bigcup \partial\Omega_h \\
& \text{For}\ \ n = 0,1,\dots,N-1: & \\
\text{(i)} & q^n_{ij} \frac{\Phi^{n+1}_{ij} - \Phi^n_{ij}}{\Delta t} - (L^n_h \Phi)_{ij} = F^n_{ij}, & (x_i,y_j) \in \Omega_h \\
& \Phi^{n+1}_{ij} = 0, & (x_i,y_j) \in \partial\Omega_h \\
\text{(ii)} & \frac{2(U^{n+\frac12}_{ij} - U^n_{ij})}{\Delta t} - \delta_{x\bar{x}} U^{n+\frac12}_{ij} - \delta_{y\bar{y}} U^n_{ij} = \frac{P^{n+1}_{ij} - P^n_{ij}}{\Delta t}, & (x_i,y_j) \in \Omega_h \\
\text{(iii)} & \frac{2(U^{n+1}_{ij} - U^{n+\frac12}_{ij})}{\Delta t} - \delta_{x\bar{x}} U^{n+\frac12}_{ij} - \delta_{y\bar{y}} U^{n+1}_{ij} = \frac{P^{n+1}_{ij} - P^n_{ij}}{\Delta t}, & (x_i,y_j) \in \Omega_h \\
& U^{n+\frac12}_{ij} = U^{n+1}_{ij} = 0, & (x_i,y_j) \in \partial\Omega_h
\end{array} \tag{5}
$$

where $(L^n_h v)_{i,j} := [\delta_x(a^n_{i-\frac12,j}\delta_{\bar{x}} v^n_{ij}) + \delta_y(d^n_{i,j-\frac12}\delta_{\bar{y}} v^n_{ij}) + \delta_x(b^n_{ij}\delta_{\hat{y}} v^n_{ij}) - \delta_y(b^n_{ij}\delta_{\hat{x}} v^n_{ij})]/h^2$, if $(x_i,y_j) \in \Omega_h$, and $(L^n_h v)_{i,j} := 0$, if $(x_i,y_j) \in \partial\Omega_h$, $P^n_{i,j} := p(x_i,y_j,t^n,\Phi^n_{i,j})$, $\delta_x v_{ij} = (v_{i+1,j} - v_{i,j})/h$, $\delta_{\bar{x}} v_{ij} = (v_{i,j} - v_{i-1,j})/h$, $\delta_y v_{ij} = (v_{i,j+1} - v_{i,j})/h$, $\delta_{\bar{y}} v_{ij} = (v_{i,j} - v_{i,j-1})/h$, $\delta_{x\bar{x}} v_{ij} = (v_{i+1,j} - 2v_{i,j} + v_{i-1,j})/h^2$, $\delta_{y\bar{y}} v_{ij} = (v_{i,j+1} - 2v_{i,j} + v_{i,j-1})/h^2$, $\Delta_h v_{ij} := \delta_{x\bar{x}} v_{ij} + \delta_{y\bar{y}} v_{ij}$. Also

$a^n_{i+\frac12,j} := a(x_{i+\frac12}, y_j, t^n, \frac{\Phi^n_{i+1,j}+\Phi^n_{i,j}}{2}, \frac{\Phi^n_{i+1,j}-\Phi^n_{i,j}}{h}, \frac{(\Phi^n_{i+1,j+1}+\Phi^n_{i,j+1})-(\Phi^n_{i+1,j-1}+\Phi^n_{i,j-1})}{4h})$,

$a^n_{i-\frac12,j} := a(x_{i-\frac12}, y_j, t^n, \frac{\Phi^n_{i,j}+\Phi^n_{i-1,j}}{2}, \frac{\Phi^n_{i,j}-\Phi^n_{i-1,j}}{h}, \frac{(\Phi^n_{i,j+1}+\Phi^n_{i-1,j+1})-(\Phi^n_{i,j-1}+\Phi^n_{i-1,j-1})}{4h})$,

$d^n_{i,j+\frac12} := d(x_i, y_{j+\frac12}, t^n, \frac{\Phi^n_{i,j+1}+\Phi^n_{i,j}}{2}, \frac{(\Phi^n_{i+1,j+1}+\Phi^n_{i+1,j})-(\Phi^n_{i-1,j+1}+\Phi^n_{i-1,j})}{4h}, \frac{\Phi^n_{i,j+1}-\Phi^n_{i,j}}{h})$,

$d^n_{i,j-\frac12} := d(x_i, y_{j-\frac12}, t^n, \frac{\Phi^n_{i,j}+\Phi^n_{i,j-1}}{2}, \frac{(\Phi^n_{i+1,j}+\Phi^n_{i+1,j-1})-(\Phi^n_{i-1,j}+\Phi^n_{i-1,j-1})}{4h}, \frac{\Phi^n_{i,j}-\Phi^n_{i,j-1}}{h})$,

$b^n_{ij} := b(x_i, y_j, t^n, \Phi^n_{ij}, \frac{\Phi^n_{i+1,j}-\Phi^n_{i-1,j}}{2h}, \frac{\Phi^n_{i,j+1}-\Phi^n_{i,j-1}}{2h})$, $F^n_{ij} := F(x_i, y_j, t^n, \Phi^n_{ij}, U^n_{ij})$,

$q^n_{ij} := q(x_i, y_j, t^n, \Phi^n_{ij}, \frac{\Phi^n_{i+1,j}-\Phi^n_{i-1,j}}{2h}, \frac{\Phi^n_{i,j+1}-\Phi^n_{i,j-1}}{2h})$.

The implementation of the explicit Euler-ADI finite difference scheme (5) is straightforward: For $n \geq 1$, given Φ^n_{ij}, U^n_{ij}, we compute Φ^{n+1}_{ij}, in stage (i). Then, we compute $U^{n+\frac12}_{ij}$ in stage (ii) by solving for each j one $J \times J$ tridiagonal linear system, and then U^{n+1}_{ij} in stage (iii) by solving again for each i one $J \times J$ tridiagonal linear system. So, the total number of operations required to advance the solution by one time step is $O(J^2)$. The operations may be readily accelerated using M processors, by solving, in each one of the the stages (ii) and (iii), J/M tridiagonal systems of size $J \times J$ on each processor (assuming that J is a multiple of M).

Implementing (5) is very time consuming because of the stability condition $\Delta t = O(h^2)$ which is the required by the explicit Euler discretization of the first p.d.e. of (2). Hence, in practice, we modify (5) as follows: We let $\Delta t = O(h)$ denote a (large) time step that is used in the ADI scheme $(5.ii)$ and $(5.iii)$ and let $t^n = n\Delta t$. Given Φ^n_{ij} and U^n_{ij}, we first compute Φ^{n+1}_{ij} using the explicit Euler scheme $(5.i)$ repeatedly with the (small) time step Δt_{Euler}, where $\Delta t = M\Delta t_{Euler}$, $M = O(N)$, evaluating the coefficient functions $q,\ a,\ d$, and f at $t^\nu = t^n + \nu\Delta t_{Euler}$, for $\nu = 0,1,\dots,M$, Φ^ν_{ij}, and U^n_{ij} (for f). We found that the accuracy of the scheme was increased by using the extrapolated values $\frac32\Phi^\nu_{ij} - \frac12\Phi^{\nu-1}_{ij}$ for the $\phi,\ \partial_x\phi,\ \partial_y\phi$ variables in the coefficient b.

J	$\|\cdot\|_\infty$ errors	order	$\|\cdot\|_2$ errors	order
	$\phi : 1.90628e-04$	$---$	$8.62755e-05$	$---$
50	$u : 7.85678e-04$	$---$	$4.08244e-04$	$---$
	$\phi : 8.44834e-05$	2.006	$3.65035e-05$	2.121
75	$u : 3.73204e-04$	1.835	$1.91513e-04$	1.866
	$\phi : 3.92623e-05$	1.889	$1.70245e-05$	1.881
112	$u : 1.60779e-04$	2.076	$8.18122e-05$	2.097
	$\phi : 1.76024e-05$	1.978	$7.40845e-06$	2.052
168	$u : 7.36724e-05$	1.924	$3.72721e-05$	1.938
	$\phi : 8.12544e-06$	1.906	$3.40779e-06$	1.915
252	$u : 3.16138e-05$	2.086	$1.59319e-05$	2.096
	$\phi : 3.71516e-06$	1.930	$1.51073e-06$	2.006
378	$u : 1.42479e-05$	1.965	$7.16154e-06$	1.972
	$\phi : 1.74010e-06$	1.870	$6.87133e-07$	1.942
567	$u : 6.28515e-06$	2.018	$3.15364e-06$	2.022

Table 1: Errors and order of convergence of the modified explicit Euler-ADI scheme.

3. Numerical experiments

We first performed a numerical experiment in order to determine the experimental order of convergence of the modified scheme. We took $\Omega = [0,1]\times[0,1]$, $T = 1$, $r(\theta) = 1 + \delta_\gamma \cos(4\theta)$, $\theta = \arctan(\phi_x\phi_y)$, (in order to avoid singularities at zeros of ϕ_x) $a = d = r^2(\theta)$, $b = -r(\theta)r'(\theta)$, $q = (1 + \delta_\gamma \cos(4\theta)/(m(1 + \delta_\mu \cos(4\theta)))$ $f = \phi(1-\phi)u/(1 + 0.25u)$, $p = \phi^3(10 - 15\phi + 6\phi^2)$, and constants $m = 1$, $\delta_\gamma = 0.03$, $\delta_\mu = 0.03$. We added a suitable nonhomogeneous term so that the solution of the associated initial-boundary value problem with Neumann boundary conditions was $(\phi, u) = (e^{-t}\cos(x(x-1))\cos(y(y-1)), e^{-t}\cos(\pi x)\cos(\pi y))$.

Table 1 shows the errors and the experimental orders of convergence of the numerical solution at $T = 1$ in the discrete maximum norm $\|\cdot\|_\infty$ and also in the discrete ℓ_2 norm $\|\cdot\|_2$. We computed with $h = 1/(J+1)$, where $J = 50, 75, \ldots, 567$. The large time step Δt was taken equal to h (i.e. $N = J$), while the small time step Δt_{Euler} was computed with a factor of safety as $\Delta t_{Euler} = 0.1\Delta t/N$. (Hence $\Delta t_{Euler} = 0.1h^2$). For two consecutive values $h_1,\ h_2$ of h, giving errors $e_1,\ e_2$, respectively, the rate of convergence was computed as $\log(e_2/e_1)/\log(h_2/h_1)$. It is evident that the orders of convergence are very close to 2 for both variables ϕ and u.

With this scheme we also performed realistic numerical experiments where we took (cf. Wang, [4]) on $\Omega = [0,1]\times[0,1]$, $\phi_0(x,y) = \frac{1}{2}\left[1 + \tanh\frac{\rho - R_0}{2\sqrt{2}\varepsilon}\right]$,

$$u_0(x,y) = \begin{cases} t_s & \rho < R_0 \\ \frac{\left[\ln\left(\frac{\rho}{R_0}\right) + t_s\ln\left(\frac{\rho}{R_{00}}\right)\right]}{\ln\left(\frac{R_0}{R_{00}}\right)} & R_0 \le R_{00} \\ -1 & \rho \ge R_{00} \end{cases}, \ \rho = \sqrt{x^2+y^2},$$

$r(\theta) = 1 + \delta_\gamma \cos(4\theta)$, $\theta = \arctan(\phi_y/\phi_x)$, $a = r^2(\theta)$, $d = r^2(\theta)$, $b = -r(\theta)r'(\theta)$, $q = (1+\delta_\gamma\cos(4\theta))/(m(1+\delta_\mu\cos(4\theta)))$, $f = \frac{1}{\varepsilon^2}(\phi(1-\phi)(\phi-\frac{1}{2}+30\varepsilon\alpha S\frac{u}{1+0.25u}\phi(1-\phi))$, $p = \phi^3(10-15\phi+6\phi^2)/S$. In these formulas S, m and ε are constants representing, respectively, the dimensionless supercooling of the melt, the ratio of the capillary to the kinetic length, and the average interface thickness parameter. We considered an isotropic case ($\delta_\gamma = \delta_\mu = 0$), a semi-anisotropic case ($\delta_\gamma = 0,\ \delta_\mu = 0.05$), and two anisotropic cases ($\delta_\gamma = 0.05,\ \delta_\mu = 0$), ($\delta_\gamma = 0.05,\ \delta_\mu = 0.05$). In all cases we took $t_s = 0.01,\ R_0 = 0.1,\ R_{00} = 2R_0,\ S = 0.8,\ m = 0.1,\ a = 70,\ \varepsilon = 1/400$. We computed up to $T = 0.8$ taking in all cases $h = 10^{-3}$ and $\Delta t = 2.75\ 10^{-5}$. Successive contours plotted every 1000 Δt time steps of the interface between the two phases are shown in Figure 3. The results clearly show the effect of anisotropy when $\delta_\mu \neq 0$ and dendrites forming when $\delta_\gamma \neq 0$. The cases ($\delta_\gamma = \delta_\mu = 0$) and ($\delta_\gamma = 0.05,\ \delta_\mu = 0.05$) were computed by Wang, [4] and our numerical results agree well with hers.

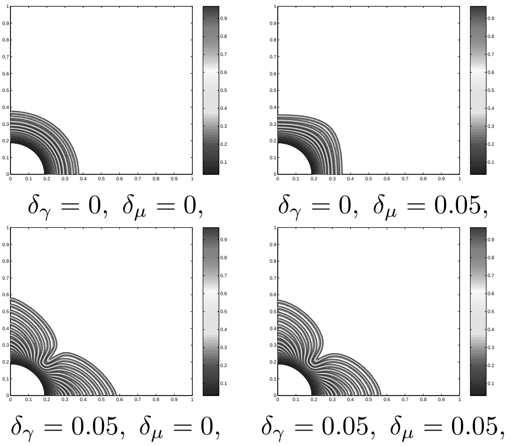

Figure 1: Evolution of the interface in four cases. (Shown are the succesive contours of the interface every 1000 $\Delta t-$time steps.)

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