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PHASE-FIELD MODELING OF DENDRITIC INTERACTION IN 2D*

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The phase-field method is used to investigate numerically the evolution of spherical grains into supercooled melt in the two-dimensional case. The interaction of different configurations of multiple grains is examined. The evolution of the grain shapes and the propagation speed of the primary dendritic tips are analyzed.

1. Introduction. Dendritic growth have been the subject of many theoretical, numerical and experimental investigations [1]–[7]. The isothermal dendritic growth experiment of Glicksman, Koss and Winsa [1], conducted under microgravity conditions, have clearly demonstrated that naturally growing dendrites are characterized by steady-state propagation of the primary tips and nonlinear time-dependant evolution of secondary and tertiary side-branches on a microscopic scale (from 10^{-6} to $10^{-5}m$). Accurate modeling of dendritic processes on the mesoscopic scale, defined from 10^{-4} to 10^{-3} m, is not only important for the prediction of the final structure of a solidified material, but also for feeding local information back to the macroscopic model (10^{-1} m).

The phase-field formulation of solidification problems is a computational tool for modeling complicated solid-liquid interfaces. The advantage is that the interface between phases is not explicitly tracked. It is given implicitly by the so-called phase-field, i.e., the level set of a scalar function ϕ of space and time, called phase-field function. It varies smoothly from -1 in the liquid to $+1$ in the solid phase. An evolution equation for the phase-field function is solved instead and the solid-liquid interface is defined by the level set $\phi = 0$. Another advantage of this approach is that the accurate computation of interface normals and curvatures is completely avoided.

The goal of this paper is to apply the method described in [2] to the problem for modeling the growth of an assemblage of equiaxed dendritic grains on a mesoscopic scale. A mesoscopic unit cell typically contains of the order of 10 equiaxed dendritic grains. Of primary interest are the predictions of the evolution of the grain shapes and the growth interactions between multiple grains.

2. The problem. The phase-field model of the dendritic growth, used in [2], [3], [4], [5], is given by the system of nonlinear equations:

$$\frac{\partial u}{\partial t} = D\triangle u + \frac{1}{2}\frac{\partial \phi}{\partial t}\ , \tag{1}$$

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$$\tau\frac{\partial\phi}{\partial t}=\nabla(W^2\nabla\phi)+\partial_x[|\nabla\phi|^2W\partial_{\phi_x}W]+\partial_y[|\nabla\phi|^2W\partial_{\phi_y}W]+\phi(1-\phi^2)-\lambda u(1-\phi^2)^2 \tag{2}$$

for the dimensionless temperature $u(x,y,t)$ and for the phase field function $\phi(x,y,t)$, $(x,y)\in\Omega$, $0<t\le t_k$. Here:

- $u=(T-T_m)/(L/c_p)$ is the dimensionless temperature;
- T and T_m are the temperature and the melting temperature respectively;
- L is the latent heat of fusion;
- c_p is the specific heat at constant pressure;
- D is the thermal diffusivity;
- λ is a dimensionless parameter that controls the coupling between u and ϕ;
- $W=\delta\,A_s$, $A_s=(1-3\epsilon)+4\epsilon\dfrac{\phi_x^4+\phi_y^4}{|\nabla\phi|^4}$ and ϵ is the anisotropy strength;
- δ is the characteristic length;
- $\tau=\tau_0A_s^2$ and τ_0 is the characteristic time.

We investigate Neumann boundary conditions:

$$\frac{\partial u}{\partial n}=0,\quad \frac{\partial\phi}{\partial n}=0,\quad \forall\,t>0,\quad \forall(x,y)\in\partial\Omega \tag{3}$$

and Dirichlet boundary conditions:

$$u=u_0,\quad \phi=-1,\quad \forall\,t>0,\quad \forall(x,y)\in\partial\Omega\ , \tag{4}$$

where u_0 is the dimensionless undercooling.

To close the problem, we pose appropriate initial conditions, which correspond to the number of the interacting seeds. In the case of a single spherical seed, $K^0=\{(x,y):(x-l)^2+(y-l)^2\le r^2\}$, posed at time $t=0$ in the center of the square $\Omega^0=\{[0,2l]\times[0,2l]\}$, the initial conditions are:

$$u(x,y,0)=0,\ \forall(x,y)\in K^0,\quad u(x,y,0)=u_0,\ \forall(x,y)\in\Omega^0\setminus K^0\ , \tag{5}$$

$$\phi(x,y,0)=1,\ \forall(x,y)\in K^0,\quad \phi(x,y,0)=-1,\ \forall(x,y)\in\Omega^0\setminus K^0. \tag{6}$$

3. Numerical method. To solve the systems (1)-(3) and (1), (2), (4) with the appropriate initial conditions of type (5), (6), we use the method of lines – we make finite difference discretization in space and solve the resulting ODE system in time.

3.1. Semidiscretization in space. Because of the symmetry, the computational domain is

$$\Omega=\{0\le x\le l,\quad 0\le y\le x\},\quad K=\Omega\bigcap K^0.$$

We use the finite difference method on regular mesh $\overline{\omega_h}=\{(ih,jh):i=\overline{0,n},j=\overline{0,i}\}$. in both directions. The discretization error is $O(h^2)$ for the case of Dirichle boundary conditions and $O(h)$ for the case of Neumann boundary conditions. The resulting system of ODE is:

$$\frac{dU}{dt}=\Theta_1(U(t))+\frac{1}{2}\frac{d\Phi}{dt},\qquad U(0)=U^{(0)},$$

$$\frac{d\Phi}{dt} = \Theta_2(\Phi(t)), \qquad \Phi(0) = \Phi^{(0)},$$

$$U(t) = (U^t_{0,0}, U^t_{1,0}, .., U^t_{n,0}, U^t_{1,1}, U^t_{2,1}, .., U^t_{n,1}, .., U^t_{n,n})^T$$

$$\Phi(t) = (\Phi^t_{0,0}, \Phi^t_{1,0}, .., \Phi^t_{n,0}, \Phi^t_{1,1}, \Phi^t_{2,1}, .., \Phi^t_{n,1}, .., \Phi^t_{n,n})^T$$

3.2. Discretization in time. To solve the ODE system we use a second order explicit modification of the Runge-Kutta method [8] with extended region of stability. The time step is chosen automatically so as to guarantee stability and a given desired accuracy at the end of the time interval. Applied to the system:

$$y\prime = f(y), \qquad y(0) = y_0$$

it reads:

$$y^{j+1} = y^j + p_1 k^j_1 + p_2 k^j_2 + p_3 k^j_3,$$

where

$$\begin{aligned} p_1 &= 1/4, & k^j_1 &= \tau_j f(y^j), \\ p_2 &= 15/32, & k^j_2 &= \tau_j f(y^j + 2k^j_1/3), \\ p_3 &= 9/32, & k^j_3 &= \tau_j f(y^j + k^j_1/3 + k^j_2/3). \end{aligned}$$

The step τ_j satisfies the criteria for accuracy and stability respectively:

$$\max_{0\le i\le s} |(k^j_2 - k^j_1)_i|/(|(y^j)_i + E|) \le 6.2\alpha, \tag{7}$$

$$\max_{0\le i\le s} |(3k^j_3 - 2k^j_2 - k^j_1)_i| \le 5 \max_{0\le i\le s} |(k^j_2 - k^j_1)_i|. \tag{8}$$

Here α is the desired accuracy, E is a positive parameter ($E = 10^{-2}$ in our computations).

4. Numerical experiments. The first set of numerical experiments was devoted to find a strategy for increasing the computational efficiency of the modified Runge-Kutta method. The common strategy is to find the optimal time step (to decrease or to increase the previous one by a factor of q, usually $q = 1.1$) while the two conditions (7) and (8) are fulfilled. It is good, when it is applied to one equation of the kind (1) or (2). For the system (1), (2) it must be changed.

The new strategy must be consistent with the specific peculiarities of the mathematical model and of the evolution process. They are : the very different nature and structure of the equations (1) and (2); the discontinuity of the initial conditions (5), (6); the imposed (in equation (2)) steady-state profile of the phase-field function along the axes of the tip growth.

Regarding these peculiarities it is predictable (and the numerical experiments confirm this) that in the beginning of the process the time step τ_j varies significantly, but it becomes and remains constant when the steady-state profile of ϕ is attained. That's why we begin with small initial time step (about 10^{-4}) and keep it small by permitting only one increase of it per iteration, in order to avoid the big variations of it. When τ_j becomes constant we do not examine the conditions (7) and (8) at every time step. This strategy increases significantly the efficiency of the method.

In the second set of experiments the influence of the boundary conditions (3) and (4) on the solution was investigated. It was done in the case of one spherical seed posed in the center of the domain. The computations were made until the tip reached the boundary. We obtaine identical shapes and dimensionless tip velocities in both cases.

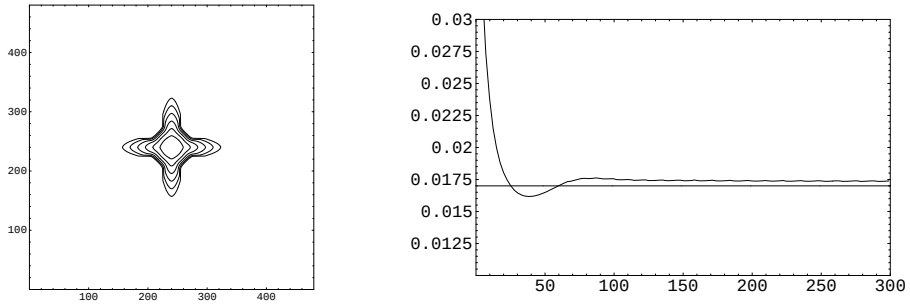

Figure 1: Evolution (left) and the tip velocity (right) of one seed

In the last set of experiments we examine the interaction of multiple grains. Everywhere in the experiments below the computational domain is: $\Omega = \{(x, y) : 0 \leq x \leq 240, 0 \leq y \leq x\}$. The radius of the seeds is $r = 4$, the spatial step is $h = 0.4$. The undercooling is $u_0 = -0.55$, the thermal diffusivity is $D = 4$, the anisotropy is $\epsilon = 0.05$ and $\delta = 1$.

Fig. 1 shows the evolution of one spherical seed and its corresponding dimensionless tip velocity. It is done for comparison with the case of multiple interacting grains.

Fig. 2 shows the evolution of 5 interacting seeds (only a quarter of the real picture) and the dimensionless tip velocity of the free, non-interacting tips. The initial conditions in this case are:

$$u(x, y, 0) = 0,\ \forall (x, y) \in K, \quad u(x, y, 0) = u_0,\ \forall (x, y) \in \Omega \setminus K$$
$$\phi(x, y, 0) = 1,\ \forall (x, y) \in K, \quad \phi(x, y, 0) = -1,\ \forall (x, y) \in \Omega \setminus K,$$

where

$$K = \{(x, y) : (x - 240)^2 + (y - 240)^2 \leq r^2 \ \cup \ (x - 160)^2 + (y - 160)^2 \leq r^2\}$$

Fig. 3 shows the evolution of 9 interacting seeds (a quarter of the picture) and the dimensionless tip velocity of the free, non-interacting tips. In this case

$$K=\{(x, y):(x-240)^2+(y-240)^2\leq r^2\cup(x-200)^2+(y-200)^2\leq r^2\cup(x-240)^2+(y-200)^2\leq r^2\}$$

5. Conclusions. The last set of experiments shows:

– the velocities of the dendrite tips which, because of their geometry position, do not interact with the other dendrite tips, comes to the same stationary state as in the case of one free dendrite (compare the speeds in the Fig. 1-3);

– propagation of primary tips only is observed in all our experiments. This confirm the observation of all known for us investigations, that in the frame of the phase-field model (1)-(2) secondary and tertiary side-branching is possible only if some noise is added in the model. This is the next aim of our investigations.

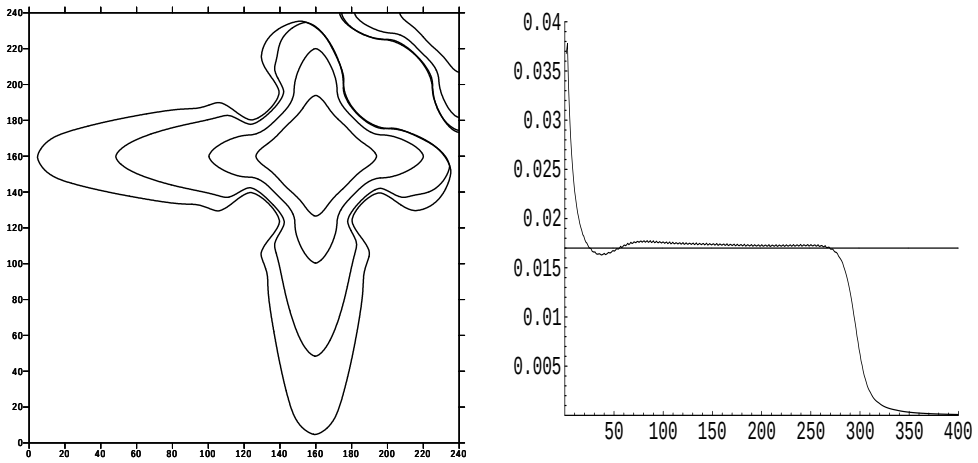

Figure 2: Evolution of 5 seeds (left) and the tip velocity (right)

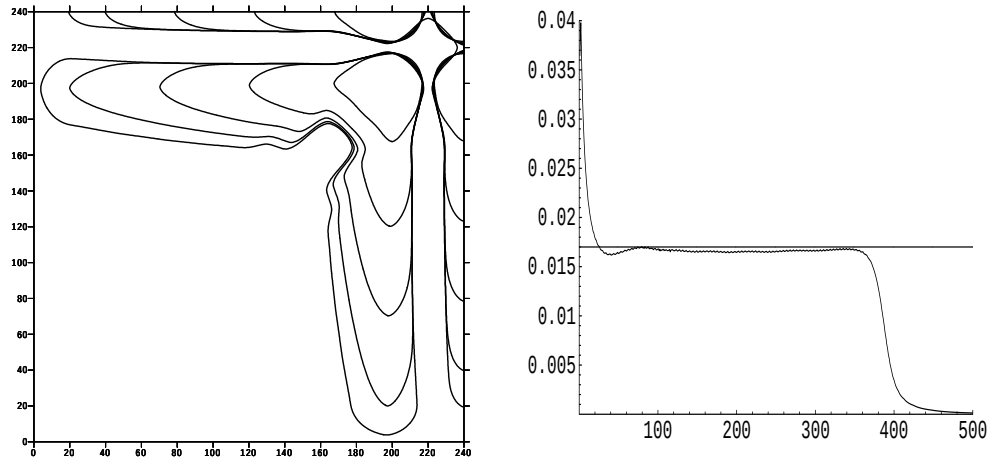

Figure 3: Evolution of 9 seeds (left) and the tip velocity (wright)

REFERENCES

[1] M. E. Glicksman, M. B. Koss, E.A. Winsa. Dendritic growth velocities in microgravity. *Phys. Rev. Lett.*, **73** (1994), 536–576.
[2] V. Slavov, St. Dimova, O. Iliev. Phase-field method for 2D dendritic growth. *Lect. Notes in Comp. Sci.*, **2902** (2004), 404–411.
[3] C. Beckermann, H. Diepers, I. Steinbach, A. Karma, X. Tong. Modeling melt convection in phase-field simulations of solidification. *J. Comput. Phys.*, **154** (1999), 468–496.
[4] A. Karma, W.-J. Rappel. Phase-field method for computationally efficient modeling of solidification with arbitrary interface kinetics. *Phys. Rev.*, **E 53** (1996), 3017–3020.
[5] A. Karma, W.-J. Rappel. Quantitative phase-field modeling of dendritic growth in two and three dimensions. *Phys. Rev.*, **E 57** (1998), 4323–4349.
[6] X. Tong, C. Beckermann, A. Karma, Q. Li. Phase-field simulations of dendritic crystal growth in a forced flow. *Phys.Rev.*, **E 63** (2001), 061601-1–061601-15.
[7] Q. Li, C. Bckermann. Scaling behaviour of three dimensional dendrites. *Phys. Rev.*, **E 57** (1998), 3176–3188.
[8] V. Novikov, E. Novikov. Stability control of explicit one-step methods for integration of ordinary differential equations. *Dokl. Akad. Nauk SSSR*, **272** (1984), 1058–1062.

МЕТОД НА ФАЗОВОТО ПОЛЕ ЗА МОДЕЛИРАНЕ ВЗАИМОДЕЙСТВИЕТО НА ДЕНДРИТИ В ДВУМЕРНИЯ СЛУЧАЙ

В. Славов, Ст. Димова

Методът на фазовото поле е използван за числено изследване на еволюцията на сферични зародиши в преохладен разплав. Изследвано е взаимодействието на различни конфигурации от зародиши и скоростта на нарастване на първичните им разклонения.