Features in simulation of crystal growth using the hyperbolic PFC equation and the dependence of the numerical solution on the parameters of the computational grid

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Abstract: We investigate the three-dimensional mathematical model of crystal growth called PFC (Phase Field Crystal) in a hyperbolic modification. This model is also called the modified model PFC (originally PFC model is formulated in parabolic form) and allows to describe both slow and rapid crystallization processes on atomic length scales and on diffusive time scales [1,2]. The modified phase field crystal model describes a continuous field of atomic density $\phi(x,t)$ and it can be expressed by the following equation:

$$\tau\frac{\partial^2\phi}{\partial t^2}+\frac{\partial\phi}{\partial t}=\nabla^2\mu, \tag{1}$$

where t is the time, τ is the relaxation time of the atomic flux to its stationary state, and μ represents the chemical potential, obtained from the free-energy functional

$$\mathcal{F}[\phi,\nabla\phi,\nabla^2\phi]=\int_\Omega\left[f(\phi)-|\nabla\phi|^2+\frac{1}{2}(\nabla^2\phi)^2\right]\mathrm{d}\Omega, \tag{2}$$

associated to the domain Ω. The chemical potential can be obtained as the variational derivative of the free-energy functional $\mathcal{F}$, namely

$$\mu(\phi)=\frac{\delta\mathcal{F}}{\delta\phi}=f'(\phi)+2\nabla^2\phi+\nabla^4\phi. \tag{3}$$

The function f represents the homogeneous part of the free energy density. It takes on the form

$$f(\phi)=\frac{1-\epsilon}{2}\phi^2+\frac{\alpha}{3}\phi^3+\frac{1}{4}\phi^4. \tag{4}$$

Here, $\epsilon=(T_c-T)/T_c$ is the undercooling, where T and T_c are the temperature and critical temperature of transition, respectively. α is a coefficient which means a measure of metastability.
The solution of this equation is possible only by numerical methods. Previously, authors created the software package for the solution of the Phase Field Crystal problem, based on the method of isogeometric analysis (IGA) [4] and

PetIGA program library [5].
Using the modified PFC model for the simulation allows description of fast and slow dynamics of structure rearrangement from homogeneous unstable phase to the emerged periodic structure [3]. We consider that if the element size is larger than lattice parameter of the emerged structure on the interface, then the type of finite elements and its shape functions predetermine the behavior of the interface front movement, because of approximating of the atomic density inside the element using inappropriate functions. In this report, we show solutions for both stationary and non-stationary problems which confirm our assumption of a necessary condition for the computational cell size: to be at least less then the lattice parameter.

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