PRISMS-PF Application Formulation: dendriticSolidification

This example application implements a simple model of dendritic solidification based on the CHiMaD Benchmark Problem 3, itself based on the model given in the following article:
"Multiscale Finite-Difference-Diffusion-Monte-Carlo Method for Simulating Dendritic Solidification" by M. Plapp and A. Karma, *Journal of Computational Physics*, 165, 592-619 (2000)

This example application examines the non-isothermal solidification of a pure substance. The simulation starts with a circular solid seed in a uniformly undercooled liquid. As this seed grows, two variables are tracked, an order parameter, ϕ, that denotes whether the material a liquid or solid and a nondimensional temperature, u. The crystal structure of the solid is offset from the simulation frame for generality and to expose more readily any effects of the mesh on the dendrite shape.

1 Governing Equations

Consider a free energy density given by:

$$\Pi = \int_{\Omega} \left[\frac{1}{2} W^2(\hat{n}) |\nabla \phi|^2 + f(\phi, u) \right] \, dV \tag{1}$$

where ϕ is an order parameter for the solid phase and u is the dimensionaless temperature:

$$u = \frac{T - T_m}{L/c_p} \tag{2}$$

for temperature T, melting temperature T_m, latent heat L, and specific heat c_p. The free energy density, $f(\phi, u)$ is given by a double-well potential:

$$f(\phi, u) = -\frac{1}{2}\phi^2 + \frac{1}{4}\phi^4 + \lambda u \phi \left(1 - \frac{2}{3}\phi^2 + \frac{1}{5}\phi^4 \right) \tag{3}$$

where λ is a dimensionless coupling constant. The gradient energy coefficient, W, is given by

$$W(\theta) = W_0[1 + \epsilon_m \cos[m(\theta - \theta_0)]] \tag{4}$$

where, W_0, ϵ_m, and θ_0 are constants and θ is the in-plane azimuthal angle, where $\tan(\theta) = \frac{\partial \phi}{\partial y} / \frac{\partial \phi}{\partial x}$.

The evolution equations are:

$$\frac{\partial u}{\partial t} = D \nabla^2 u + \frac{1}{2} \frac{\partial \phi}{\partial t} \tag{5}$$

$$\tau(\hat{n}) \frac{\partial \phi}{\partial t} = -\frac{\partial f}{\partial \phi} + \nabla \cdot \left[W^2(\theta) \nabla \phi \right] + \frac{\partial}{\partial x} \left[|\nabla \phi|^2 W(\theta) \frac{\partial W(\theta)}{\partial \left(\frac{\partial \phi}{\partial x} \right)} \right] + \frac{\partial}{\partial y} \left[|\nabla \phi|^2 W(\theta) \frac{\partial W(\theta)}{\partial \left(\frac{\partial \phi}{\partial y} \right)} \right] \tag{6}$$

where

$$\tau(\hat{n}) = \tau_0[1 + \epsilon_m \cos[m(\theta - \theta_0)]] \tag{7}$$

$$D = \frac{0.6267 \lambda W_0^2}{\tau_0} \tag{8}$$

The governing equations can be written more compactly using the variable μ, the driving force for the phase transformation:

$$\frac{\partial u}{\partial t} = D\nabla^2 u + \frac{\mu}{2\tau} \tag{9}$$

$$\tau(\hat{n})\frac{\partial \phi}{\partial t} = \mu \tag{10}$$

$$\mu = -\frac{\partial f}{\partial \phi} + \nabla \cdot \left[W^2(\theta)\nabla\phi\right] + \frac{\partial}{\partial x}\left[|\nabla\phi|^2 W(\theta)\frac{\partial W(\theta)}{\partial\left(\frac{\partial\phi}{\partial x}\right)}\right] + \frac{\partial}{\partial y}\left[|\nabla\phi|^2 W\theta)\frac{\partial W(\theta)}{\partial\left(\frac{\partial\phi}{\partial y}\right)}\right] \tag{11}$$

The $\frac{\partial W(\theta)}{\partial\left(\frac{\partial\phi}{\partial x}\right)}$ and $\frac{\partial W(\theta)}{\partial\left(\frac{\partial\phi}{\partial y}\right)}$ expressions can be evaluated using the chain rule, using θ as an intermediary (i.e. $\frac{\partial W(\theta)}{\partial\left(\frac{\partial\phi}{\partial x}\right)} = \frac{\partial W(\theta)}{\partial\theta}\frac{\partial\theta}{\partial\left(\frac{\partial\phi}{\partial x}\right)}$ and $\frac{\partial W(\theta)}{\partial\left(\frac{\partial\phi}{\partial y}\right)} = \frac{\partial W(\theta)}{\partial\theta}\frac{\partial\theta}{\partial\left(\frac{\partial\phi}{\partial y}\right)}$). Also, the last two terms can be expressed using a divergence operator, allowing them to be grouped with the second term, which will simplify matters later. Carrying out these transformations yields:

$$\mu = \left[\phi - \lambda u\left(1-\phi^2\right)\right]\left(1-\phi^2\right) + \nabla\cdot\left[\left(W^2\frac{\partial\phi}{\partial x} + W_0\epsilon_m m W(\theta)\sin\left[m\left(\theta-\theta_0\right)\right]\frac{\partial\phi}{\partial y}\right)\hat{x}\right.$$
$$\left. + \left(W^2\frac{\partial\phi}{\partial y} - W_0\epsilon_m m W(\theta)\sin\left[m\left(\theta-\theta_0\right)\right]\frac{\partial\phi}{\partial x}\right)\hat{y}\right] \tag{12}$$

2 Model Constants

W_0: Controls the interfacial thickness, default value of 1.0.
τ_0: Controls the phase transformation kinetics, default value of 1.0.
ϵ_m: T the strength of the anisotropy, default value of 0.05.
D: The thermal diffusion constant, default value of 1.0.
$\Delta : \frac{T_m - T_0}{L/c_p}$: The level of undercooling, default value of 0.75.
θ_0: The rotation angle of the anisotropy with respect to the simulation frame, default value of 0.125 ($\sim$7.2°).

3 Time Discretization

Considering forward Euler explicit time stepping, we have the time discretized kinetics equation:

$$u^{n+1} = u^n + \Delta t\left(D\nabla^2 u^n + \frac{\mu^n}{2\tau}\right) \tag{13}$$

$$\phi^{n+1} = \phi^n + \frac{\Delta t \mu^n}{\tau} \tag{14}$$

$$\mu^{n+1} = \left[\phi^n - \lambda u \left(1-(\phi^n)^2\right)\right]\left(1-(\phi^n)^2\right) + \nabla \cdot \Bigg[\left(W^2 \frac{\partial \phi^n}{\partial x} + W_0 \epsilon_m m W(\theta^n) \sin\left[m\left(\theta^n - \theta_0\right)\right] \frac{\partial \phi^n}{\partial y} \right) \hat{x}$$
$$+ \left(W^2 \frac{\partial \phi^n}{\partial y} - W_0 \epsilon_m m W(\theta^n) \sin\left[m\left(\theta^n - \theta_0\right)\right] \frac{\partial \phi^n}{\partial x} \right) \hat{y} \Bigg] \quad (15)$$

4 Weak Formulation

$$\int_\Omega w u^{n+1} \, dV = \int_\Omega w \underbrace{\left(u^n + \frac{\mu^n \Delta t}{2\tau}\right)}_{r_u} + \nabla w \cdot \underbrace{\left(-D \Delta t \nabla u^n\right)}_{r_{ux}} \, dV \quad (16)$$

$$\int_\Omega w \phi^{n+1} \, dV = \int_\Omega w \underbrace{\left(\phi^n + \frac{\Delta t \mu^n}{\tau}\right)}_{r_\phi} \, dV \quad (17)$$

$$\int_\Omega w \mu^{n+1} \, dV = \int_\Omega w \underbrace{\left[\phi^n - \lambda u \left(1-(\phi^n)^2\right)\right]\left(1-(\phi^n)^2\right)}_{r_\mu}$$
$$+ \nabla w \cdot \underbrace{\left[- \left(W^2 \frac{\partial \phi^n}{\partial x} + W_0 \epsilon_m m W(\theta^n) \sin\left[m\left(\theta^n - \theta_0\right)\right] \frac{\partial \phi^n}{\partial y} \right) \hat{x} - \left(W^2 \frac{\partial \phi^n}{\partial y} - W_0 \epsilon_m m W(\theta^n) \sin\left[m\left(\theta^n - \theta_0\right)\right] \frac{\partial \phi^n}{\partial x} \right) \hat{y} \right]}_{r_{\phi x}} \, dV \quad (18)$$

The above values of r_u, r_{ux}, r_ϕ, and $r_{\phi x}$ and r_μ are used to define the residuals in the following parameters file:
applications/dendriticSolification/parameters.h