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)

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

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

where, W_0, ϵ_m, and θ_0 are constants and θ is the in-plane azimuthal angle, where $\tan(\theta) = \frac{n_y}{n_x}$, where n_y and n_x are components of the normal vector $\hat{n} = \frac{\nabla \phi}{|\nabla \phi|}$.

The evolution equations are:

$$\frac{\partial u}{\partial t} = -\frac{\delta \Pi}{\delta \phi} = D \nabla^2 u + \frac{1}{2} \tau(\hat{n}) \frac{\partial \phi}{\partial t} \tag{5}$$

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

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:

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

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

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

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, default value of 0.125 ($\sim$7.16°).

3 Time Discretization

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

$$u^{n+1} = \left(u^n - \frac{\mu^n \Delta t}{\tau}\right) + D\Delta t \nabla^2 u^n \tag{12}$$

$$\phi^{n+1} = \left(\phi^n - \frac{\Delta t \mu^n}{\tau}\right) \tag{13}$$

$$\mu^{n+1} = \left(\frac{\partial f^n}{\partial \phi}\right) - \nabla \cdot \left[\left(W^2\frac{\partial \phi^n}{\partial x} - W\frac{\partial W}{\partial u^n}\frac{\partial \phi^n}{\partial y}\right)\hat{x} + \left(W^2\frac{\partial \phi^n}{\partial y} + W\frac{\partial W}{\partial u}\frac{\partial \phi^n}{\partial x}\right)\hat{y}\right] \tag{14}$$

4 Weak Formulation

$$\int_\Omega w u^{n+1}\, dV = \int_\Omega w \underbrace{\left(u^n - \frac{\mu^n \Delta t}{\tau}\right)}_{r_u} + \nabla w \underbrace{(-D\Delta t \nabla u^n)}_{r_{ux}}\, dV \tag{15}$$

$$\int_\Omega w \phi^{n+1}\, dV = \int_\Omega w \underbrace{\left(\phi^n - \frac{\Delta t \mu^n}{\tau}\right)}_{r_\phi}\, dV \tag{16}$$

$$\int_\Omega w \mu^{n+1}\, dV = \int_\Omega w \underbrace{\left(\frac{\partial f^n}{\partial \phi}\right)}_{r_\mu} + \nabla w \cdot \underbrace{\left[\left(W^2\frac{\partial \phi^n}{\partial x} - W\frac{\partial W}{\partial u^n}\frac{\partial \phi^n}{\partial y}\right)\hat{x} + \left(W^2\frac{\partial \phi^n}{\partial y} + W\frac{\partial W}{\partial u}\frac{\partial \phi^n}{\partial x}\right)\hat{y}\right]}_{r_{\phi x}}\, dV \tag{17}$$

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