

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:

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

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

$$u = \frac{T - T_m}{L/c_p} \quad (2)$$

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:

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

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

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

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:

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

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

where

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

$$D = \frac{0.6267 \lambda W_0^2}{\tau_0} \quad (8)$$

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

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

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

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

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 ($\sim 7.16^\circ$).

3 Time Discretization

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

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

$$\phi^{n+1} = \phi^n + \frac{\Delta t \mu^n}{\tau} \quad (13)$$

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

4 Weak Formulation

$$\int_{\Omega} w u^{n+1} dV = \int_{\Omega} w \underbrace{\left(u^n + \frac{\mu^n \Delta t}{2\tau} \right)}_{r_u} + \nabla w \cdot \underbrace{(-D \Delta t \nabla u^n)}_{r_{ux}} dV \quad (15)$$

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

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

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