Two-Dimensional Dendritic Growth Using Phase-Field Model Design Document

CS 294-73 Group H 2015-Nov-24

1 Discretization Methods and Numerical Schemes

Recall the governing equations:

$$\begin{cases} \frac{\partial u}{\partial t} = D\nabla^{2}u + \frac{1}{2}\frac{\partial\phi}{\partial t} \\ \tau \frac{\partial\phi}{\partial t} = \phi(1-\phi)(\phi - \frac{1}{2} + \tilde{n}(u)) - \frac{\partial}{\partial x}(WW'\frac{\partial\phi}{\partial y}) \\ + \frac{\partial}{\partial y}(WW'\frac{\partial\phi}{\partial x}) + \nabla(W^{2}) \cdot \nabla\phi + W^{2}\nabla^{2}\phi \end{cases}$$
(1)
$$W = W_{0}(1 + \mu\cos(a_{0}(\theta - \theta_{0})) \\ \theta = tan^{-1}(\frac{\partial\phi}{\partial y}/\frac{\partial\phi}{\partial x}) + \pi(1 - sign(\frac{\partial\phi}{\partial x}))$$

A 2nd order central difference scheme will be used for spatial discretization while a 4th order Runge-Kutta scheme for time integration.

The final computational solution consists of time dependent phase field (ϕ) and dimensionless temperature field (u) in the form of vtk files.

2 Software Design

The following existing classes will be directly utilized:

Point, Box, RectMDarray

RK4

VisitWriter, WriteRectMDArray

CH_Timer

A new class <code>DendriticGrowth</code> is defined, along with a modified version of the original RK4. Inside <code>DendriticGrowth</code>, public member data and functions contain ϕ and u fields, as well as update and increment functions for both fields. As <code>DendriticGrowth</code> is the only input class for RK4, class setup in RK4 is modified accordingly.

3 Algorithm and Flow Chart

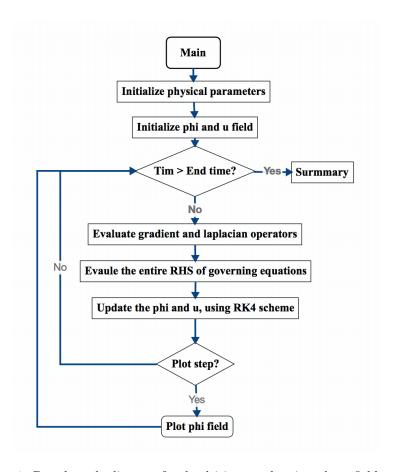


Figure 1: Pseudo code diagram for dendritic growth using phase-field model

- 1. Initialize the modeling parameters including timestep dt, end time t, grid dh, domain size L, etc.;
 - 2. Initialize the ϕ and u field;
- 3. Evaluate the gradient and laplacian operators by 2nd order central difference scheme;
 - 4. Evaluate the orientation angle θ and W;
 - 5. Evaluate RHS of ϕ and u euquations, update ϕ and u using RK4;
 - 6. Plot intermidiate time step contour of ϕ and u.