

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

CS 294-73 Group H

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1 Discretization Methods and Numerical Schemes

Recall the governing equations:

$$\begin{cases} \frac{\partial u}{\partial t} = & D\nabla^2 u + \frac{1}{2} \frac{\partial \phi}{\partial t} \\ \tau \frac{\partial \phi}{\partial t} = & \phi(1 - \phi)(\phi - \frac{1}{2} + \tilde{n}(u)) - \frac{\partial}{\partial x}(WW' \frac{\partial \phi}{\partial y}) \\ & + \frac{\partial}{\partial y}(WW' \frac{\partial \phi}{\partial x}) + \nabla(W^2) \cdot \nabla \phi + W^2 \nabla^2 \phi \\ W = & W_0(1 + \mu \cos(a_0(\theta - \theta_0))) \\ \theta = & \tan^{-1}(\frac{\partial \phi}{\partial y} / \frac{\partial \phi}{\partial x}) + \pi(1 - \text{sign}(\frac{\partial \phi}{\partial x})) \end{cases} \quad (1)$$

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

VisitWriter, WriteRectMDarray

CH_Timer

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

3 Algorithm and Flow Chart

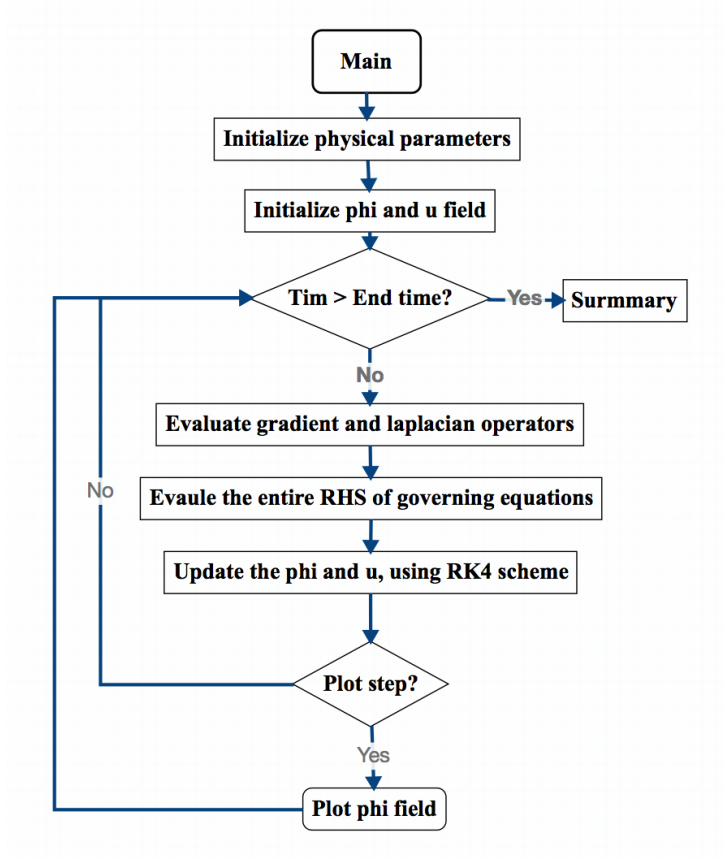


Figure 1: Pseudo code diagram for dendritic growth using phase-field model

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 euqations, update ϕ and u using RK4;
6. Plot intermidiate time step contour of ϕ and u .