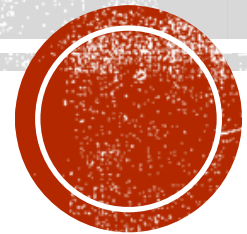


PHASE FIELD METHODS

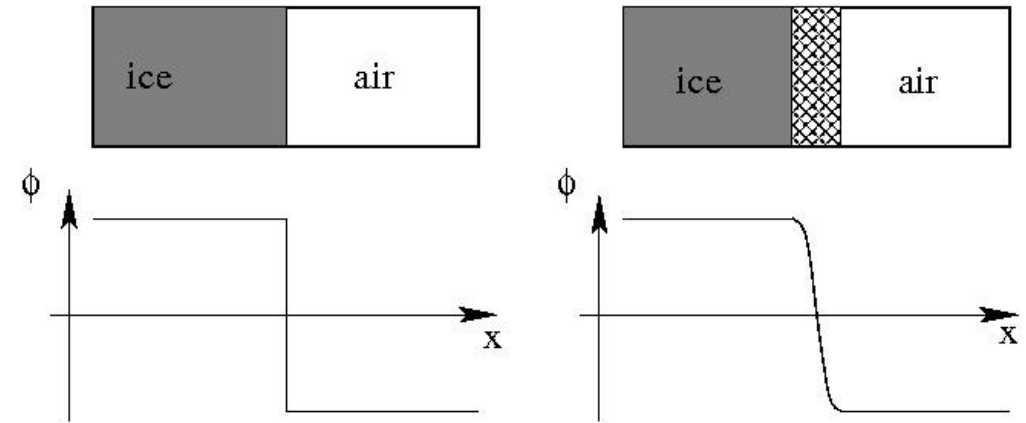
Derrick Shields

Kevin Caputo

Jesse Scarborough



- Solving problems involving complex and diffuse interfaces using free energy
- Models systems where shape of interface are important
- Can turn sharp interfaces into diffuse interfaces using phase field parameters
- Important in material science



WHAT IS PHASE FIELD MODELING?



- Sharp interface problems do not adequately describe most physical phenomena
- Written in terms of conserved and non-conserved variables that are continuous and smooth
- Allows for highly localized variations at an interface

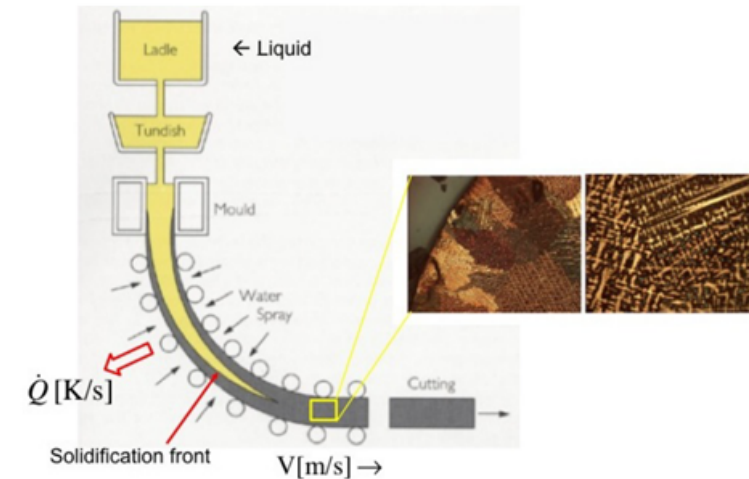


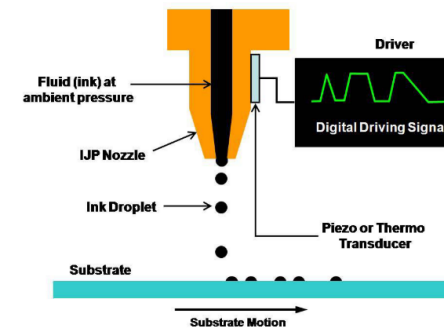
Figure 1.3: Typical industrial layout for thin slab casting. Liquid is enters from top, is cooled by splashing water and is directed –as it solidifies– at some speed (V) to the right. Most steels will then be cut and thermo-mechanically treated to improve their strength properties. In spite of the post solidification treatment that the metal may receive, the so called "as-cast" structure (inset) that is established initially is always, to some extend, present in the final product.

MOTIVATION FOR PHASE FIELD MODELING



- Impact of droplet on solid surface
- Drop coalescence and retraction in viscoelastic fluids
- Flow induced polymerization

Dynamics of drop formation from a capillary tube: inkjet printing



IMPORTANT APPLICATIONS



ADVANTAGES OF PHASE FIELD MODELING

- Able to compute geometric quantities easily
- Codes can be converted from two to three dimensions easily
- Can handle topology changes easily



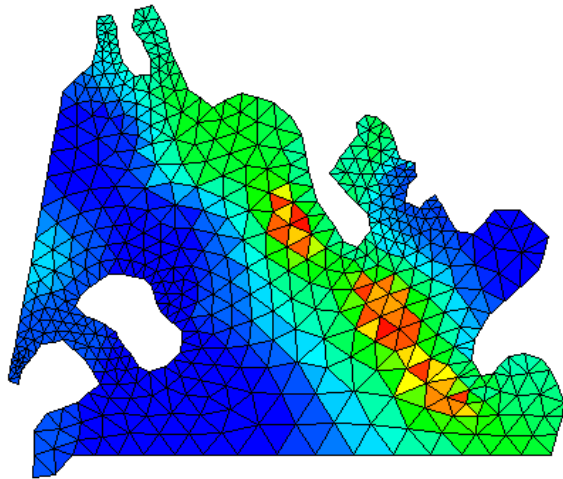
DISADVANTAGES OF PHASE FIELD MODELING

- Requires large number of grid points near interface
- Most applications limited to observation of shape
- Large domains can be computationally challenging

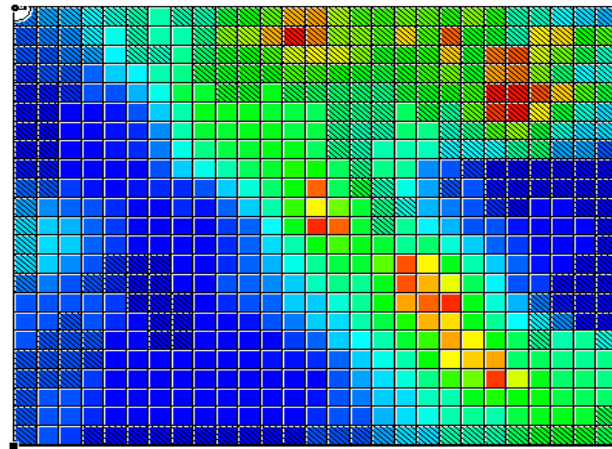


WAYS OF SOLVING PHASE FIELD MODELS

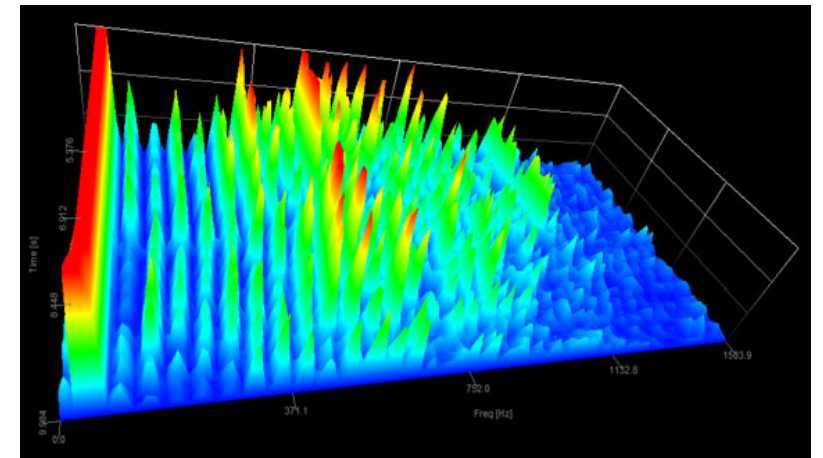
Finite element



Finite difference



Fourier spectral analysis



PHASE FIELD MODELING VS. LEVEL SET METHOD

Both phase field models and level set methods...

- Solve for diffuse interfaces
- Have fixed meshes
- Use an order parameter



PHASE FIELD MODELING VS. LEVEL SET METHOD

Phase field modeling...

- Can solve for three phases
- Allows for fluid-structure interaction and phase separation models
- More computationally intensive than level set
- Tends to be more accurate
- Is developed from physics standpoint
- Best when the shape of the interface is important



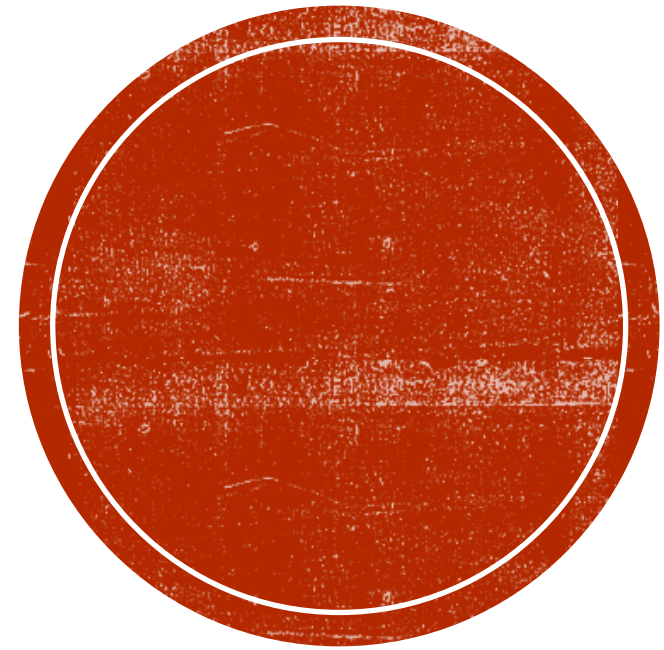
PHASE FIELD MODELING VS. LEVEL SET METHOD

Level set methods...

- Only solve for two phases
- Less computationally intensive
- Developed from mathematical perspective

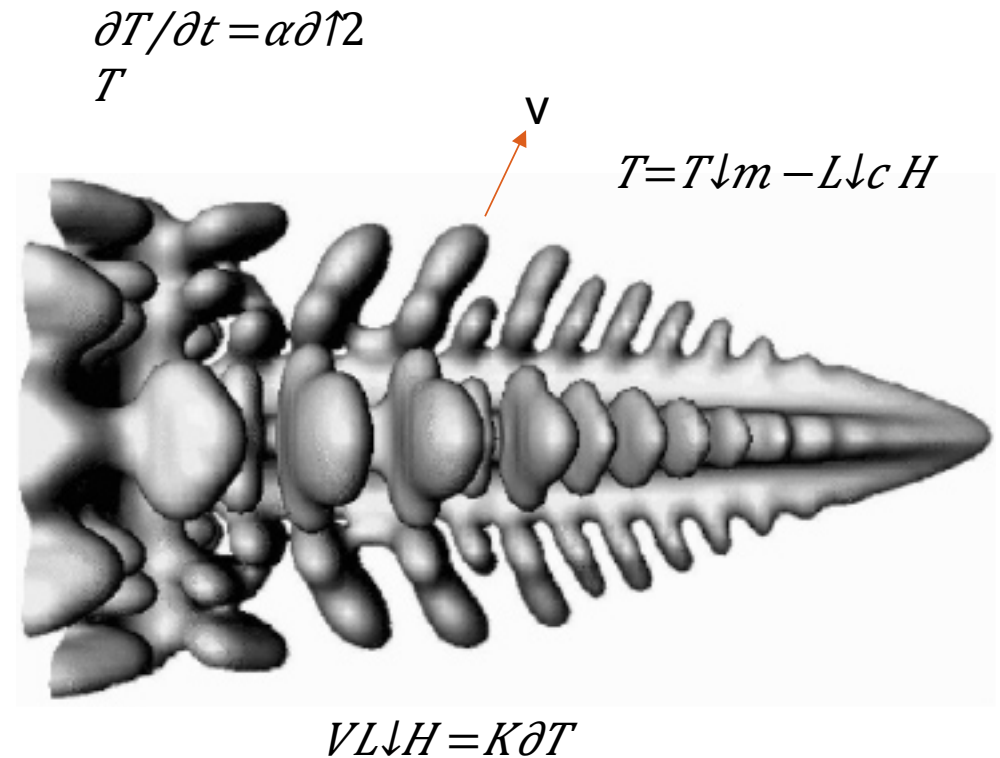


HISTORICAL PERSPECTIVE



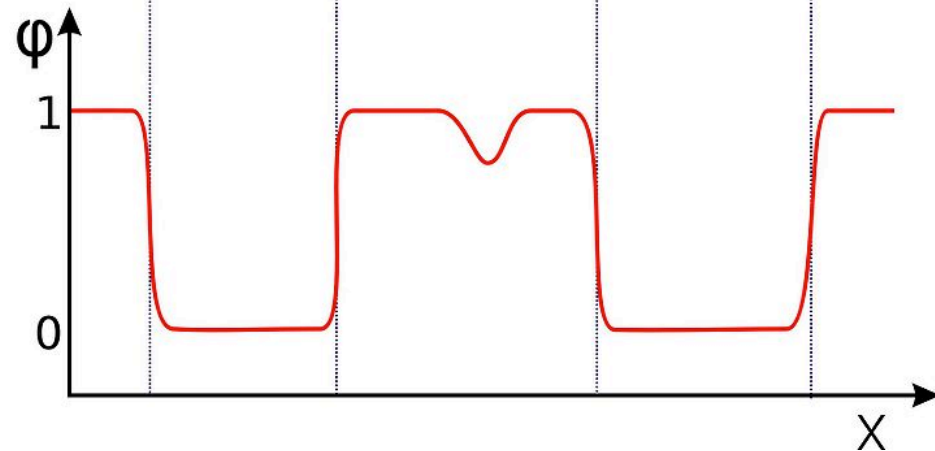
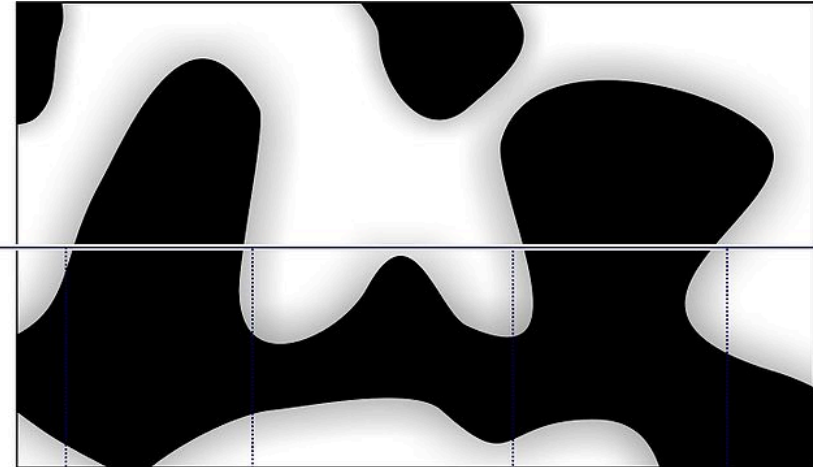
BEFORE PHASE FIELD

- Track boundary by predicting local normal velocity at a point - solve diffusion equation in both solid and liquid
- Boundary conditions on interfaces are evolving with time
- Free boundary problem where one equation depends on the other
- Must breakup/mesh surface to solve the problem. Move the mesh a certain distance over a certain time and solve the equations again



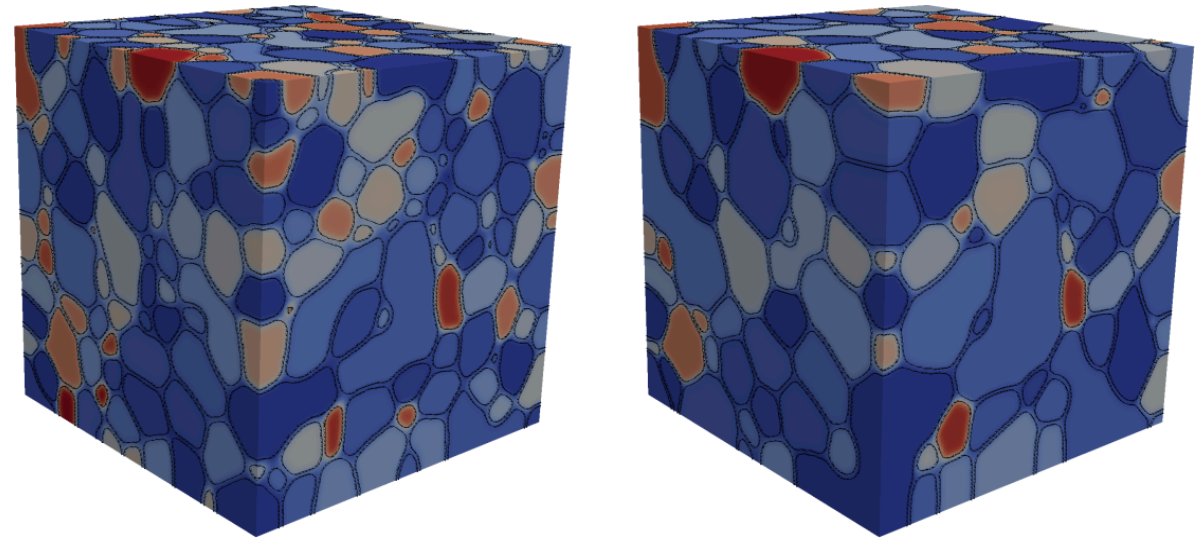
PHASE FIELD BEGINNING

- Developed more than a century ago by Van Der Waals and more than 40 years ago independently by Cahn and Hilliard
 - local interfacial velocity was determined
 - Limited when dealing with 3D systems
- Method was first introduced through modeling solidification of a pure melt



PHASE FIELD EVOLUTION

- Complexity created incentives for numerical calculations
- Much value in predicting the evolution of arbitrary morphologies and complex microstructures
 - Used in many industries
 - Both practical and theoretical
- Does not require explicitly tracking the positions of the interface



PHASE FIELD APPLICATIONS

- Microstructure evolution is common in many fields as the microstructure plays a critical role in determining the physical properties of a material
- Applications began to expand to grain growth modeling and coarsening
- More recently, phase field models have developed to thin films and surfaces, dislocation dynamics, crack propagation, and electromigration

Solidification

Pure liquid

Pure liquid with fluid flow

Binary alloys

Multicomponent alloys

Nonisothermal Solidification

Solid-State Phase Transformations

Spinodal phase separation

Precipitation of cubic ordered intermetallic

Cubic-tetragonal transformations

Hexagonal to orthorhombic transformations

Ferroelectric transformations

Phase transformations under an applied stress

Martensitic transformations in a single and polycrystals

Coarsening and Grain Growth

Coarsening

Grain growth with phases

Anisotropic grain growth

Other Applications

Phase transformations in thin films

Surface-stress induced pattern formation

Spiral growth

Crystal growth under stress

Crack propagation

Electromigration

TWO MODELS

Solidification Models

- Field variables or phase fields are introduced for the sole purpose of avoiding tracking the interface
- Solidification and original models belong to this type

Physical Order Parameters

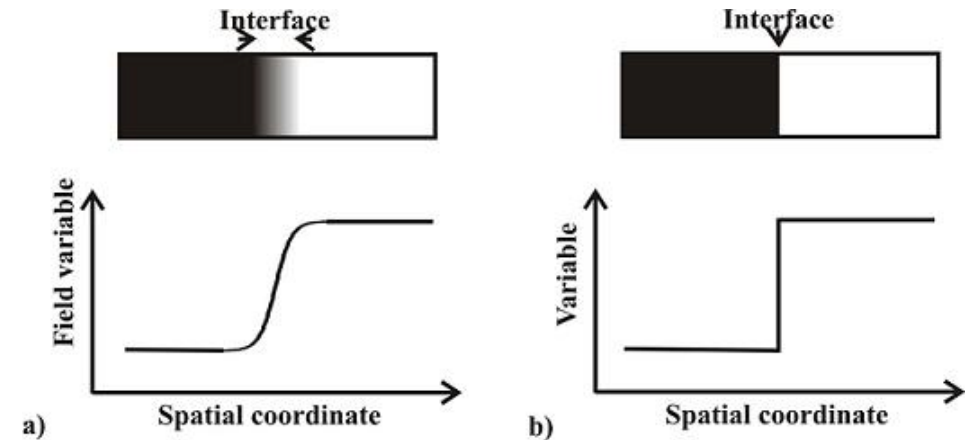
- Field variables correspond to well-defined physical order parameters
- These models assume that the microstructure evolution during a given process is governed by the phase field equations and that all the thermodynamic and kinetic coefficients can be related to microscopic parameters
- Mostly used for solid-state transformations

VARIATION IN MODELS

- The main difference among models lies in the treatment of various contributions to the total free energy
- Two types of variables: conserved and nonconserved
- In each model, the evolution of an order parameter can be obtained by solving the Cahn-Hilliard and Allen-Cahn equations

$$\partial\phi/\partial t = -M[\partial f/\partial\phi - \epsilon\downarrow\phi\uparrow\downarrow \nabla\uparrow\downarrow\phi]$$

$$\partial\phi/\partial t = M\nabla\uparrow\downarrow [\partial f/\partial\phi - \epsilon\downarrow\phi\uparrow\downarrow \nabla\uparrow\downarrow\phi]$$



PHASE FIELD METHOD TODAY

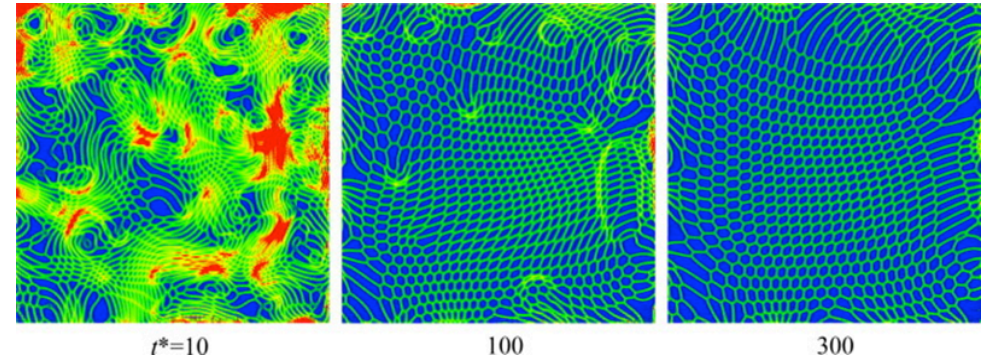
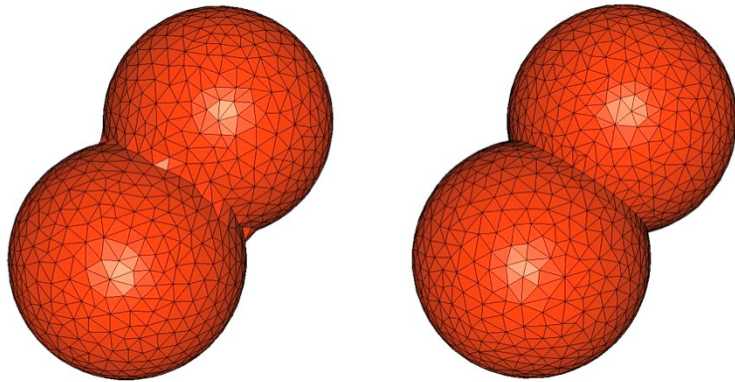


Fig. Dislocation network formation, fcc crystal during annealing. N. Zhou, C. Shen, M.J. Mills, Y. Wang (2007)

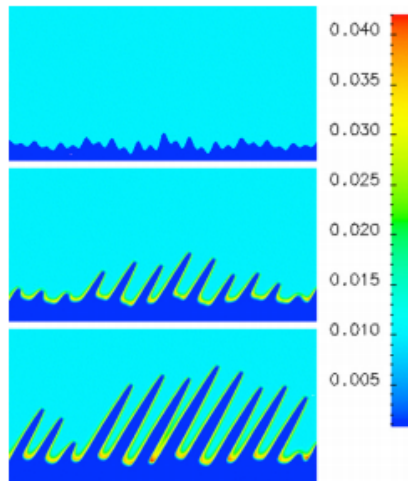


Fig.. Precipitation from an austenite grain boundary. Singer

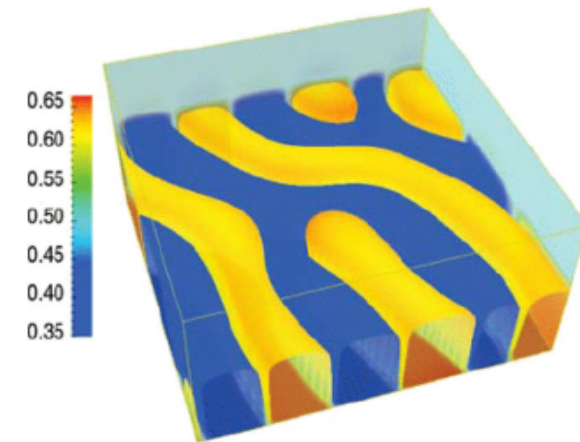
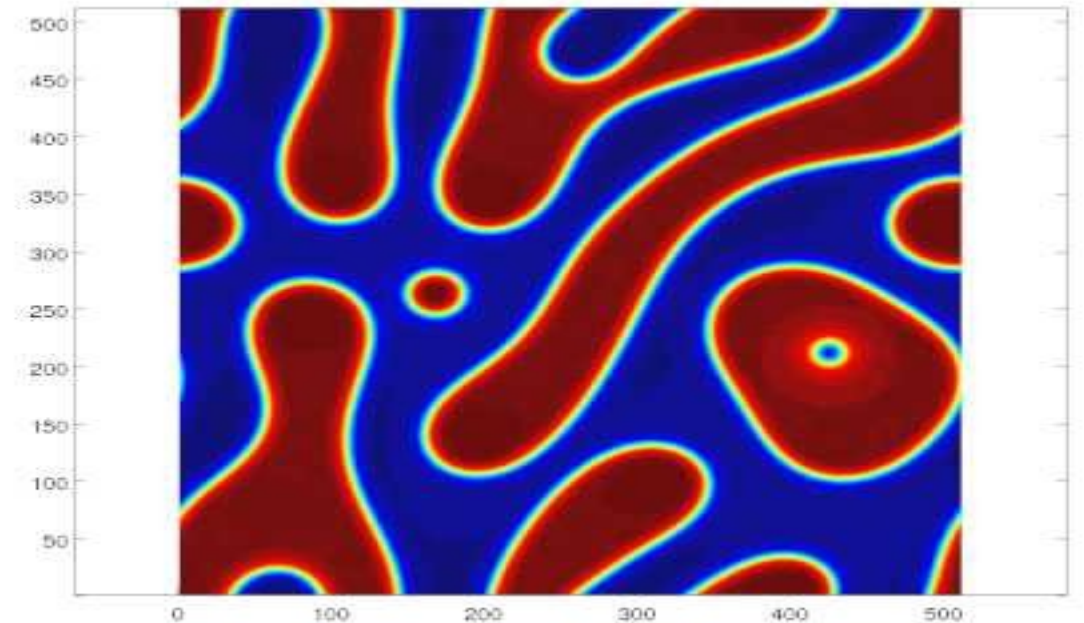


Fig. 3D eutectic growth. Lewis et al.

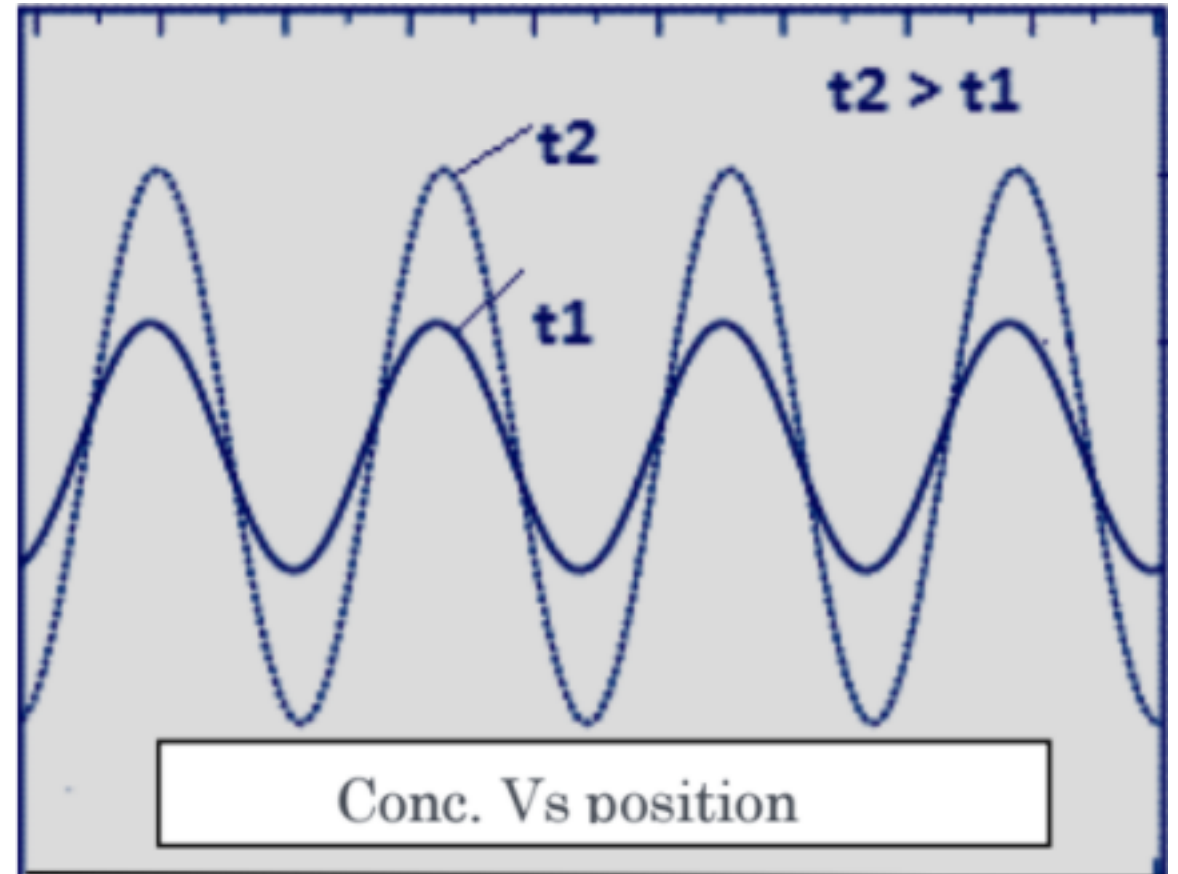
SPINODAL DECOMPOSITION

- Mechanism in which a solution of two or more components separate into distinct regions with distinct chemical and physical properties.
- One of the few phase transformations in solids for which there is any plausible quantitative theory
- There is no thermodynamic barrier to reaction inside spinodal region, meaning decomposition is determined solely by diffusion
- Provides a means of producing a very finely dispersed microstructure that can significantly enhance the physical properties of the material



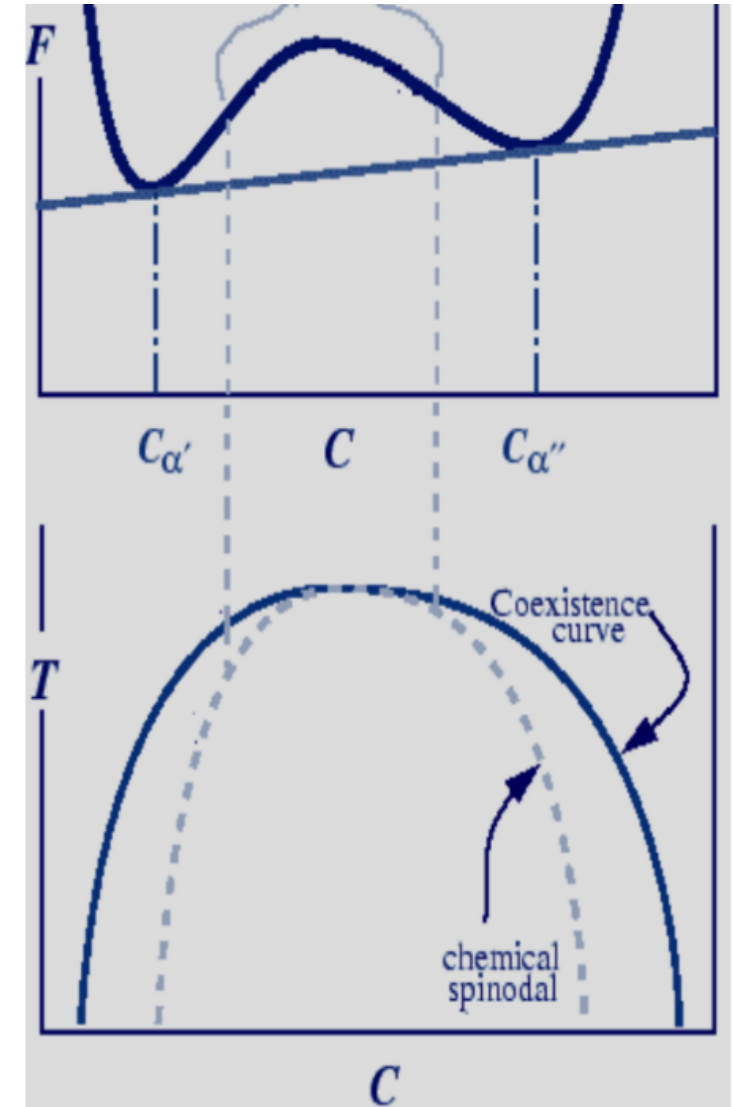
SPINODAL DECOMPOSITION

- In a binary mixture spinodal decomposition occurs when delocalized small amplitude fluctuations grow spontaneously
- The local concentration fluctuations lead to phase change in the thermodynamically unstable state
- This mechanism does not occur in the whole two-phase region but in a smaller region which is given by spinodal curve.



SPINODAL DECOMPOSITION

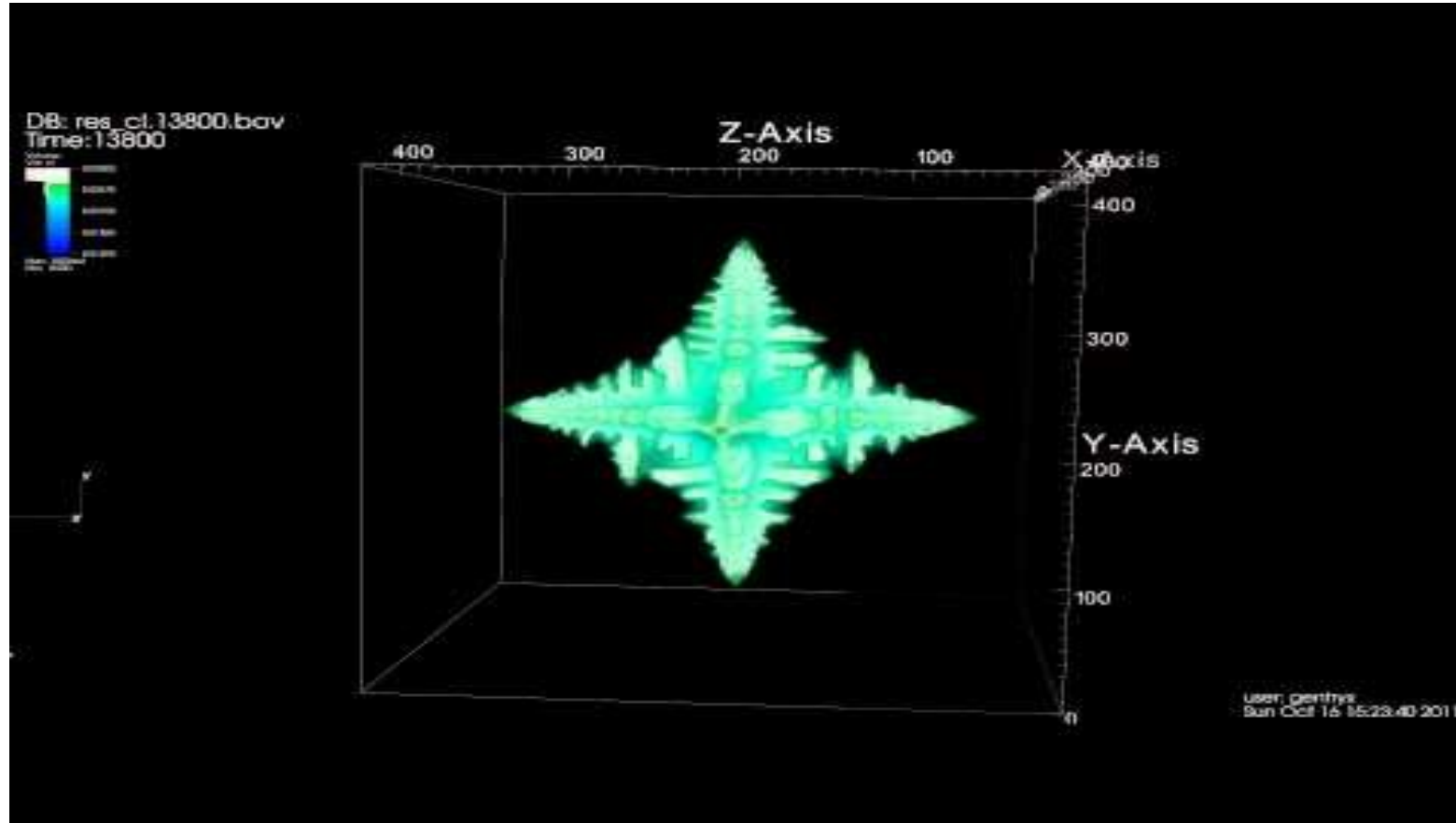
- Plot of free energy vs composition for a binary mixture. The points of inflection enclose the region in which spinodal decomposition will occur at that temperature
- The spinodal curve is found by finding points of inflection at different temperatures
- Phase separation in spinodal curve is spinodal decomposition
- Phase separation between spinodal curve and coexistence curve takes place via nucleation
- Outside of spinodal curve, localized large amplitude fluctuations must form in order to start transformation



DENDRITIC GROWTH

- A dendrite is a crystal with a tree-like structure
 - Process known as the solidification or freezing
 - The resulting micro-structures from solidification impact numerous properties of the solid material.
-
- <http://math.nist.gov/mcsd/savg/vis/dendrite/>
 - Computations using phase field method have provided some of the most realistic simulations of this complicated phenomenon
 - Simulations use diffusion in the bulk phases and surface energy and kinetic effects at the solid/liquid interface
-
- <http://math.nist.gov/mcsd/Reports/95/yearly/node15.html>

DENDRITIC GROWTH



The video shows the concentration of copper (in an aluminium 2 wt% copper alloy) in the liquid phase changes as the dendrite solidifies

<http://www.phase-trans.msm.cam.ac.uk/dendrites.html>



FREE ENERGY MINIMIZATION

$$F(\phi) = \int f(\phi) dV$$

$$F(\phi) = \int (f(\phi) + \varepsilon^2 |\partial\phi|^2) dV$$

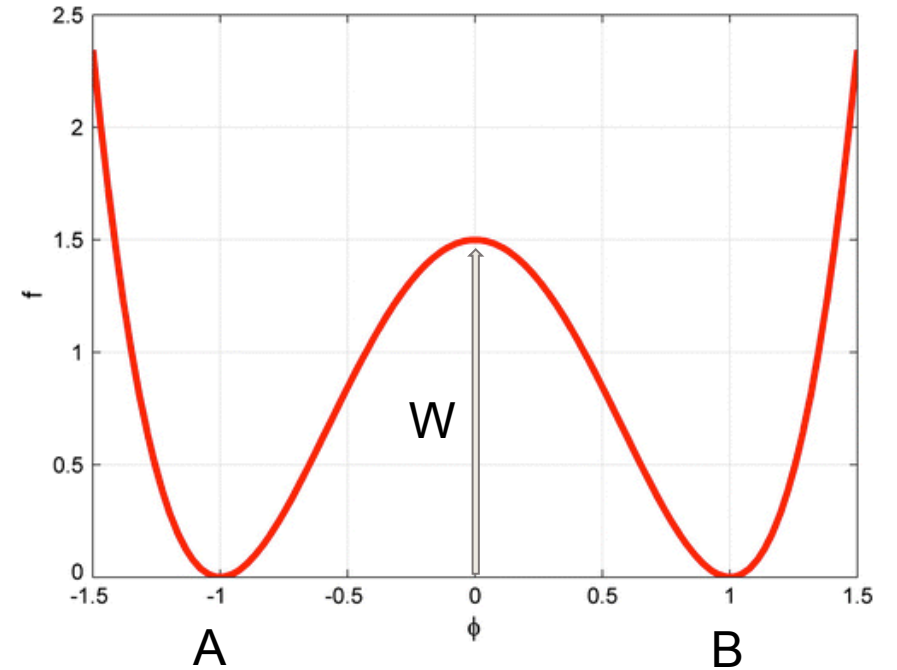


Cahn Hilliard (conserved)

Allen-Cahn (non-conserved)

$$\frac{\partial\phi}{\partial t} = M \partial^2 \left(\frac{\partial f}{\partial \phi} - 2\varepsilon^2 \partial^2 \phi \right)$$

$$\frac{\partial\phi}{\partial t} = M \left(\frac{\partial f}{\partial \phi} - 2\varepsilon^2 \partial^2 \phi \right)$$



DERIVATION OF PHASE FIELD EQUATIONS

Free Energy Functional

$$F(\phi) = \int_{\Omega} (f(\phi) + \epsilon^2 |\nabla \phi|^2) dV$$

$$\delta F / \delta \phi = 0 \quad \longrightarrow \quad \frac{\partial f}{\partial \phi} - 2\epsilon^2 \nabla^2 \phi = 0$$

$$F(\phi) = \int_{\Omega} (f(\phi) + \epsilon^2 |\nabla \phi|^2) dV$$

$$\delta F(\phi) = \delta \int_{\Omega} (f(\phi) + \epsilon^2 |\nabla \phi|^2) dV$$

FUNCTIONAL DERIVATIVE

Functional derivative acts like a differential operator

$$\delta F(\phi) = \int \left(\delta f(\phi) + \delta \epsilon \left(\frac{d\phi}{dx} \right) \right) dV$$

$$\delta F(\phi) = \int \left(\frac{\partial f(\phi)}{\partial \phi} \delta \phi + \epsilon \delta \left(\frac{d\phi}{dx} \right) \right) dV$$

$$\delta F(\phi) = \int \left(\frac{\partial f(\phi)}{\partial \phi} \delta \phi + \epsilon \frac{d}{dx} \left(\frac{d\phi}{dx} \delta \phi \right) \right) dV$$

$$\delta F(\phi) = \int \left(\frac{\partial f(\phi)}{\partial \phi} \delta \phi + \epsilon \frac{d}{dx} \left(\frac{d\phi}{dx} \delta \phi \right) \right) dV$$

➤ Integrate by parts

$$= 2\epsilon \int \nabla^2 \phi \, (\delta\phi) - \int \nabla^2 (2\epsilon \nabla^2 \phi / dx^2) (\delta\phi) dV$$

➤ Assume phi doesn't vary at the boundaries

$$\delta F(\phi) = \int \nabla^2 (\partial f(\phi) / \partial \phi - 2\epsilon \nabla^2 \phi / dx^2) \delta\phi dV$$

➤ For generalized form, setting expression in parenthesis equal to zero

$$\begin{aligned} \delta F / \delta \phi &= \partial f / \partial \phi - 2\epsilon \nabla^2 \phi / dx^2 \\ \phi &= 0 \end{aligned}$$

$$\delta F / \delta \phi = \partial f / \partial \phi - 2\epsilon^2 \nabla^2 \phi = 0$$

➤ Define free energy density

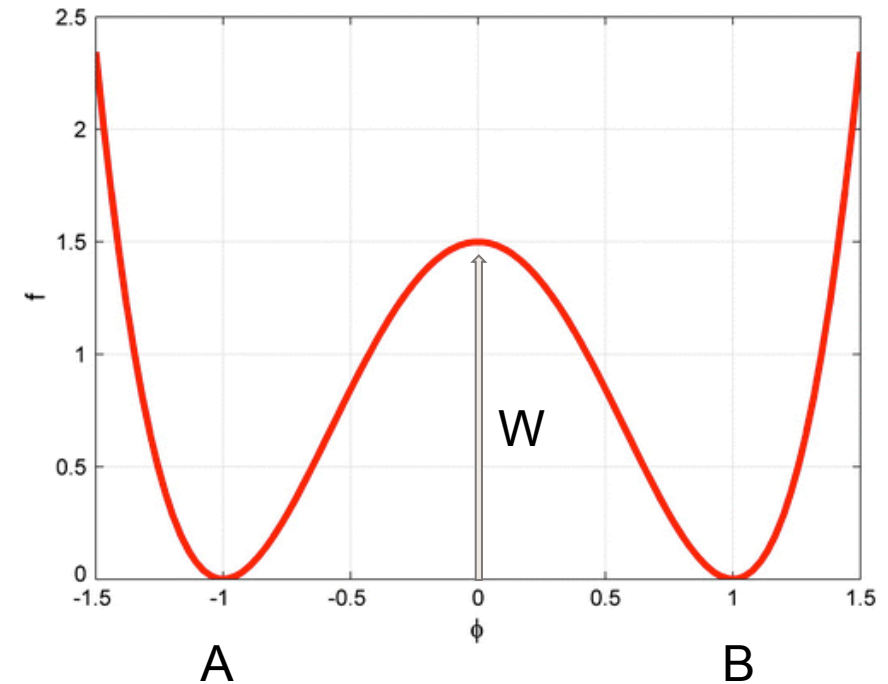
$$f(\phi) = W\phi^2(1-\phi)^2$$

$$2W\phi(1-\phi)(1-2\phi) - 2\epsilon^2 \frac{d^2 \phi}{dx^2} = 0$$

➤ Composition Profile

$$\phi(x) = \frac{1}{2} (1 + \tanh(x/2l))$$

$$l = (2/W)^{1/2} \epsilon$$



CONSERVED ORDER PARAMETER

➤ Introduce Lagrange multiplier

$$F(\phi) = \int dV (f(\phi) + \epsilon \nabla^2 \phi - \lambda(\phi - \phi_0))$$

➤ Repeat the process

$$\lambda = \partial f / \partial \phi - 2\epsilon \nabla^2 \phi$$

➤ If we wish to describe diffusion

$$J = -M \Delta \lambda = -M \nabla^2 (\partial f / \partial \phi - 2\epsilon \nabla^2 \phi)$$


DESCRIBING DIFFUSIVE PROCESSES

$$J = -M \nabla \lambda = -M \nabla (\partial f / \partial \phi - 2 \epsilon \nabla^2 \phi)$$

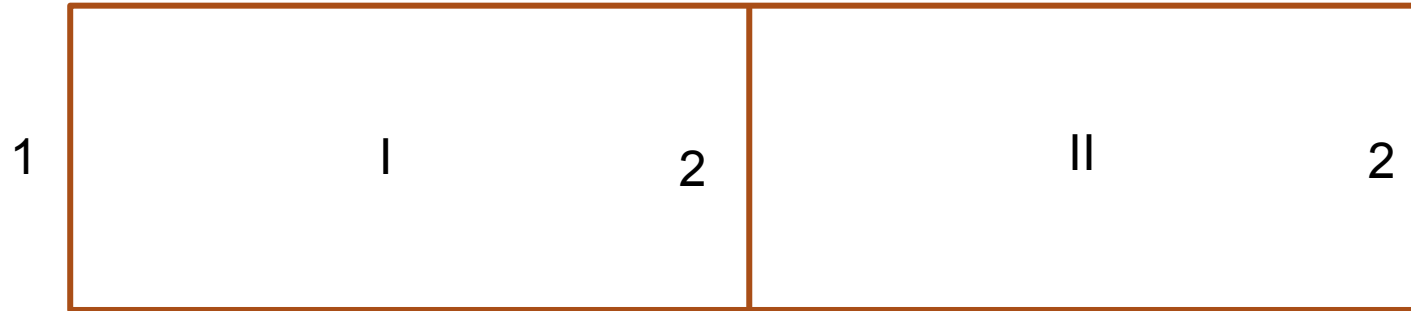
$$\partial \phi / \partial t = -\nabla \cdot J$$

$$\partial \phi / \partial t = M \nabla^2 (\partial f / \partial \phi - 2 \epsilon \nabla^2 \phi)$$

Cahn-Hilliard 

Allen-Cahn  $\partial \phi / \partial t = -M \lambda = -M (\partial f / \partial \phi - 2 \epsilon \nabla^2 \phi)$

HAND CALCULATION



$$@t=0^- \quad | \quad \phi|_3 = 1, \phi|_1 = 1$$

$$@t=0^+ \quad | \quad \phi|_3 = 0, \phi|_1 = 1$$

➤ Allen-Cahn non-conserved equation

$$(1/M) \partial \phi / \partial t = (K \nabla^2 \phi - \partial f / \partial \phi)$$

➤ Take free energy density to be the following

$$f(\phi) = W \phi^2$$

$$K \nabla^2 \phi - s \phi = 2W\phi$$

DEFINING MATRICES

- Taking transient and diffusion coefficients to be values such that our matrices are simplified, while taking barrier height to be 1

Local Matrices

$$I = K \downarrow II = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

$$I = S \downarrow II = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Global Matrices

$$\begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{Bmatrix}$$

$$\begin{bmatrix} 0 & -1 & 0 & 0 \\ -1 & 2 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{Bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{Bmatrix}$$

EQUATIONS

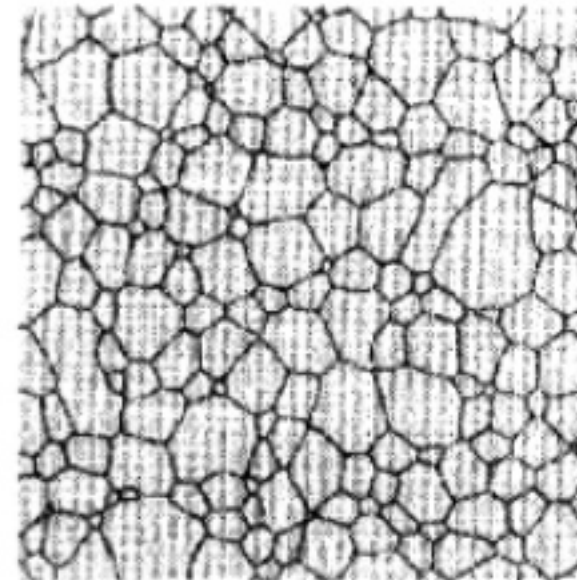
$$k \phi_{j,t+\Delta t} - s \frac{1}{\Delta t} (\phi_{j,t+\Delta t} - \phi_{j,t}) = 2 \phi_{j,t+\Delta t}$$

$$\phi_{j,t+\Delta t} [k - 1/\Delta t s] = 2 \phi_{j,t+\Delta t} - 1/\Delta t s \phi_{j,t}$$

$$[k - 1/\Delta t s] = k^*$$

$$2 \phi_{j,t+\Delta t} - 1/\Delta t s \phi_{j,t} = \phi_{j,t+\Delta t}^*$$

$$k^* \phi_{j,t+\Delta t} = \phi_{j,t+\Delta t}^*$$



FIRST TIME STEP

For $\Delta t=0.1$

$$k^* = [2 - 1/0.1 \ 2] = -18$$

$$\phi^*_{t+\Delta t} = 2\phi_{t-\Delta t} + \phi_{t-2\Delta t} + \phi_{t-3\Delta t} - 1/\Delta t \cdot s \cdot \phi_{t-2\Delta t}$$

$$\phi^*_{t+\Delta t} = 2(1) + 1 + 1 - 1/0.1 (2)(1)$$

$$-18\phi_{t+\Delta t} = -16$$

$$\phi_{t+\Delta t} = 0.889$$

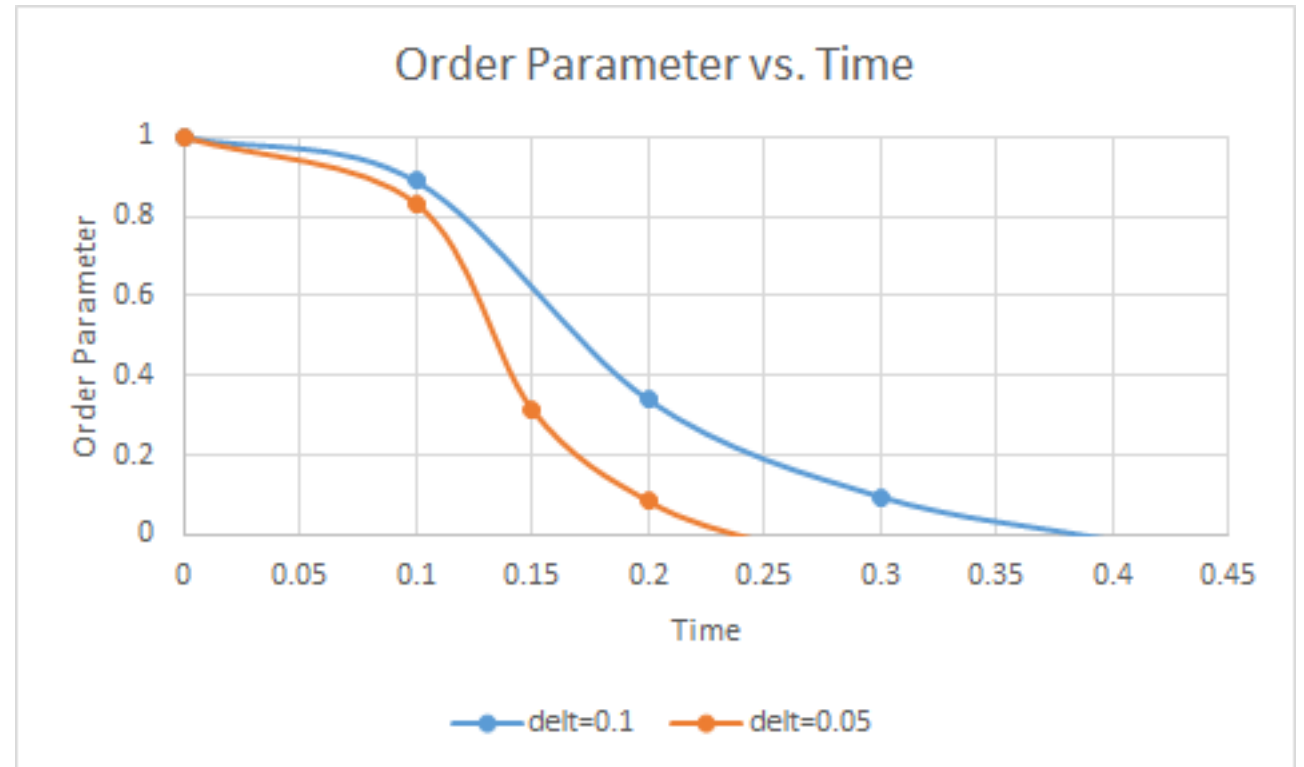


NEXT TIME STEP

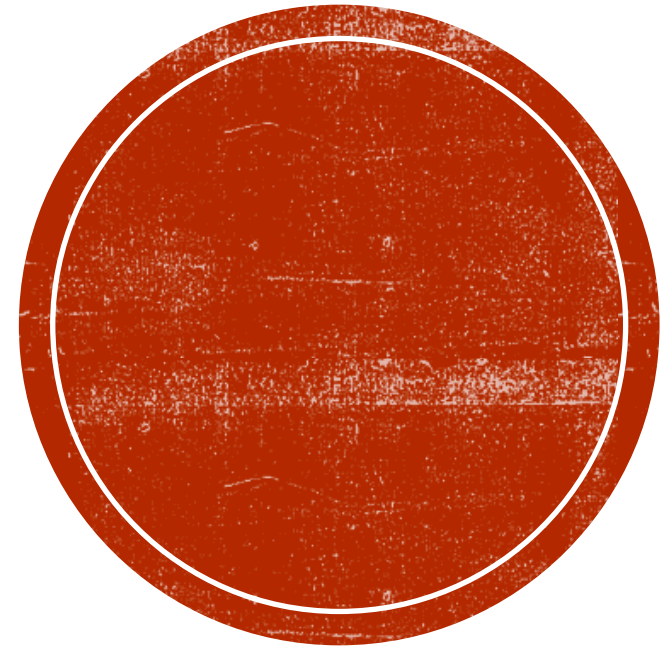
$$-18\phi \downarrow t+\Delta t = \phi \uparrow^* \downarrow t+\Delta t$$

$$\phi \uparrow^* \downarrow t+\Delta t = (2)(0.889) + 0 + 1 - 1/2 (2)(0.889)$$

$$\phi \downarrow t+\Delta t = 0.34$$



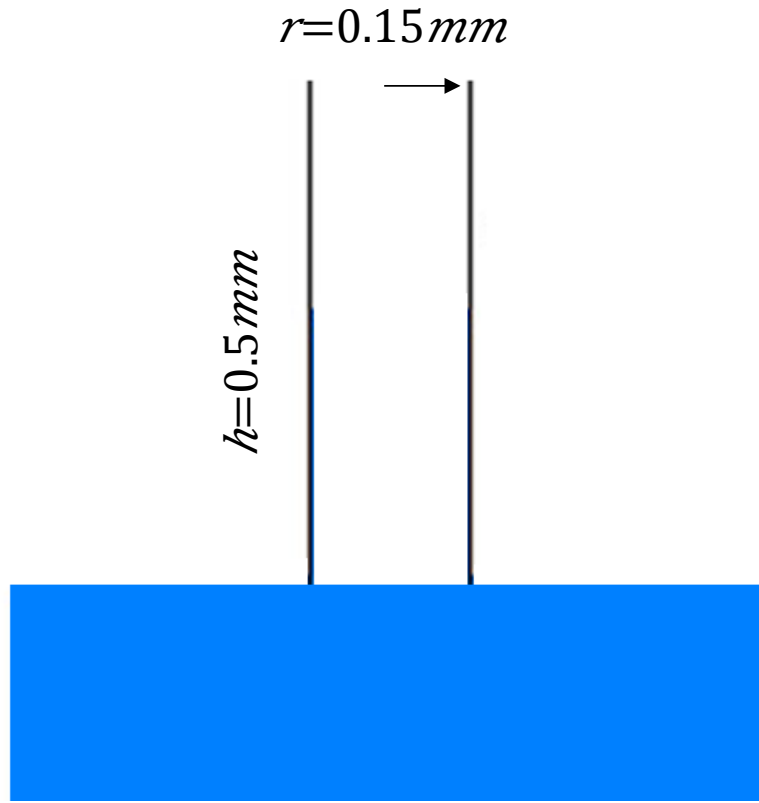
**NUMERICAL
L
EXAMPLES**





CAPILLARY TUBE IN COMSOL





GEOMET RY OF PROBLE M





PHASE SEPARATION

- Cahn-Hilliard Equation

$$\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = \nabla \cdot (\gamma \lambda / \epsilon \nabla^2 \nabla \psi)$$

Where $\psi = -\nabla \cdot \epsilon \nabla^2 \nabla \phi + (\phi^2 - 1)\phi$



UPDATING VARIABLES WITH ORDER PARAMETER

$$V \downarrow f1 = 1 - \phi / 2$$

$$V \downarrow f2 = 1 + \phi / 2$$

$$\rho = \rho \downarrow air + (\rho \downarrow water - \rho \downarrow air) V \downarrow f2$$

$$\mu = \mu \downarrow air + (\mu \downarrow water - \mu \downarrow air) V \downarrow f2$$



MOMENTUM BALANCE

Continuity condition

$$\nabla \cdot u = 0$$

Momentum Transport (Navier-Stokes)

$$\rho \frac{\partial u}{\partial t} + \rho (u \cdot \nabla) u = \nabla \cdot [-pI + \mu(\nabla u + (\nabla u)^T)] + F_{\text{ext}} + \rho g$$

Where $F_{\text{ext}} = G \nabla \phi$ and $G = \lambda [-\nabla^2 \phi + \phi(\nabla^2 - 1)/\epsilon^2] = \lambda/\epsilon^2 \psi$



BOUNDARY CONDITIONS

Initial conditions

Reservoir full of water

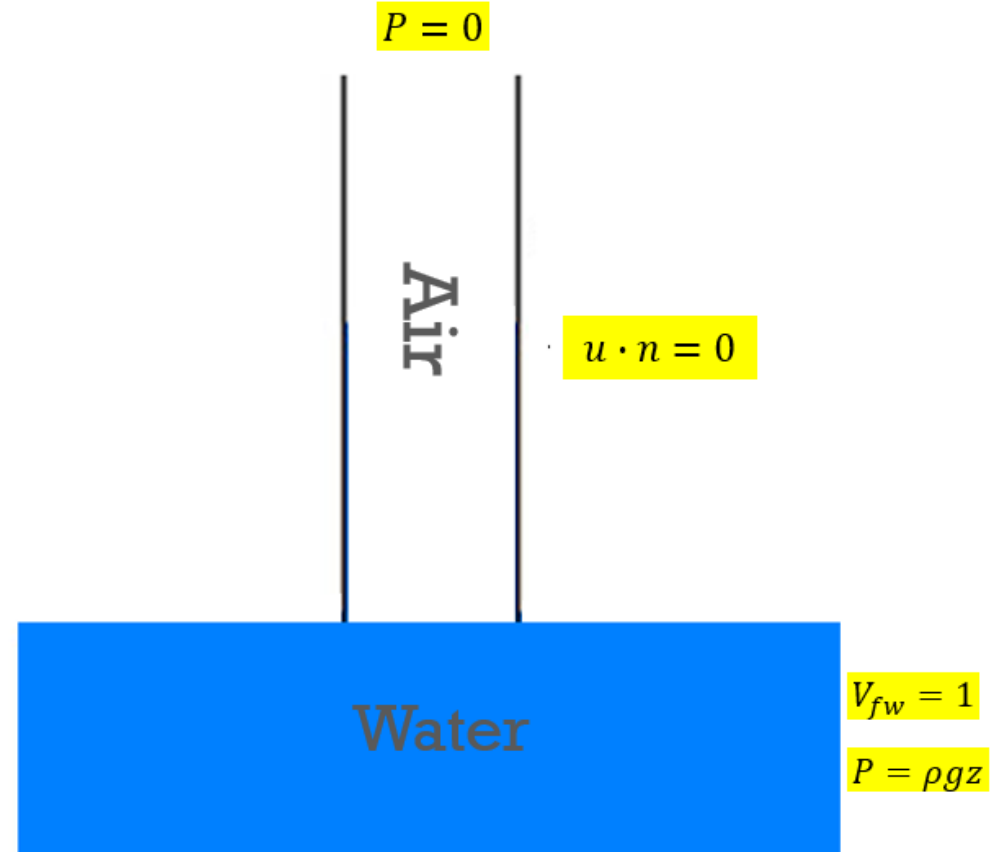
Capillary tube full of air

Boundary conditions

$P = 0$ at top of capillary tube

$P = \rho g z$ on right side of reservoir

No slip condition on walls of capillary tube



Settings Properties

Size

Build Selected Build All

Label: Size

Element Size

Calibrate for:

General physics

Predefined Custom

Extra fine

Element Size Parameters

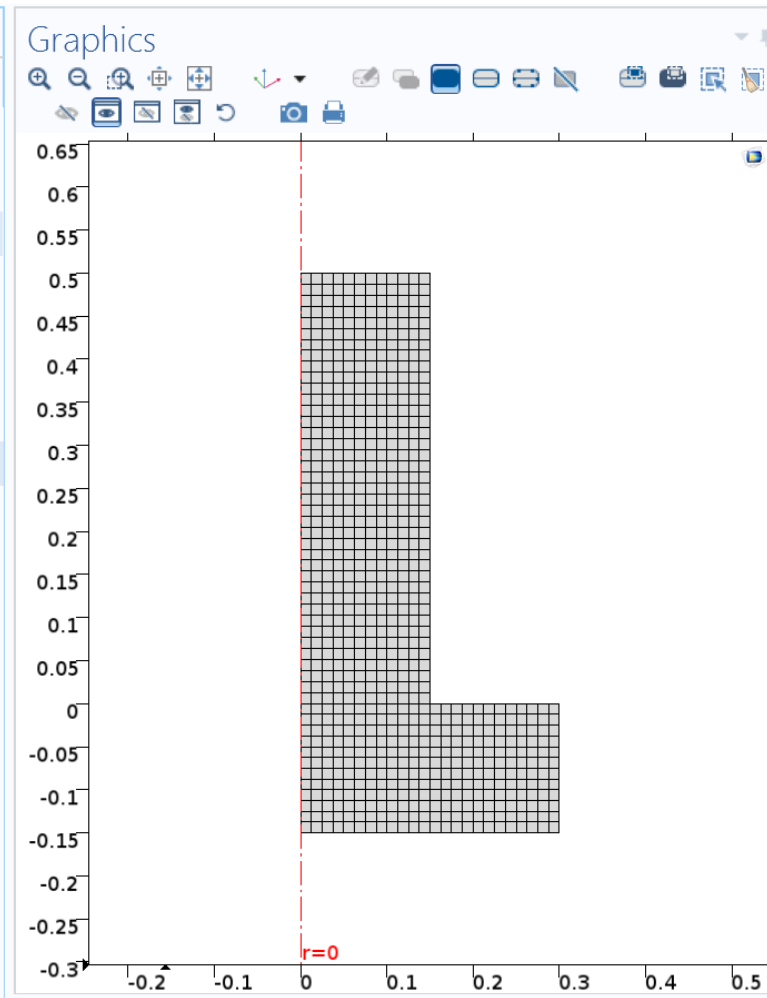
Maximum element size: 0.013 mm

Minimum element size: 4.88E-5 mm

Maximum element growth rate: 1.2

Curvature factor: 0.25

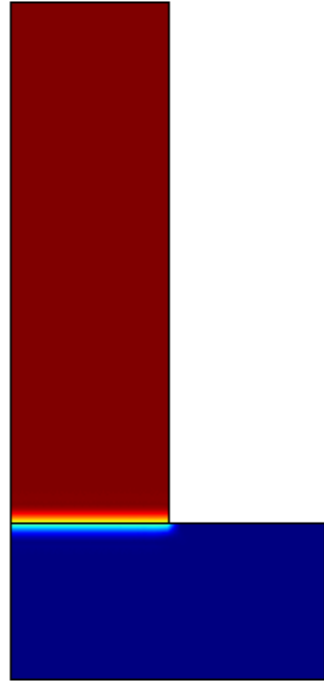
Resolution of narrow regions: 1



GRID SIZE SELECTION

- Rectangular grid system
- Too fine of a grid took too long to compute
- Too coarse and the water did not move





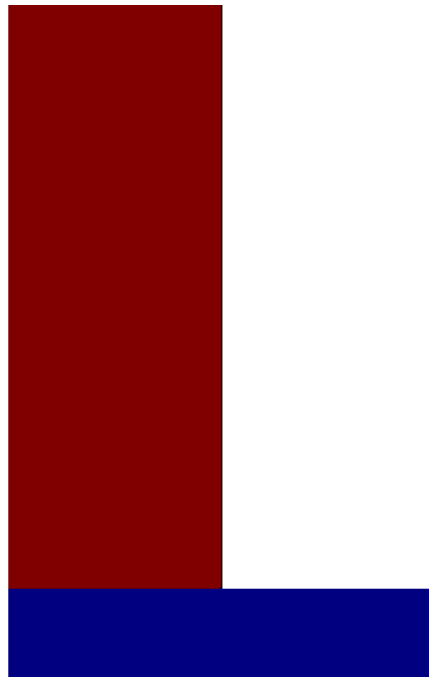
SOLUT
ION



COMPUTATION TIME – LEVEL SET VS. PHASE FIELD

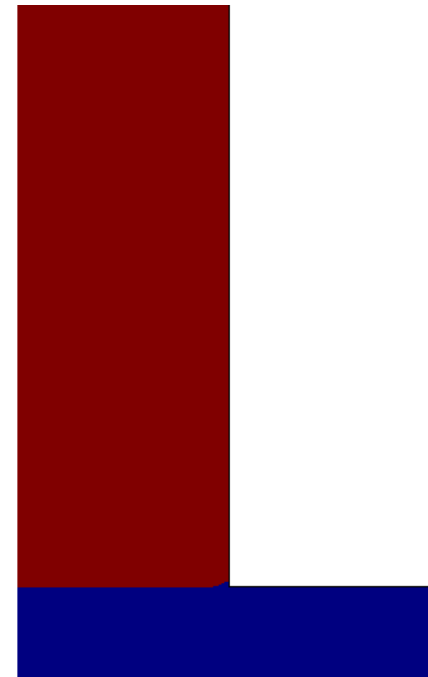
Level Set

- 13 minutes and 20 seconds



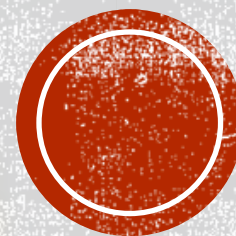
Phase field

- 10 minutes and 50 seconds



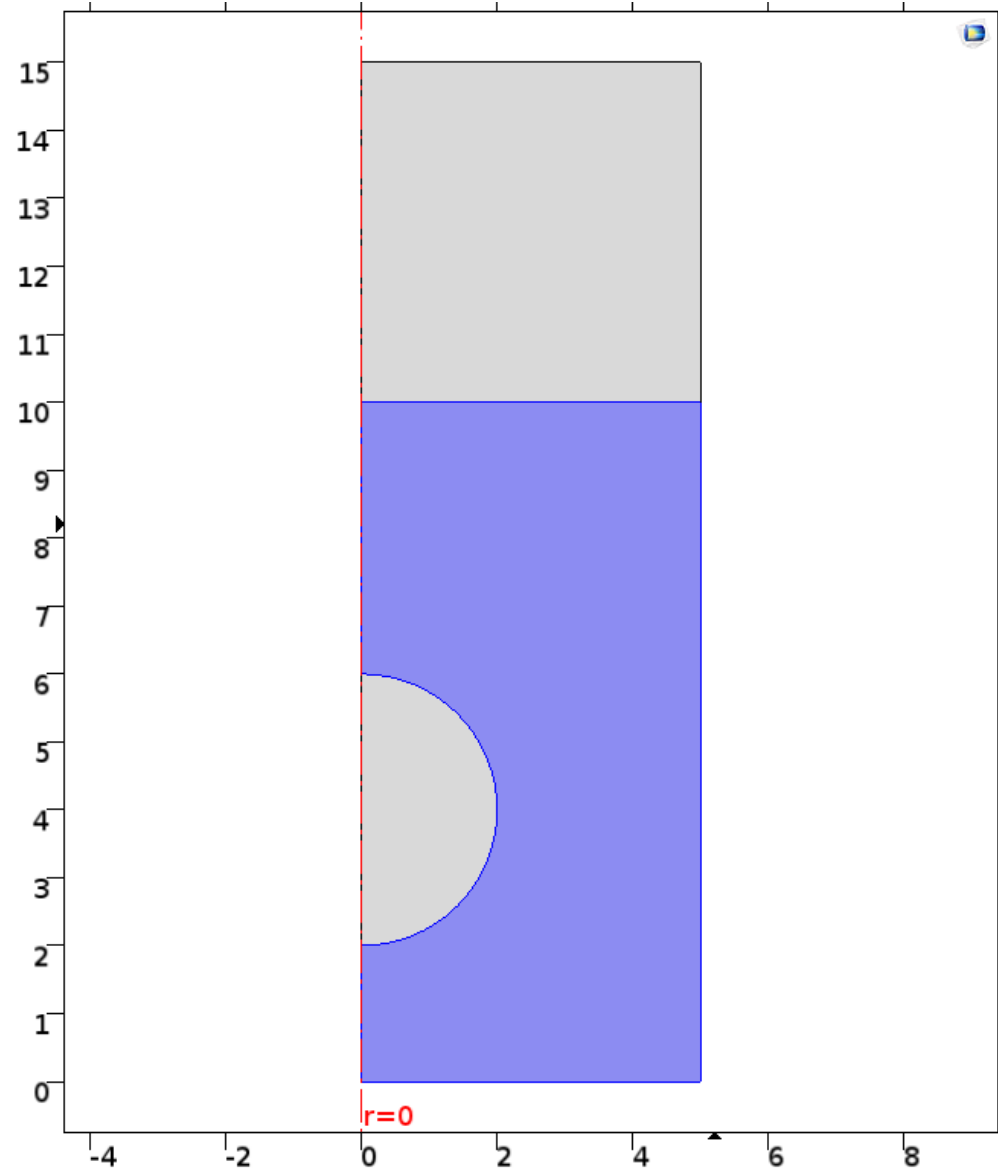


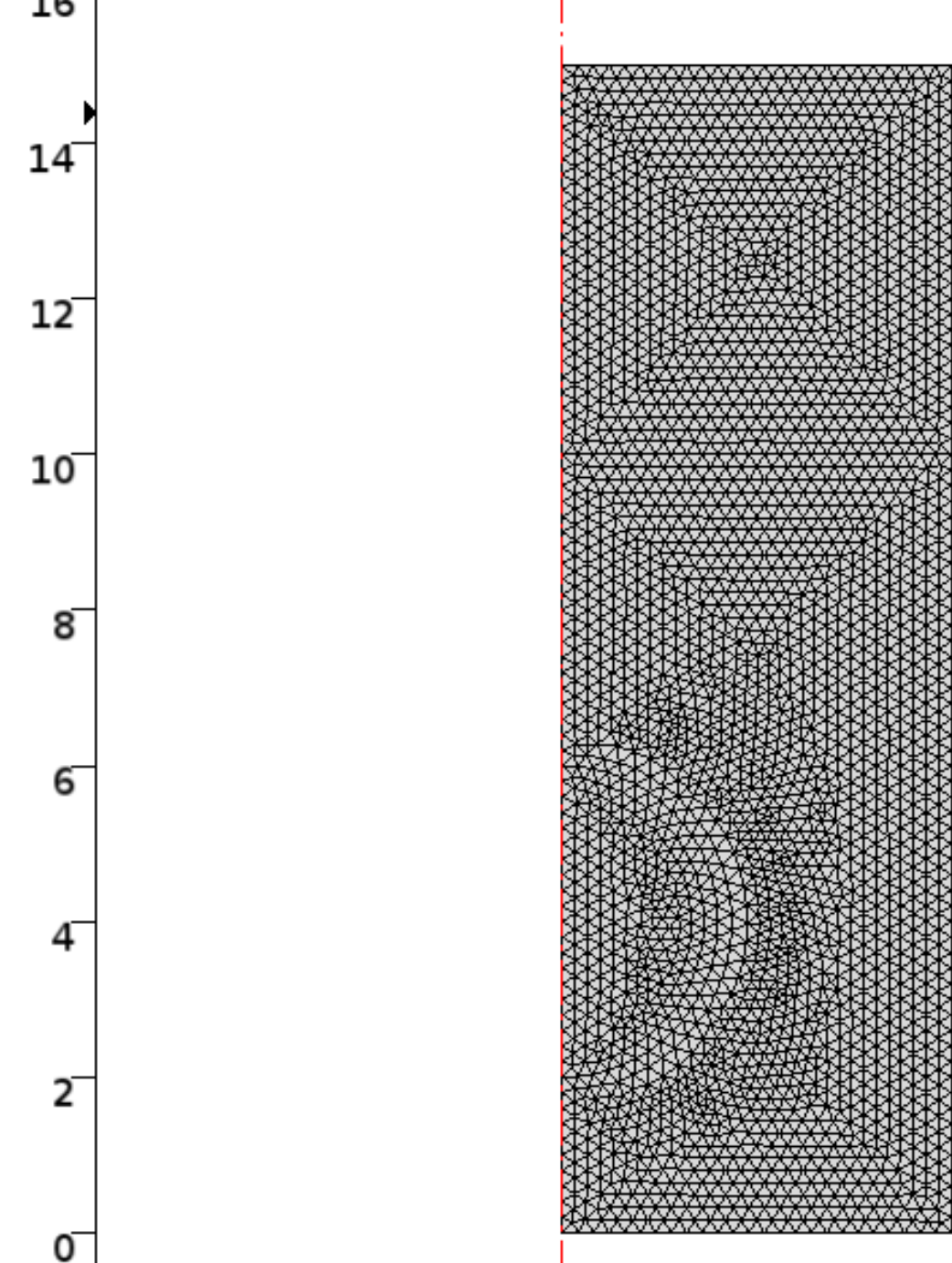
RISING OIL BUBBLE



PROBLEM DESCRIPTION

- Geometry adapted for phase field from COMSOL Manual (designed for level set)
- Uses both Navier-Stokes and Cahn-Hilliard
- Has many important applications





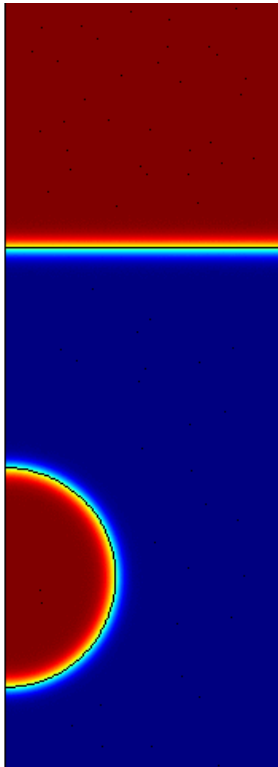
GRID SELECTION

- Free triangular grid
- Most dense around phase interface

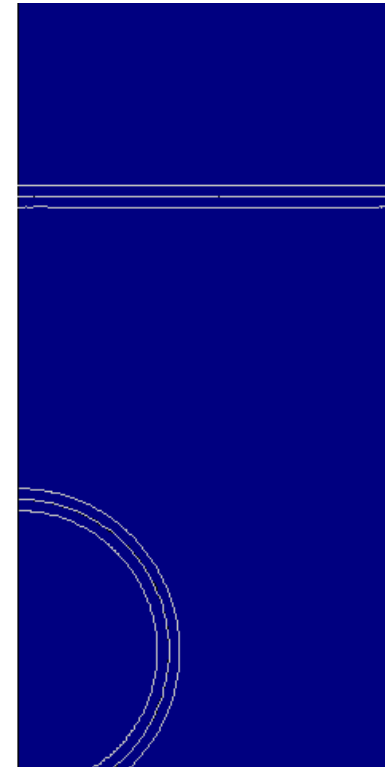


SOLUTION ANIMATIONS

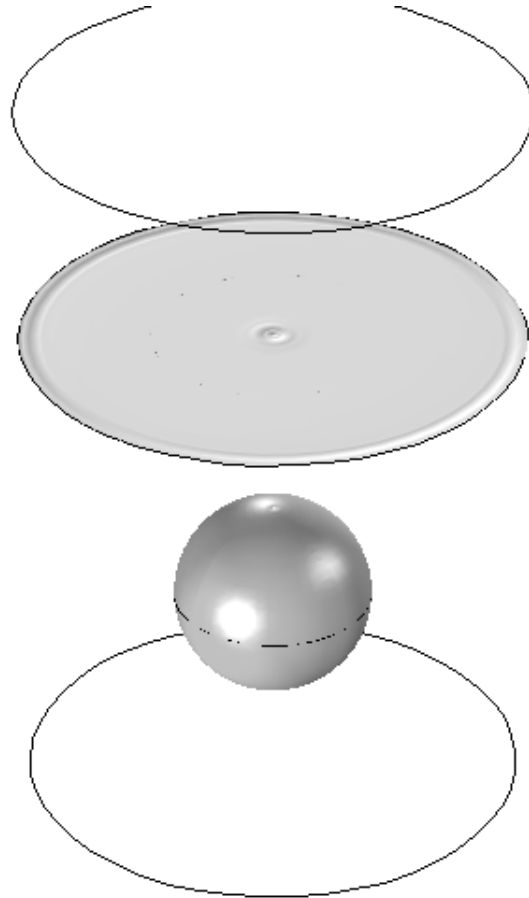
Volume Fraction



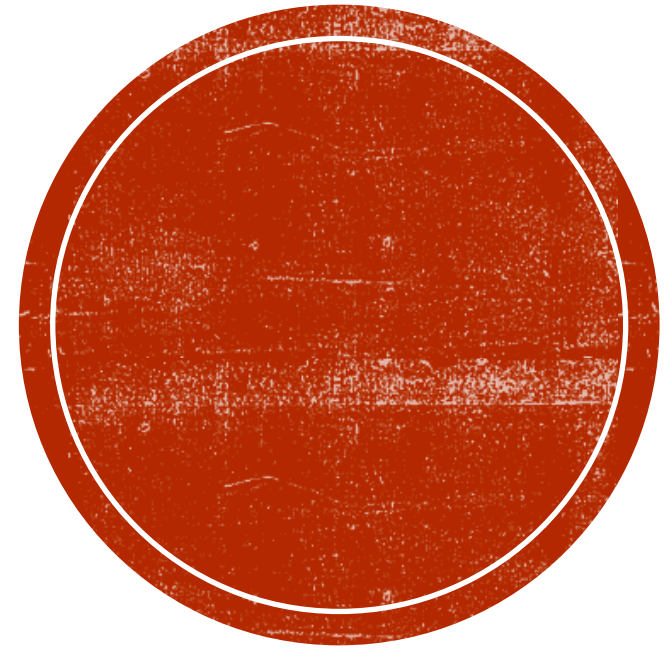
Velocity



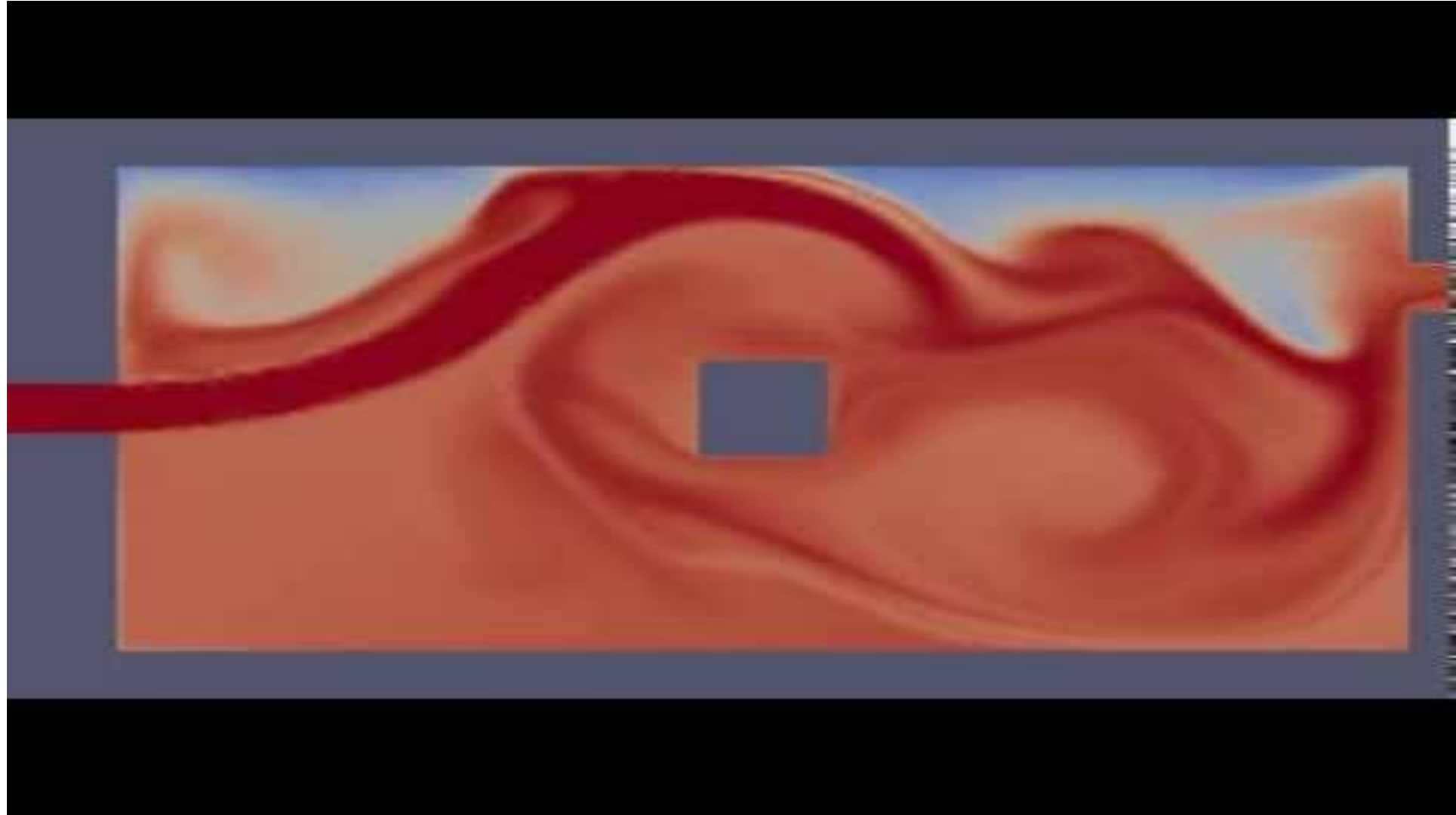
BONUS ANIMATION: 3D VOLUME FRACTION



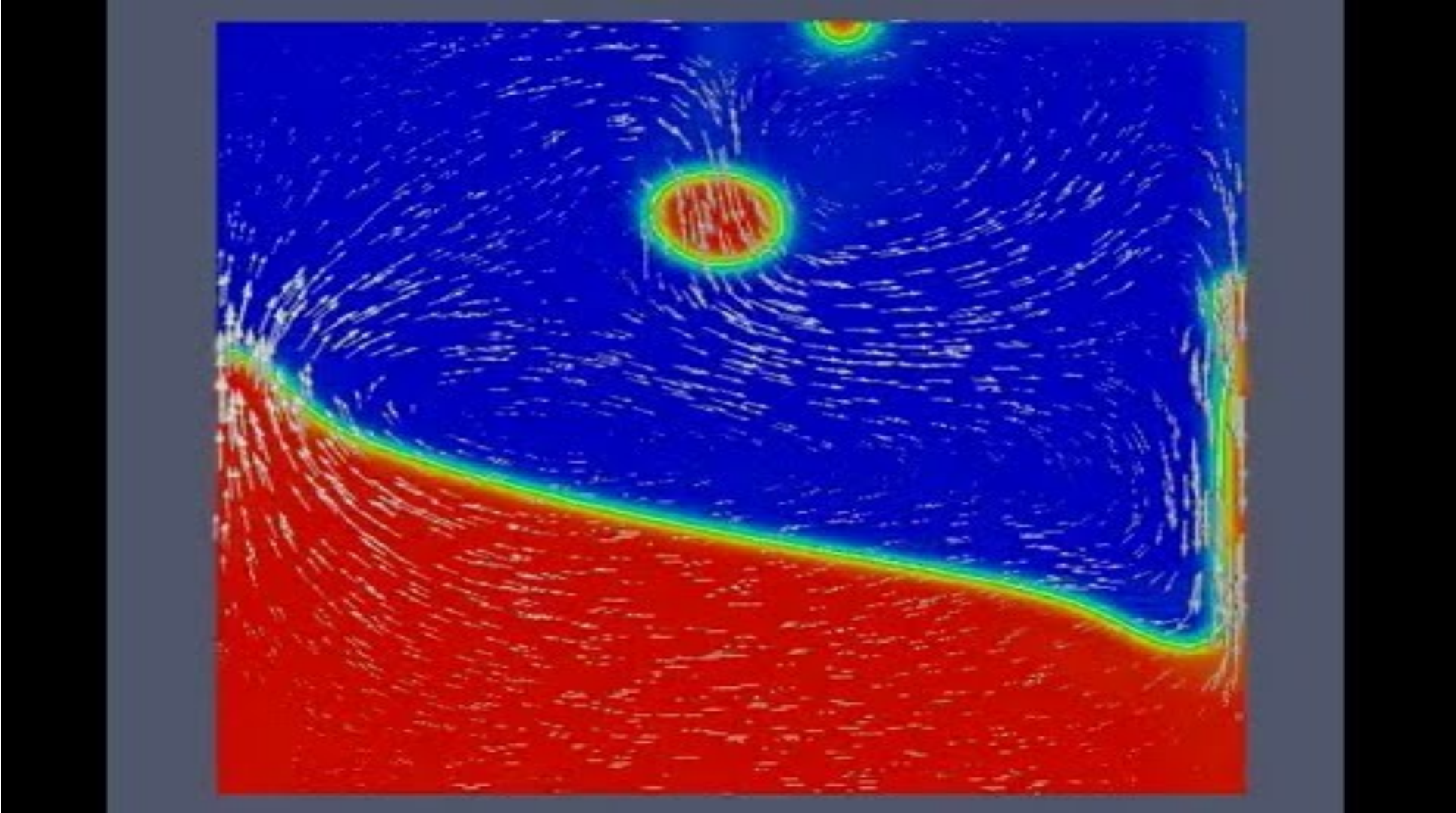
EXAMPLE APPLICATIONS



NAVIER-STOKES PHASE FIELD FOR TWO MISCIBLE FLUIDS



NAVIER-STOKES-CAHN-HILLARD SIMULATION OF A DAM BREAK



EXAMPLE APPLICATIONS

- Example using the Phase Field Model for the spinodal decomposition of Iron-Chromium Alloy at 500°C during one week.
- The simulation assumes a two-dimensional 25nm × 25nm surface.
- The reactions are simple and depend solely on concentrations. Therefore, we can use the Cahn-Hilliard equation.

$$\frac{\partial c}{\partial t} = \nabla M(c) \nabla \left(\frac{\partial f_{loc}(c)}{\partial c} - \kappa \nabla^2 c \right).$$

c is the mole fraction of chromium (unitless)

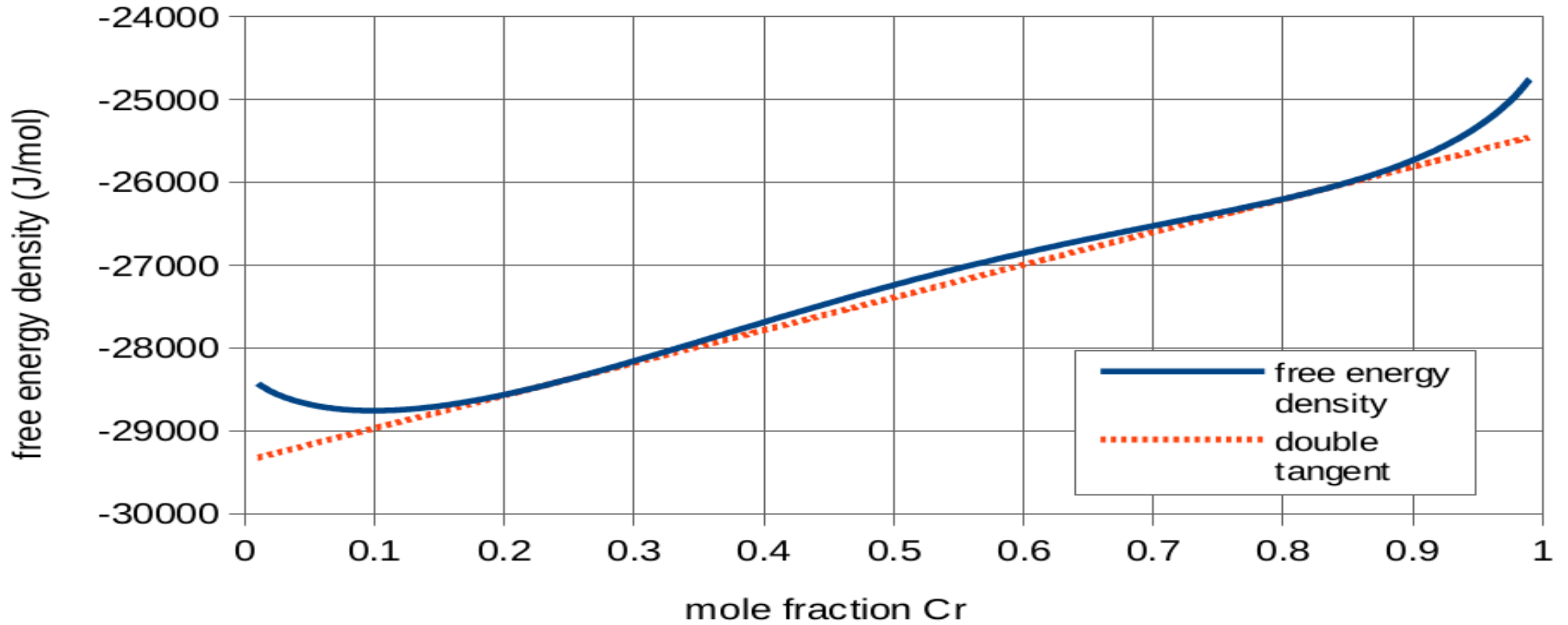
$M(c)$ is the mobility of chromium ($\text{m}^2\text{mol}/\text{Js}$)

$f_{loc}(c)$ is the free energy density (J/mol)

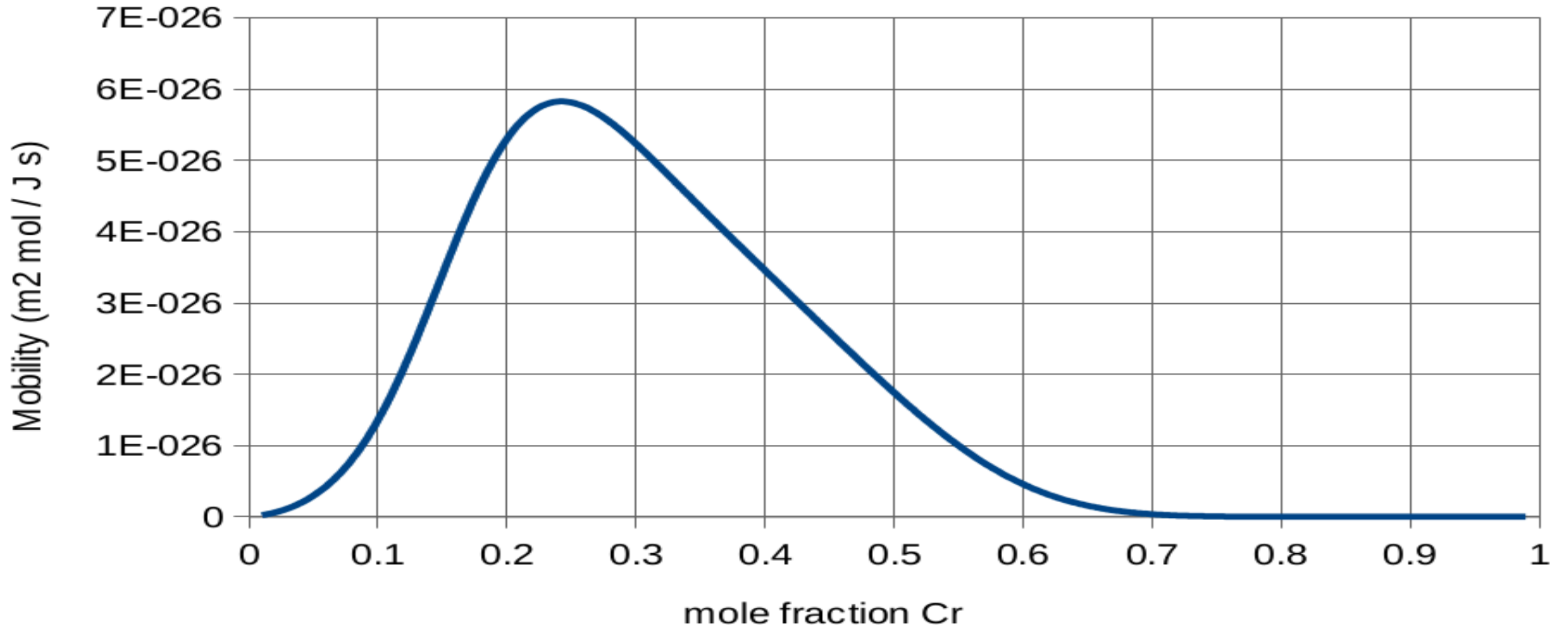
κ is the gradient energy coefficient (Jm^2/mol).



FREE ENERGY DENSITY



INITIAL MOBILITY CURVE

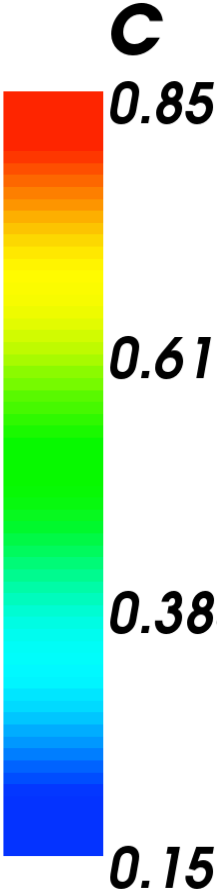
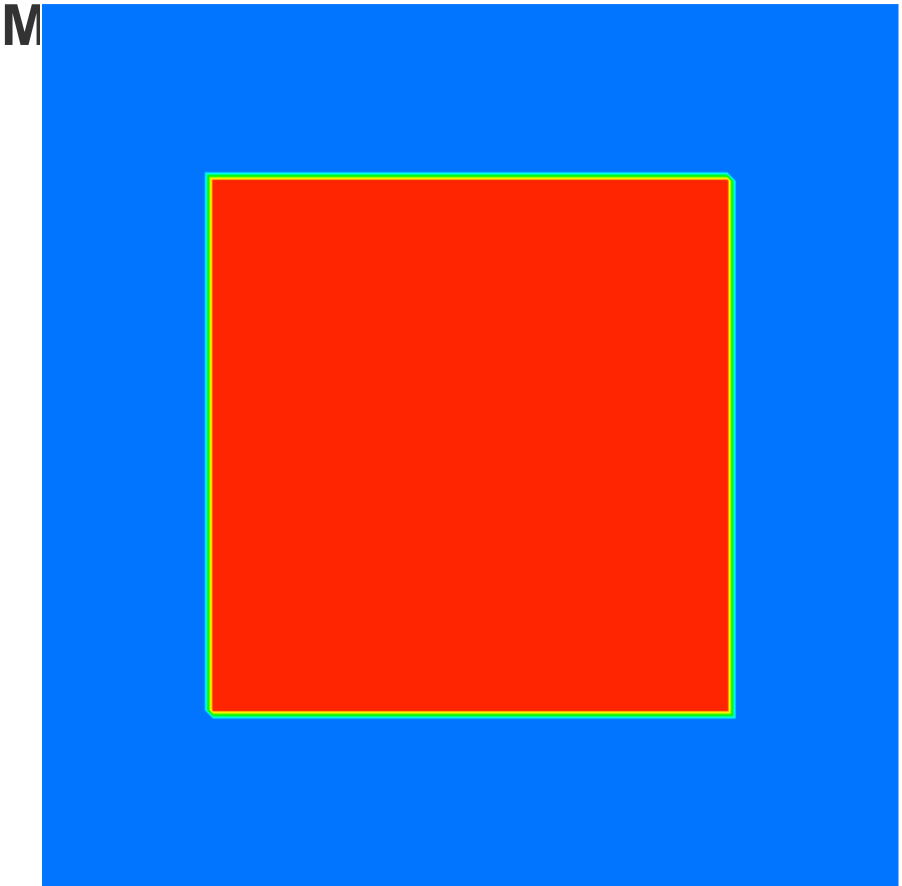


EXAMPLE APPLICATION

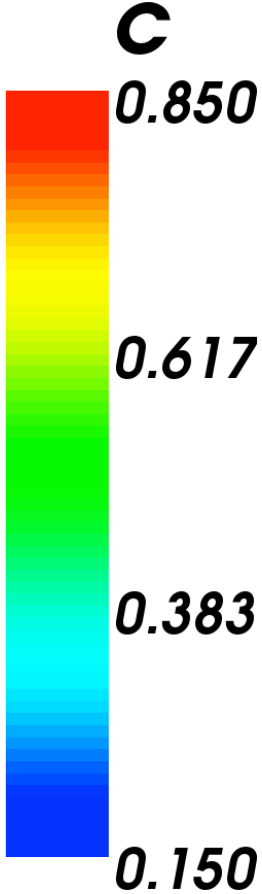
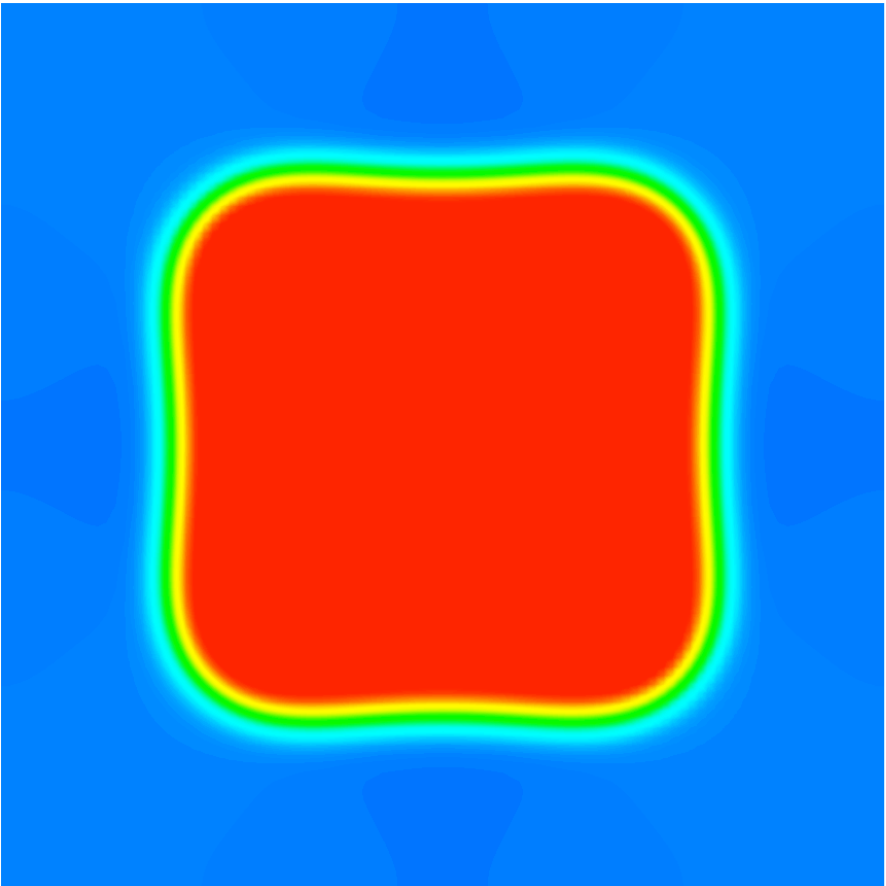
- We expect three things from this simulation:
- First, the surface should decompose into the iron and chromium phases at the equilibrium concentrations.
- Second, the decomposed surface will minimize energy by minimizing the interface contact between the two phases. It does this by shaping the regions as circles or large stripes.
- Third, most phase field problems reduce the free energy of the surface in an s-curve shape. That is, at the beginning and end of the simulation, there is relatively little change in the free energy of the surface, but there is a rapid decrease somewhere in the middle.



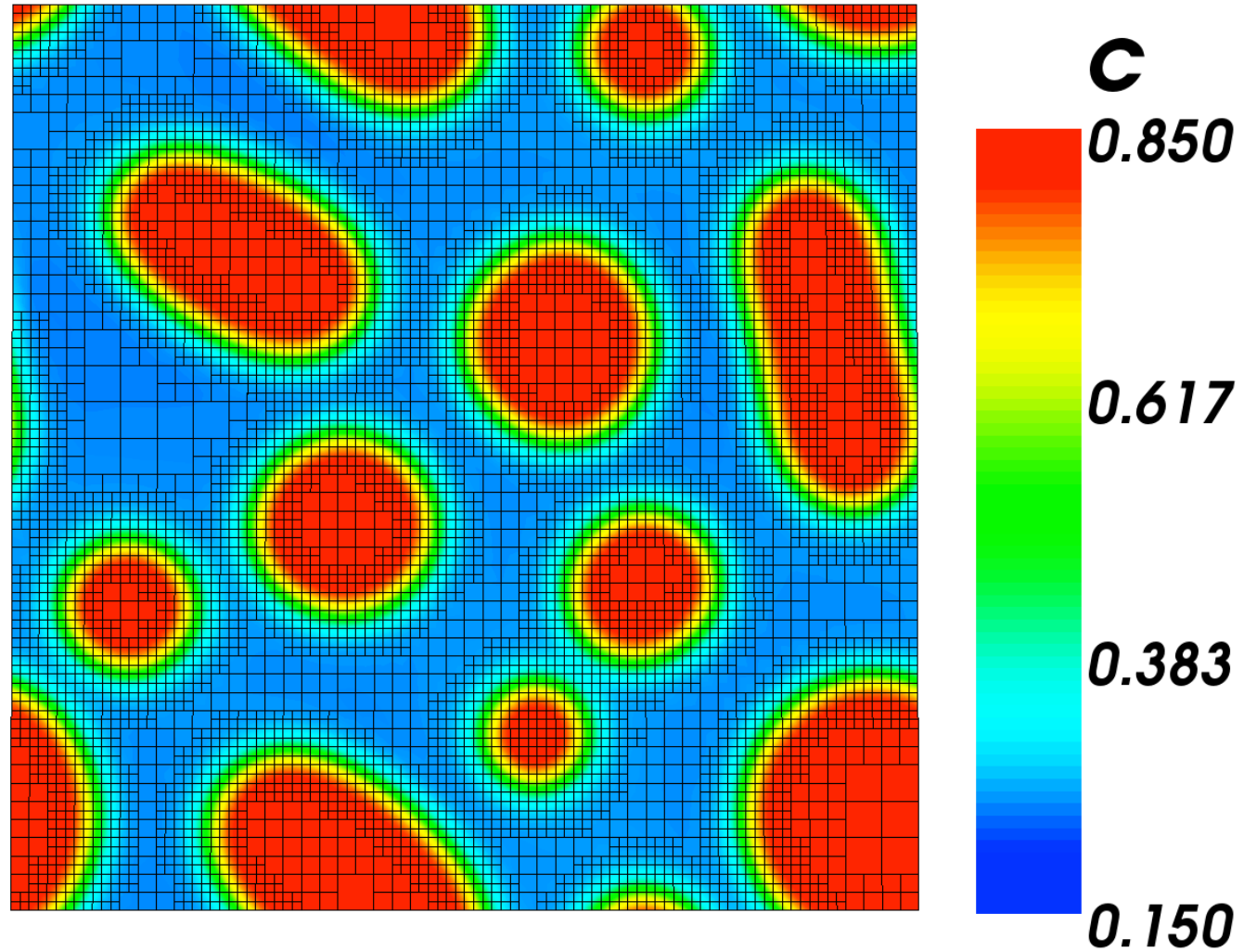
STEP 1: MAKE A SIMPLE TEST MODEL



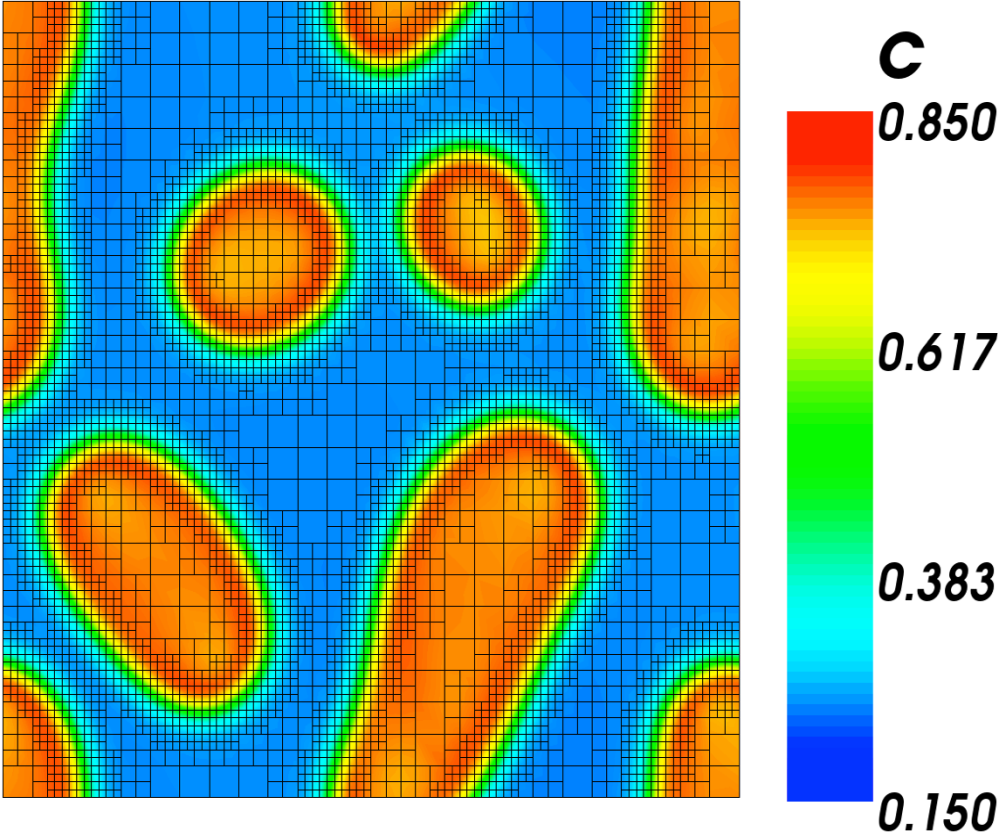
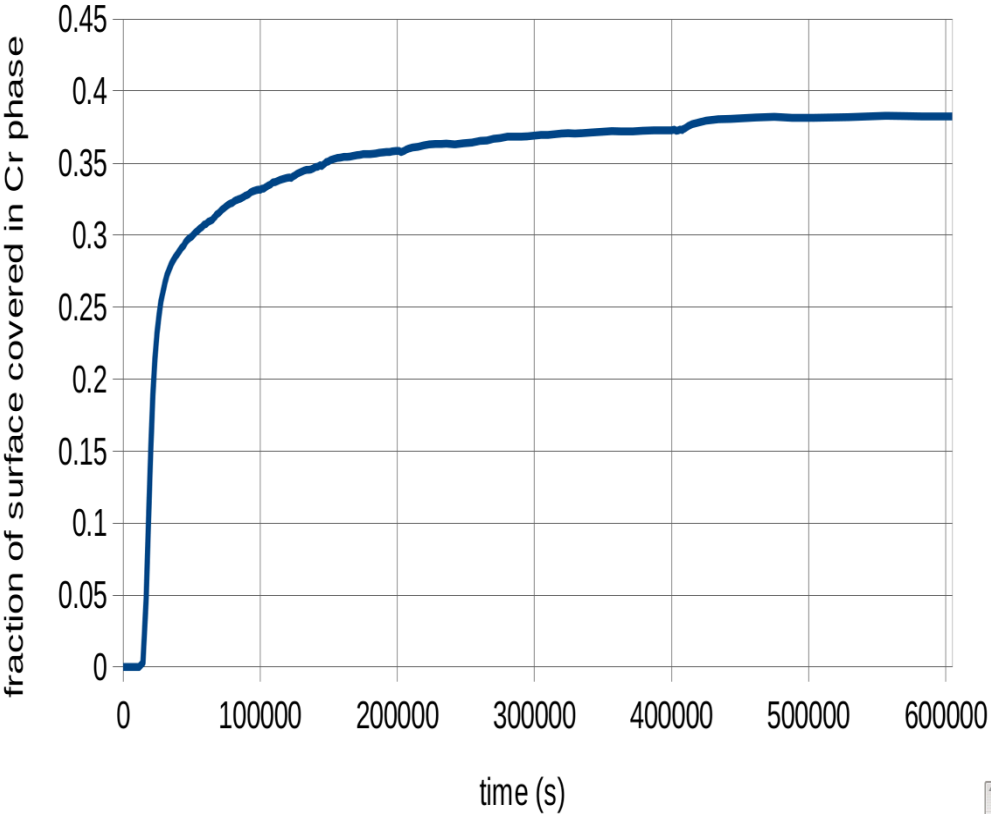
STEP 2: MAKE A FASTER TEST



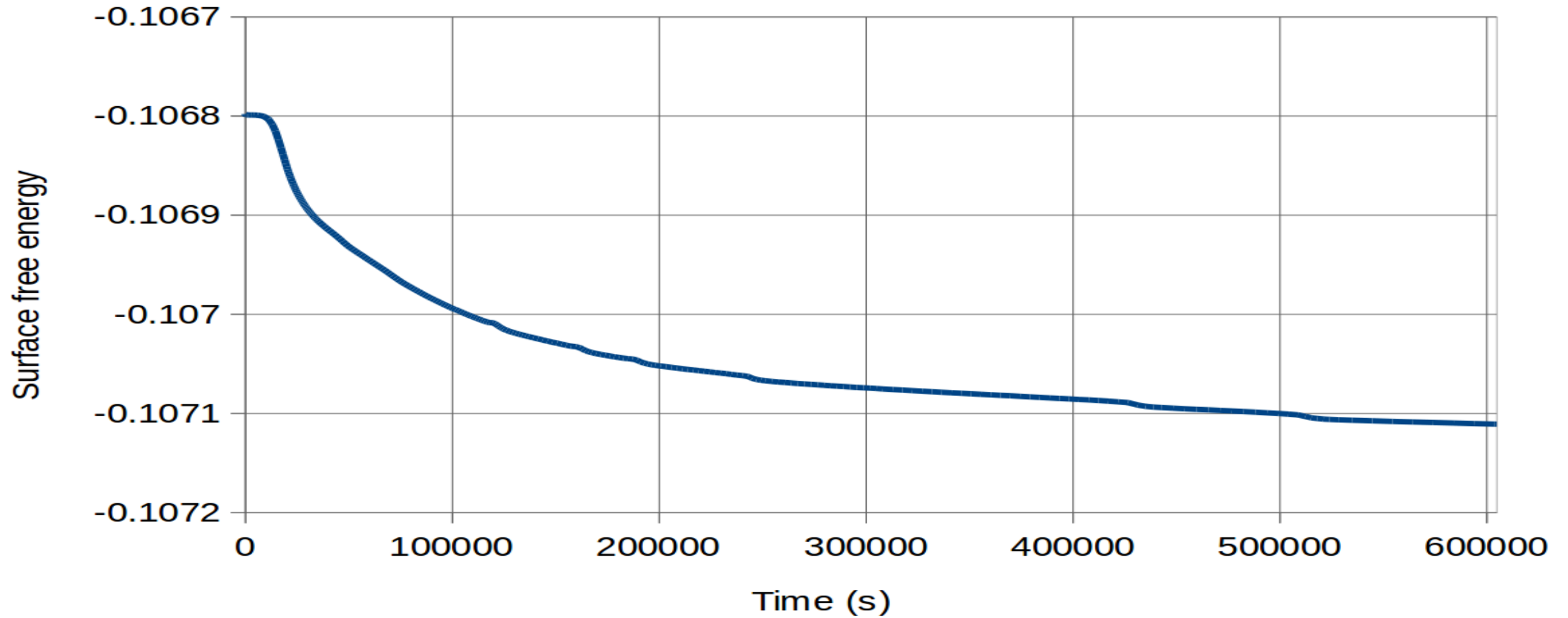
STEP 3: ADD PHASE DECOMPOSITION TO THE MODEL



STEP 5: CREATE A FUNCTION OF MOBILITY



STEP 5: CHECK THE SURFACE ENERGY CURVE



NAIVER-STOKES-CAHN-HILLARD RISING BUBBLES

