Phase-Field Models

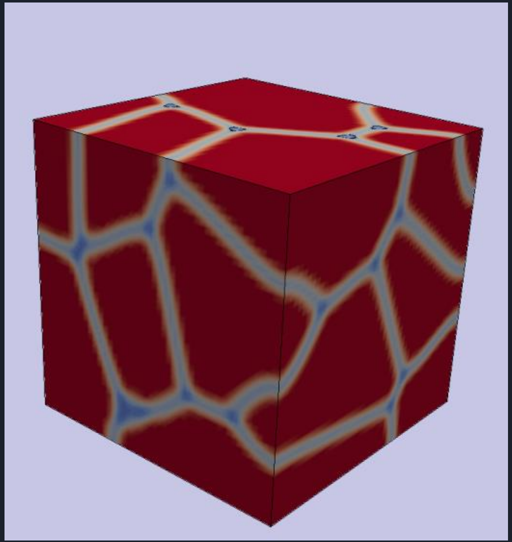
Faras Al Balushi
Timothy Duffy

★ Introduction
★ Historical background
★ General principle
★ Governing equations
★ Hand-calculation example
★ Numerical example

- ★ Introduction
- ★ Historical background
- ★ General principle
- ★ Governing equations
- ★ Hand-calculation example
- ★ Numerical example

Introduction to Phase Field Modeling

- Mathematical model used to solve interfacial problems
- Provide quantitative modeling of the evolution of microstructure and physical properties at the mesoscale
- Solve for problems where the shape of the interface is important
- Used widely in material science



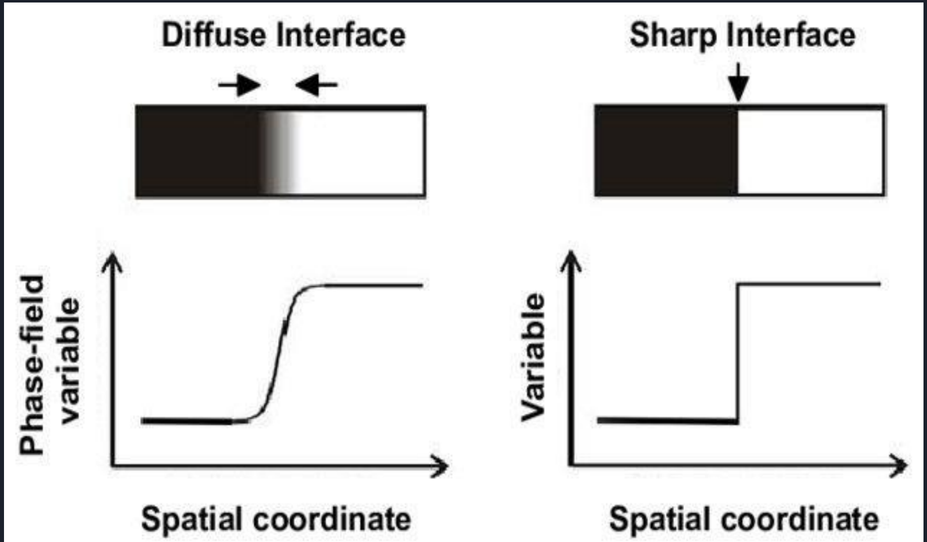
Openphase.de

Applications in Which Phase Field Models Are Used:

- Solidification dynamics
- Viscous fingering
- Droplet on solid interface
- Fracture dynamics
- Phase transformation

Advantages of Phase Field Models:

- Able to turn sharp interfaces to diffuse interfaces
- No explicit tracking of the interface
- Can solve for problems involving three phases
- Can be converted from 2D to 3D easily
- Provide more accurate solutions



Disadvantages of Phase Field Models:

- Large number of grid points needed near the interface
- Computationally-intensive
- Applications are limited to shape observation

- ★ Introduction
- ★ Historical background
- ★ General principle
- ★ Governing equations
- ★ Hand-calculation example
- ★ Numerical example

Historical Background

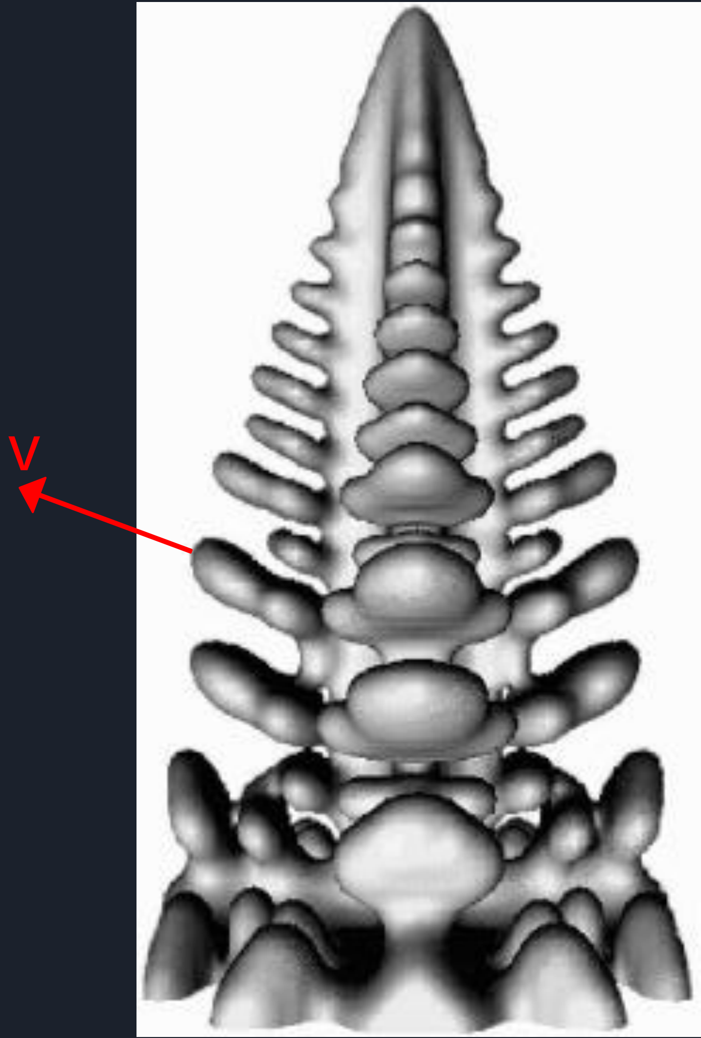
- Van Der Waals
- Cahn-Hilliard
- Landau-Ginzburg

Before Phase Field Models

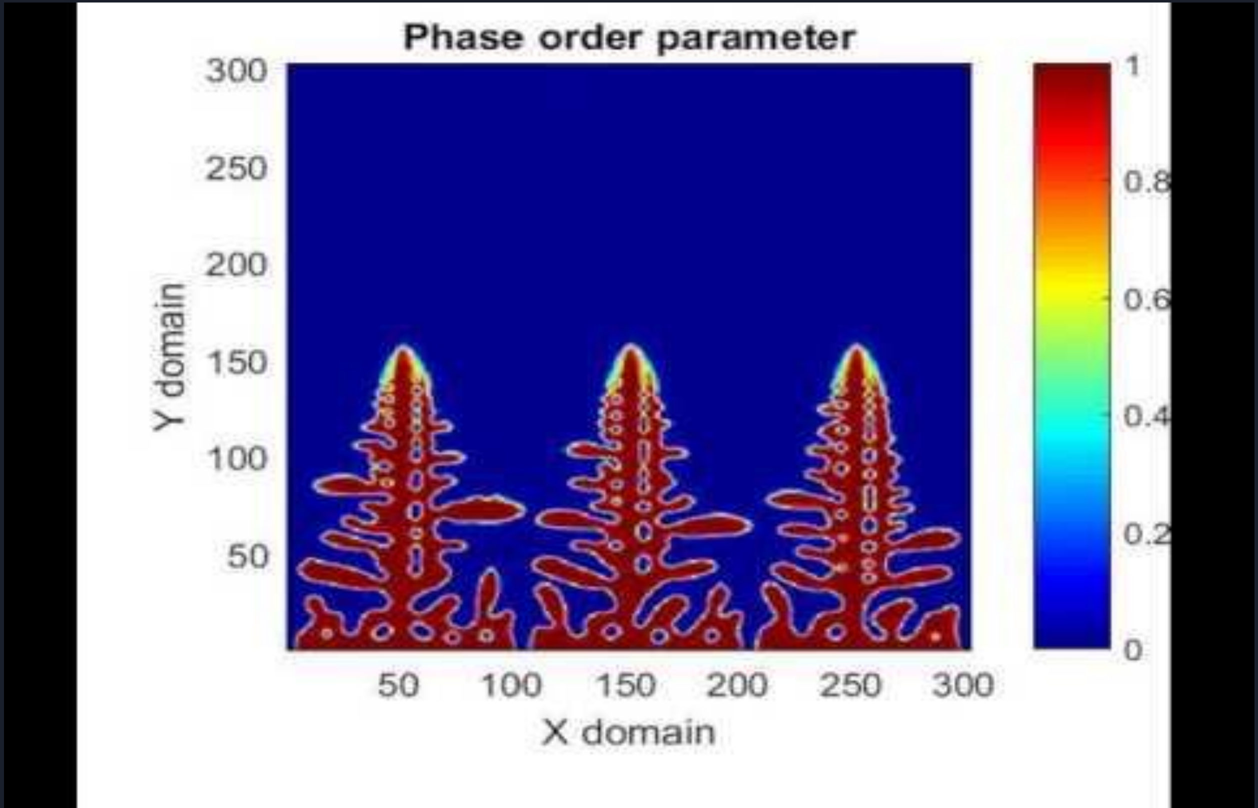
$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

$$T_1^L = T_0 - l\,H$$

$$LV = k[\![\nabla T]\!]$$



Dendrite Growth Using Phase Field Models



Phase-Field Models at Penn State:

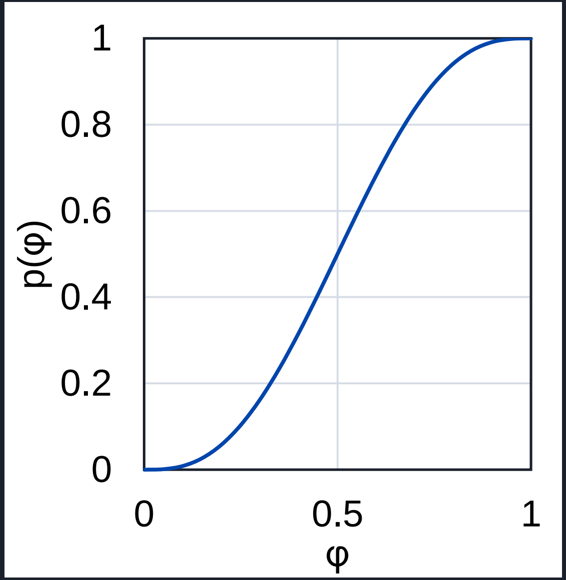
→ Dr. Long-Qing Chen

- Professor of Material Science and Engineering
- Research area:
  - Phase-field methods and software development
  - Co-evolution of microstructures and properties
- Projects:
  - Phase-field modeling of dielectric degradation and breakdown
  - Phase-field Model of Microstructure Evolution in Ti-Alloys

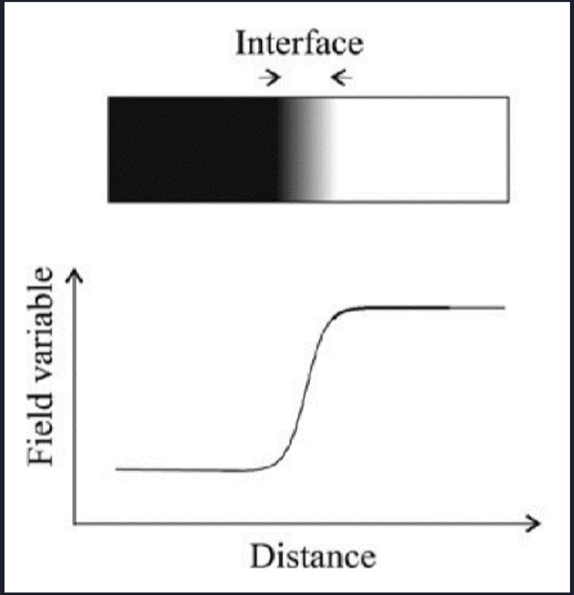
- ★ Introduction
- ★ Historical background
- ★ General principle
- ★ Governing equations
- ★ Hand-calculation example
- ★ Numerical example

General Principles

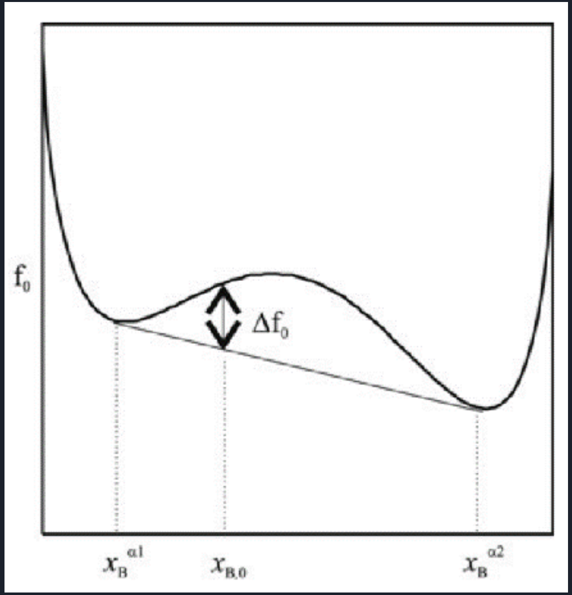
Phase Field Variables



Diffuse Interface



Free Energy- Double Well



The phase field variable φ represents a state that a system can evolve towards

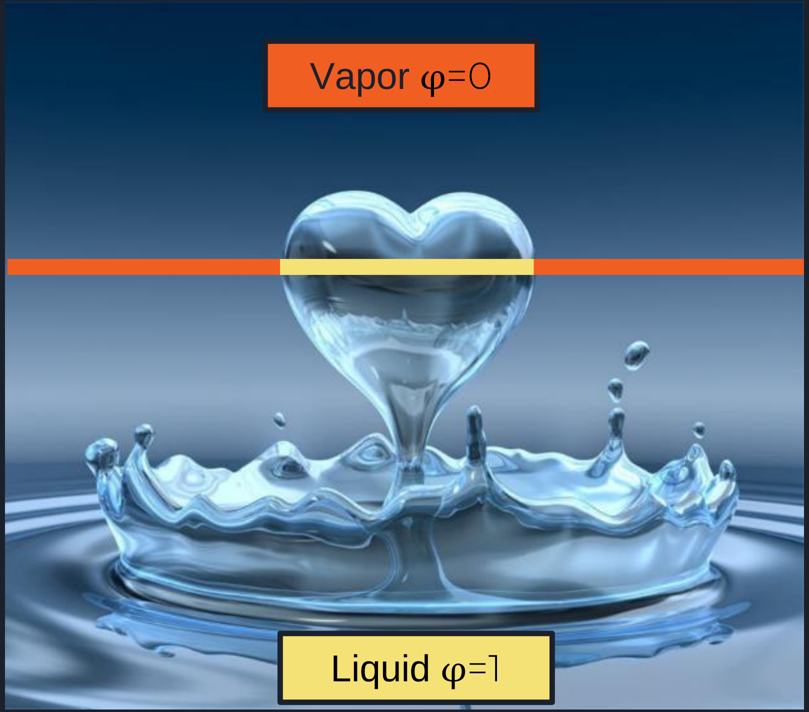
Commonly:

$$0 \leq \varphi \leq 1$$

or

$$-1 \leq \varphi \leq 1$$

e.g. phase, spin, crystal lattice, composition



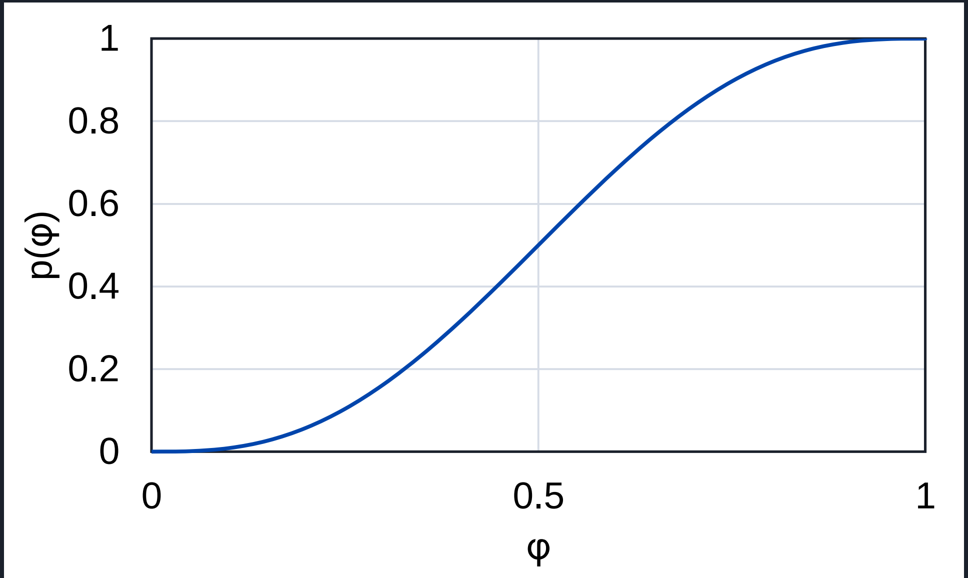
The phase field variables φ provide a tool to interpolate between the parameters of two phases

For parameters such as heat capacity, conductivity, etc.

Allows us to perform Multiphysics problems with interfaces

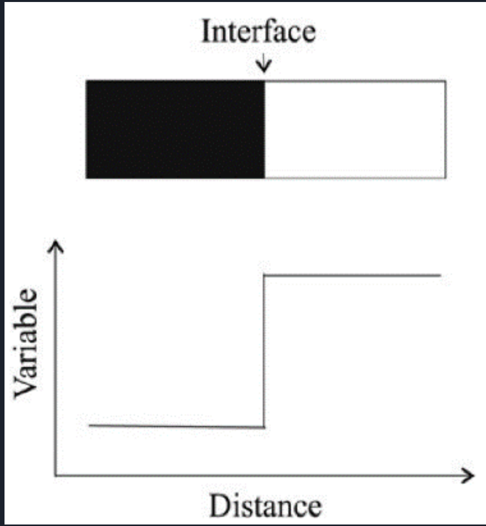
Common interpolation function:

$$p(\phi) = \phi^3(6\phi^2 - 15\phi + 10)$$



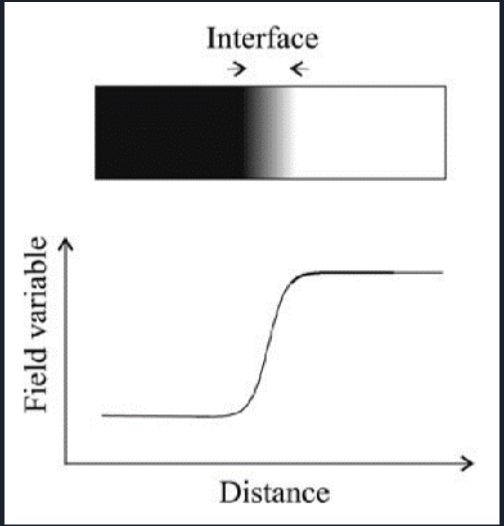
Diffuse Interface- No tracking required!

Sharp Boundary



- Discontinuous properties between the interface
- Location of interface is part of the unknowns

Diffuse Boundary



- Continuous properties across interface
- Don't need to track interface during solve

Moehlans et al. (2008)

Free Energy Double-Well

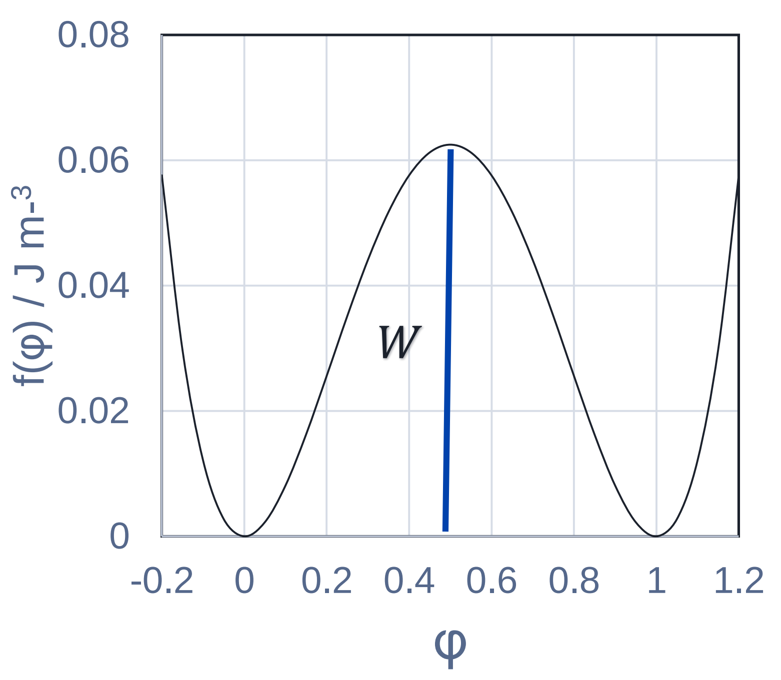
Minimization of free energy

$$F = F_{\text{bulk}} + F_{\text{int}} + \cancel{F_{\text{el}}} + \cancel{F_{\text{fys}}} + \dots$$

$$F = \int_V \left[\overbrace{f(\phi, c, T)}^{\text{Penalizes intermediate phases}} + \underbrace{\frac{\epsilon_C^2}{2} |\nabla c|^2 + \frac{\epsilon_\phi^2}{2} |\nabla \phi|^2}_{\text{Penalizes sharp interface}} \right] \mathrm{dV}$$

Interfacial gradient $\quad \epsilon_\phi = \sqrt{6 \sigma l}$

Double-Well height $\quad W = 3 \dfrac{\sigma}{l}$



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

Calphad: Thermodynamic Database for Phase Diagrams/ Free Energy Functions

CALculation of **PHA**se **D**iagrams

Longer run times for more quantitative solution

Commonly used in binary/ternary alloy systems

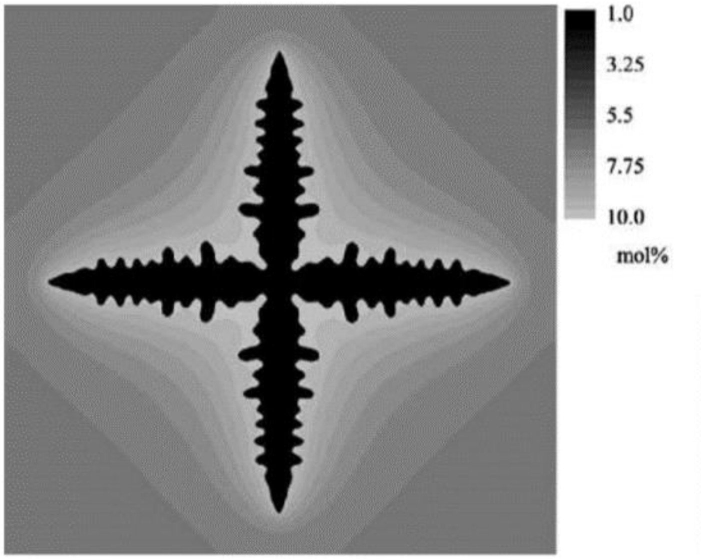


Fig. 5. Silicon concentration profile in the dendrite growth of Al–6.7 mol%Si–1.1 mol%Mg alloy.

Kobayashi (2003)

Governing Equations

Cahn Hilliard

$$\frac{\partial c}{\partial t} = \nabla M_c \nabla \frac{\delta \mathrm{F}}{\delta c}$$

Conserved variables

Allen- Cahn/
time-dependent Ginzburg-Landau

$$\frac{\partial \phi}{\partial t} = -M_\phi \frac{\delta \mathrm{F}}{\delta \phi}$$

Non-conserved variables

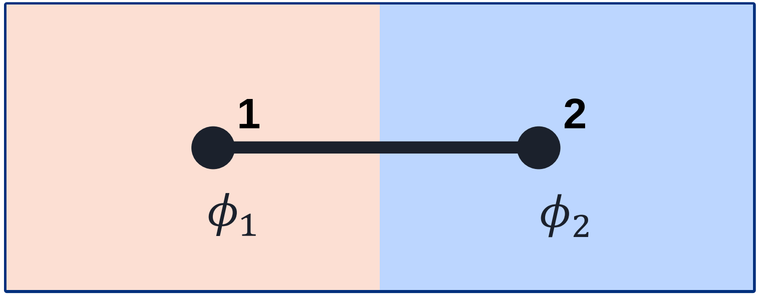
$$\frac{\delta \mathrm{F}}{\delta \phi} = \frac{\partial f}{\partial \phi} - {\epsilon_\phi}^2 \nabla^2 \phi$$

Hand Calculation Example: Allen Cahn 1D

Initially:

Phase α

Phase β



How does this develop over time?

Allen- Cahn:

$$\frac{\partial \phi}{\partial t} = -M_\phi \left(\frac{\partial f}{\partial \phi} - {\epsilon_\phi}^2 \frac{\partial^2 \phi}{\partial x^2} \right)$$

Hand Calculation Example

Rearranged:

$$\underline{\frac{1}{M_\phi}\frac{\partial \phi}{\partial t}} + \underline{\frac{\partial f}{\partial \phi}} = \epsilon_\phi{}^2 \underline{\frac{\partial^2 \phi}{\partial x^2}}$$

Takes the Form:

$$\left(\frac{1}{M_\phi}\int_V \underline{b^T b}\mathrm{dV}\right)\underline{\dot{\phi}} + \int_V \underline{b^T b}\mathrm{dV}\underline{\left(\frac{\partial f}{\partial \phi}\right)} + \int_V \underline{a^T}\epsilon_\phi^2 \underline{a}\mathrm{dV}\underline{\phi} = 0$$

*No Flux

Substitute Shape Functions:

$$\frac{SAL}{2M_\phi}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\begin{Bmatrix}\dot{\phi}_1\\ \dot{\phi}_2\end{Bmatrix} + \frac{SAL}{2}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\begin{Bmatrix}\partial f/\partial \phi_1\\ \partial f/\partial \phi_2\end{Bmatrix} + \frac{\epsilon_\phi{}^2 A}{L}\begin{bmatrix}1 & -1\\ -1 & 1\end{bmatrix}\begin{Bmatrix}\phi_1\\ \phi_2\end{Bmatrix} = 0$$

We use semi-implicit time stepping

$$\frac{SAL}{2M_\phi}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}\begin{Bmatrix}\dot{\phi}_1\\\dot{\phi}_2\end{Bmatrix}+\frac{SAL}{2}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}\begin{Bmatrix}\partial f/\partial\phi_1\\\partial f/\partial\phi_2\end{Bmatrix}+\frac{{\epsilon_\phi}^2A}{L}\begin{bmatrix}1 & -1\\-1 & 1\end{bmatrix}\begin{Bmatrix}\phi_1\\\phi_2\end{Bmatrix}=0$$

$\partial f/\partial\phi$ term is too costly to calculate at t+1, so we use it's historic value

Substitute with: $\dot{\phi}_1=\dfrac{\phi_1^{t+1}-\phi_1^t}{\Delta\mathrm{t}}$

$$\frac{SAL}{2M_\phi\Delta\mathrm{t}}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}\begin{Bmatrix}\phi_1^{t+1}-\phi_1^t\\\phi_2^{t+1}-\phi_2^t\end{Bmatrix}+\frac{SAL}{2}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}\boxed{\begin{Bmatrix}\partial f/\partial{\phi_1}^t\\\partial f/\partial{\phi_2}^t\end{Bmatrix}}+\frac{{\epsilon_\phi}^2A}{L}\begin{bmatrix}1 & -1\\-1 & 1\end{bmatrix}\begin{Bmatrix}\phi_1^{t+1}\\\phi_2^{t+1}\end{Bmatrix}=0$$

One last rearrangement:

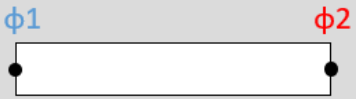
$$\underbrace{\boxed{\frac{SAL}{2M_\phi \Delta t}}}_{\text{C1}}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}\begin{Bmatrix}\phi_1^{t+1}-\phi_1^t\\\phi_2^{t+1}-\phi_2^t\end{Bmatrix}+\underbrace{\boxed{\frac{{\epsilon_\phi}^2 A}{L}}}_{\text{C2}}\begin{bmatrix}1 & -1\\-1 & 1\end{bmatrix}\begin{Bmatrix}\phi_1^{t+1}\\\phi_2^{t+1}\end{Bmatrix}+\underbrace{\boxed{\frac{SAL}{2}}}_{\text{C3}}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}\begin{Bmatrix}\partial f/\partial {\phi_1}^t\\\partial f/\partial {\phi_2}^t\end{Bmatrix}=0$$

$$\text{C1}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}\begin{Bmatrix}\phi_1^{t+1}\\\phi_2^{t+1}\end{Bmatrix}+\text{C2}\begin{bmatrix}1 & -1\\-1 & 1\end{bmatrix}\begin{Bmatrix}\phi_1^{t+1}\\\phi_2^{t+1}\end{Bmatrix}=\text{C1}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}\begin{Bmatrix}\phi_1^{t}\\\phi_2^{t}\end{Bmatrix}-\text{C3}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}\begin{Bmatrix}\partial f/\partial {\phi_1}^t\\\partial f/\partial {\phi_2}^t\end{Bmatrix}$$

$$\left.\begin{aligned}\phi_1^{t+1}&=\frac{\text{C1}\,\phi_1^t+\text{C2}\,\phi_2^{t+1}-\text{C3}\,\partial f/\partial {\phi_1}^t}{\text{C1}+\text{C2}}\\[2ex]\phi_2^{t+1}&=\frac{\text{C1}\,\phi_2^t+\text{C2}\,\phi_1^{t+1}-\text{C3}\,\partial f/\partial {\phi_2}^t}{\text{C1}+\text{C2}}\end{aligned}\right\}\quad \textit{System of 2 equations}$$

Time Stepping in MS Excel

1D Phase-Field Model



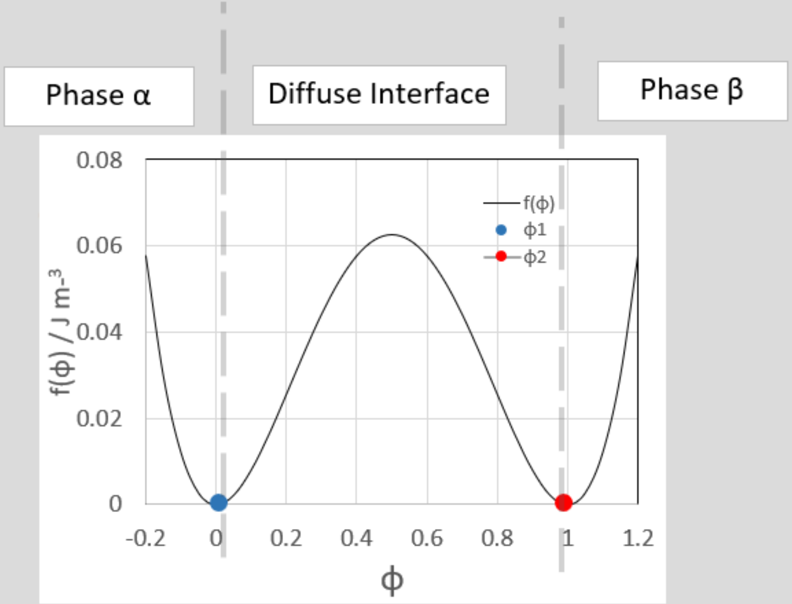
Δt	ϕ1	∂f/∂ϕ1		ϕ2	∂f/∂ϕ2
0	0.30	0.17		0.70	-0.17
1	0.22	0.19		0.78	-0.19
2	0.13	0.17		0.87	-0.17
3	0.06	0.10		0.94	-0.10
4	0.02	0.04		0.98	-0.04
5	0.01	0.02		0.99	-0.02
6	0.01	0.02		0.99	-0.02
7	0.01	0.02		0.99	-0.02
8	0.01	0.02		0.99	-0.02
9	0.01	0.02		0.99	-0.02
10	0.01	0.02		0.99	-0.02

C2	0.01

Interfacial energy term/ gradient coefficient

ϕ1	f(ϕ1)
0.01	0.000

ϕ2	f(ϕ2)
0.99	0.000

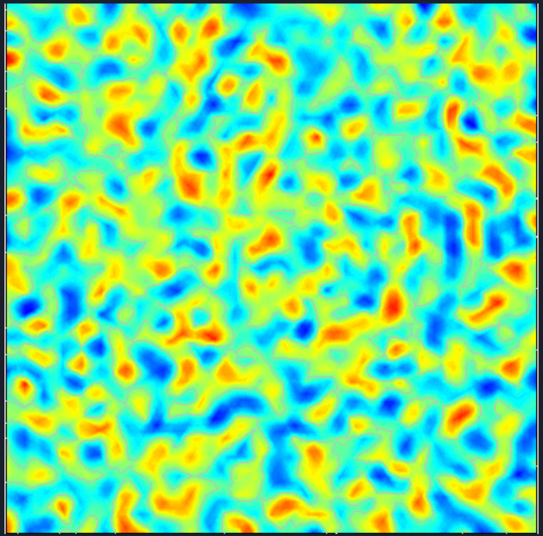


Numerical Example: COMSOL

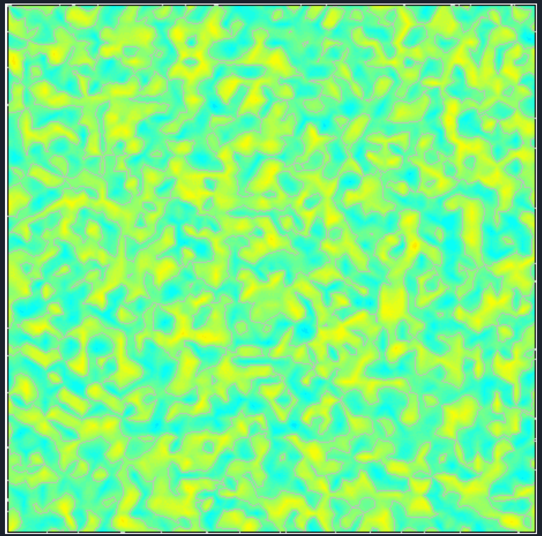
COMSOL Example: Grain Growth

Random starting grid,
Average ϕ = 0.5 (equal parts phase A and phase B)

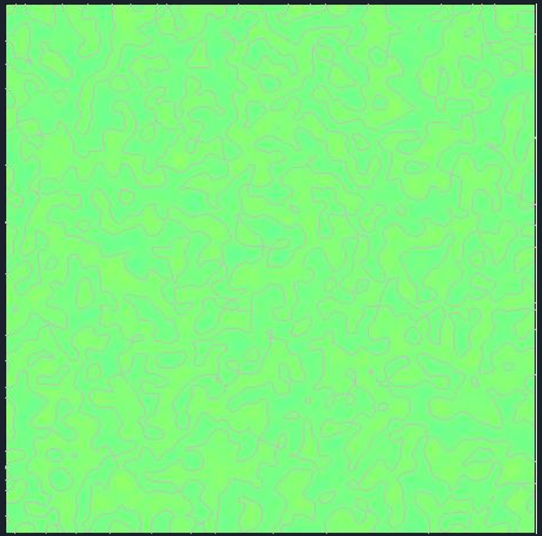
Surface Tension = 1 mN/m



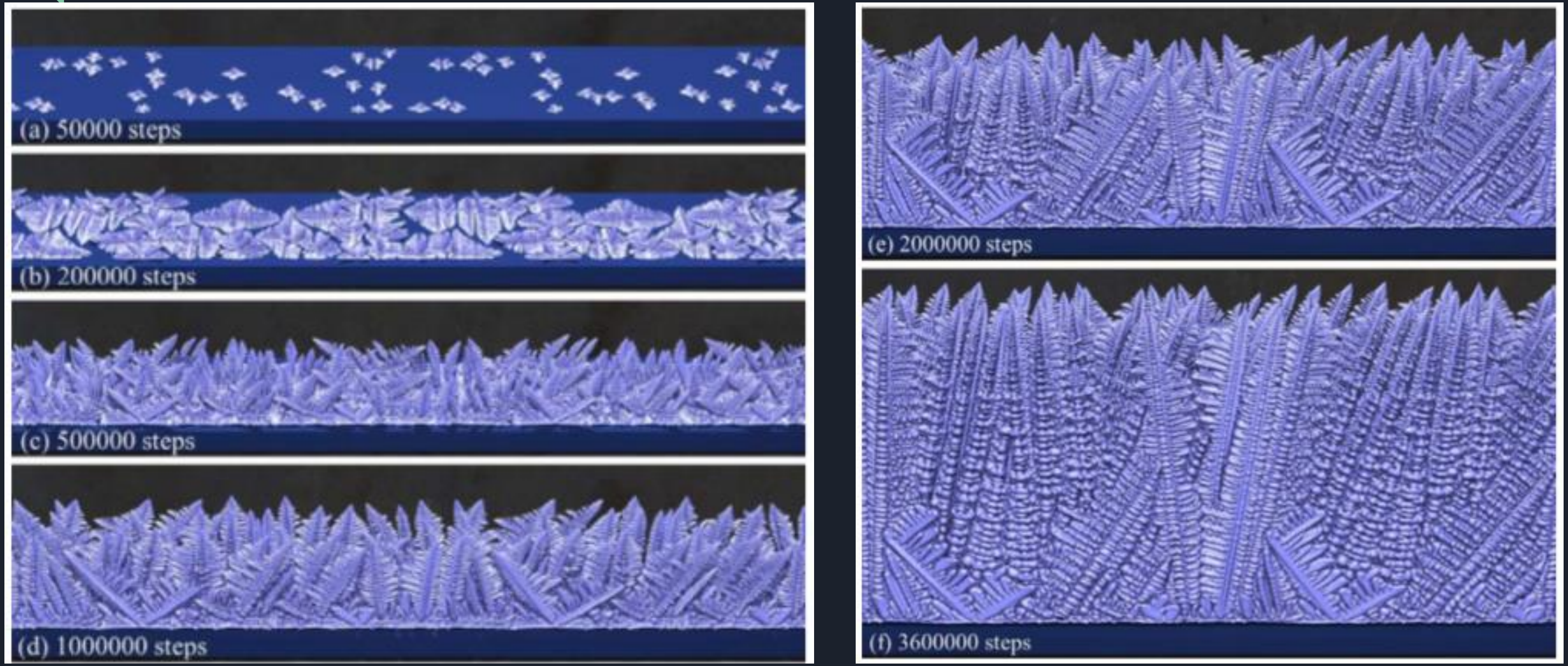
Surface Tension =100 mN/m



Surface Tension =1 N/m

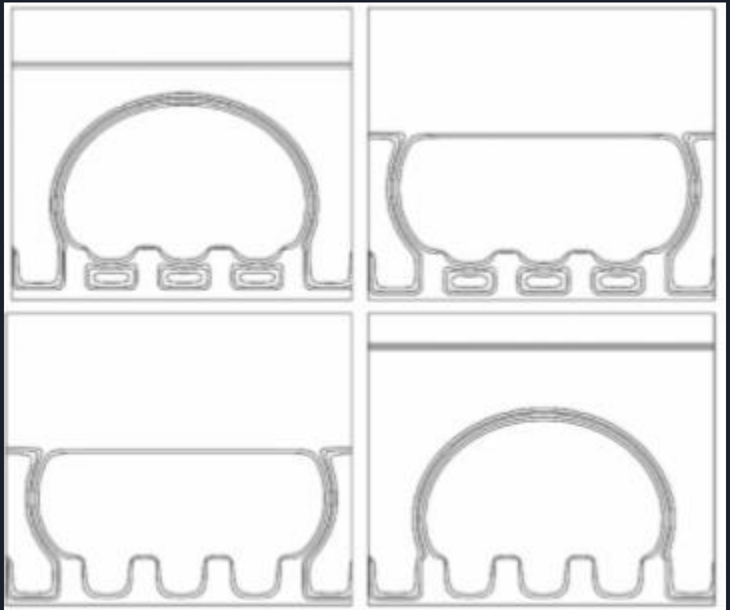


Dendrite growth:
Allen Cahn +Heat Equation w/ Latent heat of solidification

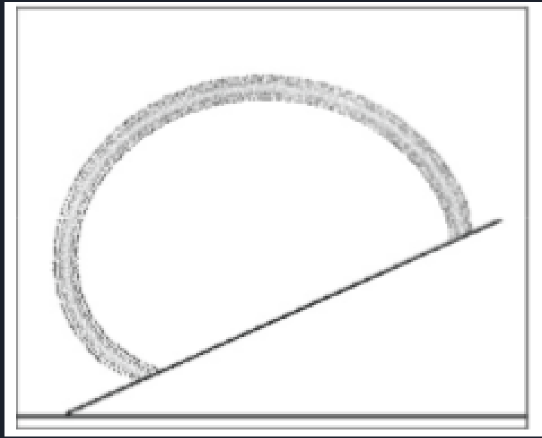


Takaki (2014)

Wetting Phenomena on rough surfaces



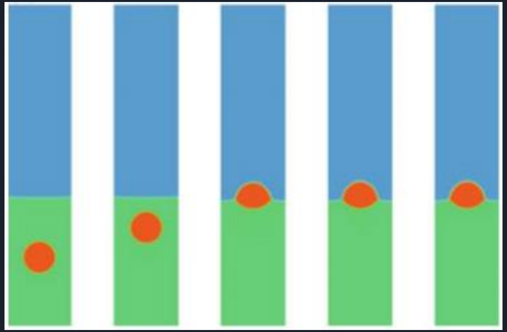
- Prescribe droplet volume
- Add appropriate free energy terms



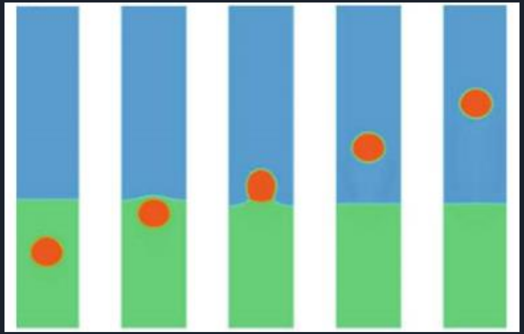
Turco et al. (2008)

Cahn-Hilliard+ Navier Stokes: 3-Phase Flow

A



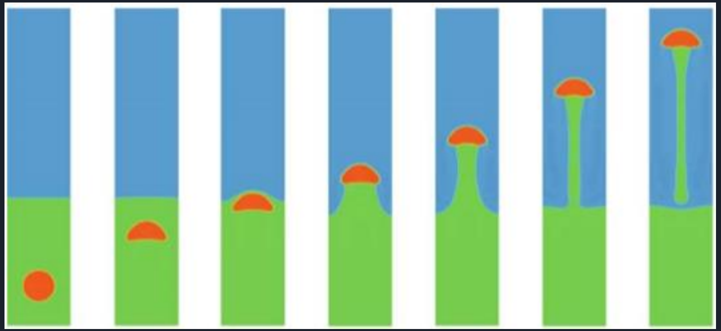
B



Air bubble crossing water-oil interface

- bubble radius increases for each case

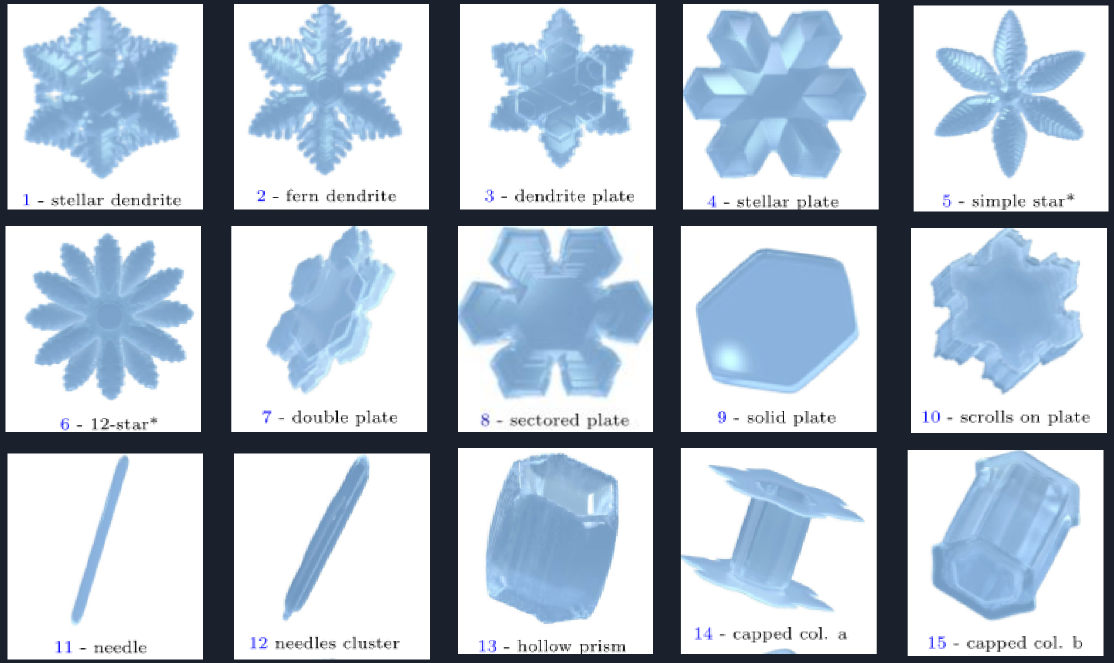
C



Boyer et al. (2010)

Snowflake growth ☺

- Two-phases (ice, vapor)
- Two coupled non-conserved phase field equations



Demange et al. (2017)

Thank you!

Do you have any question?

References

S. B. Biner, *Programming Phase-Field Modeling*. Cham: Springer International Publishing, 2017.

W. J. Boettinger, J. A. Warren, C. Beckermann, and A. Karma, “Phase-Field Simulation of Solidification,” *Annu. Rev. Mater. Res.*, vol. 32, pp. 163–194, 2002.

F. Boyer, C. Lapuearta, S. Minjeaud, and B. Piar, “Cahn-Hilliard/Navier-Stokes Model for the Simulation of Three-Phase Flows,” *Transp. Porous Media*, vol. 82, pp. 463–483, 2010.

G. Demange, H. Zapolsky, R. Patte, and M. Brunel, “A phase field model for snow crystal growth in three dimensions,” *npj Comput. Mater.*, pp. 3–15, 2017.

H. Kobayashi, M. Ode, S. G. Kim, W. T. Kim, and T. Suzuki, “Phase-field model for solidification of ternary alloys coupled with thermodynamic database,” *Scr. Mater.*, vol. 48, pp. 689–694, 2003.

N. Moelans, B. Blanpain, and P. Wollants, “An introduction to phase-field modeling of microstructure evolution,” *Calphad*, vol. 32, no. 2, pp. 268–294, 2008.

T. Takaki, “Phase-field Modeling and Simulations of Dendrite Growth,” *ISIJ Int.*, vol. 54, no. 2, pp. 437–444, 2014.

A. Turco, F. Alouges, and A. DeSimone, “Wetting on rough surfaces and contact angle hysteresis: numerical experiments based on a phase field model,” *ESAIM Math. Model. Numer. Anal.*, vol. 43, pp. 1027–1044, 2009.