



MSE6701H, Multiscale Materials Modeling and Simulation

- ✓ Electronic DFT
- ✓ Atomistic MD
- Mesoscale PF

Lecture 10

Governing equation for microstructure evolution & Solutions

Guisen Liu (刘桂森)

➤ Mesoscale models

- I. Why model microstructure evolution?
- II. What can Phase Field method do?
- III. Basics for Phase Field method: Principles & how?
 1. Microstructure in PFM
 2. Driving forces for microstructure evolution
 3. Governing equation for microstructure evolution



- Microstructure: composition (c_n) , phase (η_p) , phase interfaces
- Total free energy: short-range chemical interactions + interface energy

$$F = \int \left[f(c_1, c_2, \dots, c_n, \eta_1, \eta_2, \dots, \eta_p) + \sum_{i=1}^n \alpha_i (\nabla c_i)^2 + \sum_{i=1}^3 \sum_{j=1}^3 \sum_{k=1}^p \beta_{ij} \nabla_i \eta_k \nabla_j \eta_k \right] d^3r + \boxed{\iint G(r - r') d^3r d^3r'} \quad \text{Nonlocal long-range interactions}$$
$$+ E_{elastic} + E_{electric} + E_{magnetic}$$

Total free energy functional

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- Total free energy: volume integration of local **free energy density**

$$F[\phi(\mathbf{x}, t)] = \int f[\phi(\mathbf{x}, t), \nabla\phi(\mathbf{x}, t)] dV$$

- $f[\phi(\mathbf{x}, t), \nabla\phi(\mathbf{x}, t)]$: $g = \nabla\phi(\mathbf{x}, t)$ is small for diffuse interface

- Taylor expansion $f[\phi, \nabla\phi]$ at $g = \nabla\phi(\mathbf{x}, t)$


$$f[\phi(\mathbf{x}, t), g] = f[\phi(\mathbf{x}, t), 0] + \left(\frac{\partial f}{\partial g} \right) \bigg|_{g=0} g + \frac{1}{2} \left(\frac{\partial^2 f}{\partial g^2} \right) \bigg|_{g=0} g^2 + \mathcal{O}(g^2)$$

$\equiv f[\phi], E_{\min}$ for positive E_{int}
Equilibrium, no interface

$\equiv 0$, for $f[\phi, g=0]$
to be minimum

**Unknown
coefficient α**

$$\Rightarrow f[\phi, \nabla\phi] = f[\phi(\mathbf{x}, t)] + \frac{\alpha}{2} |\nabla\phi(\mathbf{x}, t)|^2 \Rightarrow F[\phi(\mathbf{x}, t)] = \int_V \left[f(\phi) + \frac{\alpha}{2} |\nabla\phi|^2 \right] dV$$

1. Microstructure in PFM
2. Driving forces for microstructure evolution  decrease of free energy \rightarrow governing equation
3. **Governing equation for microstructure evolution**
 - **Conserved variable: Cahn-Hilliard Equation**
 - **Non-conserved variable: Allen-Cahn equation**
 - **Functional and variation**

1. Cahn-Hilliard equation for evolution of conserved field variables
2. Allen-Cahn equation for evolution of non-conserved field variables
3. Discussion, outlook and summary
 - Advantages & Limitations of PFM

➤ **Goals today**

- ✓ Understand the governing equation
- ✓ Numerically solve evolution equation (Partial Differential Equation)
- ✓ Pros and Cons for PF

1.1 Conserved field variables: concentration or density 7

- A binary mixture of components A + B, local densities

$$c_A(\mathbf{x}, t), c_B(\mathbf{x}, t): c_A(\mathbf{x}, t) + c_B(\mathbf{x}, t) = 1.$$

- Field variable: only one concentration $c(\mathbf{x}, t)$

$$c_A(\mathbf{x}, t) := c(\mathbf{x}, t); \quad c_B(\mathbf{x}, t) := 1 - c(\mathbf{x}, t).$$

- Flux: $\mathbf{J} = -M\nabla(\mu_A - \mu_B)$

- M : mobility
- μ_i : chemical potential of component i .
- Difference of chemical potentials: variation of a corresponding free energy functional

$$\mu_A - \mu_B = \frac{\delta F[c(\mathbf{x}, t)]}{\delta c(\mathbf{x}, t)} \Rightarrow \mathbf{J} = -M\nabla\left(\frac{\delta F[c(\mathbf{x}, t)]}{\delta c(\mathbf{x}, t)}\right).$$

- Under assumption of mass conservation

$$\frac{\partial c(\mathbf{x}, t)}{\partial t} = -\nabla \cdot \mathbf{J} = \nabla \cdot M\nabla\left(\frac{\delta F[c(\mathbf{x}, t)]}{\delta c(\mathbf{x}, t)}\right)$$

1.2 Cahn-Hilliard equation for conserved field variable 8

$$\frac{\partial c(\mathbf{x}, t)}{\partial t} = -\nabla \cdot \mathbf{J} = \nabla \cdot M \nabla \left(\frac{\delta F[c(\mathbf{x}, t)]}{\delta c(\mathbf{x}, t)} \right) + \xi_c(\mathbf{x}, t) \leftarrow \text{Thermal noise}$$

Differential time derivative of concentration: Evolution of the field variable

Variational derivative of total free energy functional

Local variation of the field variable (composition, concentration etc.): $\delta c(\mathbf{x}, t)$



Variation of the **total** free energy $\delta F[c(\mathbf{x}, t)]$

$$\frac{\partial c(\mathbf{x}, t)}{\partial t} = \nabla \cdot \left(M \nabla \frac{\delta F}{\delta c(\mathbf{x}, t)} \right) + \xi_c(\mathbf{x}, t)$$

➤ Fick's Law (1st, 2nd)

$$\mathbf{J} = -D \frac{\partial C}{\partial x}, \quad \frac{\partial C}{\partial t} = -\nabla \cdot \mathbf{J} = D \frac{\partial^2 C}{\partial^2 x}$$

- **J: flux**
- **C: concentration**
- **D: diffusion coefficient**

➤ Generalized Fick's law

$$\mathbf{J} = Mf$$

$$f = -\nabla \mu = -\nabla \frac{\delta F}{\delta C(r, t)}, \quad \mu = \frac{\delta F}{\delta C(r, t)}$$

$$\frac{\partial C}{\partial t} = -\nabla \cdot \mathbf{J} = \nabla \cdot \left[M \nabla \frac{\delta F}{\delta C(r, t)} \right]$$

- $\mu = \delta F / \delta C(r, t)$: **chemical potential**
- f : **driving force, gradient of μ**
- M : **mobility of atom migration**

1.4 Example (1)

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➤ Typical total free energy functional: $F[c(\mathbf{x},t)] = \int_V \left[f[c] + \frac{k}{2} |\nabla c|^2 \right] d\mathbf{x}$

- Local energy density (double well function)

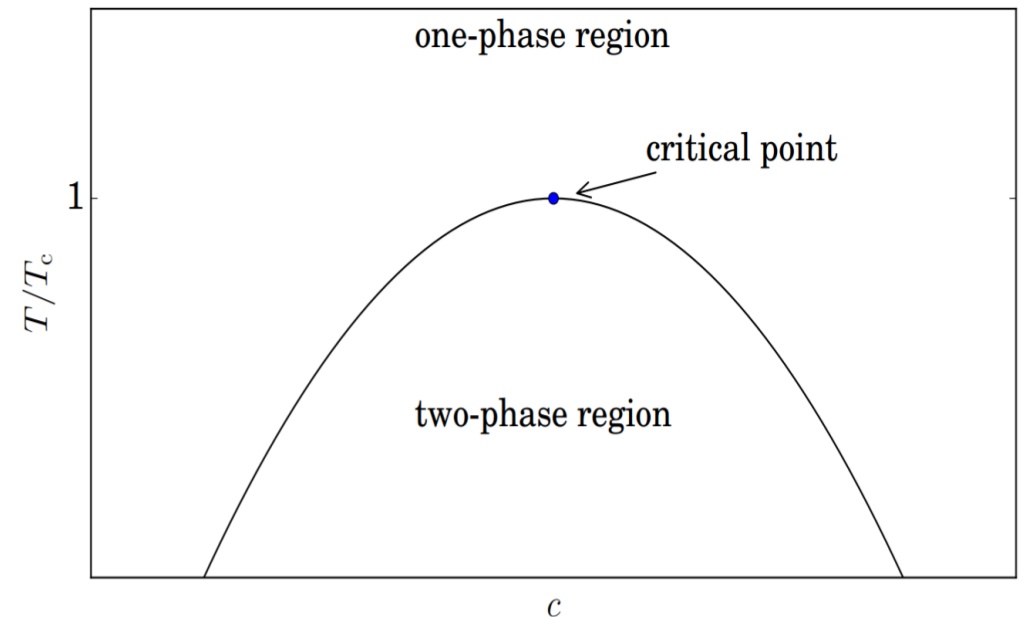
$$f[c] = \frac{\alpha}{2} c^2 + \frac{\beta}{4} c^4, \beta > 0$$

- α : depends on temperature (T), and it determines whether a phase separation will occur.
 - $T < T_c$: two-phase (super cooling)
 - $T > T_c$: one-phase region

$$\Rightarrow \delta F = \int_V \left[f'(c) \delta c - \frac{\partial}{\partial x} (k \nabla c) \delta c \right] d\mathbf{x}$$

$$\Rightarrow \frac{\partial c(\mathbf{x},t)}{\partial t} = \nabla \cdot M \nabla \left(\frac{\delta F}{\delta c} \right)$$

$$= \nabla \cdot M \nabla [\alpha c(\mathbf{x},t) + \beta c(\mathbf{x},t)^3 - k \Delta c(\mathbf{x},t)]$$



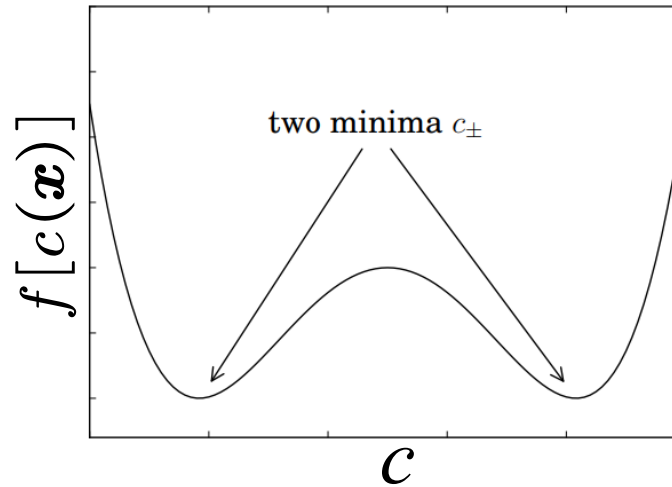
1.4 Example (2)

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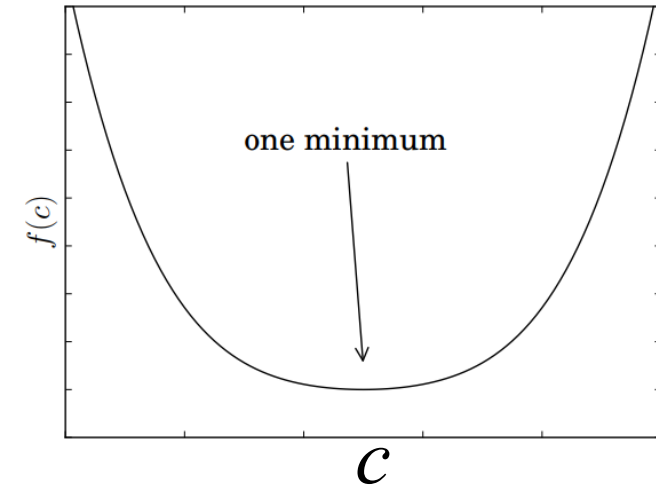
$$f[c(\mathbf{x})] = \frac{\alpha}{2}c^2 + \frac{\beta}{4}c^4, \beta > 0$$

$$\frac{\partial f}{\partial c} = c(\beta c^2 + \alpha)$$

$T < T_c, \alpha < 0$



$T > T_c, \alpha > 0$



$$F[c] = \int_V \left[f[c] + \frac{k}{2} |\nabla c|^2 \right] d\mathbf{x}$$

$$\frac{\partial c(\mathbf{x}, t)}{\partial t} = \nabla \cdot M \nabla \left(\frac{\delta F[c]}{\delta c} \right) = \nabla \cdot M \nabla [\alpha c(x, t) + \beta c(x, t)^3 - k \Delta c(x, t)]$$

1.4 Example (3)

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➤ Decrease of the free energy?

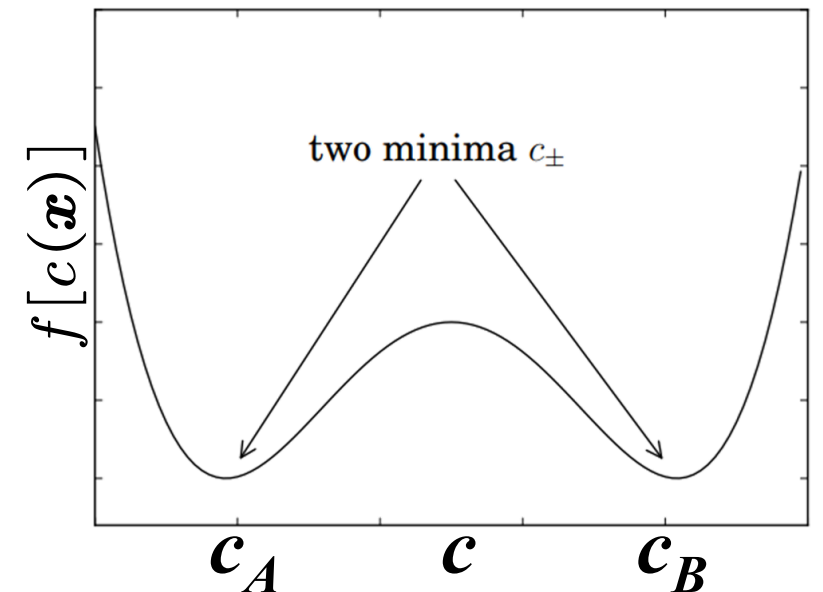
$$\begin{aligned}\frac{dF[c]}{dt} &= \int_V \frac{\delta F[c]}{\delta c(\mathbf{x},t)} \frac{\partial c}{\partial t} d\mathbf{x} = \int_V \frac{\delta F[c]}{\delta c} \nabla \cdot M \nabla \left(\frac{\delta F[c]}{\delta c} \right) d\mathbf{x} \\ &= - \int_V \nabla \frac{\delta F[c]}{\delta c} \cdot M \nabla \left(\frac{\delta F[c]}{\delta c} \right) d\mathbf{x} = - \int_V M \left[\nabla \left(\frac{\delta F[c]}{\delta c} \right) \right]^2 d\mathbf{x} \leq 0\end{aligned}$$

$$F[c] = \int_V \left[f[c] + \frac{\kappa}{2} |\nabla c|^2 \right] d\mathbf{x}$$

$$\frac{\partial c(\mathbf{x},t)}{\partial t} = \nabla \cdot M \nabla \left(\frac{\delta F[c]}{\delta c(\mathbf{x},t)} \right)$$

➤ Minimization of $F[c]$?

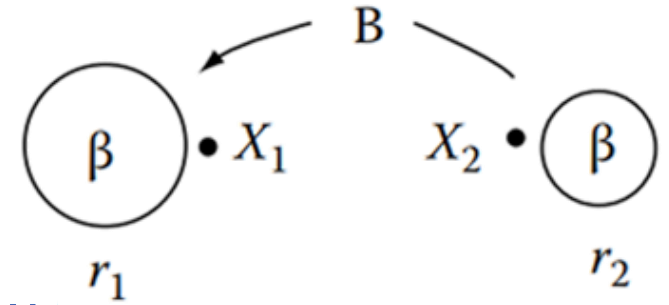
- Minimize $f[c(\mathbf{x})]$: evolve to either c_A or c_B
- Minimize $\frac{\kappa}{2} |\nabla c|^2$: reduce interfaces between regions with c_A or c_B ➔ coarsening, regions with c merge to larger regions with less interfaces.



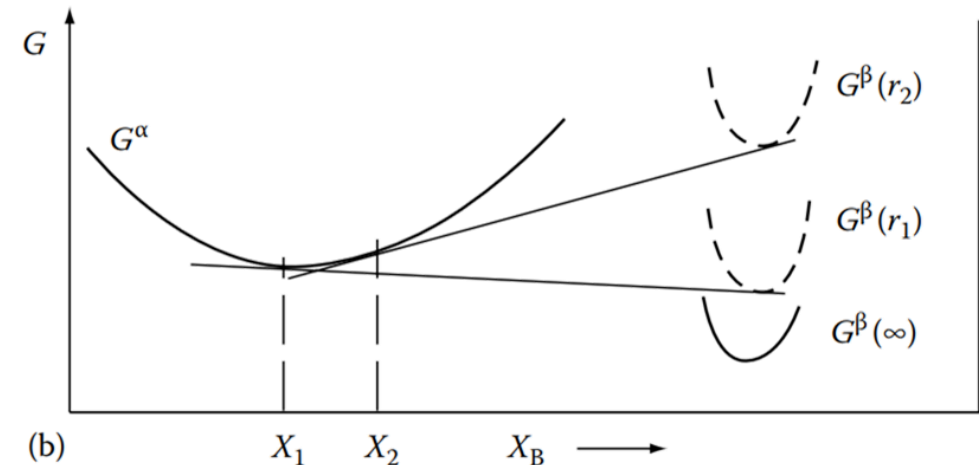
1.5 Example: particle coarsening

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- Two spherical precipitates: smaller r_2 vs larger r_1
 - Solution concentration X ____?____ with increasing r .
 - solute gradient (X) → solute diffuse along ____?____.
- ➔ small particles shrink & disappear, large particles grow.



- Coarsening rate $\dot{r} \propto k/r^2$, with $k \propto D\gamma X_e$
 - Volume diffusion controlled $r^3 = r_0^3 + kt$
 - D : Diffusion coefficient.
 - γ : Interface energy
 - X_e : equilibrium solubility of large particles
 - D, X_e exponentially increase with T



D.A. Porter, K.E. Easterling, Phase transformations in metals and alloys (revised reprint), CRC press 2009.

Variational derivative



$$\frac{\partial \phi_p(\mathbf{x}, t)}{\partial t} = M \cdot - \frac{\delta F}{\delta \phi_p(\mathbf{x}, t)} + \xi_p(\mathbf{x}, t)$$

Evolution rate = $M \cdot$ **Driving force**

Thermal noise

Analogy: velocity = $\dot{\mathbf{r}} =$ **Force** \cdot time/mass = $-\nabla E \cdot$ const

*(Time Dependent or Non-conserved) Ginzburg-Landau equation

S.M. Allen, J.W.J.A.m. Cahn, A microscopic theory for antiphase boundary motion and its application to antiphase domain coarsening, 27(6) (1979) 1085-1095.

$$\frac{\partial \phi_p(\mathbf{x}, t)}{\partial t} = M \cdot - \frac{\delta F}{\delta \phi_p(\mathbf{x}, t)} \quad F[\phi] = \int_V \left[f[\phi] + \frac{\alpha}{2} |\nabla \phi|^2 \right] d\mathbf{x}$$

$$\Rightarrow \frac{\partial \phi(\mathbf{x}, t)}{\partial t} = - \underset{\substack{\uparrow \\ \text{Mobility for boundary migration}}}{M} \frac{\delta F[\phi(\mathbf{x}, t)]}{\delta \phi(\mathbf{x}, t)} = - M \left[\frac{\partial f(\phi)}{\partial \phi} - \alpha \nabla^2 \phi(\mathbf{x}, t) \right]$$

Mobility for boundary migration

- Condition for minimum total energy

$$\Leftrightarrow \frac{\delta F[\phi(\mathbf{x}, t)]}{\delta \phi(\mathbf{x}, t)} = 0 = \frac{\partial f(\phi)}{\partial \phi} - \alpha \nabla^2 \phi(\mathbf{x}, t)$$

$$|\nabla \phi|^2 = \left(\frac{\partial \phi}{\partial x} \right)^2 + \left(\frac{\partial \phi}{\partial y} \right)^2 + \left(\frac{\partial \phi}{\partial z} \right)^2$$

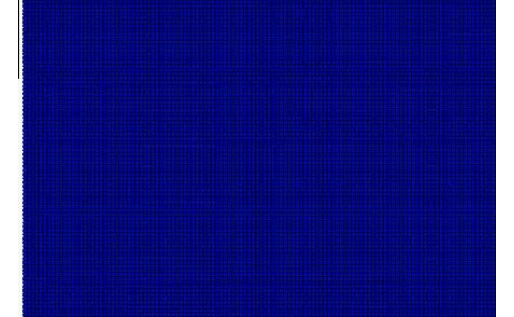
$$\Delta \phi = \nabla^2 \phi = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2}$$

(Laplacian operator)

- Energy depends on ϕ and $\nabla \phi$
- Driving force depends on 2nd derivative of ϕ w.r.t. x

2.2 Mobility Coefficient M

$$\frac{\partial \phi(\mathbf{x}, t)}{\partial t} = -M \frac{\delta F[\phi(\mathbf{x}, t)]}{\delta \phi(\mathbf{x}, t)}$$



- Kinetic nature, time-scale
- Anisotropic nature: migration rate of the interface is sensitive to interface orientation (kinetics controlled)
- Coupling the dynamics between multiple order parameters

$$\frac{\partial \phi_i(\mathbf{x}, t)}{\partial t} = - \sum_{j \neq i} M_{ij} \frac{\delta F[\phi_1, \phi_2, \dots]}{\delta \phi_j(\mathbf{x}, t)}$$

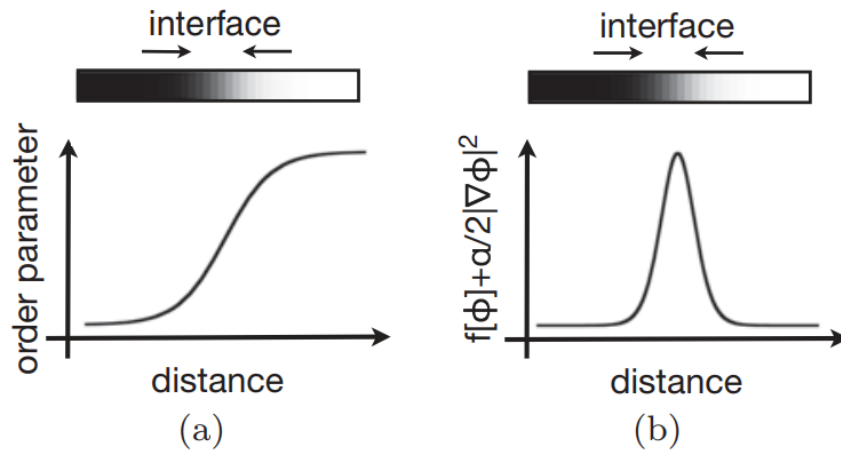


Figure 12.1 (a) A schematic view of the one-dimensional diffuse interface. Plotted is the variation of the order parameter through an interface, $\phi(x)$. (b) Schematic drawing of the integrand of the energy expression from Eq. (12.5), showing the peak in free-energy density in the interface.

➤ Discretization

- **Each grid point: a certain volume $v = a^3$**
- **throughout the grid volume: same ϕ**

➤ Boundary condition

- **Fixed $\phi_1 = 1$**
- **Fixed $\phi_{15} = -1$**

	ϕ_1	ϕ_2	ϕ_3	ϕ_4	ϕ_5	ϕ_6	ϕ_7	ϕ_8	ϕ_9	ϕ_{10}	ϕ_{11}	ϕ_{12}	ϕ_{13}	ϕ_{14}	ϕ_{15}
$t=0$	1	1	1	1	1	0.9	0.5	0	-0.5	-0.9	-1	-1	-1	-1	-1

Figure 12.2 A one-dimensional model showing the values of the order parameter at $t = 0$.

2.3 Example (2): numerical solution

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- **Solid-liquid in equilibrium**

$$f[\phi(x,t)] = 4U \left(-\frac{1}{2} \phi^2 + \frac{1}{4} \phi^4 \right)$$

To model the **phenomenological** behavior of a system with two phases of equal energy

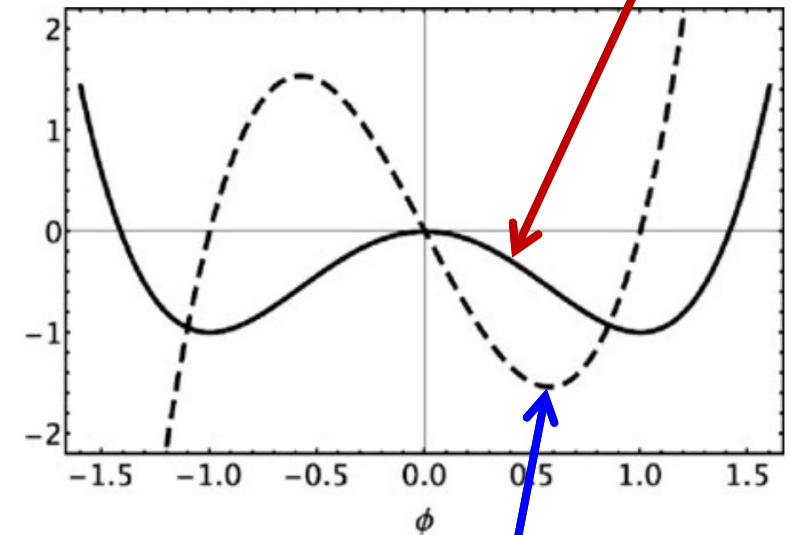
- **Finite difference method:**

$$\frac{d\phi_i}{dx} = \frac{\phi_{i+1} - \phi_{i-1}}{2a}, \quad \frac{d^2\phi_i}{dx^2} = \frac{\phi_{i+1} + \phi_{i-1} - 2\phi_i}{a^2}$$
$$\Rightarrow \frac{\partial\phi_i}{\partial t} = -M \left[4U(-\phi_i + \phi_i^3) - \alpha \left(\frac{\phi_{i+1} + \phi_{i-1} - 2\phi_i}{a^2} \right) \right]$$

Numerical methods: Finite difference/element method, Fast Fourier Transformation method

$$\frac{\partial\phi(\mathbf{x},t)}{\partial t} = -M \left[\frac{\partial f(\phi)}{\partial\phi} - \alpha \nabla^2 \phi(\mathbf{x},t) \right]$$

Double well chemical energy density $f(\phi)$



$$\frac{\partial f(\phi)}{\partial\phi} = 4U(-\phi + \phi^3), U = 1$$

2.3 Example (3): numerical solution

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$$\frac{\partial \phi_i}{\partial t} = -M \left[4U(-\phi_i + \phi_i^3) - \alpha \left(\frac{\phi_{i+1} + \phi_{i-1} - 2\phi_i}{a^2} \right) \right]$$

- Integrate the **equation of motion** (1st order Taylor expansion):

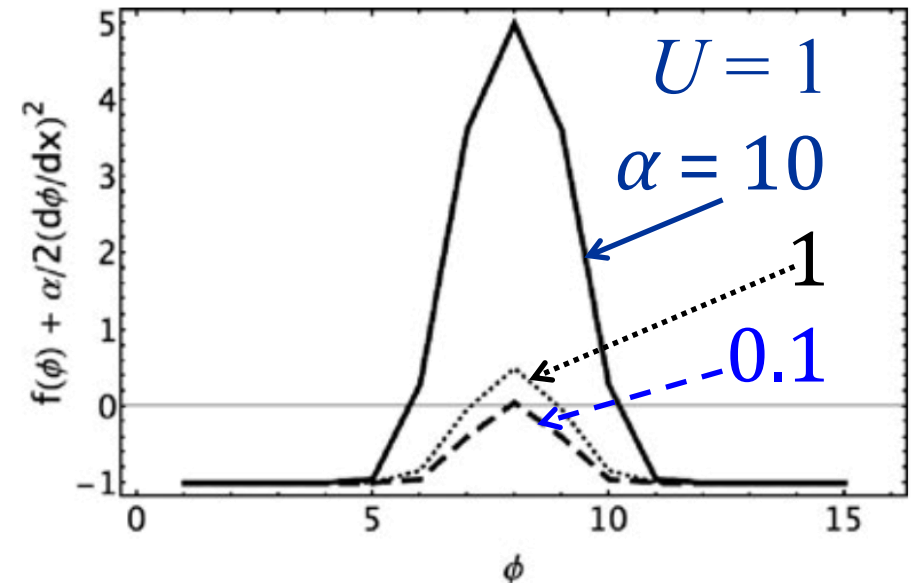
$$\phi_i(t + \delta t) = \phi_i(t) + \frac{\partial \phi_i}{\partial t} \delta t.$$

δt : accuracy, efficiency
(Euler equation)

EOM in PF	EOM in MD
Decrease of total free energy	Accurate integration

- Kinetic parameter **$M = 1$** for convenience

$$f[\phi_i] + \frac{\alpha}{2} \left(\frac{d\phi_i}{dx} \right)^2$$
$$= 4U \left(-\frac{1}{2} \phi_i^2 + \frac{1}{4} \phi_i^4 \right) + \frac{\alpha}{2} \left(\frac{\phi_{i+1} - \phi_{i-1}}{2a} \right)^2$$



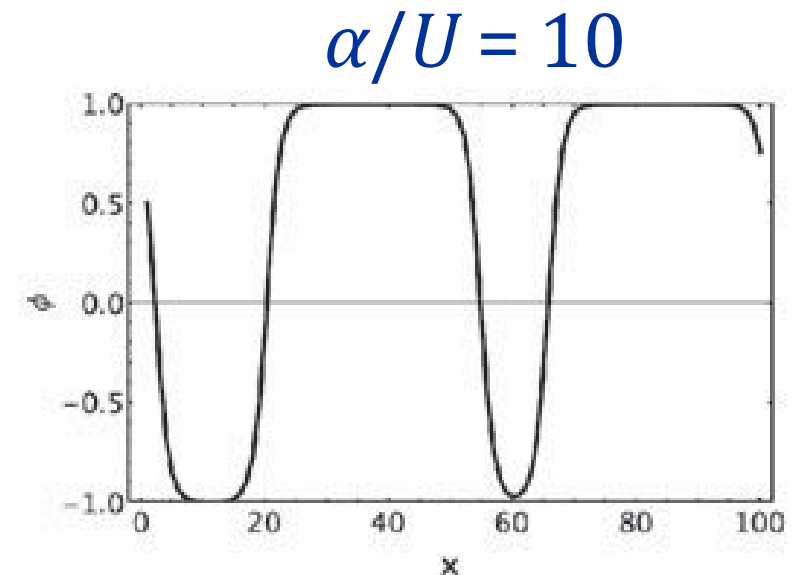
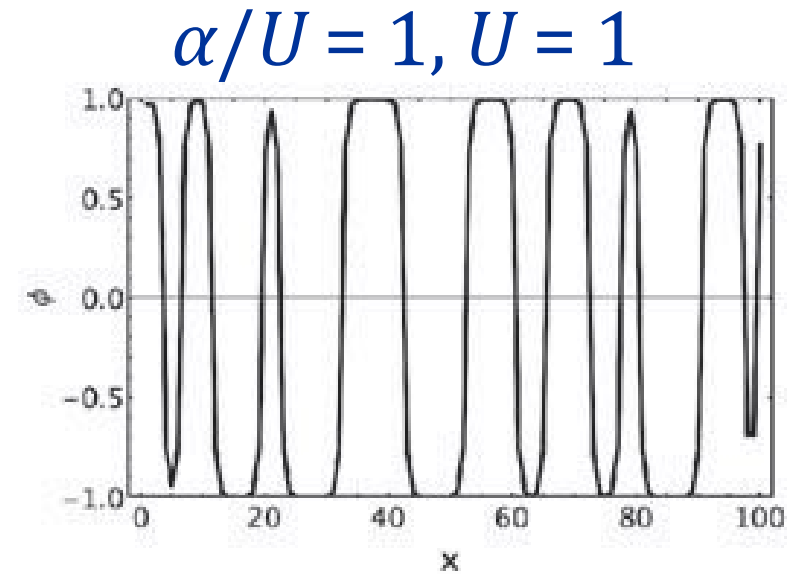
2.3 Example (4): numerical solution

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$$\left. \begin{array}{l} 1. \phi_i, \frac{d\phi_i}{dx} \Rightarrow F\left[\phi_i, \frac{d\phi_i}{dx}\right] \\ 2. \phi_i, \frac{d^2\phi_i}{dx^2} \Rightarrow \frac{\partial\phi_i}{\partial t} \end{array} \right\} \Rightarrow \phi_i(t + \delta t) = \phi_i(t) + \frac{\partial\phi_i}{\partial t} \cdot \delta t$$

➤ Periodic boundary condition

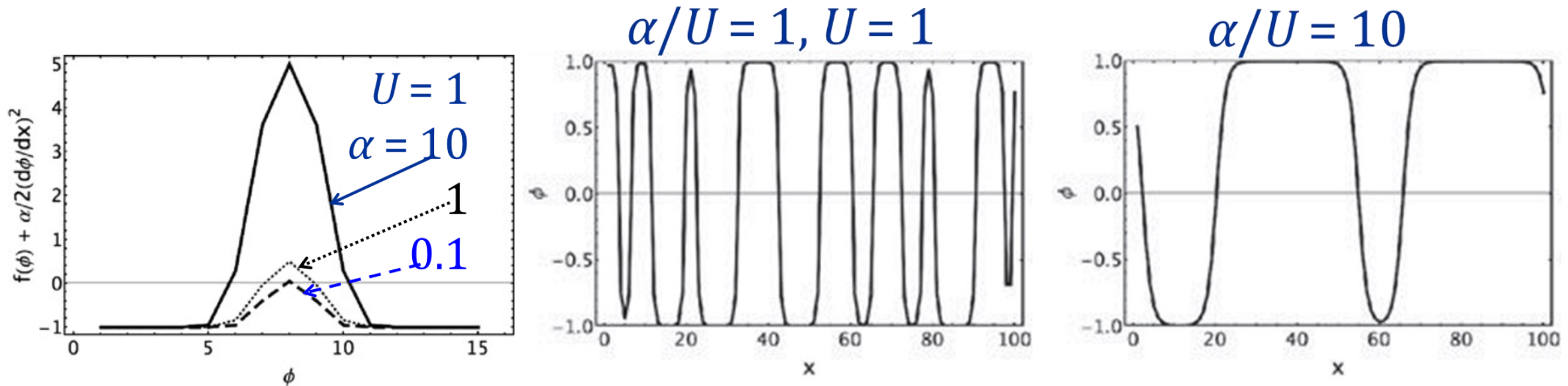
1. Initialize $\phi(x)$ at each mesh grid at $t = 0$, random $[-0.1, 0.1]$
2. Calculate $F[\phi_i, d\phi_i/dx]$ & $d\phi_i/dt$ for each grid point at time t
3. Update new $\phi(x)$ at $t + \delta t$
4. Go to 2 and repeat **till F converges to a minimum** $\Leftrightarrow d\phi_i/dt \approx 0$



2.3 Example (5): discussion

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- Influence of interface energy?



$d\phi_i/dt \approx 0$, but not at equilibrium

- Equilibrium: no interfaces to minimize the interface energy
- Q: $\alpha = 0$?

- Condition for minimum total energy (equilibrium)

$$\Leftrightarrow \frac{\delta F[\phi(\mathbf{x}, t)]}{\delta \phi(\mathbf{x}, t)} = 0 \Rightarrow \frac{\partial f(\phi)}{\partial \phi} - \alpha \nabla^2 \phi(\mathbf{x}, t) = 0$$

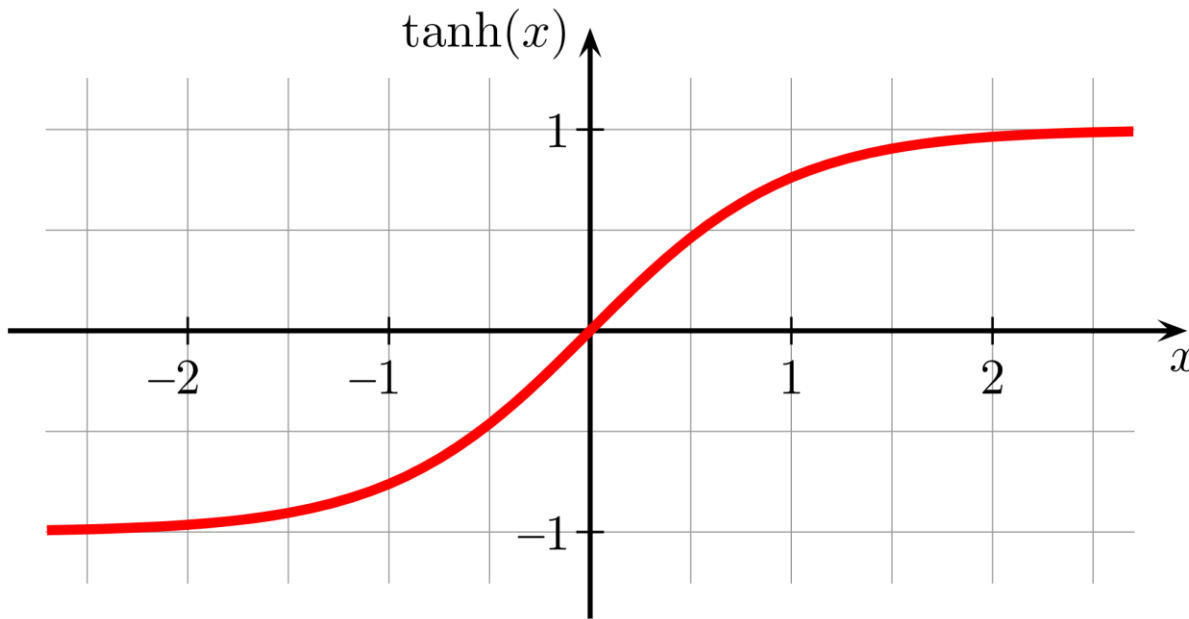
- Interface located in yz plane at $x = 0$, with $f[\phi(x, t)] = 4U\left(-\frac{1}{2}\phi^2 + \frac{1}{4}\phi^4\right)$

- Free energy per unit area $\frac{F}{A} = \int_x \left[4U\left(-\frac{1}{2}\phi^2 + \frac{1}{4}\phi^4\right) + \frac{\alpha}{2} \left(\frac{\partial \phi}{\partial x}\right)^2 \right] dx$

- $\frac{\delta(F/A)}{\delta \phi} = 0 \Rightarrow 4U[-\phi(x) + \phi^3(x)] - \alpha \left[\frac{\partial^2 \phi(x)}{\partial x^2} \right] = 0$

$$\frac{\delta(F/A)}{\delta\phi} = 0 \Rightarrow 4U[-\phi(x) + \phi^3(x)] - \alpha \left[\frac{\partial^2 \phi(x)}{\partial x^2} \right] = 0$$

$$\Rightarrow \phi(x) = \tanh(x\sqrt{2U/\alpha})$$



- Minimum interface energy?

$$\frac{F}{A} = \frac{4\sqrt{2}}{3} \sqrt{U\alpha}$$

- Interface width?

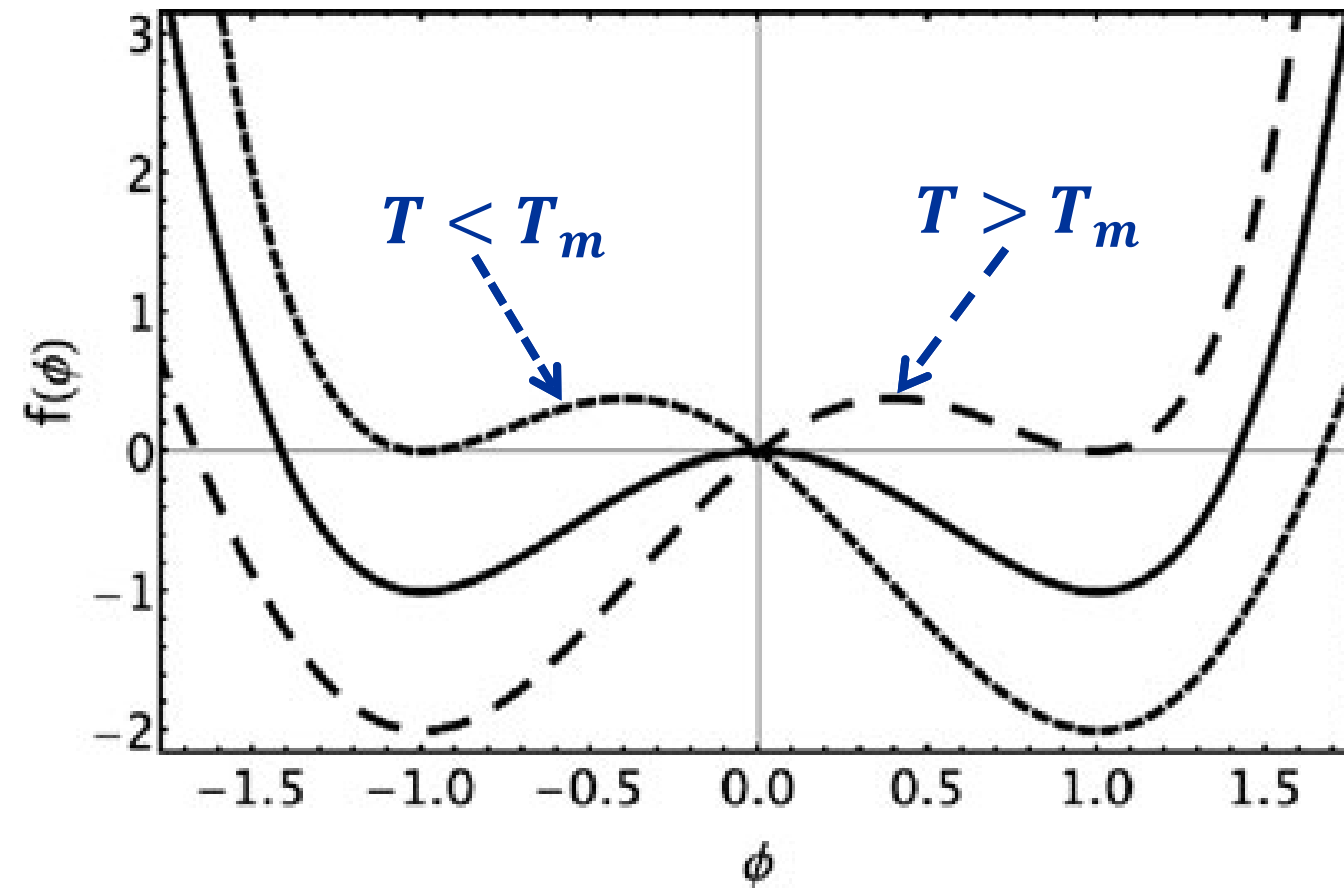
$$w \propto \sqrt{\alpha/U}$$

1. Cahn-Hilliard equation for evolution of conserved field variables
2. Allen-Cahn equation for evolution of non-conserved field variables
3. **Discussion, outlook and summary**
 - **Advantages & Limitations of PFM**

3.1 phase preference

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$$f[\phi] = 4U \left(-\frac{1}{2}\phi^2 + \frac{1}{4}\phi^4 \right) + \frac{15\gamma}{8} \left(\phi - \frac{2}{3}\phi^3 + \frac{1}{5}\phi^5 \right) (T - T_m), \gamma > 0.$$



- $T = T_m$: $f[\phi = 1] = f[\phi = -1]$
solid liquid
- $T \neq T_m$: one phase is preferred
- **Accurate free energy model?**
 - thermodynamic calculations such as CALPHAD
 - database

3.2 multi-phase system (1)

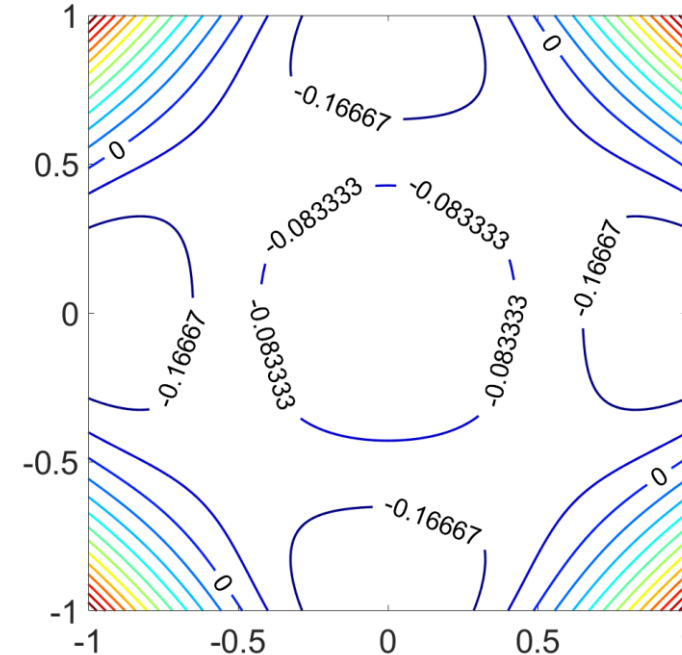
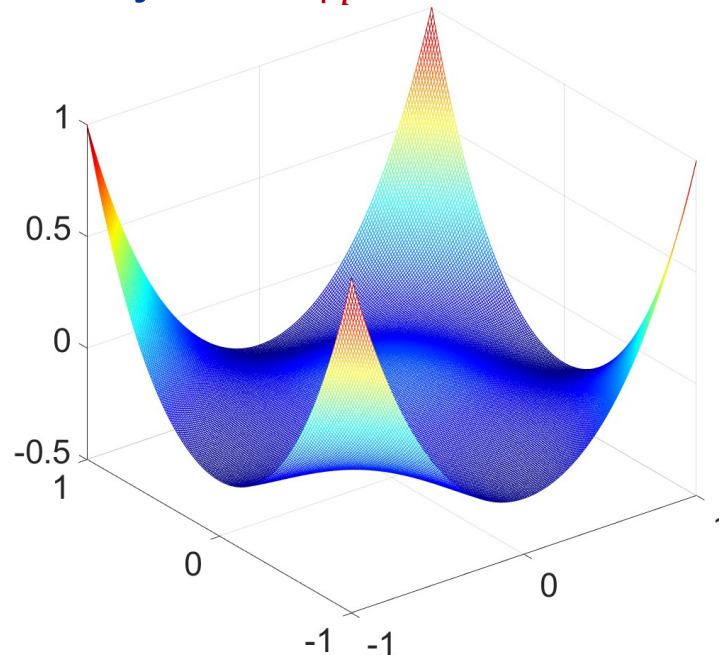
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- Example: grain growth--many “phases” with same composition, each phase (ϕ_i) represents a grain with a different orientation.
- Free energy
 - arbitrary # of order parameters for different orientations
 - Distinct minima, each has only one ϕ_i is non-zero.

$$f[\{\phi_i\}] = -\frac{\gamma}{2} \sum_{i=1}^P \phi_i^2 + \frac{\beta}{4} \left(\sum_{i=1}^P \phi_i^2 \right)^2 + \left(\lambda - \frac{\beta}{2} \right) \sum_{i=1}^P \sum_{j \neq i=1}^P \phi_i^2 \phi_j^2$$

$P=2, \beta=\lambda=1$

other options?

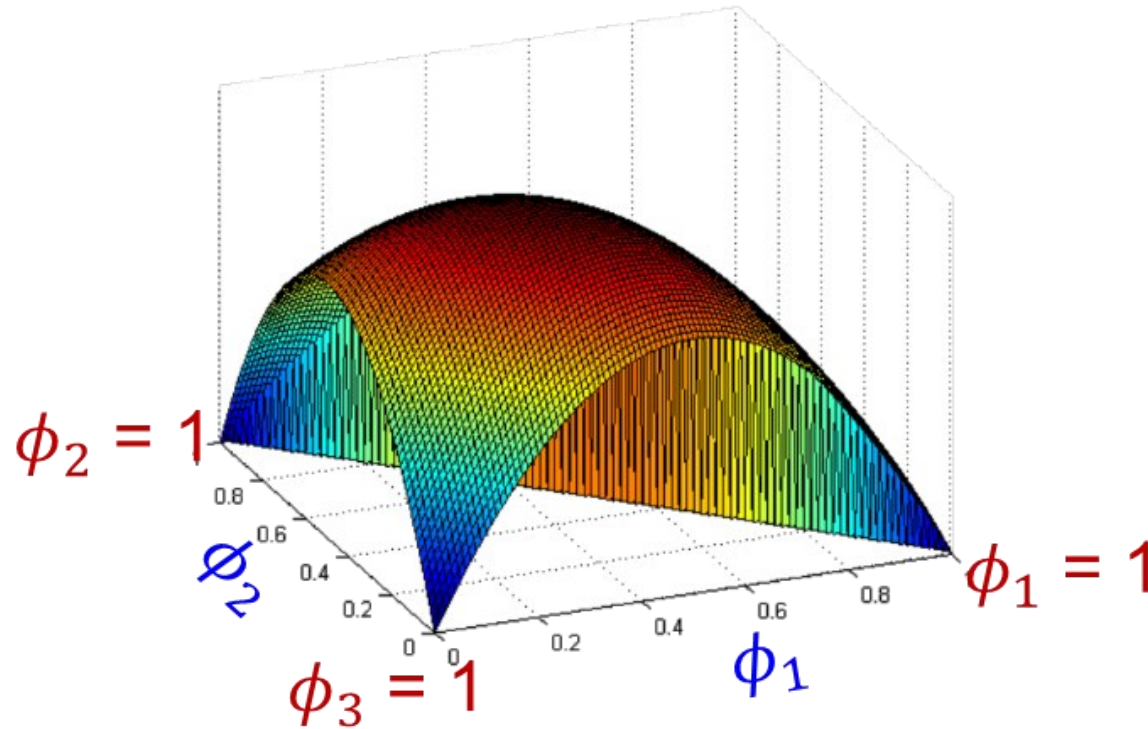


3.2 multi-phase system (2)

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- Free energy: Distinct minima, each has only one ϕ_i approaching unity or zero (pure phase)

$$f[\{\phi_i\}] = U(|\phi_1\phi_2| + |\phi_2\phi_3| + |\phi_3\phi_1|)$$



- Modeling meso-(micro-) scale microstructure
 - **Based on thermodynamic principles**

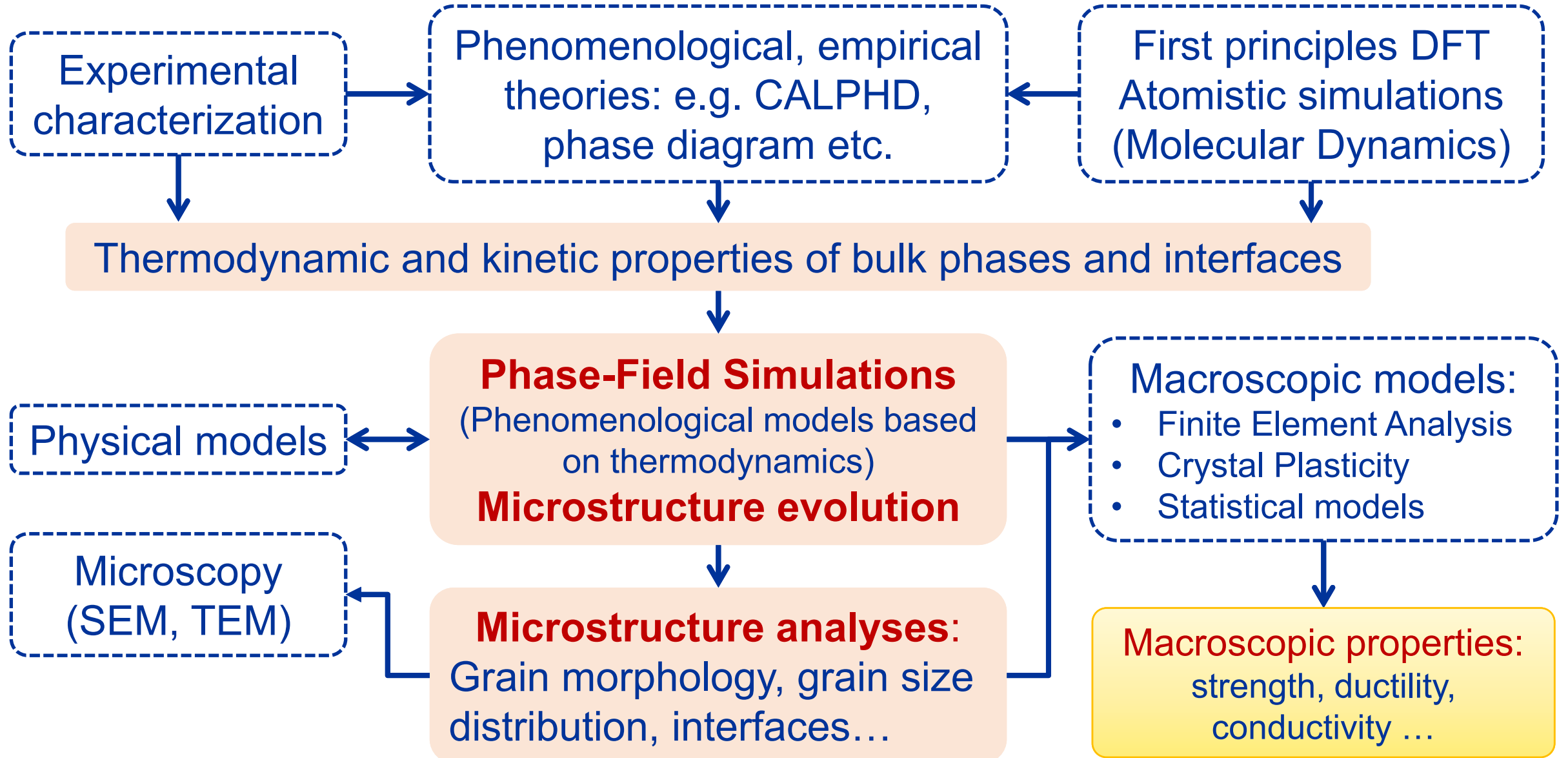
- Current topics
 - Realistic, complex, multi component systems
 - More realistic description of free energy**

 - **Quantitative aspects**

- Accurately reproduce bulk properties, and interfaces as observed
 - **Effective model description and parameters**
 - Numerical issues
- Provide insights into evolution of complex morphologies (i.e. grain assemblies, twin evolution etc.)
 - Effect of individual bulk and interface properties on results
- Predictive ability ?
 - **Depends on availability and accuracy of input data**
 - Requires composition and orientation dependence

3.4 Quantitative PFM (2)

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- Different kinds of input data
 - Bulk phase stabilities, bulk phase diagram information (CALPHAD)
 - Interfacial energy and mobility
 - Elastic properties, crystal structure, lattice parameters
 - Diffusion mobilities/coefficients (DICTRA mobilities)
- Orientation and composition dependence
 - Anisotropy, segregation, solute drag
 - Very important for microstructure evolution, but difficult to measure/calculate

**Coupling phase-field with
thermodynamic databases**

- **Microstructure in PFM**
 - **Field variables (conserved, non-conserved)**
- **Driving forces for microstructure evolution**
 - **Decrease of free energy**
 - **Free energy**
- **Governing equation for microstructure evolution**
 - **Conserved variable (Cahn-Hilliard Equation)**
 - **Non-conserved (Allen-Cahn equation)**
- **Solve the governing equation to obtain microstructure**
 - **Determine parameters (atomic scale models, experiments)**
 - **Initialize variables, apply boundary conditions**
 - **Numerical solutions**



上海交通大学

材料科学与工程学院

School of Materials Science and Engineering, SJTU

Next Week:

Hands-On Phase Filed Method



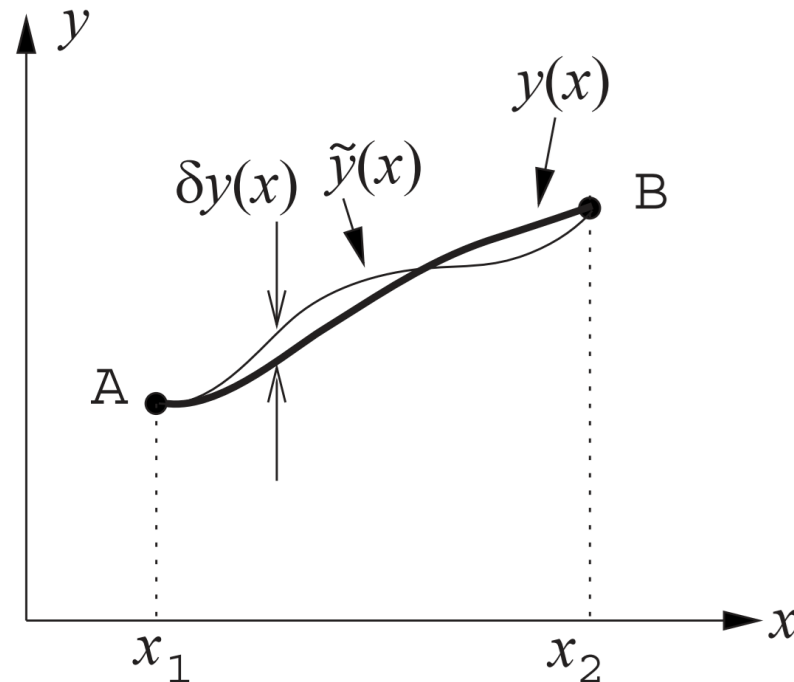
- **Functional:** functions of a function. i.e.

$$I[y(x)] = \int_{x_1}^{x_2} F[x, y(x), y'(x)] dx, \quad y'(x) \equiv dy(x)/dx$$

- **Variation:** small change in $y(x) \rightarrow$ variation of the functional

$$\tilde{y}(x) = y(x) + \delta y(x)$$

$$\delta I = I[\tilde{y}(x)] - I[y(x)]$$



- The **calculus of variations**: find an extremum (maximum or minimum) of a quantity that is expressible as an **integral**.
- Explicit expression of variation?

$$\delta I = I[y(x) + \delta y(x)] - I[y(x)]$$

- Define the infinitesimal $\delta y(x) = \epsilon \phi(x)$,
 - $\phi(x)$: an arbitrary continuous and sufficiently smooth function
 - ϵ : an infinitesimal number.

- Taylor expand $I[\tilde{y}(x)] = \int_{x_1}^{x_2} F(x, y(x) + \epsilon \phi(x), y'(x) + \epsilon \phi'(x)) dx$
$$= \int_{x_1}^{x_2} \left[F(x, y(x), y'(x)) + \frac{\partial F}{\partial y} \epsilon \phi(x) + \frac{\partial F}{\partial y'} \epsilon \phi'(x) + \mathcal{O}(\epsilon^2) \right] dx$$
$$= I[y(x)] + \epsilon \int_{x_1}^{x_2} \left[\frac{\partial F}{\partial y} \phi(x) + \frac{\partial F}{\partial y'} \phi'(x) \right] dx + \mathcal{O}(\epsilon^2)$$

- Variation of the integral:
$$\begin{aligned}\delta I &= \epsilon \int_{x_1}^{x_2} \left[\frac{\partial F}{\partial y} \phi(x) + \frac{\partial F}{\partial y'} \phi'(x) \right] dx \\ &= \int_{x_1}^{x_2} \left[\frac{\partial F}{\partial y} \delta y(x) + \frac{\partial F}{\partial y'} \delta y'(x) \right] dx\end{aligned}$$

- Integration by parts:

$$\begin{aligned}\delta I &= \epsilon \int_{x_1}^{x_2} \frac{\partial F}{\partial y} \phi(x) dx + \epsilon \int_{x_1}^{x_2} \frac{\partial F}{\partial y'} d\phi(x) \\ &= \epsilon \int_{x_1}^{x_2} \frac{\partial F}{\partial y} \phi(x) dx + \epsilon \left[\frac{\partial F}{\partial y'} \phi(x) \right]_{x_1}^{x_2} - \epsilon \int_{x_1}^{x_2} \frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right) \phi(x) dx\end{aligned}$$

- If constrain $y(x_1), y(x_2)$ to be constant (fixed boundary condition), then

$$\begin{aligned}\delta I &= \epsilon \int_{x_1}^{x_2} \left[\frac{\partial F}{\partial y} - \frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right) \right] \phi(x) dx \\ &= \int_{x_1}^{x_2} \left[\frac{\partial F}{\partial y} - \frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right) \right] \delta y(x) dx\end{aligned}$$

$$I[y(x)] = \int_{x_1}^{x_2} F[x, y(x), y'(x)] dx$$

$$\delta I = \int_{x_1}^{x_2} g(x) \delta y(x) dx \Rightarrow \frac{\delta I}{\delta y(x)} = g(x) = \frac{\partial F}{\partial y} - \frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right)$$

- Impossible to change only one $y(x_i)$ without change neighboring $y(x_i \pm dx)$ due to continuity
- variations: local change in function $\delta\phi(\mathbf{x})$
 \Rightarrow variation in total energy $\delta F[\phi(\mathbf{x}), \nabla\phi(\mathbf{x})]$
- 局部区域函数值的变化对泛函值的影响的大小
- Functional derivative: change of I divided by the change of area under the curve $y(x)$

$$\frac{\delta I}{\delta y(x)} = \frac{\partial F}{\partial y} - \frac{d}{dx} \left(\frac{\partial F}{\partial y'} \right) = \lim_{\Delta x \rightarrow 0} \frac{\partial I_n}{\partial y_k} \frac{1}{\Delta x}$$

