上海交通大学
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MSE6701H, Multiscale Materials Modeling and Simulation

- ✓ Electronic DFT
- ✓ Atomistic MD
- • Mesoscale PF

Lecture 14

Governing equation for microstructure evolution & Solutions

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Review: Introduction to Phase Field Modeling(PFM)

- **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**

Review: energy functional

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

$$F = \int \left[f(c_1, c_2, \ldots, c_n, \eta_1, \eta_2, \ldots, \eta_p) + \sum_{i=1}^{n} \alpha_i (\nabla c_i)^2 + \sum_{i=1}^{3} \sum_{j=1}^{3} \sum_{k=1}^{p} \beta_{ij} \nabla_i \eta_k \nabla_j \eta_k \right] d^3r + \boxed{\iint G(r - r')\, d^3r\, d^3r'}$$

Nonlocal long-range interactions

$$+ E_{elastic} + E_{electric} + E_{magnetic}$$

Total free energy functional

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

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

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

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

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

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

Unknown coefficient α

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

III. Basics for Phase-Field method

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

Contents

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

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

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

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

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

- Flux: $\mathbf{J}=-M\nabla(\mu_B-\mu_A)$
  - M: mobility
  - μ_i: chemical potential of component i.
  - Difference of chemical potentials: variation of a corresponding free energy functional

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

- Under assumption of mass conservation

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

1.2 Cahn-Hilliard equation for conserved field variable

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

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 $\delta F[c(\mathbf{x},t)]$

1.3 Analogy: Fick's law for diffusion

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

➢ Fick's Law (1st, 2nd)

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

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

➢ Generalized Fick's law

$$\mathbf{J} = Mf$$

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

$$\frac{\partial C}{\partial t} = -\nabla\bullet J = \nabla\bullet(M\nabla\frac{\delta F}{\delta C(r,t)})$$

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

1.4 Example (1)

- Typical total free energy functional: $F[c(\boldsymbol{x},t)]=\int_V\left[f[c]+\frac{k}{2}|\nabla c|^2\right]d\boldsymbol{x}$
  - Local energy density (double well function)

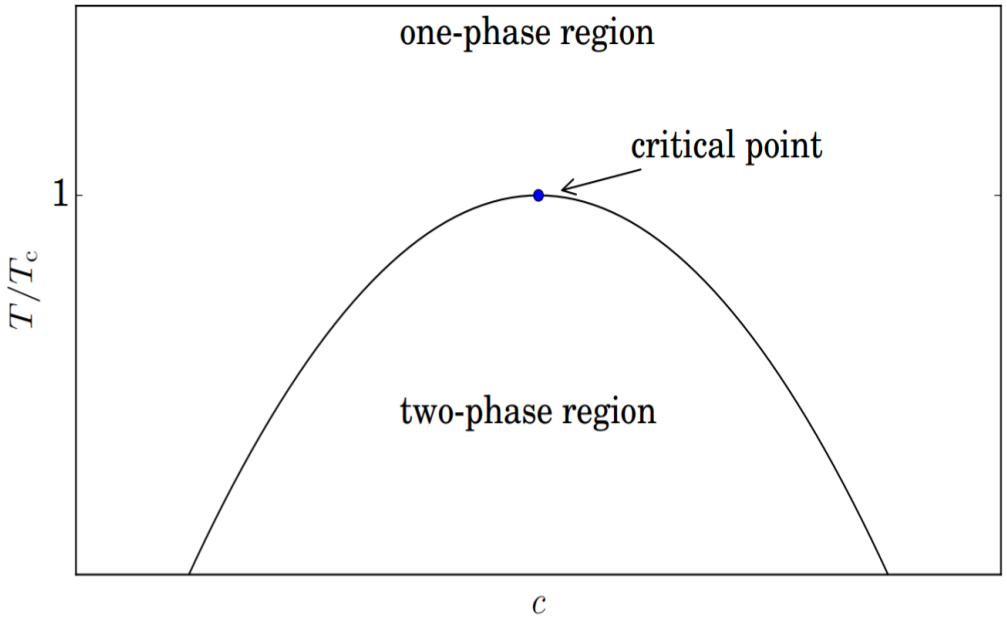
$$f[c]=\frac{\alpha}{2}c^2+\frac{\beta}{4}c^4,\beta>0$$

  - 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**

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

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

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

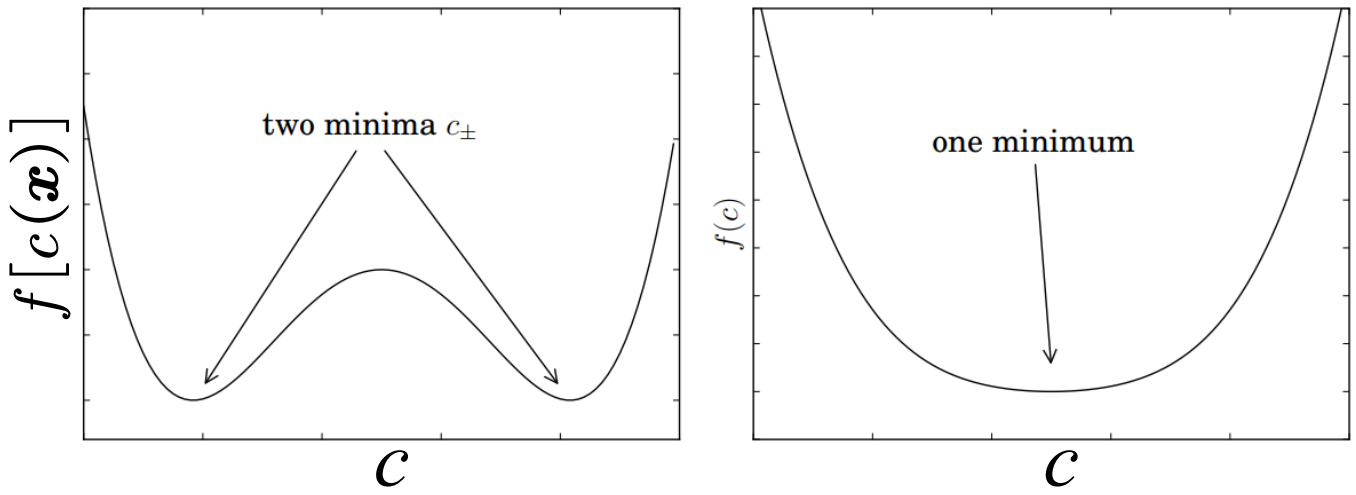


1.4 Example (2)

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

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

$T < T_c$, $\alpha < 0$ **$T > T_c$, $\alpha > 0$**



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

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

1.4 Example (3)

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

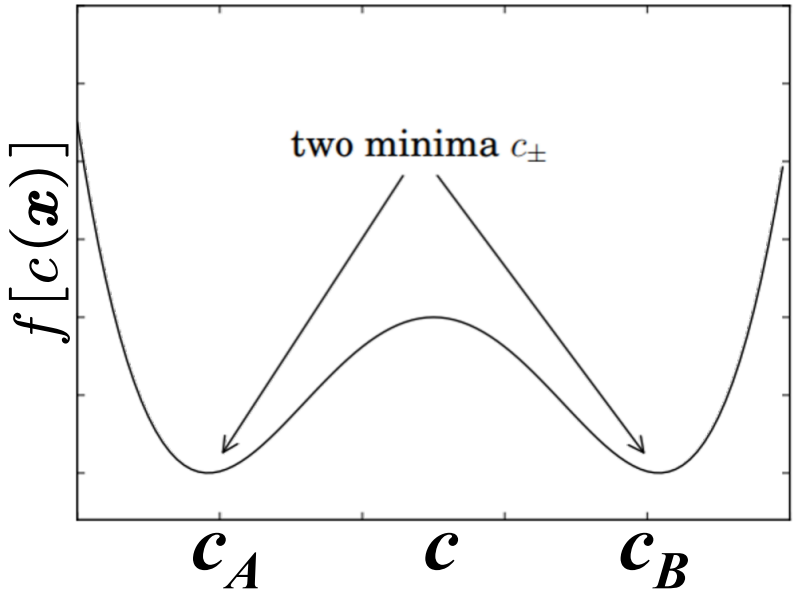
$$\frac{\partial c(\boldsymbol{x},t)}{\partial t}=\nabla\cdot M\nabla\left(\frac{\delta F[c]}{\delta c(\boldsymbol{x},t)}\right)$$

- Decrease of the free energy?

$$\frac{dF[c]}{dt}=\int_V\frac{\delta F[c]}{\delta c(\boldsymbol{x},t)}\frac{\partial c}{\partial t}d\boldsymbol{x}=\int_{\boldsymbol{V}}\frac{\delta F[c]}{\delta c}\nabla\cdot M\nabla\left(\frac{\delta F[c]}{\delta c}\right)d\boldsymbol{x}$$

$$=-\int_V\nabla\frac{\delta F[c]}{\delta c}\cdot M\nabla\left(\frac{\delta F[c]}{\delta c}\right)d\boldsymbol{x}=-\int_V M\left[\nabla\left(\frac{\delta F[c]}{\delta c}\right)\right]^2d\boldsymbol{x}\leqslant 0$$

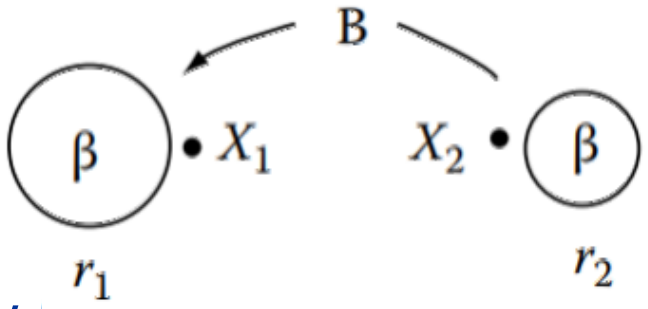
- Minimization of $F[c]$?
  - Minimize $f[c(\boldsymbol{x})]$: evolve to either c_A or c_B
  - Minimize $\frac{\kappa}{2}|\nabla c|^2$: reduce interfaces between regions with c_A or c_B ➔ coarsening, regions with c merge to larger regions with less interfaces.



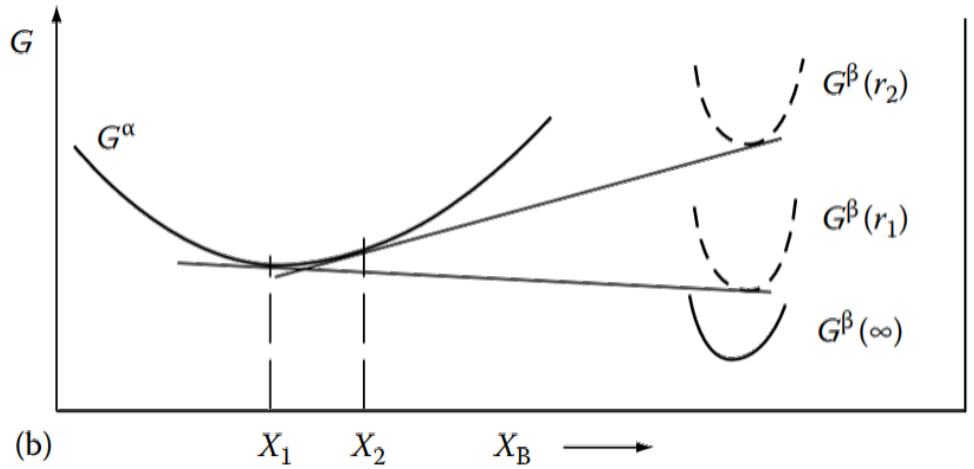
1.5 Example: particle coarsening

- 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 press2009.

2.1 Allen-Cahn equation for non-conserved field variables

Variational derivative

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

Evolution rate = *M* · Driving force **Thermal noise**

Analogy: velocity = $\dot{\mathbf{r}}$ = Force · 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.

2.1 Allen-Cahn equation for non-conserved field variables

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

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

Mobility for boundary migration

- Condition for minimum total energy

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

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

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

(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*

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

- 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

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

2.3 Example (1): one-dimensional interface

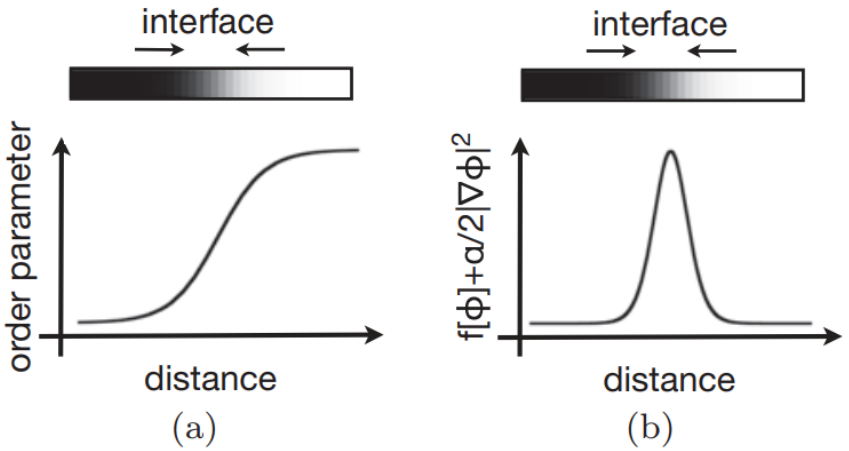


Figure 12.1 (a) A schematic view of the one-dimensional diffuse interface. Plotted is the variation of the order parameter through an interface, $\phi(x)$. (b) Schematic drawing of the integrand of the energy expression from Eq. (12.5), showing the peak in free-energy density in the interface.

	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 $t = 0$.

- **Discretization**
  - **Each grid point: a certain volume v = a^3**
  - **throughout the grid volume: same ϕ**
- **Boundary condition**
  - **Fixed $\phi_1 = 1$**
  - **Fixed $\phi_{15} = -1$**

2.3 Example (2): numerical solution

- **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:**

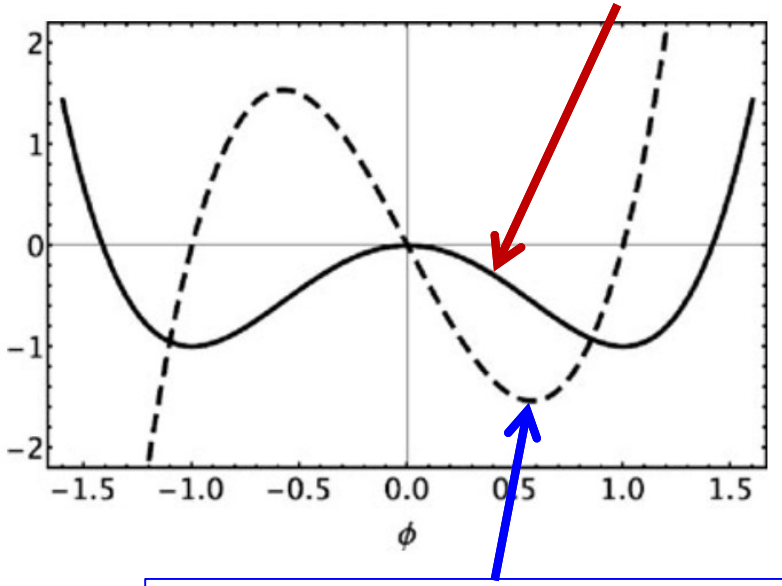
$$\frac{d\phi_i}{dx} = \frac{\phi_{i+1} - \phi_{i-1}}{2a}, \quad \frac{d^2\phi_i}{dx^2} = \frac{\phi_{i+1} + \phi_{i-1} - 2\phi_i}{a^2}$$

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

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

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

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

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

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

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

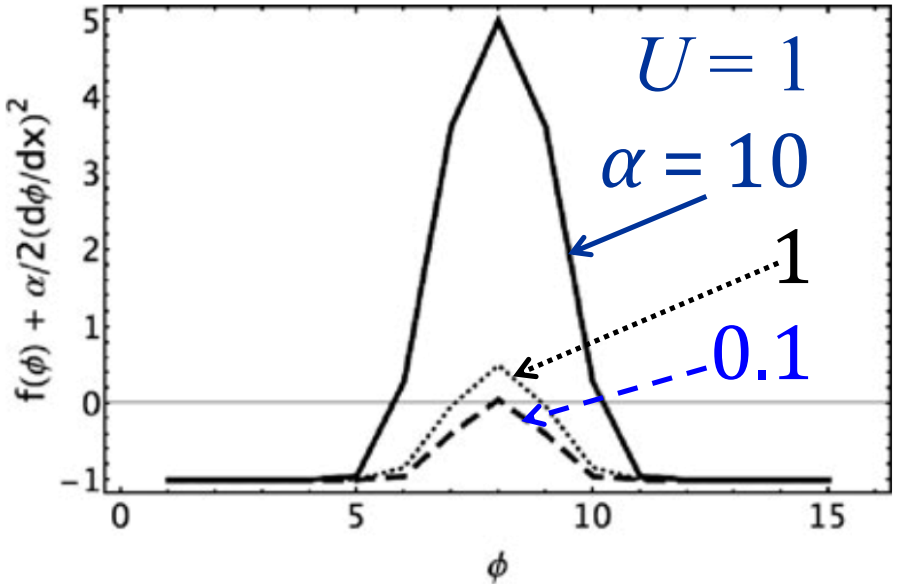
δt: accuracy, efficiency
(Euler equation)

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

- Kinetic parameter M = 1 for convenience

$$f[\phi_i] + \frac{\alpha}{2}\left(\frac{d\phi_i}{dx}\right)^2$$

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

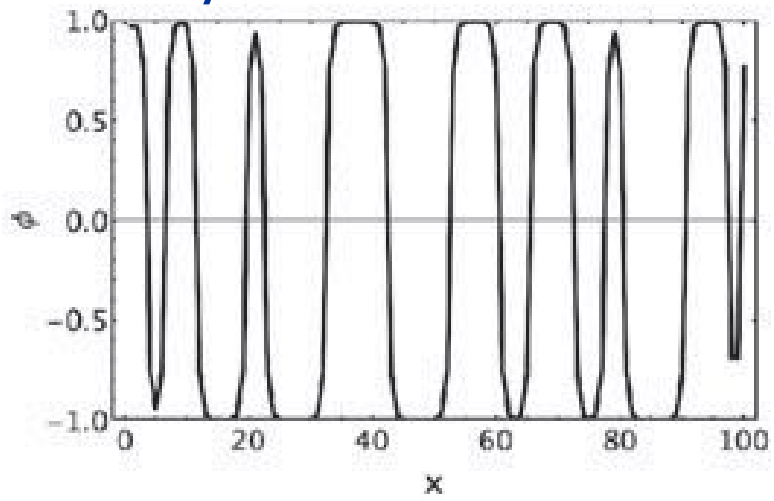


2.3 Example (4): numerical solution

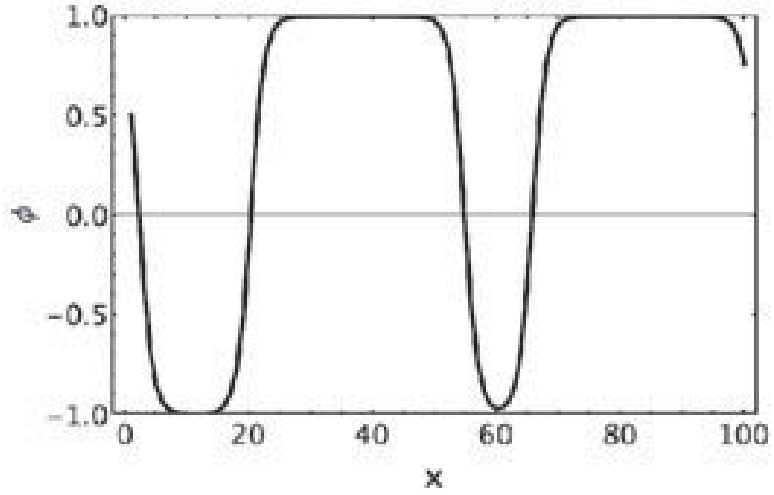
$$\left.\begin{array}{l} 1.\ \phi_i, \dfrac{d\phi_i}{dx} \Rightarrow F\left[\phi_i, \dfrac{d\phi_i}{dx}\right] \\ 2.\ \phi_i, \dfrac{d^2\phi_i}{dx^2} \Rightarrow \dfrac{\partial \phi_i}{\partial t} \end{array}\right\} \Longrightarrow \phi_i(t+\delta t) = \phi_i(t) + \frac{\partial \phi_i}{\partial t}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

- 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** $\Leftrightarrow d\phi_i/dt \approx 0$

$\alpha/U = 1, U = 1$

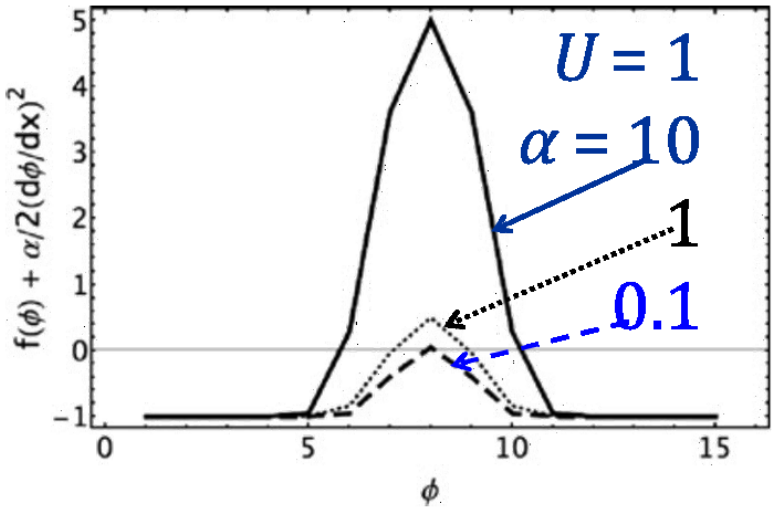


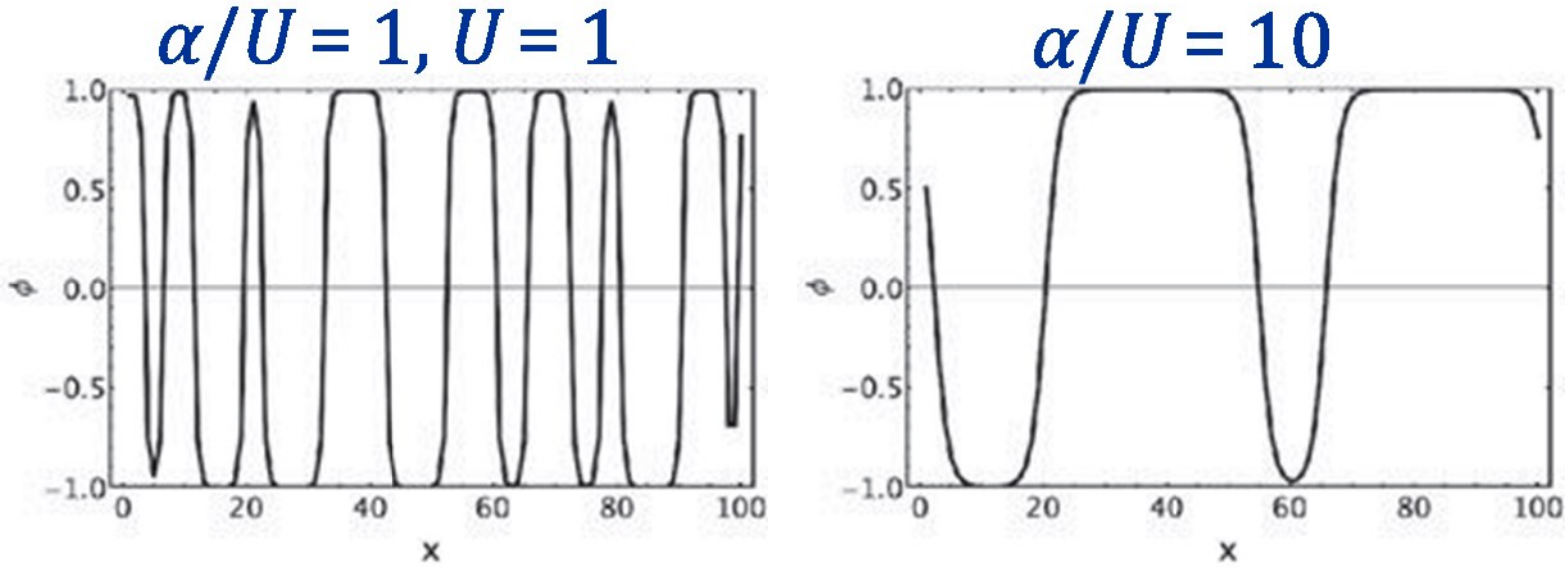
$\alpha/U = 10$



2.3 Example (5): discussion

- **Influence of interface energy?**





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

- **Equilibrium: no interfaces to minimize the interface energy**

2.4 Example: analytical solution (for simple interface model)

- Condition for minimum total energy (equilibrium)

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

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

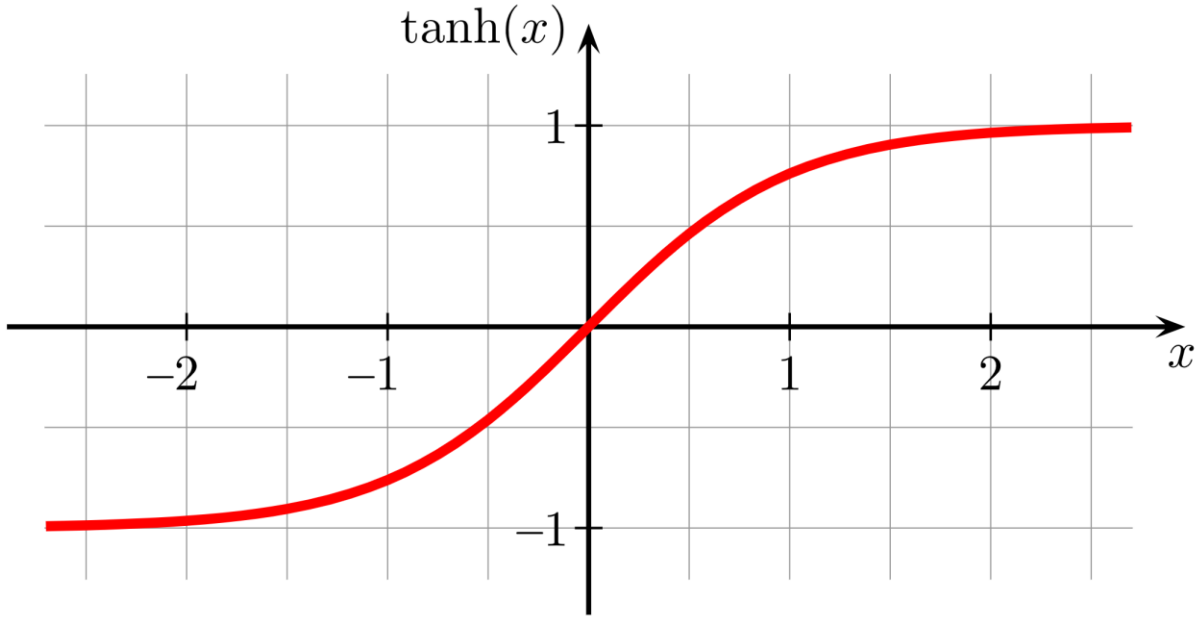
- Free energy per unit area $\frac{F}{A} = \int_x \left[4U\left(-\frac{1}{2}\phi^2 + \frac{1}{4}\phi^4\right) + \frac{\alpha}{2}\left(\frac{\partial\phi}{\partial x}\right)^2\right]dx$

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

2.4 Example: analytical solution for equilibrium interface

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

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



- Minimum interface energy?

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

- Interface width?

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

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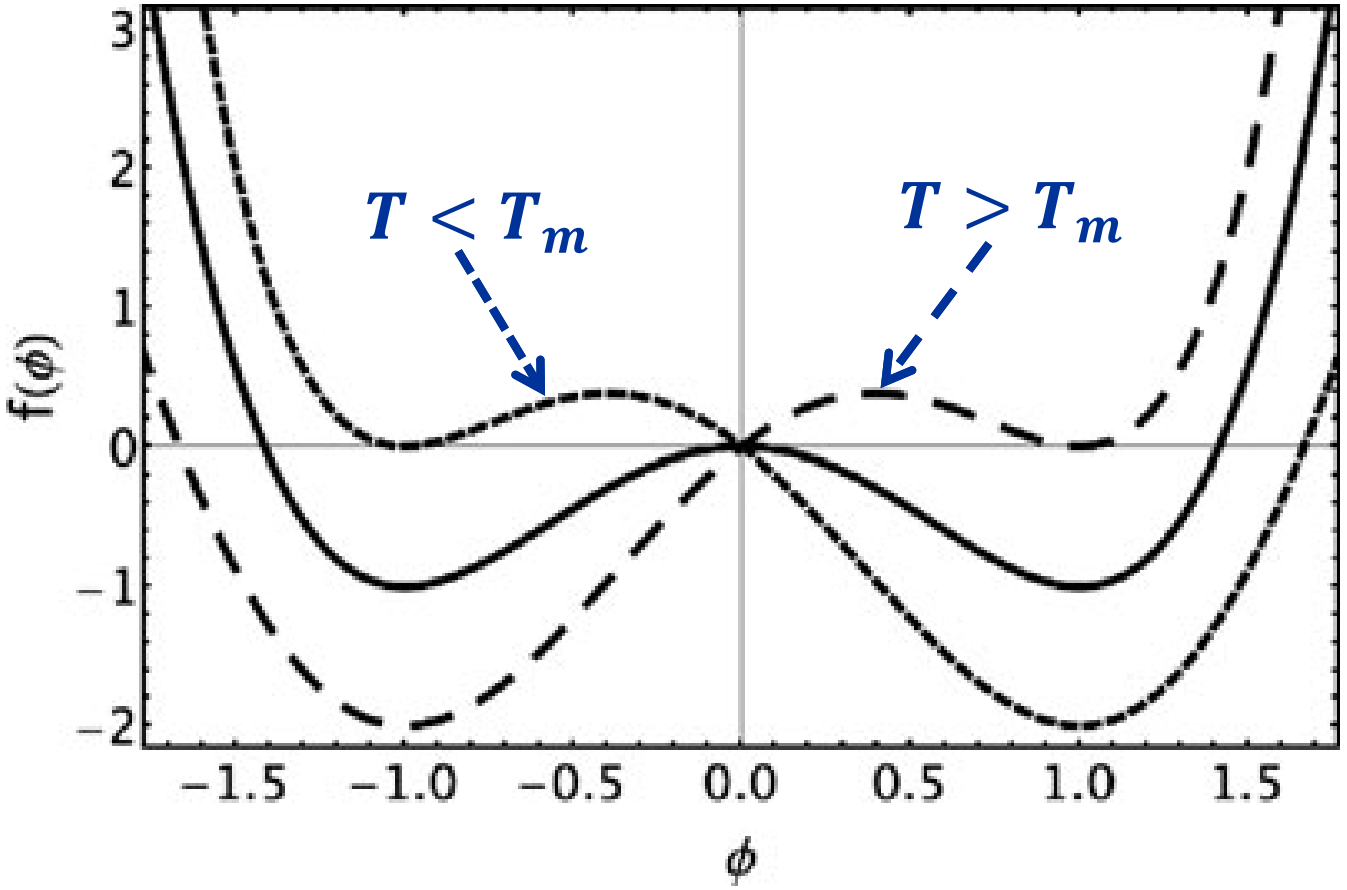
3.1 phase preference

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



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

3.2 multi-phase system (1)

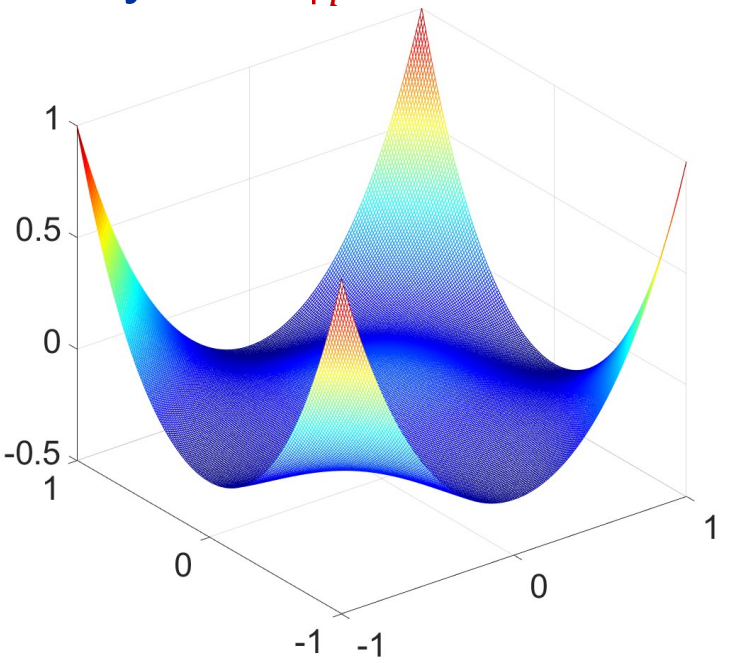
- Example: grain growth--many “phases” with same composition, each phase (ϕ_i) represents a grain with a different orientation.
- Free energy
  - arbitrary # of order parameters for different orientations
  - Distinct minima, each has only one ϕ_i is non-zero.

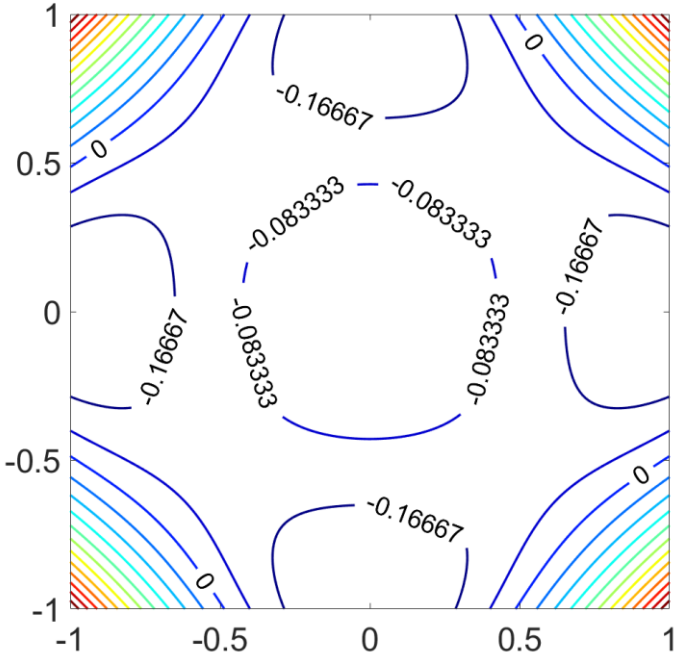
$$f[\{\phi_i\}] = -\frac{\gamma}{2}\sum_{i=1}^{P}\phi_i^2 + \frac{\beta}{4}\left(\sum_{i=1}^{P}\phi_i^2\right)^2$$

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

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

other options?

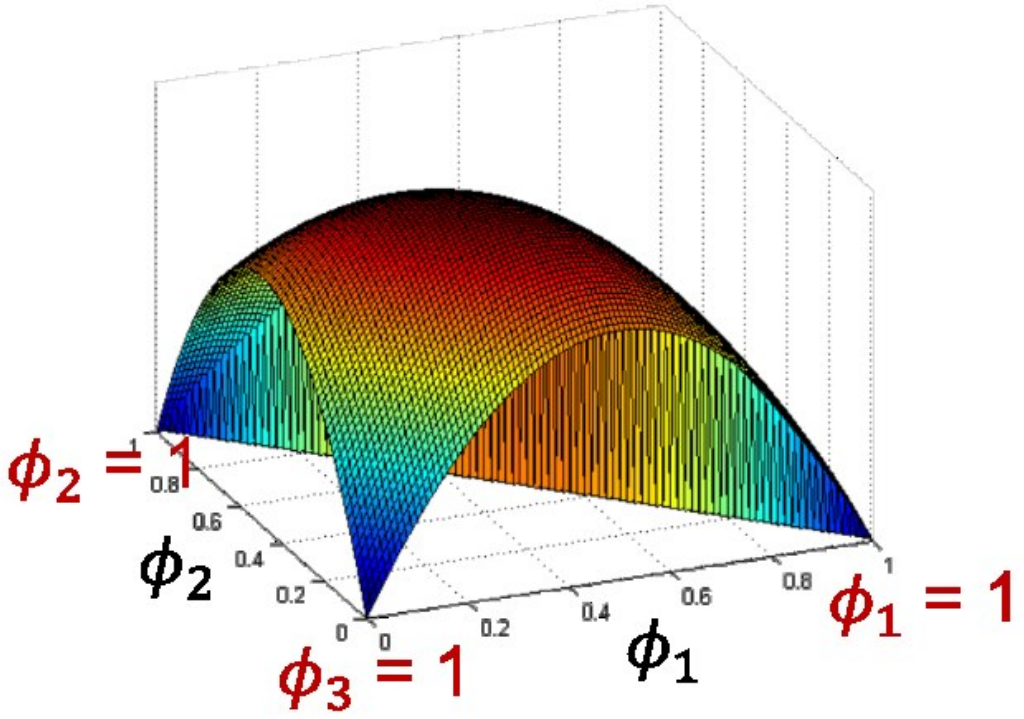




3.2 multi-phase system (2)

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

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



3.3 Current state of Phase Field Modeling

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

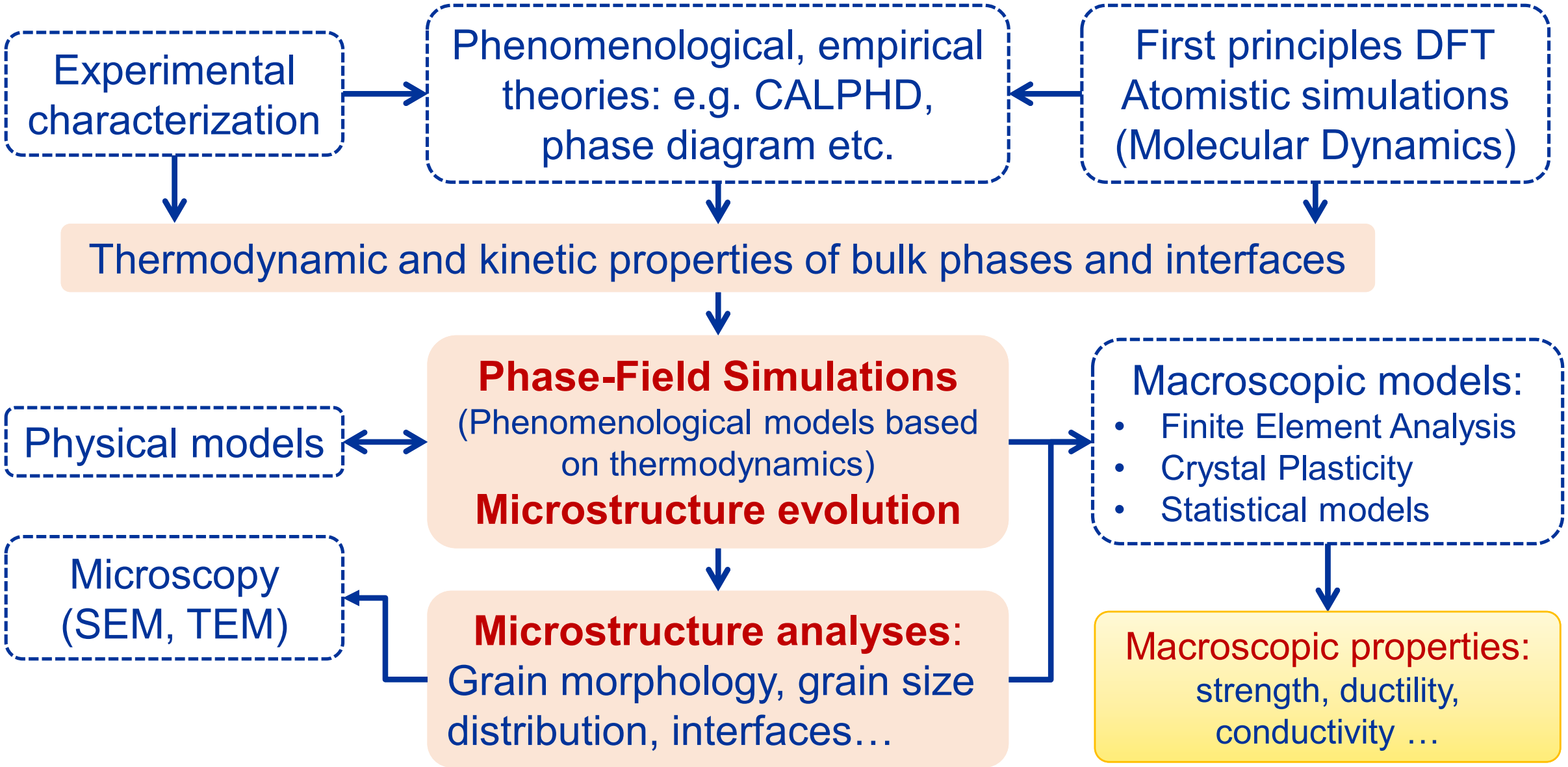
- Current topics
  - Realistic, complex, multi component systems

    More realistic description of free energy
  - **Quantitative aspects**

3.4 Quantitative PFM (1)

- 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)



3.5 Parameter assessment

- 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

Summary for PFM

- **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

Homework

1. Derive the Allen-Cahn equation.
2. For a one dimensional interface with given parabolic chemical energy density, i.e., the free energy density is given by

$$f[\phi(x,t)] = f_0\phi(1-\phi) + \frac{\alpha}{2}|\nabla\phi|^2,$$

   1) Numerically solve the equilibrium interface structure, e.g., the thickness and the energy of the equilibrium interface.
   2) Compare with analytical solution if existed.

- Due: Jan 5, 2022

Next Week:

Hands-On Phase Filed Method

Appendix: functional, variation

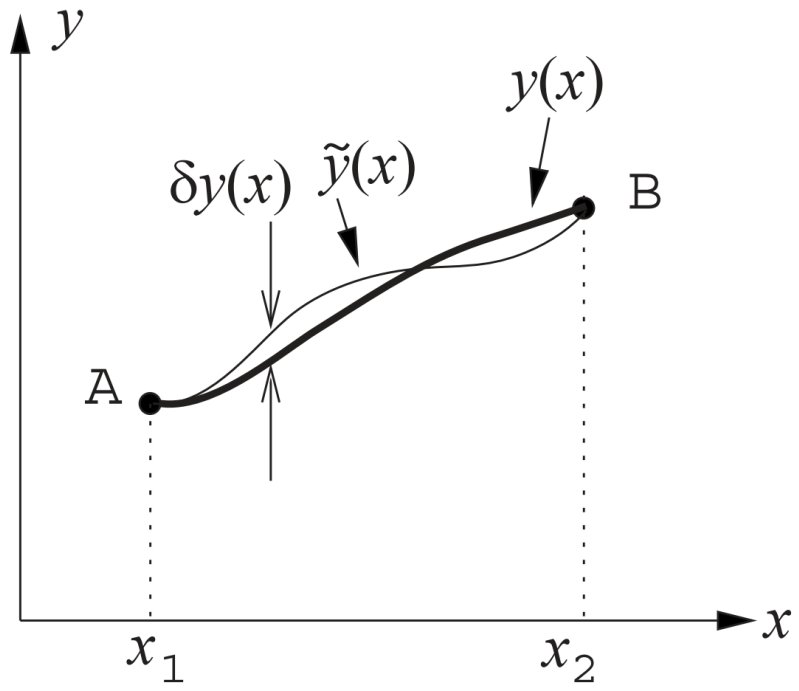
- Functional: functions of a function. i.e.

$$I[y(x)] = \int_{x1}^{x2} F[x, y(x), y'(x)]dx, \quad y'(x) \equiv dy(x)/dx$$

- Variation: small change in $y(x)$ → variation of the functional

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

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



Appendix: calculus of variations

- 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

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

Appendix: calculus of variations

- 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:

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

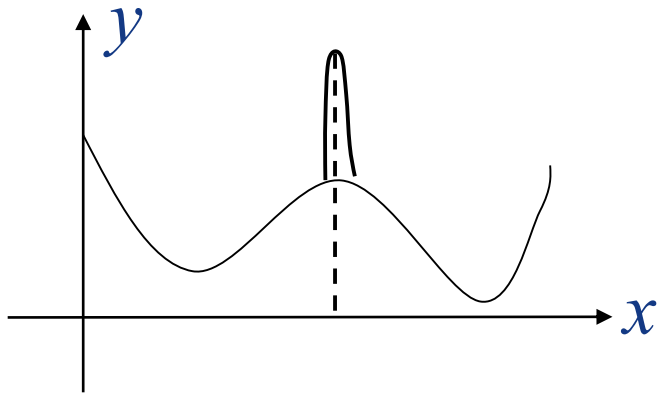
- If constrain $y(x_1), y(x_2)$ to be constant, then

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

Appendix: variational (functional) derivative

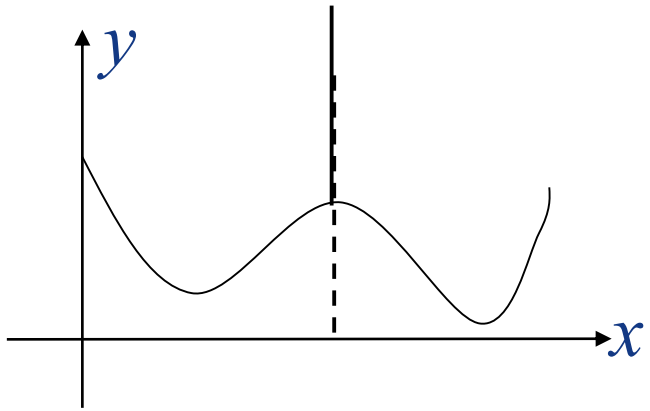
$$I[y(x)] = \int_{x1}^{x2} F[x, y(x), y'(x)]dx$$

$$\delta I = \int_{x1}^{x2} g(x)\delta y(x)dx \Rightarrow \frac{\delta I}{\delta y(x)} = g(x)$$



$$\lim_{\epsilon \to 0} \frac{\text{variation of the functional } \delta I}{[\text{change in function } \cdot \text{ variantion region width}]}$$

- Impossible to change only one $y(x_i)$ without change neighboring $y(x_i \pm dx)$ due to continuity



- Variations: local change in function $\boldsymbol{\delta y(x)}$
  - ➔ variation in total energy

局部区域函数值的变化对泛函值的影响的大小