

# Phase-field method: basics and application in materials science

## 1 Introduction

The key task in materials science is to understand the processing-microstructure-property relation, where microstructure bridges processing and property. Experimental studies of materials can detect uncorrelated information about processing, microstructure and property. For example, in tensile test of steels, one can set different strain-rates and temperatures, observe microstructures at different deformation stages, get different stress-strain curves. However, we can hardly have in-situ visualization of microstructure evolution (e.g. phase morphology change and dislocation motion) due to current technical limit. Besides, how can we correlate different strain-rates, temperature, dislocation densities and stresses... to reveal the mechanism behind? Such demands in materials science trigger the power of materials modelling and simulation.

Phase-field is a simulation method which has been widely used for liquid-solid phase transition, solid-solid phase transition, dislocation evolution, etc. This practical is designed to provide elementary experience on phase-field method. we will learn the basic equations of phase-field (which are a set of partial differential equations) in section 2, solve partial differential equations by finite volume method in section 3 and try some phase-field applications in section 4.

## 2 Phase-field model

Although phase-field model may be presented in different forms for different applications, they are all based on a common set of fundamentals: representation of microstructure, the thermodynamic and kinetic equations for governing microstructure evolution.

### 2.1 Microstructure description

In a phase-field model, a microstructure is described using one or more variables called *order parameters*. Literally and historically, an order parameter is a measure of the degree of order across the boundaries in a phase transition system. However, it is an ambiguous concept because it is not always straight forward to tell what can be counted as degree of order and what cannot be. Since phase-field has been extending to more and more applications, we can understand an order parameter in phase-field in the following way: a field variable which changes its value across the boundaries. For example, for a phase-A/phase-B transition, we can describe the microstructure as:  $\eta = 0$  stands for phase-A,  $\eta = 1$  for phase-B, and  $0 < \eta < 1$  across the phase-A/phase-B interface<sup>1</sup>, as shown in Fig.1. It does not necessary to be phase transition, although it is called *phase-field*. It can be grain-A/grain-B in the same phase, the order parameter represents crystalline orientation in this case. We can also use phase-field for dislocation loop motion:  $\eta = 0$  stands for slipped region inside the loop,  $\eta = 1$  for outside the loop, and  $0 < \eta < 1$  for dislocation line.

It is import to distinguish the conservativeness of order parameters, for the reason we

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<sup>1</sup> $\eta$  is actually a field variable  $\eta(\vec{r}, t)$ , where  $\vec{r}$  is the space and  $t$  is the time. For simplicity,  $(\vec{r}, t)$  is often ignored in many literatures.

will see in section 2.3. In other words, order parameters can be either conserved or non-conserved depends on if the total amount of  $\eta$  changes with time. Order parameter in phase-field model for pure material solidification is an example of non-conserved order parameter, because all liquid phase ( $\eta = 0$ ) can be transited to solid phase ( $\eta = 1$ ). Spinodal decomposition, meaning a parent phase simultaneously separates into two daughter phases with different compositions but the same crystal structure, is an example of conserved order parameter. Because in this case order parameters are the local composition of elements, and the global composition (total composition) of any element should be the same at any time.

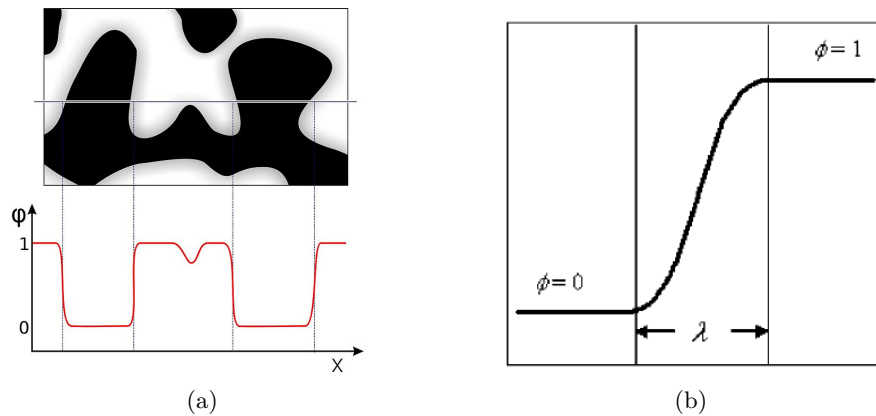


Figure 1: (a) a two phase microstructure and its phase-field model representation by the field  $\phi$ ; (b) a qualitative plot of interface with a thickness roughly  $\lambda$ .

## 2.2 Thermodynamics

It seems  $0 \leq \eta \leq 1$  can represent many different physical systems, how to tell which system it represents? The answer is in the thermodynamic formulation. The key formulation idea of phase-field is, first constructing the total energy of the system (thermodynamics), then evolving the system by minimizing the total energy (kinetics). Different total energy formulations or even the same formulation with different coefficients represent different systems. A general formula of the total free energy<sup>2</sup> can be written as

$$F = F_{bulk} + F_{grad} + F_{elas} + F_{plas} + F_{surf} + \dots \quad (1)$$

where

$$F_{bulk} = \int \left( f_{bulk}(c_1, \dots, c_p, \phi_1, \dots, \phi_q) \right) d\vec{r}$$

$$F_{grad} = \int (f_{grad}) d^3r = \int \left( \sum_{i=1}^3 \sum_{j=1}^3 \sum_{k=1}^p \frac{K_{c_{ij}}}{2} \nabla_i c_k \nabla_j c_k + \sum_{i=1}^3 \sum_{j=1}^3 \sum_{k=1}^q \frac{K_{\phi_{ij}}}{2} \nabla_i \phi_k \nabla_j \phi_k \right) d\vec{r}$$

<sup>2</sup>Strictly speaking, Gibbs energy (more common in chemistry) should be used in the case of constant temperature and pressure, while Helmholtz energy (more common in physics) in the case of constant temperature and volume. In most phase-field models, however, pressure and volume are assumed to be constant. Under this assumption, the Gibbs energy and Helmholtz energy are the same. In general, the free energy symbol  $F$  is used in phase-field models. It is not always stated clearly whether it refers to Gibbs or Helmholtz energy, also not important.

in which  $c$  is conserved field,  $\phi$  is non-conserved field,  $F_{bulk}$  is bulk free energy,  $F_{grad}$  is gradient energy.  $K_c$  and  $K_\phi$  are the gradient energy coefficients. Mathematically  $F$  is called *functional* which means a function of functions, because  $f_{bulk}$  is a function of  $c$  and  $\phi$ ,  $f_{grad}$  is function of  $\nabla c$  and  $\nabla \phi$ , while  $F$  is function of  $f_{bulk}$  and  $f_{grad}$ . We only give expressions of  $F_{bulk}$  and  $F_{grad}$  because all phase-field models have these two parts. We do not give expressions of other energy terms. Because on one hand, their presence depends on specific problem. On the other hand, their formulas differ case by case. We therefore will emphasize  $F_{bulk}$  and  $F_{grad}$  in detail, while just provide simple examples to other energy terms.

### 2.2.1 The bulk free energy density

Bulk free energy, as the name implies, is the free energy of homogeneous "bulk" materials. There are two common ways to construct the bulk free energy density formulation. One way is to directly use the formulation from thermodynamic models. Another way is to use phenomenological Landau energy. In this practical, for simplicity, we always use the phenomenological Landau energy and assume constant temperature and pressure. Taking the example of a two-phase system, the Landau free energy density can be constructed as:

$$f_{bulk} = f_0 c^2 (1 - c)^2 \quad \text{or} \quad f_{bulk} = f_0 \phi^2 (1 - \phi)^2 \quad (2)$$

where  $f_0$  is an energy density coefficient currently unknown. From calculation of phase diagrams, we can get the plot of bulk energy density for a specific system, as illustrated in Fig.2.  $c = 0 (\phi = 0)$  means the free energy density of purely one phase,  $c = 1 (\phi = 1)$  means the free energy density of purely the other phase. It is impossible, also not important, to know the absolute value of free energy, what is important is the relative free energy density. Because it tells us what is relatively energetically-favorable. In Fig.2 the free energy density is given with respect to pure phase, so  $f_{bulk} = 0$  for pure phases, and the energetically-favorable situation is therefore coexistence of two phases. However, coexistence of two phases appears in many materials, what distinguishes them? It is the  $\Delta f$ . Different systems have different  $\Delta f$  values. By fitting  $f_0$  according to  $\Delta f$ , the bulk energy density is therefore constructed for a specific system.

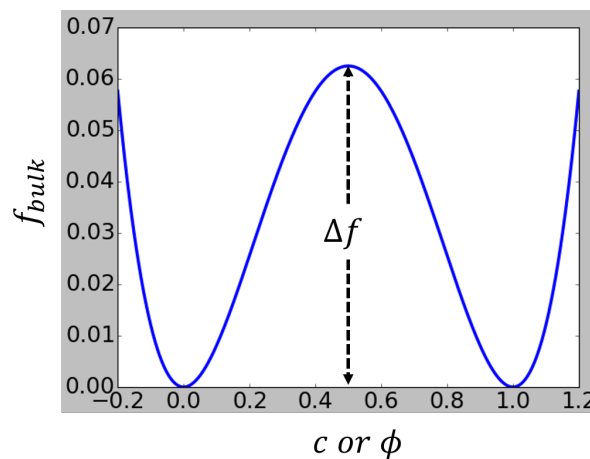


Figure 2: Bulk energy density of a two-phase system

### 2.2.2 The gradient energy density

As can be seen in Fig.1, real microstructure is not homogenous, there are inhomogeneous regions between pure phases, which are actually interfaces. It is easy to imagine the interfaces in real materials are as sharp as a few atom layers. However, in phase-field the interface is diffusive and the thickness is much wider than a few atom layers, which seems to be intuitively unphysical. It turns out that on one hand the diffusive interface is a numeric advantage. Because if it is a sharp interface (numerically a line), we have to always trace the line in order to know where the interface is. On the other hand we can still make it a physical system as long as we construct the interface energy correctly. In the interface region  $0 < c(\text{or } \phi) < 1$ , we will have some bulk energy according to Fig.2. However, if comparing that bulk energy with experimental interface energy, we will find there is still some part of energy missing. But what is missing? The interface region is inhomogeneous, it is natural to think about the energy increment due to inhomogeneity. The mathematical language for "inhomogeneity" could be "the presence of gradient". Therefore, to compensate the interface energy, a gradient energy is introduced into phase-field.

Isotropic gradient energy density of a two-phase system can be expressed as :

$$f_{grad} = \frac{K_c}{2} |\nabla c|^2 \quad \text{or} \quad f_{grad} = \frac{K_\phi}{2} |\nabla \phi|^2 \quad (3)$$

Putting bulk energy and gradient energy together gives the interface energy:

$$f_{inte} = f_0 c^2 (1 - c)^2 + \frac{K_c}{2} |\nabla c|^2 \quad \text{or} \quad f_{inte} = f_0 \phi^2 (1 - \phi)^2 + \frac{K_\phi}{2} |\nabla \phi|^2 \quad (4)$$

We have to first search for interface energy determined by experiments or lower level calculation. After that, find a proper value for  $K_c$  or  $K_\phi$  by trial and error. The correct  $K_c$  or  $K_\phi$  should not only let numeric interface energy roughly agree with experimental interface energy, but also keep a proper interface thickness and numerics stable.

### 2.2.3 Other energy terms

As mentioned, the presence and formula of other energy terms differ case by case. We just give elastic energy density as an example:

$$f_{elas} = \frac{1}{2} C_{ijkl} \epsilon_{ij}^{el} \epsilon_{kl}^{el} \quad (5)$$

where  $\sigma_{ij}^{el}$  is the elastic stress and  $\epsilon_{ij}^{el}$  is the elastic strain.

## 2.3 Kinetics

In all phase-field models, the temporal and spatial evolution of the field variables follows the same set of kinetic equations<sup>3</sup>. All conserved fields,  $c_p$ , evolve with time according to the Cahn-Hilliard equation, whereas the non-conserved fields,  $\phi_q$ , are governed by the Allen-Cahn equation.

$$\begin{aligned} \frac{\partial c_p}{\partial t} &= \nabla_i \left( M_{pqij} \nabla_j \frac{\delta F}{\delta c_q} \right) \\ \frac{\partial \phi_p}{\partial t} &= -L_{pq} \frac{\delta F}{\delta \phi_q} \end{aligned} \quad (6)$$

<sup>3</sup>In the present subsection 2.3, we use subscripts "q" and "p" refer to different  $c$  and  $\phi$ , while subscripts "i" and "j" refer to coefficient anisotropy of a specific  $c$  and  $\phi$ .

where  $M_{pqij}$  and  $L_{pq}$  are interface mobility coefficients. For simplicity, we only consider homogeneous and isotropic coefficients in this practical. Eq.6 is reduced to:

$$\begin{aligned}\frac{\partial c_p}{\partial t} &= M \nabla^2 \frac{\delta F}{\delta c_p} \\ \frac{\partial \phi_p}{\partial t} &= -L \frac{\delta F}{\delta \phi_p}\end{aligned}\tag{7}$$

$\frac{\delta F}{\delta \phi}$  (the same for  $\frac{\delta F}{\delta c}$ ) is called *functional derivative* which relates the change of  $\phi$  to the change of  $F$ .  $\frac{\delta F}{\delta \phi} = 0$ , which means at the same time  $\frac{\partial \phi}{\partial t} = 0$ , gives a local minimum of  $F$ <sup>4</sup>. In other word, the microstructure stop evolving when the total energy is at local minimum. The expression of  $\frac{\delta F}{\delta \phi}$  is given as:

$$\begin{aligned}F &= \int f(\vec{r}, \phi, \nabla \phi) d\vec{r} \\ \frac{\delta F}{\delta \phi} &= \frac{\partial f}{\partial \phi} - \nabla \cdot \frac{\partial f}{\partial (\nabla \phi)}\end{aligned}\tag{8}$$

<sup>4</sup>Actually the first variation  $\delta F = 0$  is only the necessary condition for a local minimum, the sufficient condition requires the second variation  $\delta^2 F$  is strongly positive. However, having an analytical proof of whether the second variation  $\delta^2 F$  is strongly positive is vary complicated. Instead, an easier way is to just trace  $F$  during running the simulation. It is possible to get a local maximum in simulations if the coefficients are not selected properly. In this case, we have to reconsider the coefficients.

### 3 Finite volume method

Finite volume method is a method for representing and solving partial differential equations. 'Finite volume(control volume)' refers to the small volume surrounding each node at the center of a grid. Schematic plot of a control volume is shown in Fig.3. The whole domain is discretized into many control volumes. Finite volume method solves partial differential equations in the integral form. Because of this, divergence terms can be converted to surface integrals which are fluxes through the surfaces of each control volume. If fluxes at interior control volumes are conservative, the total flux evolution of the whole domain is actually determined by boundary flux.

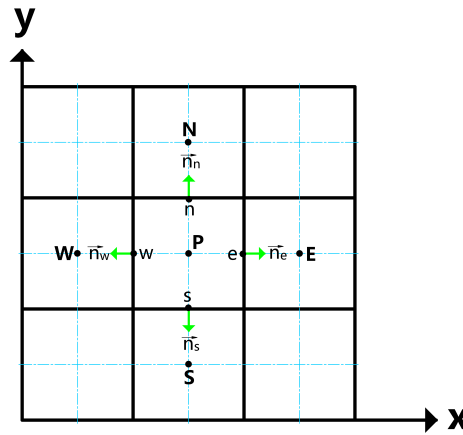


Figure 3: Schematic plot of a 2D mesh. "P,E,W,N,S" are control volume centers, "e(east),w(west),n(north),s(south)" indicate orientation surrounding "P". " $\vec{n}$ " stands for normal vector.

In the rest of this section, we will study a general partial differential equation to see how exactly finite volume method works. The physical meaning of this equation will be explained firstly, followed by discretization of each term. After that, we will solve the system of linear equations and evaluate the solution.

#### 3.1 General conservation equation

A general conservation equation is expressed as

$$\underbrace{\frac{\partial(\rho\phi)}{\partial t}}_{\text{transient}} = - \underbrace{\nabla \cdot (\vec{u}\phi)}_{\text{convection}} + \underbrace{\left( \nabla \cdot (\Gamma \nabla) \right)^m}_{\text{diffusion}} \phi + \underbrace{S}_{\text{source(sink)}} \quad (9)$$

where the variable  $\phi$  represents the unknown quantity in the equation.  $\rho$ ,  $m$ ,  $\vec{u}$  and  $\Gamma$  are coefficients. These coefficients can be arbitrary functions of any parameters or variables in the system. The equation tells that three reasons cause the evolution of  $\phi$ : convection, diffusion and source(sink). Convection means bulk-flow of  $\phi$  driven by external force, while diffusion means inter-flow due to gradient of  $\phi$  itself. Neither convection nor diffusion generates(disappears)  $\phi$ , they only transport it. However, Source(sink) means immediate generation(disappear) of  $\phi$ . Imagine a boy farts in an isolated classroom, so he is a source

of odor. Then other people smell it because of diffusion. Unfortunately, other people are actually sinks. Finally, a girl cannot stand it so opens windows and winds transport it out, which is convection.

### 3.2 Discretization

We first write the Eq.9 in the integral form as (we set  $m = 1$  for simplicity)

$$\int_V \frac{\partial(\rho\phi)}{\partial t} dV = \int_V -\nabla \cdot (\vec{u}\phi) dV + \int_V \nabla \cdot (\Gamma \nabla \phi) dV + \int_V S dV \quad (10)$$

For transient term, we always discretize as

$$\int_V \frac{\partial(\rho\phi)}{\partial t} dV \simeq \frac{(\rho\phi_P - \rho\phi_P^{\text{old}})\Delta V}{\Delta t} \quad (11)$$

where  $\Delta V$  is the volume of control volume,  $\Delta t$  is the time interval.  $\phi_P$  is the  $\phi$  value of present control volume.

For convection term, the discretization is given by

$$\begin{aligned} -\int_V \nabla \cdot (\vec{u}\phi) dV &= -\int_A (\vec{u}\phi) \cdot \vec{n} dA \quad (\text{Divergence theorem}) \\ &\simeq -\sum_g \phi_g (\vec{u} \cdot \vec{n}_g) A_g \end{aligned} \quad (12)$$

where  $g$  means boundaries of control volume (could be  $e$ ,  $w$ ,  $n$  or  $s$ ).  $\vec{n}_g$  is the outer normal vector of each boundary.  $\phi_g$  is  $\phi$  value at each boundary center.  $A_g$  is the area of each boundary.

For diffusion term, we constantly discretize as

$$\begin{aligned} \int_V \nabla \cdot (\Gamma \nabla \phi) dV &= \int_A \Gamma (\nabla \phi \cdot \vec{n}) dA \\ &\simeq \sum_g \Gamma ((\nabla \phi)_g \cdot \vec{n}_g) A_g \end{aligned} \quad (13)$$

For source(sink) term, we discretize as

$$\int_V S dV \simeq S \Delta V = (S_0 + S_1 \phi_P) \Delta V \quad (14)$$

where we decompose  $S$  to  $(S_0 + S_1 \phi_P)$  for stability concern.  $S_0$  is independent of  $\phi$  while  $S_1$  may depend on  $\phi$ .

After discretization, Eq.(9) becomes a system of linear equations as

$$\frac{(\rho\phi_P - \rho\phi_P^{\text{old}})\Delta V}{\Delta t} = -\sum_g \phi_g (\vec{u} \cdot \vec{n}_g) A_g + \sum_g \Gamma ((\nabla \phi)_g \cdot \vec{n}_g) A_g + (S_0 + S_1 \phi_P) \Delta V \quad (15)$$

### 3.3 Approximation

As can be seen in Eq.(15), unknowns are  $\phi_P$ ,  $\phi_g$  and  $(\nabla \phi)_g$ . However, we only want to get  $\phi_P$  (values at control volume center). Besides, it is impossible to solve the system with too many unknowns. So, we approximate  $\phi_g$  and  $(\nabla \phi)_g$  using  $\phi$  values at control volume center.  $\phi_g$  can be approximated as

$$\phi_g = \alpha_g \phi_P + (1 - \alpha_g) \phi_G \quad (16)$$

where  $\alpha_g$  is weighting factor determined by the interpolation scheme (see appendix A).  $\phi_G$  (could be  $\phi_E$ ,  $\phi_W$ ,  $\phi_N$  or  $\phi_S$ ) is the  $\phi$  value at adjacent control volume center of boundary  $g$ . For example, if  $g$  is  $e$ , then  $\phi_G$  is  $\phi_E$ .  $((\nabla\phi)_g \cdot \vec{n}_g)$  can be approximate as

$$((\nabla\phi)_g \cdot \vec{n}_g) \simeq \frac{\phi_G - \phi_P}{d_{GP}} \quad (17)$$

After the approximation of both  $\phi_g$  and  $((\nabla\phi)_g \cdot \vec{n}_g)$ , we can further derive Eq.(15) as

$$\begin{aligned} \frac{(\rho\phi_P - \rho\phi_P^{\text{old}})\Delta V}{\Delta t} = & - \sum_g (\vec{n}_g \cdot \vec{u}) [\alpha_g \phi_P + (1 - \alpha_g) \phi_G] A_g \\ & + \sum_g \Gamma \frac{(\phi_G - \phi_P)}{d_{GP}} A_g \\ & + (S_0 + S_1 \phi_P) \Delta V \end{aligned} \quad (18)$$

As shown in Eq.(18), now the only unknowns are  $\phi_G$  (values at control volume centers). For conveniency, We rearrange Eq.(18) as

$$a_P \phi_P = \sum_g a_G \phi_G + b_P \quad (19)$$

where

$$\begin{aligned} a_P &= \frac{\rho\Delta V}{\Delta t} + \sum_g (a_A + C_g) - \Delta V S_1 \\ a_G &= D_g - (1 - \alpha_g) C_g \\ b_P &= \Delta V S_0 + \frac{\rho\Delta V \phi_P^{\text{old}}}{\Delta t} \end{aligned}$$

### 3.4 Boundary condition

The "boundary" here does not mean the boundary of each control volume, but the boundary of whole domain. In a 1D case with  $I$  control volumes ( $CV_0, \dots, CV_{I-1}$ ), we will have  $I$  linear equations as Eq.(19) and  $I + 2$  unknowns ( $\phi_{-1}, \phi_0, \dots, \phi_{I-1}, \phi_I$ ). To solve this linear equation system, we have to prescribe  $\phi_{-1}$  and  $\phi_I$  which are  $\phi$  values of virtual control volumes. Once the  $\phi_g$  or  $((\nabla\phi)_g \cdot \vec{n}_g)$  or both are prescribed at boundaries of the whole domain,  $\phi_{-1}$  and  $\phi_I$  can be derived from Eq.16 and 17. This is why we need boundary condition. Then we substitute  $\phi_{-1}$  and  $\phi_I$  into Eq.(19) and solve linear equation. In this way of inserting boundary conditions, the structure of Eq.(19) can be maintained. If  $V$  is the domain on which the given equation is to be solved and  $\partial V$  denotes its boundary, the general form for boundary condition is:

$$a\phi_g + b\nabla\phi_g \cdot \vec{n} = \text{constant} \quad \text{on } \partial V \quad (20)$$

where  $a, b$  are coefficients. Some specific boundaries can be derived from Eq.(20). If  $a = 0$  and  $b \neq 0$ , it is Neumann boundary condition. If  $b = 0$  and  $a \neq 0$ , it is Dirichlet boundary condition. If  $a \neq 0$  and  $b \neq 0$ , it is Robin boundary condition (fixed flux boundary).



### 3.5 Assessment

We should of course let our numerical results as "good" as possible. "Good" involves many issues like accuracy, computational cost, etc. The most important ones are conservativeness, transportiveness and convergence.

Conservativeness means the flux(both advection and diffusion fluxes) leaving boundary of a controlled volume should equal the flux entering the same boundary of adjacent controlled volume.

Stability requires both boundedness and convergence. Boundedness states that in the absence of sources(sinks), finally the internal values should be bounded by its boundary values, as shown in Eq.(21). Imagine a conductive bar isolated from surrounding and with boundary temperatures of  $100K$  and  $1000K$ . We can easily find it unrealistic that the temperature inside is below  $100K$  or over  $1000K$ . However, boundedness does not necessarily mean convergence. For example,  $\sin(\theta)$  is bounded between  $-1$  and  $1$  but not convergent. To overcome the oscillation, another rule should be satisfied, which is, all coefficients of  $\phi$  in the Eq.(19) should have the same sign (usually all positive). Physically this implies that an increase(decrease) of  $\phi$  value at one control volume should result in an increase(decrease) at neighbouring control volume.

$$\frac{\sum |a_G|}{|a_P|} \begin{cases} \leq 1 & \text{for all controlled volumes} \\ < 1 & \text{for one controlled volume at least} \end{cases} \quad (21)$$

Transportiveness is described quantitatively by Peclet number in Eq.(29) and qualitatively by Fig.4. If it is a pure diffusion, the contribution from  $W$  to  $P$  and  $E$  to  $P$  are the same(Fig.4(a)). In the convection-diffusion case(Fig.4(b)),  $W$  contributes to  $P$  by convection and diffusion, while  $E$  contributes to  $P$  only by diffusion. However, if the convection is strong enough, diffusion must be neglected. Taking the previous fart example, if windows are open, students near upwind windows cannot smell it. Because the convection of wind is much stronger than the diffusion of fart. Our schemes should also reflect these physical realities.

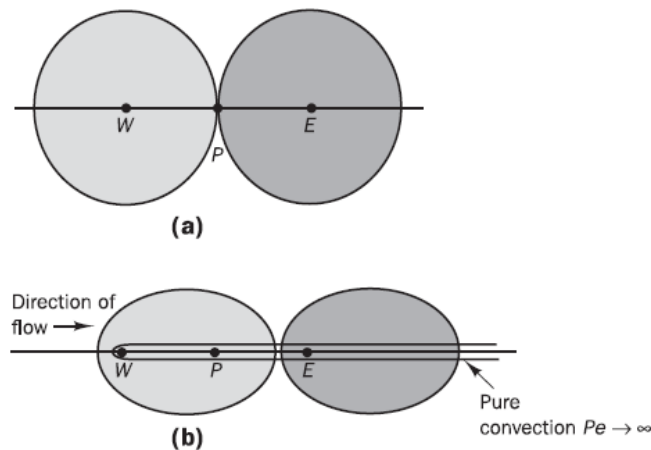


Figure 4: Distribution of  $\phi$  at different Peclet numbers: (a) pure convection,  $Pe \rightarrow 0$ ; (b) diffusion and convection

### 3.6 Explicit and implicit

Explicit scheme calculates the state of a system at a later time from the state of the system at the current time, while implicit scheme finds a solution by solving an equation involving both the current state of the system and the later one. Eq.(19) is actually the implicit form. If we add superscript "old" to  $\phi_G$  in Eq.(19)(and above derivations accordingly of course), it will change to explicit scheme. For implicit scheme, we can set any space and time intervals without caring about stability, but the computational cost is expensive. For explicit scheme, space and time intervals are constrained by some relations in order to maintain stability, but the computational cost is small.

## 4 Fipy

FiPy(finite volume python package) is an object oriented, partial differential equation solver, written in Python, based on a standard finite volume method. Below is an example showing implementation of a general partial differential equation.

$$\frac{\partial(\rho\phi)}{\partial t} = -\nabla \cdot (\vec{u}\phi) + \nabla \cdot (\Gamma\nabla)\phi + a\phi^2 + b\phi + c \quad (22)$$

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```

from fipy import *

#mesh
dx = 0.1
Lx = 10.
nx = 100
nx = int(Lx/dx)
mesh = Grid1D(dx=dx, nx=nx)
x = mesh.cellCenters[0]

#field variable
phi = CellVariable(mesh=mesh, hasOld=1)

#initial condition
phi0 = GaussianNoiseVariable(mesh=mesh, mean=0.0, variance=1.0, hasOld=0)
phi.setValue(value = phi0.value)

#boundary condtion
phi.faceValue.constrain(value=0., where=mesh.facesLeft)
phi.faceGrad.constrain(value=1., where=mesh.facesRight)

#equation coefficients
rho = 1. ; u = (20.,) ; Gamma = 5. ; a = 1. ; b = 1. ; c = 1.

#equation
s0 = c
s1 = a * phi + b
eq = TransientTerm(coeff=rho) == - ConvectionTerm(coeff=u) \
    + DiffusionTerm(coeff=Gamma) \
    + ImplicitSourceTerm(coeff=s1) \
    + s0

#viewer
viewer = Viewer(phi)

#solver
dt = 1.e-2
steps = 100
for step in range(steps):
    phi.updateOld()
    res = 1.e5
    while res > 1.e-3:
        res = eq.sweep(var=phi, dt=dt)
    viewer.plot()

```

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Task1: 1D single-component solidification.

1D single-component solidification can be described by one non-conserved order parameter, where  $\phi = 0$  for liquid and  $\phi = 1$  for solid. The total energy functional is given as:

$$F = \int \left( f_0 \phi^2 (1 - \phi)^2 + \frac{K_\phi}{2} |\nabla \phi|^2 \right) d\vec{r}$$

and governing equation:

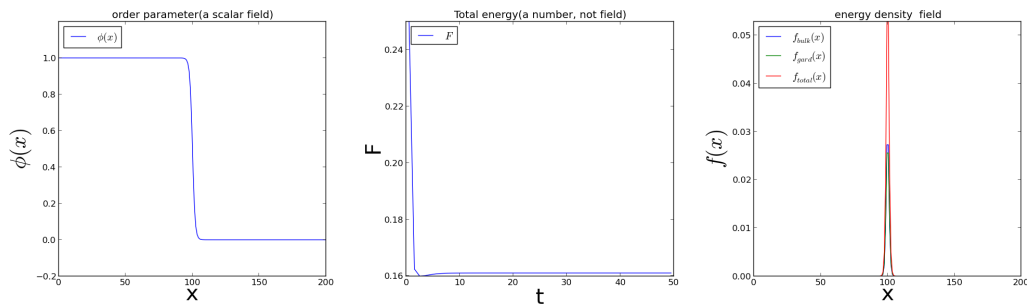
$$\frac{\partial \phi}{\partial t} = -L \frac{\delta F}{\delta \phi}$$

with dimensionless coefficients:

$$f_0 = 1., \quad K_\phi = 1., \quad L = 1., \quad dx = 1., \quad dt = 1.$$

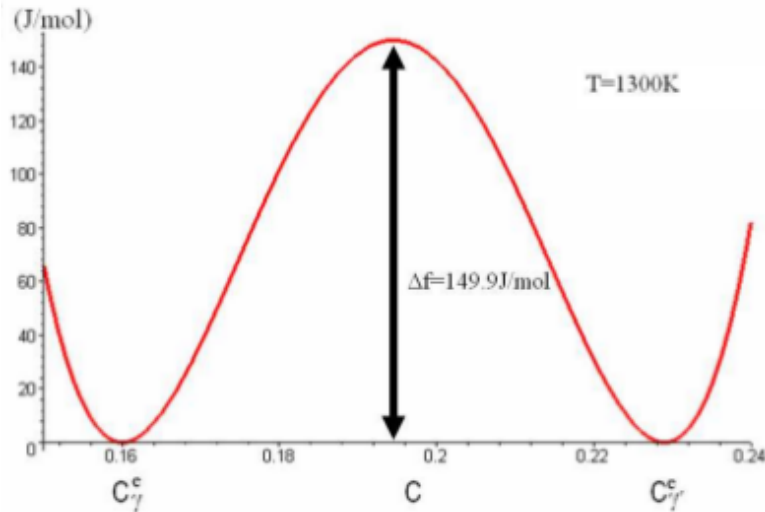
Please write down the analytical expression of  $\frac{\delta F}{\delta \phi}$ .

Keep  $dx = 1$  and  $dt = 1$ , change  $f_0$ ,  $K_\phi$ , and  $L$  one by one and see what will happen. Understanding of  $f_0$ ,  $K_\phi$ , and  $L$  helps to determine them if they are unknown in task 2 and task 3. A tip is to plot the evolution as figures below so that the influence of different  $f_0$ ,  $K_\phi$ , and  $L$  are visible. Maybe reuse the codes in Fipy tutorial or section 4.



Task 2. Determination of bulk energy density coefficient.

We consider a Ni-Al binary system with two phases:  $\gamma$  and  $\gamma'$ . The bulk energy density plot is shown in the following figure.



where  $c$  is the composition of Al element.  $c_{\gamma}^e$  and  $c_{\gamma'}^e$  are the equilibrium composition of Al in  $\gamma$  and  $\gamma'$  phase, respectively. If the bulk energy density is constructed as:

$$f_{bulk} = f_0(c_{\gamma'}^e - c)^2(c - c_{\gamma}^e)^2 \quad (23)$$

Please determine the rough value of  $f_0$ .

Task 3. Determination of gradient energy density coefficient.  
The gradient energy density therefore is:

$$f_{grad} = \frac{K_c}{2} |\nabla c|^2 \quad (24)$$

and the governing equation is:

$$\frac{\partial c}{\partial t} = M \nabla^2 \frac{\delta F}{\delta c} \quad (25)$$

If the following coefficients are given:

molar volume  $V_m = 1 \times 10^{-5} \text{ m}^3 \text{ mol}^{-1}$

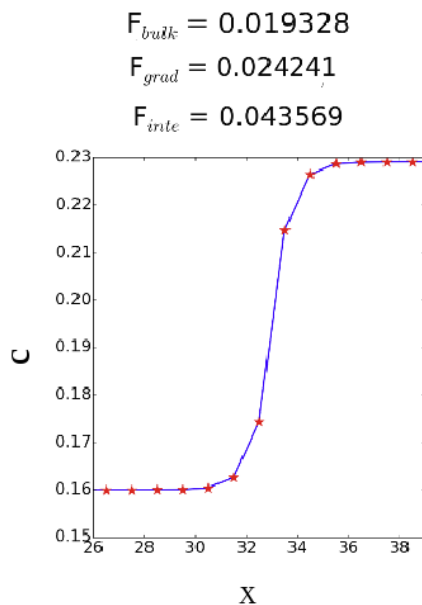
interface mobility  $M = 1 \times 10^{-17} \text{ mol}^2 \text{ J}^{-1} \text{ m}^{-1} \text{ s}^{-1}$

time scale  $dt = 1 \text{ s}$

length scale  $dx = 1 \times 10^{-8} \text{ m}$

experimental interface energy  $F_{inte} = 5 \sim 50 \times 10^{-3} \text{ Jm}^{-2}$

Please find a proper value for  $K_c$  in the range of  $1 \times 10^{-7} \sim 1 \times 10^{-5} \text{ Jm}^{-1}$  by setting up a 1D simulation. Maybe plot the interface and show the numeric interface energy and thickness in your simulation, like the following figure:



Please extend the simulation to 2D and use  $c = 0.195$  plus a gaussian noise as initial condition, and plot the 2D order parameter figure at time step  $t = 1000dt$ .

## Appendix A

The central differencing scheme,

$$\alpha_g = \frac{1}{2} \quad (26)$$

The upwind scheme,

$$\alpha_g = \begin{cases} 1 & \text{if } Pe_g > 0 \\ 0 & \text{if } Pe_g < 0 \end{cases} \quad (27)$$

The hybrid scheme,

$$\alpha_g = \begin{cases} \frac{Pe_g - 1}{Pe_g} & \text{if } Pe_g > 2 \\ \frac{1}{2} & \text{if } |Pe_g| < 2 \\ -\frac{1}{Pe_g} & \text{if } Pe_g < -2 \end{cases} \quad (28)$$

More schemes can be found in some numerical books.

$Pe_g$  is called 'Peclet number' expressed as

$$Pe_g = C_g / D_g \quad (29)$$

where  $C_g$  and  $D_g$  represent the convective strength and diffusive conductance, respectively, given by

$$C_g = A_g (\vec{u} \cdot \vec{n}_g) \quad (30)$$

$$D_g = \frac{A_g \Gamma}{d_{GP}} \quad (31)$$

where  $d_{GP}$  is the distance connecting centers of adjacent control volumes.