Numerical sessions
The Allen-Cahn-Hilliard equation in Python

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Chapter 1

2D Allen-Cahn equation in Fourier space

1.1 Free energy functional

We use the following free energy functional:

$$F = \int f(\phi) + \frac{\alpha}{2}|\nabla\phi|^2 \; dV \tag{1.1}$$

where the homogeneous free energy density is

$$f(\phi) = 16\,\Delta f\,\phi^2\;(1-\phi)^2 \tag{1.2}$$

The equilibrium profile of a one-dimensional interface is

$$\phi_{eq}(x) = \frac{1}{2}(1 + th(2x/\delta)) \tag{1.3}$$

where $\delta = \sqrt{\alpha/(2\Delta f)}$ is the interface width. The associated interfacial energy is

$$\gamma = \frac{2}{3}\sqrt{2\,\alpha\,\Delta f} \tag{1.4}$$

Introducing the grid spacing d, the discretised non-dimensional free energy $\tilde{F} = F/(d^3\,\Delta f)$ becomes:

$$\tilde{F} = \sum \tilde{f}(\phi) + \frac{\tilde{\alpha}}{2}|\tilde{\nabla}\phi|^2 \tag{1.5}$$

where $\tilde{f(\phi)} = f(\phi)/\Delta f$, $\tilde{\alpha} = \alpha/(\Delta f\, d^2)$ and $\tilde{\nabla}\phi$ is the non-dimensional gradient operator equal, for example, to $\phi((n+1)d) - \phi(nd)$. $\tilde{\delta} = \delta/d$ is the dimensionless interface width that should be equal to 3–5 for numerical reasons.

The adimensional interface free energy and interfacial width are related to the adimensional gradient term through:

$$\tilde{\gamma} = \gamma/(d\,\Delta f) = \frac{2\sqrt{2}}{3}\sqrt{\tilde{\alpha}} \tag{1.6}$$

$$\tilde{\delta} = \sqrt{\tilde{\alpha}/2} \tag{1.7}$$

1.2 Allen-Cahn equation

$$\frac{d\phi}{dt} = -L\,\frac{\delta F}{\delta\phi} \tag{1.8}$$

where

$$\frac{\delta F}{\delta\phi} = f'(\phi) - \alpha\Delta\phi \tag{1.9}$$

We assume that the characteristic decay time t_{exp} for a long wavelength fluctuation around $\phi = 0$ is know. Using $f(\phi) \approx \frac{1}{2}f''(0)\phi^2$, and neglecting the heterogeneous term, we have

$$\frac{d\phi}{dt} \approx -L\,f''(0)\,\phi \tag{1.10}$$

and finally $L = 1/(f''(0)\,t_{exp})$.

Using the dimensionless time $\tilde{t} = t/t_{exp}$, the adimensional Allen-Cahn writes:

$$\frac{d\phi}{d\tilde{t}} = -\tilde{L}\,(\tilde{f}'(\phi) - \tilde{\alpha}\tilde{\Delta}\phi) \tag{1.11}$$

where we have used the kinetic parameter $\tilde{L} = 1/\tilde{f}''(0)$ and the discrete laplacian $\tilde{\Delta} = d^2\Delta$.

As you know, life is much more easy in Fourier space. The Allen-Cahn equation in Fourier space writes:

$$\frac{d\hat{\phi}}{d\tilde{t}} = -\tilde{L}\,\left(\left\{\tilde{f}'(\phi(\tilde{r}))\right\}_{\tilde{k}} + \tilde{k}^2\,\tilde{\alpha}\,\hat{\phi}\right) \tag{1.12}$$

The first order Euler spectral scheme is already programmed:

$$\hat{\phi}(t+dt) - \hat{\phi}(t) = -\tilde{L}\, dt \left(\left\{ \tilde{f}'(\phi(\tilde{r})) \right\}_{\tilde{k},t} + \tilde{k}^2\, \tilde{\alpha}\, \hat{\phi}(t) \right) \tag{1.13}$$

Question 1 : How can we ensure to have about 3 grid points inside the interface ?

Question 2 : Obtain an equilibrium flat profile and compute the adimensional interfacial free energy.

Question 3 : Start a simulation with a circle and study the evolution of the average phase field. What do you get?

From the velocity we get $\frac{1}{2} R \frac{dR}{dt} = -\alpha L \frac{D-1}{2}$ so we have

$$R^2(t) = R_0^2 - \alpha\, L\, \frac{D-1}{2}\, t. \tag{1.14}$$

Because $D = 2$, we get for the adimensional radius:

$$\tilde{R}^2(t) = \tilde{R}_0^2 - \frac{\tilde{\alpha}}{2\tilde{f}''(0)}\, \tilde{t} \tag{1.15}$$

Because $\langle \phi \rangle = \pi \tilde{R}^2 / N^2$, we predict a linear decrease of $\langle \phi \rangle$ with a slope given by $\frac{\pi}{N^2} \frac{\tilde{\alpha}}{2\tilde{f}''(0)}$. Example: $N = 100$, $\alpha = 18$, $\tilde{f}''(0) = 32$, slope$=\frac{9\pi}{32N^2} = 1.963\, 10^{-5}$.

Question 4 : What is the maximum time step that can be used ?

Question 5 : Program the semi implicit spectral scheme and analyse its stability and accuracy. (You may used the simulation of a circle decreasing in size.)
Note: the semi-implicit scheme is obtained by evaluating $\hat{\phi}$ in the right hand side of Eq. **??** at time $t + dt$.

$$\hat{\phi}(t+dt) - \hat{\phi}(t) = -\tilde{L}\, dt \left(\left\{ \tilde{f}'(\phi(\tilde{r})) \right\}_{\tilde{k},t} + \tilde{k}^2\, \tilde{\alpha}\, \hat{\phi}(t+dt) \right) \tag{1.16}$$

Question 6 : Start the simulation with the constant value of 0.5 for phi plus a small noise of amplitude 0.01. What is the obtained microstructural evolution ?

Question 7 : *Homework. Test of the spatial discretization scheme.* I want to repeat a calculation after increasing the number of grid points in the interface, keeping the real width of the interface, the interfacial energy, the decay time and the real box size constant. What shall I do ?

Question 8 : *Homework. Test of the errors related to the real interfacial width.* I want to repeat the calculation after decreasing the real interfacial width, but keeping constant the number of grid points in the interface, the interfacial energy, the decay time and the real box size. What shall I do ?

Question 9 : Code Cahn-Hilliard equation in a semi-implicit scheme.

Question 10 : Express elastic energy in Fourier space assuming homogeneous elastic constants. Add the elastic contribution to the kinetic equation.