1 Phase Field model

We postulate the free energy of the system as

$$F = \int_\Omega f(C)d\Omega + \int_\Gamma f_\Gamma(C)d\Gamma = \int_\Omega \left(\frac{\gamma}{\epsilon}\Psi(C) + \frac{\gamma\epsilon}{2}|\nabla C|^2\right) d\Omega + \int_\Gamma \gamma_{sl} + (\gamma_{sg} - \gamma_{sl})w(C)d\Gamma. \quad (1)$$

where the first term is the bulk energy $\Psi(C) = \frac{1}{4}(C-1)^2(C+1)^2$, $C = C(\mathbf{x}, t)$ is a concentration, the second term the interfacial energy and the boundary integral term is the solid substrate energy in dry ($w(C=-1)=1$) and wet ($w(C=1)=0$) state. $C = C(\mathbf{x}, t)$ is a scalar field, which represents the two phases i.e. liquid state $C = 1$ and gas state $C = -1$. The volume integral (Ω) represents the bulk free energy and the surface integral (Γ) the free energy contribution from the surface. γ is the surface tension coefficient and ϵ is the interface thickness. γ_{sg} and γ_{sl} is the surface tension of the solid in dry (gas-solid) and wet (liquid-solid) state, respectively.

1.1 Chemical potential ϕ

Find the integral equation for the chemical potential ϕ, where $\delta F/\delta C = \int_\Omega \phi d\Omega + \int_\Gamma \phi_\gamma d\Gamma$ by making a variation in F [Nm] with respect to the order parameter/concentration C and the wetting boundary conditions (integral). Scale the chemical potential with γ/ϵ and the volume/$\mathbf{x}$ with a characteristic length of the system e.g. drop size L to make the equation dimensionless.

1.2 Derive the equilibrium interface thickness

Assume a flat interface along one dimension in equilibrium i.e. constant chemical potential $\phi = 0$. Neglect the boundary term and find the equilibrium interface profile $C(x) = \tanh \frac{x}{\sqrt{2}\epsilon}$

1.3 Surface tension calculation

Find the effective surface tension coefficient from the free energy at equilibrium (assume a flat one-dimensional interface) i.e. $\int_{-\infty}^{\infty} F(C(x))dx$

1.4 Substrate boundary conditions

Use the equilibrium solution to find the form of the polynomial for $g(C)$ in the surface integral by assuming the Neumann boundary condition on C at the substrate equals the variation in the substrate free energy i.e. $\gamma\epsilon\nabla C \cdot \mathbf{n} = \phi_\gamma$, with $\mathbf{n}$ the interface normal.

1.5 Decrease in free energy

Assume any variation δC must balance a diffusive Fickean flux $\mathbf{J} = M\nabla\phi$ we get the mass conscerving Cahn-Hilliard equation,

$$\frac{\partial C}{\partial t} + \mathbf{u}\nabla C = \nabla \cdot \mathbf{J} = \nabla \cdot (M\nabla\phi). \quad (2)$$

What is the sign of M that ensures that the free energy F decreases in time, albeit the laws of thermodynamics (assume $\mathbf{u} = 0$). (Hint: Use the variation δC from the Cahn-Hilliard equation into the variation of F with respect to C.)

1.6 Numerical simulation

We will by end of the week put a repository with a solver of the Cahn-Hilliard equation. Perform simulations with the code
i) Initialize the domain with a condition for $C = 1$ in the left half and $C = -1$ right half. Test if you get the analytical equilibrium thickness. How does the solution change when you change the Cahn number?
ii) Try to make an initial condition around $C = 0$ with some small disturbance. How does the solution behave?