1 Phase field modeling

Given is the following energy functional

$$F\left[\phi(x,y,t)\right] = \int_{-\infty}^{\infty} \underbrace{\left(\frac{U}{2}\left[a^2\left((\partial_x\phi)^2 + (\partial_y\phi)^2\right) + g(\phi)\right] + \mu_0 h(\phi)\right)}_{f(\phi,\partial_x\phi,\partial_y\phi)} dx,$$

where a and U are constants of the dimension length and energy respectively. $f(\phi, \partial_x\phi, \partial_y\phi)$[1] denotes the local free energy density and μ the bulk free energy density difference between the two phases. Depending on the sign of μ, this can either favor the growth of the one or the other phase. $g(\phi) = \phi^2(1-\phi)^2$ is the double well potential and $h(\phi) = \phi^2(3-2\phi)$ is the interpolation function. Please note, that for the reason of phase-stability we have to demand $|\mu| < U/6$.

Variational principles provide the phase field equation

$$\begin{aligned}
\frac{1}{M_\phi}\frac{\partial\phi}{\partial t} &= -\frac{\delta F}{\delta\phi} \\
&= \partial_x \frac{\partial f}{\partial\left(\partial_x\phi\right)} + \partial_y \frac{\partial f}{\partial\left(\partial_y\phi\right)} - \frac{\partial f}{\partial\phi} \\
&= U\left(a^2(\partial_x^2\phi + \partial_y^2\phi) - \frac{1}{2}\frac{\partial g(\phi)}{\partial\phi}\right) - \mu\frac{\partial h(\phi)}{\partial\phi}. \qquad (1)
\end{aligned}$$

1.1 Stability of the homogenous and time independent solutions

We look for constant solutions of Eq. 1

$$0 = \frac{U}{2}\frac{\partial g(\phi)}{\partial\phi} + \mu\frac{\partial h(\phi)}{\partial\phi}$$

Calculation of the partial derivatives of the polynomial functions leads to

$$\begin{aligned}
\frac{\partial g(\phi)}{\partial\phi} &= 2\phi(1-\phi)(1-2\phi) \\
\frac{\partial h(\phi)}{\partial\phi} &= 6\phi(1-\phi)
\end{aligned}$$

[1] ∂_x is an abbreviation for the partial derivative with respect to x, i.e. $\partial_x \equiv \partial/\partial x$

Inserting in the equation above yields

$$\begin{aligned}
0 &= U\phi(1-\phi)(1-2\phi) + \mu 6\phi(1-\phi)\\
0 &= \phi(1-\phi)(1-2\phi) + \frac{6\mu}{U}\phi(1-\phi)\\
0 &= \phi(1-\phi)\left(1-2\phi+\frac{6\mu}{U}\right)\\
\Rightarrow & \phi_1 = 0; \phi_2 = 1; \phi_3 = \frac{1}{2} + \frac{3\mu}{U};
\end{aligned}$$

Stability of the solutions:

- $\phi_1 = 0$ is a global (local) minimum if $\mu_0 > 0$ ($\mu_0 < 0$), i.e. stabile (meta stabile)
  - $\phi_2 = 1$ is local (global) minimum if $\mu_0 > 0$ ($\mu_0 < 0$), d.h. meta stabile (stabile)
  - $\phi_3 = \frac{1}{2} + 3\mu_0/U$ is for positive and negative μ unstable ($|\mu| < U/6$)

1.2 Phase-field profile function

We show that

$$\phi_0(x,t) = \frac{1}{2}\left(1+\tanh\frac{(x-vt)}{2a}\right) \tag{2}$$

is a heterogeneous solution of the phase field equation (1) if $v = 6M_\phi a\mu$. Note that from $\partial_x(\tanh(x)) = 1-\tanh^2(x)$ we can deduct the following property of this solution $\partial_x\phi_0 = \phi_0(1-\phi_0)/a$.

Calculation of the derivatives:

$$\begin{aligned}
\frac{\partial\phi_0}{\partial x} &= \frac{1}{2}\frac{\partial}{\partial x}\left(1+\tanh\frac{(x-vt)}{2a}\right) = \frac{1}{4a}\left(1-\tanh^2\frac{(x-vt)}{2a}\right)\\
&= \frac{1}{4a}\left(1+\tanh\frac{(x-vt)}{2a}\right)\left(1+1-1-\tanh\frac{(x-vt)}{2a}\right)\\
&= \frac{1}{4a}\left(1+\tanh\frac{(x-vt)}{2a}\right)\left(2-\left(1+\tanh\frac{(x-vt)}{2a}\right)\right)\\
&= \frac{1}{a}\frac{1}{2}\left(1+\tanh\frac{(x-vt)}{2a}\right)\left(1-\frac{1}{2}\left(1+\tanh\frac{(x-vt)}{2a}\right)\right)\\
&= \frac{1}{a}\phi_0(1-\phi_0) && (3)\\
\frac{\partial^2\phi_0}{\partial x^2} &= \frac{1}{a}\frac{\partial}{\partial x}\left[\phi_0(1-\phi_0)\right] = \frac{1}{a}\frac{\partial}{\partial\phi_0}\left[\phi_0(1-\phi_0)\right]\frac{\partial\phi_0}{\partial x}\\
&= \frac{1}{a^2}\phi_0(1-\phi_0)(1-2\phi_0), && (4)\\
\frac{\partial\phi_0}{\partial t} &= -v\frac{\partial\phi_0}{\partial x} = -\frac{v}{a}\phi_0(1-\phi_0). && (5)
\end{aligned}$$

Where the second derivative has been calculated using the chain rule $\frac{\partial f(\varphi(x))}{\partial x} = \frac{\partial f}{\partial \varphi}\frac{\partial \varphi}{\partial x}$. Inserting in the nonlinear partial differential equation

$$
\begin{aligned}
-\frac{v}{a}\phi_0\left(1-\phi_0\right) = M_\phi U & \underbrace{\left[a^2\frac{1}{a^2}\phi_0\left(1-\phi_0\right)\left(1-2\phi_0\right) - \phi(1-\phi)(1-2\phi)\right]}_{=0} \\
& - M_\phi \mu 6\phi_0\left(1-\phi_0\right) \\
\Leftrightarrow \quad -v = -6M_\phi a\mu. &
\end{aligned}
$$

1.3 Interface energy density

The interface energy density γ in the phase-field model corresponds to the total free energy of the heterogeneous solution $\gamma = F[\phi_0(x,t)]$:

$$
\begin{aligned}
F &= \frac{U}{2}\int_{-\infty}^{\infty}\left(a^2\left(\frac{\partial\phi_0}{\partial x}\right)^2 + \phi_0^2(1-\phi_0)^2\right)dx \\
&= \frac{U}{2}\int_{-\infty}^{\infty}\left(a^2\left(\frac{1}{a}\phi_0\left(1-\phi_0\right)\right)^2 + \phi_0^2(1-\phi_0)^2\right)dx \\
\left[dx = \frac{a}{\phi_0(1-\phi_0)}d\phi_0\right] &= aU\int_0^1 \frac{\phi_0^2(1-\phi_0)^2}{\phi_0(1-\phi_0)}d\phi_0 \\
&= aU\int_0^1 \phi_0(1-\phi_0)d\phi_0 \\
&= aU\left(\frac{1}{2}\phi_0^2 - \frac{1}{3}\phi_0^3\right)\Big|_0^1 = \frac{aU}{6}
\end{aligned}
$$

1.4 Calibration of the field model

We calibrate the phase field model according to the 1D considerations above, i.e. we switch from the parameters a, U, M_ϕ to the parameters $\xi = 2a$ for the phase-field width, $\Gamma = aU/6$ for interface energy density and $M = M_\phi a^2 U$ for the kinetic coefficient $M[\mathrm{m}^2/\mathrm{s}]$. The calibrated phase-field model provide the following relation between the driving force μ and the resulting stationary interface velocity v

$$
v = \frac{M}{\Gamma}\mu_0 = K\mu_0.
$$

With these parameters we obtain the following phase-field equation

$$
\frac{1}{M}\partial_t\phi = \underbrace{\partial_x^2\phi + \partial_y^2\phi}_{\mathrm{Laplace-Operator}} - \frac{2}{\xi^2}\partial_\phi g(\phi) - \frac{\mu}{3\Gamma\xi}\partial_\phi h(\phi).
$$