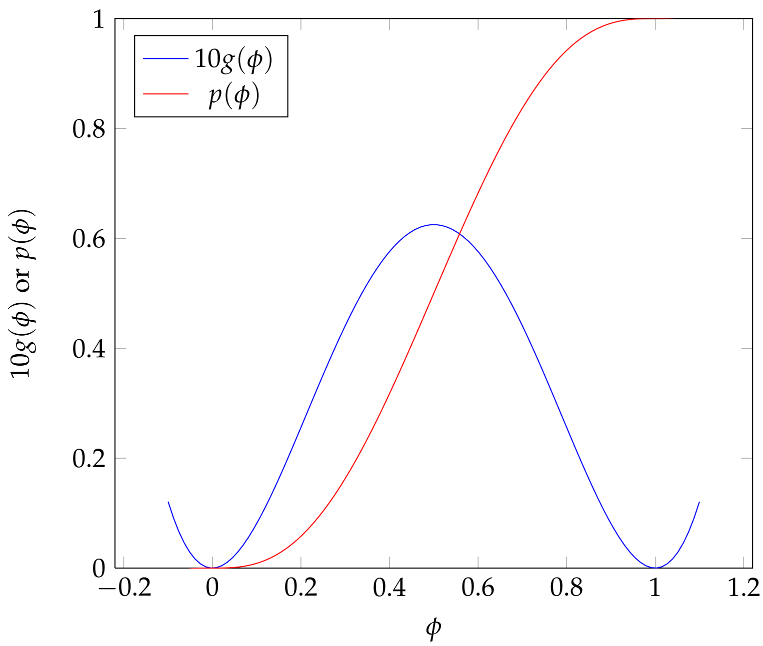
$$F = \int_V \left[f(\phi, T) + \frac{\varepsilon^2}{2} |\nabla\phi|^2 \right] dV$$

$$\frac{\partial\phi}{\partial t} = M\left[\varepsilon^2\nabla^2\phi - \frac{\partial f(\phi,T)}{\partial\phi}\right] \tag{1}$$

$$\frac{\partial u}{\partial t} = D\nabla^2 u + \frac{1}{2}\frac{\partial\phi}{\partial t} \tag{2}$$

$$u \equiv \frac{T - T_m}{L/c_P}$$

$$\begin{aligned} f(\phi,T) &= [1 - p(\phi)]\, f_S(T) + p(\phi) f_L(T) + Qg(\phi) \\ &= f_S(T) + p(\phi)[f_L(T) - f_S(T)] + Qg(\phi) \qquad (3) \\ p(\phi) &= \phi^3\left(6\phi^2 - 15\phi + 10\right) \\ g(\phi) &= \phi^2(1-\phi)^2 \end{aligned}$$



Simplifications on $f(\phi, T)$:

1. Set solid as standard state, so that, for all T:

$$f_S(T) \equiv 0.$$

2. Use the common approximation for alloys at $T \approx T_m$:

$$\begin{aligned}\Delta f_{\text{melt}} = f_L(T) - f_S(T) &\approx \frac{L(T_m - T)}{T_m} \\ &= -\frac{L^2}{c_P T_m} u \\ &= -\kappa u\end{aligned}$$

where $\kappa = L^2/(c_P T_m)$.

Therefore, changing from T to u and substituting into (3), we have

$$f(\phi, u) = -\kappa u p(\phi) + Q g(\phi). \tag{4}$$

In one dimension, the interface thickness δ is given by

$$\delta = \frac{\varepsilon}{\sqrt{2Q}}$$

and the surface free energy σ is

$$\sigma = \frac{\varepsilon\sqrt{Q}}{3\sqrt{2}}.$$

To introduce anisotropy, let $\varepsilon = \varepsilon(\hat{\boldsymbol{n}})$, where $\hat{\boldsymbol{n}}$ is the unit vector normal to the to the interface. Following Baragard,

$$\varepsilon^2(\hat{\boldsymbol{n}}) = \varepsilon_0^2(1 - 3\varepsilon_c)\left[1 + \frac{4\varepsilon_c}{1 - 3\varepsilon_c}\left(n_x^4 + n_y^4 + n_z^4\right)\right]$$

where ε_c is a constant, ε reduces to ε_0 in the isotropic case, and $\hat{\boldsymbol{n}}$ is taken as $-\nabla\phi/|\nabla\phi|$, so that

$$n_x^4 + n_y^4 + n_z^4 = \frac{(\partial\phi/\partial x)^4 + (\partial\phi/\partial y)^4 + (\partial\phi/\partial z)^4}{|\nabla\phi|^4}.$$

Numerical Analysis

Finding the derivative of Eqn. (4) and substituting into (1), we have

$$\frac{\partial\phi}{\partial t} = M\varepsilon^2\nabla^2\phi + 2M\phi\Big[15\kappa u\phi(\phi - 1)^2 - Q(1 - \phi)\,(1 - 2\phi)\Big]$$

which is to be integrated numerically, coupled with Eqn. (2). Let $h(\phi, u)$ be the second term on the right hand side of the above equation, so

$$\frac{\partial\phi}{\partial t} = M\varepsilon^2\nabla^2\phi + h(\phi, u)$$