

The assignment consists of four exercises 1a), 1b), 2a) and 2b). Please hand in a separate matlab file for each exercise. It is best to read an exercise till the end before starting the implementation procedure. The exercises should be done with the help of matlab. Please write the answers to the questions given in the exercises in your matlab files as comments. You can create a comment line starting it with the percent sign. Additionally to this pdf file you will be also provided two matlab files. They are not finished and are meant as a help in order to save your time and as guidance. You can use these files as a starting point. However, everyone can feel free to write his own implementations, too.

Here are some basics about matlab:

- accessing the n-th entry of a one dimensional array: $x(n)$
- accessing the element in the m-th row and n-th column of a two dimensional array: $x(m, n)$
- setting the 7-th to 13-th elements of a one dimensional array to 42: $x(7 : 13) = 42$
- multiplication of an array with 7: $x = x * 7$
- elementwise multiplication of two arrays (note the dot!) : $a = b .* c$
- defining a function with x as input:

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function[result] = F(x)
    result = ..;
end
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- using the defined function to set y: $y = F(x)$

1 WBM model

- a) Implement the following evolution equation for the phase field variable ϕ :

$$\dot{\phi} = M_{\phi} \left[\epsilon^2 \nabla^2 \phi - g'(\phi) \cdot W + g(\phi)(G_0 - G_1) \frac{36}{\eta} \right] \quad (1)$$

where $g(\phi) = \phi^2(1 - \phi)^2$ is the double well potential, $g'(\phi)$ is its derivative with respect to ϕ , $G_{0/1}$ are the constant Gibbs energy functions of the bulk phases 0 and 1 given by:

$$G_0 = 0 \frac{J}{m^3} \quad (2)$$

$$G_1 = -1e6 \frac{J}{m^3} \quad (3)$$

and the parameters $M_{\phi} = 1e - 10 \frac{m^4}{J_s}$, $W = 1e12 \frac{J}{m^4}$, $\epsilon^2 = 1 \frac{J}{m^2}$ and $\eta = 20dx$. Use a one dimensional space discretisation consisting of $N = 100$ cells with a

cell width of $dx = 1e - 6m$, the discrete Laplace operator ¹:

$$(\nabla^2 \phi)_i = \frac{1}{dx^2} (\phi_{i-1} - 2\phi_i + \phi_{i+1}) \quad (4)$$

with the boundary conditions $(\nabla^2 \phi)_1 = (\nabla^2 \phi)_{N_x} = 0$. For the time discretisation use the time step $dt = 1e - 3s$ and integrate the evolution equation for $N_t = 1000$ steps using Euler integration:

$$\phi^n = \phi^{n-1} + dt \cdot \dot{\phi}^{n-1} \quad (5)$$

Try to answer the following questions before starting the implementation:

- which phase is represented by ϕ , phase 0 or phase 1?
- which phase will grow, and which will shrink?

Depending on your answers choose a reasonable initial state for ϕ such, that the interface moves from left to right. In the case it does not work, try the following initialisation:

$$\begin{aligned} \phi_{[1: \frac{N_x}{2}]} &= 0 \\ \phi_{[\frac{N_x}{2} + 1: N_x]} &= 1 \end{aligned}$$

Once you know which phase will grow position the interface such that in the beginning of the calculation 10% of the system belong to the growing phase and 90% are occupied by the shrinking one.

b) Exchange the constant Gibbs energy functions by concentration dependent ones:

$$G_0(c) = \left[\frac{13e4}{2} (c - 10)^2 + 1e6 \right] \frac{J}{m^3} \quad (6)$$

$$G_1(c) = \left[\frac{5e4}{2} (c - 20)^2 + 1e5 \right] \frac{J}{m^3} \quad (7)$$

Additionally to the phase field variable ϕ introduce a concentration variable c with the above discretisation. For the initial concentration state, assume the phase concentrations:

$$\begin{aligned} c_0 &= 13at.\% \\ c_1 &= 20at.\% \end{aligned} \quad (8)$$

and set the concentration field c as an average of the two phase concentration fields using the phase field variable as the averaging weight. If you think, that ϕ stands for phase 0 use:

$$c = \phi \cdot c_0 + (1 - \phi) \cdot c_1 \quad (9)$$

¹ $(\cdot)_i^n$ stands for the variable's value at i-th cell in the n-th time step

or

$$c = \phi \cdot c_1 + (1 - \phi) \cdot c_0 \quad (10)$$

if you think that it stands for phase 1.

Implement the diffusion equation:

$$\dot{c} = D \nabla^2 \mu \quad (11)$$

with the coefficient $D = 1e - 15 \frac{m^5(at.\%)^2}{J_s}$ and the chemical potential $\mu = \frac{\partial G}{\partial c}$. Assume linear mixing of Gibbs energies similar to equations (9,10).

Implement the following scheme:

$$\phi^n, c^n \rightarrow \dot{\phi}^n \rightarrow \dot{c}^n \rightarrow \phi^{n+1} \rightarrow c^{n+1} \quad (12)$$

and integrate it for $N_t = 20000$ steps.

How does the interface velocity evolve? Can you explain why does it behave this way? Change the initial concentration $c_0 = 10$ and repeat the calculation. What do you observe? Can you explain your observation?

2 MPF model²

a) Implement the phase field evolution equation:

$$\dot{\phi} = M_\phi \left[\sigma \left(\nabla^2 \phi - \frac{72}{\eta^2} g'(\phi) \right) + \frac{6}{\eta} \phi (1 - \phi) (G_0 - G_1) \right] \quad (13)$$

Set the interface energy $\sigma = 1 \frac{J}{m^2}$ and interface width $\eta = 20dx$. For other parameters, discretisation and initial conditions use the same specifications as in the WBM part.

Compare the solution with that of 1.a part. Repeat the calculation 1.a) with $W = \frac{72\sigma}{\eta^2}$.

b) Exchange the constant Gibbs energy functions by phase concentration dependent ones from 1.b). Please note the difference between the total composition c and the phase compositions $c_{0/1}$. Since the concentration dependent Gibbs energy functions now depend on the phase concentrations, you will need to store them, too, additionally to the concentration field c . For the driving force dG use $dG_{0/1}(c_{0/1})$ instead of $dG_{0/1}(c)$. In order to determine the phase concentrations use the partitioning condition:

$$c_1 = \frac{c + (1 - \phi) \cdot c_s \cdot \left(\frac{m_{01}}{m_{10}} - 1 \right)}{\phi + (1 - \phi) \frac{m_{01}}{m_{10}}} \quad (14)$$

$$c_0 = c_s + \frac{m_{01}}{m_{10}} (c_1 - c_s) \quad (15)$$

²Even though MPF stands for “multi phase field” we will limit ourselves to a dual phase system.

to split the total concentration into phase concentrations. The partitioning condition makes use of linearised (concentration - temperature) phase diagrams, where the two phase region is framed by two intersecting lines. Each of the lines marks the 'edge' between a single phase bulk region and the two phase interface region. The two lines meet in the point (c_s, T_S) . The slopes of the lines $m_{01} = 0.7 \frac{K}{at.\%}$ and $m_{10} = 1 \frac{K}{at.\%}$ can be calculated from a linearised phase diagram via:

$$m_{01/10} = \frac{T_s - T}{c_s - c_{0/1}^{eq}} \quad (16)$$

The partitioning is based on the assumption, that the ratio $\frac{m_{01}}{m_{10}}$ is constant for any phase concentration values, close enough to the equilibrium phase concentrations $c_{0/1}^{eq}$:

$$\frac{c_s - c_0^{eq}}{c_s - c_1^{eq}} = \frac{c_s - c_0}{c_s - c_1} \quad (17)$$

thus only the intersection composition $c_s = 25at.\%$ is needed for the partitioning condition.

Implement the scheme:

$$\phi^n, c^n, c_0^n, c_1^n \rightarrow \dot{\phi}^n \rightarrow \dot{c}^n \rightarrow \phi^{n+1} \rightarrow c^{n+1} \rightarrow c_0^{n+1}, c_1^{n+1} \quad (18)$$

and integrate it for $N_t = 20000$ steps.

3 Appendix: derivation of the driving force coefficient function

In both models, the coefficients in front of the driving force term must be chosen such, that the term disappears in the bulk and the integral over the interface is equal the driving force itself. The first condition is satisfied in both models by the choice of the coefficient function $g(\phi)$ in the case of the WBM model and $\phi \cdot (1 - \phi)$ in the case of the MPF model. The missing constant factor can be derived by demanding:

$$\int_{\eta} F(\phi(x)) dx = 1 \quad (19)$$

where $F(\phi(x))$ is the coefficient function that is to be formulated. Factorising $F(\phi(x)) = F_{const} \cdot F_{\phi}(\phi(x))$ yields:

$$\begin{aligned} \int_{\eta} F_{const} F_{\phi}(\phi(x)) dx &= 1 \\ \Leftrightarrow F_{const} &= \frac{1}{\int_{\eta} F_{\phi}(\phi(x)) dx} \end{aligned} \quad (20)$$

In the case of the WBM model we can identify:

$$\int_{\eta} F_{\phi}(\phi(x))dx = \int_{\eta} g(\phi(x))dx \quad (21)$$

Using the steady state profile of the phase field function we execute the variable substitution $x \rightarrow \phi^3$:

$$\begin{aligned} \phi(x) &= \frac{1}{2} \tanh\left(\frac{3x}{\eta}\right) + \frac{1}{2} \\ \Rightarrow dx &= \frac{\eta}{6} \frac{d\phi}{\phi(1-\phi)} \end{aligned} \quad (22)$$

Applying this variable substitution to the above integral (21) yields:

$$\begin{aligned} \int_0^{\eta} g(\phi)dx &= \int_0^1 \phi^2(1-\phi)^2 \frac{\eta}{6} \frac{d\phi}{\phi(1-\phi)} \\ &= \int_0^1 \phi(1-\phi) \frac{\eta}{6} d\phi \\ &= \frac{1}{36} \eta \end{aligned} \quad (23)$$

In the case of the MPF model the phase field dependent function is given by $F_{\phi}(\phi) = \phi(1-\phi)$. Therefore we end up with:

$$\begin{aligned} \int_0^{\eta} \phi(1-\phi)dx &= \int_0^1 \phi(1-\phi) \frac{\eta}{6} \frac{d\phi}{\phi(1-\phi)} \\ &= \int_0^1 \frac{\eta}{6} d\phi \\ &= \frac{1}{6} \eta \end{aligned} \quad (24)$$

³ $\frac{d}{dx} \tanh(x) = 1 - \tanh^2(x)$