Friedrich-Alexander-Universität
Faculty of Engineering

Department Materials Science

WW8: Materials Simulation

Practical: Phase-Field Method

Basics and Application in Materials Science

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Supervision:

Contents

1 Introduction

Phase-field simulation is a versatile application in the toolbox of materials simulation. It is often used for simulations of phase transitions, dislocation evolution, fracture simulations etc. The following practicals aim is to get a practical introduction into the subject. In two separate tasks a 1D single-component solidification simulation, calculation of a bulk energy density coefficient and gradient energy density coefficient are going to be conducted.

2 Task 1: 1D Single-Component Solidification

To simulate a 1D single-component solidification we utilize the following energy density:

$$F = \int \left(f_0 \phi^2 (1-\phi)^2 + \frac{K_\phi}{2} |\nabla \phi|^2 \right) d\vec{r} \tag{1}$$

As soldification is a a non-conservative process, the kinetics are governed by the Allen-Cahn equation (for the homogeneous, isotropic case).

$$\frac{\partial \phi}{\partial t} = -L \frac{\delta F}{\delta \phi} \tag{2}$$

Here the functional derivative $\frac{\delta F}{\delta \phi}$ of an energy functional eq. 3a can be evaluated as eq. 3b.

$$F = \int f(\vec{r}, \phi, \nabla \phi) d\vec{r} \tag{3a}$$

$$\frac{\delta F}{\delta \phi} = \frac{\partial f}{\partial \phi} - \nabla \cdot \frac{\partial f}{\partial (\nabla \phi)} \tag{3b}$$

Solving the functional derivative from eq. 2 yields:

$$\frac{\delta F}{\delta \phi} = 2 f_0 \phi (1-\phi)^2 + 2 f_0 \phi^2 (\phi - 1) - K_\phi \nabla^2 \phi \Leftrightarrow \tag{4a}$$

$$\Leftrightarrow 2\phi^3 - 4\phi^2 + 2\phi \tag{4b}$$

Inserting the result into eq. 2 results in:

$$\frac{\partial\phi}{\partial t} = -L\big[f_0(2\phi^3 - 4\phi^2 + 2\phi) - K_\phi\nabla^2\phi\big] \tag{5}$$

As the governing equation for solving the PDE we apply Dirichlet boundary conditions $\phi_1 = 0; \phi_n = 1$ and discretize the partial derivative $\frac{\partial\phi}{\partial t}$ as:

$$\frac{\partial\phi}{\partial t} \approx \frac{\phi_{next} - \phi}{\Delta t} = -L\big[f_0(2\phi^3 - 4\phi^2 + 2\phi) - K_\phi\nabla^2\phi\big] \Leftrightarrow \tag{6a}$$

$$\Leftrightarrow \phi_{next} = -\Delta t L\big[f_0(2\phi^3 - 4\phi^2 + 2\phi) - K_\phi\nabla^2\phi\big] \tag{6b}$$

and $\nabla^2\phi(x)$ is discretized according to the (forward) finite differences scheme:

$$\nabla^2\phi(x_i) \approx \frac{\phi(x_{i+2}) - 2\phi(x_{i+1}) + \phi(x_i)}{\Delta x} \tag{7}$$

where x_i is the node at which the value is computed and Δx is the node distance. The initial result is plotted in fig. 2. As can be seen in 2 f_0 seems to be reciprocally proportional energy functional over time. With decreasing value the transition region (where ϕ changes from 0 to 1) becomes broader. The opposite effect can be observed in fig. 2 with variation of K_ϕ. Additional the energy density functional seems to become broader but only changes its peak value for increased K-values. L does not seem to have any influence on the ϕ, the energy or energy density - see fig. 2 .

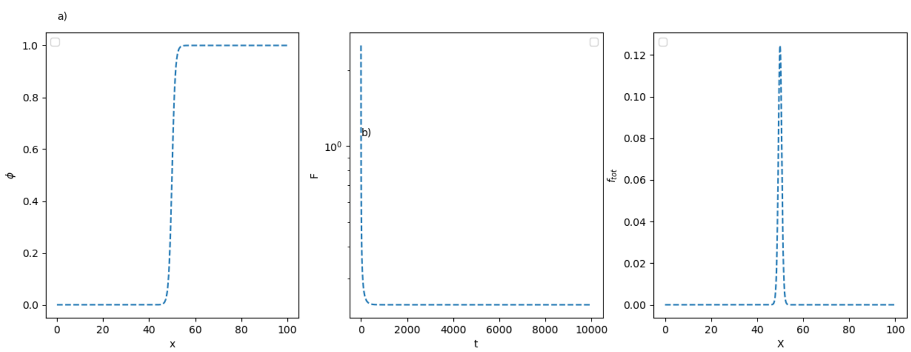

Figure 1: Initial results of the 1D single-component solidification simulation.

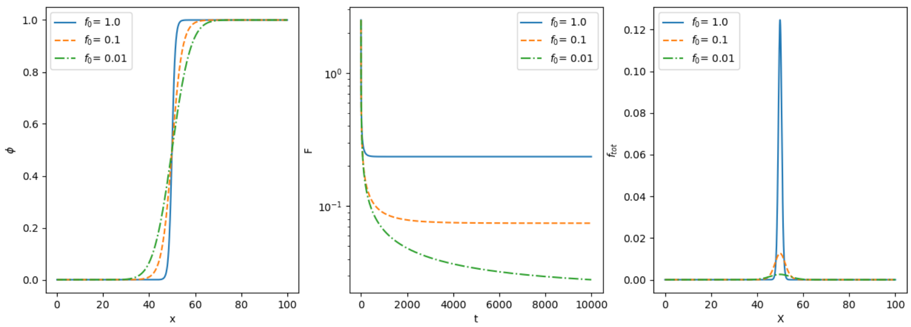

Figure 2: Results of the 1D single-component solidification simulation with various f_0 values.

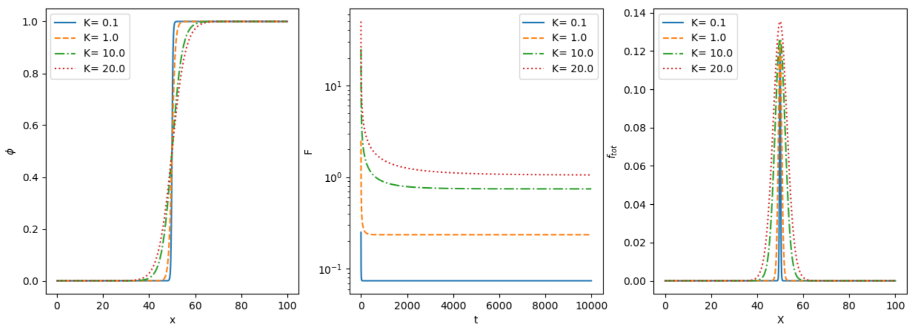

Figure 3: Results of the 1D single-component solidification simulation with various K values.

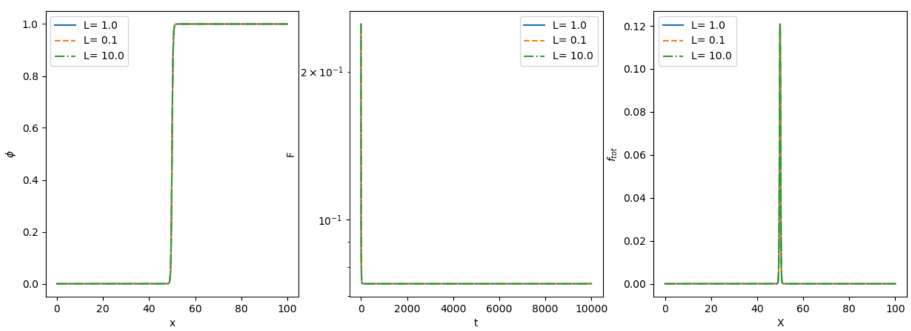

Figure 4: Results of the 1D single-component solidification simulation with various L values.