Manual for using FFT solver for evolution of Cahn-Hilliard model for precipitation

Dasari Mohan and M P Gururajan

November 3, 2021

1 Introduction

This is a multi-phase multicomponent phase-field solver for precipitate evolution. The solver is based on a Fourier spectral discretization of space and forward time marching scheme.

2 Infile

The input parameters required for the solver are derived from an infile. This contains information about the domain geometry, the thermodynamic functions(free energy), material properties such as the interfacial energies and their anisotropies as well as boundary conditions. It could also contain special flags related to the running of the solver. The following is a basic description of the keys in the infile. **Each key must end with a semicolon**. Additionally, all lines beginning with "#" will be treated as comments in the infile.

```
##Geometrical dimensions of the simulation domain
DIMENSION = 2;
MESH_X = 256;
MESH_Y = 256;
MESH_Z = 1;
##Discretization, space and time
DELTA_X = 0.4;
DELTA_Y = 0.4;
DELTA_Z = 0.0;
DELTA_t = 0.2;
##Number of phases and composition
NUMPHASES = 2;
NUMCOMPONENTS = 2;
#Running and saving information
NTIMESTEPS = 10;
NSMOOTH = 10;
SAVET = 100;
## Component and Phase names
COMPONENTS = {Cu, Al};
PHASES = {beta, alpha};
##Gas constant and molar volume
```

```
R = 1.0;
V = 1.0;
##FILEWRITING and OUTPUTTING TO SCREEN
## WRITEFORMAT ASCII/BINARY
##TRACK_PROGRESS: interval of writing out the progress of the
    ↪ simulation to stdout.
WRITEFORMAT = ASCII;
TRACK_PROGRESS = 10;
##Model-specific parameters: Preipitate growth (FFT)
#AtomicMobility = {Diagonal:0/1, phase, 11,22,33, 12, 13, 23...};
AtomicMobility = {1, 0, 1};
AtomicMobility = {1, 1, 1};
##L={12, 13, 14, 23, 24...}
L_phi = {1.0};
##K={12, 13, 14, 23, 24...}
Kappa_phi = {1.0};
##K={12, 13, 14, 23, 24...}
Kappa_c = {1.0};
##A from free energy expression
A_fm = {1.0};
##B from free energy expression
B_fp = {1.0};
ceq = {0, 0, 1.0};
ceq = {0, 1, 1.0};
ceq = {1, 1, 0.0};
ceq = {1, 0, 0.0};
cfill = {0, 0, 1.0};
cfill = {0, 1, 1.0};
cfill = {1, 1, 0.0};
cfill = {1, 0, 0.0};
```

2.1 Simulation geometry, spatial and temporal discretization

```
##Geometrical dimensions of the simulation domain
DIMENSION = 2;
MESH_X = 100;
MESH_Y = 100;
MESH_Z = 1;
```

- DIMENSION: This can take values 2,3 for 2D and 3D simulations respectively. This is a required key in the solver and not mentioning this key might lead to unexpected results

- MESH_X,MESH_Y,MESH_Z: These are the number of grid points in the domain(and not the physical lengths) in the respective X, Y, Z directions. When DIMENSION is 2, the value of MESH_Z will redundant and will be taken as 1.

```
##Discretization, space and time
DELTA_X = 2.0;
DELTA_Y = 2.0;
DELTA_Z = 2.0;
DELTA_t = 0.08;
```

- The values DELTA_X, DELTA_Y, DELTA_Z correspond to the grid resolution in the X, Y, Z directions respectively. Similarly, DELTA_t corresponds to the temporal discretization(time-step).

2.2 Phases and Components information

```
##Number of phases and composition
NUMPHASES = 2;
NUMCOMPONENTS = 2;
```

- The keys are self-explanatory. NUMPHASES corresponds to the number of phases in the domain, while NUMCOMPONENTS corresponds to the number of components(2, for binary, 3 for ternary etc.)

- These keys are absolutely necessary, please fill carefully for successful running of your codes.

```
COMPONENTS = {Cu, Al};
PHASES = {beta, alpha};
```

- COMPONENTS refers to the tuple that consists of the names of the components. The names are separated by commas and the entire tuple needs to placed within {} followed by a semicolon.

- Similarly, PHASES refers to the names of the phases in the domain.

2.3 Number of iterations, smoothing time-steps and writing interval

```
#Running and saving information
NTIMESTEPS = 10000;
NSMOOTH = 10;
SAVET = 1000;
```

- NTIMESTEPS: Total number of iterations that you wish the solver to run. This is not the total time

- NSMOOTH: The number of pre-conditioning steps for smoothening sharp phase-field profiles that are initialised at the start of the simulation

- SAVET: Writing interval, i.e, frequency of writing files of the respective fields

2.4 Material parameters

```
##Gas constant and molar volume
R = 1.0;
V = 1.0;
```

- The values "R" and "V" will refer to the gas constant and the molar volume respectively

```
#DIFFUSIVITY={Diagonal:0/1, phase, 11,22,33..(K-1) diagonal
    ↪ elements, 12, 13, 23...(rest of the elements; rowwise)}
DIFFUSIVITY = {1, 0, 1};
```

- The DIFFUSIVITY key refers to the inter-diffusivity matrix which has the tuple in the following form. The first element can taken in values 0/1, "1" refers to as a diagonal matrix and "0" is a full matrix.

- The following element refers to the phase number referring to the phases in the list PHASES. This can take values from 0 to NUMPHASES-1.

- The following elements are the values in the inter-diffusivity matrix. The first elements are the diagonal terms in the matrix, while the following elements correspond rowwise to the off-diagonal terms in the diffusivity matrix.

- If the first element in the tuple is "1", i.e. the matrix is diagonal irrespective of the number of entries in the tuple only the entries corresponding to the diagonal elements in the matrix will be read in.

```
##GAMMA = {12, 13, 14, 23, 24...}
GAMMA = {1.0};
```

- The GAMMA key refers to the interfacial energy $\gamma_{\alpha\beta}$ between the phases $\alpha\beta$. The elements in tuple correspond to all combination of phases forming the interfaces from the list of phases in PHASES numbered from 0 to NUMPHASES-1.

- The elements are numbered in the order $12, 13, 14, 23, 24 \ldots N(N-1)$, $N = NUMPHASES$ where "12" corresponds to the value of the interfacial energy between phase 1 and 2; γ_{12}.

- In the tuple only combinations $\alpha\beta$ are included where $\alpha < \beta$ as the value of the interfacial energy of the $\alpha\beta$ interface is $\gamma_{\alpha\beta}$ which is the same as $\gamma_{\beta\alpha}$.

- Therefore, the total number of elements in the tuple is $\frac{N(N-1)}{2}$.

```
ceq = {0, 0, 1.0};
ceq = {0, 1, 1.0};
ceq = {1, 1, 0.0};
ceq = {1, 0, 0.0};
cfill = {0, 0, 1.0};
cfill = {0, 1, 1.0};
cfill = {1, 1, 0.0};
cfill = {1, 0, 0.0};
```

- The key "ceq" refers to the equilibrium compositions of the phases. The considered equilibrium is between the last phase NUMPHASES-1 and any of the other phase.

- The first two elements of the tuple "ceq={}" are numbers between 0 and N = NUMPHASES-1, which correspond to the list of N phases.

- Thereafter, the tuple consists in order, the compositions of the K = NUMCOMPONENTS-1 components.

- The required values are corresponding to all combinations "ceq=$\{a, a, 0, 1 \ldots K\}$" and secondly "ceq=$\{a, N-1, 0, 1 \ldots K\}$" where $a \in [0, N-1]$. The former corresponds to the composition of the "a" phase in equilibrium with the "N-1" phase, and the latter set corresponds to the composition of the "N-1" phase in equilibrium with the "a" phase.

- The remaining possibilities can be skipped.

- The key "cfill" is of the same type as "ceq" and is utilized while initializing the domain. It is safe to start with having the "cfill" the same as "ceq", unless one wants to start with a supersaturation.

2.5 Model specific parameters

The following parameters are corresponding to the phase-field model formalism for precipitate growth (*Acta Materialia 57, 3947, 2009*).

The microstructure is described by composition $c(\boldsymbol{r}, t)$ and order parameter $\phi(\boldsymbol{r}, t)$. The order parameter is defined such that $\phi(\boldsymbol{r}, t) = 0$ represents matrix (m) phase and $\phi(\boldsymbol{r}, t) = 1$ represents precipitate (p) phase.

The free energy of the system F is

$$F = N_V \int_\Omega \left[f(\phi, c) + \kappa_\phi (\nabla \phi)^2 + \kappa_c (\nabla c)^2 \right] d\Omega. \tag{1}$$

where $f(\phi, c)$ is the bulk free energy per atom, κ_ϕ and κ_c are gradient energy parameters for ϕ and c, respectively. N_V is the number of atoms per unit volume.

The bulk free energy density $f(\phi, c)$ is given by

$$f(\phi, c) = f^m(c)(1 - W(\phi)) + f^p(c)W(\phi) + P\phi^2(1 - \phi)^2 \tag{2}$$

where P, is height of the energy barrier between the m-phase and p-phase.

$f^m(c)$ and $f^p(c)$ are free energies of m (matrix) and p (precipitate) phases, respectively and is given by

$$f^m(c) = Ac^2 \tag{3}$$

$$f^p(c) = B(1-c)^2 \tag{4}$$

where A and B are positive constants.

$W(\phi)$ is an interpolation function, given by

$$w(\phi) = \begin{cases} 0; & \text{for } \phi < 0 \\ \phi^3(10 - 15\phi + 6\phi^2); & \text{for } 0 \leq \phi \leq 0 \\ 1; & \text{for } \phi > 1 \end{cases} \tag{5}$$

The microstructure evolution is governed by evolution of coupled Allen-Cahn equation and Cahn–Hilliard equation

$$\frac{\partial \phi}{\partial t} = -L_\phi \frac{\delta(F/N_V)}{\delta \phi} \tag{6}$$

$$\frac{\partial c}{\partial t} = \nabla \cdot M \nabla \mu \tag{7}$$

where L_ϕ is the relaxation coefficient, M is the atomic mobility and μ is the chemical potential is given by

$$\mu = \frac{\delta(F/N_V)}{\delta c} \tag{8}$$

The precipitate evolution is governed by

$$\frac{\partial \phi}{\partial t} = -L_\phi \left(\frac{\partial f}{\partial \phi} - 2\kappa_\phi \nabla^2 \phi \right) \tag{9}$$

$$\frac{\partial c}{\partial t} = M\nabla^2 \left(\frac{\partial f}{\partial c} - 2\kappa_c \nabla^2 c \right) \tag{10}$$

The evolution equations 9 and 10 are solved using semi-implicit Fourier spectral method with periodic boundary conditions. Euler forward difference scheme is employed for the time derivative.

Considering $g_c = \frac{\partial f}{\partial c}$ and $g_\phi = \frac{\partial f}{\partial \phi}$ Applying the spatial Fourier transform and the discretized form of evolution equations are given below

for equaiton 9

$$\frac{\partial \tilde{\phi}}{\partial t} = -L_\phi \left[\tilde{g}_\phi - 2\kappa_\phi k^2 \tilde{\phi} \right] \tag{11}$$

$$\frac{\tilde{\phi}(\boldsymbol{k}, t + \Delta t) - \tilde{\phi}(\boldsymbol{k}, t)}{\Delta t} = -L_\phi \tilde{g}_\phi(\boldsymbol{k}, t) + 2L_\phi \kappa_\phi k^2 \tilde{\phi}(\boldsymbol{k}, t + \Delta t) \tag{12}$$

rearranging above equation

$$\tilde{\phi}(\boldsymbol{k}, t + \Delta t) = \frac{\tilde{\phi}(\boldsymbol{k}, t) - \Delta t L_\phi \tilde{g}_\phi(\boldsymbol{k}, t)}{1 + 2\Delta t \kappa_\phi L_\phi k^2} \tag{13}$$

for equaiton 10

$$\frac{\partial \tilde{c}}{\partial t} = M \left[-k^2 \tilde{g}_c - 2\kappa_c k^4 \tilde{c} \right] \tag{14}$$

$$\frac{\tilde{c}(\boldsymbol{k}, t + \Delta t) - \tilde{c}(\boldsymbol{k}, t)}{\Delta t} = -M k^2 \tilde{g}_c(\boldsymbol{k}, t) - 2M\kappa_c k^4 \tilde{c}(\boldsymbol{k}, t + \Delta t) \tag{15}$$

rearranging above equation

$$\tilde{c}(\boldsymbol{k}, t + \Delta t) = \frac{\tilde{c}(\boldsymbol{k}, t) - \Delta t M k^2 \tilde{g}_c(\boldsymbol{k}, t)}{1 + 2\Delta t \kappa_c M k^4} \tag{16}$$

~represents the variable in the Fourier space. $\boldsymbol{k}$ is the wave vector $(= 2\pi/L)$ and $k = |\boldsymbol{k}|$. Equations 13 and 16 gives the evolution of the precipitate. Characteristic length L', energy E' and time T' are used to get non-dimensional evolution equations. Composition is scaled as

$$c = \frac{c' - c'_m}{c'_p - c'_m} \tag{17}$$

where c' is alloy composition, c'_m is composition of matrix and c'_p is composition of precipitate. The above scaling gives composition variable value zero in matrix and one in precipitate.

The details of model specific parameters in `Input.in` file are given below

- `AtomicMobility`: Atomic mobility (M) in equation 10. The present model takes the atomic mobility in precipitate (phase index 0) as input in the simulations

- `L_phi`: Relaxation coefficient (L_ϕ) in equation 9

- `Kappa_phi`: Gradient energy coefficient for order parameter ϕ (κ_ϕ) in equation 9

- `A_fm`: Positive constant in free energy of matrix given in equation 3

- `B_fp`: Positive constant in free energy of precipitate given in equation 4