Code: 1 Spinodal_Semi_implicit.m
Free energy functional, G

$$\frac{G}{N_v} = \int f_0(c) + \kappa\,|\,\nabla C\,|^2\,dv$$

where
$f_0(c) = Ac^2(1-c)^2$

where c is a conserved order parameter
The evolution equation is given by

$$\frac{\delta c}{\delta t} = M(\nabla C)^2\left(\frac{\delta \frac{G}{N_v}}{\delta c}\right)$$

$$\frac{\partial c}{\partial t} = M(\nabla C)^2\left(\frac{\delta\left(\frac{G}{N_v}\right)}{\delta c}\right)$$

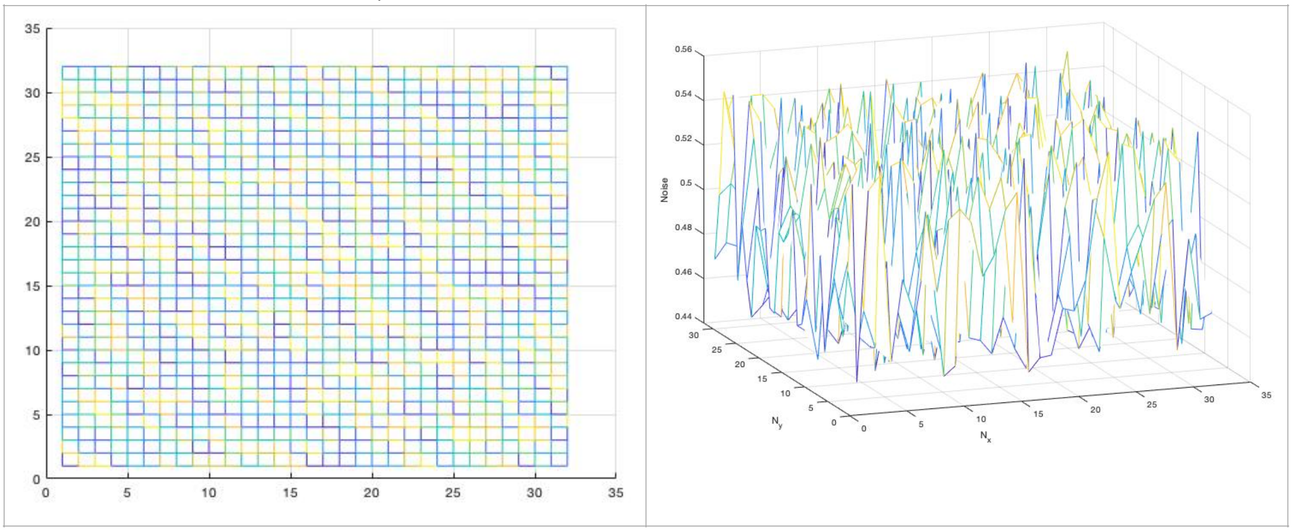
$$= M(\nabla C)^2\left[\frac{\partial f_0}{\partial C} - 2\kappa\nabla^2 C\right]$$

$$= M\,\nabla^2 g(c) - 2\kappa M\,\nabla^4 C$$

where $\mu = \left(\frac{\delta\left(\frac{G}{N_v}\right)}{\delta c}\right)$ and $g(c) = \frac{\partial f_0}{\partial C}$

Finally:

$$\tilde{c}^{(t+\Delta t)} = \frac{\tilde{c}^t - M \times (k_x^2 + k_y^2) \times \Delta t \times \tilde{g}}{1 + 2\kappa M(k_x^2 + k_y^2)^2 \times \Delta t}$$



Code 2: Regular_Soln_Model.m

Non dimensional formula for the regular solution model

$$\frac{\Delta G}{RT} = \Omega x \frac{(1-x)}{RT} + [xln(x) + (1-x)ln(1-x)]$$

Non dimensionalize: \Delta G/RT as dg

$$dg = \frac{\Delta G}{RT}$$

Non dimensionalizing: \Omega/RT as \alpha

$$dg = \alpha x(1-x) + ds$$

Non dimensional entropy of mixing

$$ds = xln(x) + (1-x)ln(1-x)$$

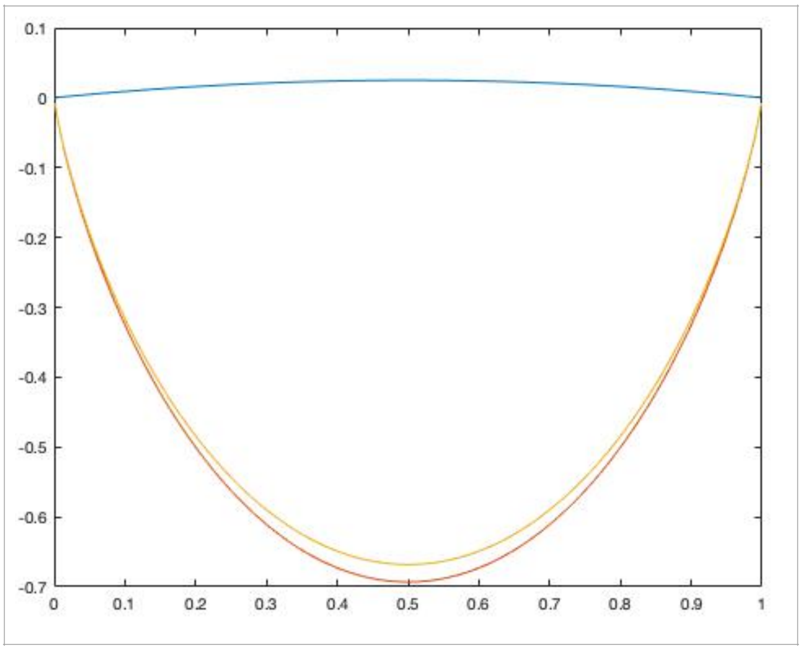
For alpha = 0.1: Since this is positive there will be a phase separation and it will be dominated by temperature

Note: For higher values of alpha (like 1.5, 2.5) the temperature will be low.

Blue line = dg_a is positive

Red line = Entropy line (lowest)

Yellow line = Non dimensionalized free energy (Occurs due to addition of the blue line to the red line)



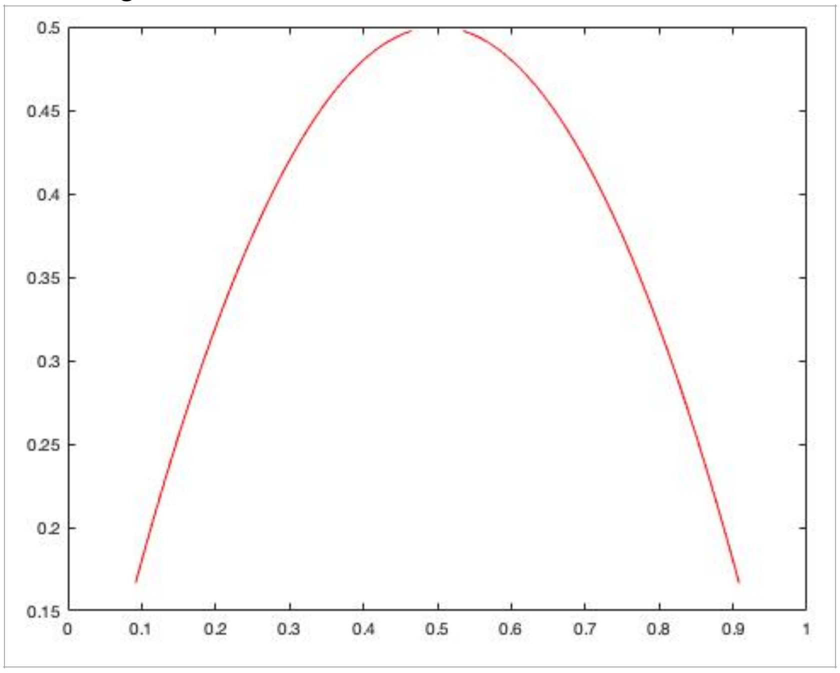
$$\begin{aligned}
\Delta G_{\text{mix}} &= G_{\text{sol}} - G^0 \\
&= (X_A\mu_A + X_B\mu_B) - (X_A\mu_A^0 + X_B\mu_B^0) \\
&= X_{\text{A}}(\mu_A - \mu_A^0) + X_{\text{B}}(\mu_B - \mu_B^0) \\
&= X_{\text{A}}(\text{RT } ln X_A + X_{\text{B}}) + X_{\text{B}}(\mu_B - \mu B^0) \\
&= X_{\text{A}} \text{ RT } ln \ X_{\text{A}} + X_{\text{B}} \text{ RT } ln \ X_B
\end{aligned}$$

Refer: https://www.tf.uni-kiel.de/matwis/amat/td_kin_ii/kap_1/backbone/r_se8.pdf

Code 3: Spinodal.m and S.m

Construction of a phase diagram and spinodal
For a non dimensionalized regular solution model

Explanation of the code is given in the code.



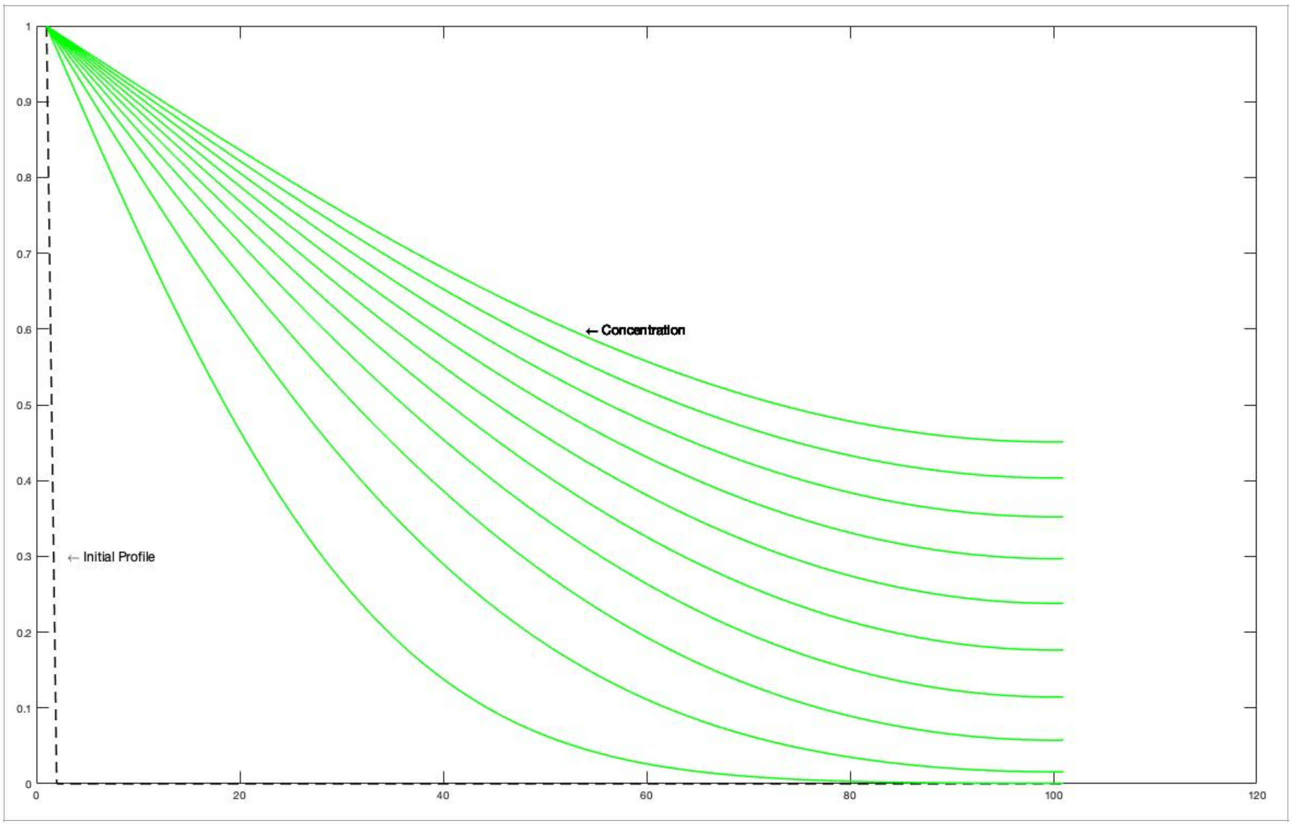
Code 4: explicit_1D.m

The code explains, the case when the concentration is fixed at a position and the diffusion equation is solved using explicit method. The concentration at the fixed location is kept constant over time and initialize at time t = 0. The initial boundary conditions are:

$c = 0$ at $t = 0$

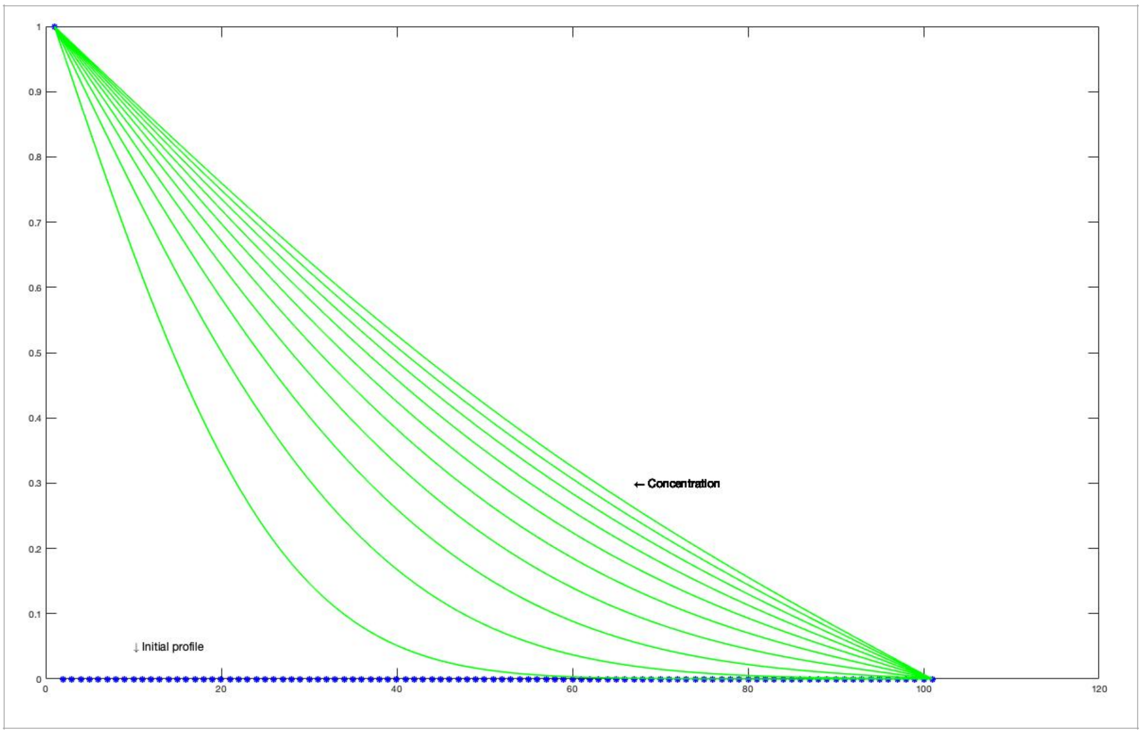
$c = c_0$ at $x = 0$,

Refer: Page 21: https://www.dartmouth.edu/~cushman/courses/engs43/Chapter2.pdf



Code 5: implicit_1D_noflux.m

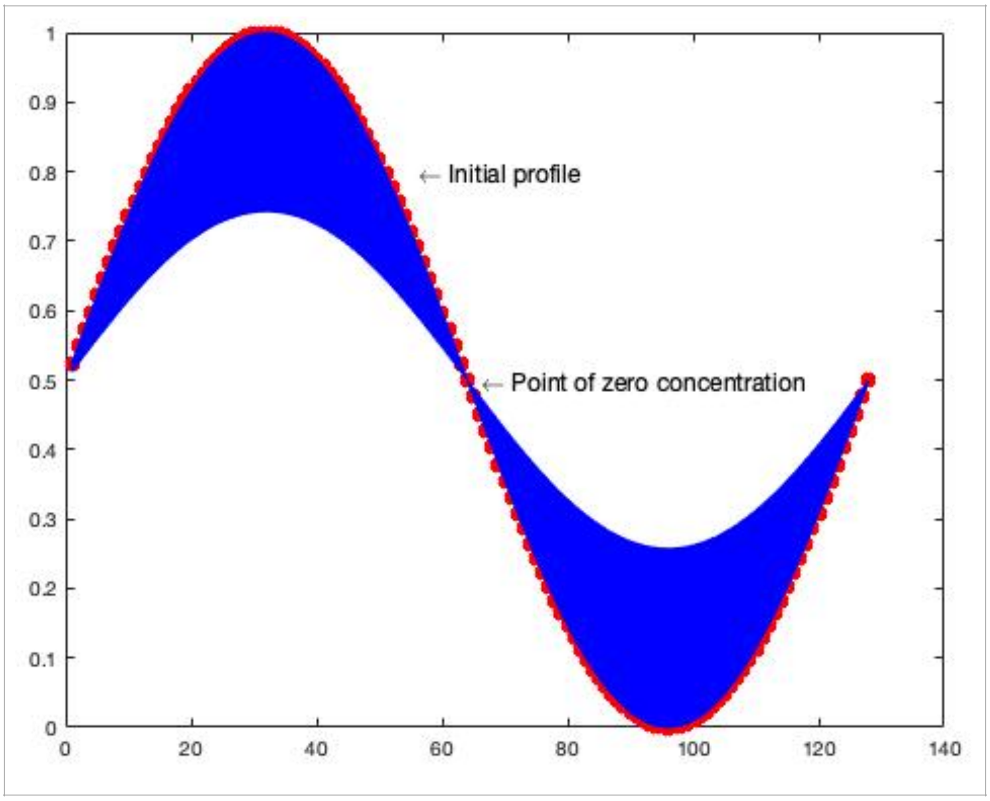
The code implements a diffusion equation with no flux and boundary condition with an implicit scheme.



Refer: http://www.atmos.albany.edu/facstaff/brose/classes/ATM623_Spring2015/Notes/Lectures/Lecture16%20--%20Numerical%20methods%20for%20diffusion%20models.html

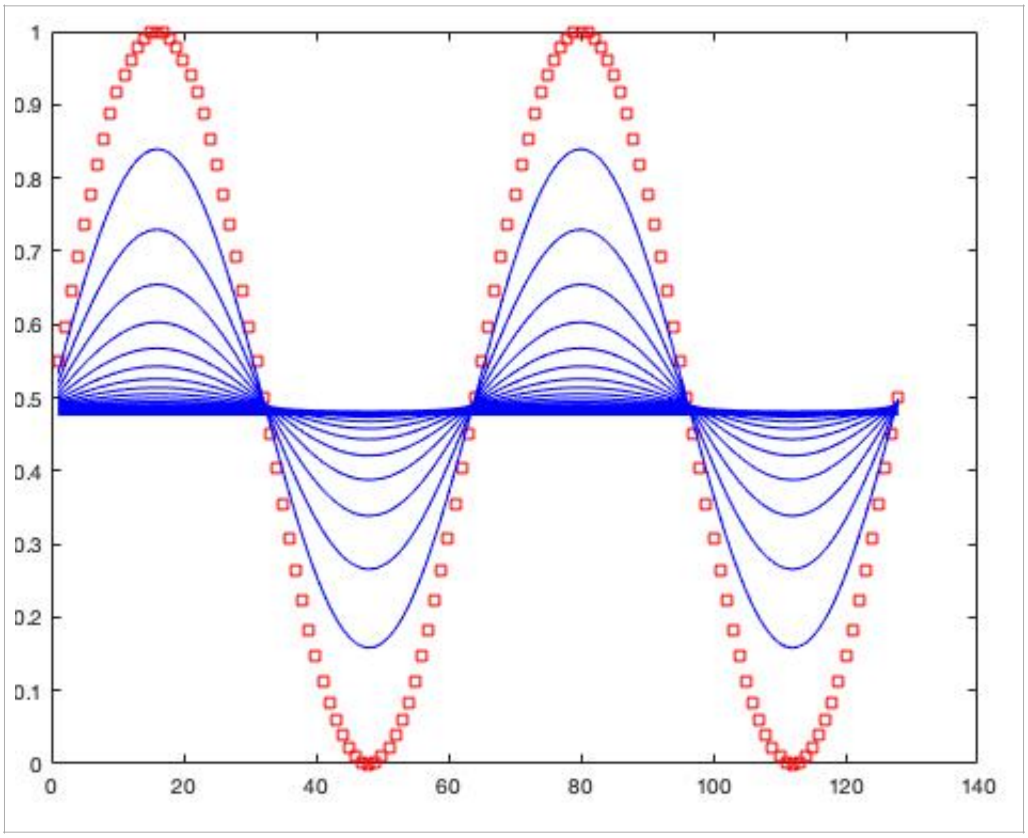
Code 6: Diffusion_eq_1D_PBC.m

The code implements a 1D diffusion equation that is solved using a periodic boundary condition.

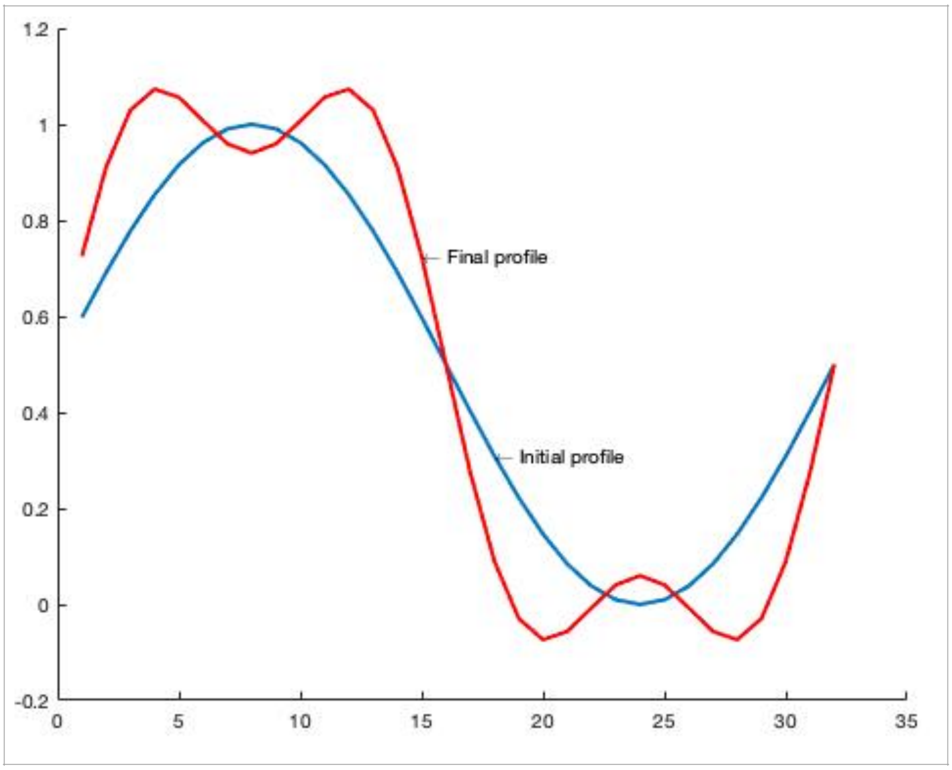


Code 7: Diffusion_eq_1D_implicit.m

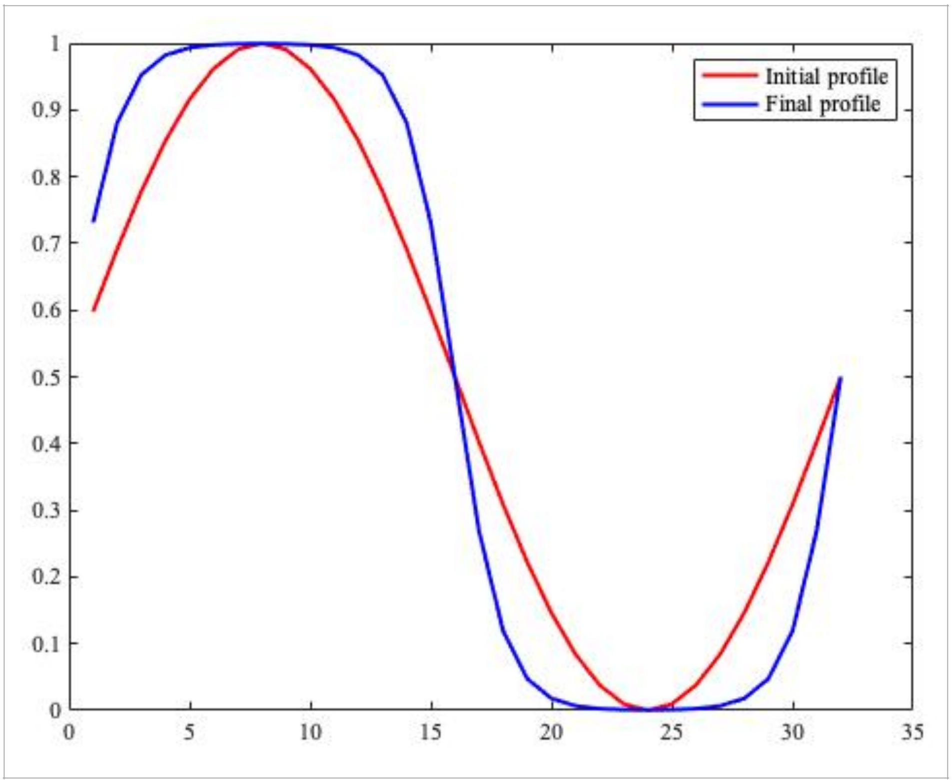
The code implements a 1D diffusion equation using implicit spectral method



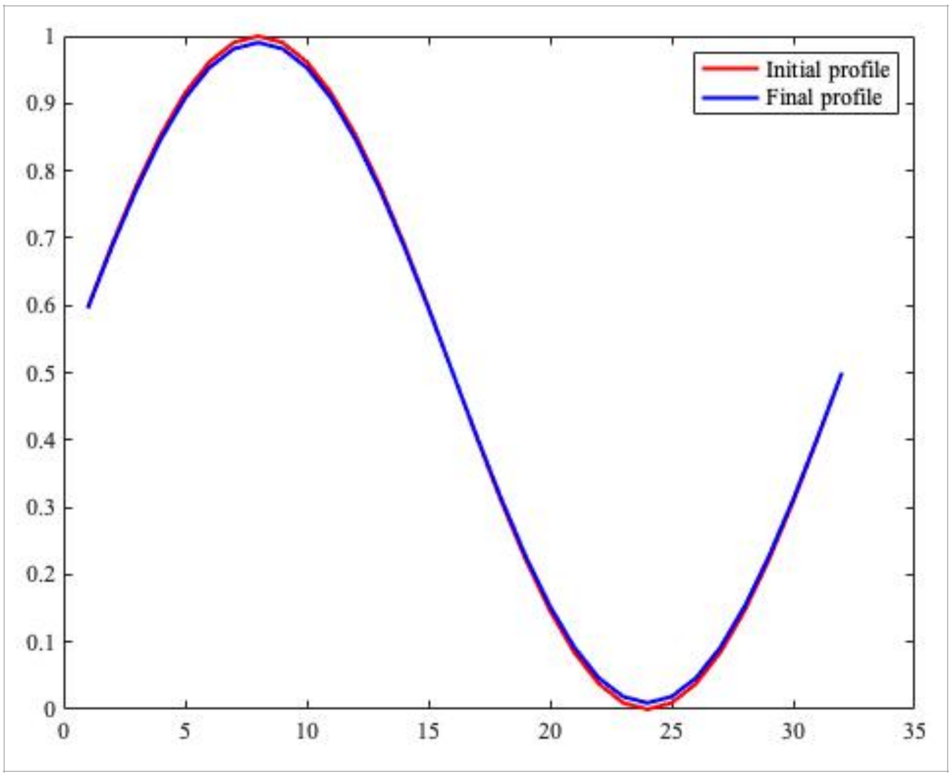
Code 8: Cahn_Hilliard_explicit_PBC.m
Solution for Cahn-Hilliard equation by applying finite difference explicit method and periodic boundary conditions.



Code 9:
cahn_Hilliard_semi_implicit_spectral.m
Solution for Cahn-Hilliard equation using semi-implicit spectral technique



diffusion_eq_implicit_technique.m
Solution to 1D Diffusion equation using Implicit technique.



Code 10: Allen_Cahn.m

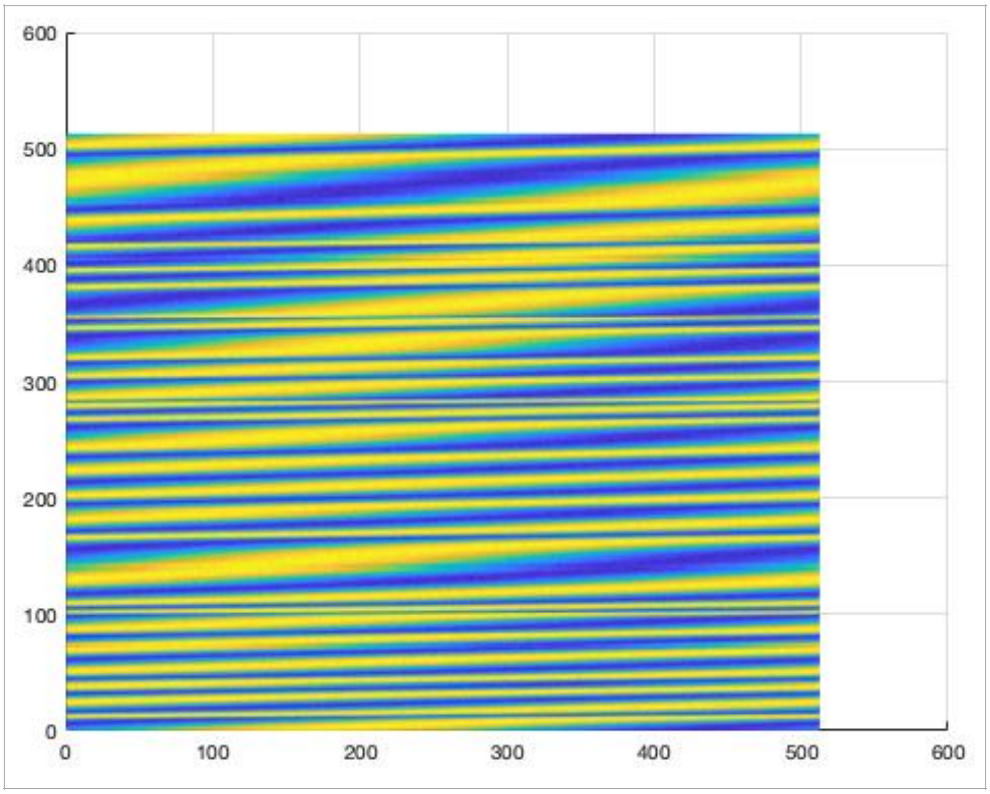
Allen-Cahn equation solved by the semi-implicit fourier spectral method.

Semi-Implicit fourier spectral is given by:

$$\tilde{\phi}^{t+\Delta t} - \tilde{\phi}^{t} = -2\kappa k^{2} L \tilde{\phi}^{t} \Delta t - L \Delta t \tilde{g}^{t}$$

$$\tilde{\phi}^{t+\Delta t} = \frac{\tilde{\phi}^{t} - L \Delta t \tilde{g}^{t}}{1 + 2\kappa k^{2} L}$$

where k^{2} = k_{x}^{2} + k_{y}^{2}



600
500
400
300
200
100
0
0
100
200
300
400
500
600