Allen Cahn Phase Field Solver

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1 ALLEN CAHN PHASE FIELD EQUATION SOLVER : 2D

Importing the required library

[1]:
```
import numpy as np
import matplotlib.pyplot as plt
```

Define the Physical parameters

[2]:
```
h = 1                   # Grid size in x and y directions
N = 64                  # Grid Dimension in x and y directions
L = N * h               # Boundary Dimension
k = 1                   # Relaxation rate
eps = 4                 # Gradient Energy
U = 1                   # Free Energy Multiplier
a = 0.01                # Initialization parameter
```

Defining the arrays representing grid space in x and y directions

[3]:
```
x = np.arange(64)       # Defining an array to store grid points in x direction
y = x                   # Defining an array to store grid points in x direction
```

Defining the time step size and no of time steps

[4]:
```
dt = 0.001              # Defining the time step size
nsteps = 5000           # Defining the no of time steps
```

Defining the functions to compute the bulk free energy density

$$f(\phi) = U(\phi - 1)^2(\phi + 1)^2$$

[5]:
```
def f(xi): return np.square(xi - 1) * np.square(xi + 1)
```

Defining the function to compute the first derivative of the free energy function w.r.t ϕ

$$\frac{\partial f(\phi)}{\partial \phi} = 4U\phi(\phi^2 - 1)$$

[6]:
```
def f1(xj): return 4 * xj * (np.square(xj) - 1)
```

Initializing the phase field distribution

Filling the phase field array phi with random numbers between -a/2 and a/2

[7]:
```
phi = np.random.uniform(low=-a / 2, high=a / 2, size=(N, N))
```

Defining arrays for applying the Periodic boundary conditions

$$\phi(x, y) = \phi(x + L, y) = \phi(x, y + L)$$

[8]:
```
plus = np.append(np.arange(1, N), 0)
minus = np.append(N - 1, np.arange(0, N - 1))
```

Initializing an array to store the value of free energy functional over time

[9]:
```
Fplot = np.arange(nsteps)
```

1.1 Allen Cahn phase field evolution equation

Solving the Allen Cahn phase field equation

$$\frac{\partial \phi}{\partial t} = -k\frac{\delta F[\phi]}{\delta \phi} = -k[\frac{\partial f}{\partial \phi} - 2\epsilon\nabla^2\phi]$$

[ ]:
```
for i in range(nsteps):
```

1.2 Laplacian approximation using Central Difference method

Using Central difference Method to compute the numerical approximation of the laplacian of phase field in 2D

$$\nabla^2\phi = \frac{\phi(x+h, y) + \phi(x, y+h) + \phi(x-h, y) + \phi(x, y-h) - 4\phi(x, y)}{h^2}$$

[ ]:
```
def laplacephi(phi): return (phi[:, plus] + phi[:, minus] + phi[plus, :] +
↪phi[minus, :] - 4 * phi) / (h * h)
```

1.3 Derivative approximation using Central Difference method

Derivative of phase field in x direction, using Central Difference Method with periodic boundary conditions

$$\frac{\partial f}{\partial x} = \frac{\phi(x+h,y) - \phi(x-h,y)}{2h}$$

[ ]:
```
def phidx(phi) : return (phi[:, plus] - phi[:, minus]) / (2 * h)
```

Derivative of phase field in y direction, using Central Difference Method with periodic boundary conditions

$$\frac{\partial f}{\partial y} = \frac{\phi(x,y+h) - \phi(x,y-h)}{2h}$$

[ ]:
```
def phidy(phi): return (phi[plus, :] - phi[minus, :]) / (2 * h)
```

1.4 Free energy functional

Computing the numerical approximation of free energy functional in 2D

$$F[\phi] = \int_V [f(\phi) + \epsilon|\nabla\phi|^2] dV$$

[ ]:
```
F = sum(sum(f(phi))) * U + sum(sum(np.square(phidx(phi)) + np.
↪square(phidy(phi)))) * eps
```

Storing the Free energy functional value for plotting

[ ]:
```
Fplot[i] = F
```

1.5 Variation of free energy functional

Computing variation of F with respect to ϕ, this is also referred as the driving force.

$$\frac{\delta F[\phi]}{\delta\phi} = [\frac{\partial f}{\partial\phi} - 2\epsilon\nabla^2\phi]$$

[ ]:
```
Fdphi = f1(phi) * U - 2 * eps * laplacephi(phi)
```

1.6 Evolution equation

Computing evolution of the phase field using Allen-Cahn equation

$$\phi(x, y; t + \Delta t) = \phi(x, y; t) - k\frac{\partial f}{\partial \phi}$$

$$+\frac{2k\epsilon\Delta t}{h^2}[\phi(x + h, y; t) + \phi(x, y + h; t) + \phi(x - h, y; t) + \phi(x, y - h; t) - 4\phi(x, y; t)]$$

[ ]:
```
phi = phi - k * dt * Fdphi
```

1.7 Results

Plotting the final phase field distribution

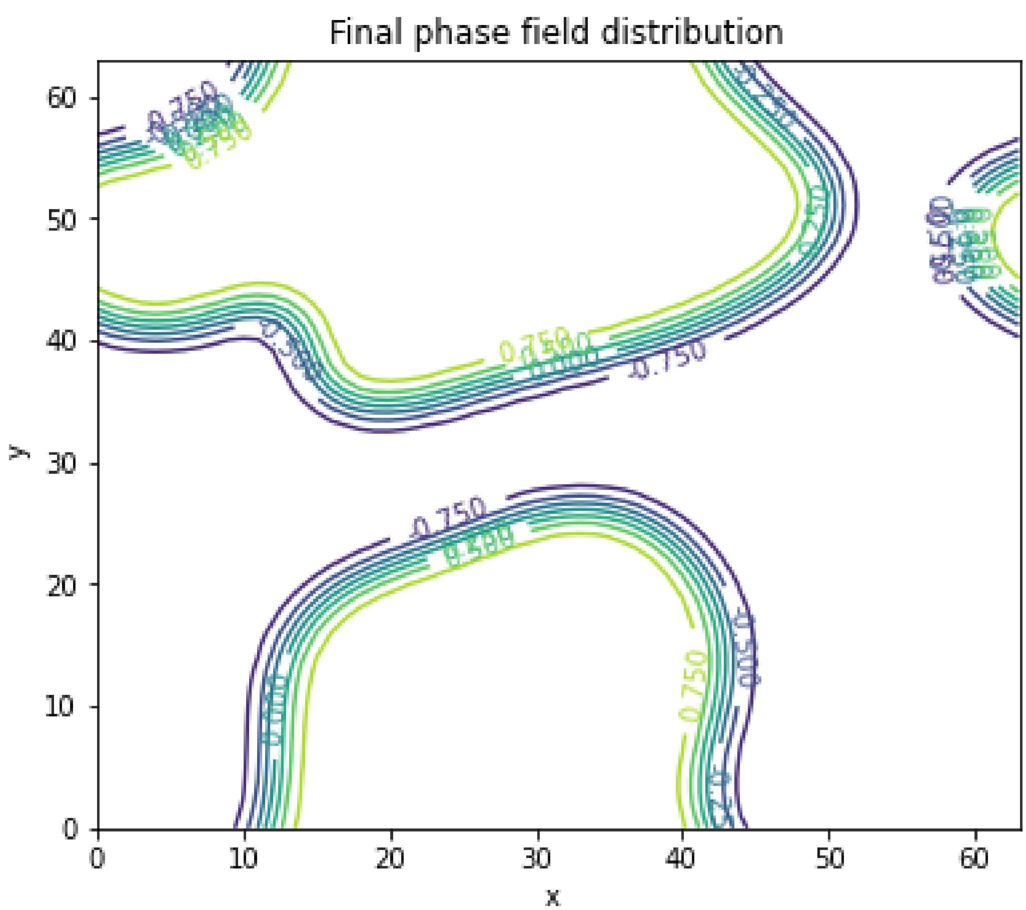
[11]:
```
plt.close('all')

fig = plt.figure(figsize=(6, 5))
left, bottom, width, height = 0.1, 0.1, 0.8, 0.8
ax = fig.add_axes([left, bottom, width, height])

X, Y = np.meshgrid(x, y)

cp = ax.contour(X, Y, phi)
ax.clabel(cp, inline=True,
              fontsize=10)
ax.set_title('Final Phase Field Distribution')
ax.set_xlabel('x ')
ax.set_ylabel('y ')
plt.show()
```

1.7.1 Final Phase field distribution



Plotting the Free energy functional over time

[12]:
```
plt.close('all')

t = np.arange(nsteps)
plt.plot(t, Fplot)
plt.show()
```

1.7.2 Free Energy functional over time