Cahn Hillard Phase Field Solver

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1 CAHN HILLARD PHASE FIELD EQUATION SOLVER : 2D

Importing the required library

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

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
eps = 4                  # Gradient Energy
U = 1                    # Free Energy Multiplier
a = 0.01                 # Initialization parameter
M = 1                    # Diffusion Coefficient
delta = 10**-8           # Tolerance
```

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 = 30000           # 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)
```

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

$$\frac{\partial^2 f}{\partial \phi^2} = 4U(3\phi^2 - 1)$$

[7]:
```
def f2(xk): return 12*np.square(xk) - 4
```

Defining a function to compute third derivative of free energy function w.r.t ϕ

$$\frac{\partial^3 f}{\partial \phi^3} = 24U\phi$$

[8]:
```
def f3(xl): return 24*(xl)
```

Initializing the phase field distribution

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

[9]:
```
phi = np.random.uniform(low=-a / 2, high=a / 2, size=(N, N))
phi1 = np.random.uniform(low=-a+1 / 2, high=a+1 / 2, size=(N, N))
```

Defining arrays for applying the Periodic boundary conditions

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

[10]:
```
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

[11]:
```
Fplot = np.arange(nsteps)
```

1.1 Cahn Hillard phase field evolution equation

Solving the Cahn-Hillard phase field equation

$$\frac{\partial \phi}{\partial t} = \nabla . \left[M \nabla \left(\frac{\delta F[\phi]}{\delta \phi} \right) \right] = M \nabla^2 \left[\frac{\partial f}{\partial \phi} - 2\epsilon \nabla^2 \phi \right]$$
$$\frac{\partial \phi}{\partial t} = M \left[\frac{\partial^2 f}{\phi^2} \nabla^2 \phi + \frac{\partial^3 f}{\phi^3} (\nabla \phi)^2 - 2\epsilon \nabla^4 \phi \right] \equiv g[\phi]$$

[ ]:
```
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

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

[ ]:
```
# Defining a function to compute numerical approximation of Laplacian of phase␣
↪field in 2D using Central Difference method

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

1.3 Central Difference approximation of $\nabla^4 \phi$

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

[ ]:
```
 # Defining a function to compute numerical approximation of Laplacian of␣
↪Laplace using Central Difference Method in 2D
   def llphi(phi) : return ( lphi(phi)[:, plus] +  lphi(phi)[:, minus] + ␣
↪lphi(phi)[plus, :] +lphi(phi)[minus, :] - 4 *  lphi(phi)) / (h * h)
```

1.4 Derivative approximation using Central Difference method

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

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

[ ]:
```
# Derivative of phase field in x direction : dphi/dx, using Central Difference␣
↪Method

    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

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

[ ]:
```
 # Derivative of phase field in y direction : dphi/dy, using Central Difference␣
↪Method

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

1.5 Free energy functional

Computing the numerical approximation of free energy functional in 2D

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

Here ϕ is a two dimensional function, i.e. $\phi(x,y)$. So gradient of $\phi(x,y)$ will have two components $\frac{\partial\phi(x,y)}{x}$ and $\frac{\partial\phi(x,y)}{y}$.

Using this we get the norm of the gradient of the phase fiel as

$$|\nabla\phi(x,y)| = \sqrt{\left(\frac{\partial\phi(x,y)}{x}\right)^2 + \left(\frac{\partial\phi(x,y)}{y}\right)^2}$$

[ ]:
```
    # Computing the numerical approximation of free energy functional in 2D

    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
```

1.6 Computing the numerical approximation $g[\phi]$

$$g[\phi] \equiv \frac{\partial^2 f}{\phi^2}\nabla^2\phi + \frac{\partial^3 f}{\phi^3}(\nabla\phi)^2 - 2\epsilon\nabla^4\phi$$

[ ]:
```
# Computing the numerical approximation of g[phi]

Gdphi = np.multiply (f2(phi),lphi(phi))*U + np.multiply(f3(phi),(np.
↪square(phidx(phi)) + np.square(phidy(phi))))*U - 2 * eps * llphi(phi)
```

1.7 Evolution equation

Computing evolution of the phase field using Cahn-Hillard equation

$$\phi(x,y;t+\Delta t) = \phi(x,y;t) + \frac{\Delta t}{2}.(g[\phi(x,y;t) + g[\phi(x,y;t+\Delta t)]])$$

1.8 Implicit Euler Method Algorithm

STEP 1 : Compute the predictor

$$\phi_0 = \phi(t) + g[\phi(t)].\Delta t$$

STEP 2 : Compute the corrector

$$\phi_1 = \phi(t) + (g[\phi(t)] + g[\phi_0(t)]).\frac{\Delta}{2}t$$

STEP 3 : Compute the error

$$If\ max|\phi_1 - \phi_0| < \delta,\ return\ with\ \phi(x,y;t+\Delta t) := \phi_1$$

STEP 4 : Update the predictor value

$$Else\ set\ \phi_0 := \phi_1\ and\ go\ to\ \textbf{STEP 2}$$

[12]:

```
# Computing evolution of the phase field using Cahn-Hillard equation

# Uncomment this line and comment the lines below this line to run the␣
↪Explicit euler method

#phi = phi + M * dt * Gdphi

# Computing the predictor STEP: 1

phi0 = phi + M * dt * Gdphi

# Setting the initial value for error

error = 1


# Implicit Euler Method

while LA.norm(error) > delta :

    # Computing g[phi_0] to compute the corrector STEP: 2

    Gdphi0 = np.multiply (f2(phi0),lphi(phi0))*U + np.multiply(f3(phi0),(np.
↪square(phidx(phi0)) +np.square(phidy(phi0))))*U - 2 * eps * llphi(phi0)

    # Computing phi_1 corrector STEP: 2

    phi1 = phi + (Gdphi + Gdphi0)*(dt/2)

    # Computing the error STEP: 3

    error = phi1 - phi0

    # Updating the phase field value STEP: 4

    phi0 = phi1

# Computing the phase field in new time step

phi = phi1
```

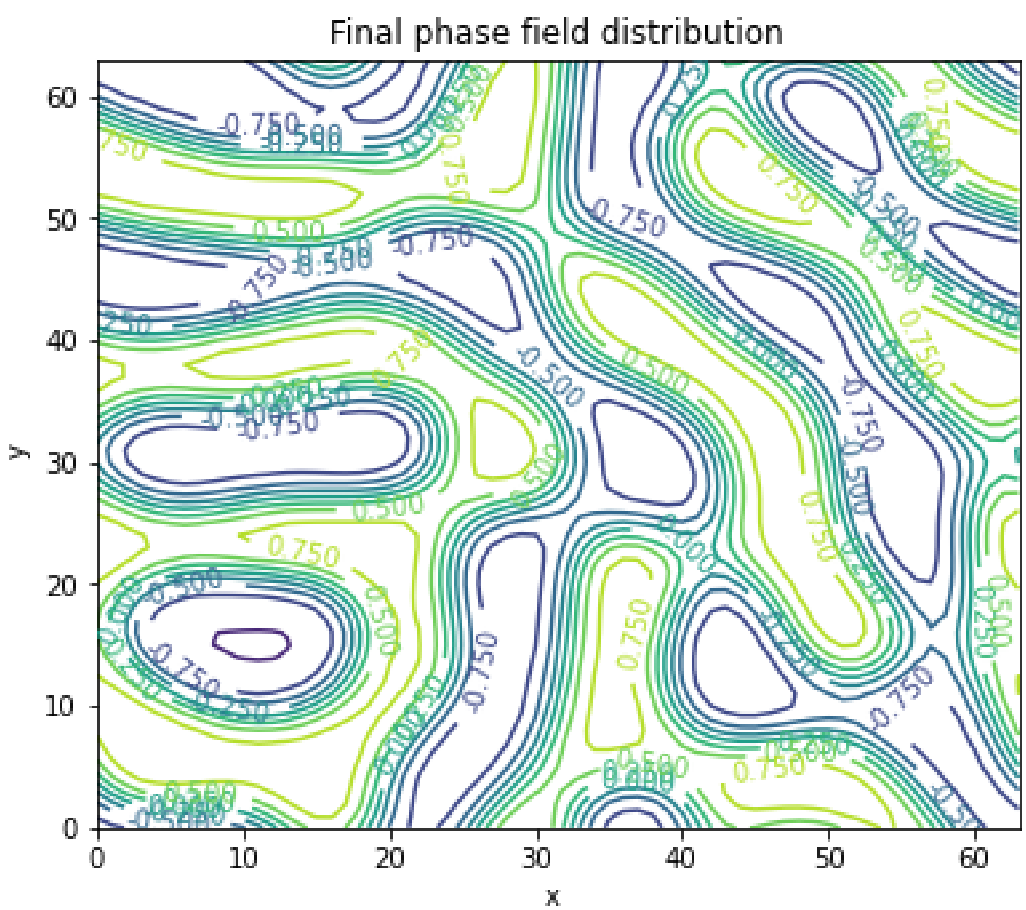
1.9 Plotting the final phase field distribution

[13]:
```python
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()
```



1.10 Plotting the Free energy Functional over time

[14]:
```
plt.close('all')

t = np.arange(nsteps)
plt.plot(t/1000, Fplot/1000)
plt.title("Free energy Functional vs time")
plt.xlabel("time")
plt.ylabel("F/10^3")
plt.show()
```