Solving the Cahn-Hilliard Equation with Finite Difference and Spectral Methods

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Background of Cahn-Hilliard Equation

Cahn-Hilliard Equation

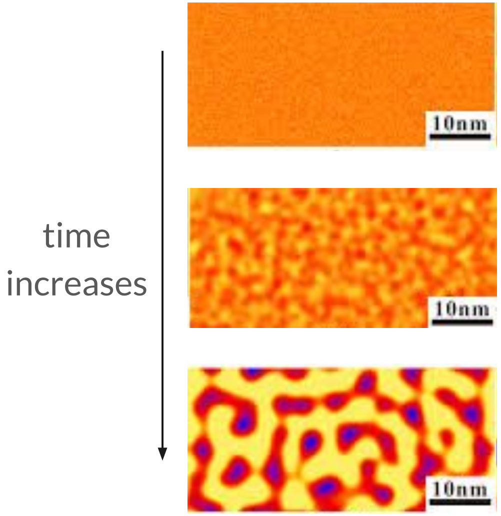
$$\boxed{\frac{\partial c}{\partial t} = D\nabla^2(c^3 - c - \gamma\nabla^2 c)}$$

Ginzburg-Landau Free Energy Functional

$$f = \frac{1}{2}\gamma|\nabla c|^2 + \frac{1}{4}(c^2 - 1)^2$$

Time Evolution of order parameter $c(\vec{x})$

$$\frac{\partial c}{\partial t} = D\nabla^2\frac{\delta f}{\delta c}$$



J. Zhou et al. Journal of Micromechanics and Molecular Physics. (2016)

Project Goals

- **Finite Differences Method**
  - **Spatial Method**
    - 2^{nd} Order Central Difference
    - 4^{th} Order Central Difference
  - **Temporal Method**
    - 1^{st} Order Explicit Euler
    - 4^{th} Order Explicit Runge-Kutta
    - 1^{st} Order Implicit Euler
    - 2^{nd} Order Implicit Crank-Nicolson
- **Spectral Method**
  - 1^{st} Order Explicit
  - 1^{st} Order Semi-Implicit
  - 4^{th} Order Explicit Runge-Kutta

Problem Parameters

Spatial Domain: [-25,25]

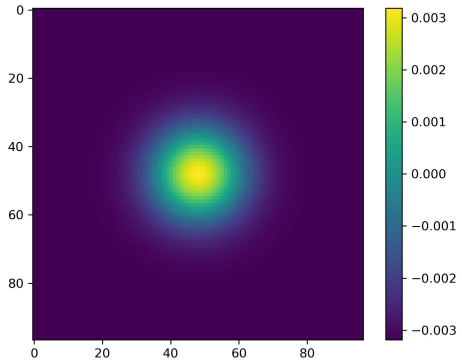
Temporal Domain: [0,60]

Constants: D = 1, ɣ = 1

Boundary conditions: Periodic

Grid Size: 25, 50, 75, 100

Initial Conditions : Bivariate Normal Distribution



Finite Differences

Laplacian

$$\nabla^2_{N^2\times N^2} = I_{N\times N} \otimes D^2_{N\times N} + D^2_{N\times N} \otimes I_{N\times N}$$

Second Order Central Difference

$$\frac{\partial^2 c[i][j]}{\partial x^2} \approx \frac{c[i][j+1] - 2c[i][j] + c[i][j-1]}{dx^2}$$

$$D^2 = \frac{1}{dx^2}\begin{bmatrix} -2 & 1 & 0 & 0 & \dots & 0 & 1 \\ 1 & -2 & 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & -2 & 1 & 0 \\ 0 & 0 & \dots & 0 & 1 & -2 & 1 \\ 1 & 0 & \dots & 0 & 0 & 1 & -2 \end{bmatrix}$$

Fourth Order Central Difference

$$\frac{\partial^2 c[i][j]}{\partial x^2} \approx \frac{-c[i][j+2] + 16c[i][j+1] - 30c[i][j] + 16c[i][j-1] - c[i][j-2]}{12dx^2}$$

$$D^2 = \frac{1}{12dx^2}\begin{bmatrix} -30 & 16 & -1 & 0 & \dots & -1 & 16 \\ 16 & -30 & 16 & -1 & \dots & 0 & -1 \\ -1 & 16 & -30 & 16 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 16 & -30 & 16 & -1 \\ -1 & 0 & \dots & -1 & 16 & -30 & 16 \\ 16 & -1 & \dots & 0 & -1 & 16 & -30 \end{bmatrix}$$

Temporal Schemes - Explicit Methods

$$\frac{\partial c}{\partial t} = \nabla^2(c^3 - c - \nabla^2 c)$$

First Order Forward Euler

$$\frac{c^{k+1} - c^k}{dt} = \nabla^2((c^k)^3 - (c^k) - \nabla^2(c^k))$$

$$c^{k+1} = c^k + dt\nabla^2((c^k)^3 - (c^k) - \nabla^2(c^k))$$

Fourth Order Runge-Kutta

$$k_1 = dtf(c^k)$$

$$k_2 = dtf(c^k + \frac{k_1}{2})$$

$$k_3 = dtf(c^k + \frac{k_2}{2})$$

$$k_4 = dtf(c^k + k_3)$$

$$c^{k+1} = c^k + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

Temporal Schemes - Implicit Methods

$$\frac{\partial c}{\partial t} = \nabla^2(c^3 - c - \nabla^2 c)$$

First Order Backward Euler

$$\frac{c^{k+1} - c^k}{dt} = \nabla^2((c^{k+1})^3 - (c^{k+1}) - \nabla^2(c^{k+1}))$$

$$\underbrace{[I + dt\nabla^2 + dt\nabla^2\nabla^2]}_{A}\, c^{k+1} = \underbrace{c^k + dt\nabla^2(c^{k+1})^3}_{b}$$

Second Order Crank-Nicolson

$$\frac{c^{k+1} - c^k}{dt} = \frac{1}{2}\nabla^2((c^k)^3 - (c^k) - \nabla^2(c^k)) + \frac{1}{2}\nabla^2((c^{k+1})^3 - (c^{k+1}) - \nabla^2(c^{k+1}))$$

$$\underbrace{[I + \frac{dt}{2}\nabla^2 + \frac{dt}{2}\nabla^2\nabla^2]}_{A}\, c^{k+1} = \underbrace{c^k + \frac{dt}{2}\nabla^2(c^{k+1})^3 + \frac{dt}{2}\nabla^2((c^k)^3 - (c^k) - \nabla^2(c^k))}_{b}$$

Spectral Methods

Cahn-Hilliard Equation in Fourier Space $$\frac{\partial \tilde{c}}{\partial t} = -k^2(\tilde{g} + k^2\tilde{c})$$ $$g = c^3 - c$$

First Order Forward Euler

$$\frac{\tilde{c}^{j+1} - \tilde{c}^j}{dt} = -k^2(\tilde{g}^j + k^2\tilde{c}^j)$$

$$\tilde{c}^{j+1} = \tilde{c}^j - dtk^2(\tilde{g}^j + k^2\tilde{c}^j)$$

Fourth Order Runge-Kutta

$$f(\tilde{g}^j, \tilde{c}^j) = -k^2(\tilde{g}^j + k^2\tilde{c}^j)$$

$$d_1 = dt f(\tilde{g}^j, \tilde{c}^j)$$
$$d_2 = dt f(\tilde{g}_1^{j+1/2}, \tilde{c}^j + d_1/2)$$
$$d_3 = dt f(\tilde{g}_2^{j+1/2}, \tilde{c}^j + d_2/2)$$
$$d_4 = dt f(\tilde{g}_1^{j+1}, \tilde{c}^j + d_3)$$

$$\tilde{c}^{j+1} = \tilde{c}^j + \frac{1}{6}(d_1 + 2d_2 + 2d_3 + d_4)$$

First Order Semi-implicit

$$\frac{\tilde{c}^{j+1} - \tilde{c}^j}{dt} = -k^2(\tilde{g}^j + k^2\tilde{c}^{j+1})$$

$$\tilde{c}^{j+1} = \frac{\tilde{c}^j - dtk^2\tilde{g}^j}{1 + k^4 dt}$$

Comparison of Central Difference Methods

Spatial Method (with 1st Order Forward Euler)	Runtimes (s)
2nd Order Central Difference	80.86
4th Order Central Difference	99.05

Spatial Method (with 4th Order Explicit Runge-Kutta)	Runtime (s)
2nd Order Central Difference	208.45
4th Order Central Difference	246.97

Comparison of Explicit/Implicit Time Methods

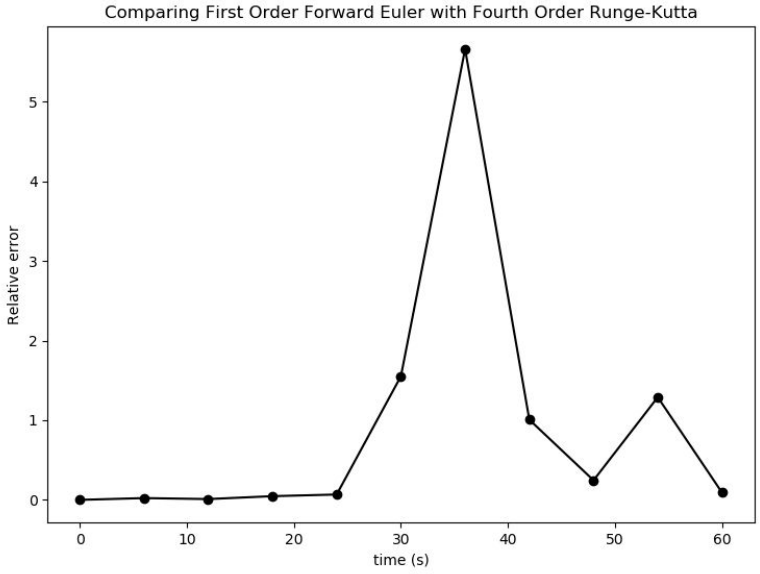
Temporal Methods (with 4^{th} Order Central Difference)	**dt_{max} (s)**	**Runtimes (s)**
1^{st} Order Explicit Euler	0.001	89.14
4^{th} Order Explicit Runge-Kutta	0.001	232.44
1^{st} Order Implicit Euler	0.1	794.64
2^{nd} Order Crank Nicolson	0.5	179.08

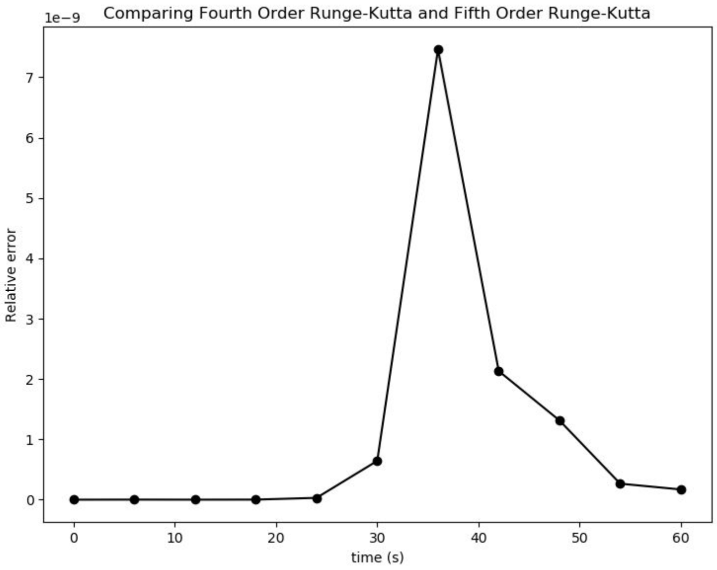
Linear Cahn-Hilliard Equation

$$\frac{\partial c}{\partial t} = \nabla^2(-c - \nabla^2 c)$$

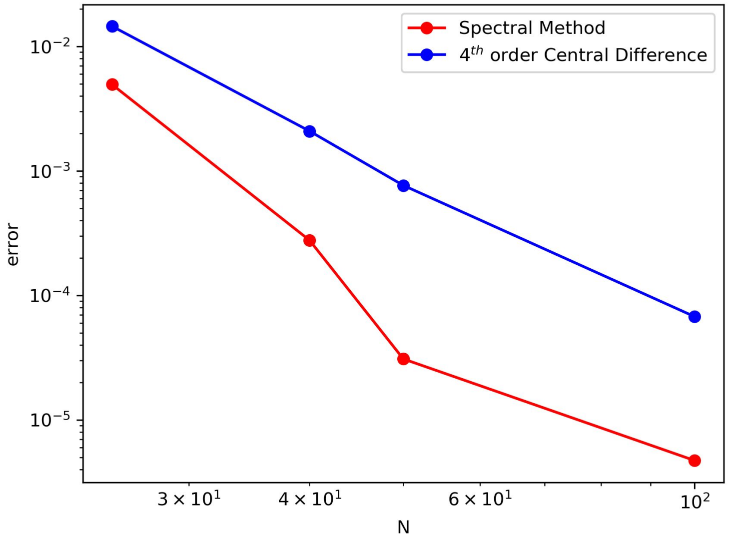
Integration Scheme	dt (s)	**Runtime (s)**
First Order Backward Euler	1	10.01
Second Order Crank Nicolson	2	7.29

Comparison of Explicit Methods





Comparison of Finite Differences and Spectral



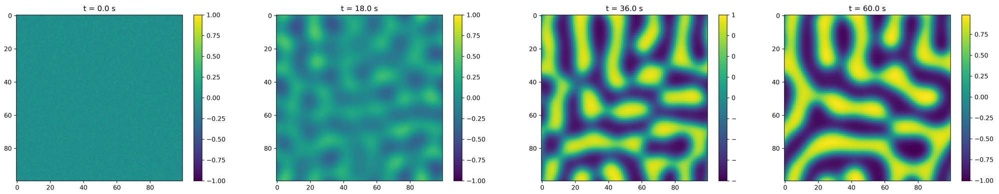
$dt = 0.0004s$ Temporal method: 4th order Runge-Kutta

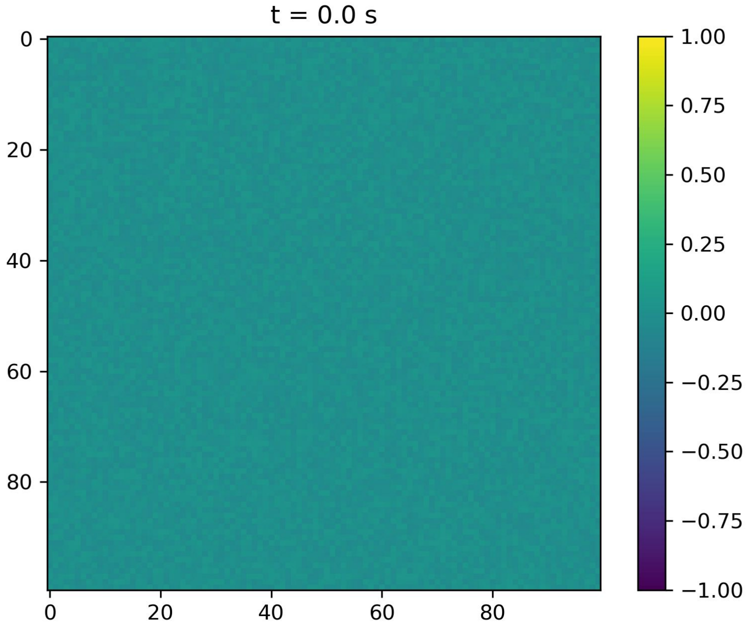
Number of grid points in one direction (N)	Runtime of 4th order Central Difference (s)	Runtime of Spectral Method (s)
25	32.55	87.16
40	54.72	119.91
50	73.50	146.53
100	233.98	381.69

Metric for accuracy: 4th order Central Difference with N=200, dt =0.00008s

Optimal Method with Random Initial Conditions

Simulated phase separation using random initial fluctuations bounded by 0.05, spectral in space, RK4 in time, on a 100 x 100 grid for $L = 50$, $T = 60$. Color represents phase concentration. x and y values correspond to *jth* and *ith* entries in *c[i][j]* matrix, respectively.





Summary of Results

- 4CD > 2CD
- Explicit methods > implicit methods for Cahn-Hilliard
- Implicit methods > explicit methods for Linear Cahn-Hilliard
- Constructed an estimate for the ‘truth’ with a conservative bound on the error
- Spectral methods > finite differences for Cahn-Hilliard with periodic BCs