Numerical Analysis of the Cahn-Hillard Equation with Runge-Kutta Methods

APC 523 Final Project

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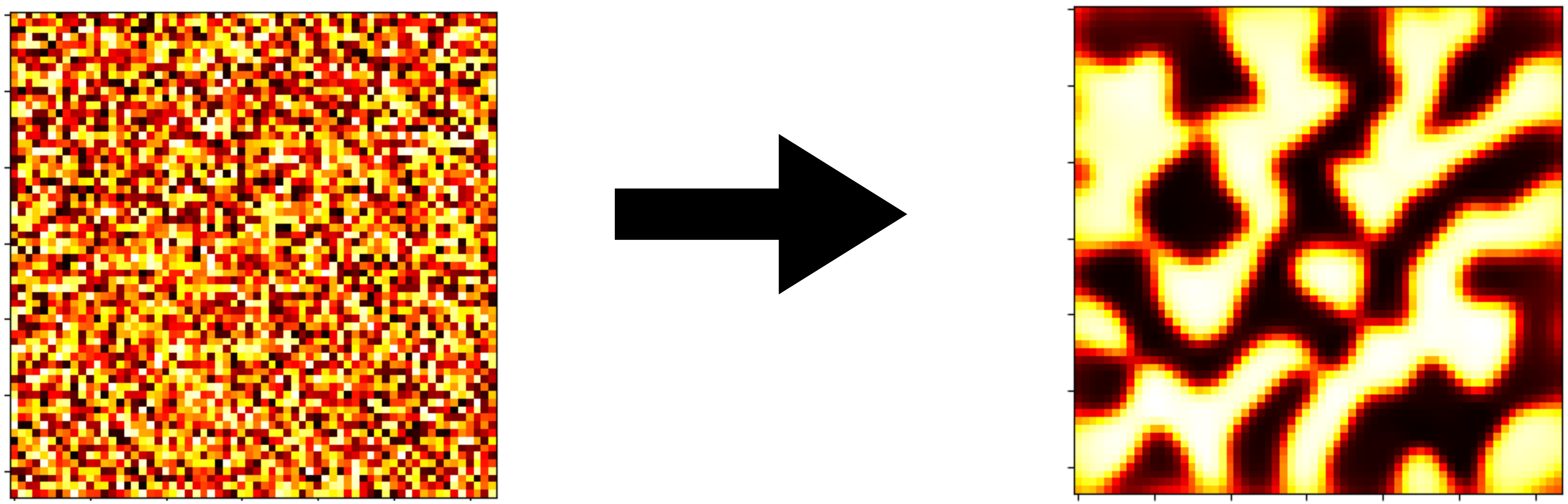
Spinodal Decomposition

Introduction to Highly Disordered Materials

- Spontaneous phase transition in binary materials from homogenous mix to islands rich in one component and matrix rich in the other



- Governed by the Cahn-Hillard Equation

$$\frac{\partial \mathbf{c}}{\partial t}(\mathbf{x}, t) = \nabla \cdot [M(\mathbf{c}) \cdot \nabla \mu(\mathbf{c})], \quad \mathbf{c} \in \Omega, \ t > 0$$

Intuition of Cahn-Hillard Equation

Reduces total energy of the system

$$E(\mathbf{c}, t) = \int_{\Omega} \frac{\kappa}{2} |\nabla \mathbf{c}|^2 + f(\mathbf{c}, t) d\mathbf{x}$$

System will reduce energy by minimizing these values

Coarsening
Reduce the number of interfaces between the two components

Separation
Find concentrations that minimize the local atomic energy

Intuition of Cahn-Hillard Equation

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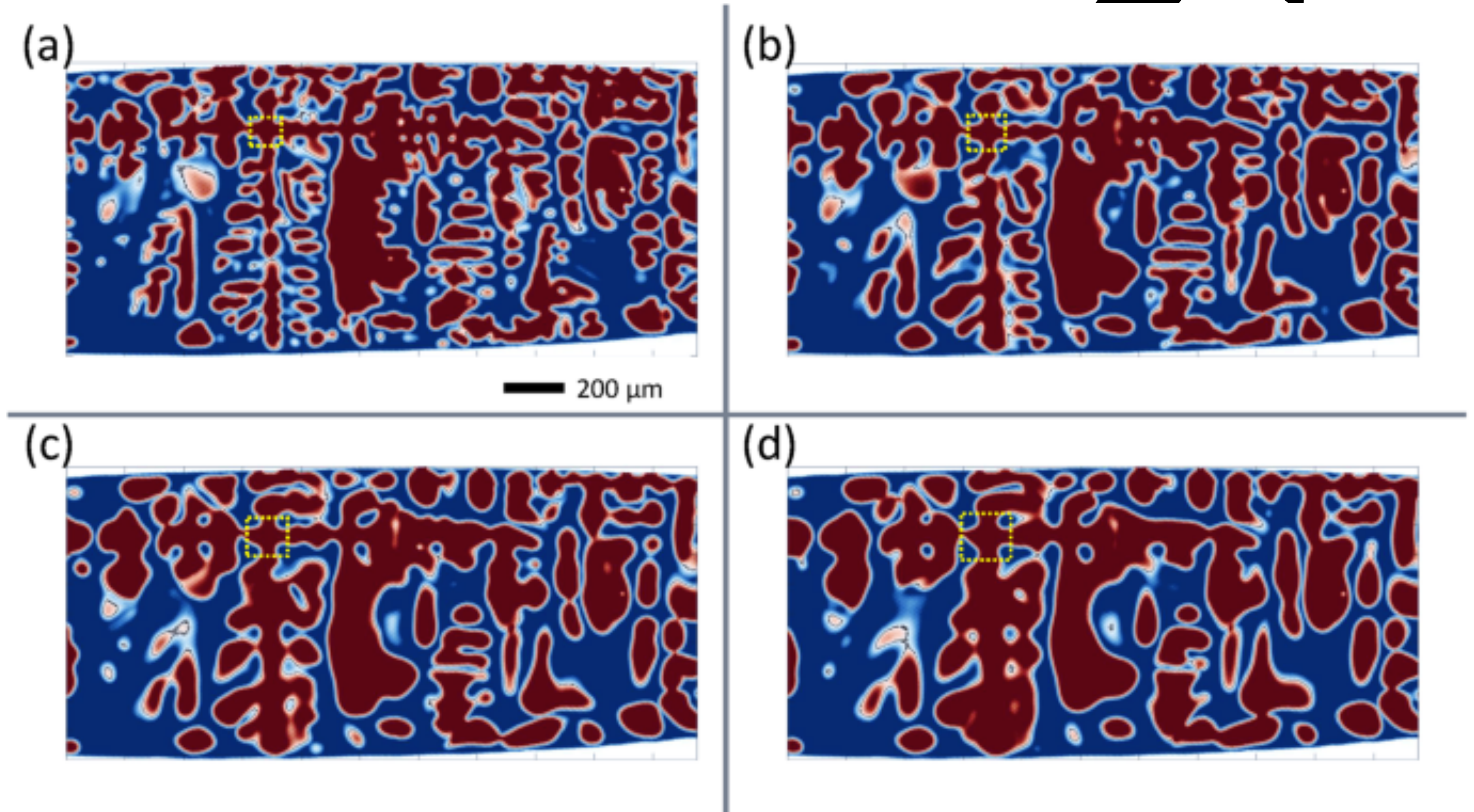
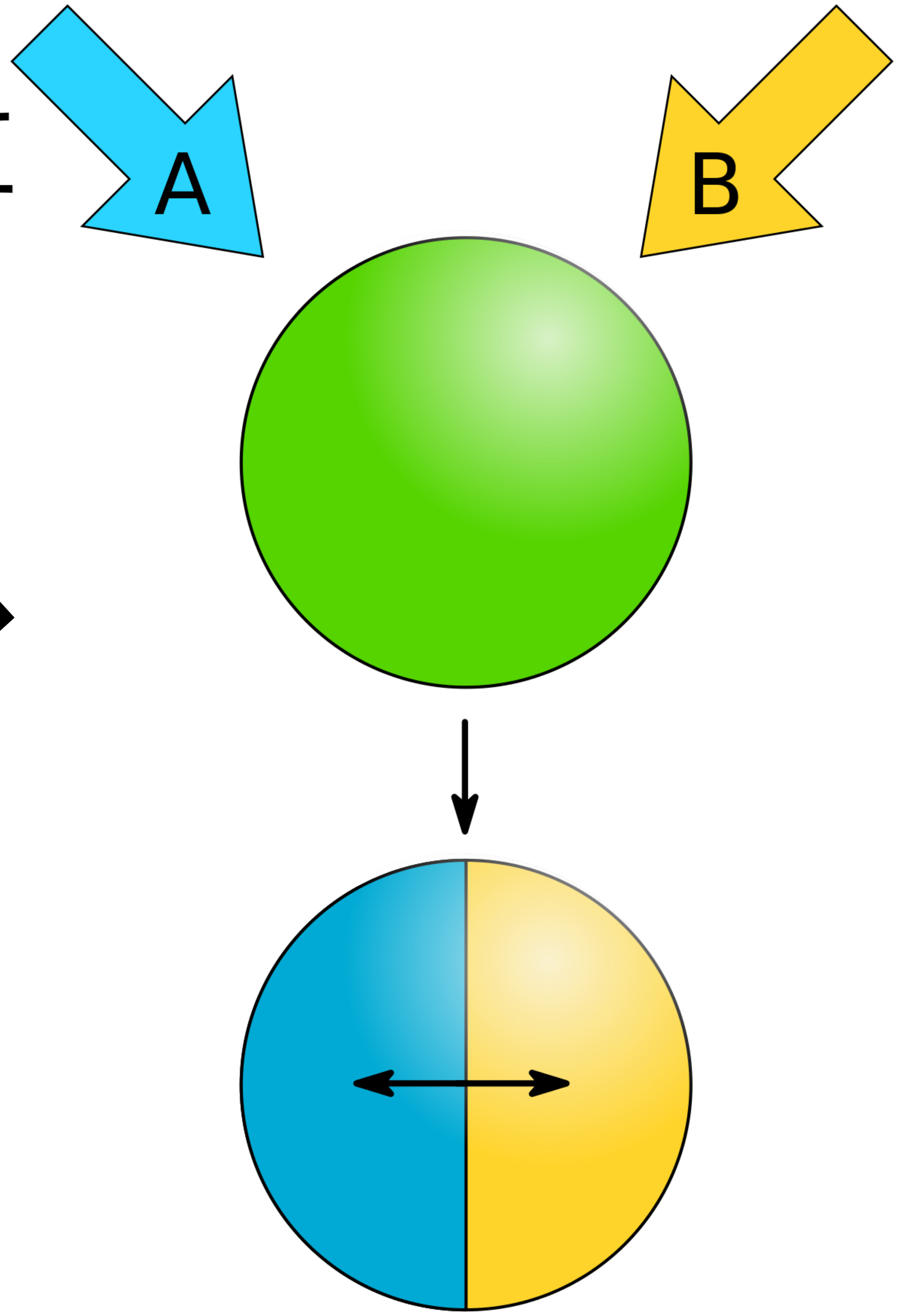




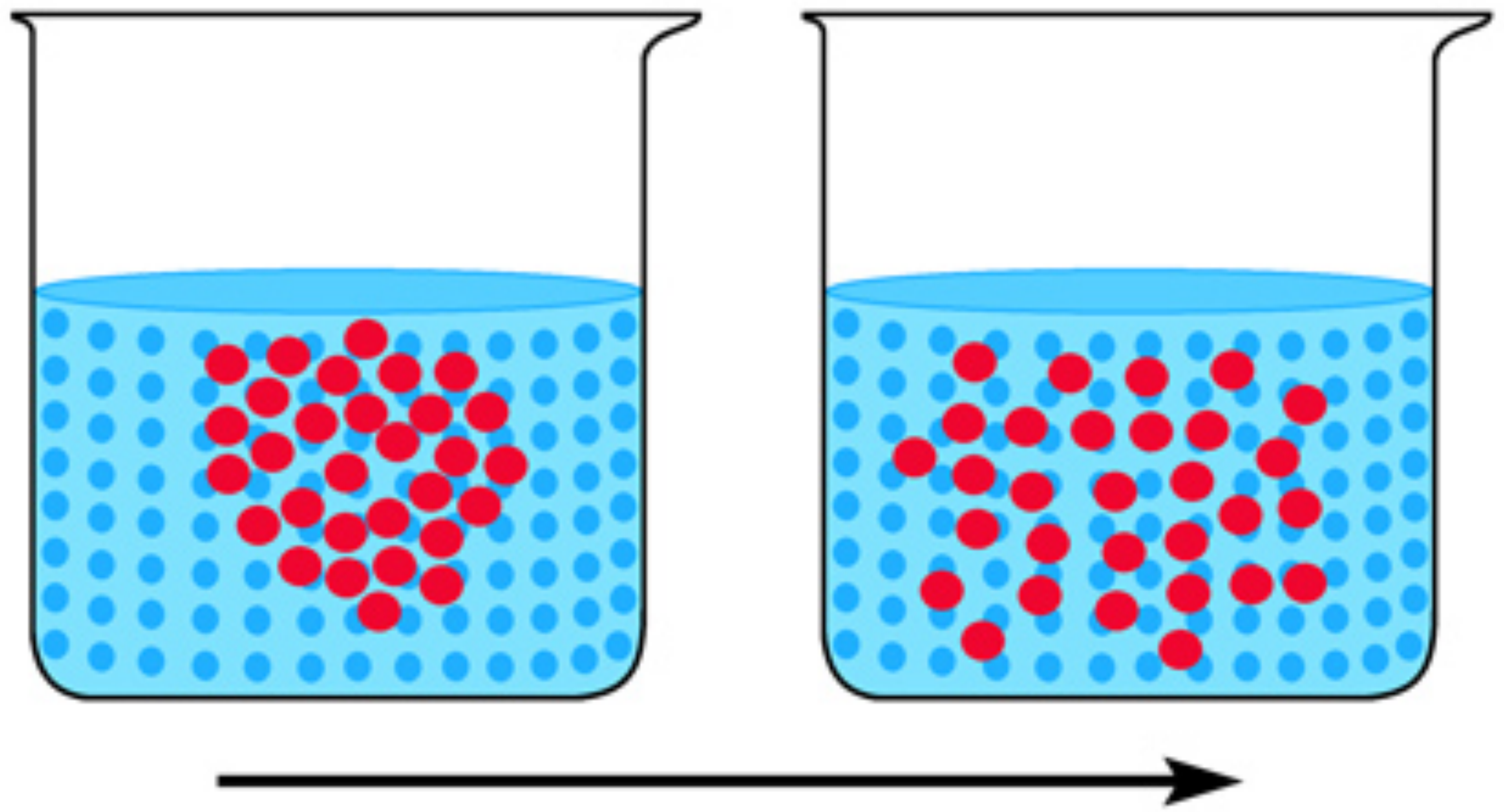
Derivation of Cahn-Hillard Equation

Frick's First and Second Laws

Movement of a component (diffusive flux) is related to concentration gradient.

Isolated systems chemical potential drives configuration change

$$J = -M(\mathbf{x}, t) \cdot \nabla \mu(\mathbf{c}, t)$$



Particles diffusing from high to low concentration

Diffusing component must obey the *conservation of mass* and the continuity equation

$$0 = \frac{\partial \mathbf{c}}{\partial t}(\mathbf{x}, t) + \nabla J$$

$$\frac{\partial \mathbf{c}}{\partial t}(\mathbf{x}, t) = \nabla \cdot [M(\mathbf{c}) \cdot \nabla \mu(\mathbf{c})],$$

Derivation of *Modified* Cahn-Hillard Equation

Chemical potential is the rate of change of energy!

$$\frac{\partial \mathbf{c}}{\partial t}(\mathbf{x}, t) = \nabla \cdot [M(\mathbf{c}) \cdot \nabla \mu(\mathbf{c})],$$

$$0 = \frac{\partial \mathbf{c}}{\partial t}(\mathbf{x}, t) - \nabla \left(M(\mathbf{x}, t) \cdot \nabla \frac{\partial E(\mathbf{c}, t)}{\partial c} \right)$$

$$0 = \frac{\partial \mathbf{c}}{\partial t}(\mathbf{x}, t) - \nabla \left(M(\mathbf{x}, t) \cdot \nabla \left(-\kappa \nabla^2 \mathbf{c} + \frac{df(\mathbf{c}, t)}{d\mathbf{c}} \right) \right)$$

$$\frac{\partial \mathbf{c}}{\partial t}(\mathbf{x}, t) = \nabla \left(M(\mathbf{x}, t) \cdot \nabla \left(\frac{\partial f(\mathbf{c}, t)}{\partial \mathbf{c}} - \kappa \nabla^2 c \right) \right)$$

Equilibrium of *Modified* Cahn-Hillard Equation

Minimize total energy by coarsening and minimize f(c)

$$\frac{\partial \mathbf{c}}{\partial t}(\mathbf{x}, t) = \nabla \left(M(\mathbf{x}, t) \cdot \nabla \left(\frac{\partial f(\mathbf{c}, t)}{\partial \mathbf{c}} - \kappa \nabla^2 c \right) \right)$$

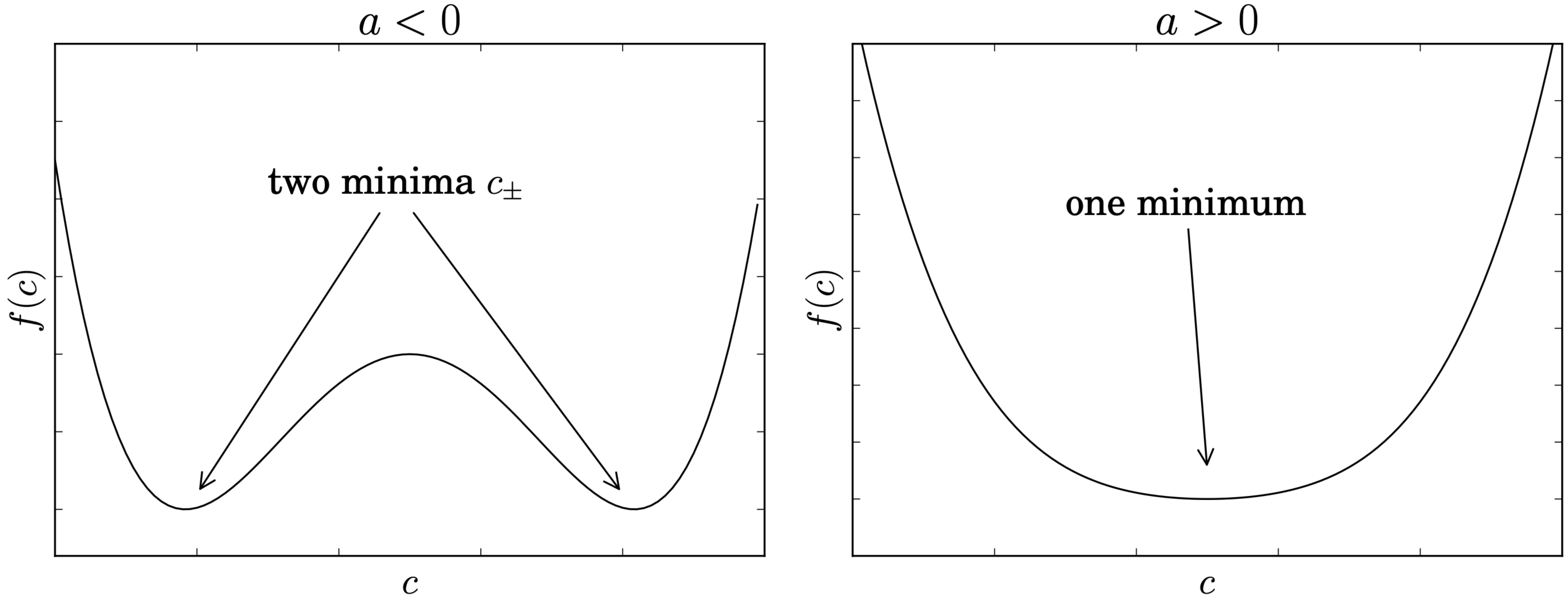
Reasonable approximation of real local energy binary system is a polynomial double well potential

$$f(\mathbf{c}, t) = \frac{a(t)\mathbf{c}^2}{2} + \frac{b(t)\mathbf{c}^4}{4}$$

Equilibrium of *Modified* Cahn-Hillard Equation

Spinodal Decomposition occurs when a < 0

$$f(\mathbf{c}, t) = \frac{a(t)\mathbf{c}^2}{2} + \frac{b(t)\mathbf{c}^4}{4}$$



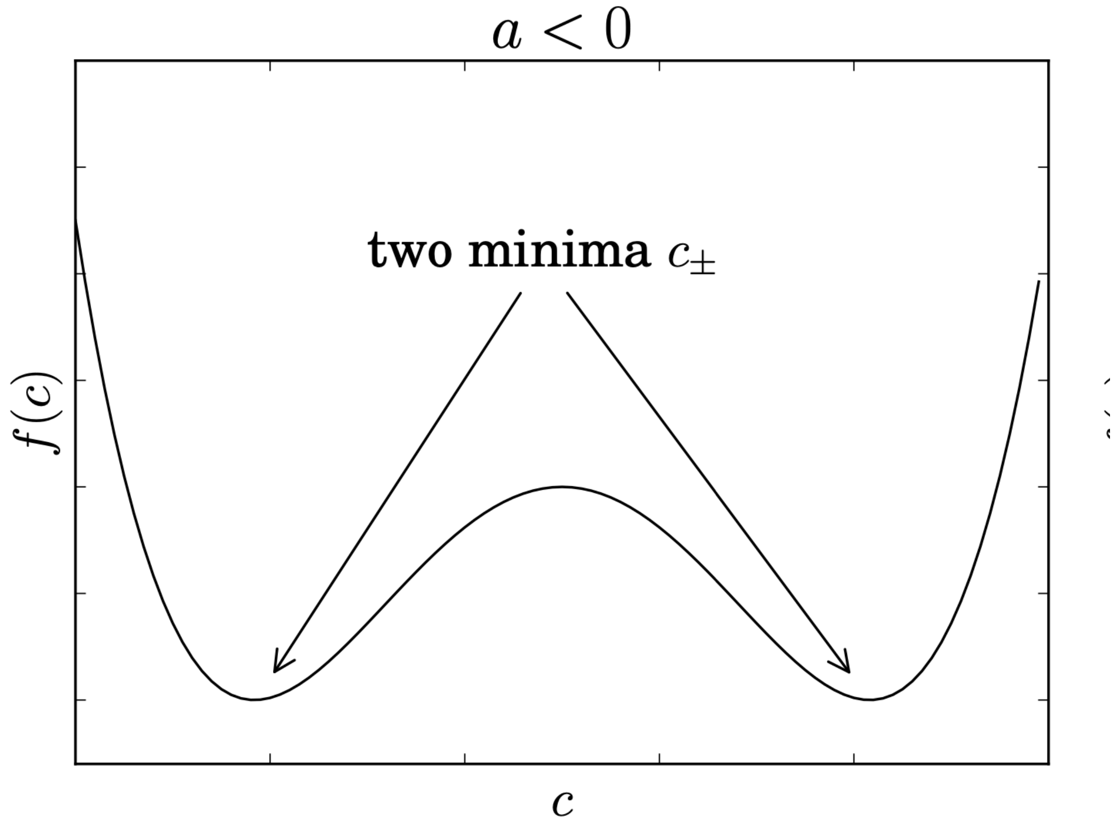
Simple *Modified* Cahn-Hillard Equation

System will quickly separate and slowly coarsen

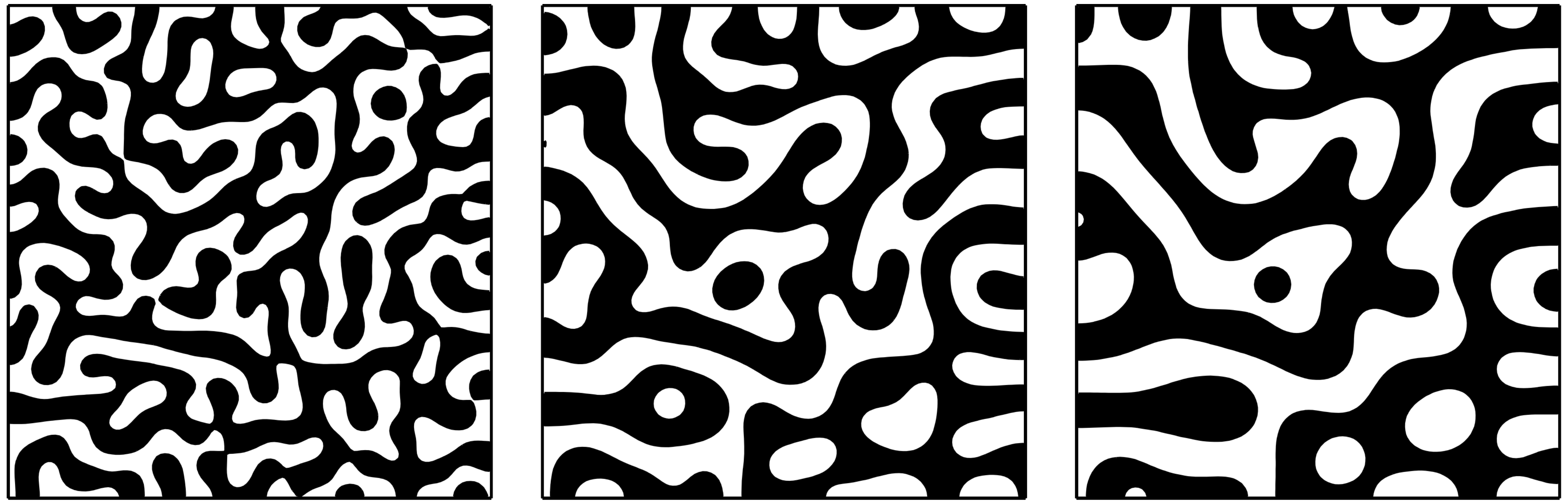
$$\frac{\partial \mathbf{c}}{\partial t}(\mathbf{x}, t) = \nabla(M_0(\mathbf{x}, t) \cdot \nabla \mu(\mathbf{c}, t))$$

$$\mu(\mathbf{c}, t) = b\mathbf{c}^3 + a\mathbf{c} - \kappa \nabla^2 \mathbf{c}$$

Quickly system separates into two minima at -1 and 1



Slowly the system will reduce barriers via coarsening



Numerical Scheme Methodology for Cahn-Hillard Equation

Stiff non-linear fourth order partial differential equation

<u>Need schemes with following traits:</u>

- *Symplectic* inheriting decreasing energy

- *Time adaptivity* due to the drastically different time scales of separation and coursing

- Ideally be *L-stable*

Finite Difference Spatial Discretization

2nd Order Central Finite Difference for Simplicity

$$\frac{\partial \mathbf{c}}{\partial t}(\mathbf{x}, t) = M_0 \Delta_h f'(\mathbf{c}) - M_0 \kappa \Delta_h^2 \mathbf{c} \tag{17}$$

where

$$\Delta_h f'(\mathbf{c}) = \frac{f'(\mathbf{c}_{i-1,j}) - 2f'(\mathbf{c}_{i,j}) + f'(\mathbf{c}_{i+1,j})}{h^2} + \frac{f'(\mathbf{c}_{i,j-1}) - 2f'(\mathbf{c}_{i,j}) + f'(\mathbf{c}_{i,j+1})}{h^2} \tag{18}$$

$$\Delta_h \mathbf{c} = \frac{\mathbf{c}_{i-1,j} - 2\mathbf{c}_{i,j} + \mathbf{c}_{i+1,j}}{h^2} + \frac{\mathbf{c}_{i,j-1} - 2\mathbf{c}_{i,j} + \mathbf{c}_{i,j+1}}{h^2} \tag{19}$$

$$\Delta_h^2 \mathbf{c} = \frac{\mathbf{c}_{i-2,j} - 4\mathbf{c}_{i-1,j} + 6\mathbf{c}_{i,j} - 4\mathbf{c}_{i+1,j} + \mathbf{c}_{i+2,j}}{h^4} + \frac{\mathbf{c}_{i,j-2} - 4\mathbf{c}_{i,j-1} + 6\mathbf{c}_{i,j} - 4\mathbf{c}_{i,j+1} + \mathbf{c}_{i,j+2}}{h^4} \tag{20}$$

Benefit: Preserves the non-linearity of functional f

Finite Difference Spatial Discretization

Von Neumann Stability Analysis

Assume linear solution requiring linearization of *f*(c) around a minima

$$\mathbf{c}(\mathbf{x}, t) = c_0 e^{ikx} e^{\Omega_r t} e^{i\Omega_i t}$$

$$\Omega = -\frac{8M_0}{h^2}\sin^2\left(\frac{kh}{2}\right) - \frac{16M_0\kappa}{h^4}\sin^4\left(\frac{kh}{2}\right)$$

Always negative! Not producing periodic oscillations and decreasing

Runge Kutta Temporal Schemes

A Family of Multi-Stage Explicit and Implicit Schemes

Recall given a Butcher table, we have

$$
\begin{array}{c|cccc}
c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\
c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\
\hline
 & b_1 & b_2 & \cdots & b_s
\end{array}
$$

$$
\begin{aligned}
y_{n+1} &= y_n + h \sum_{i=1}^{s} b_i k_i \\
k_1 &= f(t_n, y_n), \\
k_2 &= f(t_n + c_2 h, y_n + h(a_{21} k_1)), \\
k_3 &= f(t_n + c_3 h, y_n + h(a_{31} k_1 + a_{32} k_2)), \\
&\;\;\vdots \\
k_i &= f\left(t_n + c_i h, y_n + h \sum_{j=1}^{i-1} a_{ij} k_j\right).
\end{aligned}
$$

Explicit 1 Stage Runge Kutta

$C_1 = M_0\kappa\frac{\Delta t}{h^4}$ and $C_2 = M_0\frac{\Delta t}{h^2}$

Stability of Forward Euler Scheme + FD

$$\frac{\partial \mathbf{c}}{\partial t} = \frac{\mathbf{c}_{ij}^{n+1} - \mathbf{c}_{ij}^{n}}{\Delta t} \qquad \frac{\partial \mathbf{c}}{\partial t}(\mathbf{x}, t) = M_0\Delta_h f'(\mathbf{c}) - M_0\kappa\Delta_h^2\mathbf{c}$$

The stability condition for the FE scheme is $(1+\Omega_r\Delta t)^2 + \Omega_i^2\Delta t^2 < 1$

$$\Omega_r\Delta t = -16C_1\mathrm{sin}^4\left(\frac{kh}{2}\right) - 8C_2\mathrm{sin}^2\left(\frac{kh}{2}\right) > -16C_1 - 8C_2 > -2$$

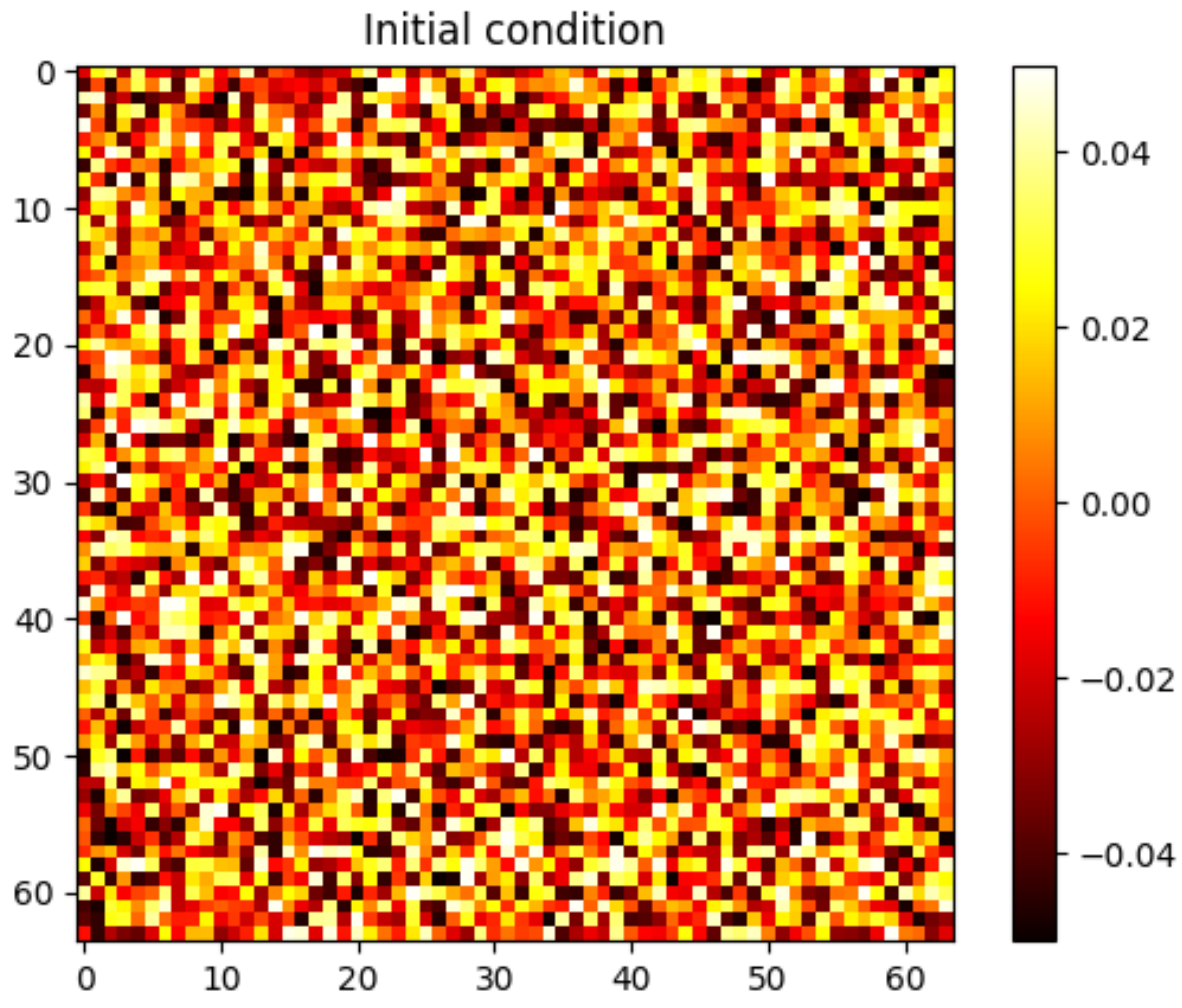
$$2C_1 + C_2 < \frac{1}{4}$$

Extremely restrictive conditions due to stiffness! Doubling spatial mesh requires time step to increase by 16!

Initial Condition for ALL Schemes

Implement Periodic Neumann Boundary Conditions

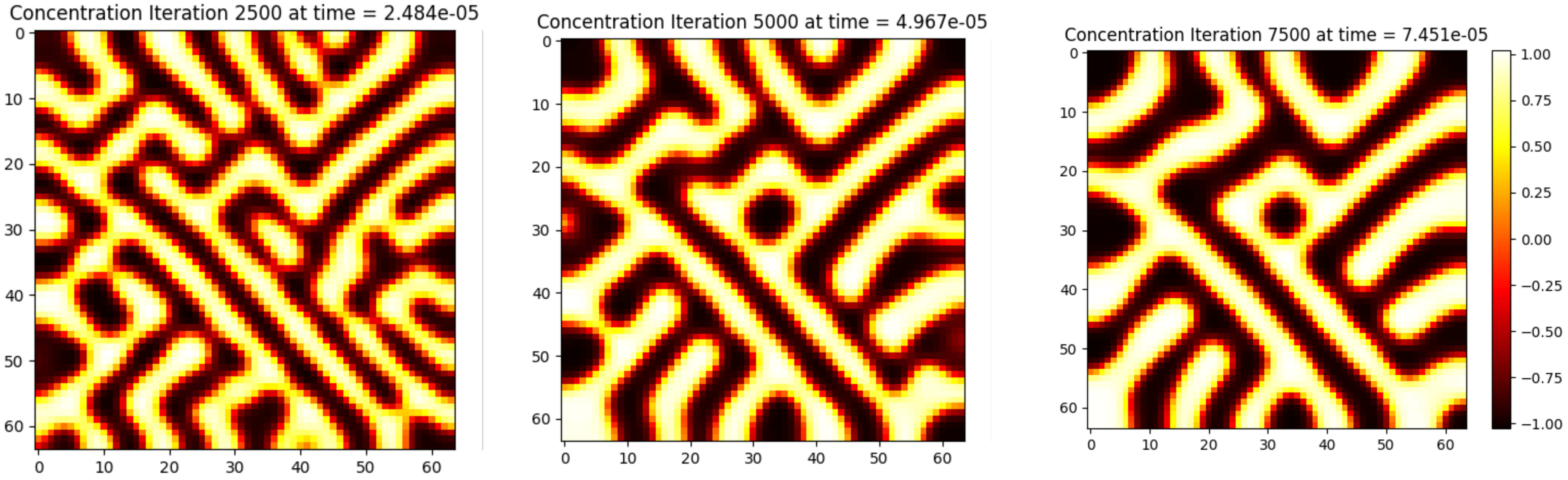
Uniformly random distribution around 0



Explicit 1 Stage Runge Kutta Results

Dynamics of Cahn-Hillard with Forward Euler Scheme + FD

Restricted simulation to 1000 time steps/iterations. Time steps must be 10% of Courant for stability

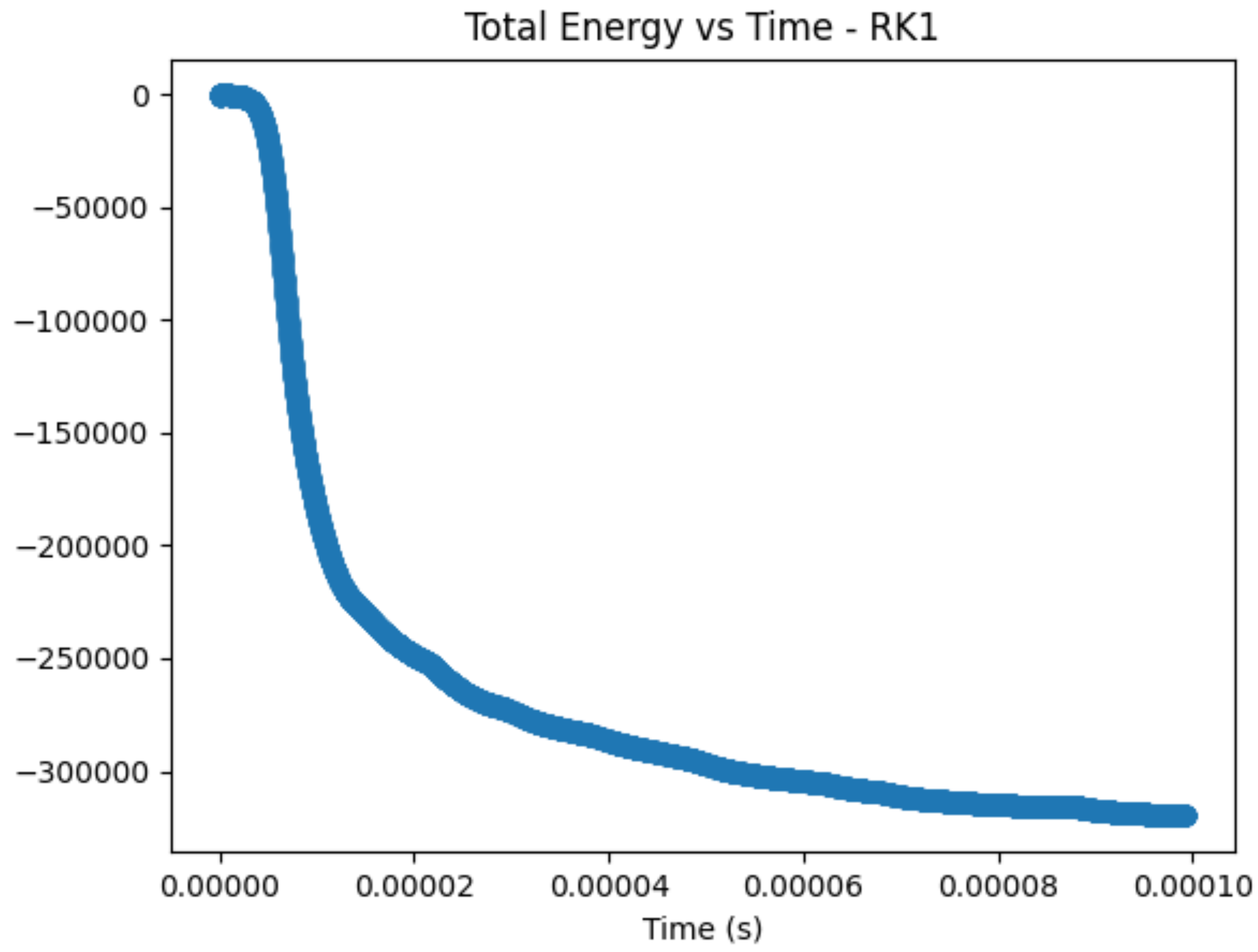


Dynamics are correct but time steps are too small for slow coarsening process

Explicit 1 Stage Runge Kutta Results

Dynamics of Cahn-Hillard with Forward Euler Scheme + FD

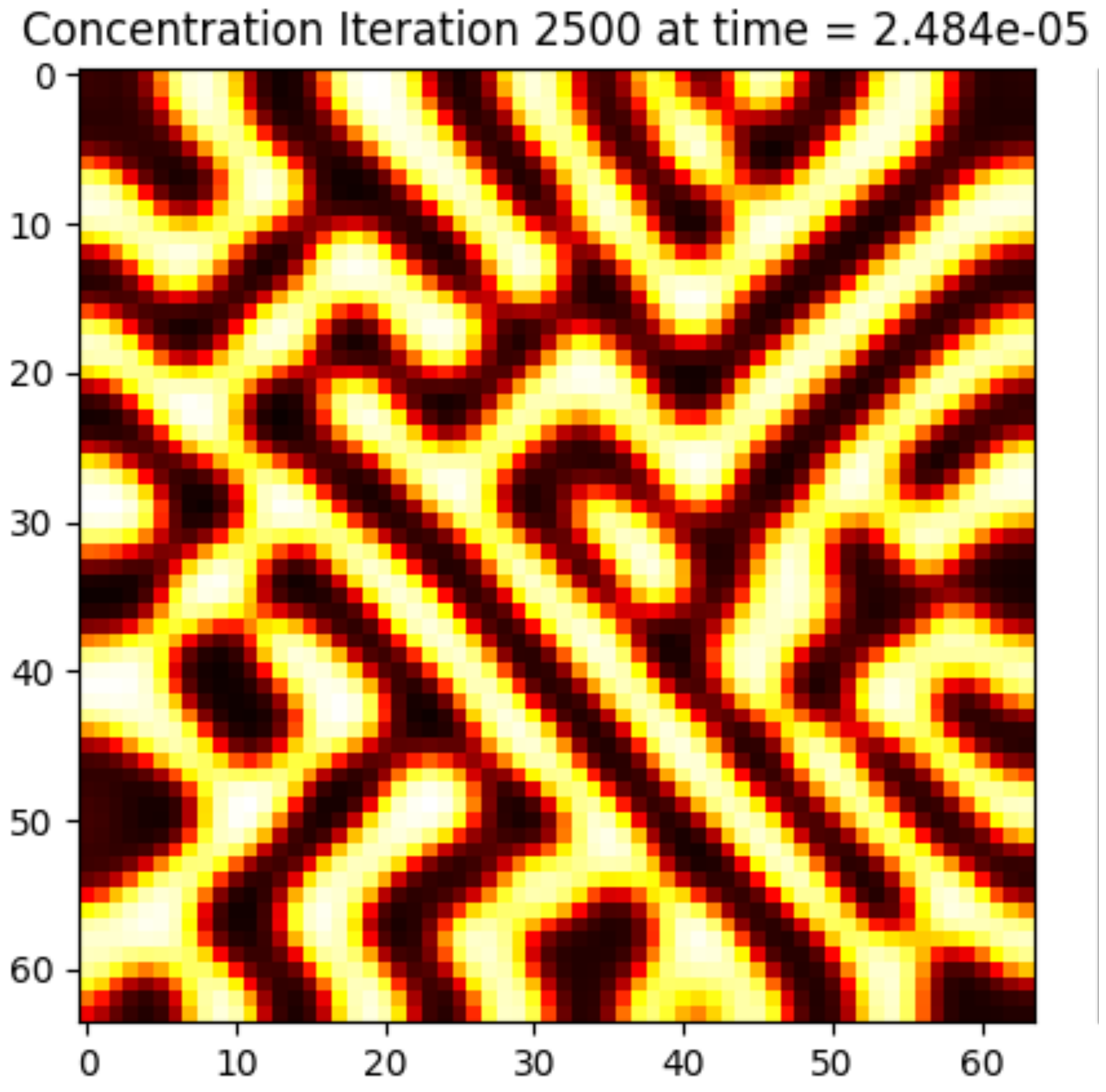
Inherits Decreasing Energy as Expected

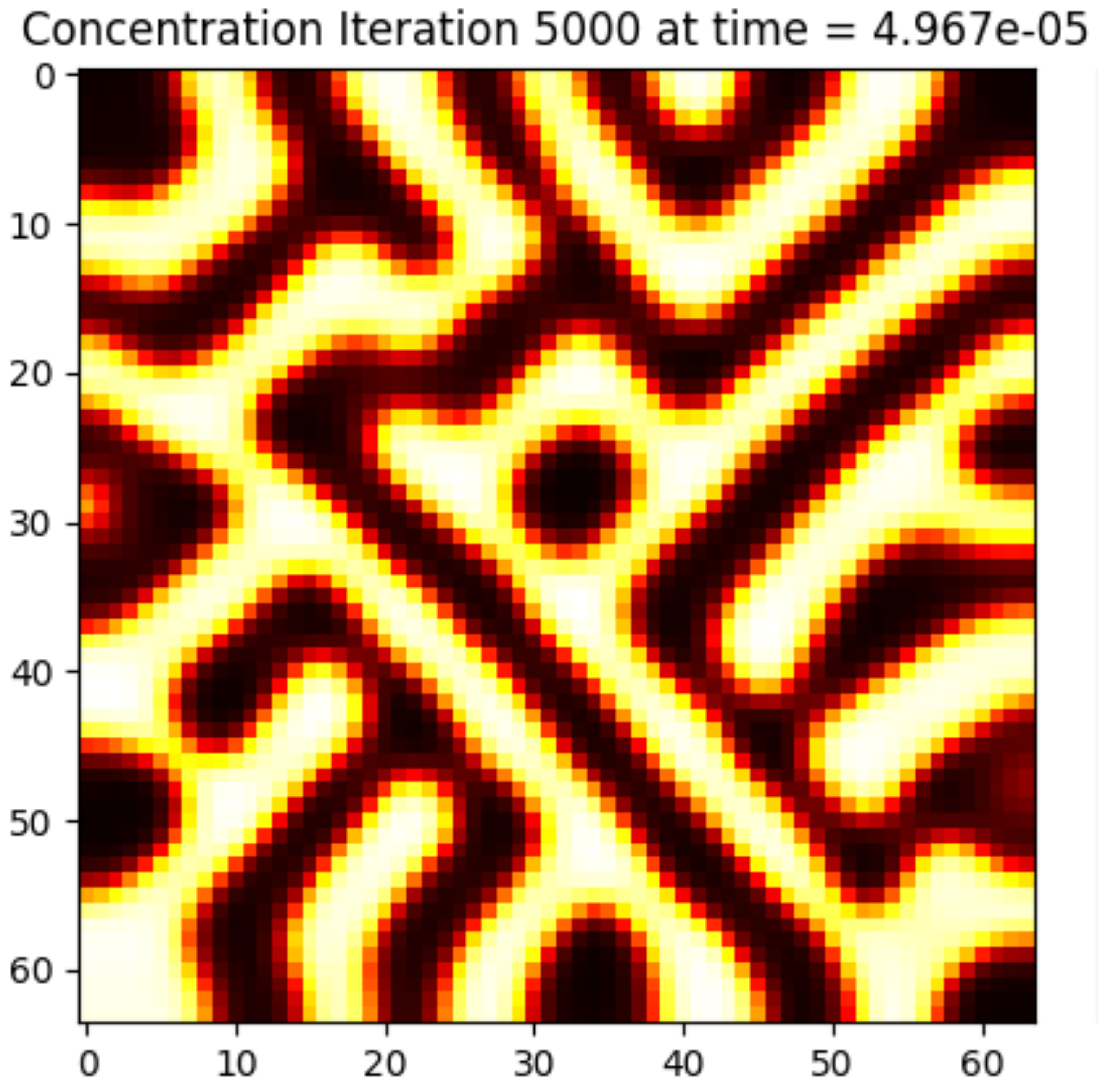


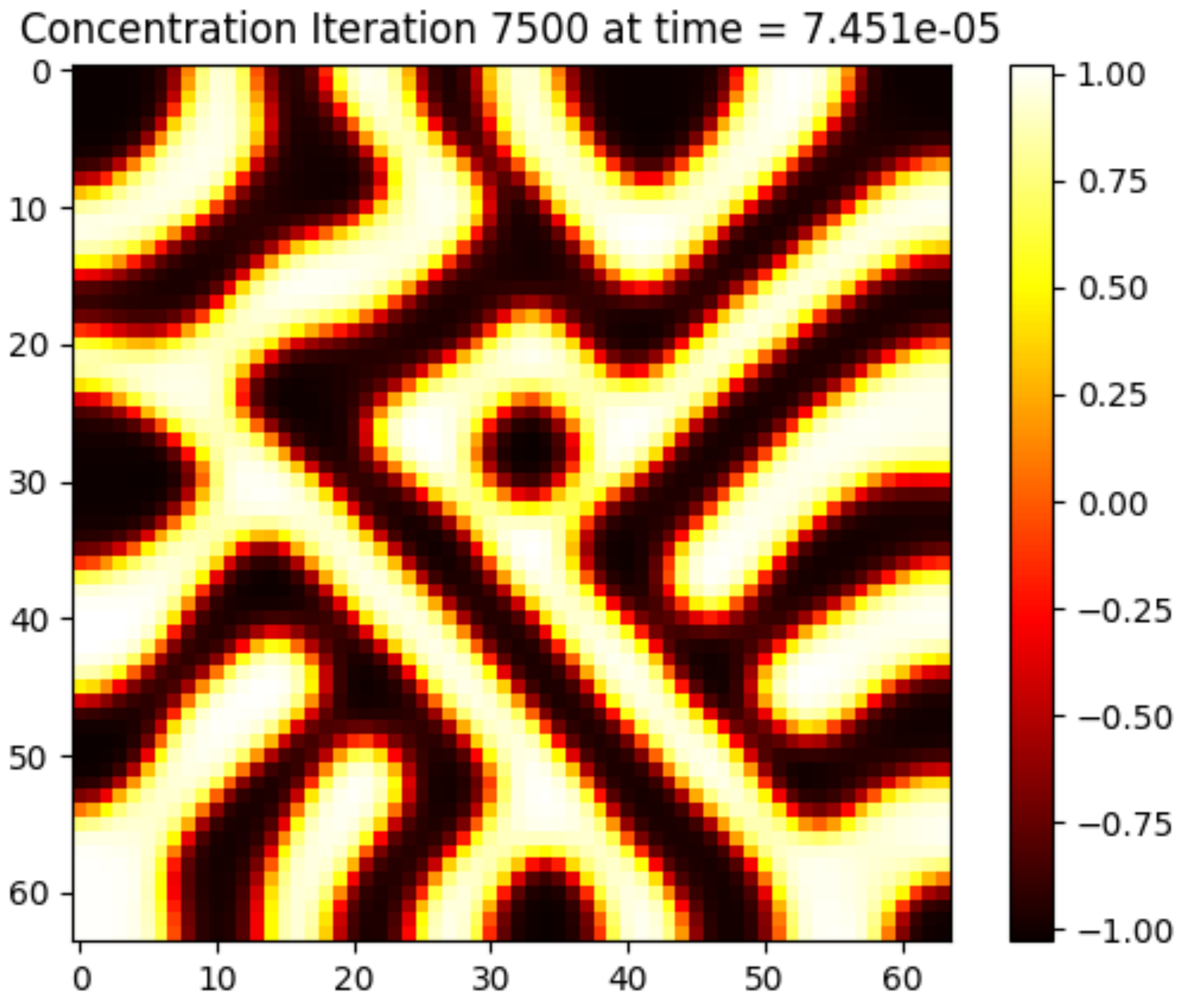
Explicit 4 Stage Runge Kutta Results

Dynamics of Cahn-Hillard with THE Range Kutta Scheme + FD

Restricted simulation to 1000 time steps/iterations. Time steps must be 30% of Courant for stability





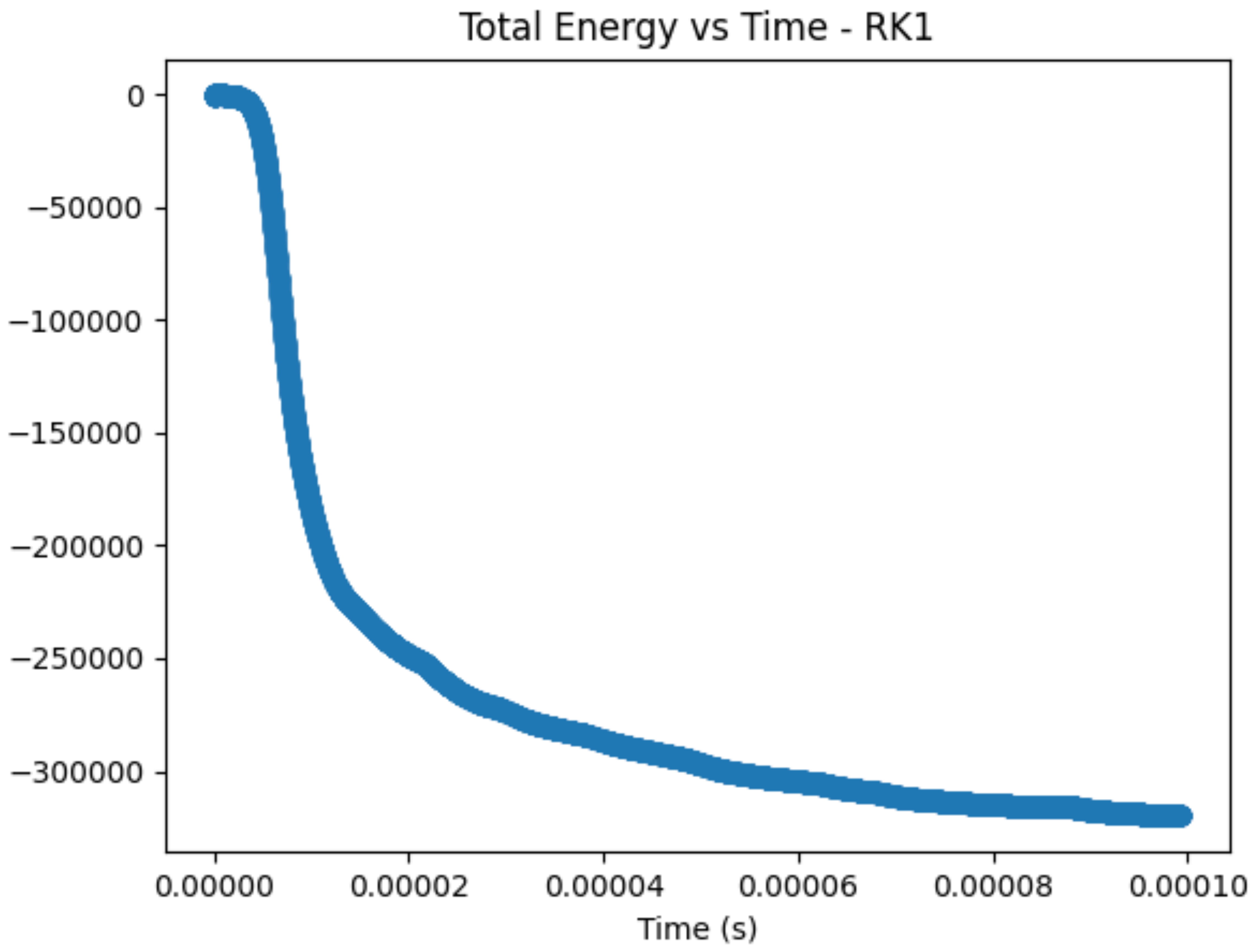


Dynamics are identical to RK1 but slightly larger time steps

Explicit 1 Stage Runge Kutta Results

Dynamics of Cahn-Hillard with Forward Euler Scheme + FD

Inherits Decreasing Energy as Expected



Implicit 1 Stage Runge Kutta

Stability of Backward Euler Scheme + FD

$$\frac{\partial \mathbf{c}^{n+1}}{\partial t} = \frac{\mathbf{c}_{ij}^{n+1} - \mathbf{c}_{ij}^{n}}{\Delta t}.$$

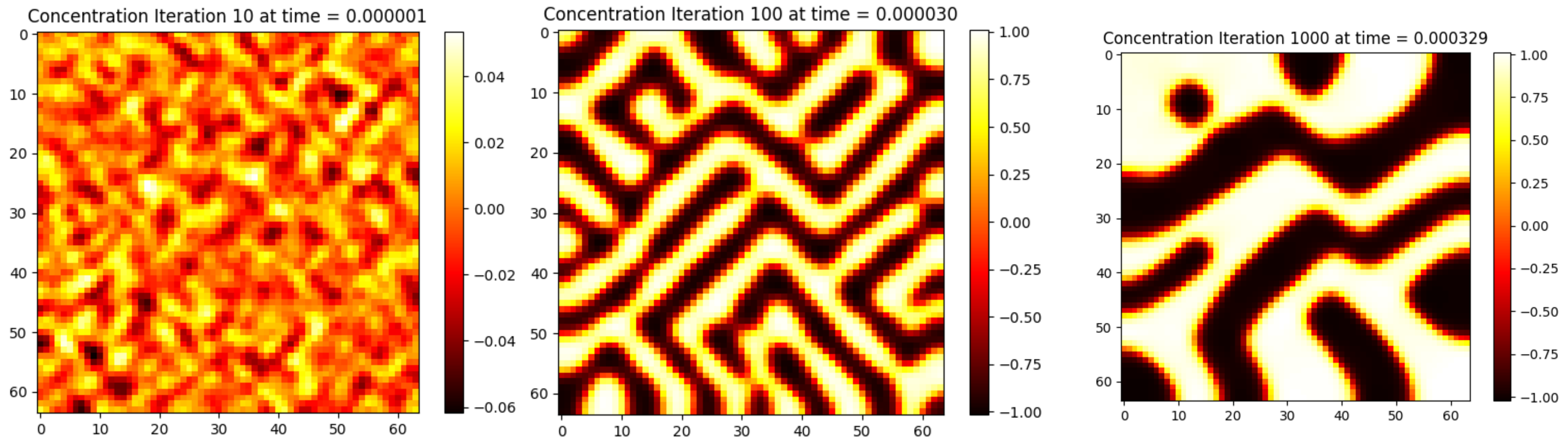
Generally L-stable but requires linearized Raphson-Newton method (nonlinear solvers) at each stage

Able to include time adaptivity! Double time steps if less than 10% change between solutions

Implicit 1 Stage Runge Kutta Results

Dynamics of Cahn-Hillard with Backward Euler Scheme + FD

Restricted simulation to 1000 time steps/iterations. Time steps are dynamics

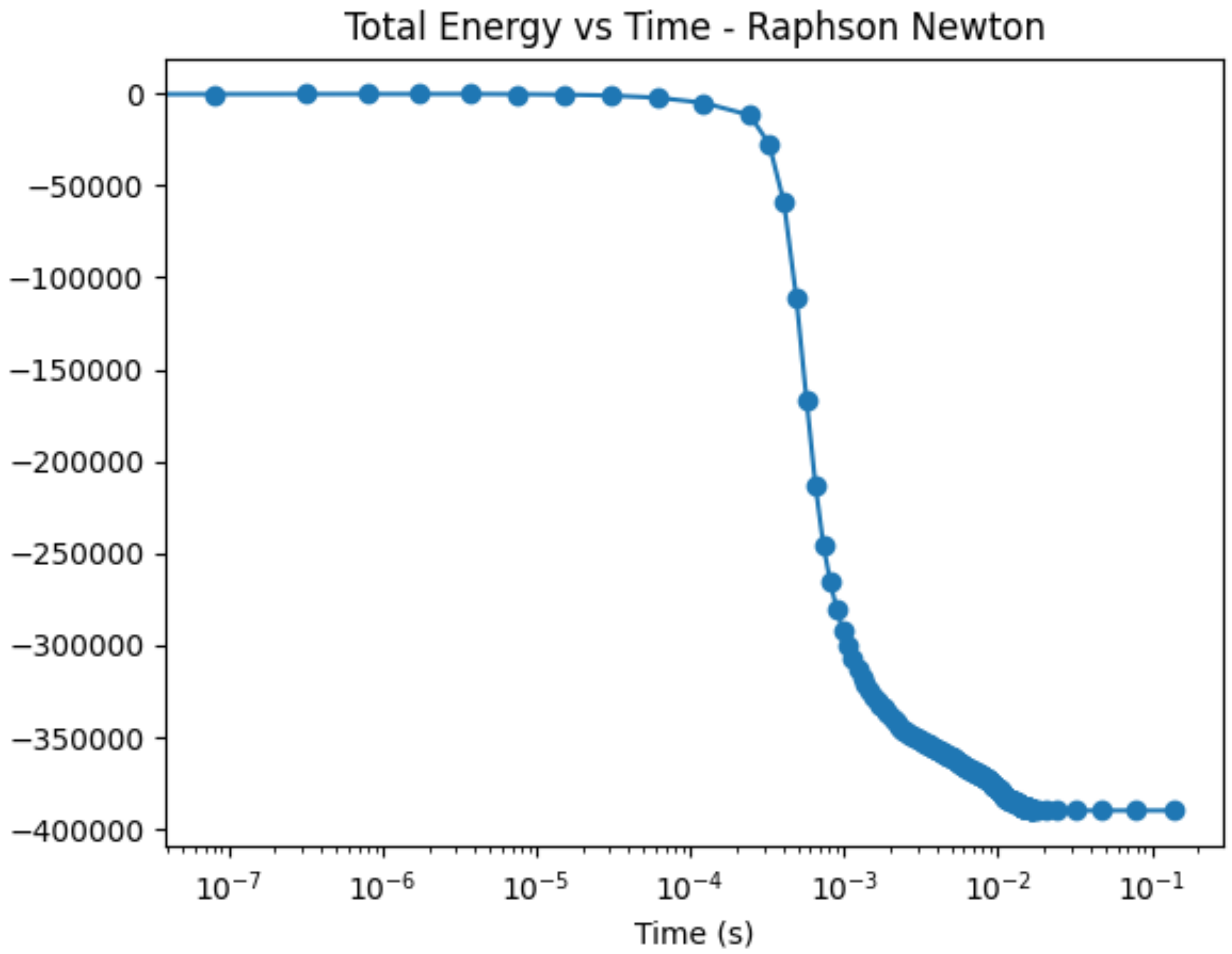


Dynamics are correct and can cover larger time scales!

Implicit 1 Stage Runge Kutta Results

Dynamics of Cahn-Hillard with Forward Euler Scheme + FD

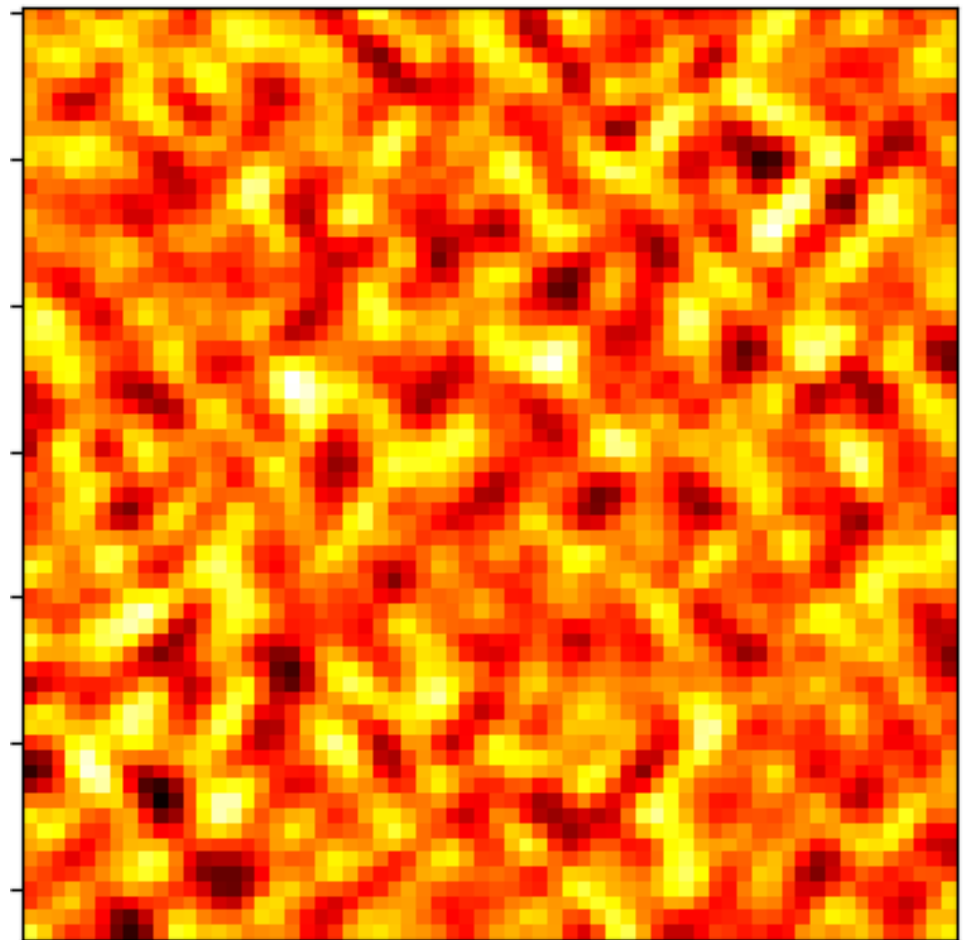
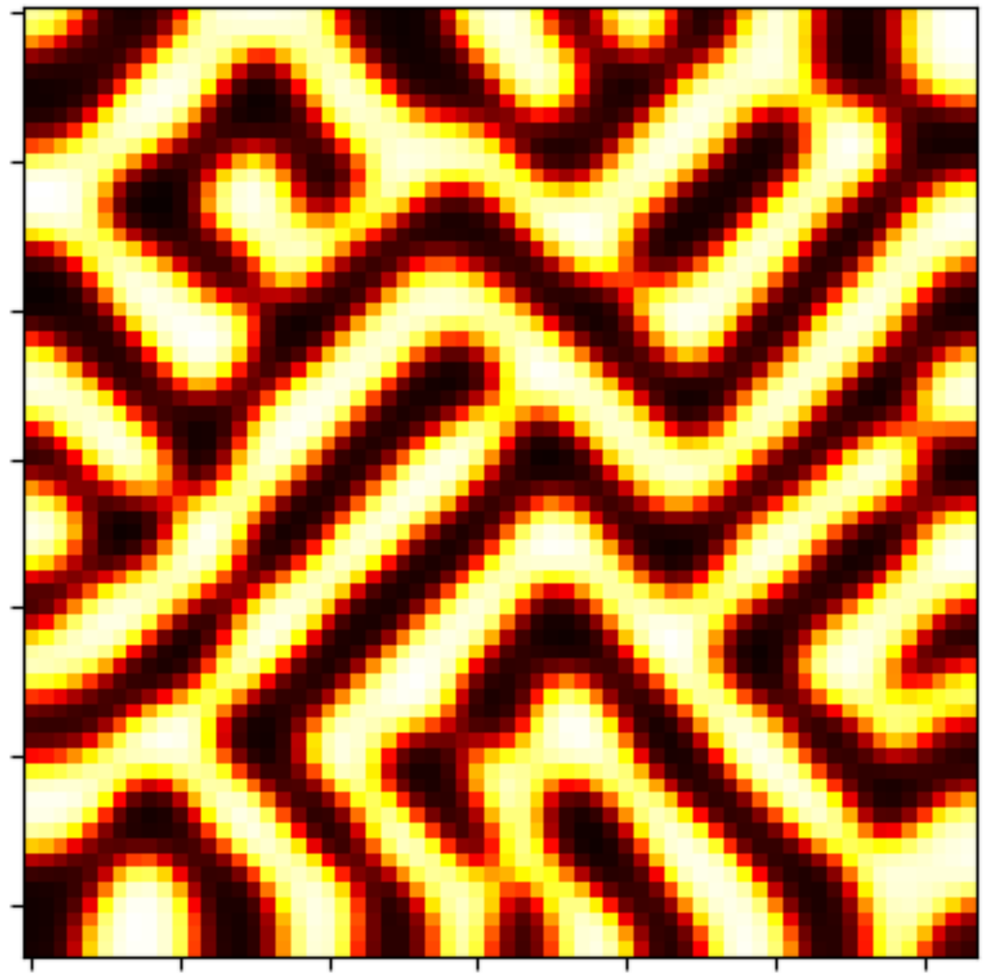
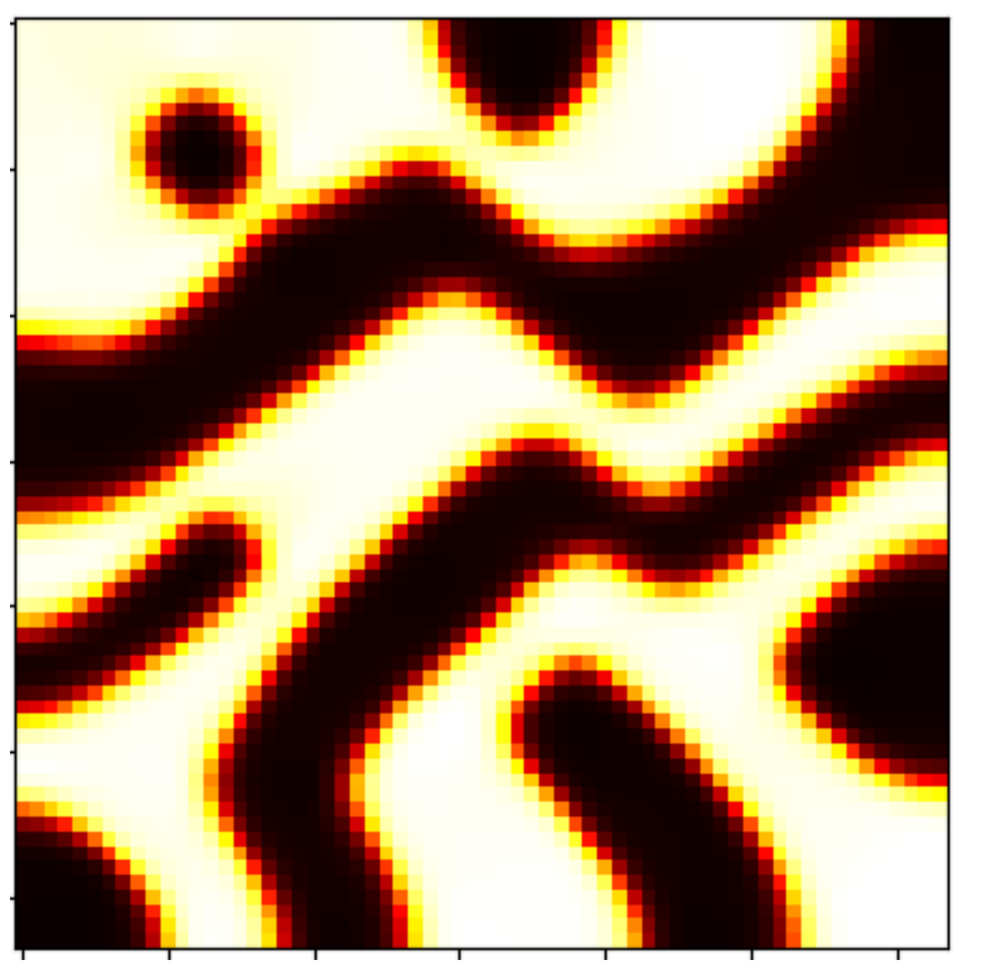
Inherits Decreasing Energy as Expected and covers orders of magnitudes to time



TakeAways and Next Steps

Cahn-Hillard Equation Requires Adaptable Schemes

- Explicit schemes cannot capture long time dynamics due to stiffness
- Implicit schemes are more flexible but require non-linear solvers
- Form of Cahn-Hillard equation determines time dynamics and which numerical schemes to use
- Adding complexities such as new geometries, non periodic boundary conditions, and temporal constants requires a mix of numerical schemes

References

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