Simulation of Multiphase Liquid

Final Project of APC 523

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MAE

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Statement of the Problem

Volume fraction of each component $\sum_i \phi_i(\mathbf{x}) = 1 \qquad 0 \le \phi_i \le 1$

Free energy density $\bar{f} = \sum_i \phi_i \ln \phi_i + \frac{1}{2} \sum_{i,j} \chi_{ij} \phi_i \phi_j - \frac{\lambda^2}{2} \sum_{i,j} \chi_{ij} \nabla \phi_i \cdot \nabla \phi_j \qquad \overline{F} = \int_V \mathrm{d}^3 \mathbf{x} \bar{f}(\mathbf{x})$

Chemical potential density $\bar{\mu}_j = \frac{\delta \overline{F}}{\delta \phi_j} = 1 + \ln \phi_j + \sum_k \chi_{jk} (1 + \lambda^2 \nabla^2) \phi_k$

Diffusion equation $\frac{\partial \phi_i}{\partial t} = D \nabla \cdot \left[\phi_i \sum_j \left(\delta_{ij} - \phi_j \right) \nabla \bar{\mu}_j \right]$

Non-dimensionalized diffusion equation $\frac{\partial \phi_i}{\partial \bar{t}} = \overline{\nabla} \cdot \left[\phi_i \sum_j \left(\delta_{ij} - \phi_j \right) \overline{\nabla} \bar{\mu}_j \right]$

Let the length unit x be the length of the box L and the time unit $\tau = \frac{L^2}{D}$

Statement of the Problem

To solve $\frac{\partial \phi_i}{\partial \bar{t}} = \overline{\nabla} \cdot \left[\phi_i \sum_j \left(\delta_{ij} - \phi_j \right) \overline{\nabla} \overline{\mu}_j \right]$, we first simplify the diffusion equation

Let $\overline{\mu}_j = \overline{\mu}_{j1} + \overline{\mu}_{j2} = 1 + \ln \phi_j + \sum_k \chi_{jk}(1 + \lambda^2 \nabla^2)\phi_k$, where $\overline{\mu}_{j1} = 1 + \ln \phi_j$ $\quad \overline{\mu}_{j2} = \sum_k \chi_{jk}(1 + \lambda^2 \nabla^2)\phi_k$

$$\frac{\partial \phi_i}{\partial \bar{t}} = \overline{\nabla} \cdot \left[\phi_i \sum_j \left(\delta_{ij} - \phi_j \right) \frac{\overline{\nabla} \phi_j}{\phi_j} + \phi_i \sum_j \left(\delta_{ij} - \phi_j \right) \overline{\nabla} \overline{\mu}_{j2} \right]$$

$$= \overline{\nabla} \cdot \left[\overline{\nabla} \phi_i - \overline{\nabla} \left(\sum_j \phi_j \right) + \phi_i \sum_j \left(\delta_{ij} - \phi_j \right) \overline{\nabla} \overline{\mu}_{j2} \right] \qquad \sum_i \phi_i(\mathbf{x}) = 1$$

$$= \overline{\nabla}^2 \phi_i + \left[\phi_i \sum_j \left(\delta_{ij} - \phi_j \right) \overline{\nabla} \overline{\mu}_{j2} \right]$$

FFT Method

$$\frac{\partial \phi_i}{\partial \bar{t}} = \overline{\nabla}^2 \phi_i + \left[\phi_i \sum_j \left(\delta_{ij} - \phi_j \right) \overline{\nabla} \overline{\mu}_{j2} \right]$$

We use a semi-implicit time-integration scheme

$$\frac{\phi_i^{n+1} - \phi_i^n}{\overline{\Delta t}} = N_i(\phi_i^n) + L_i(\phi_i^{n+1})$$

$$N_i(\phi_i^n) = \overline{\nabla}^2 \phi_i + \left[\phi_i \sum_j \left(\delta_{ij} - \phi_j \right) \overline{\nabla} \overline{\mu}_{j2} \right] + A\overline{\lambda}^2 \overline{\nabla}^4 \phi_i \qquad L_i(\phi_i^n) = -A\overline{\lambda}^2 \overline{\nabla}^4 \phi_i$$

After Fourier transformation, we have

$$\frac{\tilde{\phi}_i^{n+1} - \tilde{\phi}_i^n}{\overline{\Delta t}} = \tilde{N}_i(\phi_i^n) + \tilde{L}_i(\phi_i^{n+1}) = \tilde{N}_i(\phi_i^n) - A\lambda^2 \overline{k}^4 \tilde{\phi}^{n+1}$$

$$\Rightarrow \tilde{\phi}_i^{n+1} = \frac{\tilde{\phi}_i^n + \tilde{N}_i(\phi_i^n)\overline{\Delta t}}{1 + A\overline{\lambda}^2 \overline{k}^4 \overline{\Delta t}}$$

Settings

$$A = 0.5 \max\{\chi_{ij}\}$$

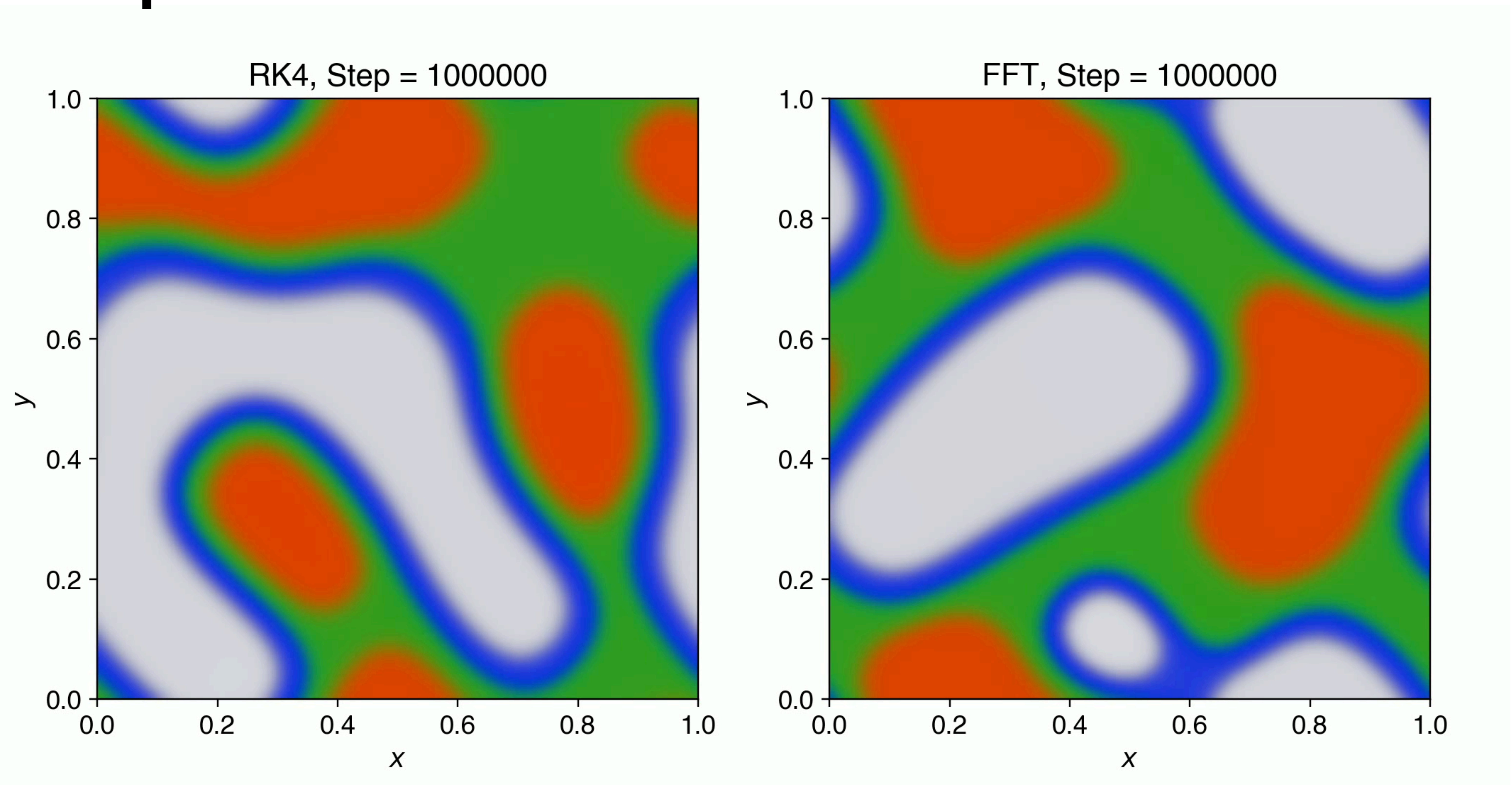
$$\overline{\lambda} = 0.45 \times 10^{-2}$$

$$\overline{\Delta t} = 0.5 \overline{\lambda}^2$$

$$\mathrm{d}\overline{x} = \frac{1}{128}$$

[1] Mao, Sheng, et al. "Designing the morphology of separated phases in multicomponent liquid mixtures." *Physical review letters* 125.21 (2020): 218003.

Comparison between RK4 and FFT

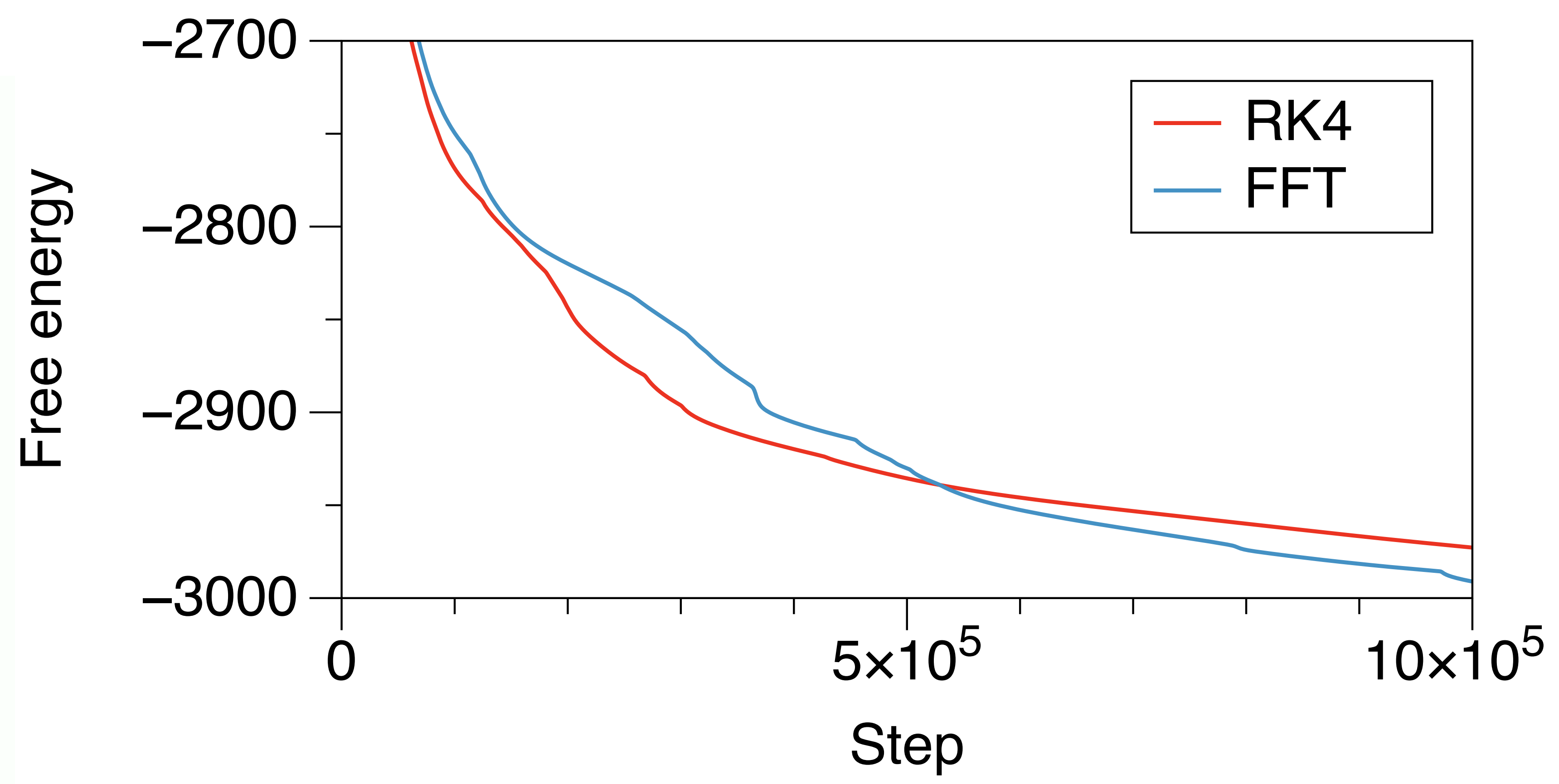


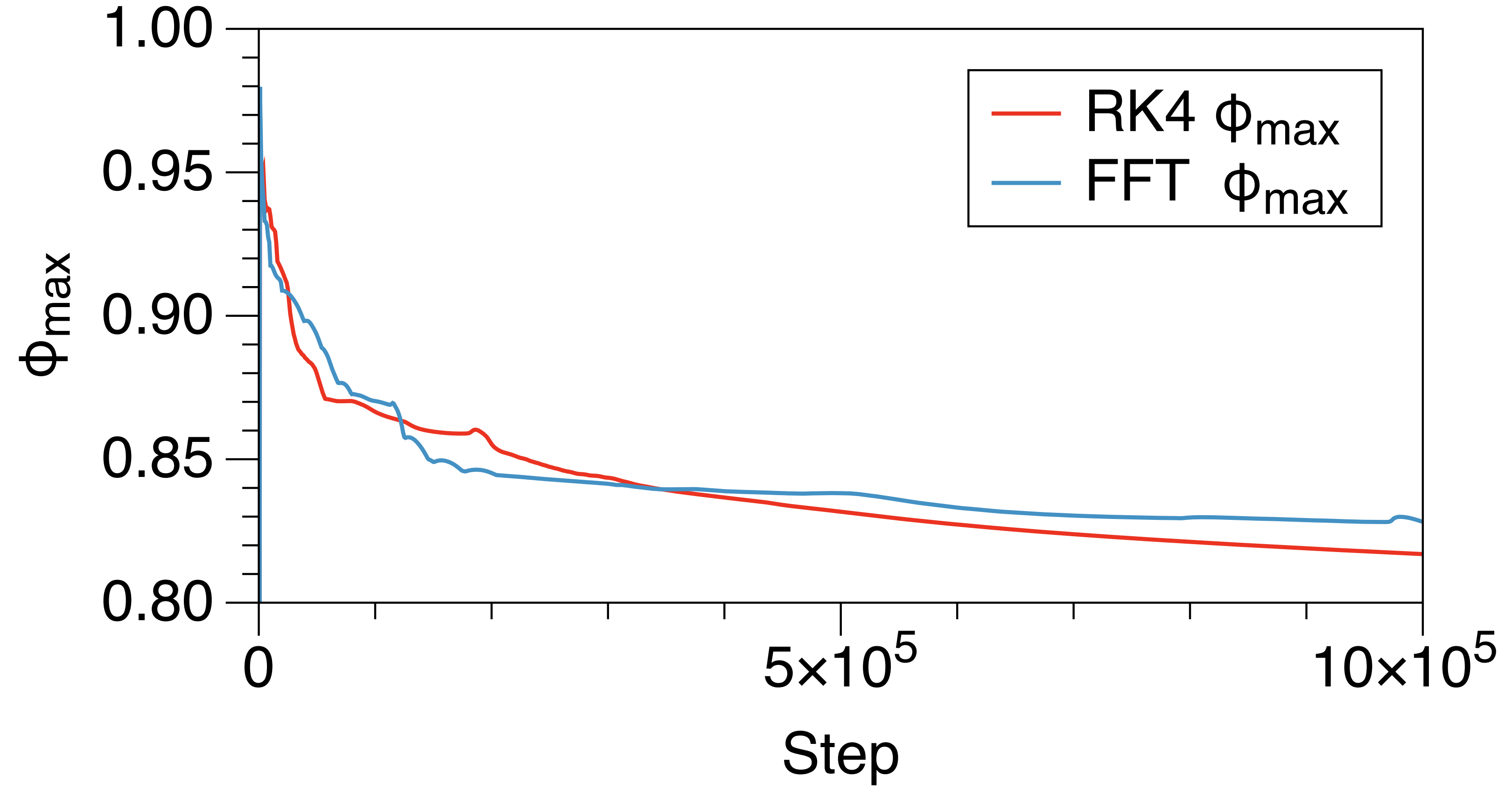
~310 steps/s

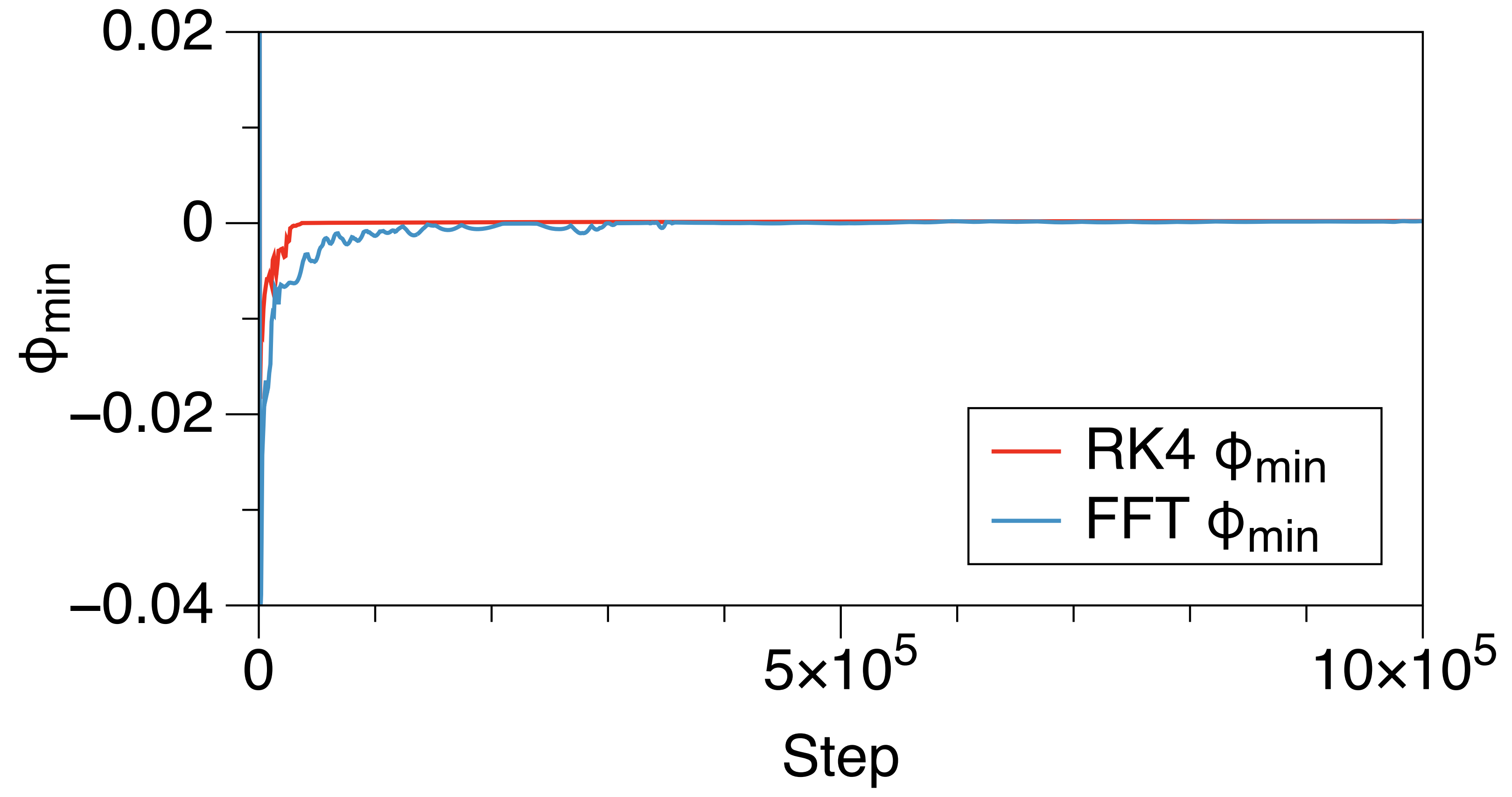
~450 steps/s

On my laptop

$$\chi_{ij} = \begin{bmatrix} 0 & 2.2 & 4.6 & 7 \\ & 0 & 2.2 & 9.4 \\ & & 0 & 2.2 \\ & & & 0 \end{bmatrix} \qquad \phi_i = \begin{bmatrix} 0.25 \text{ red} \\ 0.25 \text{ green} \\ 0.25 \text{ blue} \\ 0.25 \text{ white} \end{bmatrix}$$

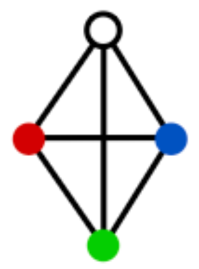




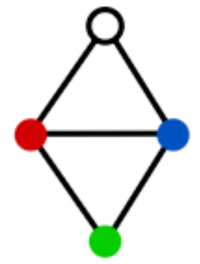


Designing Different morphologies by Changing Interactions

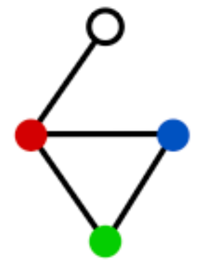
$$\phi_i = \begin{bmatrix} 0.25 \text{ red} \\ 0.25 \text{ green} \\ 0.25 \text{ blue} \\ 0.25 \text{ white} \end{bmatrix}$$



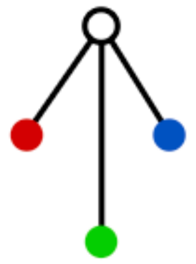
$$\chi_{ij} = \begin{bmatrix} 0 & 5 & 5 & 5 \\ & 0 & 5 & 5 \\ & & 0 & 5 \\ & & & 0 \end{bmatrix}$$



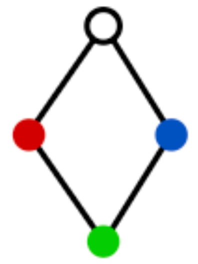
$$\chi_{ij} = \begin{bmatrix} 0 & 4 & 4 & 6 \\ & 0 & 4 & 9 \\ & & 0 & 4 \\ & & & 0 \end{bmatrix}$$



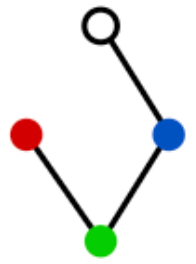
$$\chi_{ij} = \begin{bmatrix} 0 & 4 & 4 & 4 \\ & 0 & 4 & 8.2 \\ & & 0 & 8.2 \\ & & & 0 \end{bmatrix}$$



$$\chi_{ij} = \begin{bmatrix} 0 & 7.5 & 7.5 & 3.5 \\ & 0 & 7.5 & 3.5 \\ & & 0 & 3.5 \\ & & & 0 \end{bmatrix}$$



$$\chi_{ij} = \begin{bmatrix} 0 & 3 & 6.5 & 4 \\ & 0 & 3 & 6.5 \\ & & 0 & 3 \\ & & & 0 \end{bmatrix}$$



$$\chi_{ij} = \begin{bmatrix} 0 & 2.5 & 5.5 & 8.5 \\ & 0 & 2.5 & 6.5 \\ & & 0 & 2.5 \\ & & & 0 \end{bmatrix}$$

Conclusion of Coding

- The FFT method is faster than RK4 because RK4 has 4 subprocesses of iteration for each step
- Both FFT and RK4 can stabilize ϕ_i even though at the beginning of simulation we find $\phi_i < 0$ in some region
- We use float 32 instead of float 64 to accelerate the computation, which is about 1.2-1.4 times faster
- The $\ln \phi_i$ in the chemical potential μ can be simplified for calculating $\nabla \mu$, there is no need to calculate $\ln \phi_i$ explicitly as it takes longer time
- Both FFT and RK4 have similar results and they both reproduce the result in Reference [1]

[1] Mao, Sheng, et al. "Designing the morphology of separated phases in multicomponent liquid mixtures." *Physical review letters* 125.21 (2020): 218003.