Pseudospectral Solutions to 2D-Advection Diffusion Equations

Joseph Lucero

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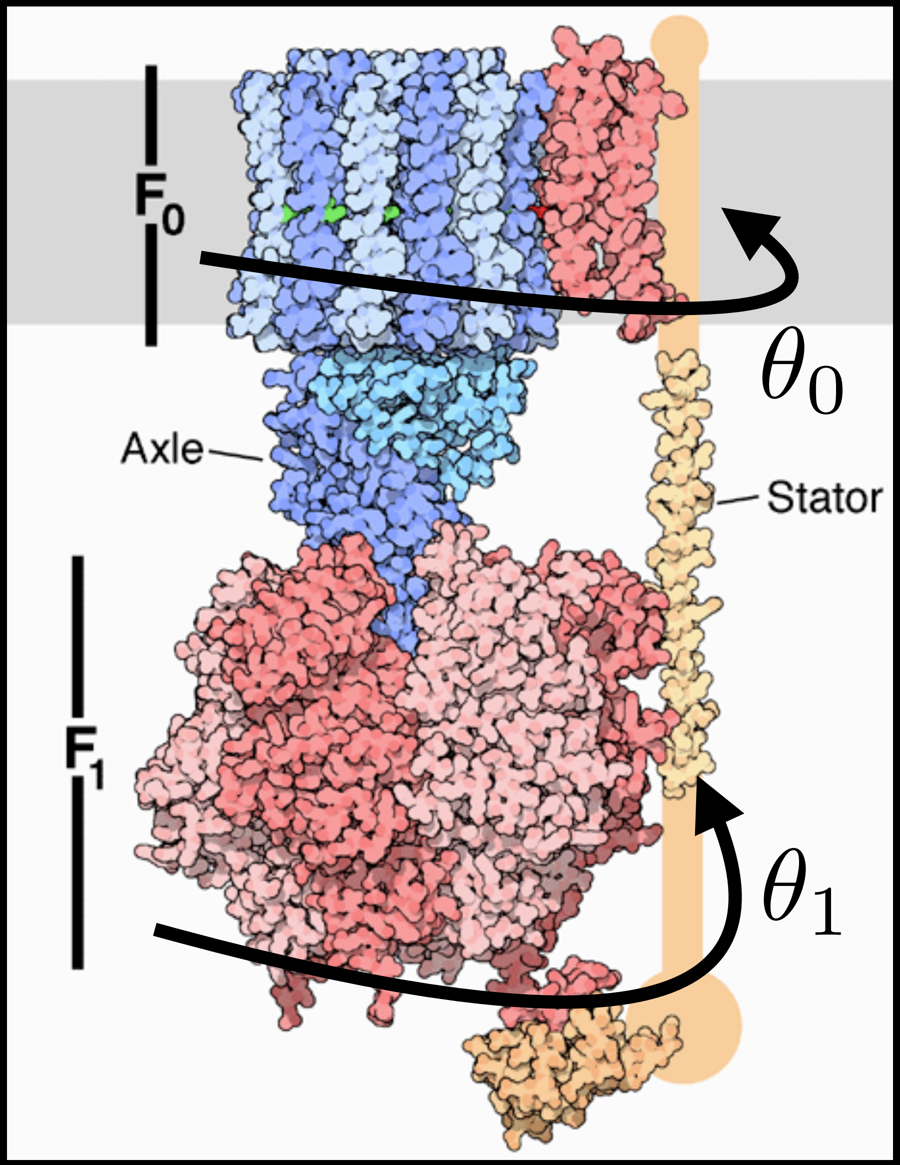
ATP Synthase and Stochastic Dynamics

- ATP Synthase is responsible for creating the energy currency that is used to power cellular processes
  - Molecular motor that is able to converts between two forms of chemical energy
- It is about 10nm in diameter
  - The energy scale of its operation is the same as the scale of thermal energy fluctuations in the environment that surrounds it
- Its motion is inherently stochastic



How do you model stochastic behaviour?

Stochastic variables

Noise term

$$\mathrm{d}\vec{\theta}(t) = \vec{\mu}(\vec{\theta}(t), t)\,\mathrm{d}t + \vec{\sigma}(\vec{\theta}(t), t) \circ \mathrm{d}\vec{W}(t)$$

Langevin Equation

Drift vector

Diffusivity

$$\langle \mathrm{d}W(t) \rangle = 0$$

$$\langle \mathrm{d}W(t)\,\mathrm{d}W(s) \rangle = \delta(t-s)\,\mathrm{d}t$$

- Use stochastic differential equations
- These are effectively ordinary differential equations with a stochastic noise term
  - Stochastic noise term satisfies certain statistical relations

The Fokker-Planck Equation

Diffusion Tensor

$$\frac{\partial P(\vec{\theta}(t),t)}{\partial t} = -\sum_i \frac{\partial}{\partial \theta_i}\left[\mu_i(\vec{\theta}(t),t)P(\vec{\theta}(t),t)\right] + \sum_i \sum_j \frac{\partial^2}{\partial \theta_i \partial \theta_j}\left[D_{ij}(\vec{\theta}(t),t)P(\vec{\theta}(t),t)\right]$$

Probability Distribution

$$\mu_i(\vec{\theta}(t),t) = \mu_i(\vec{\theta})$$

$$D_{ij}(\vec{\theta},t) = \frac{1}{2}\vec{\sigma} \otimes \vec{\sigma} = D\delta_{ij}$$

Diffusivity

$$\frac{\partial P(\vec{\theta},t)}{\partial t} = -\sum_i \frac{\partial}{\partial \theta_i}\left[\mu_i(\vec{\theta})P(\vec{\theta},t)\right] + D\sum_i \frac{\partial^2}{\partial \theta_i^2}\left[P(\vec{\theta},t)\right]$$

$$= -\nabla \cdot \left[\vec{\mu}(\vec{\theta})P(\vec{\theta},t)\right] + D\nabla^2\left[P(\vec{\theta},t)\right]$$

Advection

Diffusion

- In stochastic processes this is also known as the Forward-Kolmogorov Equation

The Fokker-Planck Equation

$$\frac{\partial P(\vec{\theta}, t)}{\partial t} = -\boldsymbol{\nabla} \cdot \left[\vec{\mu}(\vec{\theta}) P(\vec{\theta}, t)\right] + D\nabla^2 \left[P(\vec{\theta}, t)\right]$$

Characteristic Function

$$P(\vec{\theta}, t) = \left(\frac{1}{\sqrt{2\pi}}\right)^{\mathcal{N}} \int \mathrm{d}^{\mathcal{N}}\vec{\xi}\, P(\vec{\xi}, t) \exp\left[i\vec{\xi} \cdot \vec{\theta}\right]$$

$$\left\{\frac{\partial \hat{P}(\vec{\xi}, t)}{\partial t}\right\} = -\left[\boldsymbol{\nabla} \cdot \vec{\mu}(\vec{\theta})\right] \left\{\hat{P}(\vec{\xi}, t)\right\} - \left[\vec{\mu}(\vec{\theta})\right] \cdot \left\{i\vec{\xi}\hat{P}(\vec{\xi}, t)\right\} - \left\{D|\vec{\xi}|^2 \hat{P}(\vec{\xi}, t)\right\}$$

Conditions on Solutions

	$P(\vec{\theta}, t)$	$\hat{P}(\vec{\xi}, t)$
Normalization	$\int \mathrm{d}^{\mathcal{N}}\vec{\theta}\, P(\vec{\theta}, t) = 1$	$\hat{P}(\vec{0}, t) = 1$
Bounds	$P(\vec{\theta}, t) \geq 0$	$\lvert\hat{P}(\vec{\xi}, t)\rvert \leq 1$

Steady-State Distribution

$$\frac{\partial P(\vec{\theta},t)}{\partial t} = -\boldsymbol{\nabla}\cdot\left[\vec{\mu}(\vec{\theta})P(\vec{\theta},t)\right] + D\nabla^2\left[P(\vec{\theta},t)\right]$$

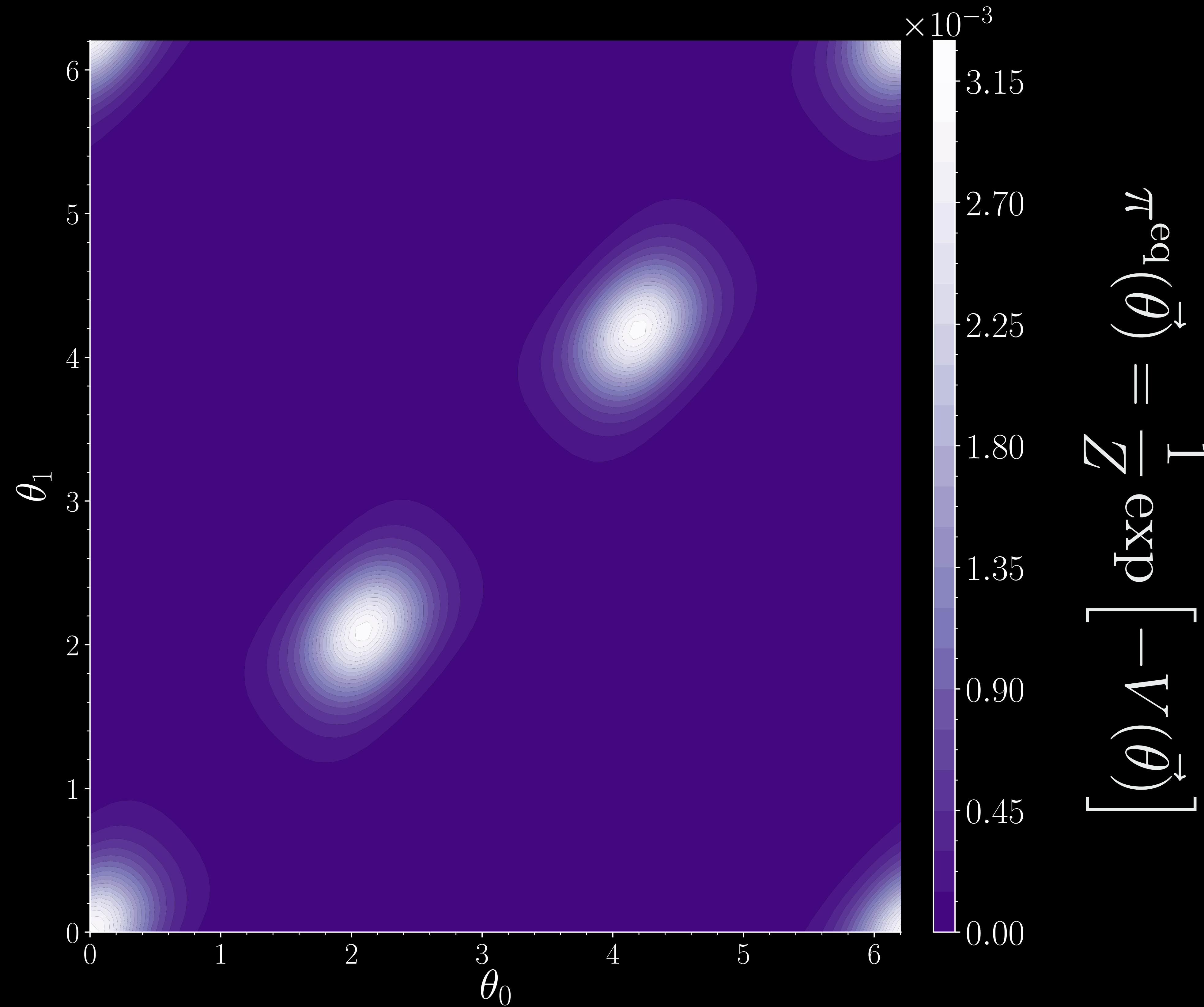
$$\mu_i(\vec{\theta}) = -D\left(\frac{\partial V(\vec{\theta})}{\partial \theta_i} - \psi_i\right)$$

$$V(\vec{\theta}) = \frac{1}{2}\Big[E_0(1-\cos(n_0\theta_0)) + E_c(1-\cos(\theta_0-\theta_1)) + E_1(1-\cos(n_1\theta_1))\Big]$$

$$\lim_{t\to\infty} P(\vec{\theta},t) = \pi^{\mathrm{eq}}(\vec{\theta}) = \frac{1}{Z}\exp\left[-V(\vec{\theta})\right]$$

Gibbs-Boltzmann Distribution

Steady-State Distribution



Numerical Schemes

$$\frac{\partial p(\vec{\theta},t)}{\partial t} = -\boldsymbol{\nabla}\cdot\left[\vec{\mu}(\vec{\theta})p(\vec{\theta},t)\right] + D\nabla^2\left[P(\vec{\theta},t)\right]$$

- Forward Time, Central Space (FTCS)

Definition 16 (IDIOT) *Anyone who publishes a calculation without checking it against an identical computation with smaller N OR without evaluating the residual of the pseudospectral approximation via finite differences is an IDIOT.*

Real Space

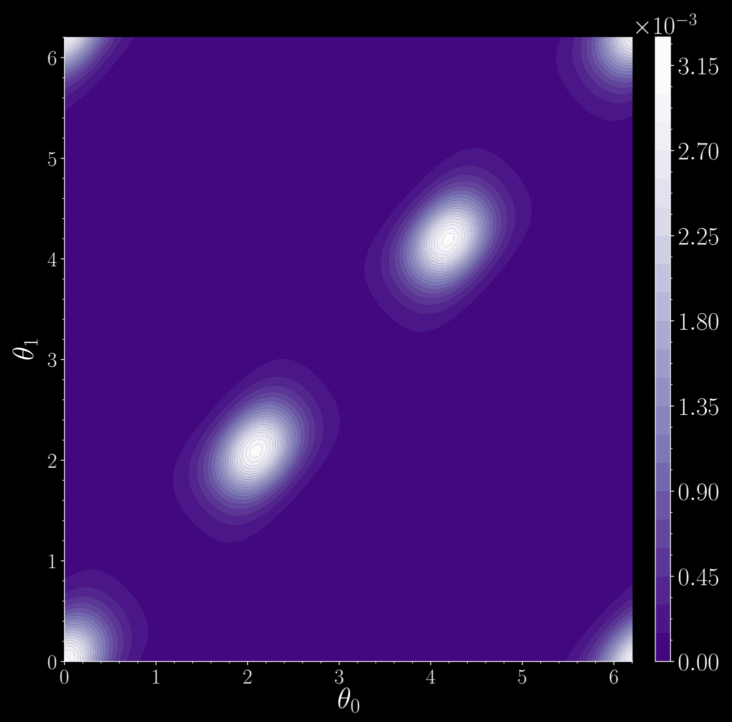
$$\left\{\frac{\partial \hat{P}(\vec{\xi},t)}{\partial t}\right\} = -\left[\boldsymbol{\nabla}\cdot\vec{\mu}(\vec{\theta})\right]\left\{\hat{P}(\vec{\xi},t)\right\} - \left[\vec{\mu}(\vec{\theta})\right]\cdot\left\{i\vec{\xi}\hat{P}(\vec{\xi},t)\right\} - \left\{D|\vec{\xi}|^2\hat{P}(\vec{\xi},t)\right\}$$

- Forward Time, Spectral Space (FTSS)
- Crank-Nicolson Forward Euler (IMEX)
- Integrating Factor RK4 (IFRK4)
- Exponential-Time Differencing RK4 (ETDRK4)

Fourier Space

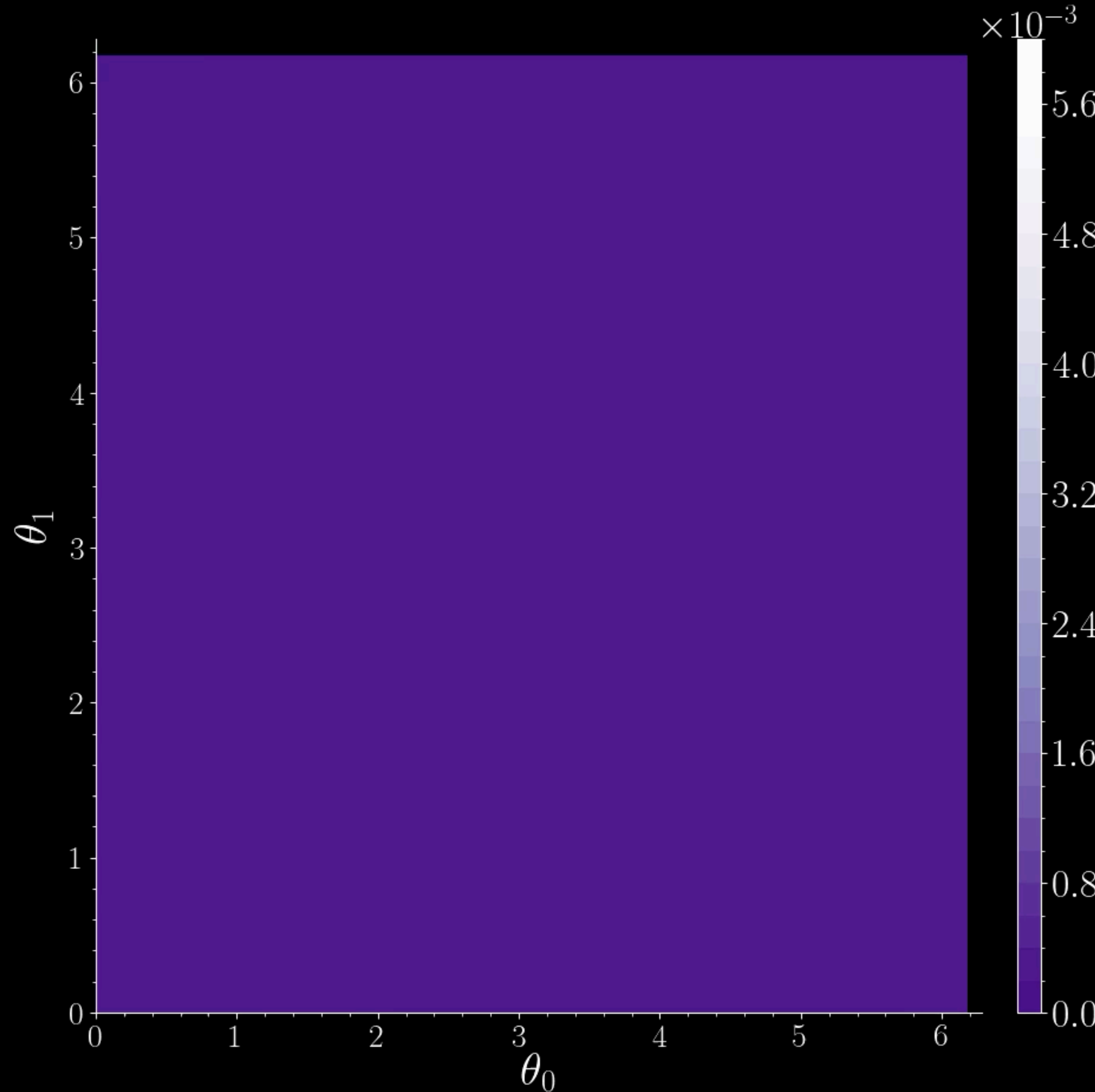
Results

Time Evolution



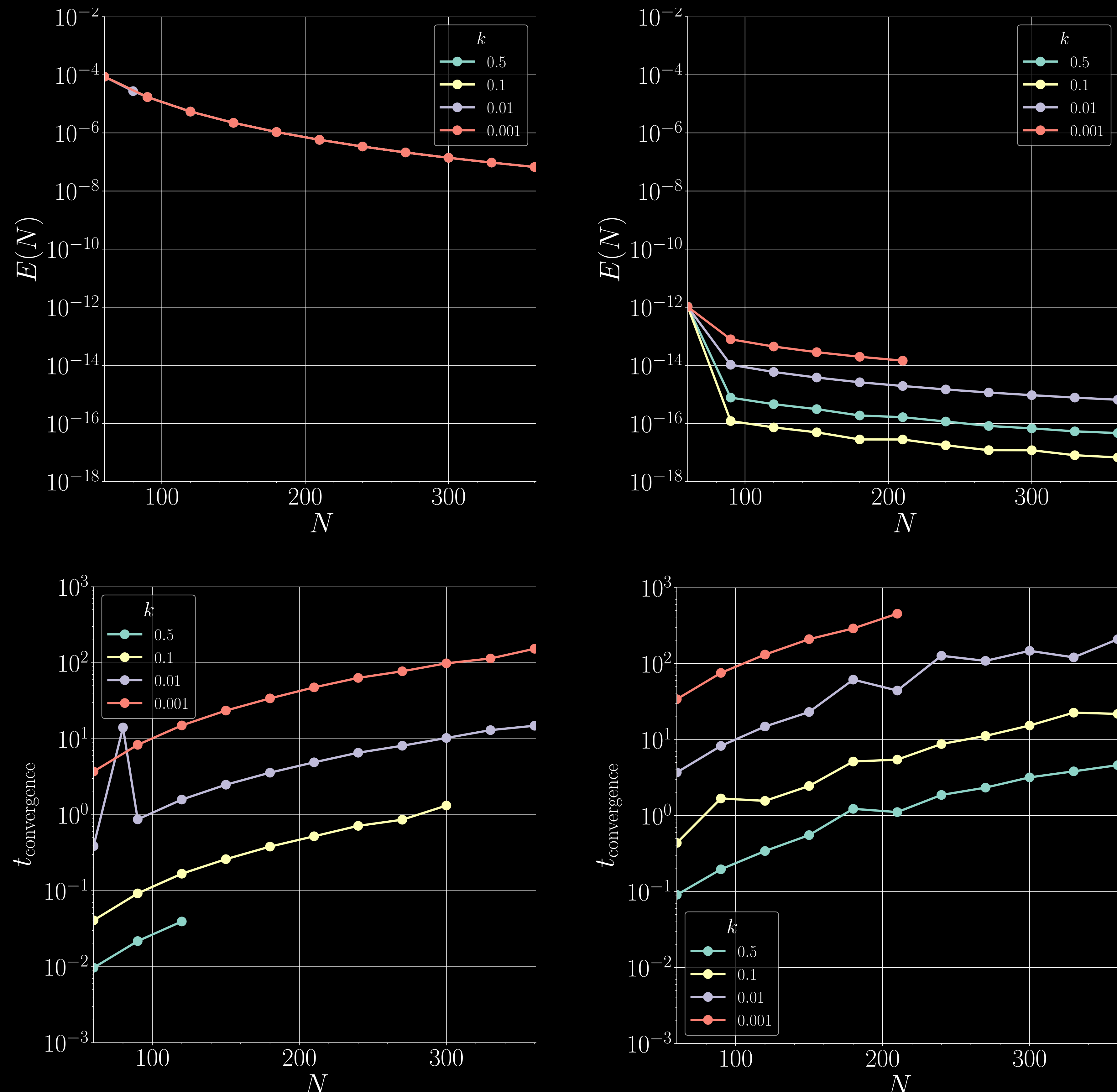
Stopping Criteria

$$\frac{1}{2}\sum_{ij}|\hat{P}_{ij}^{n-1}-\hat{P}_{ij}^{n}|<\varepsilon$$



FTCS vs. IMEX

FTCS **IMEX**



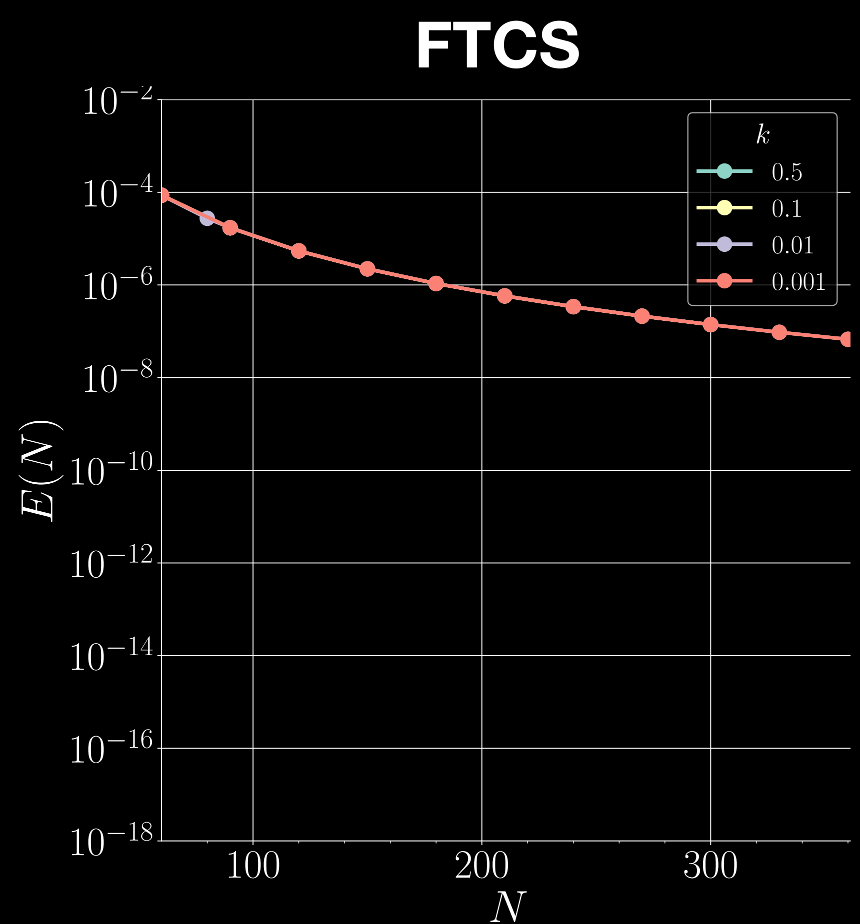
Spatial Accuracy

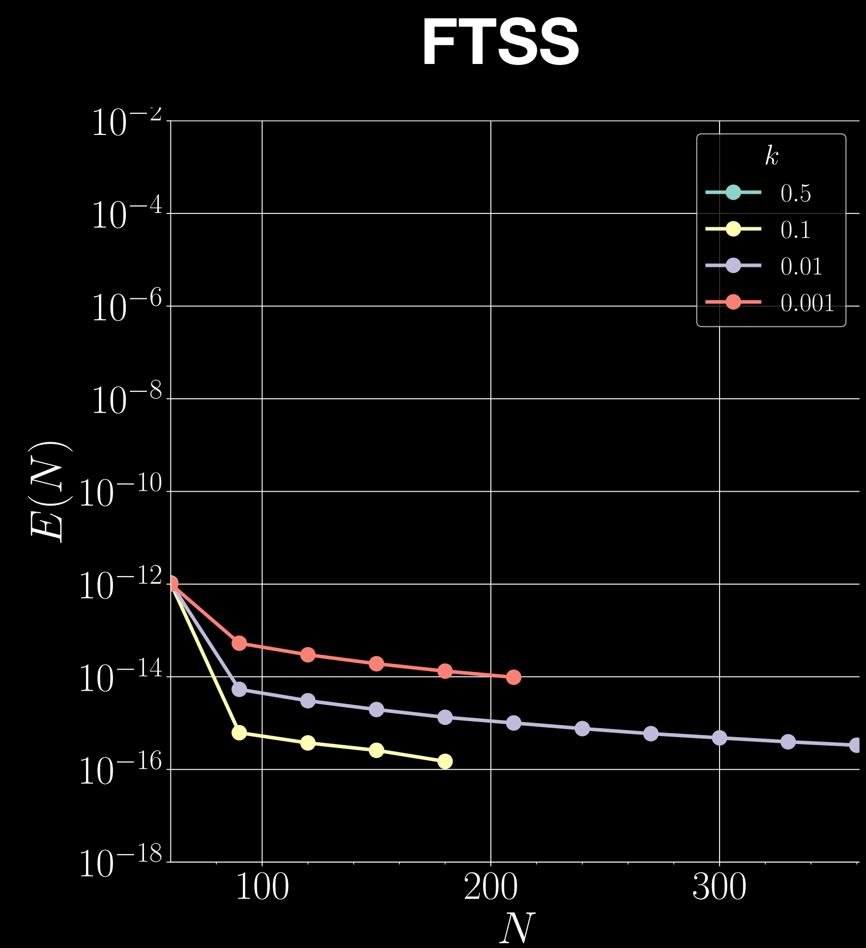
Convergence Time

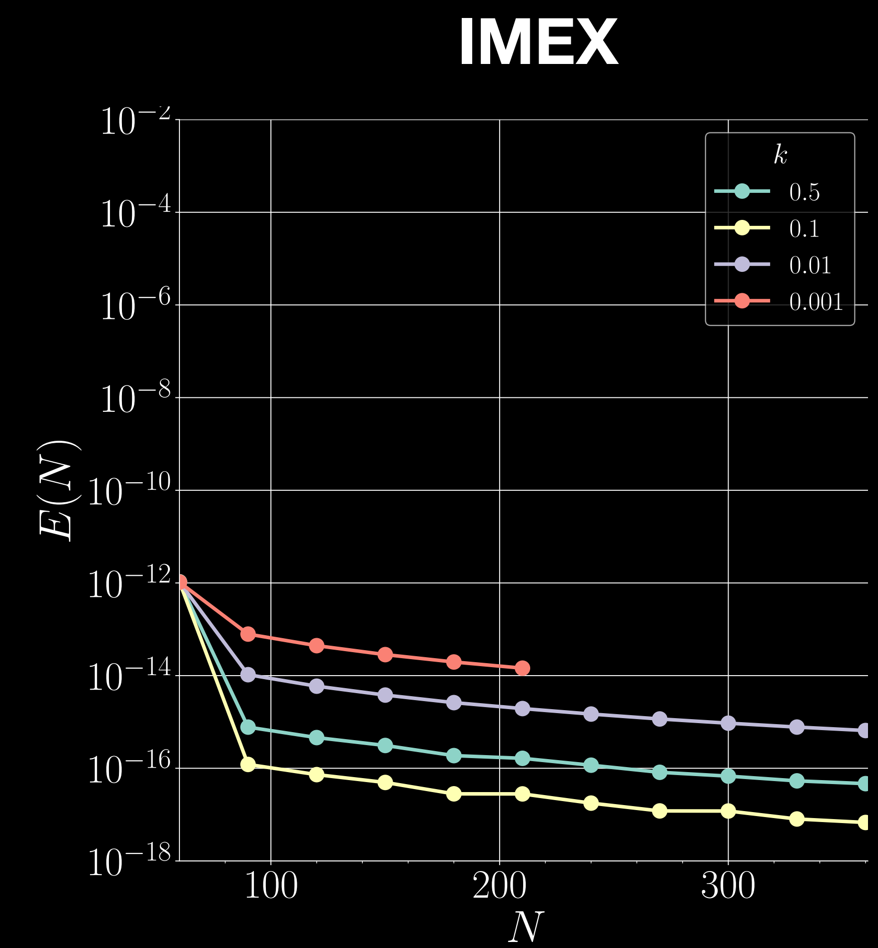
*All times reported are in minutes

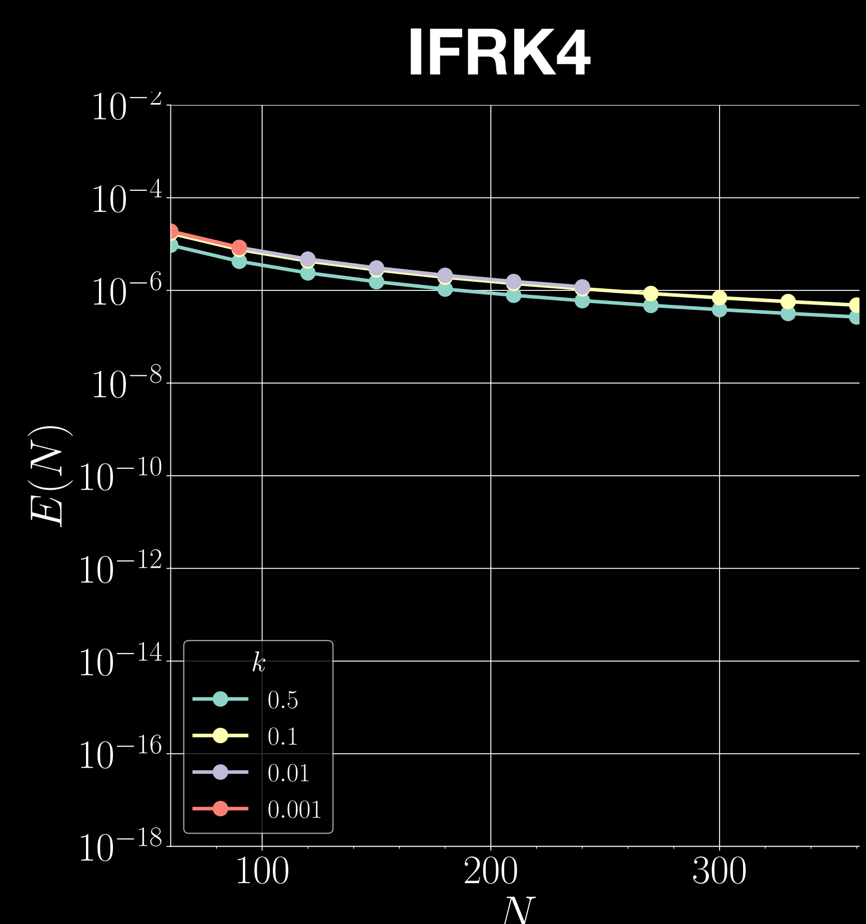
*Accuracy is measured using the inf-norm

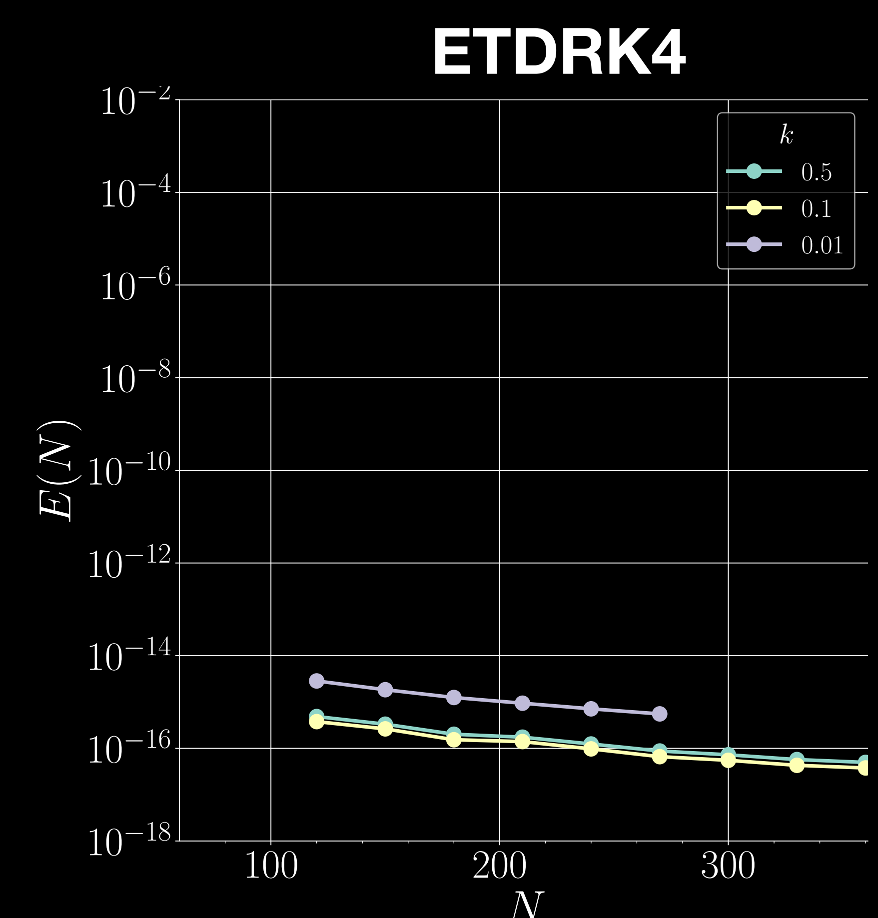
Spatial Accuracy











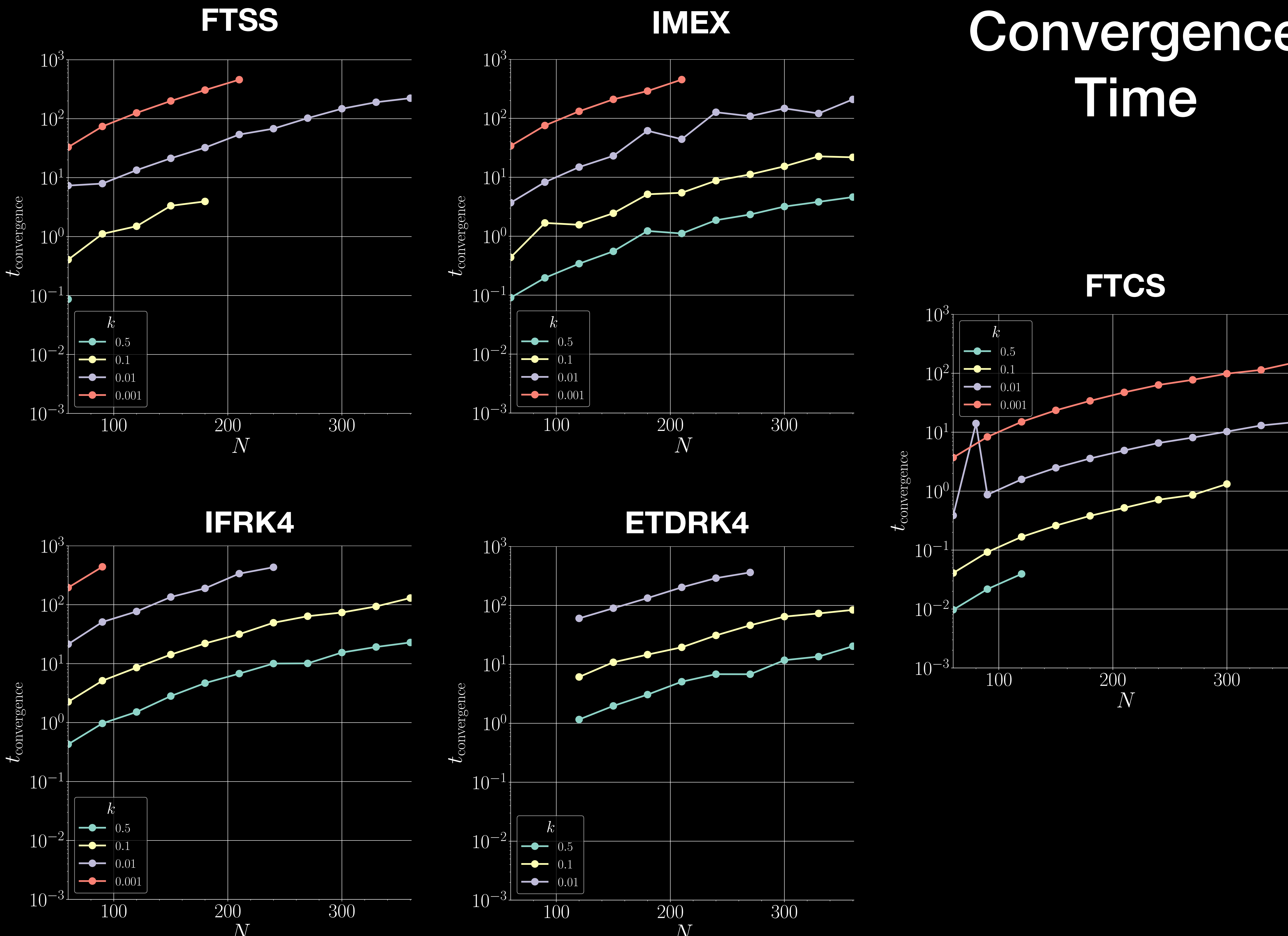
*Accuracy is measured using the inf-norm

Conclusions

- The generalized Langevin Equation (SDE) governing a set of random variables can be recast in terms of an equation of motion for the joint probability distribution of the random variables known as the Fokker-Planck Equation (FPE)
- We solved the FPE numerically using pseudo-spectral methods and showed that this improved the accuracy of solutions by more than 4 orders of magnitude relative to finite differences (!!!!)
- Was it worth all the pain and hours debugging?
    - Maybe…

Extra Slides

Convergence Time



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