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Free Space Particle-in-Fourier

For Plasma Simulation

🎙️ Introduction

Introduction

Kinetic Description of Plasma

Assumptions for plasma dominated by long-range interactions:

🧐 A continuous distribution profile $f = f(\mathbf{x}, \mathbf{v}, t)$ in the phase space ($\mathbf{x} - \mathbf{v}$ space);

🧐 Fully non-collisional because its density ρ is sufficiently low, and the interaction is mainly long-range.

Properties of $f = f(\mathbf{x}, \mathbf{v}, t)$:

Density $$\rho(\mathbf{x}, t) = Q \iiint f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}$$

Mean Flow $$n\mathbf{U}(\mathbf{x}, t) = \iiint \mathbf{v} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}$$

Pressure Tensor $$\mathbf{P}(\mathbf{x}, t) = m \iiint (\mathbf{v} - \mathbf{U})(\mathbf{v} - \mathbf{U}) f d\mathbf{v}$$

Introduction

Kinetic Description of Plasma

This leads to a kinetic description of plasma, a 6-dimensional PDE system (the so-called Vlasov / Maxwell-Boltzmann system):

$$
\begin{aligned}
0 &= \frac{Df}{Dt}(\mathbf{x}(t), \mathbf{v}(t), t) \\
&= \frac{\partial f}{\partial t} + \nabla_{\mathbf{x}} f \cdot \frac{d\mathbf{x}}{dt} + \nabla_{\mathbf{v}} f \cdot \frac{d\mathbf{v}}{dt} \\
&= \boxed{\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \left(\frac{q}{m}\mathbf{E} + \mathbf{v} \times \mathbf{B}_0\right) \cdot \nabla_{\mathbf{v}} f}
\end{aligned}
$$

Electrostatic Vlasov's Equation

where

$$
\begin{aligned}
\Delta\varphi &= -\rho \\
\mathbf{E} &= -\nabla\varphi
\end{aligned}
$$

⚛️ Particle Method for Solving Vlasov's Equation

Particle Method for Solving Vlasov's Equation

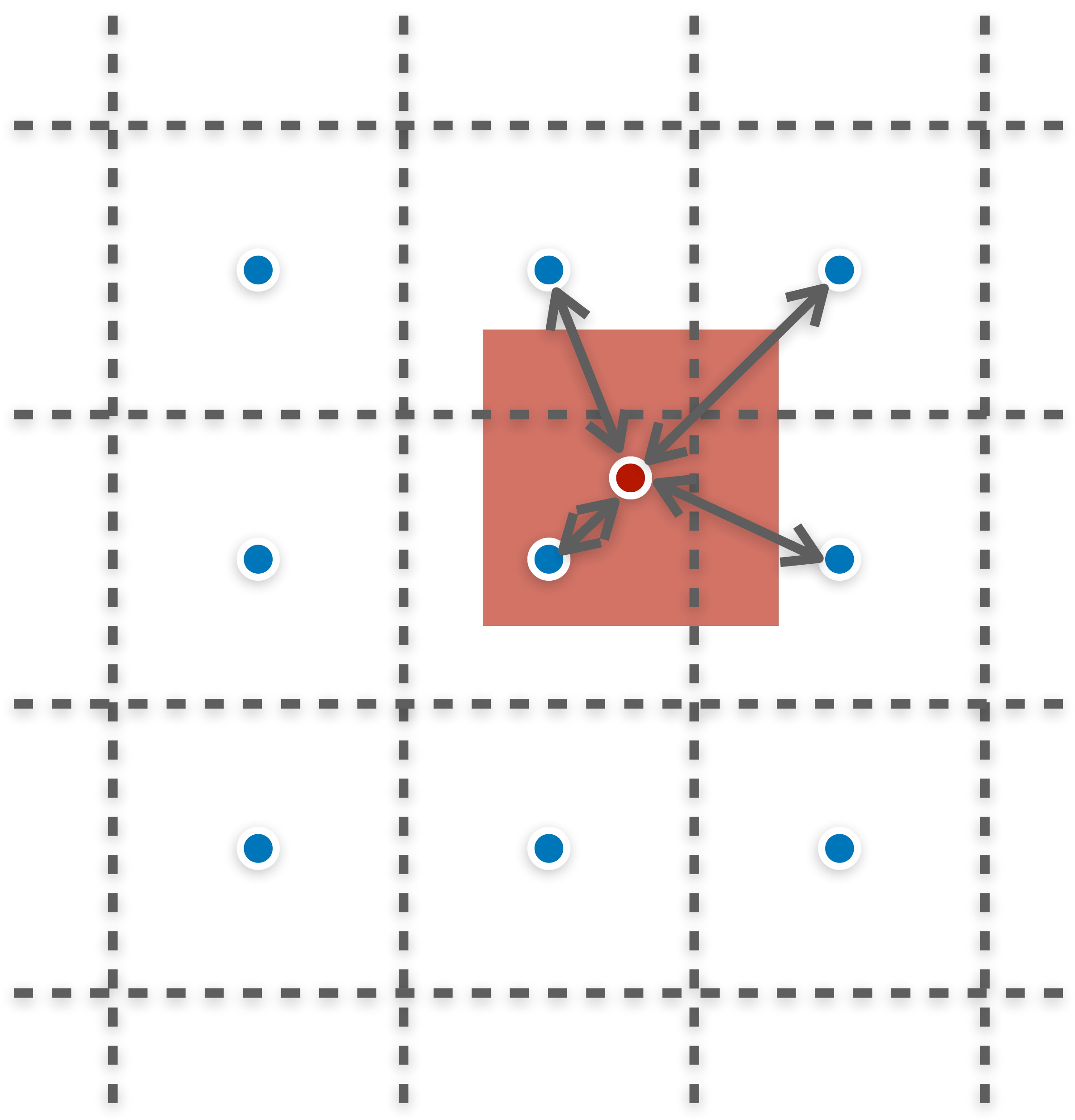
Particle-in-Cell

Normal FD or spectral method are too expensive for a 3D-3V equation;

Particle method plays a very important role in simulation: it reduces the problem to 3D, whereas the 3V part is handled by Newton's law of motion (formal proof is through taking moments of Vlasov's equation).

Algorithm outline (electrostatic):

1. Spread charge: $\rho(\mathbf{x}) = \sum_{j=1}^{N_p} qS(\mathbf{X}_j - \mathbf{x})$, where S is the shape function / interpolation function;
2. Solve Poisson's equation on grid points $\mathbf{x}$ using FD / spectral method and find $\mathbf{E}(\mathbf{x})$;
3. Interpolate electric field: $\mathbf{E}(\mathbf{X}_j) = \sum_{\mathbf{x}} \mathbf{E}(\mathbf{x})S(\mathbf{x} - \mathbf{X}_j)$
4. Push particles: $\dot{\mathbf{X}}_j = \mathbf{V}_j, \qquad \dot{\mathbf{V}}_j = q(\mathbf{E} + \mathbf{V}_j \times \mathbf{B}_0)\Big|_{\mathbf{x}=\mathbf{X}_j}$



Communication between a particle and a staggered grid

Particle Method for Solving Vlasov's Equation

Particle-in-Fourier

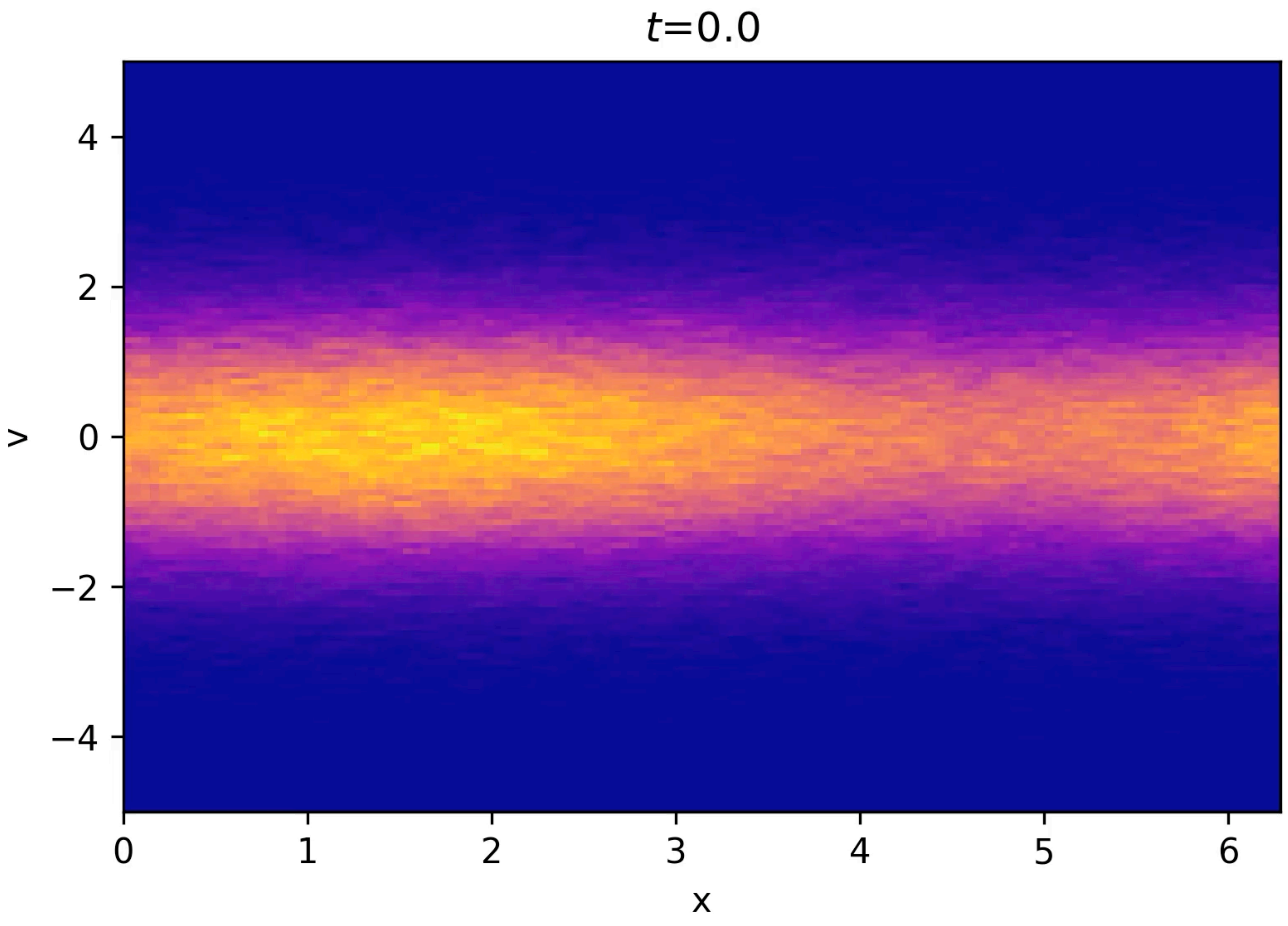
Drawbacks of PIC: Either energy or momentum can't conserve over time due to spatial discretization; High order interpolation causes extraordinary computation.

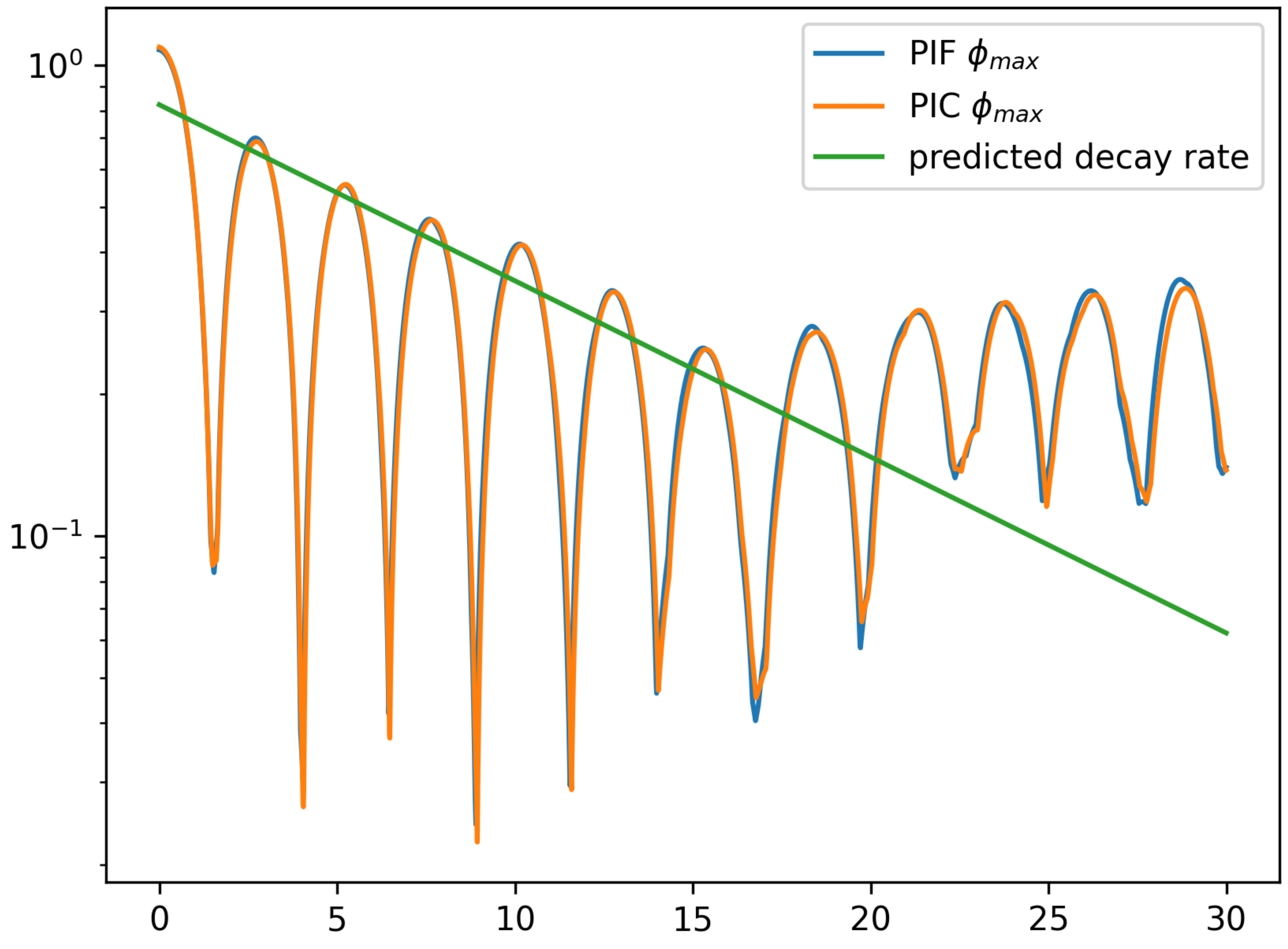
Novel Approach: Interpolate particles directly into Fourier space, and use a spectral solver.

1. Spread charge: $\hat{\rho}(\mathbf{k}) = \sum_{\mathbf{x}} \rho(\mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{x}} = q\hat{S}(\mathbf{k}) \sum_{j=1}^{N_p} e^{-i\mathbf{k}\cdot\mathbf{X}_j}$;

2. Interpolate acceleration: $\mathbf{a}_j = \mathbf{V}_j \times \mathbf{B}_0 + q \sum_{\mathbf{k}} \hat{\mathbf{E}}(\mathbf{k})\hat{S}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{X}_j}$;

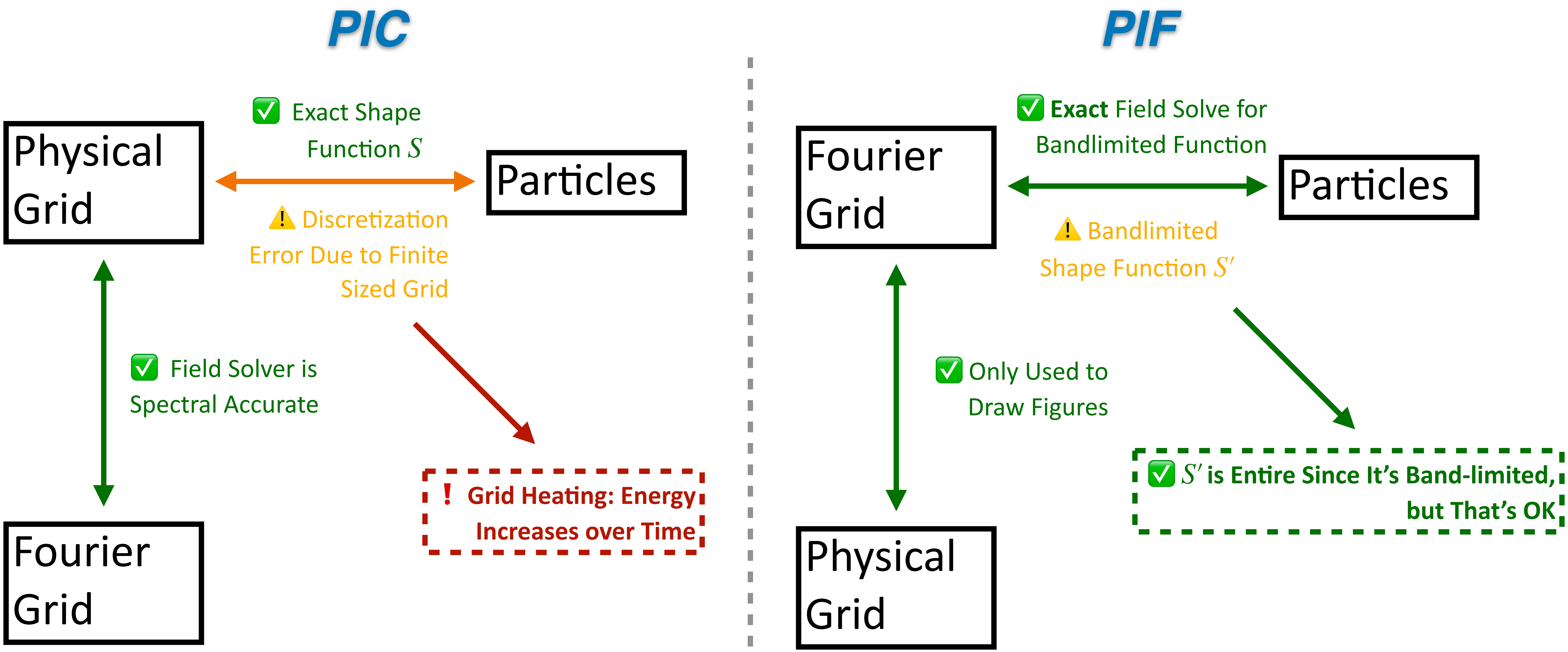
Fourier transforms of the type $\hat{f}(\mathbf{k}) = \sum_{j=1}^{N_p} f(\mathbf{X}_j) e^{\pm i\mathbf{X}_j\cdot\mathbf{k}}$ and $f(\mathbf{X}_j) = \sum_{\mathbf{k}} \hat{f}(\mathbf{k}) e^{\pm i\mathbf{X}_j\cdot\mathbf{k}}$ are handled by Non-uniform Fast Fourier Transform.


t=0.0
v
x
0
1
2
3
4
5
6
4
2
0
−2
−4


PIF ϕ_{max}
PIC ϕ_{max}
predicted decay rate
10^0
10^{-1}
0
5
10
15
20
25
30

Particle Method for Solving Vlasov's Equation

Particle-in-Fourier: Another Perspective



Particle Method for Solving Vlasov's Equation

Particle-in-Fourier

Advantages:

- 😆 Exact momentum & charge conservation;
- 😆 Energy conservation as $\Delta t \to 0$ (PIC does not conserve energy even for arbitrarily small time step);
- 😆 Arbitrary interpolation function…

Drawbacks:

- 😢 Bundled with spectral method for field solve, and thus only periodic BC using NUFFT;
- 😢 Nontrivial boundary conditions can be handled using other basis functions, but conservation properties are lost.

Can we overcome the drawbacks?

🛸 Free Space Poisson Solver

Free Space Poisson Solver

Vico-Greengard-Ferrando Scheme

Hard to numerically compute free space BC Poisson's equation since the solution is entire in $\mathbb{R}^d$;

If we specify our computational domain $\Omega = [0,1] \times [0,1]$, we find the free space solution

$$
\begin{aligned}
\varphi(\mathbf{x}) &= (g * \rho)(\mathbf{x}) \\
&= (g^L * \rho)(\mathbf{x})
\end{aligned}
$$

where $g(r,\theta) = \dfrac{-1}{2\pi} \log r$ (in 2D), and $g^L(r,\theta) = g(r,\theta)\mathrm{rect}\left(\dfrac{r}{2L}\right)$, with $L \geq \sqrt{d}$. We can thus do convolution between $g^L(\mathbf{x})$ and $\rho(\mathbf{x})$ on an enlarged domain $\tilde{\Omega} = [0,4] \times [0,4]^*$, if we choose $L = 1.5 \geq \sqrt{2}$.

🧐 Order of convergence? Surprisingly, **spectral accurate!**

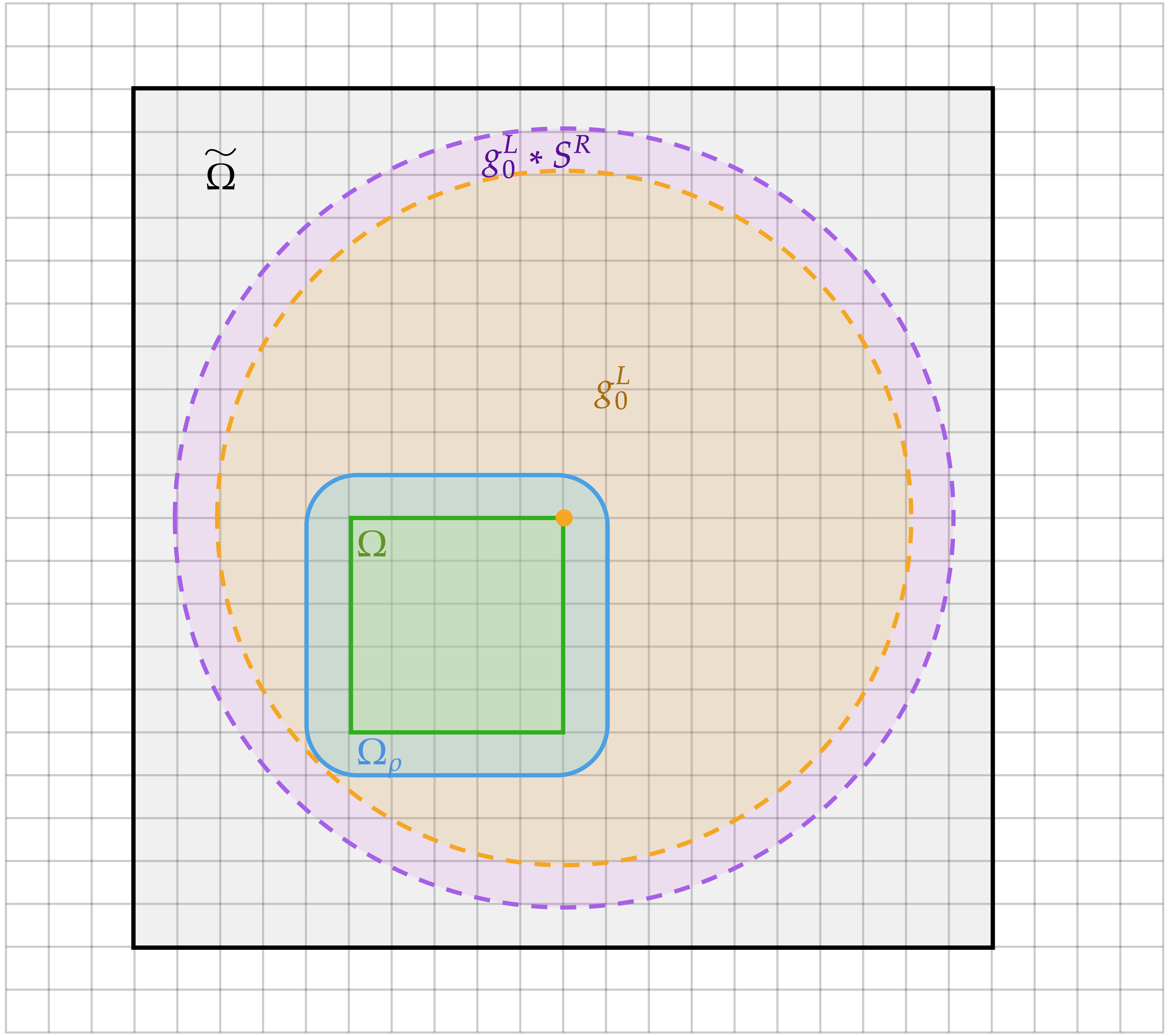
$$
G^L(s) = \mathscr{F}(g^L)(s) = \frac{1 - J_0(Ls)}{s^2} - \frac{L\log(L)J_1(Ls)}{s}
$$

* By special precomputation treatment, we could use a $[0,2] \times [0,2]$ grid to do convolution; however, the tradeoff is the method is spectral accurate only at grid points, whereas third order at arbitrary position in the domain.

💡Our Work: Free Space Particle-in-Fourier

Our Work: Free Space Particle-in-Fourier

Generalized Vico Solver for Lagrangian Particles



💡 **Basic Idea:** Replace the periodic spectral operator $1/k^2$ with Vico's kernel $G^L(\mathbf{k})$, and combine it with PIF scheme

- Define Ω as the domain where particles live in; notice that after convoluting with shape function, ρ lives in a slightly larger domain Ω_ρ.
- The mollified kernel g^L should properly cover the domain: $L \geq \sqrt{2} + R$ where R is the radius of the shape function.

$$\hat{\varphi}(\mathbf{k}) = qG^L(\mathbf{k})\hat{S}(\mathbf{k}) \sum_j \exp(-i\mathbf{k} \cdot \mathbf{X}_j)$$

$$\mathbf{a}_s = -iq^2 \sum_{\mathbf{k}} \left(\mathbf{k}G^L(\mathbf{k})\hat{S}^2(\mathbf{k}) \sum_j \exp(-i\mathbf{k} \cdot \mathbf{X}_j) \right) \exp(i\mathbf{k} \cdot \mathbf{X}_s)$$

💡 Our Work: Free Space Particle-in-Fourier

Energy Conservation for PIF with Free Space BCs (Leapfrog)

$$U_E^t = \frac{1}{2}\sum_{\mathbf{k}} \overline{\hat{\rho}^t(\mathbf{k})}\hat{\varphi}^t(\mathbf{k}), \qquad U_K^t = \frac{1}{2}\sum_j \quad \mathbf{V}_j^t \quad {}^2$$

$$U_K^{t+1} = U_K^t + \Delta t \sum_s \mathbf{V}_s^t \cdot \sum_{\mathbf{k}} \left(-i\mathbf{k}G(\mathbf{k}) \left| \hat{S}(\mathbf{k}) \right|^2 \sum_j \exp(i\mathbf{k}\cdot(\mathbf{X}_s^t - \mathbf{X}_j^t)) \right) + \mathcal{O}(\Delta t^2)$$

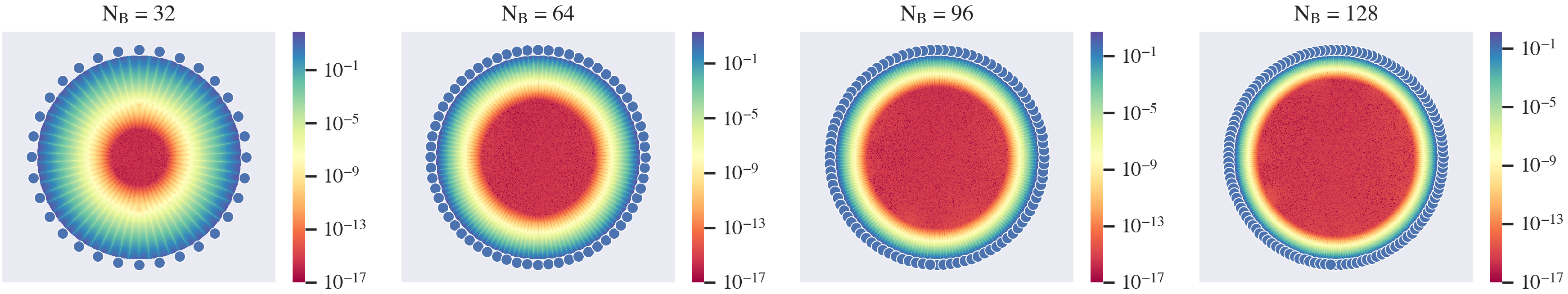
$$U_E^{t+1} = U_E^t - \sum_s \mathbf{V}_s^t \cdot \Delta t \sum_{\mathbf{k}} \left(-i\mathbf{k}G(\mathbf{k}) \left| \hat{S}(\mathbf{k}) \right|^2 \sum_j \exp(i\mathbf{k}\cdot(\mathbf{X}_s^t - \mathbf{X}_j^t)) \right) + \mathcal{O}(\Delta t^2)$$

$$\longrightarrow \quad U_K^t + U_E^t = U_K^{t+1} + U_E^{t+1} + \mathcal{O}(\Delta t^2)$$

💡 Our Work: Free Space Particle-in-Fourier

Generalization to Arbitrary Dirichlet BCs on unit circle

$$\varphi^H(\mathbf{x}) = \frac{1}{2\pi}\int_{|\mathbf{z}|=1} \frac{1-|\mathbf{x}|^2}{|\mathbf{z}-\mathbf{x}|^2}(f-\varphi^P)(\mathbf{z})\,d\theta$$



⚠️ Boundary integral method evaluates $\varphi^H(\mathbf{X}_j)$ using the above equation directly at particle positions; However, what we actually need is $(\varphi^H * S)(\mathbf{X}_j)$

💡 Our Work: Free Space Particle-in-Fourier

Generalization to Arbitrary Dirichlet BCs on unit circle

- Suppose the solution of the Poisson equation is $\varphi = \varphi^H + \varphi^P$, and we pose the following assumptions:
  - φ can be analytically extended to $B_{1+R}(0)$, where R is the radius of the shape function;
  - The charge density satisfies

$$\rho(x) = 0 \quad \forall x \in \bigcup_{x' \in C_1(0)} B_R(x')$$

- Then by Mean Value Property, we have

$$-\rho * S(x) = \Delta(\varphi * S)(x)$$
$$(\varphi * S)(x) = \varphi(x) \quad \forall x \in C_1(0)$$

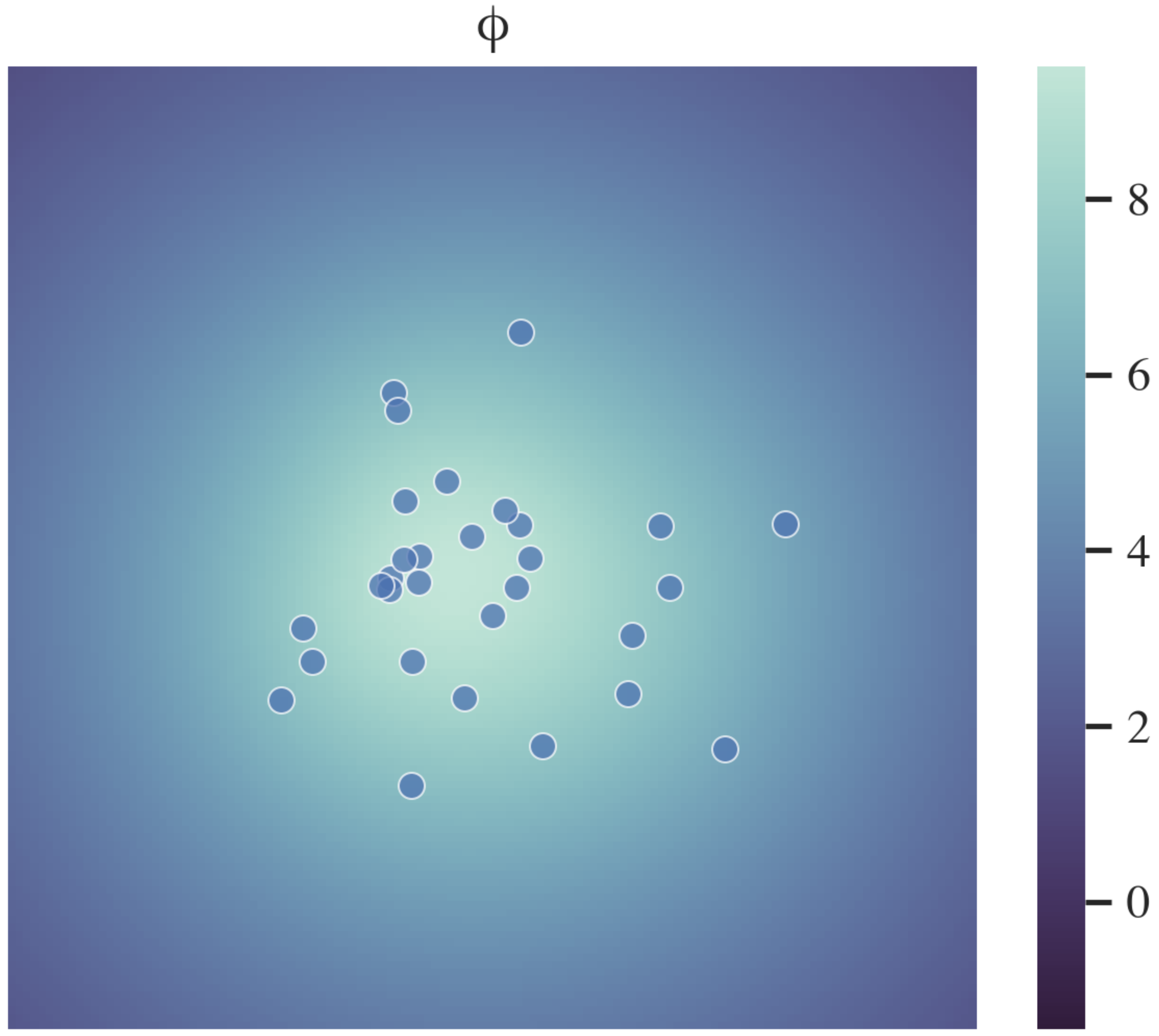
- The solution can then be easily found using boundary integral method.

Numerical Results

Numerical Results

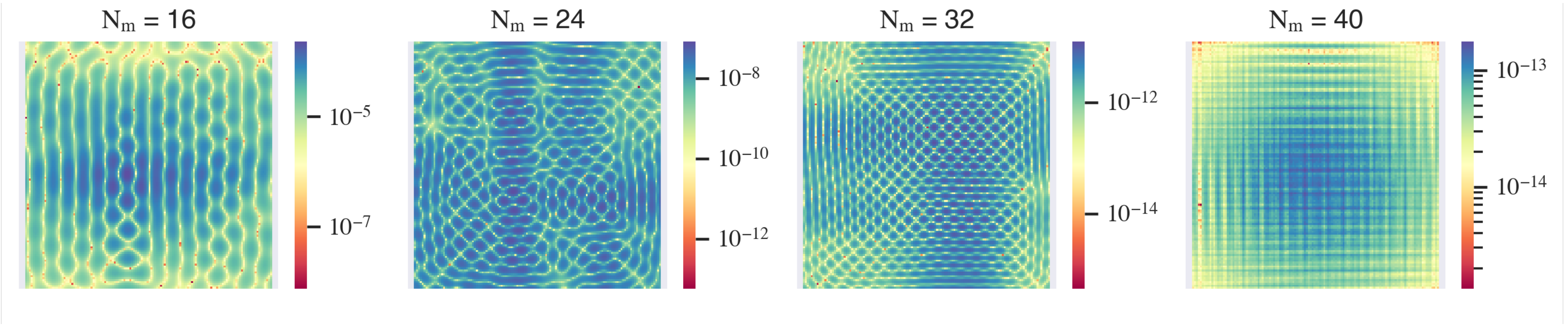
Free Space Poisson Solver

Randomly generated particles with shape function $S(r) = \dfrac{1}{\sqrt{2\pi}\sigma} \exp\left(-\dfrac{r^2}{\sigma^2}\right)$



$$\rho(\mathbf{x}) = q\sum_j S(\mathbf{X}_j - \mathbf{x}) = \frac{q}{2\pi\sigma^2}\sum_j \exp\left(-\frac{\mathbf{X}_j - \mathbf{x}\quad {}^2}{2\sigma^2}\right),$$

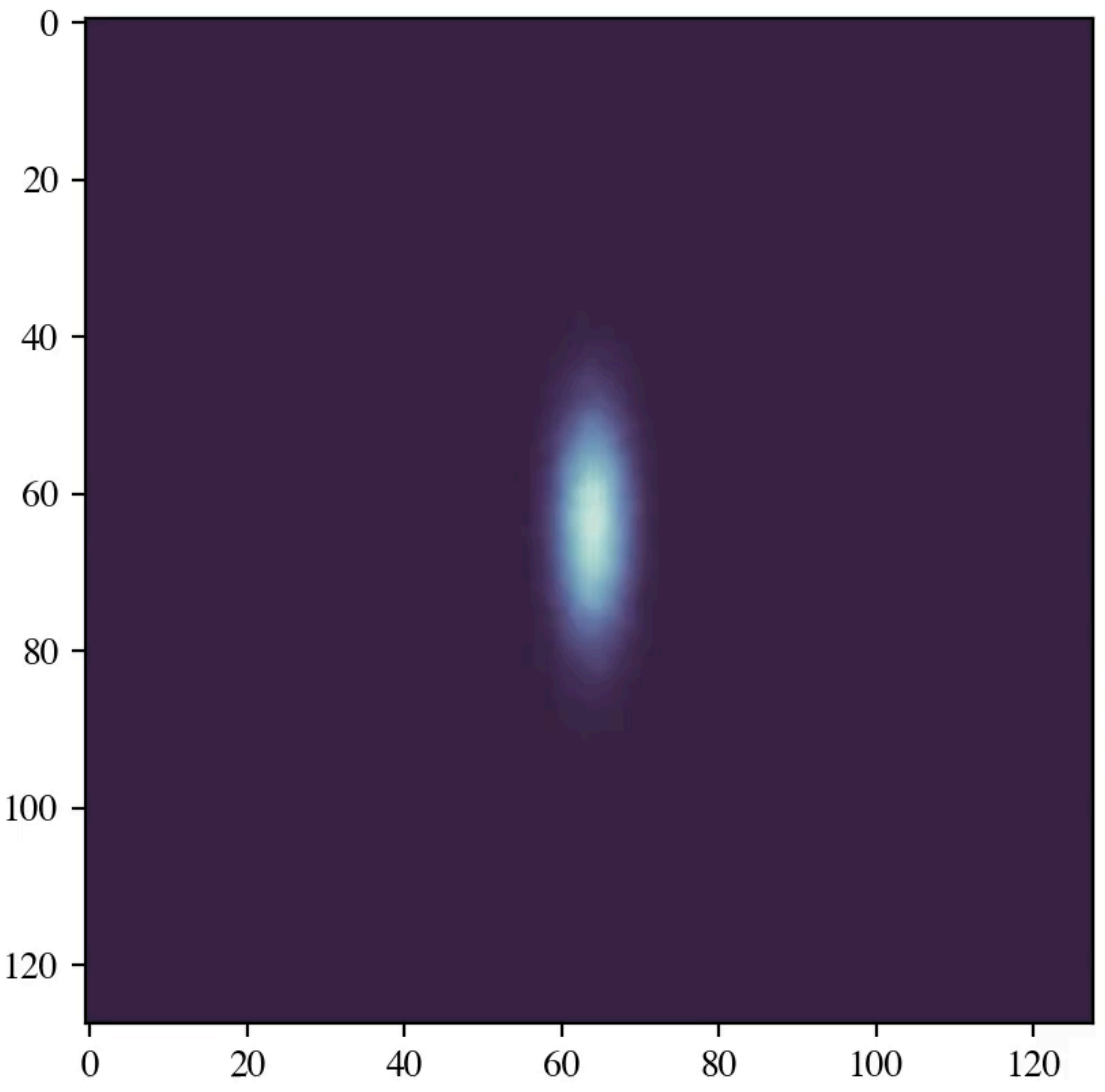
$$\varphi(\mathbf{x}) = \frac{q}{4\pi}\sum_j expi\left(\left(-\frac{\mathbf{X}_j - \mathbf{x}\quad {}^2}{2\sigma^2}\right) - \log(\quad \mathbf{X}_j - \mathbf{x}\quad {}^2)\right)$$

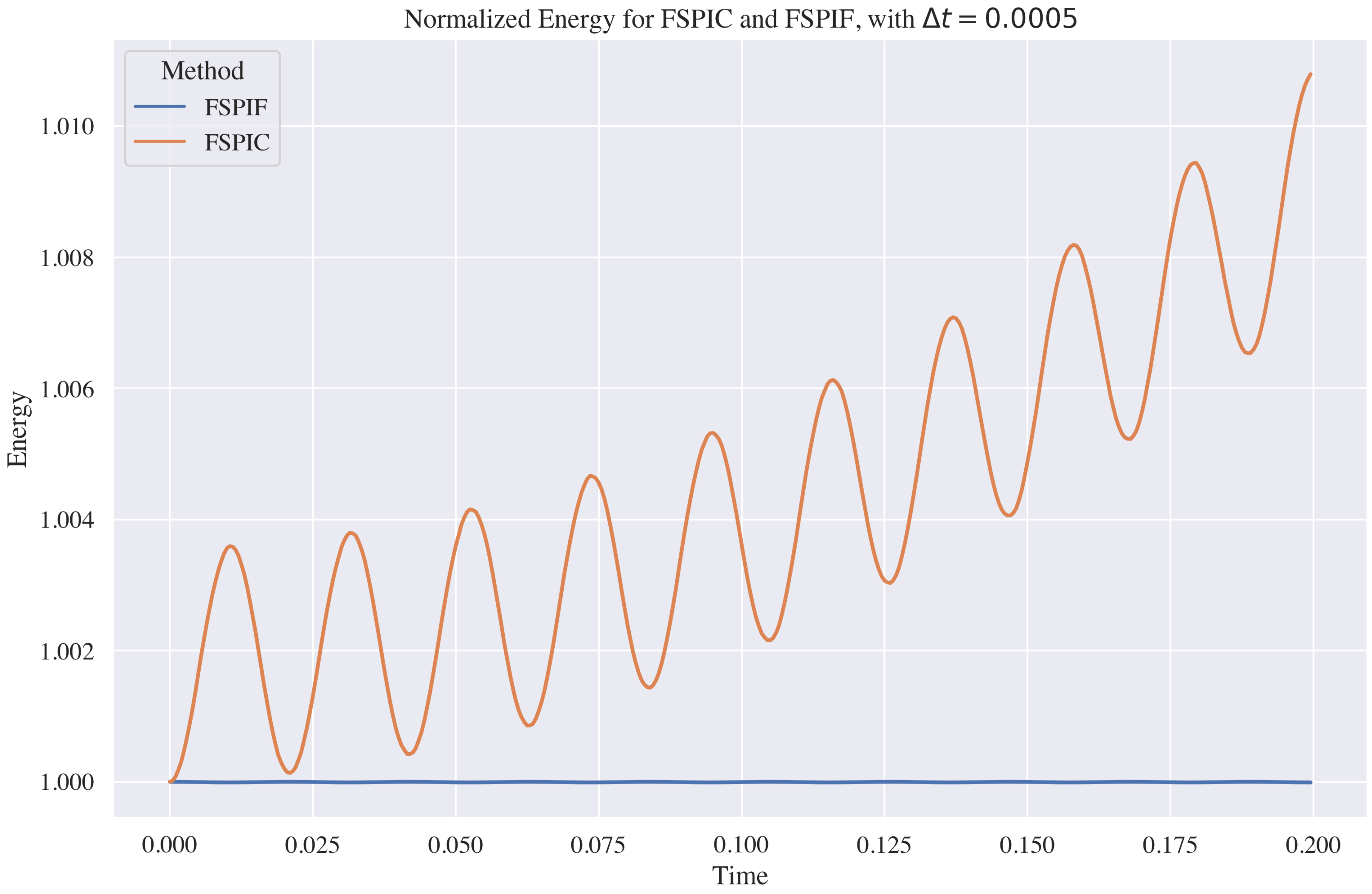


Numerical Results

Test Case: Free Space Cyclotron Beam ($B_0 \sim 50E$)

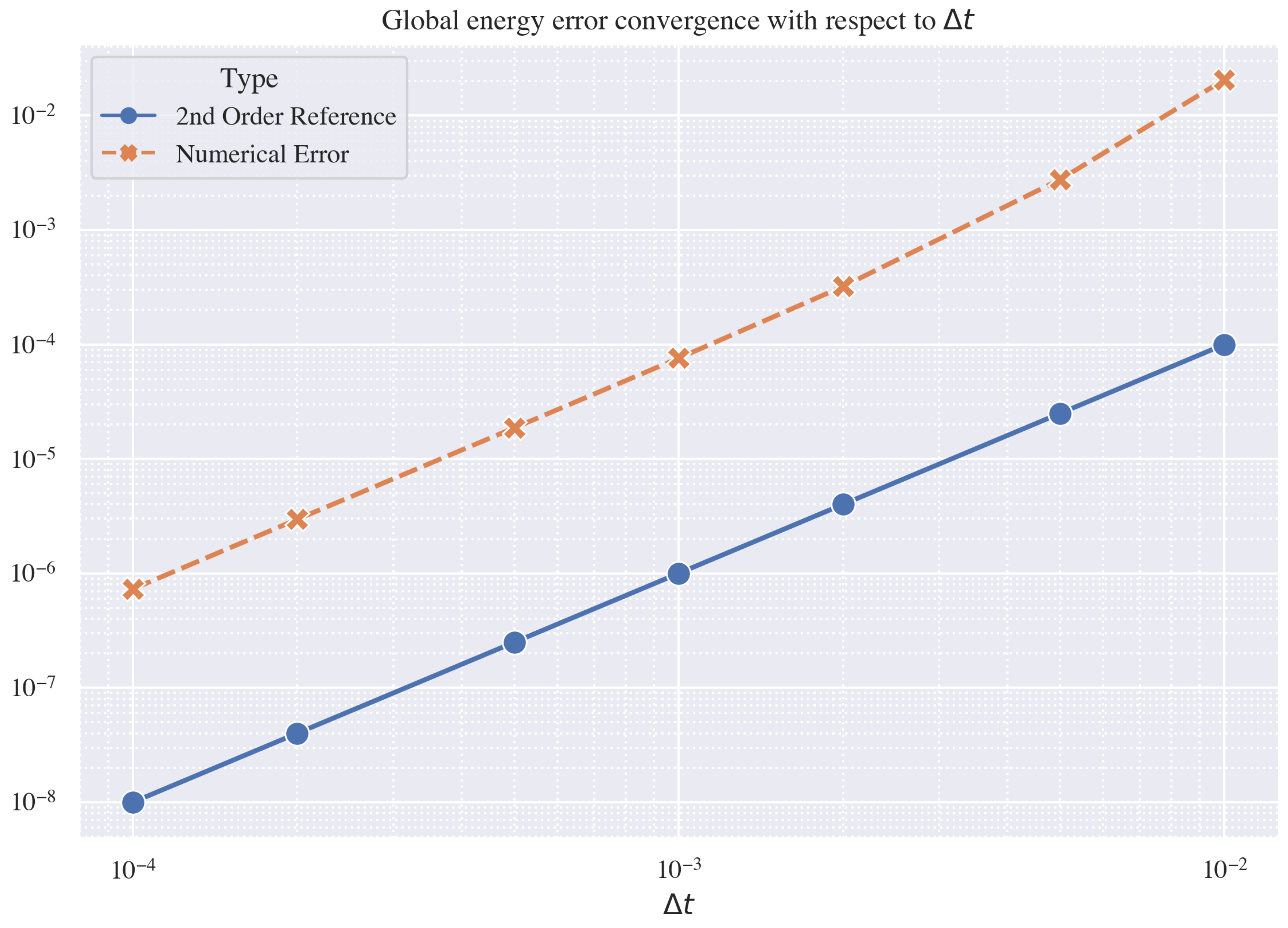
$$f(x,y,v_x,v_y,0) = \frac{n(x,y)}{2\pi} e^{-\frac{v_x^2+v_y^2}{2}} \quad \text{where} \quad n(x,y) = \frac{1}{\pi\sigma_x\sigma_y} e^{-\frac{x^2}{\sigma_x^2}} e^{-\frac{y^2}{\sigma_y^2}} \text{ with } \sigma_x = \frac{1}{30}, \sigma_y = \frac{1}{10}$$

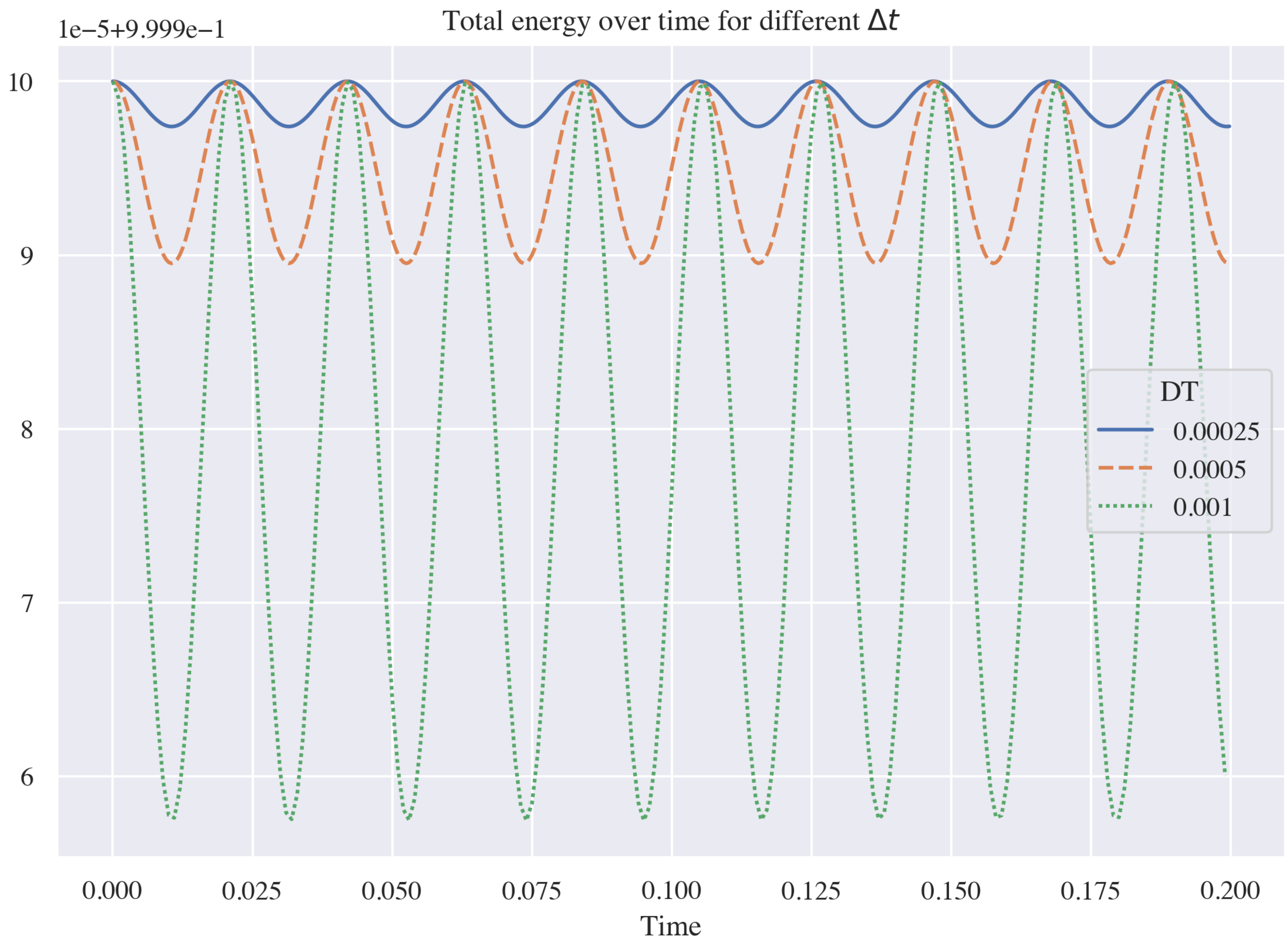




Numerical Results

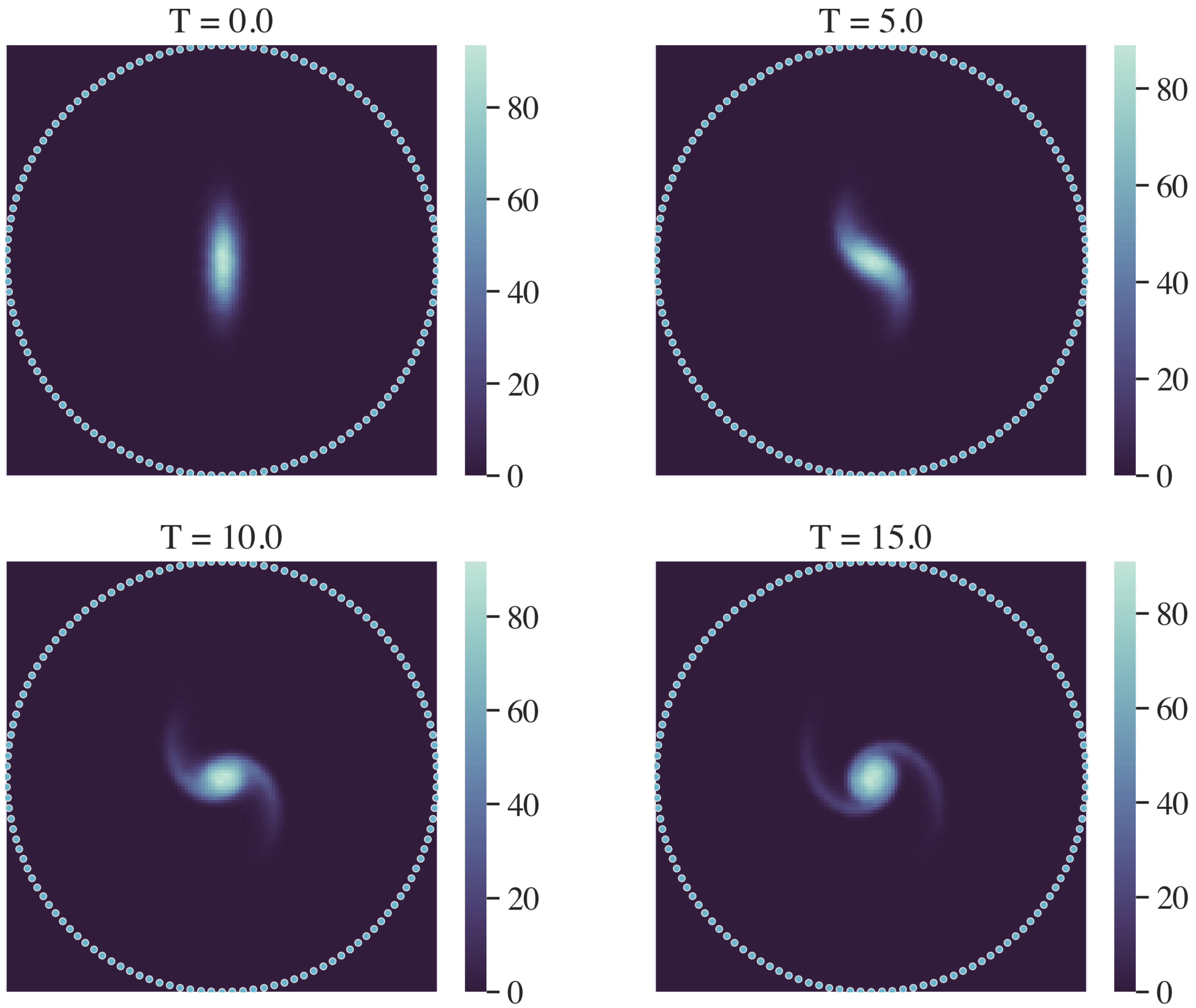
Test Case: Free Space Cyclotron Beam ($B_0 \sim 50E$)

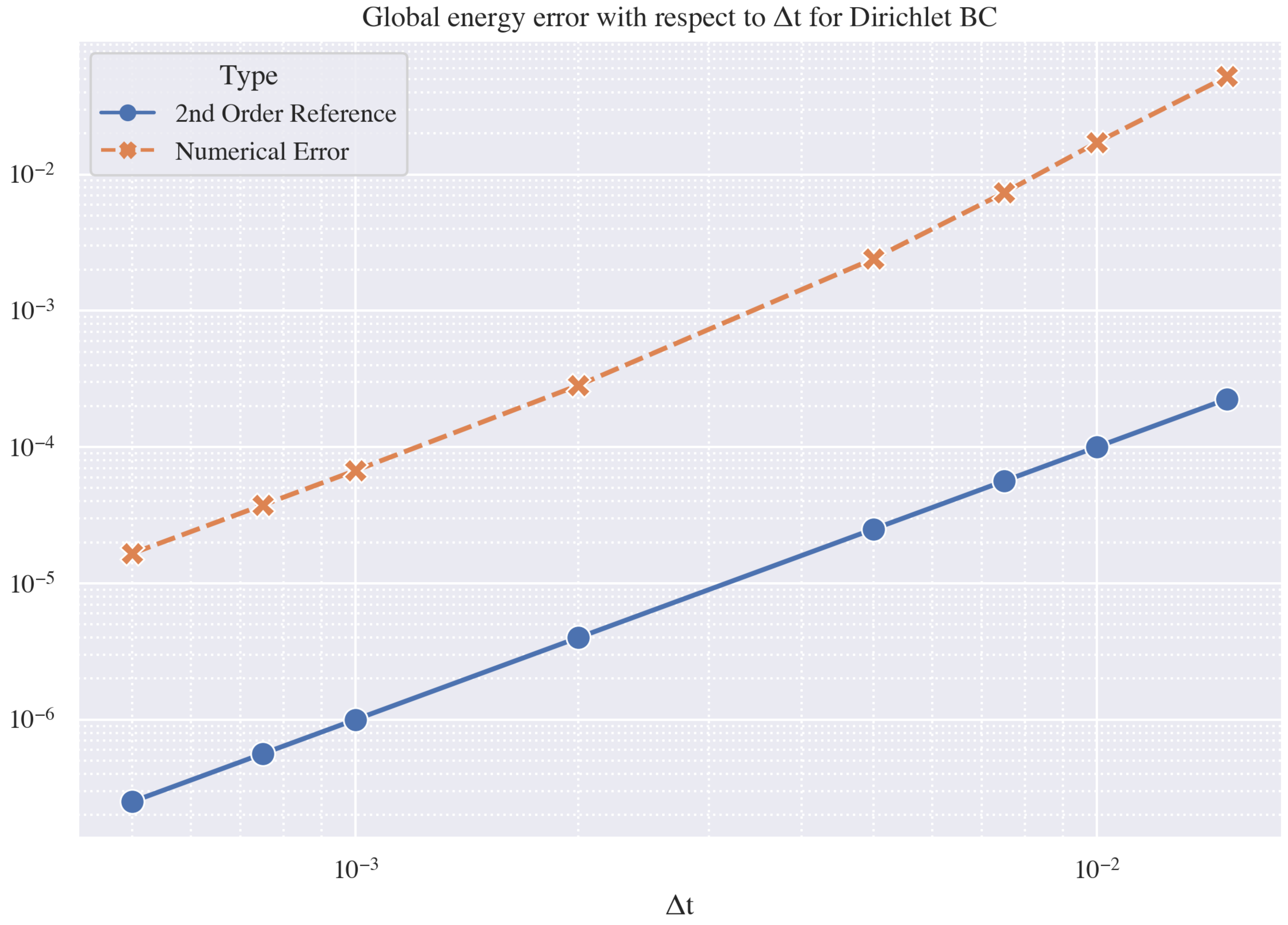




Numerical Results

Test Case: Cylinder-Confined Cyclotron Beam





Select Works Cited

1. Cerfon, Antoine J. "Vortex Dynamics and Shear Layer Instability in High Intensity Cyclotrons." *Physical Review Letters* 116, no. 17 (April 28, 2016): 174801. https://doi.org/10.1103/PhysRevLett.116.174801.
2. Evstatiev, E. G., and B. A. Shadwick. "Variational Formulation of Particle Algorithms for Kinetic Plasma Simulations." *Journal of Computational Physics* 245 (July 15, 2013): 376–98. https://doi.org/10.1016/j.jcp.2013.03.006.
3. Hairer, Ernst, and Christian Lubich. "Energy Behaviour of the Boris Method for Charged-Particle Dynamics." *BIT Numerical Mathematics* 58, no. 4 (December 2018): 969–79. https://doi.org/10.1007/s10543-018-0713-1.
4. Klöckner, Andreas, Alexander Barnett, Leslie Greengard, and Michael O'Neil. "Quadrature by Expansion: A New Method for the Evaluation of Layer Potentials." *Journal of Computational Physics* 252 (November 1, 2013): 332–49. https://doi.org/10.1016/j.jcp.2013.06.027.
5. Mitchell, Matthew S., Matthew T. Miecnikowski, Gregory Beylkin, and Scott E. Parker. "Efficient Fourier Basis Particle Simulation." *Journal of Computational Physics* 396 (November 1, 2019): 837–47. https://doi.org/10.1016/j.jcp.2019.07.023.
6. Ricketson, Lee F., and Antoine J. Cerfon. "Sparse Grid Techniques for Particle-in-Cell Schemes." *Plasma Physics and Controlled Fusion* 59, no. 2 (February 1, 2017): 024002. https://doi.org/10.1088/1361-6587/59/2/024002.
7. Vico, Felipe, Leslie Greengard, and Miguel Ferrando. "Fast Convolution with Free-Space Green's Functions." *Journal of Computational Physics* 323 (October 15, 2016): 191–203. https://doi.org/10.1016/j.jcp.2016.07.028.
8. Zou, Junyi, Eugenia Kim, and Antoine J. Cerfon. "FFT-Based Free Space Poisson Solvers: Why Vico-Greengard-Ferrando Should Replace Hockney-Eastwood." arXiv, March 15, 2021. https://doi.org/10.48550/arXiv.2103.08531.