NEOPIC: A Neural Operator Framework for Particle-based Kinetic Plasma Simulations

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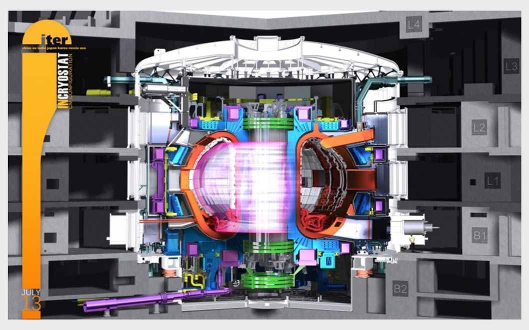
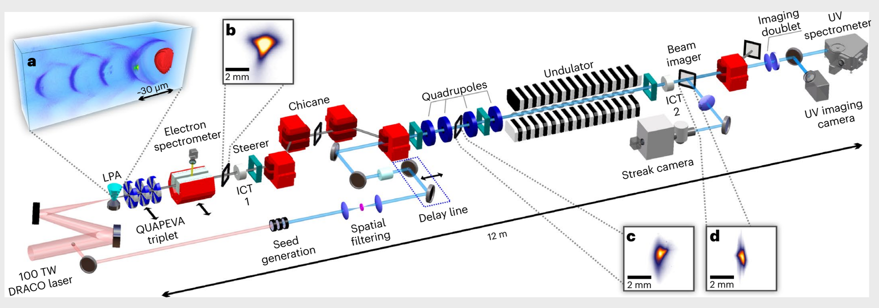
Motivation

- Kinetic plasma simulations: Nuclear fusion, Particle accelerators



Source: iter.org



Source: M. Labat et al., Nature Photonics, 2023

- Particle-in-cell (PIC): Method of choice for kinetic plasma simulations
- Issues:
  - Computational cost: large number of grid points ($\mathcal{O}(10^{11})$), particles ($\mathcal{O}(10^{12})$) and time steps ($\mathcal{O}(10^{5})$) for high-fidelity simulations
  - Numerical artifacts from grid-based solvers
- Many-query scenarios: Still unreachable with exascale supercomputers
- Need cheap surrogate models which still capture essential physics

Particle-in-Neural Operators (PINOP)

INITIALIZATION: Initialize particles positions, velocities, and charges

Neural Operator: Infer electric and magnetic fields from the particles positions and velocities

PUSH: Update particles positions and velocities

Particle equations:

$$\frac{d\mathbf{x}_k}{dt} = \mathbf{v}_k,$$
$$\frac{d\mathbf{v}_k}{dt} = \frac{q_k}{m_k}(\mathbf{E}(\mathbf{x}_k, t) + \mathbf{v}_k \times \mathbf{B}(\mathbf{x}_k, t)).$$

Field equations:

$$\nabla \times \mathbf{B} = \mu_0 (\mathbf{J} + \epsilon_0 \partial_t \mathbf{E}), \qquad \nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0},$$
$$\partial_t \mathbf{B} + \nabla \times \mathbf{E} = 0, \qquad \nabla \cdot \mathbf{B} = 0.$$
$$\rho(\mathbf{x}, t) = \sum_k q_k S(\mathbf{x} - \mathbf{x}_k), \quad \mathbf{J}(\mathbf{x}, t) = \sum_k q_k \mathbf{v}_k S(\mathbf{x} - \mathbf{x}_k).$$

Steps:

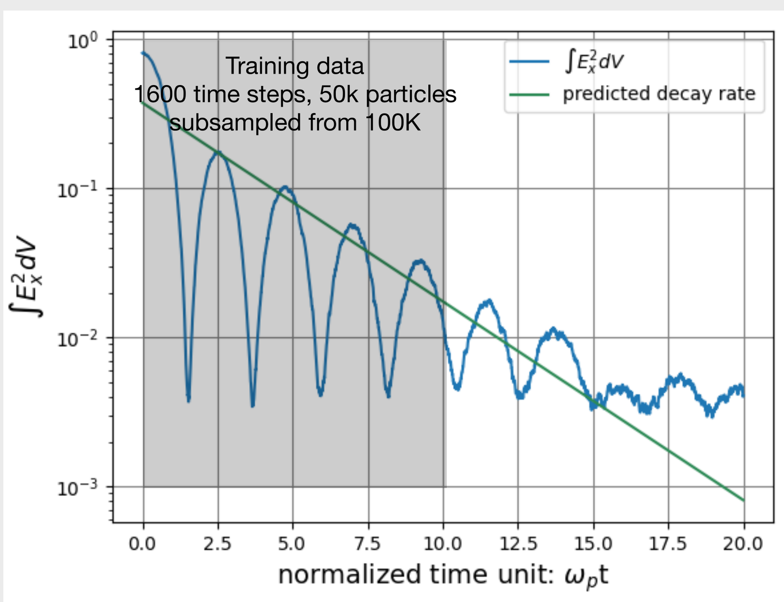
- Particle pusher: Same as in particle-based methods
- Electric and magnetic fields: Obtain from a *neural operator* instead of mesh-based or tree-based (mesh-free) field solvers by approximating the map $G : (\mathbf{x}, \mathbf{v}) \rightarrow (\mathbf{E}, \mathbf{B})$

Advantages:

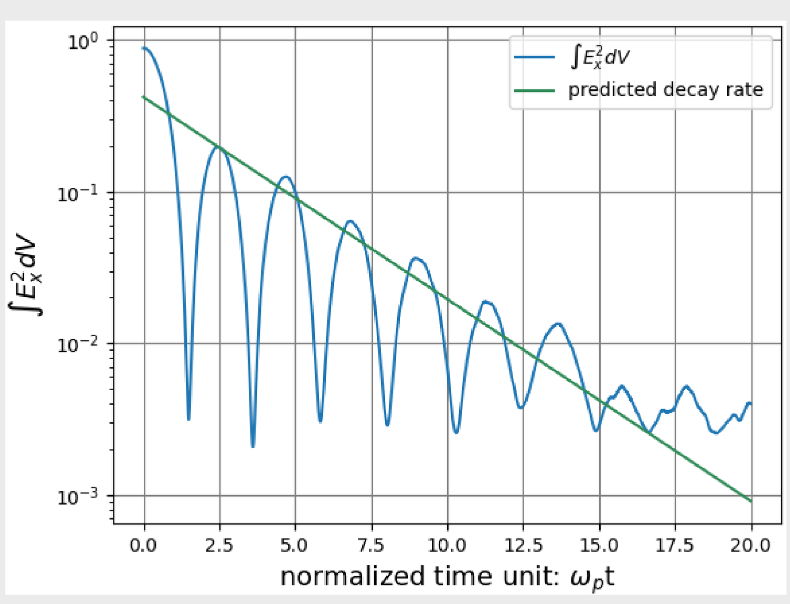
- Not constrained by Debye length and Courant-Friedrichs-Lewy time stepping restrictions
- Can use data from a variety of particle-based methods (discretization invariance)
- Can be trained and tested with different numbers of particles (resolution invariance)
- Can be interfaced with any particle-based production/community code
- Utilizes the strengths of both particle methods and AI

Preliminary results

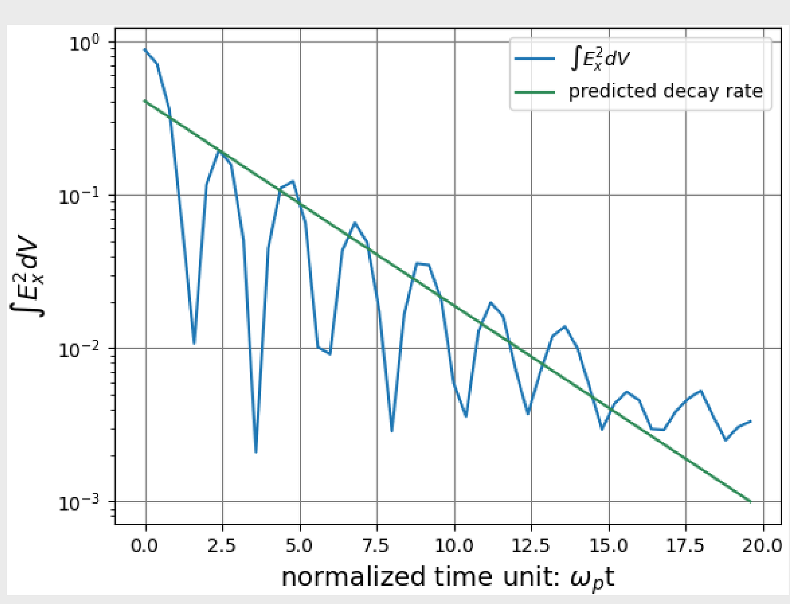
- 2D-2V electrostatic Landau damping: Trained with 50K particles and inference with 500K particles using Fourier neural operator in PINOP



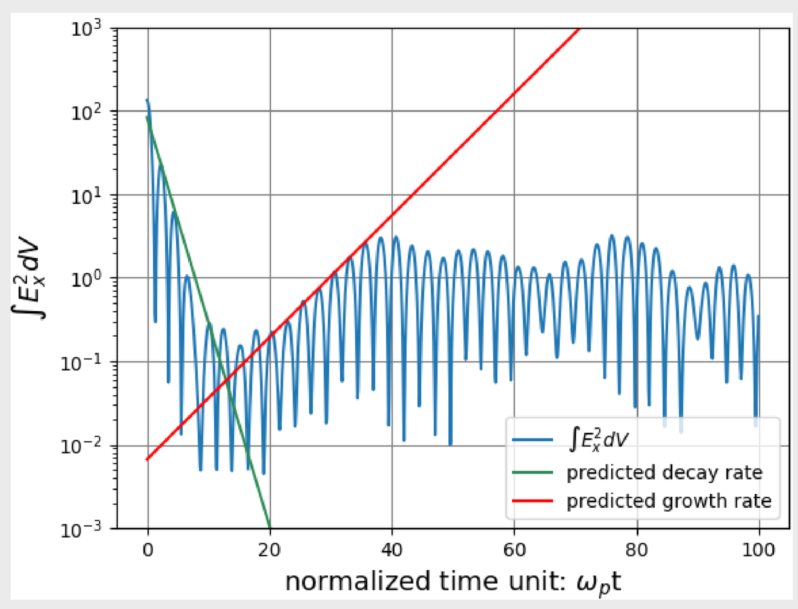
PIC



PINOP



PINOP: 80X larger time stepsize than training



PINOP: Different initial condition

Project Outlook

- Investigate other neural operator architectures (e.g. DeepONet, Graph neural operators)
- Incorporate physics to help with the generalization, long time rollouts and data requirements
- PINOP for electromagnetic kinetic plasma simulations
- HPC strategies for the PINOP scheme
  - Domain decomposition
  - Data reduction strategies
  - Interface to production particle codes

References

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This project has received funding from Helmholtz AI projects 2024 under the grant agreement number ZT-I-PF-5-242.