NEURAL INFORMATION PROCESSING SYSTEMS

Learning Efficient Hybrid Particle-continuum Representations of Non-equilibrium N-body Systems

T. Wu[1], M. Sun[1,2], H.G. J. Chou[2,3], P. Samala[1], S. Cholsaipant[1], S. Kivelson[1], J. H. Yau[1], Z. Ying[1,4], E. P. Alves[5], J. Leskovec[1], F. Fiuza[2]

[1] Computer science department, Stanford University; [2] High-energy-density division, SLAC [3] Physics department, Stanford University; [4] The department of computer science, Yale University; [5] Physics and astronomy department, UCLA

Introduction

The dynamics of physical systems is often **nonlinear** and involves the **competition** of different processes **across a wide range of spatial and temporal scales**. Particle and continuum representations could provide an efficient framework to model these systems at the disparate scales. However, **accurate modeling including both and the coupling between these representations has been a key challenge**, often limited to inaccurate or incomplete prescriptions.

In this work, we introduce Learning Hybrid Particle-Continuum (LHPC) models to **combine first-principles particle solvers, and learn the continuum dynamics and the particle-continuum coupling** with deep neural networks.

We demonstrate our method in an intense laser-plasma interaction problem involving the highly nonlinear, far-from-equilibrium dynamics associated with the coupling between multiple particle species and electromagnetic (EM-) fields. Our method paves the way for **more efficient modeling** of these interactions, critical for the design and optimization of compact accelerators for material science and medical applications.

Artist's view of particle acceleration from laser-plasma interactions

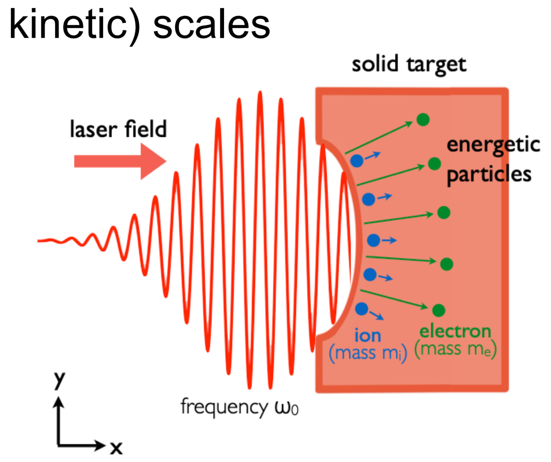
Background

Method	Pros	Cons
Continuum (fluid)	- Computationally efficient - Accurate descriptions of near-equilibrium systems	- Limited to large scales - Breaks down for non-equilibrium phenomena (small scales)
Particle (kinetic)	- First-principles descriptions of small-scale non-equilibrium phenomena	- Computationally intensive - Limited to small scales
Continuum + Deep Learning	- Accelerates simulations through coarser spatial and temporal resolutions	- Same as continuum-based approaches
Our method: Hybrid particle-continuum	- Computationally efficient - Accurate descriptions for both near- and non-equilibrium phenomena - Accurate at both large and small scales	- Requires efficient coupling the two representations

Hybrid (particle-continuum) representation

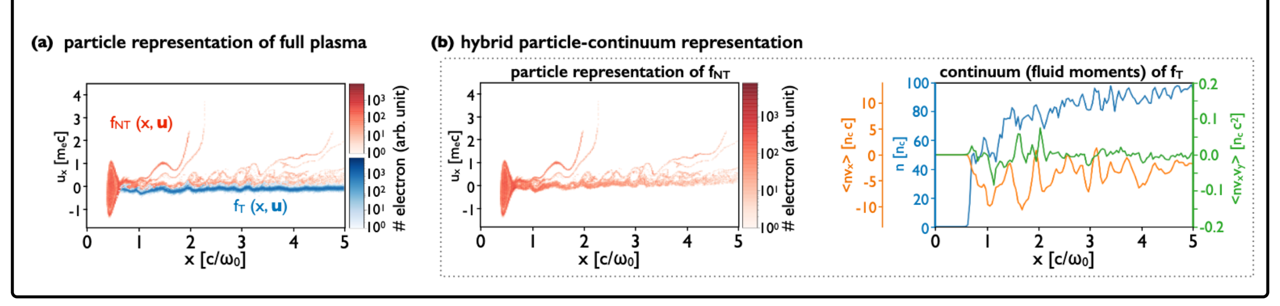
Multi-scale nonlinear dynamics of laser-plasma interactions.

Intense laser-plasma interactions generate energetic particles with rich dynamics involving both large (continuum, fluid) and small (particle, kinetic) scales



Representations of plasma dynamics (illustrated with electrons)

- Left two: longitudinal momentum (u_x)-position (x) phase space
- Right : velocity moments of the continuum (fluid)



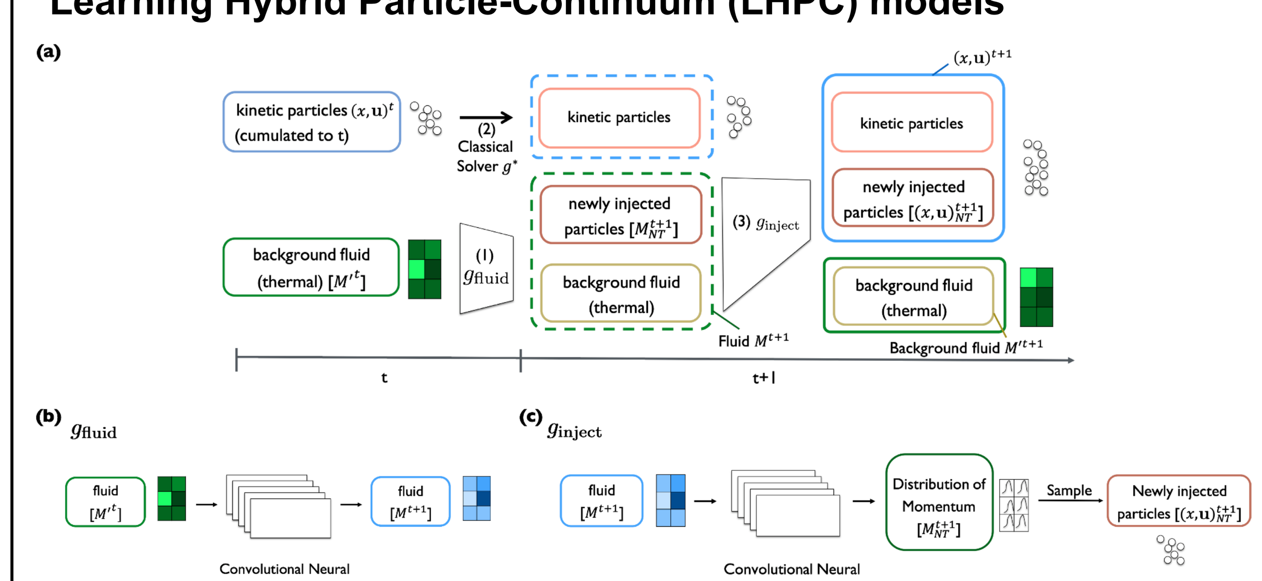
Method

General descriptions of the evolution of a dynamical system

In general, simulations of the time-evolution of a dynamical system can be described as follows. The state of the system at time t is s^t , and there exists a ground-truth evolution g^* that evolves this state:

$$s^{t+1} = g^* (s^t) \quad , \quad t = 0, 1, 2, \dots$$

Learning Hybrid Particle-Continuum (LHPC) models



We employ LHPC to model laser-plasma particle-in-cell simulations:

(1) g_{fluid}:
neural network with parameters θ evolving the continuum (fluid)

(2) g^*:
ground-truth solver that evolves the kinetic particles

(3) g_{inject}:
neural network with parameters ϕ which models the interplay of the continuum (fluid) and particle (kinetic) populations

Results

LHPC achieves

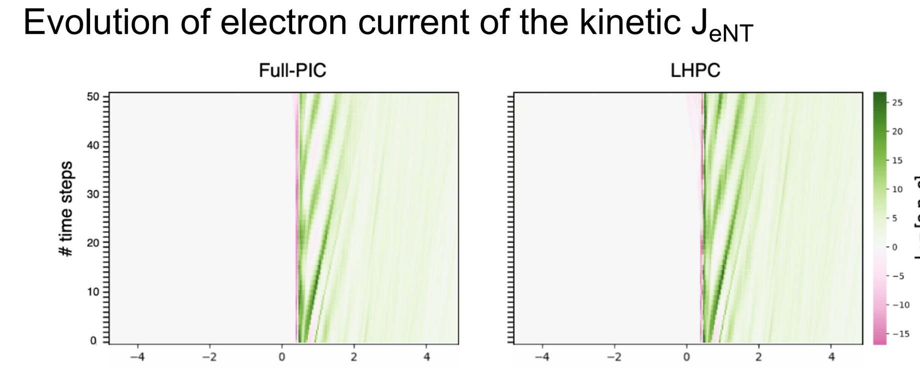
(1) **Significant error reduction** in comparison to the best-performing baseline) on:
- EM-fields: 85.4%
- Velocity moments of the kinetic population (M_{PIC}): 25.8%

(2) **8x speed-up** in comparison to the ground-truth solver

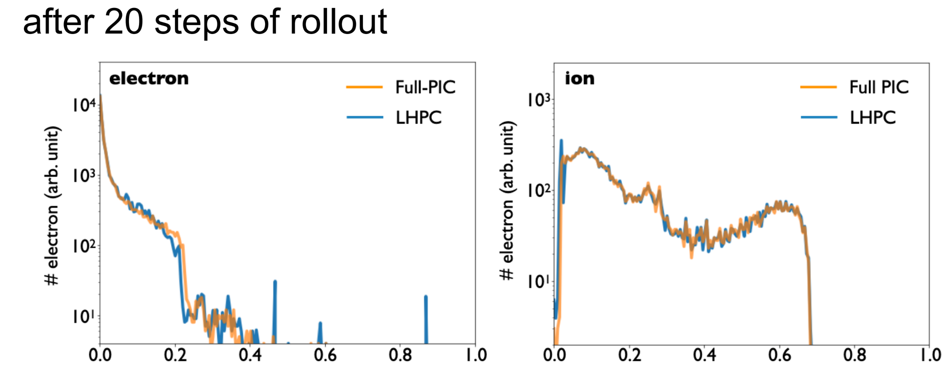
Method	Component	Error @ step 1	Error @ step 20	Error @ step 50	Speed (s/step)
GT Solver (full PIC)	–	–	–	–	9.21E-01
FNO: All-fluid	Field M_{PIC} M	5.77E-02 ± 1.52E-02 – 5.53E-03 ± 1.16E-03	9.36E-01 ± 2.00E-01 – 6.79E-02 ± 1.47E-02	2.57E+00 ± 8.56E-01 – 3.07E-01 ± 6.71E-02	7.79E-02
FNO: Bi-Gaussian	Field M_{PIC} M	2.67E-02 ± 3.23E-03 2.67E-02 ± 2.70E-03 5.85E-03 ± 1.01E-03	1.81E-01 ± 2.61E-02 2.37E-01 ± 2.98E-02 6.99E-02 ± 1.61E-02	1.22E+01 ± 8.62E+00 3.61E+01 ± 2.78E+01 7.46E+00 ± 5.38E+00	1.96E-01
Baseline: All-fluid	Field M_{PIC} M	1.97E-02 ± 7.53E-03 – **2.62E-03** ± 4.63E-04	1.83E-01 ± 5.86E-02 – **4.86E-02** ± 9.02E-03	7.16E-01 ± 3.66E-01 – **1.31E-01** ± 3.55E-02	**4.61E-02**
Baseline: Bi-Gaussian	Field M_{PIC} M	1.67E-02 ± 5.16E-03 1.86E-02 ± 4.49E-03 3.28E-03 ± 7.29E-04	1.98E-01 ± 3.34E-02 3.00E-01 ± 1.00E-01 4.95E-02 ± 6.55E-03	5.63E-01 ± 9.39E-02 7.67E-01 ± 3.49E-01 1.39E-01 ± 2.39E-02	9.34E-02
LHPC (no-coupling)	Field M_{PIC} M	**1.01E-03** ± 1.72E-04 **8.18E-03** ± 2.02E-03 4.51E-03 ± 7.12E-04	1.40E-02 ± 1.66E-03 1.53E-01 ± 5.97E-02 9.29E-02 ± 2.00E-02	1.38E-01 ± 4.52E-02 5.15E-01 ± 1.15E-01 3.26E-01 ± 7.00E-02	1.05E-01
LHPC	Field M_{PIC} M	**1.01E-03** ± 1.57E-04 **8.18E-03** ± 2.02E-03 4.51E-03 ± 7.12E-04	**1.14E-02** ± 6.76E-04 **1.16E-01** ± 6.69E-02 7.44E-02 ± 8.80E-03	**5.34E-02** ± 6.68E-03 **3.71E-01** ± 7.83E-02 1.80E-01 ± 2.88E-02	1.15E-01

LHPC accurately evolves the system in rollout (comparing against the ground-truth solver Full-PIC)

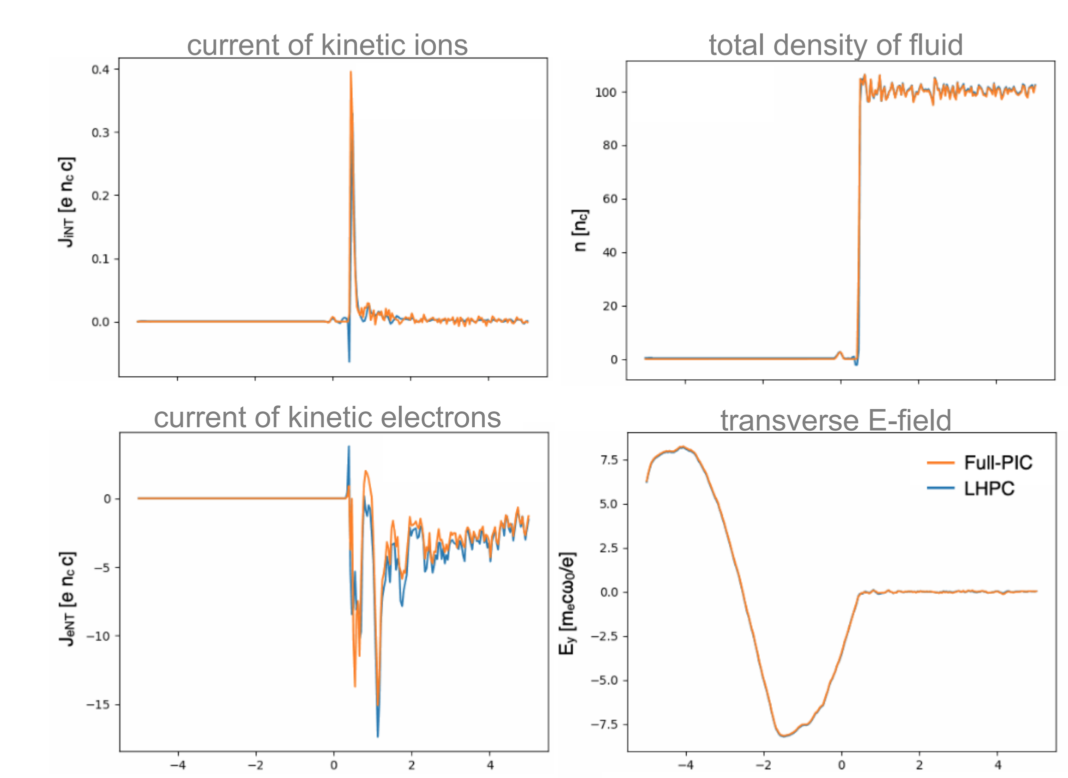
Evolution of electron current of the kinetic J_{eNT}



Comparison of energy spectrum of the kinetic particles after 20 steps of rollout



Comparison of model predictions after 20 steps of rollout



Conclusions

Our novel hybrid particle-continuum model LHPC, learns **efficient coupling of continuum and particle representations** using deep learning. In 1D particle-in-cell simulations, our method:

√ **improves speed** of classical first-principles (particle) solver by 8x
√ **improves accuracy** over baseline continuum model by 6.8x

For future work, we believe our method can:

√ generalize to higher dimensions (2D and 3D) where speed-up will be more significant
√ find accurate particle-continuum descriptions across all domains involving non-equilibrium N-body systems

QR code for our paper