Ab initio PIC simulations and data-driven techniques for multi-fidelity or reduced plasma models

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** UCLA

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Ab initio kinetic plasma simulations and the "ground truth"

Some questions

Speeding standard kinetic simulations + novel simulators

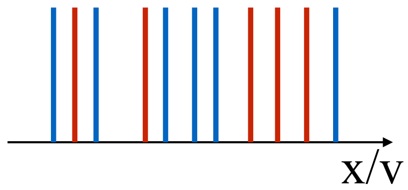
Learning advection and diffusion coefficients from PIC simulation data

Pushing PIC simulations towards capturing *ab initio* collisions: from many particles per cell to *many cells per particle*

A brief digression on plasma kinetic theory

Point like charged particles

$$N_s(\mathbf{x},\mathbf{v},t) = \sum_{i=1}^{N_0} \delta[\mathbf{x} - \mathbf{X}_i(t)]\delta[\mathbf{v} - \mathbf{V}_i(t)]$$



Equations of motion $\dot{\mathbf{X}}_i(t) = \mathbf{V}_i(t)$ $\quad m_s\dot{\mathbf{V}}_i(t) = q_s\mathbf{E}^m[\mathbf{X}_i(t),t] + \frac{q_s}{c}\mathbf{V}_i(t) \times \mathbf{B}^m[\mathbf{X}_i(t),t]$

$$\nabla \cdot \mathbf{E}^m(\mathbf{x},t) = 4\pi\rho^m(\mathbf{x},t)$$

$$\nabla \cdot \mathbf{B}^m(\mathbf{x},t) = 0$$

$$\nabla \times \mathbf{E}^m(\mathbf{x},t) = -\frac{1}{c}\frac{\partial \mathbf{B}^m(\mathbf{x},t)}{\partial t}$$

$$\nabla \times \mathbf{B}^m(\mathbf{x},t) = \frac{4\pi}{c}\mathbf{J}^m(\mathbf{x},t) + \frac{1}{c}\frac{\partial \mathbf{E}^m(\mathbf{x},t)}{\partial t}$$

$$\rho^m(\mathbf{x},t) = \sum_{e,\,i} q_s \int d\mathbf{v}\, N_s(\mathbf{x},\mathbf{v},t)$$

$$\mathbf{J}^m(\mathbf{x},t) = \sum_{e,\,i} q_s \int d\mathbf{v}\mathbf{v} N_s(\mathbf{x},\mathbf{v},t)$$

Sources for microscopic fields

D. Nicholson, Introduction to Plasma Theory, 1983

Klimontovich vs Vlasov / Boltzmann

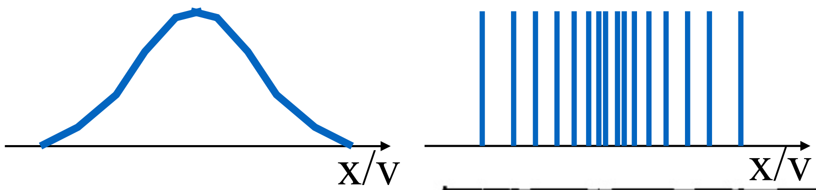
$$\frac{\partial N_s(\mathbf{x},\mathbf{v},t)}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}} N_s + \frac{q_s}{m_s}\left(\mathbf{E}^m + \frac{\mathbf{v}}{c}\times\mathbf{B}^m\right)\cdot\nabla_{\mathbf{v}} N_s = 0$$

Transport equation for N_s is the Klimontovich equation

$$f_s(\mathbf{x},\mathbf{v},t) \equiv \langle N_s(\mathbf{x},\mathbf{v},t)\rangle$$

$$N_s(\mathbf{x},\mathbf{v},t) = f_s(\mathbf{x},\mathbf{v},t) + \delta N_s(\mathbf{x},\mathbf{v},t)$$
$$\mathbf{E}^m(\mathbf{x},\mathbf{v},t) = \mathbf{E}(\mathbf{x},\mathbf{v},t) + \delta\mathbf{E}(\mathbf{x},\mathbf{v},t)$$

$$\mathbf{B}^m(\mathbf{x},\mathbf{v},t) = \mathbf{B}(\mathbf{x},\mathbf{v},t) + \delta\mathbf{B}(\mathbf{x},\mathbf{v},t)$$

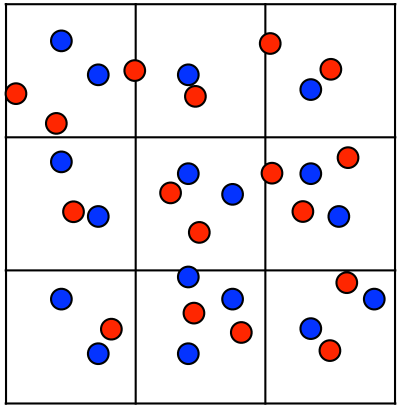


$$\frac{\partial f_s(\mathbf{x},\mathbf{v},t)}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}} f_s + \frac{q_s}{m_s}\left(\mathbf{E} + \frac{\mathbf{v}}{c}\times\mathbf{B}\right)\cdot\nabla_{\mathbf{v}} f_s = -\frac{q_s}{m_s}\left\langle\left(\delta\mathbf{E} + \frac{\mathbf{v}}{c}\times\delta\mathbf{B}\right)\cdot\nabla_{\mathbf{v}}\,\delta N_s\right\rangle$$

D. Nicholson, Introduction to Plasma Theory, 1983

Particle-in-cell/particle-mesh simulations

Solving Maxwell's equations on a grid with self-consistent charges and currents due to charged particle dynamics



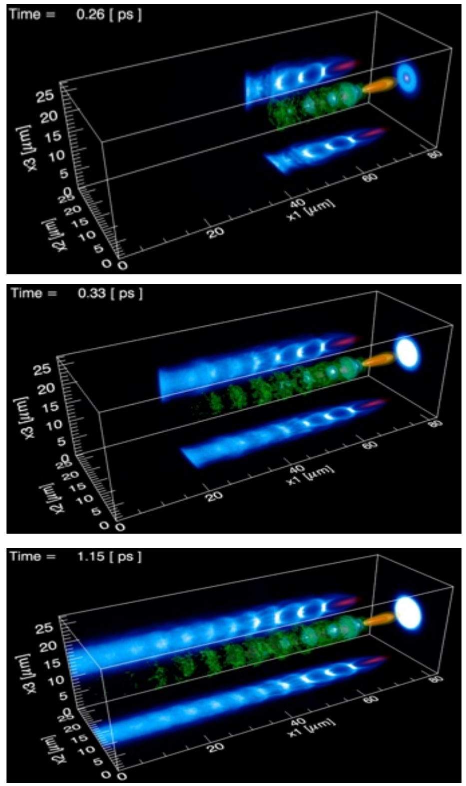
State-of-the-art

~ 10^{12} particles

~ $(12000)^3$ cells

RAM ~ 1 Gbyte - 100s TByte
Run time: hours to months
Data/run ~ few MB - 100s TByte
10's - 100's M cpu core hours/run

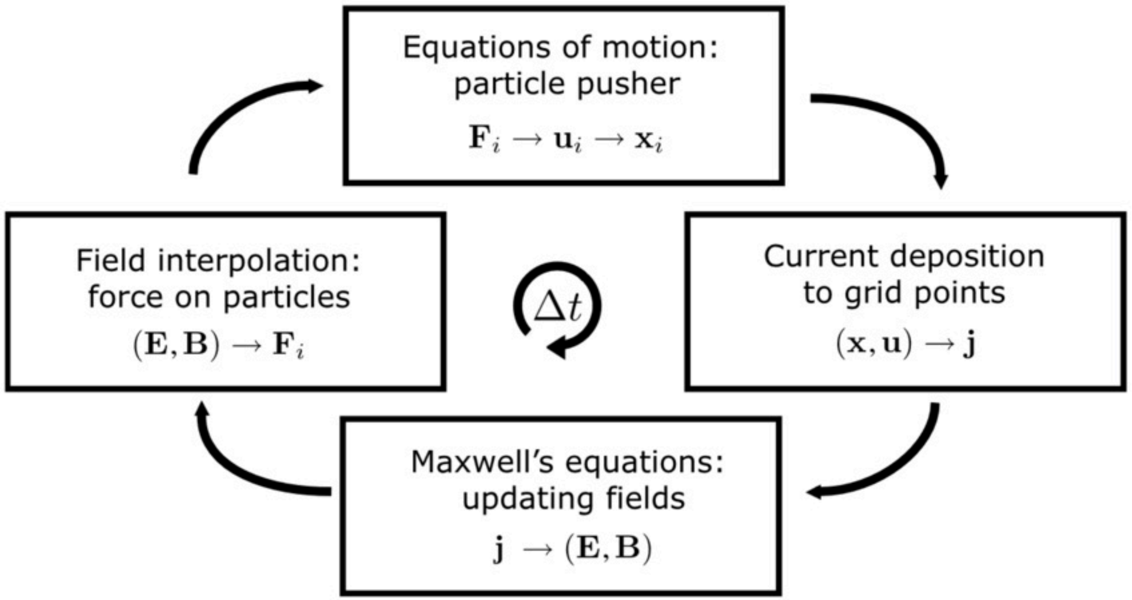
Weibel/two stream instability in astrophysics, relativistic shocks, fast igniton/inertial fusion energy, low temperature plasmas, laser-plasma interaction



Particle-in-cell (PIC) - (Dawson, Buneman, 1960's)
Maxwell's equation solved on simulation grid
Particles pushed with Lorentz force

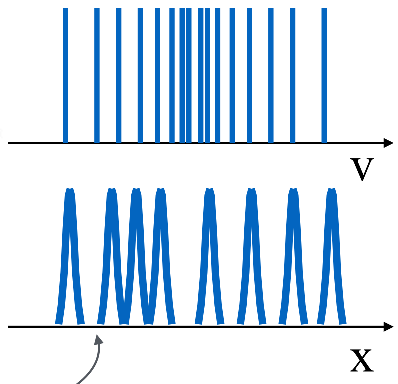
The most fundamental (classical) model in plasma physics

$$\frac{d\mathbf{p}}{dt} = \mathbf{F_L} + \boxed{\mathbf{F_{RR}}}$$



$$\frac{\partial \mathbf{E}}{\partial t} = c\nabla \times \mathbf{B} - 4\pi \mathbf{j}$$

$$\frac{\partial \mathbf{B}}{\partial t} = -c\nabla \times \mathbf{E}$$



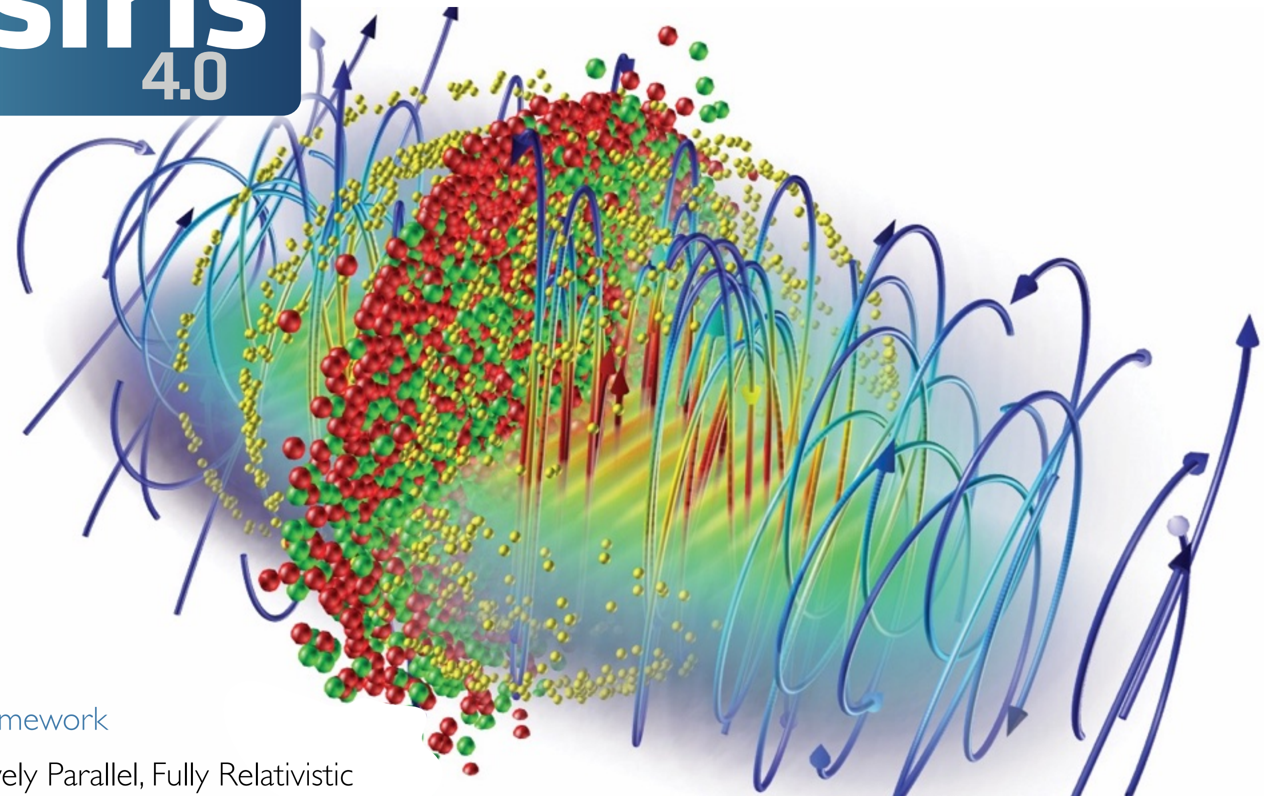
$$N_{\mathrm{PIC}}(\mathbf{x}, \mathbf{v}, t) = \sum_{i=1}^{N_0} S[\mathbf{x} - \mathbf{X}_i(t)]\delta[\mathbf{v} - \mathbf{V}_i(t)]$$

Diagram from: M.Vranic, et al. Comp. Phys. Comms. 204: 141-151 (2016)

Particle-in-cell simulations underpin many scientific advances in plasma physics

Osiris 4.0

Open-source version available



Open-access model

- 40+ research groups worldwide are using OSIRIS
- 300+ publications in leading scientific journals
- Large developer and user community
- Detailed documentation and sample inputs files available

Using OSIRIS 4.0

- The code can be used freely by research institutions after signing an MoU
- Find out more at: **http://epp.tecnico.ulisboa.pt/osiris**

OSIRIS framework

- Massively Parallel, Fully Relativistic Particle-in-Cell Code
- Parallel scalability to 2 M cores
- Explicit SSE / AVX / QPX / Xeon Phi / CUDA support
- Extended physics/simulation models

Ricardo Fonseca: ricardo.fonseca@tecnico.ulisboa.pt

A brief history of OSIRIS

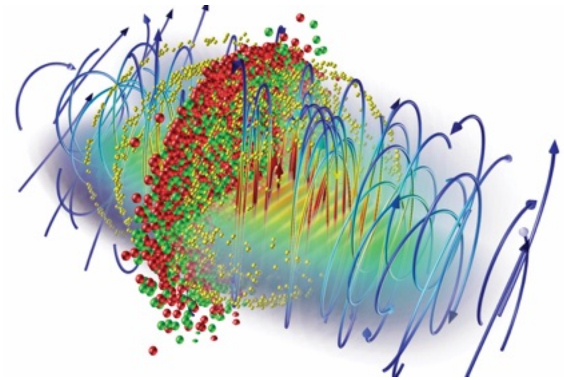
UCLA | University of Michigan | Técnico Lisboa

M. Jones LANL	J.J. Su UCLA	K. C.-Tzeng UCLA	R. Hemker UCLA	R. Fonseca IST	OSIRIS Consortium 1.0 UCLA-IST	**OSIRIS Consortium 2.0**

ISIS → PEGASUS → OSIRIS (Osiris 4.0)

Early 1980s — 1990s — Late 1990s — **Now**

+50 groups worldwide
Fully developed by universities in the US and in the EU



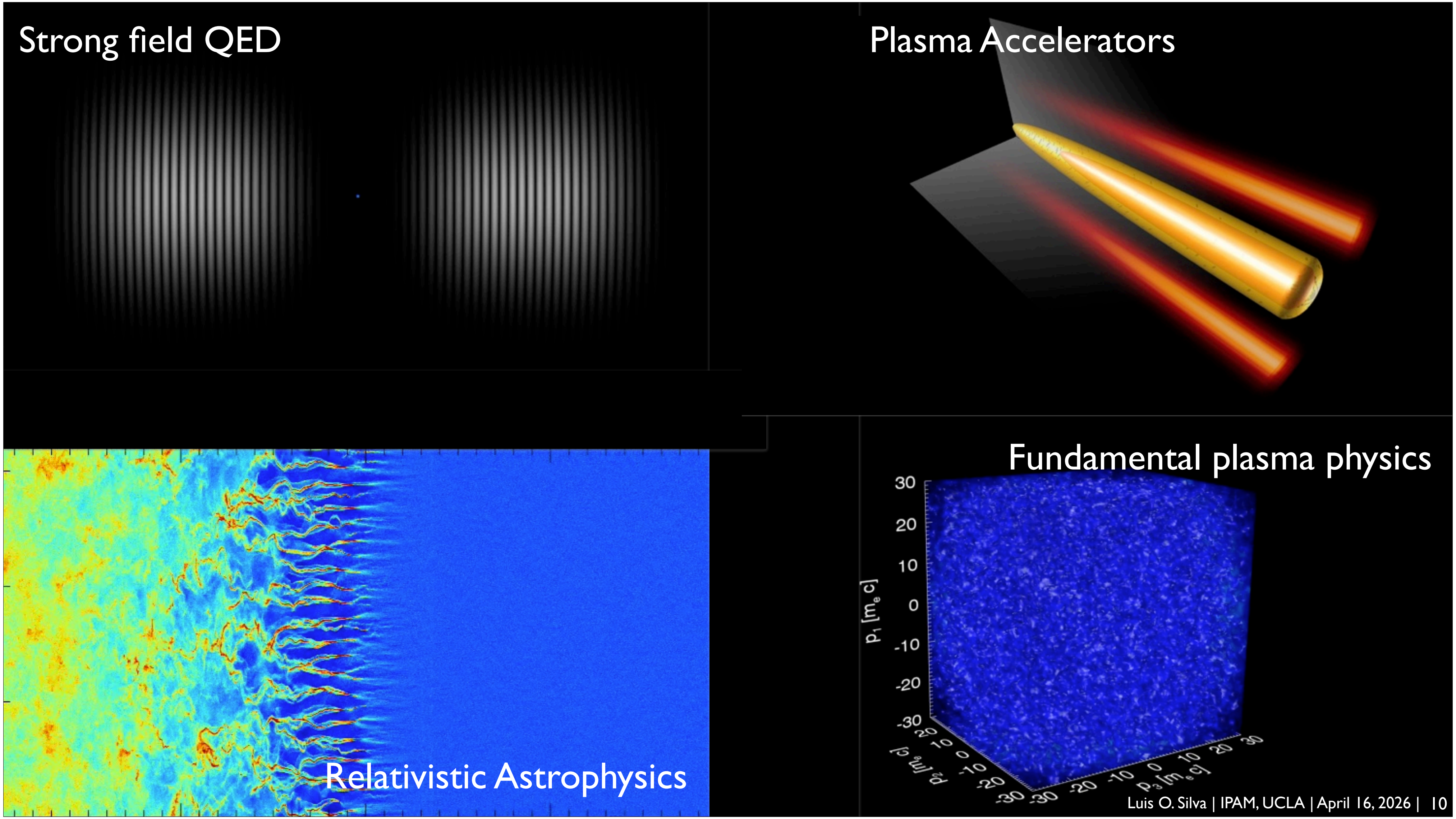
Running on all top10 machines + **open source**

Massively parallel on modern architectures, including GPUs, dynamic load balancing, large suite of field solvers + particle pushers + boundary conditions + AI

Extended physics models including QED, general relativity, spherical grids, quasi-3D, *etc.*

Physics results covering plasma accelerators, laser fusion, relativistic astrophysics, SF QED, beam physics, fundamental plasma physics, space physics, laboratory astrophysics, *etc.*

U.S. Department of Energy | NSF | erc


Strong field QED
Plasma Accelerators
Relativistic Astrophysics
Fundamental plasma physics
p_1 [m_ec]
p_2 [m_ec]
p_3 [m_ec]
30
20
10
0
-10
-20
-30

Why PIC simulations?

Very few approximations - unique source of high fidelity data

At the basis of the hierarchy of plasma physics descriptions - Klimontovich equation - can provide high resolution information to inform other scales

Well tested and benchmarked - against experiments, theory, other models

Can take advantage of large scale computational resources - across many different architectures/scales

The most fundamental (classical) physics model for plasmas- very well understood statistical mechanics/statistical properties - used across many sub-fields

Some questions

Can ML help us speed up standard plasma simulators? Early attempts: ML replaces Monte Carlo modules in PIC - Badiali et al., JPP 2022; Amaro et al., JCP 2026

Can we build faster ML based simulators? Rethinking architecture of simulators to match ML uniqueness: 1D collisional plasma model - Carvalho et al., MLST 2024

What can we learn from data-driven approaches + ML? Learning physics (following pioneering work in plasma physics by Alves et al.) e.g. collision operators: Carvalho et al., to appear PPCF (2026); *idem*, submitted JPP (2026)

Can standard plasma simulators provide “high quality data” for data-driven discovery? Capturing self-consistent collisions in PIC codes: D. Carvalho et al., in preparation

Can we understand qualitative modifications of plasma behavior from “Learning what we already know”? e.g. Waterbag vs Maxwellian; nonlinear waves vs unstable (and then turbulent) scenarios; nonrelativistic to relativistic, from conservation of enery/momentum to Casimir invariants

Ab initio kinetic plasma simulations and the "ground truth"

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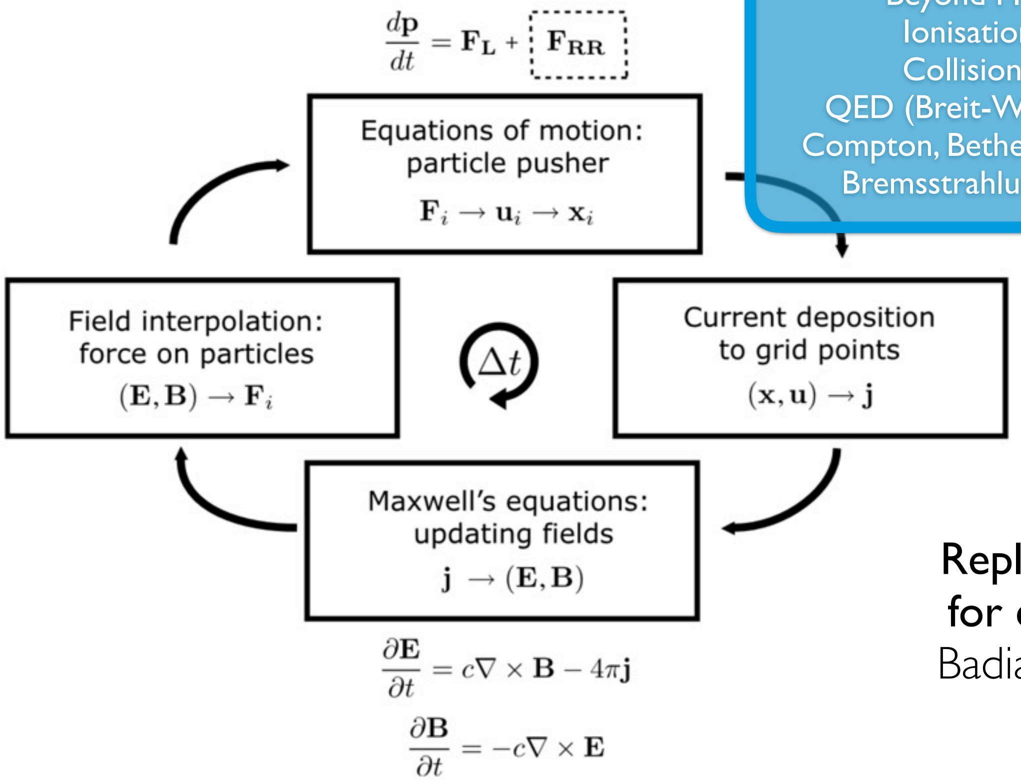
Learning advection and diffusion coefficients from PIC simulation data

Pushing PIC simulations towards capturing *ab initio* collisions: from many particles per cell to *many cells per particle*

Supplementing the PIC algorithm with additional physics



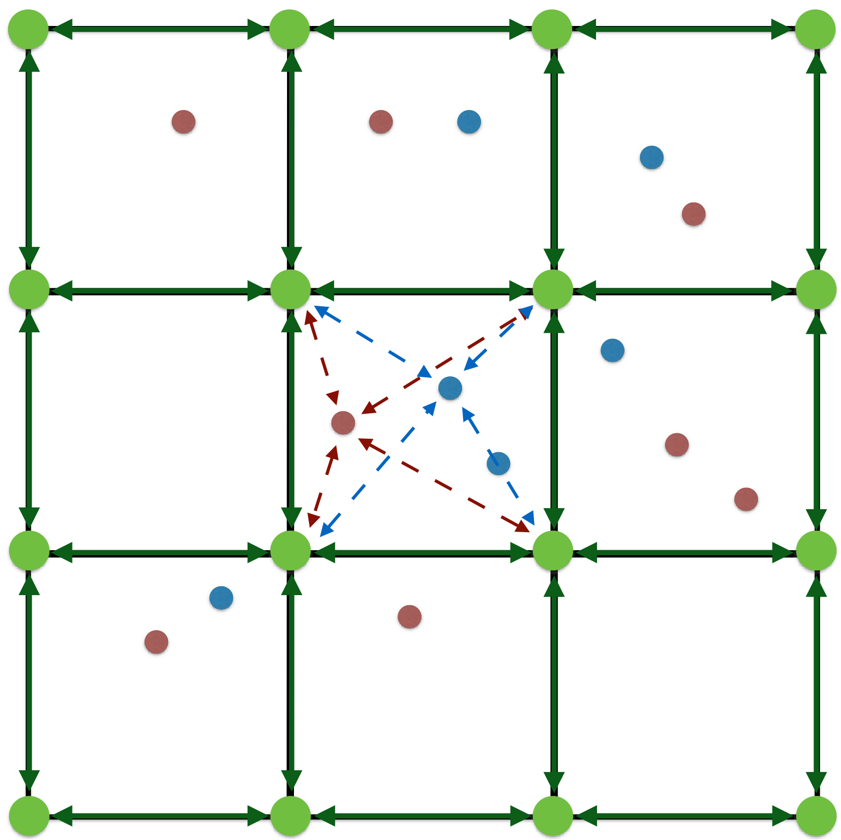
Beyond PIC:
Ionisation
Collisions
QED (Breit-Wheeler, Compton, Bethe-Heitler, Bremsstrahlung…)

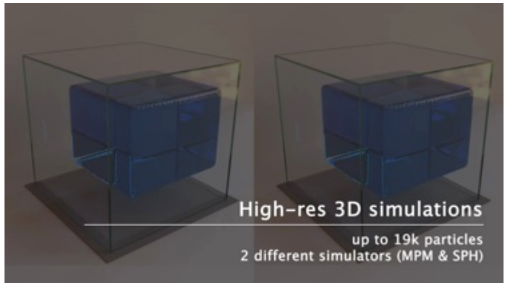
MC based techniques

Replacing look-up tables e.g. for cross sections with NN
Badiali et al., JPP 2022; Amaro et al., JCP 2026

Diagram from: M. Vranic, et al. Comp. Phys. Comms. 204: 141-151 (2016)

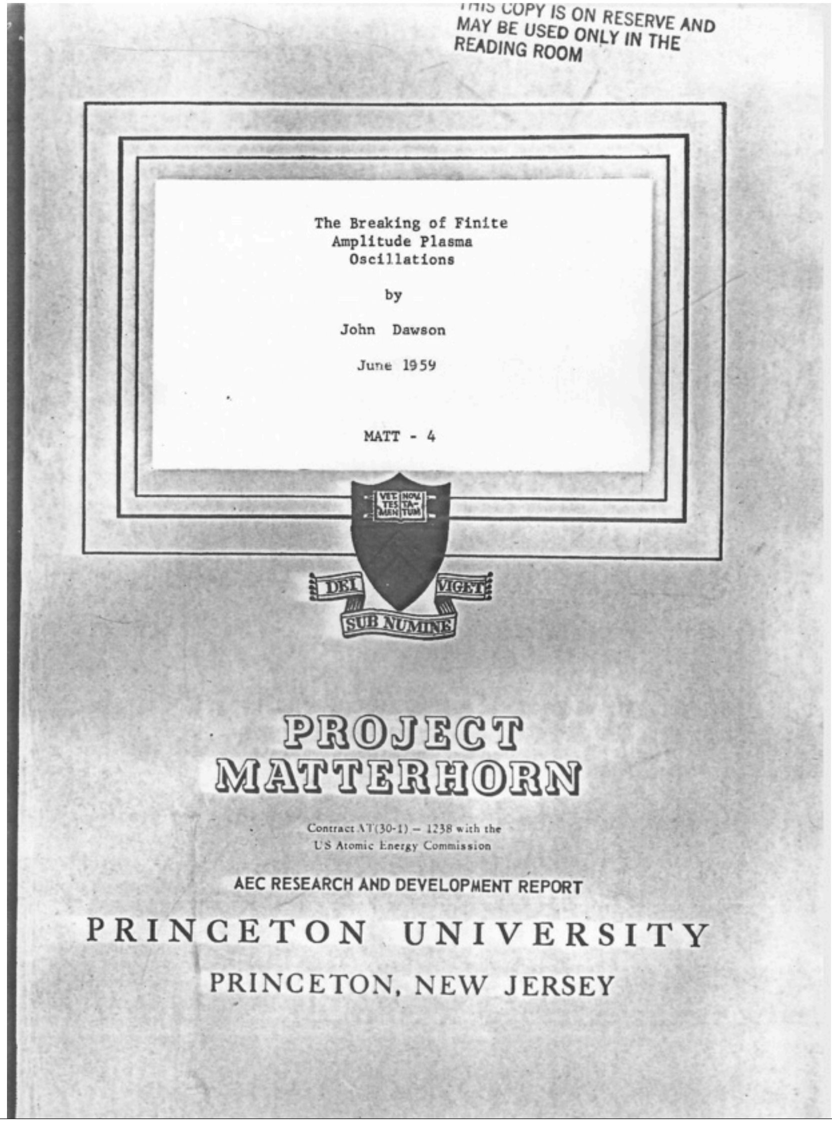
PIC codes (and others) can be seen from a graph perspective





A. Sanchez-Gonzalez et al., ICML PMLR 8459–8468 (2020)
R. Lam et al., Science 382.6677 1416-1421 (2023)

D. Carvalho et al., Mach. Learn.: Sci. Technol. 5 025048 (2024)



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The Breaking of Finite
Amplitude Plasma
Oscillations

by

John Dawson

June 1959

MATT - 4

VET TES MEN TUM NOV TA TUM

DEI SUB NUMINE VIGET

PROJECT
MATTERHORN

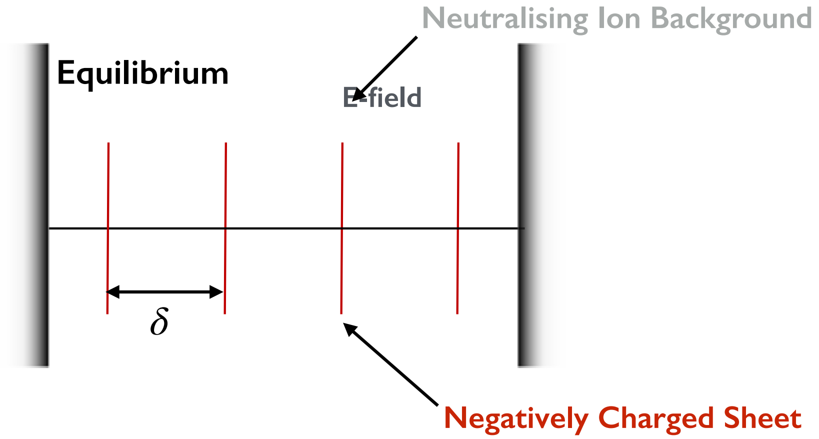
Contract AT(30-1) – 1238 with the
US Atomic Energy Commission

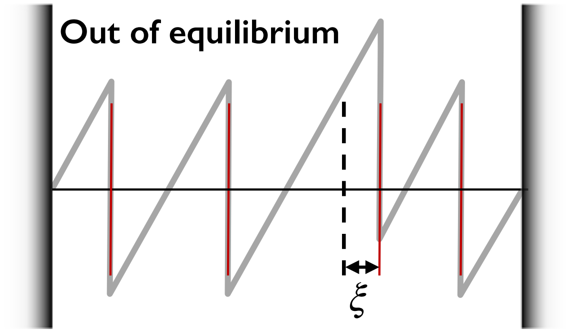
AEC RESEARCH AND DEVELOPMENT REPORT

PRINCETON UNIVERSITY

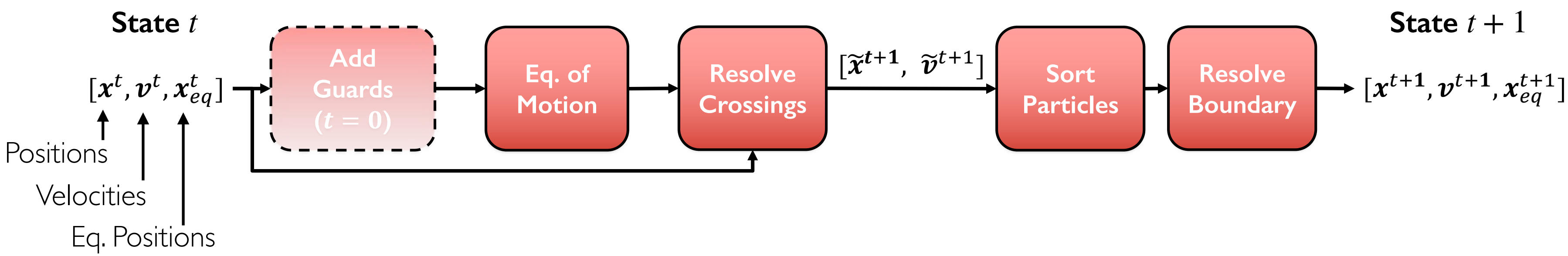
PRINCETON, NEW JERSEY

1D Plasma Electrostatic Sheet Model



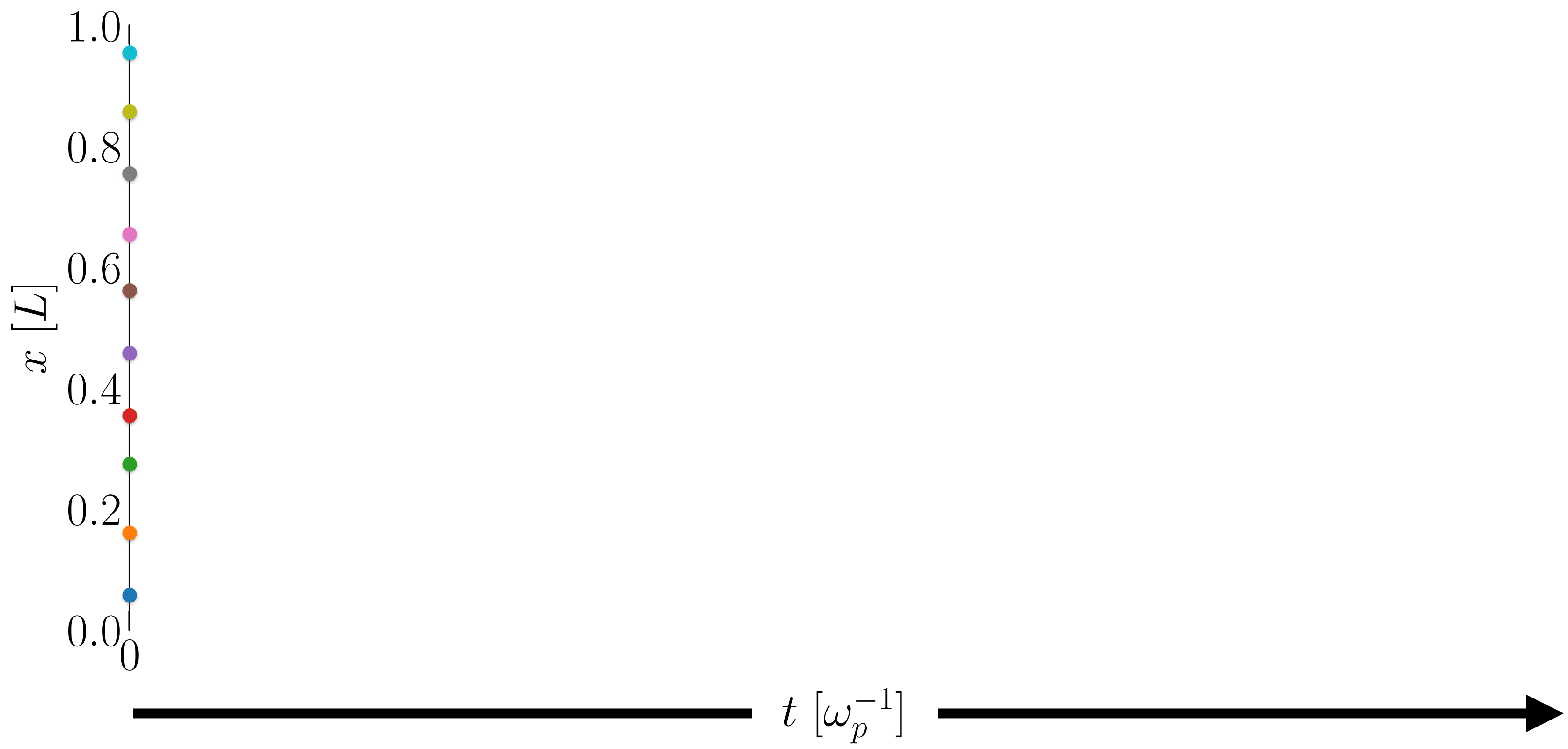


$$\ddot{\xi} = -\frac{4\pi e^2 n_0}{m_e}\xi = -\omega_p^2 \xi$$

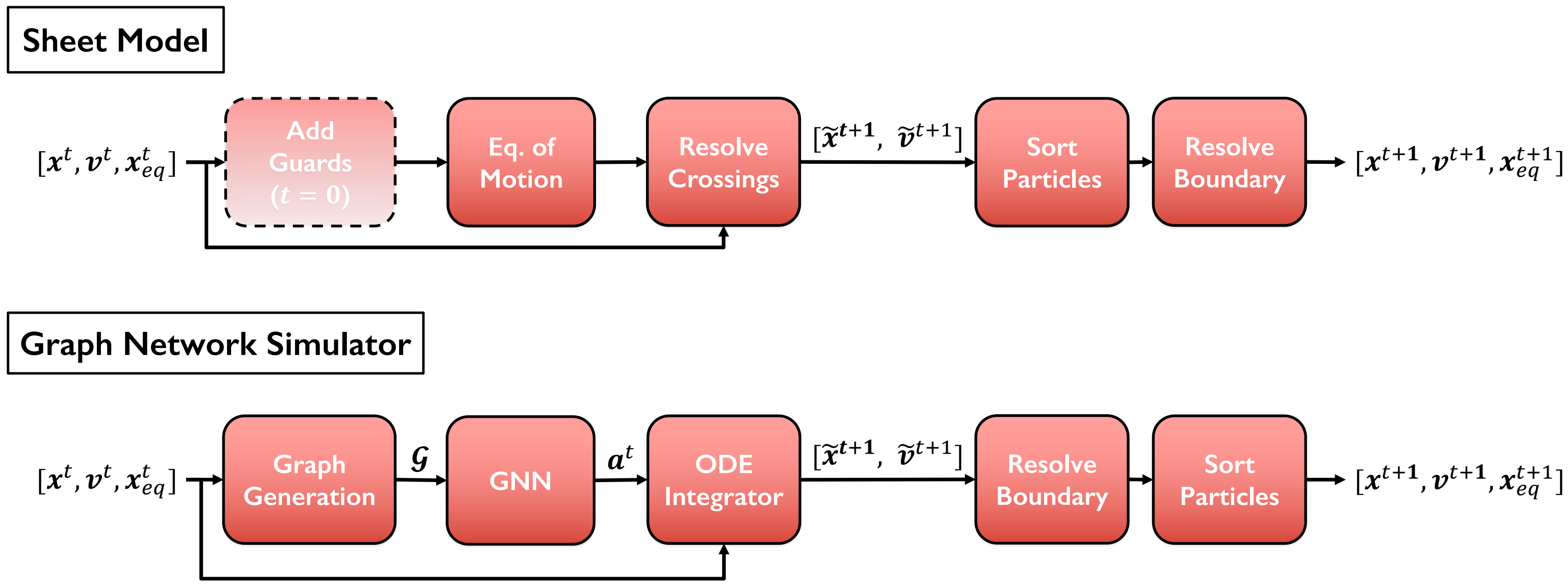


J. Dawson, Phys. Fluids 5.4, 445-459 (1962)
J. Dawson, Methods in Computational Physics 9, 1–28 (1970)

Example of Simulation



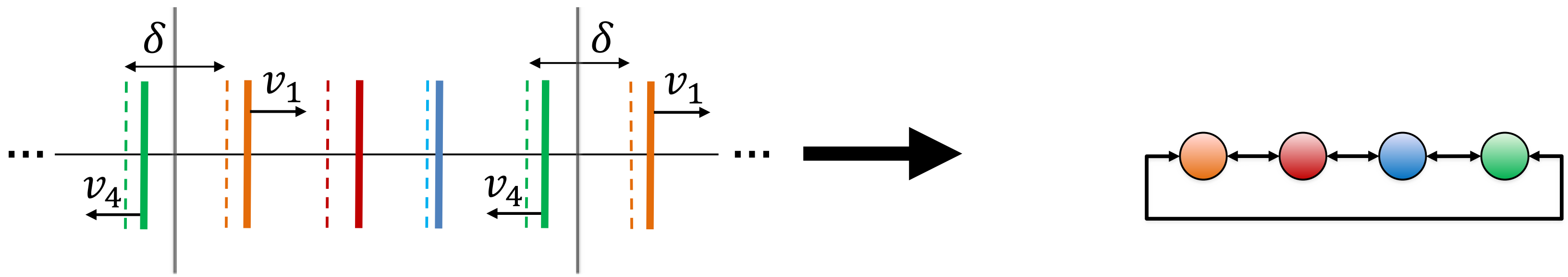
1D Plasma ESM Graph Network Simulator

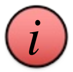


J. Dawson, Methods in Computational Physics 9, 1–28 (1970)
D. Carvalho et al., Mach. Learn.: Sci. Technol. 5 025048 (2024)

How do we represent the plasma as a graph?

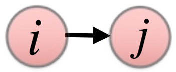
Periodic Boundaries





Node

$$\mathbf{n}_i^t = \left[\xi_i^t \ , \ v_i^t\right]$$



Edge

$$\mathbf{r}_{ji}^t = \left[x_i^t - x_j^t\right]$$

Target

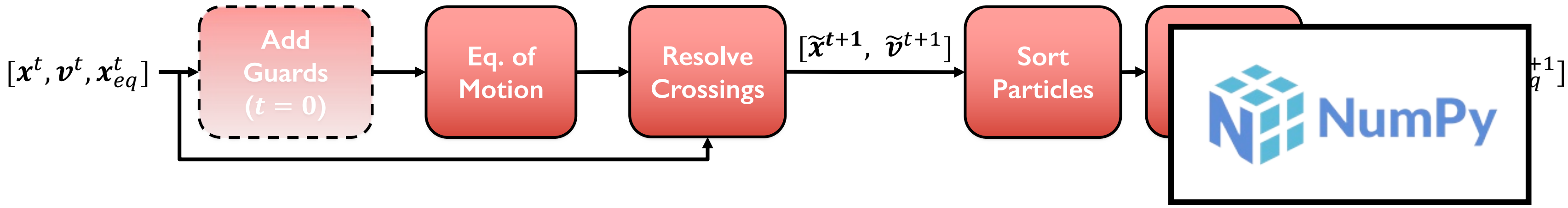
$$a_i^t = \frac{v_i^{t+1} - v_i^t}{\Delta t}$$

All values are normalised to the intersheet spacing δ

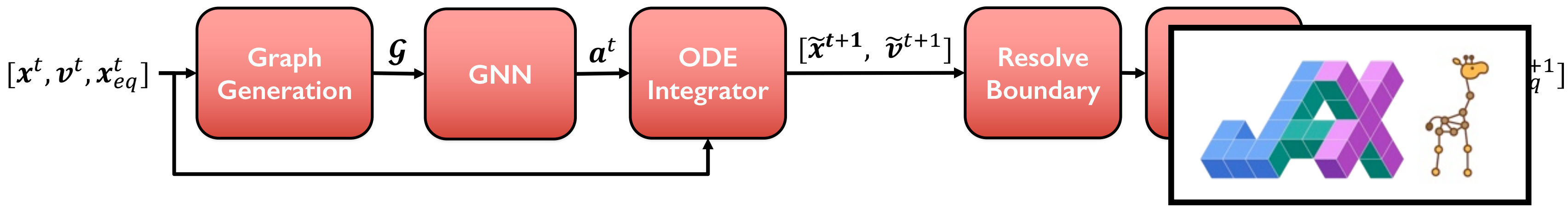
D. Carvalho et al., Mach. Learn.: Sci. Technol. 5 025048 (2024)

1D Plasma ESM Graph Network Simulator

Sheet Model



Graph Network Simulator



Code: https://github.com/diogodcarvalho/gns-sheet-model

https://github.com/google/jax

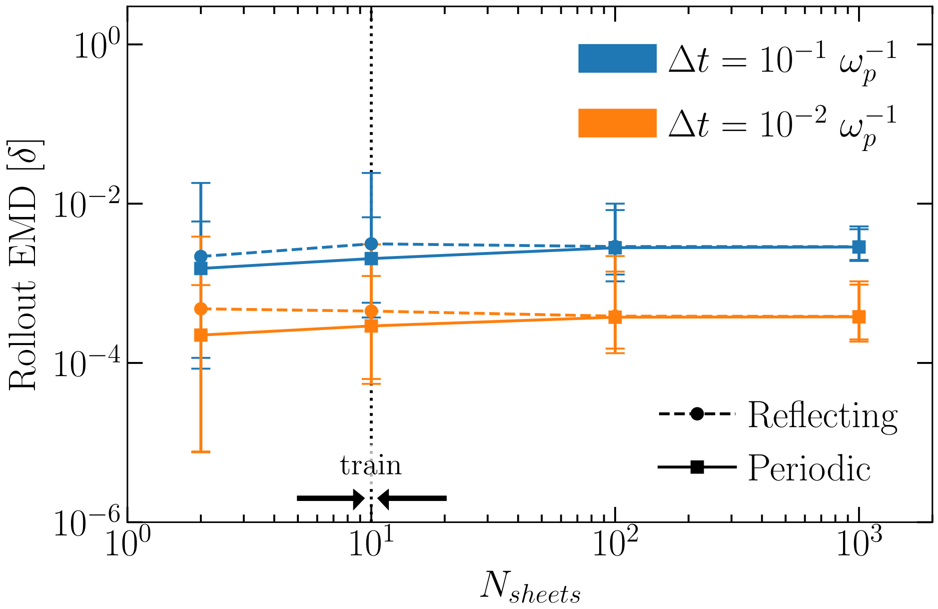
https://github.com/deepmind/jraph

J. Dawson, Methods in Computational Physics 9, 1–28 (1970)
D. Carvalho et al., Mach. Learn.: Sci. Technol. 5 025048 (2024)

GNS generalizes to different number of sheets and boundary conditions

Trained on **subsampled high temporal resolution data** $\left(\Delta t_{orig} = 10^{-4}\ \omega_p^{-1}\right)$ of **10 sheets** moving inside a **periodic box** $\left(t_{sim} = 10\ \omega_p^{-1}\right)$

Initial positions and velocities are randomly sampled from a uniform distribution



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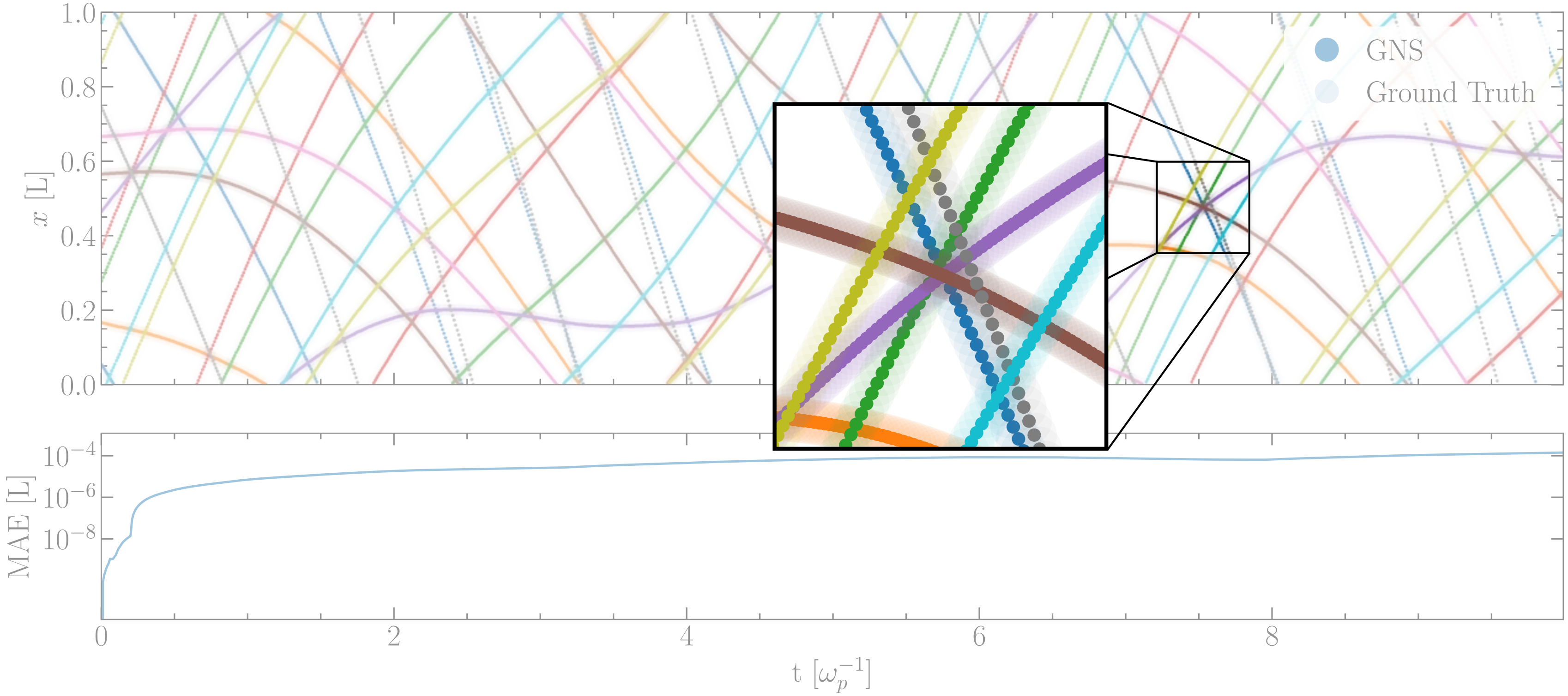
GNS rollout errors are very small

$\Delta t = 10^{-2}\ \omega_p^{-1}$ Rollout MAE $= 5.6 \times 10^{-4}\ \delta$



Example shown corresponds to the worst rollout error observed in the test set

GNS recovers a broad range of kinetic plasma processes

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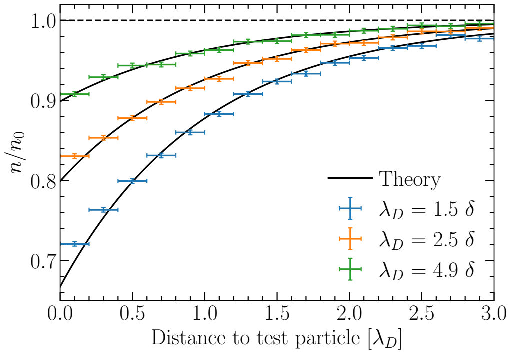
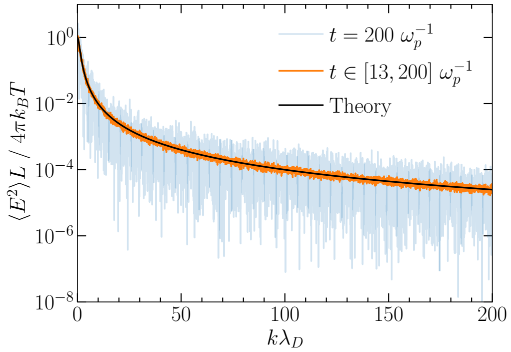
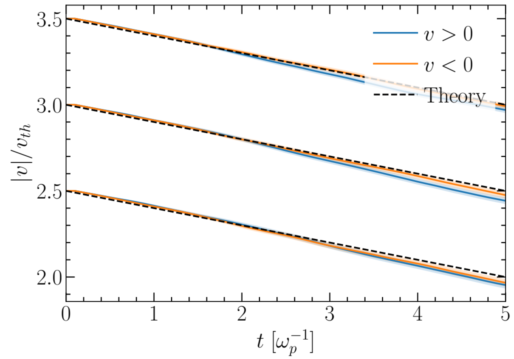
Debye Shielding



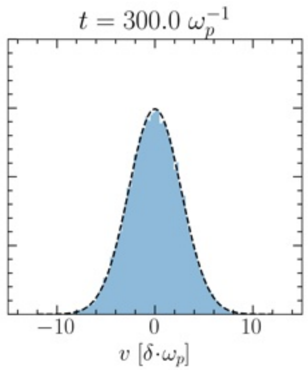
Electrostatic Fluctuations



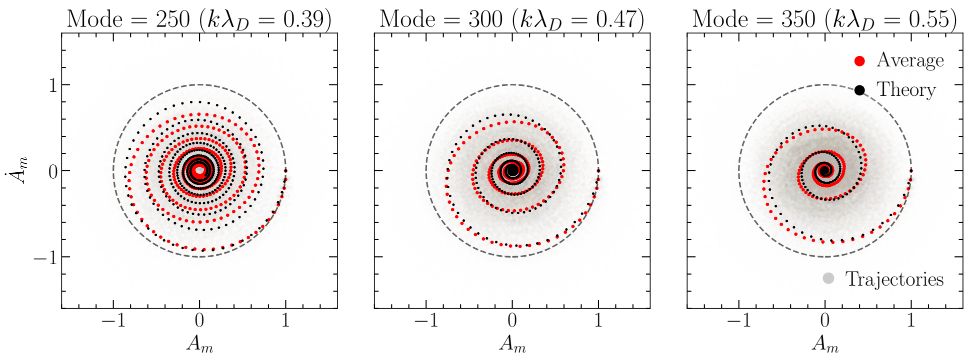
Drag on a Fast Sheet



Plasma Thermalization



Landau Damping



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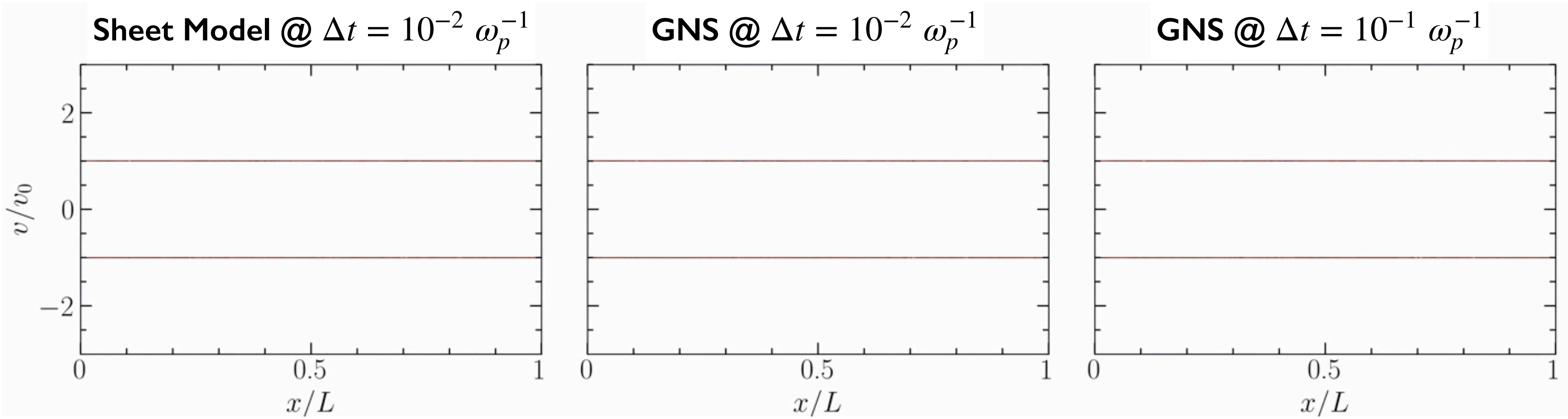
GNS recovers the two stream instability

Parameters: $N_{sheets} = 10{,}000$ $\left(\text{vs } N_{sheets}^{train} = 10\right)$ $v_0 \approx 500\ \delta \cdot \omega_p$ $\left(\text{vs } v_{max}^{train} = 20\ \delta \cdot \omega_p\right)$



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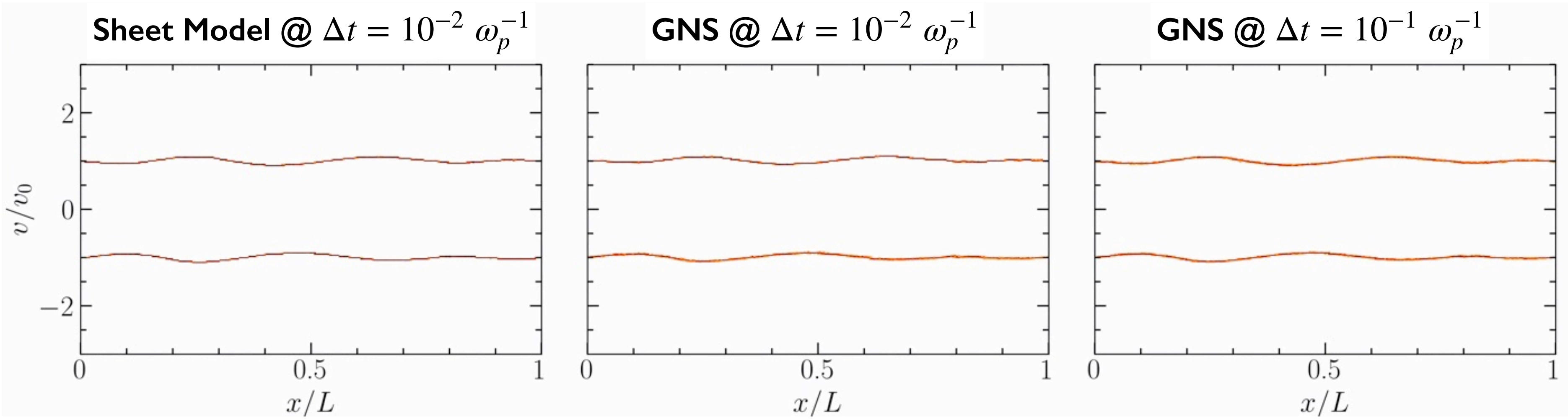

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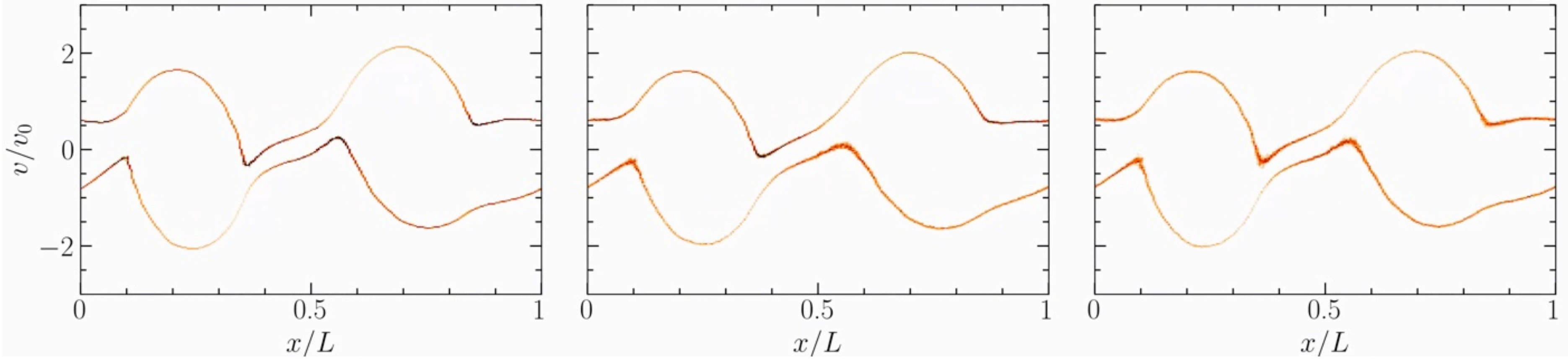
Sheet Model @ $\Delta t = 10^{-2}\ \omega_p^{-1}$ | **GNS @ $\Delta t = 10^{-2}\ \omega_p^{-1}$** | **GNS @ $\Delta t = 10^{-1}\ \omega_p^{-1}$**



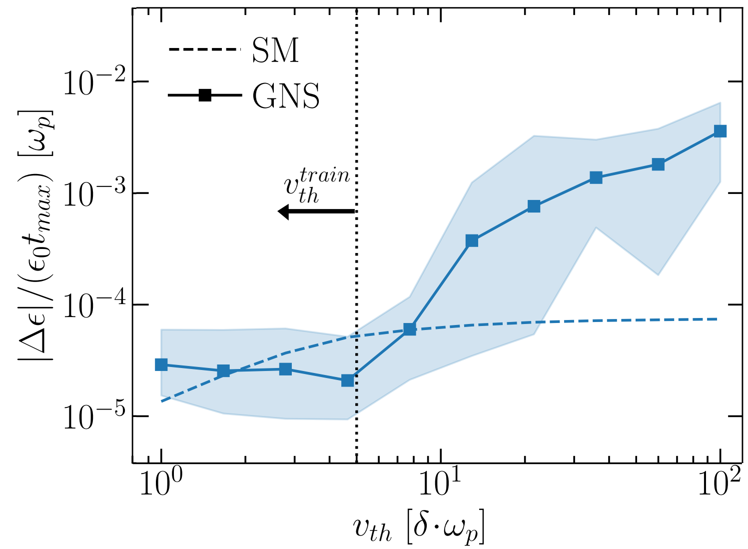
$\Delta\epsilon/\epsilon_0 \approx 10^{-6}$ | $\Delta\epsilon/\epsilon_0 \approx 10^{-2}$ | $\Delta\epsilon/\epsilon_0 \approx 10^{-2}$

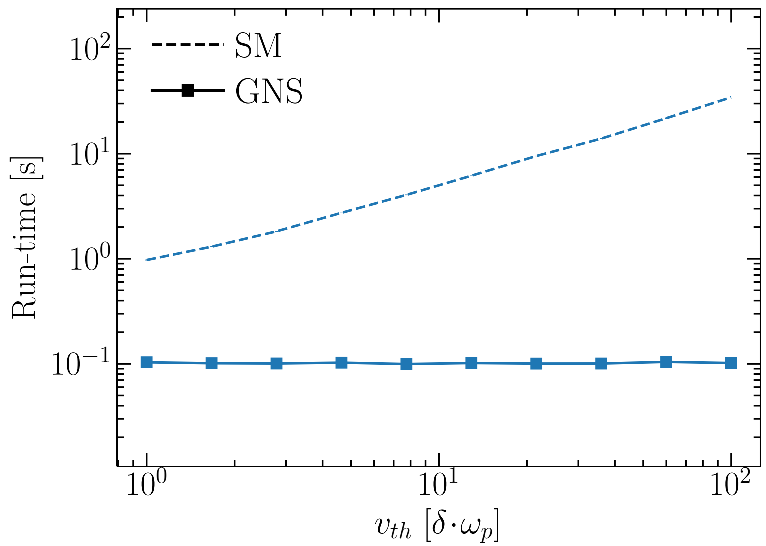
Run-Time $\approx$ 1h | Run-Time $\approx$ 1min | Run-Time $\approx$ 10s

D. Carvalho et al., Mach. Learn.: Sci. Technol. 5 025048 (2024)

GNS conserves energy similarly to Sheet Model while being significantly faster*

Parameters: $N_{sheets} = 1000$, velocities sampled from thermal distribution, $\Delta t_{GNS} = 10^{-1}\ \omega_p^{-1}$





***Note: GNS is implemented in JAX** (GPU), Sheet Model is implemented in NumPy (CPU)

D. Carvalho et al., Mach. Learn.: Sci. Technol. 5 025048 (2024)

Ab initio kinetic plasma simulations and the "ground truth"

Some questions

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Pushing PIC simulations towards capturing *ab initio* collisions: from many particles per cell to *many cells per particle*

What is the numerical ground truth in PIC simulations?

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Klimontovich + Maxwell's equations

$$\frac{\partial N}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} N - \frac{q}{m} \left(\mathbf{E}^m + \mathbf{v} \times \mathbf{B}^m \right) \cdot \nabla_{\mathbf{v}} N = 0$$

This is the particle-in-cell algorithm (with finite-size particles):

statistical mechanics is well-known (e.g. H. Okuda and C. Birdsall, (1970), A. Langdon and C. Birdsall, (1970), R. Hockney (1971), M. Touati et al. (2022))

Born-Infeld electrodynamics

Numerical collision operator has been derived in previous works (but not tested): Can this be learned from the simulation data in the weakly collisional regime? Can we then use this as a template to study conditions/regimes beyond existing theories?

Can we describe phase-space dynamics using a Fokker-Planck operator?

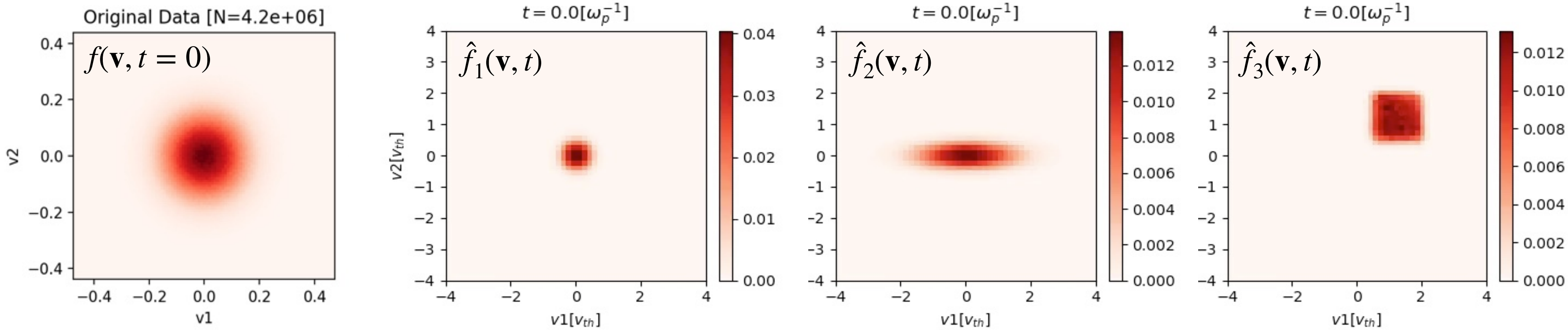
PIC (Klimontovich)

$$\frac{\partial N}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} N - \frac{q}{m}\left(\mathbf{E}^m + \mathbf{v} \times \mathbf{B}^m\right) \cdot \nabla_{\mathbf{v}} N = 0$$

?

What if we want (Fokker-Planck)?

$$\frac{\partial \hat{f}(\mathbf{v}, t)}{\partial t} = -\nabla_{\mathbf{v}} \cdot \left(\mathbf{A}\hat{f}\right) + \frac{1}{2}\nabla_{\mathbf{v}}\nabla_{\mathbf{v}} \cdot \left(\overleftrightarrow{\mathbf{D}}\hat{f}\right)$$



Thermal Plasma

How do we estimate $\mathbf{A}$ (advection) and $\overleftrightarrow{\mathbf{D}}$ (diffusion)?

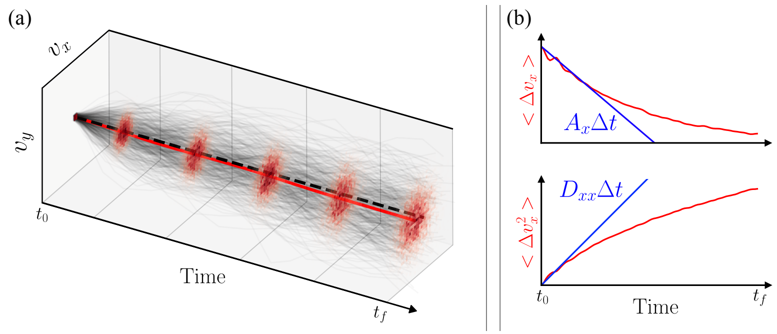
D. Carvalho et al., in submitted to JPP (2025)

How do we estimate $\mathbf{A}$ (advection) and $\overleftrightarrow{\mathbf{D}}$ (diffusion)?

Option 1: From raw particle data

The "correct" approach if possible

Not feasible for larger systems (memory-wise) unless it is done at run-time

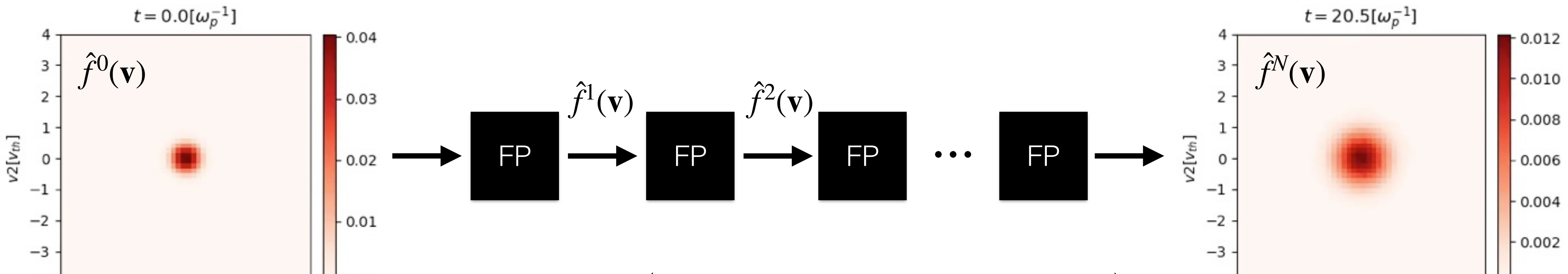


Option 2: From the phase-space evolution of sub-populations

Can be done in post-processing with a differentiable solver

Ill-posed problem: non-unique solution for coefficients

Learning advection / diffusion from evolution of sub-populations



$$\hat{f}^{t+1} = \hat{f}^t + \Delta t\left(-\nabla_{\mathbf{v}}\cdot\left(\mathbf{A}\hat{f}^t\right) + \frac{1}{2}\nabla_{\mathbf{v}}\nabla_{\mathbf{v}}\cdot\left(\overleftrightarrow{\mathbf{D}}\hat{f}^t\right)\right)$$

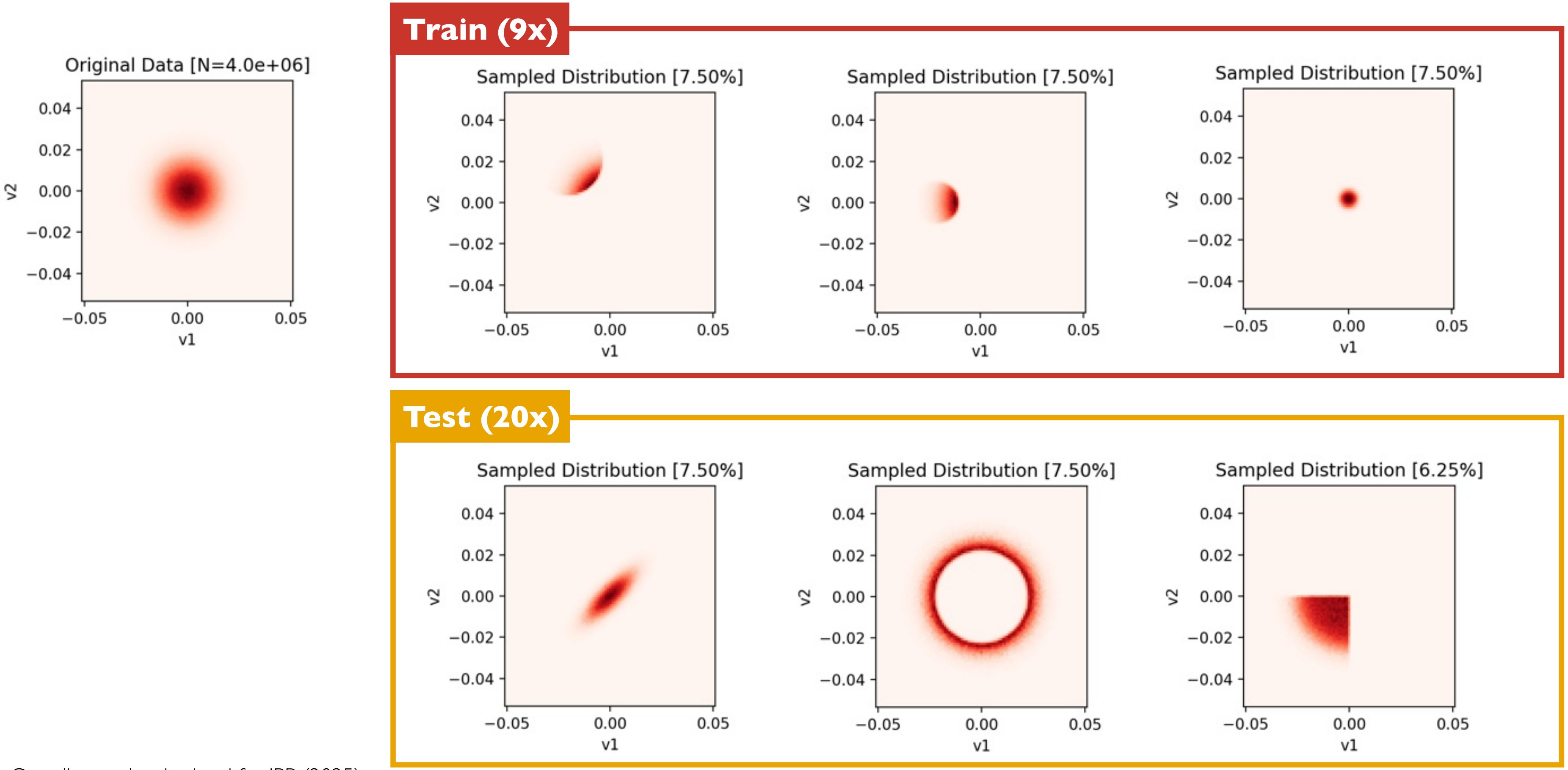
We can make the **Fokker-Planck solver differentiable** and frame this as an **optimisation task**

$$\min_{\mathbf{A},\overleftrightarrow{\mathbf{D}}} \left\| \hat{f}^N_{predicted} - \hat{f}^N_{true} \right\|$$

This is an ill-posed problem (there exists a family of solutions) → Train with multiple sub-populations

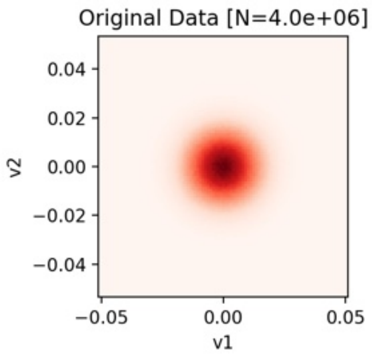
D. Carvalho et al., submitted for JPP (2025)

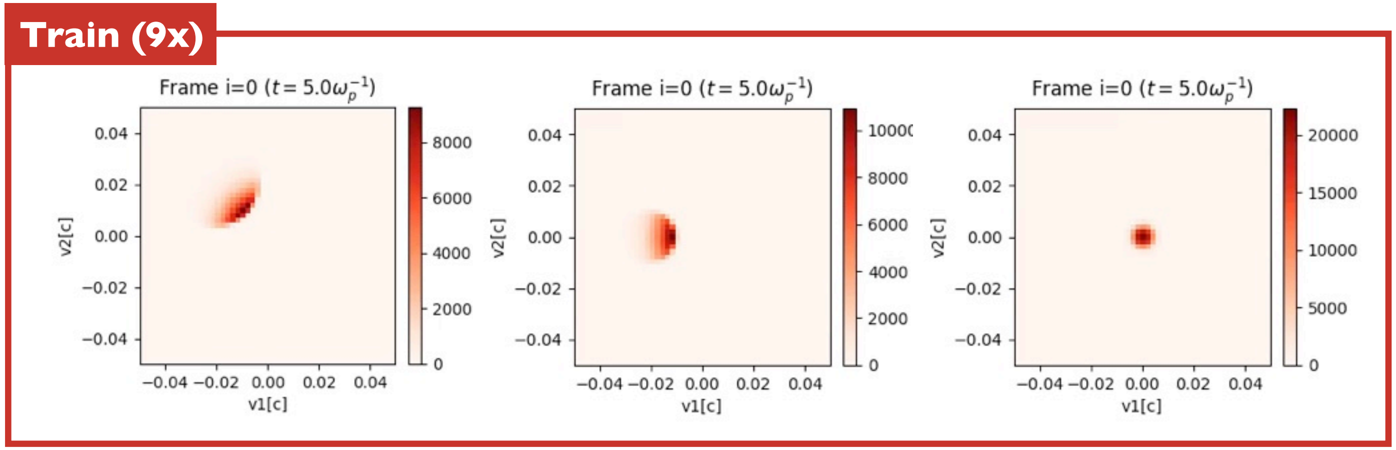
We use different sets of training and test sub-populations

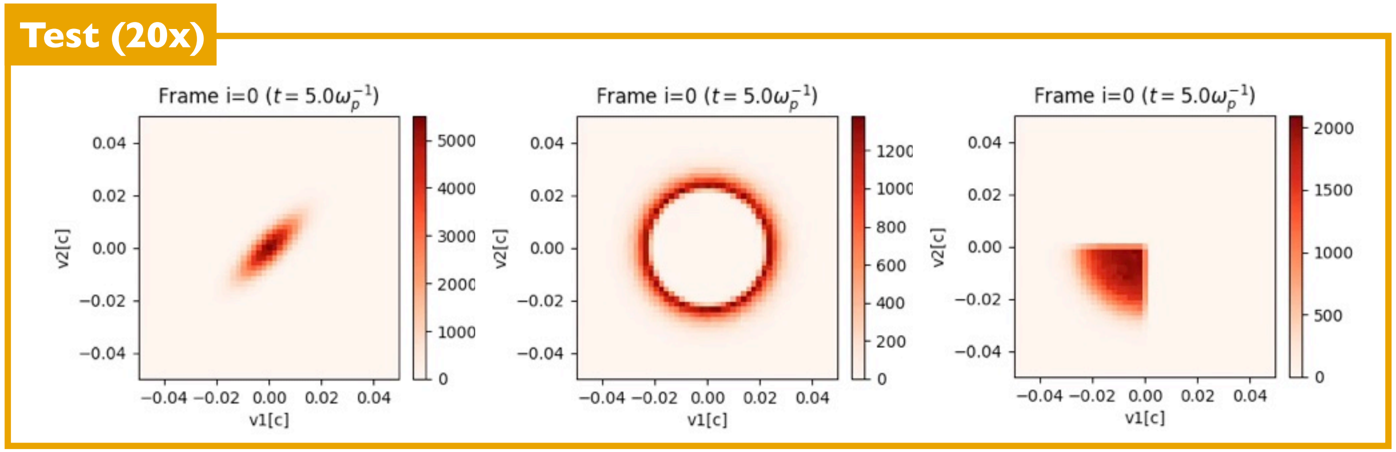


D. Carvalho et al., submitted for JPP (2025)

We use different sets of training and test sub-populations

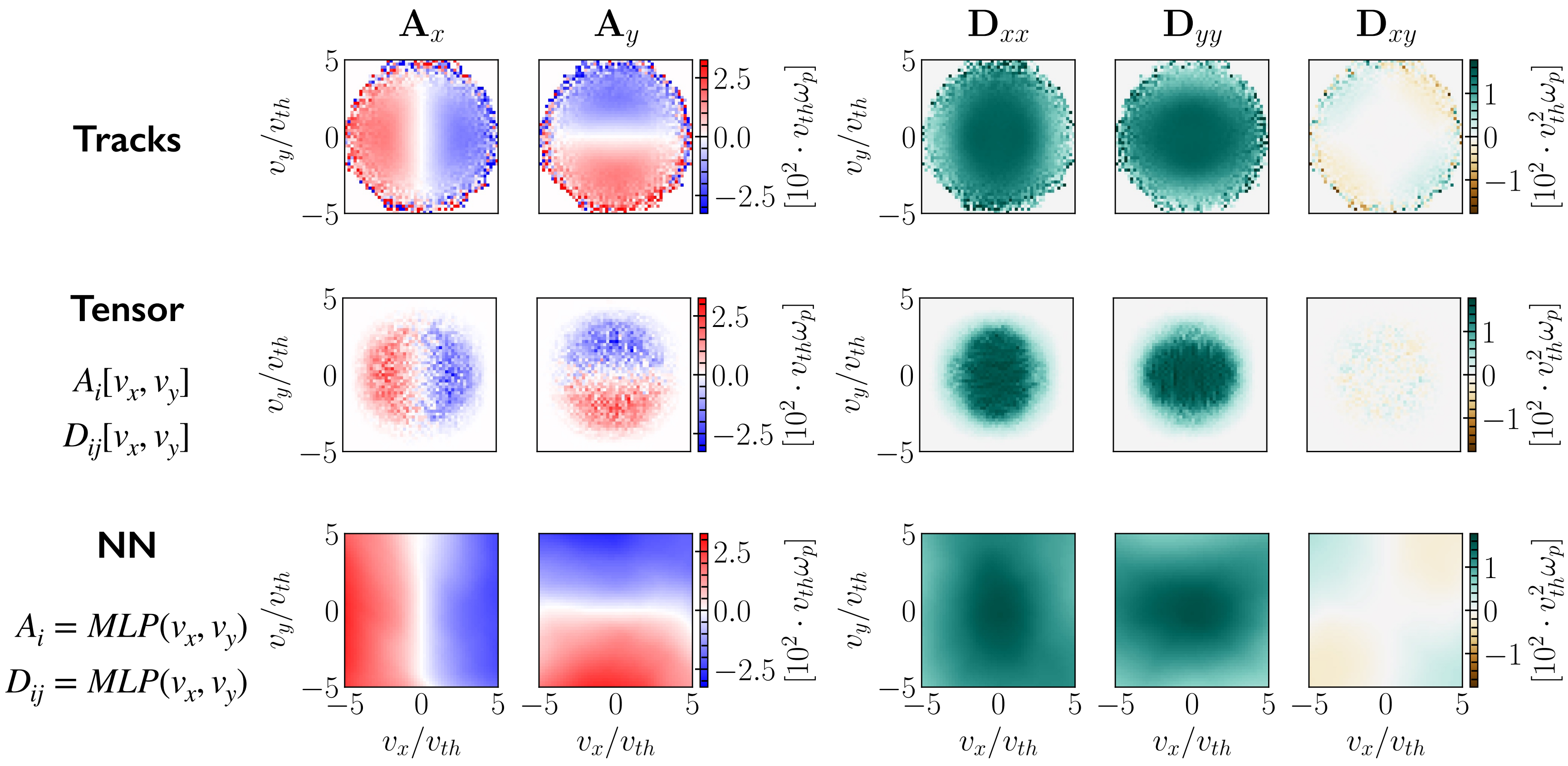






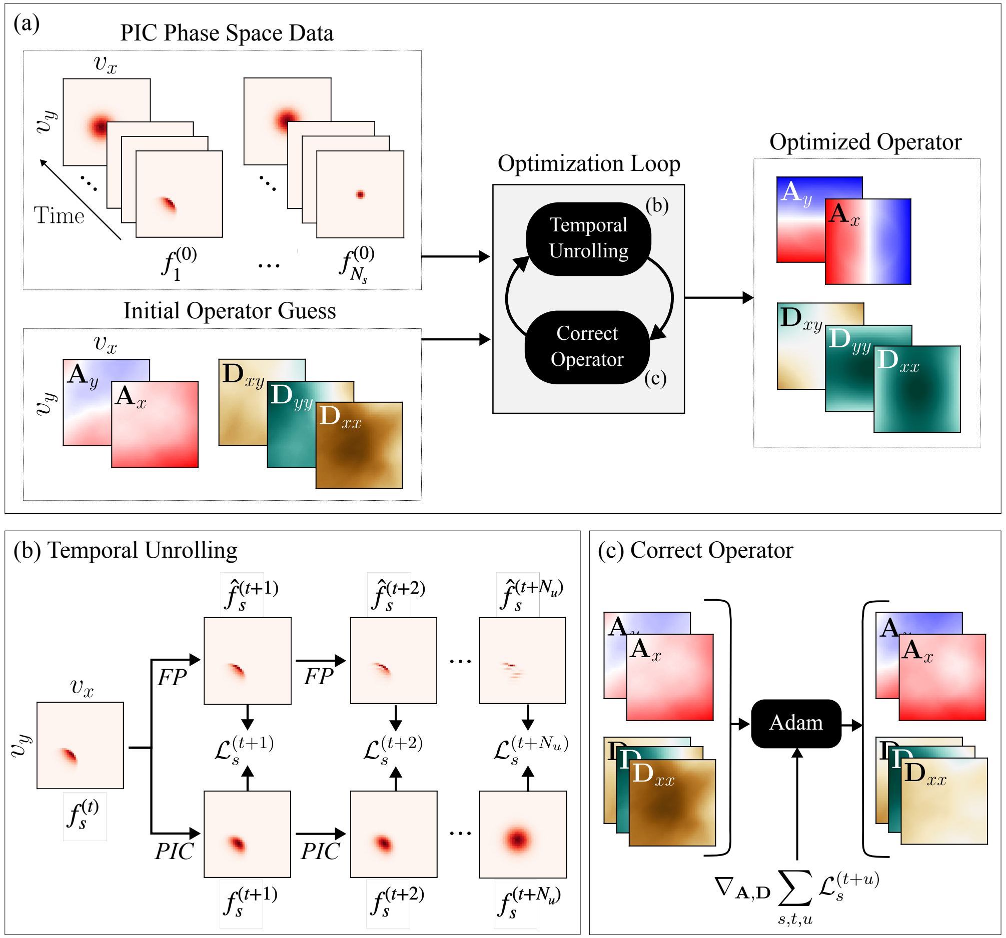
D. Carvalho et al., in submitted to JPP (2025)

We can parameterise A/D using a Tensor (discrete) or a NN (continuous)



D. Carvalho et al., in submitted to JPP (2025)

Inference of advection/diffusion from differentiable Fokker-Planck solver



D. Carvalho et al., in submitted to JPP (2025)

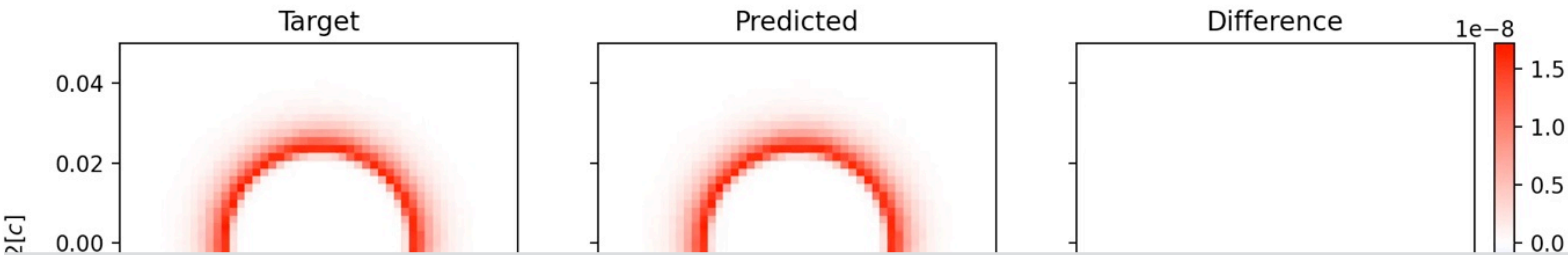
Can these operators reproduce dynamics?

$$f^{t+1} = f^t + \Delta t \left(-\nabla_{\mathbf{v}} \cdot \left(\mathbf{A} f^t\right) + \frac{1}{2} \nabla_{\mathbf{v}} \nabla_{\mathbf{v}} \cdot \left(\overleftrightarrow{\mathbf{D}} f^t \right) \right)$$

D. Carvalho et al., submitted for JPP (2025)

Can these operators reproduce dynamics? (Yes)

$$f^{t+1} = f^t + \Delta t \left(-\nabla_{\mathbf{v}} \cdot (\mathbf{A} f^t) + \frac{1}{2} \nabla_{\mathbf{v}} \nabla_{\mathbf{v}} \cdot \left(\overleftrightarrow{\mathbf{D}} f^t \right) \right)$$



Next steps

General purpose library: from phase space data, retrieve **A** and **D** (to be inserted on Fokker-Planck codes/other models) for varying plasma conditions, and from different sources of data

Sub-module to capture (PIC or other) collisions/anomalous transport coefficients for mesoscale simulations

Meta analysis: use different A and D for different plasma conditions (n, B, T) to learn more general behaviour e.g. via sparse regression

D. Carvalho et al., submitted for JPP (2025)

Ab initio kinetic plasma simulations and the “ground truth”

Some questions

Speeding standard kinetic simulations + novel simulators

Learning advection and diffusion coefficients from PIC simulation data

Pushing PIC simulations towards capturing *ab initio* collisions: from many particles per cell to *many cells per particle*

What is the (classical) ground truth?

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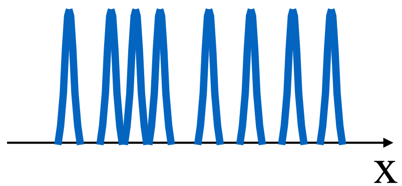
Klimontovich + Maxwell's equations

$$\frac{\partial N}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} N - \frac{q}{m} \left(\mathbf{E}^m + \mathbf{v} \times \mathbf{B}^m \right) \cdot \nabla_{\mathbf{v}} N = 0$$

This is the particle-in-cell algorithm (with finite-size particles): statistical mechanics is well-known (e.g. H. Okuda and C. Birdsall (1970), A. Langdon and C. Birdsall (1970), R. Hockney (1971), M. Touati et al. (2022)) + Born-Infeld electrodynamics

What if the cell/particle size is (shorter than) the classical electron radius r_e?



What are the challenges of running << 1 ppc?

Field initialization becomes critical + computation determined by grid (N^3 or N^2)

Numerical heating (still need to resolve Debye length) + Very small time steps (CFL) + numerical transition radiation

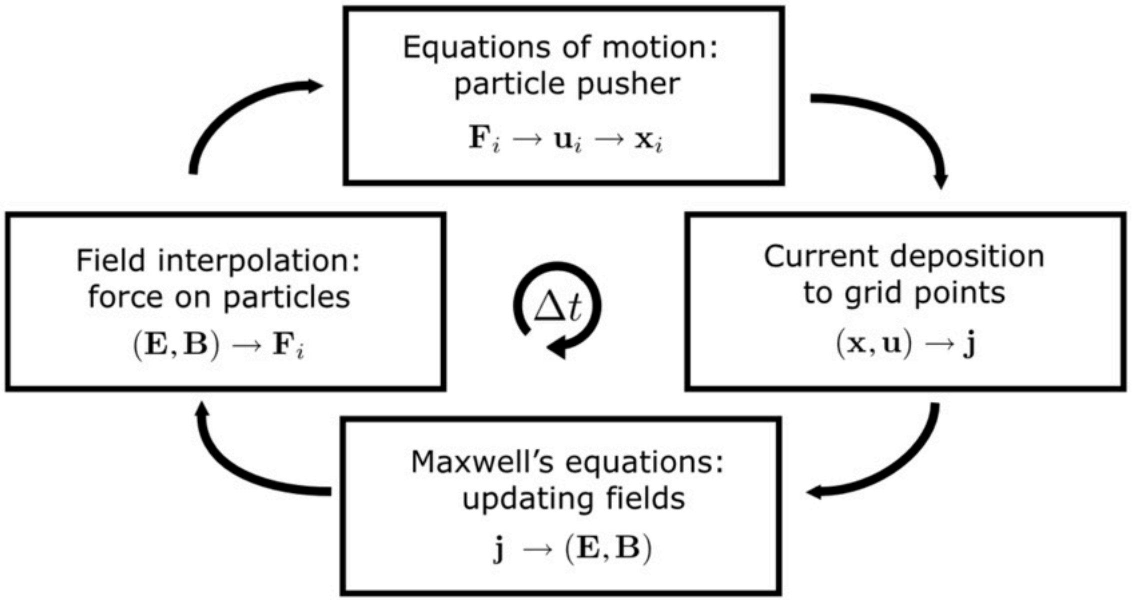
Validation against theory (but theory is very limited) or computational models (MD non relativistic)

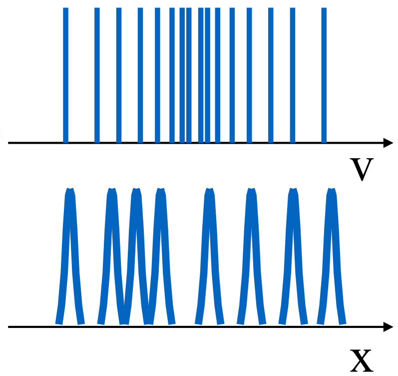
Shape functions to capture quantum effects?

D. Carvalho et al., in preparation (2025)

High resolution simulations can capture collisional dynamics

$$\frac{d\mathbf{p}}{dt} = \mathbf{F_L} + \mathbf{F_{RR}}$$





$$\frac{\partial \mathbf{E}}{\partial t} = c\nabla \times \mathbf{B} - 4\pi \mathbf{j}$$

$$\frac{\partial \mathbf{B}}{\partial t} = -c\nabla \times \mathbf{E}$$

$$N_s(\mathbf{x},\mathbf{v},t) = \sum_{i=1}^{N_0} \delta[\mathbf{x} - \mathbf{X}_i(t)]\delta[\mathbf{v} - \mathbf{V}_i(t)]$$

Nonlinear collisional absorption in laser-driven plasmas
C. D. Decker *et al.*, Phys. Plasmas 1, 4043–4049 (1994)
Disorder induced heating
M. D. Acciarri *et al.*, Plasma Sources Sci. Technol. 33 035009 (2024)

Diagram from: M. Vranic, et al. Comp. Phys. Comms. 204: 141-151 (2016)

Pushing PIC simulations to capture self-consistent (e.m.) collisions

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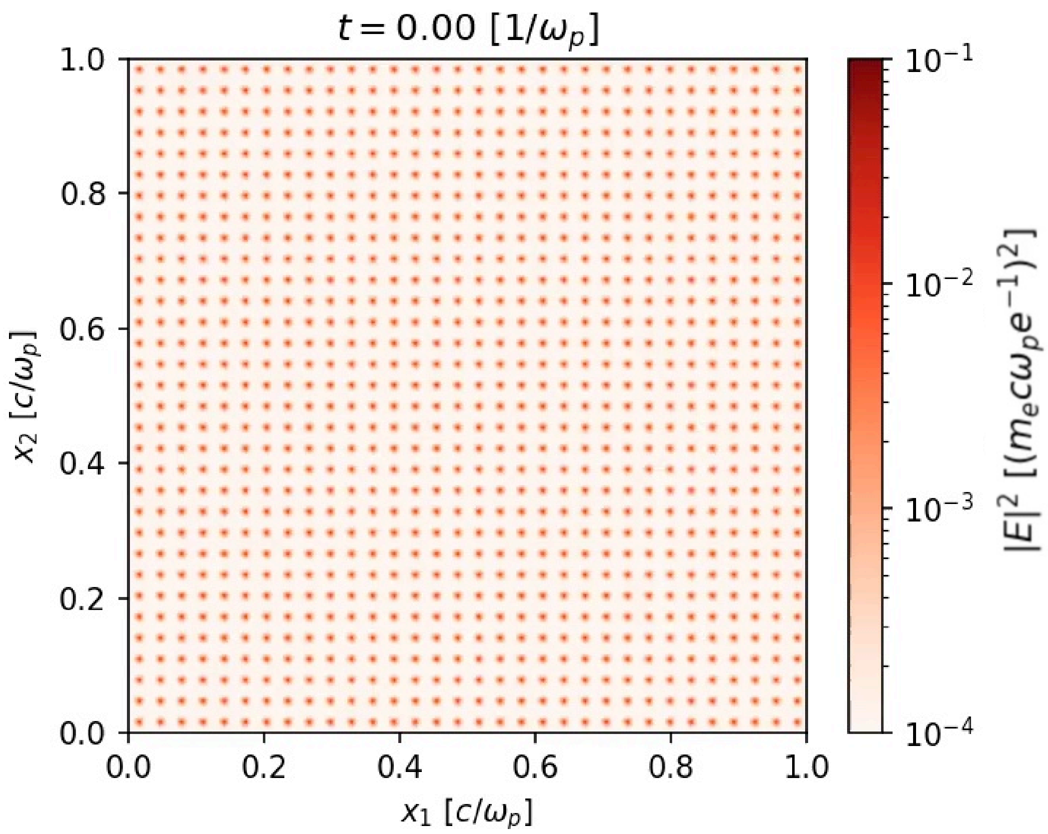
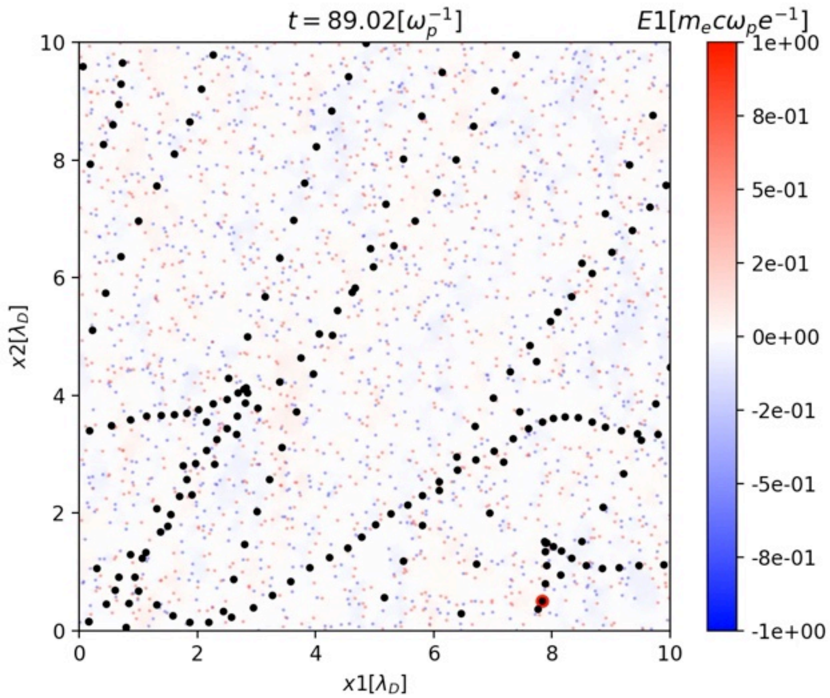
$n\lambda_D^2 \simeq 0.1$ (Average interparticle distance $\gg \lambda_D$)



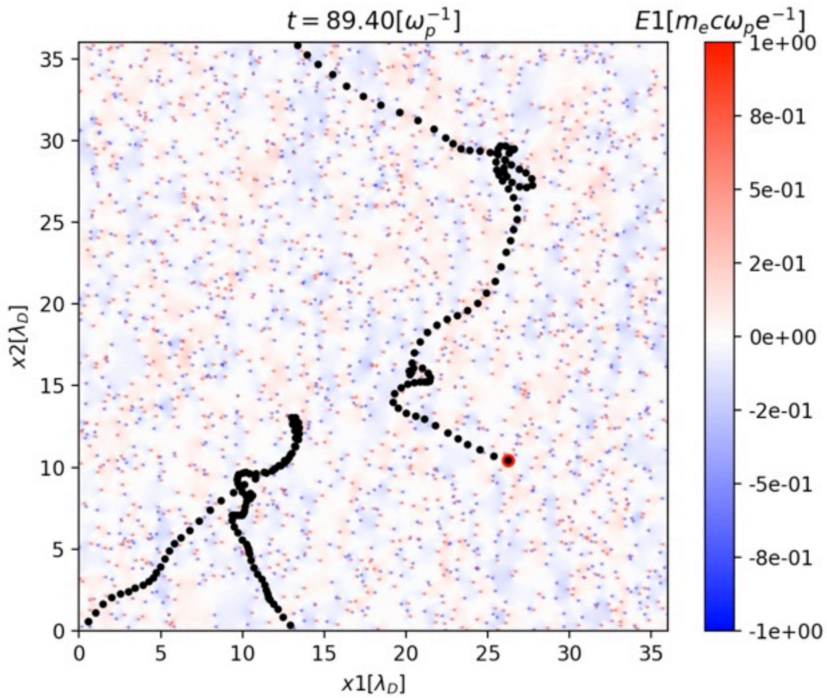
D. Carvalho et al., in preparation (2026)

Can we learn operators that describe the collisional dynamics?

$N_D^{2D} \simeq 32$



$N_D^{2D} \simeq 2.5$



D. Carvalho et al., in preparation (2026)

Summary

- Exciting opportunities from the interplay between *ab initio* PIC simulations and AI
  - Improvements in standard simulators
  - Novel approaches to standard algorithms
  - Tapping on unique properties of synthetic high fidelity PIC data
- Interplay between HPC + PIC and AI is just starting: "There are (many) unknown unknowns" (which is great for science!)

R. Ewart et al., PNAS (2025)