Graph Neural Networks for Kinetic Simulations of a 1D Plasma Sheet Model

D. D. Carvalho[1]*, D. R. Ferreira[2], L. O. Silva[1]

[1]GoLP/Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa, 1049-001 Lisbon, Portugal
[2]Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Universidade de Lisboa, 1049-001 Lisbon, Portugal

*diogo.d.carvalho@tecnico.ulisboa.pt

49th Conference on Plasma Physics

Fundação para a Ciência e a Tecnologia

Supported by the Seventh Framework Programme of the European Union

Motivation

Is it possible to develop kinetic plasma physics simulators where charged particle dynamics are fully (and correctly) predicted by a neural network? If yes, what are the advantages and limitations compared to traditional solvers? Inspired by previous works on Graph Network Simulators (GNS) for fluid simulations [2,3] we aim to provide an answer to these questions.

For this initial work [1] **we use as a test scenario the 1D Electrostatic Sheet Model** introduced by Dawson [4]. This algorithm is a predecessor of Particle in Cell codes that still models a wide range of kinetic plasma processes. We use the synchronous version of the algorithm [4] to generate both training and test data.

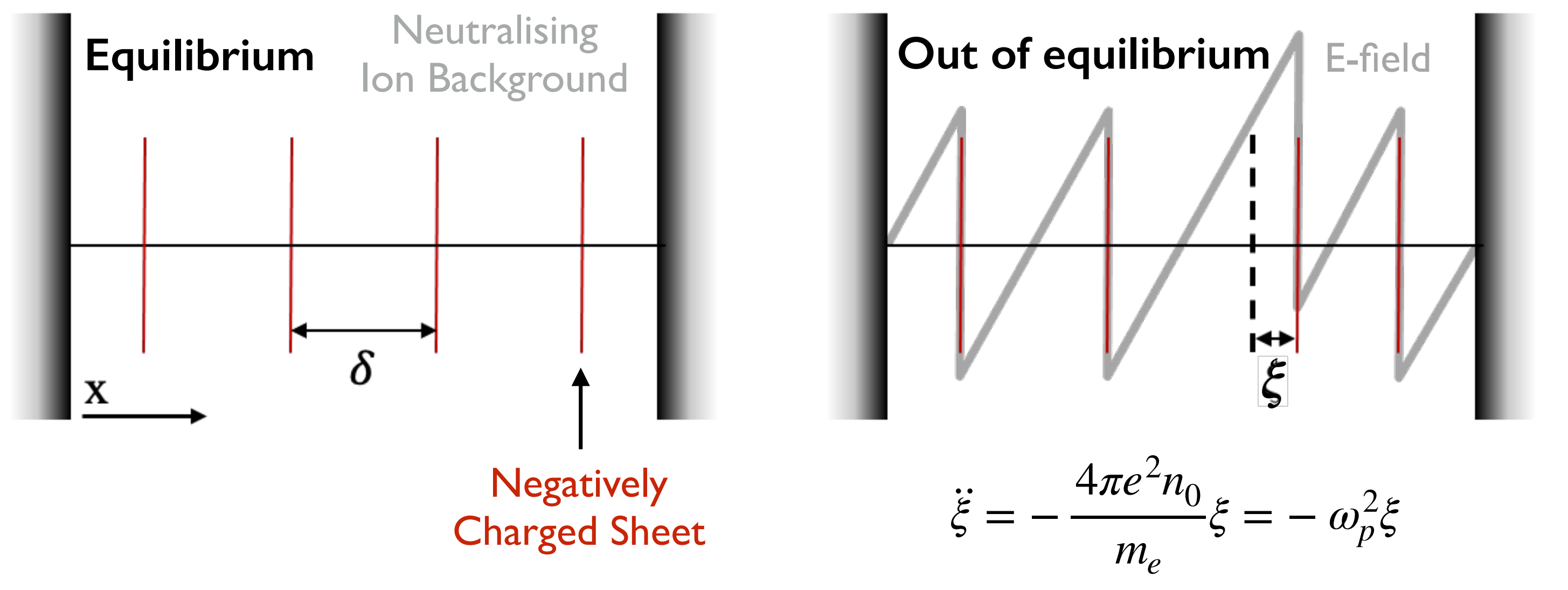

Figure 1: 1D Electrostatic Sheet Model. Plasma is represented by a set of equally negatively charged sheets moving over a neutralising ion background. Image adapted from Dawson [4].

Graph Network Simulator (GNS)

We modified the architecture of Sanchez-Gonzalez *et al.* [3] in order to embed some of the key structure and symmetries relevant for the electrostatic sheet model. Implemented in JAX [5].

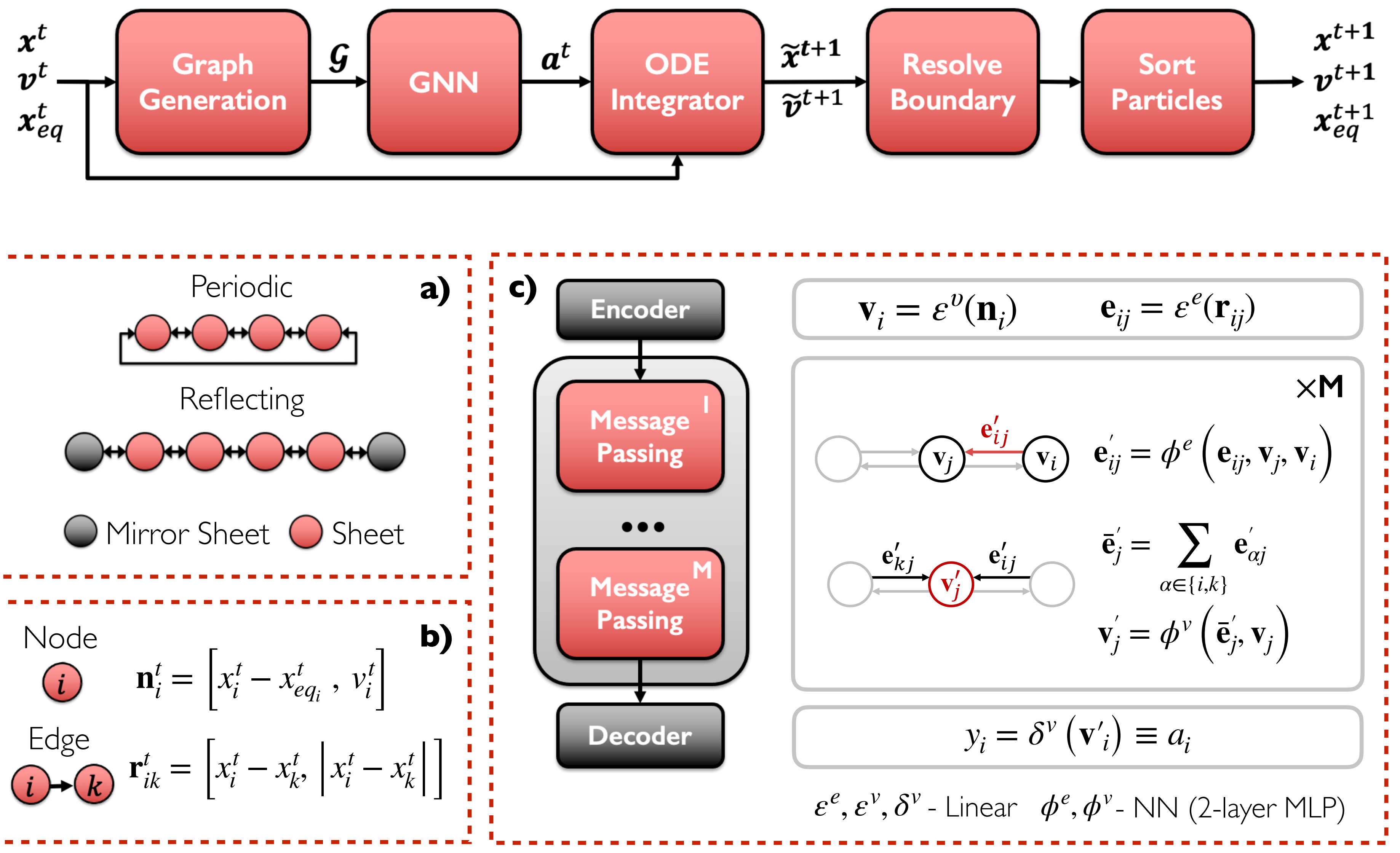

Figure 2: Schematic of Graph Network Simulator developed to simulate the 1D Electrostatic Sheet model. **a)** Graph for different boundary conditions **b)** Node/edge vectors **c)** Graph Neural Network architecture

Generalization to different system sizes and boundary conditions

The GNS was trained only on simulations consisting of 10 sheets inside a periodic box but it generalizes to different numbers of sheets and boundary conditions without retraining.

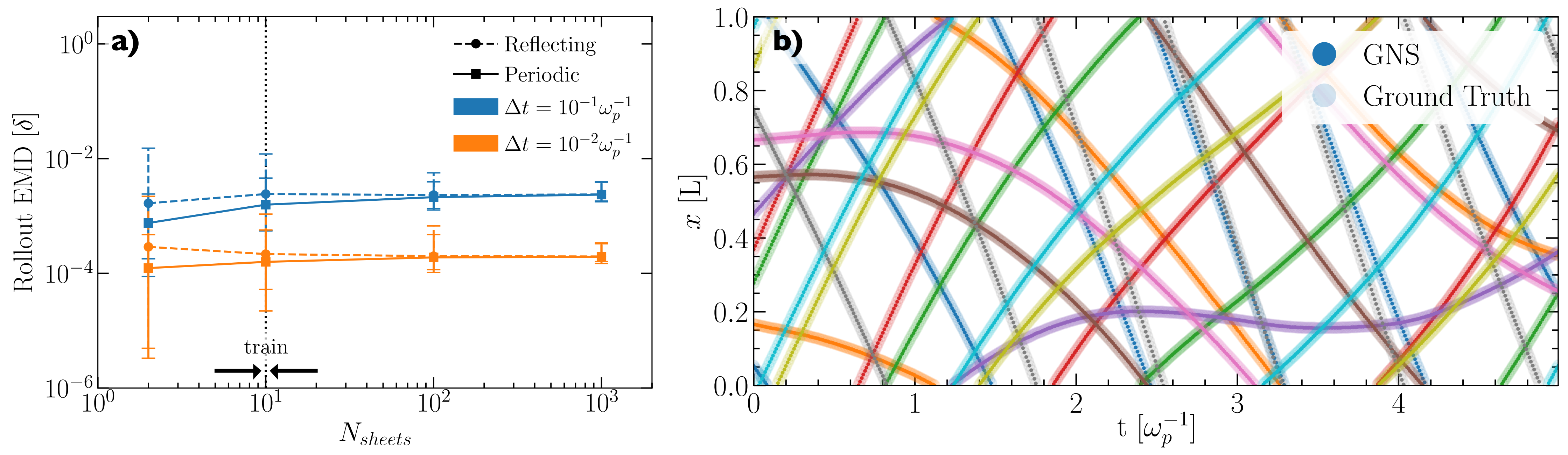

Figure 3: a) Rollout Earth Mover's Distance [6] between predicted and ground truth test set trajectories. Metric is averaged over simulations, sheets and time-steps. Error bars indicate worst/best performance. **b)** Example of predicted sheet trajectories *versus* ground truth test data. Only the initial positions and velocities are provided.

Improved energy conservation

The GNS conserves energy better than the Sheet Model (SM) at equivalent simulation time-steps.

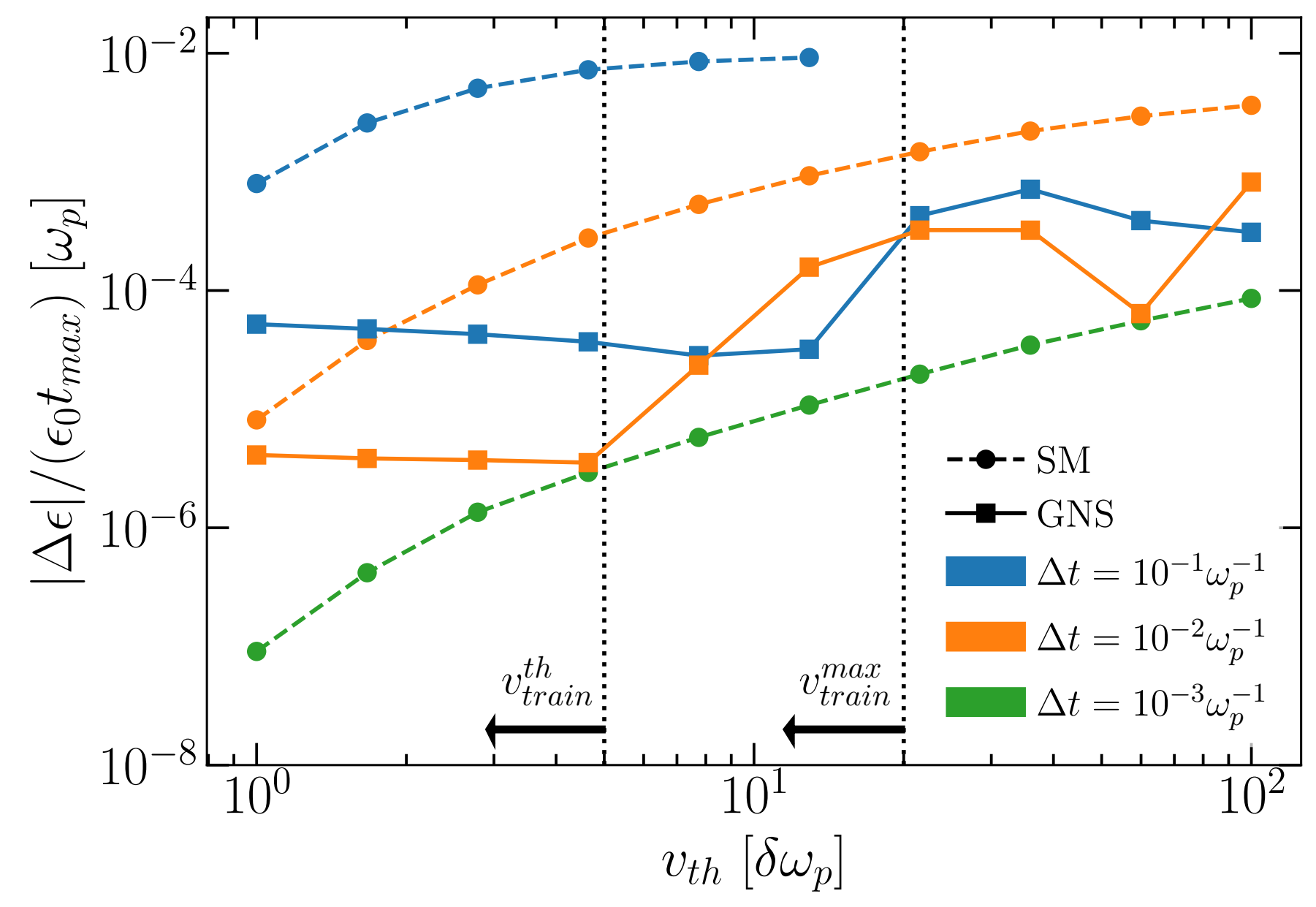

Figure 4: Comparison of energy loss rates for systems consisting of 1000 sheets with different initial thermal velocities

Recover known plasma kinetic processes

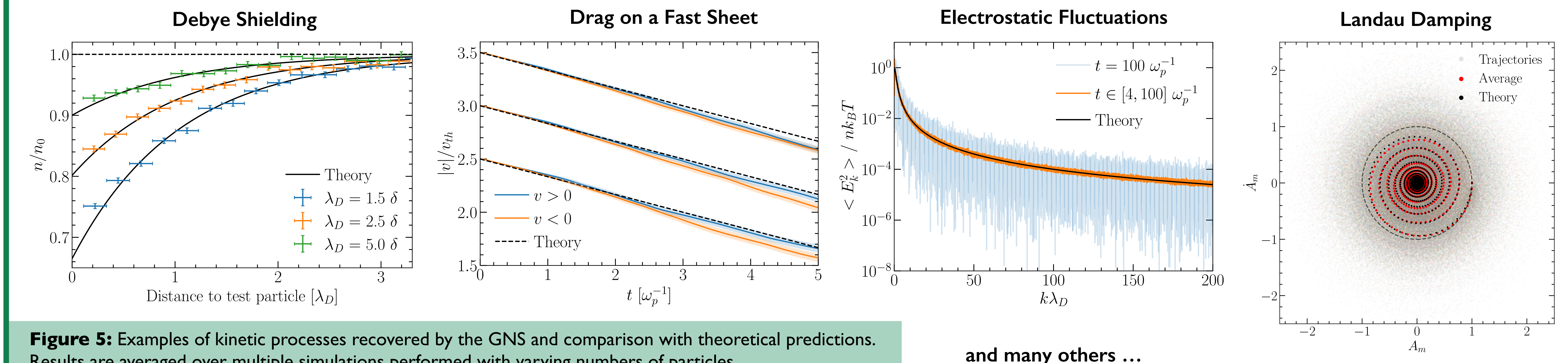

Figure 5: Examples of kinetic processes recovered by the GNS and comparison with theoretical predictions. Results are averaged over multiple simulations performed with varying numbers of particles.

and many others …

Conclusions

Developed a general purpose 1D Kinetic Plasma Simulator using Graph Neural Networks

Advantages: Better energy conservation than original Sheet Model and enables simulations at large Δt

Limitations: Simulator must run at fixed Δt and does not generalise to out of training distribution data (high v_{th})

Future work: Showcase differentiability capabilities and improve performance at high v_{th}

References

[1] D. D. Carvalho *et al.*, in preparation (2023)
[2] P. Battaglia *et al.*, arXiv:1806.01261 (2018)
[3] A. Sanchez-Gonzalez *et al.*, PMLR 119:8459-8468 (2020)
[4] J. Dawson, Phys. Fluids 5.4, 445-459 (1962); J. Dawson, Methods in Computational Physics 9 (1970)
[5] J. Bradbury *et al.*, http://github.com/google/jax (2018)
[6] C. Villani, Berlin: springer vol. 338:23 (2009)

This project was supported by the FCT under the Project No 2022.02230.PTDC (X-MASER) and Grant 2022.13261.BD and has received funding from the European Union's H2020 programme under grant agreement No 871161. Simulations were run on a local machine containing a Titan X GPU donated by NVIDIA Corporation.