Reduced Particle in Cell method for the Vlasov-Poisson system using auto-encoder and Hamiltonian neural network

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Introduction

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  - large number of particles : many degrees of freedom,
  - costly solver for particles interactions (Lorentz force),
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  - large number of particles : many degrees of freedom,
  - costly solver for particles interactions (Lorentz force),
  - multi-query context on a set of parameters (physical, geometric,...),
- + Hamiltonian structure : numerical stability,
- build a reduced model to reduce numerical costs
  - close to the original model, balance speed and precision,
  - with a Hamiltonian structure,
  - using neural networks.

Vlasov-Poisson model

- System described by the distribution $f(t,x,v;\mu)$ with time $t \in \mathcal{T} = (0,T]$, position $x \in \Omega_x = \mathbb{R}/2\pi\mathbb{Z}$, velocity $v \in \Omega_v \subset \mathbb{R}$ and parameters $\mu \in \Xi \subset \mathbb{R}^p$, $p > 0$, charge q and mass m,

$$\begin{cases} \partial_t f(t,x,v;\mu) + v\partial_x f(t,x,v;\mu) + \frac{q}{m} E(t,x;\mu)\partial_v f(t,x,v;\mu) = 0, & \text{in } \Omega_x \times \Omega_v \times \mathcal{T}, \\ \partial_x E(t,x;\mu) = \rho(t,x;\mu), & \text{in } \Omega_x \times \mathcal{T}, \end{cases}$$

  where $\rho(t,x;\mu) = q\int_{\Omega_v} f(t,x,v;\mu)\,dv$ is the electric density,

- $E(t,x;\mu)$ is the electric field, derives from electric potential $\phi(t,x;\mu)$: $-\partial_x\phi = E$,

- the Poisson equation rewrites

$$-\partial_{xx}\phi(t,x;\mu) = \rho(t,x;\mu).$$

Particle-based discretization

- Solution approximated with $N \gg 1$ particles $(x_k(t), v_k(t))$ in the phase space

$$f_N(t,x,v;\mu) = \sum_{k=1}^{N} \omega\,\delta\left(x - x_k(t)\right)\delta\left(v - v_k(t)\right)$$

- results in a $2N$-dimensional ODE

$$\begin{cases} \dfrac{d}{dt}X(t;\mu) = V(t;\mu), & \text{in } \mathcal{T} \\ \dfrac{d}{dt}V(t;\mu) = \frac{q}{m}E(X(t;\mu);\mu) & \text{in } \mathcal{T}, \end{cases}$$

where $(X)_k = x_k, (V)_k = v_k$,

- electric field computed with a mesh : Particle-In-Cell (PIC) method[1].

[1] Kraus et al. 2017.

Full order model

- Full order model of solution $u = (X\ V)^T \in \mathbb{R}^{2N}$

$$\frac{d}{dt}u(t;\mu) = J_{2N}\nabla_u\mathcal{H}(u(t;\mu))$$

with $J_{2N} = \begin{pmatrix} 0_N & I_N \\ -I_N & 0_N \end{pmatrix}$,

- $\mathcal{H} : \mathbb{R}^{2N} \to \mathbb{R}$ is the Hamiltonian (total energy)

$$\mathcal{H}(u(t;\mu)) = \underbrace{\frac{1}{2}V^T V}_{\text{kinetic energy}} + \underbrace{\frac{1}{2m}q^2\omega\Lambda^0(X(t;\mu))L^{-1}\Lambda^0(X(t;\mu))^T\mathbb{1}_N}_{\text{potential energy}}$$

with Λ^0 a particle-to-grid mapping, L a discrete Laplacian matrix,

- symplectic structure $\to$ numerical stability, physical solutions[2].

[2] Hairer, Lubich, and Wanner 2006; Cabral and Brandão Dias 2023.

Model order reduction

- Starting with $2N$-dimensional, $N \gg 1$ ODE

$$\frac{d}{dt} u(t;\mu) = J_{2N} \nabla_u \mathcal{H}(u(t;\mu))$$

- with a cost of $\mathcal{O}(N)$ for each $(t,\mu) \in \mathcal{T} \times \Xi$ is prohibitive,
- idea : find a reduced state $\bar{u}(t) \in \mathbb{R}^{2K}$, $K \ll N$ solution of

$$\frac{d}{dt} \bar{u}(t;\mu) = J_{2K} \nabla_{\bar{u}} \bar{\mathcal{H}}(\bar{u}(t;\mu))$$

with a cost of $\mathcal{O}(K)$ or $\mathcal{O}(K^2)$ and a nice map $\bar{u}(t) \mapsto u(t)$.

- Idea : two step projection[3]

$$\begin{array}{ccccc} \mathbb{R}^{2N} & \longrightarrow & \mathbb{R}^{2M} & \longrightarrow & \mathbb{R}^{2K} \\ u(t;\mu) & \longmapsto & \tilde{u}(t;\mu) & \longmapsto & \bar{u}(t;\mu) \end{array}$$

- with an intermediate state of size $2M$, $K < M \ll N$ e.g. $K = 4, M = 121$,

[3] Fresca and Manzoni 2022.

[4] Greydanus, Dzamba, and Yosinski 2019; Côte et al. 2025.

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- with an intermediate state of size $2M$, $K < M \ll N$ e.g. $K = 4, M = 121$,
- first projection = linear operator $A \in \mathcal{M}_{2N,2M}(\mathbb{R})$ such that

$$u = A\tilde{u}, \quad \tilde{u} = A^{+}u,$$

- second projection = autoencoder neural network $(\mathcal{E}_\theta, \mathcal{D}_\theta)$

$$\bar{u} = \mathcal{E}_\theta(\tilde{u}), \quad \tilde{u} \approx \mathcal{D}_\theta(\bar{u}),$$

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- reduced model captured with a Hamiltonian Neural Network (HNN)[4] $\bar{\mathcal{H}}_\theta$.

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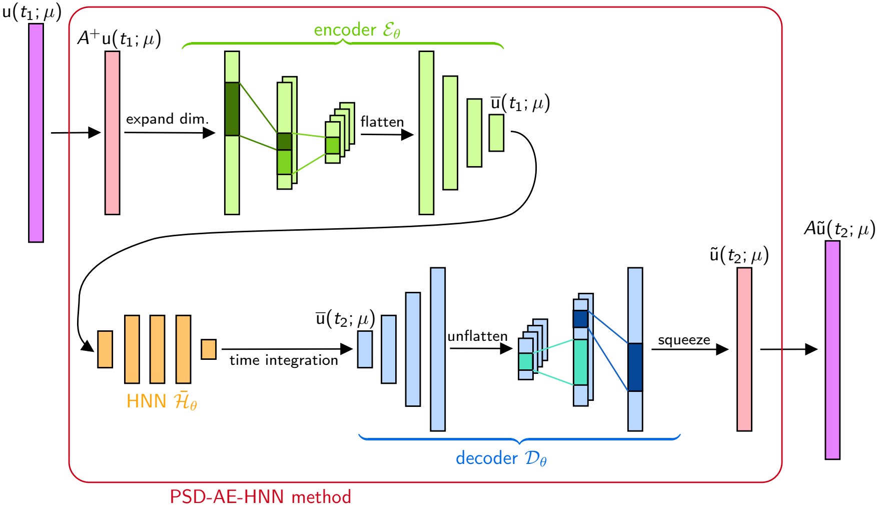
PSD-AE-HNN architecture



Linear projection

- Proper Symplectic Decomposition (PSD)[5] = Hamiltonian variant of the POD,
- the projection preserves the Hamiltonian structure,
- $A \in \mathcal{M}_{2N,2M}(\mathbb{R})$ is a symplectic matrix $A^T J_{2N} A = J_{2K}$,
- with a symplectic inverse $A^+ = J_{2K}^T A^T J_{2N}$ such that

$$A^+ A = I_{2K}$$

- built minimizing the reconstruction error

$$\underset{A^T J_{2N} A = J_{2K}}{\arg\min} \sum_{u \in U} \left\| u - AA^+ u \right\|_F$$

on a dataset U with a Singular Value Decomposition (SVD).

[5] Peng and Mohseni 2016.

Non-linear reduced model

- The autoencoder is fitted with the loss $\mathcal{L}_{\mathsf{AE}}$

$$\mathcal{L}_{\mathsf{AE}} = \sum_{u \in U} \left\| u - \mathcal{D}_\theta\left(\mathcal{E}_\theta\left(u\right)\right) \right\|_2^2$$

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- Let $\mathcal{P}$ be a (symplectic) integrator

$$\bar{u}^{n+1} \approx \mathcal{P} \left(\bar{u}^n ; \bar{\mathcal{H}}_\theta \right)$$

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$$\bar{u}^{n+1} \approx \mathcal{P}\left(\bar{u}^n; \bar{\mathcal{H}}_\theta\right)$$

- and three additional losses to couple it with the HNN

$$\mathcal{L}_{\overline{\mathsf{pred}}} = \sum_{u^n, u^{n+1} \in U} \left\| \bar{u}^{n+1} - \mathcal{P}\left(\bar{u}^n; \bar{\mathcal{H}}_\theta\right) \right\|_2^2,$$

$$\mathcal{L}_{\overline{\mathsf{stab}}} = \sum_{u^n, u^{n+1} \in U} \left\| \bar{\mathcal{H}}_\theta\left(\bar{u}^{n+1}\right) - \bar{\mathcal{H}}_\theta\left(\bar{u}^n\right) \right\|_2^2,$$

$$\mathcal{L}_{\mathsf{pred}} = \sum_{u^n, u^{n+1} \in U} \left\| u^{n+1} - \mathcal{D}_\theta\left(\mathcal{P}\left(\bar{u}^n; \bar{\mathcal{H}}_\theta\right)\right) \right\|_2^2.$$

Example

- parametrized initial condition $\mu = (\alpha \ \sigma)^T \in \Xi \subset \mathbb{R}^2$

$$f_{\text{init}}(x, v; \mu) = \underbrace{\frac{1}{4\pi}\left(1 + \alpha \cos\left(\frac{x}{2}\right)\right)}_{f_{\text{init},x}(x;\alpha)} \underbrace{\frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{v^2}{2\sigma^2}\right)}_{f_{\text{init},v}(v;\sigma)},$$

- $(\alpha, \sigma) \in [0.03, 0.06] \times [0.8, 1]$,
- electric energy $\frac{1}{2}\|E(x)\|_{L^2}$,
- $N = 10^5$, $M = 121$, $K = 3$ and $T = 20$.

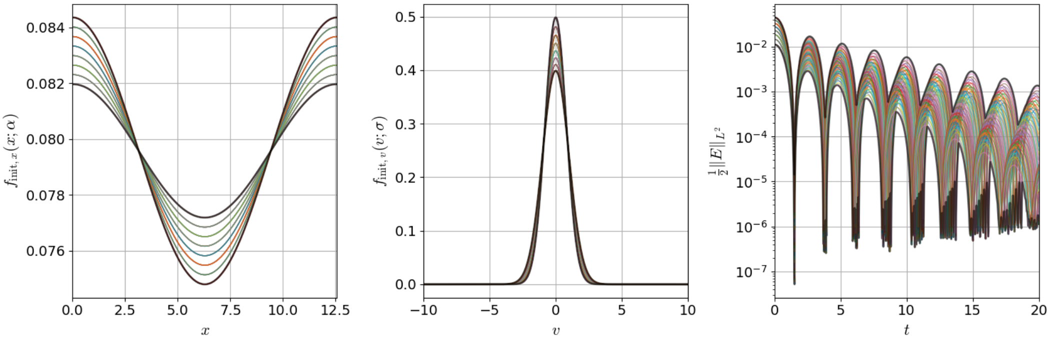

Figure: Initial condition $f_{\mathrm{init},x}(x;\alpha)$ (left), $f_{\mathrm{init},v}(v;\sigma)$ (middle) and electric energy (right) for every $\mu \in \Xi$.

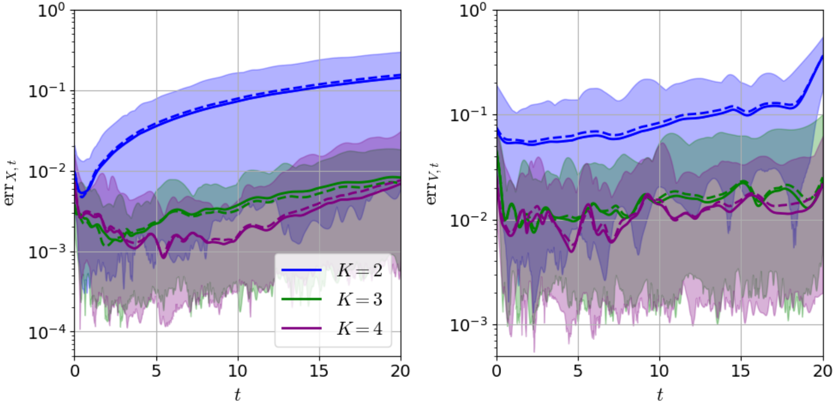

Figure: Mean relative error as a function of time (solid line) for x (left) and v (right), envelopes represents minimum and maximum errors.

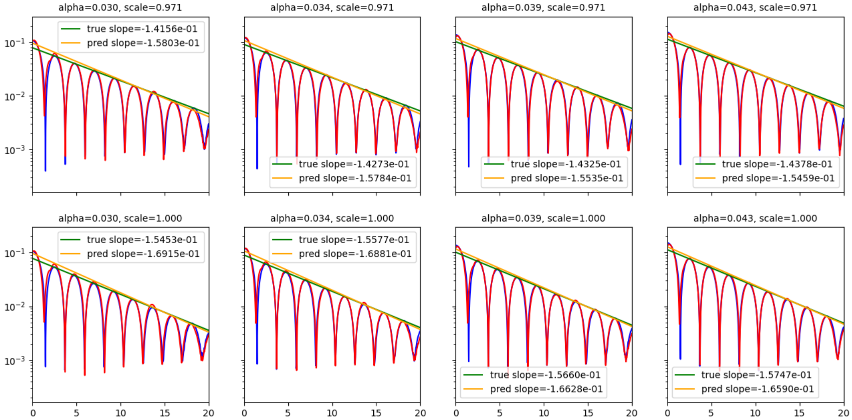

Figure: Some damping rates predictions for various $\mu \in \Xi$.

Conclusion & perspectives

- The PSD-AE-HNN is a two-stage reduction technique, Hamiltonian by design,
- generic, non-intrusive and data-driven method, easy to vectorize,
- lack of global convergence guarantees, no systematic way to improve accuracy.

- increase simulation time, 2D and 3D extensions,
- improve the AE : add some structure, dynamic projection.

- Full paper available at https://hal.science/hal-05116555

Thank you !

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