Model order reduction method for Hamiltonian dynamics using deep learning

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supervised by

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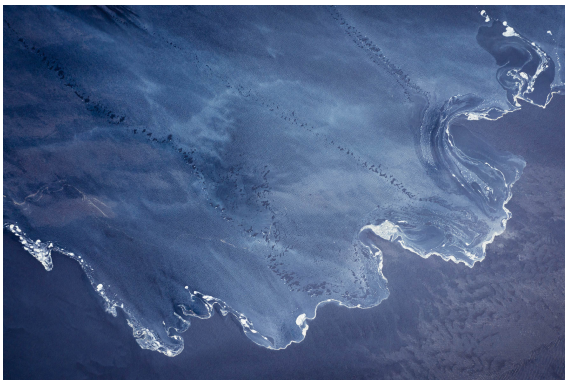
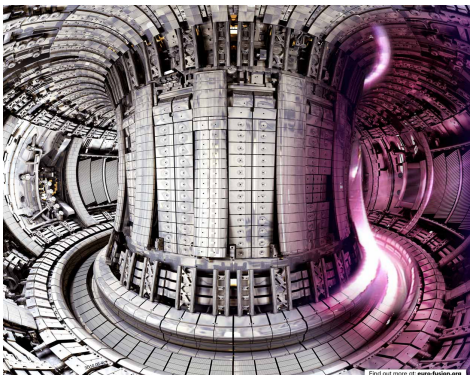
Motivation





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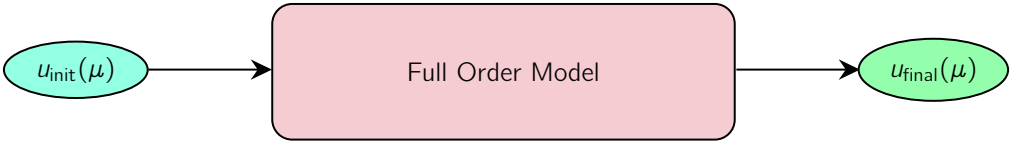
- Hamiltonian structure preserved with symplectic (implicit) methods.

- In many-query or real-time settings, solvers often fail to scale for fast resolution or repeated evaluations across multiple parameters,
- a solution: build a **Hamiltonian** Reduced Order Model (ROM) trading accuracy for computational efficiency,
- efficient over a given time and parameter domain.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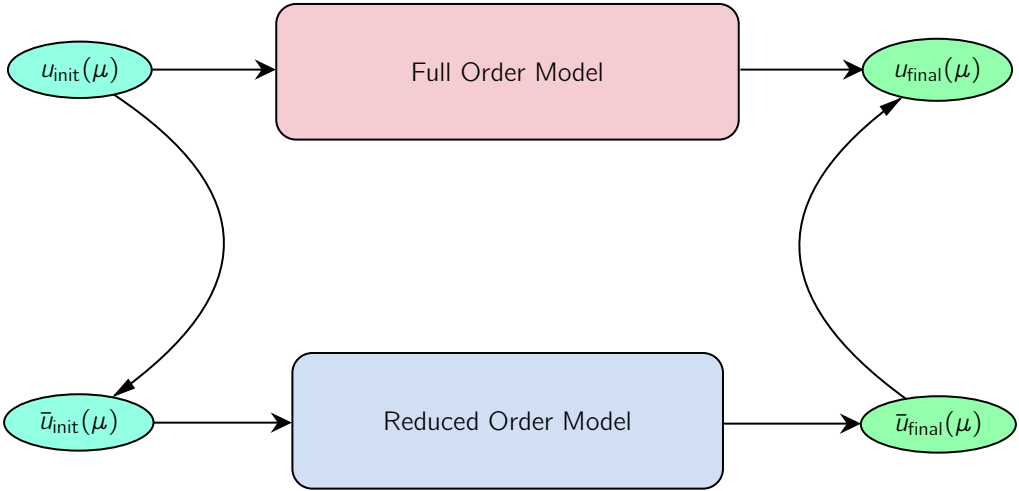
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Thesis objective

- Develop new model order reduction techniques,
  - preserving the Hamiltonian structure,
  - with deep learning (neural networks),
- test it against several Hamiltonian models,
  - mesh-based models (wave equation, shallow-water system),
  - particle-based model (Vlasov-Poisson system).

- Evolution of a field $u(x, t; \mu) \in V$ depending on space $x \in \Omega \subset \mathbb{R}^d$, time $t \in \mathcal{T} = [0, T]$ and parameters $\mu \in \Gamma \subset \mathbb{R}^p$ is given by

$$\frac{\partial u}{\partial t} = \mathcal{J}(u) \frac{\delta \mathcal{H}}{\delta u}(u),$$

  with $\delta \mathcal{H} / \delta u$ the functional derivative of $\mathcal{H}$ with respect to u,

- $\mathcal{H} : V \to \mathbb{R}$ is the **Hamiltonian** of the system, often the total energy,

- $\mathcal{J}(u) : V \to V$ is a skew-adjoint operator called the **Poisson structure operator**.

- In the canonical case, we denote $u(x,t;\mu) = (q(x,t;\mu), p(x,t;\mu)) \in \mathbb{R}^{2N}$ the canonical coordinates with generalized coordinates $q(x,t;\mu)$ and conjugate momentum $p(x,t;\mu)$,
- the Poisson structure operator $\mathcal{J}$ becomes

$$\mathcal{J} = \begin{pmatrix} 0 & \mathrm{id} \\ -\mathrm{id} & 0 \end{pmatrix},$$

- and the system rewrites

$$\frac{\partial u}{\partial t} = \mathcal{J}\frac{\delta \mathcal{H}}{\delta u}(u) \iff \begin{cases} \partial_t q = \dfrac{\delta \mathcal{H}}{\delta p}(q,p), \\ \partial_t p = -\dfrac{\delta \mathcal{H}}{\delta q}(q,p). \end{cases}$$

- Example : linear wave equation (dim. $N = 1$) on a periodic domain of length 1,

$$\partial_{tt} q(x, t; \mu) - \mu^2 \partial_{xx} q(x, t; \mu) = 0,$$

with the displacement $q(x, t; \mu)$ and the parametrized propagation speed $\mu \in \Gamma \subset \mathbb{R}$ ($p = 1$),

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  with the displacement $q(x, t; \mu)$ and the parametrized propagation speed $\mu \in \Gamma \subset \mathbb{R}$ ($p = 1$),
- the Hamiltonian (total energy) is

$$\mathcal{H}[q, p] = \frac{1}{2} \int_0^1 \left(p^2 + \mu^2 (\partial_x q)^2 \right) \, dx.$$

- denoting $p(x, t; \mu) := \partial_t q(x, t; \mu)$, the equation rewrites

$$\begin{cases} \partial_t q(x, t; \mu) = p(x, t; \mu), \\ \partial_t p(x, t; \mu) = \mu^2 \partial_{xx} q(x, t; \mu). \end{cases}$$

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$$\partial_x u(x_i, t;\mu) \approx \frac{1}{2h}[u_{i+1}(t;\mu) - u_{i-1}(t;\mu)]\,, \text{etc.},$$

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- need to preserve the Hamiltonian structure : $\mathcal{J}_h$ becomes a skew-symmetric matrix (+ Jacobi identity),
- In the canonical case, we derive a $2N$-dimensional ODE, $N \gg 1$

$$\frac{du_h(t;\mu)}{dt} = \mathcal{J}_h \nabla \mathcal{H}_h(u_h(t;\mu)),\ \mathcal{J}_h = \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix} \in \mathcal{M}_{2N}(\mathbb{R})$$

with $\mathcal{H}_h : \mathbb{R}^{2N} \to \mathbb{R}$ the (semi-discretized) Hamiltonian.

- Full order model = $2N$-dimensional ODE of solution $u(t;\mu) \in \mathbb{R}^{2N}$ and Hamiltonian $\mathcal{H} : \mathbb{R}^{2N} \to \mathbb{R}$

$$\begin{cases} \dfrac{du(t;\mu)}{dt} = \mathcal{J}_{2N} \nabla_u \mathcal{H}(u(t;\mu)), \\ u(0;\mu) = u_{\text{init}}(\mu), \end{cases}$$

  with $\mathcal{J}_{2N} = \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix} \in \mathcal{M}_{2N}(\mathbb{R})$,

- and its flow $\phi_t : \mathbb{R}^{2N} \to \mathbb{R}^{2N}$

$$\phi_t(u_{\text{init}}(\mu)) := u(t;\mu).$$

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  - preservation of the Hamiltonian along the flow

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  - time reversibility, volume preservation,
  - etc.,
- provide guarantees for long-time stability, physical relevance.

- Last step : deriving numerical solutions,

[1] Hairer et al. 2006.

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- discretization of $[0, T]$ with time steps $t^n = n\Delta t$,
- compute approximated solution at each time step with numerical integration,

$$u(t^{n+1}; \mu) = u(t^n; \mu) + \int_{t^n}^{t^{n+1}} \mathcal{J}_{2N} \nabla_u \mathcal{H}(u(t; \mu))\, dt.$$

- quadrature choice for $\int_{t^n}^{t^{n+1}} \mathcal{J}_{2N} \nabla_u \mathcal{H}(u)\, dt$ = numerical scheme,

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- quadrature choice for $\int_{t^n}^{t^{n+1}} \mathcal{J}_{2N} \nabla_u \mathcal{H}(u)\, dt$ = numerical scheme,
- need to use a symplectic numerical scheme[1] to safeguard the system properties : long time stability, physical relevance, etc.,
- in practice : implicit midpoint or Störmer Verlet.

[1] Hairer et al. 2006.

1 Hamiltonian systems

2 Model Order Reduction for Hamiltonian systems
- Proper Symplectic Decomposition (PSD)
- Deep learning based Hamiltonian reduction

3 An application to the shallow-water system

4 Reduced Particle in Cell method for the Vlasov-Poisson system

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$$\widehat{\mathcal{M}} := u_{\text{ref}}(\mu) + \{\mathcal{D}\left[\bar{u}(t;\mu)\right] \,|\, (t,\mu) \in \mathcal{T} \times \Gamma\}$$

with $\mathcal{D} : \mathbb{R}^{2K} \to \mathbb{R}^{2N}$, $K \ll N$ a reconstruction/decoding operator or **decoder**, $u_{\text{ref}}(\mu) \in \mathbb{R}^{2N}$ a reference state, $\bar{u}(t;\mu) \in \mathbb{R}^{2K}$ a **reduced state**,

- that is

$$\hat{u}(t;\mu) = u_{\text{ref}}(\mu) + \mathcal{D}\left[\bar{u}(t;\mu)\right] \approx u(t;\mu).$$

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- for illustration $N = 10^5$, $K = 30$ and $\dim(\Gamma) = 2$,

- Assume the trial manifold is a linear subspace

$$\widehat{\mathcal{M}} = \text{span}(a_i, i \in \{1, \dots, 2K\}) \iff \mathcal{D}\left[\bar{u}(t;\mu)\right] = A\bar{u}(t;\mu)\,,\ A \in \mathcal{M}_{2N,2K}(\mathbb{R})$$

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- constraint that the decoder $\bar{u} \mapsto A\bar{u}$ is a symplectic map

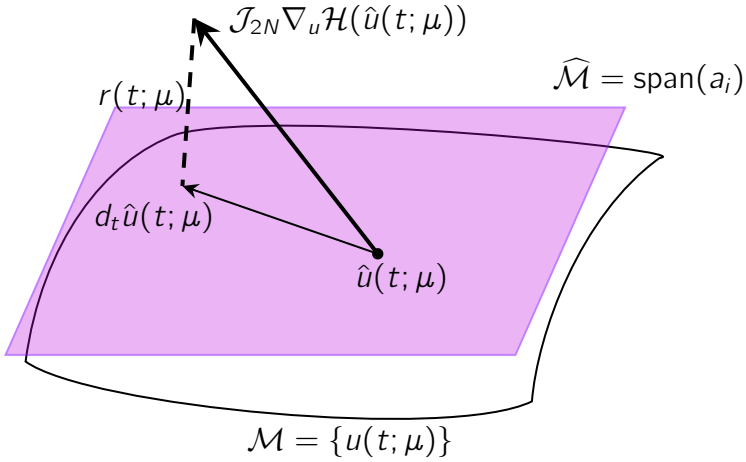
$$A^T \mathcal{J}_{2N} A = \mathcal{J}_{2K}$$

- symplectic inverse of the decoder = encoder $\mathcal{E}$

$$\mathcal{E}\left[u(t;\mu)\right] = A^+ u(t;\mu)$$

with $A^+ \in \mathcal{M}_{2K,2N}(\mathbb{R})$ such that $A^+ = \mathcal{J}_{2K}^T A^T \mathcal{J}_{2N}$ the symplectic inverse of A ($A^+ A = I_{2K}$).

- What is the dynamics of the reduced state $\bar{u}(t;\mu)$?


$\mathcal{J}_{2N}\nabla_u\mathcal{H}(\hat{u}(t;\mu))$
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$r(t;\mu)$
$d_t\hat{u}(t;\mu)$
$\hat{u}(t;\mu)$
$\mathcal{M} = \{u(t;\mu)\}$

- We define the residual $r(t;\mu)$

$$r(t;\mu) = \frac{d\hat{u}(t;\mu)}{dt} - \mathcal{J}_{2N}\nabla_u \mathcal{H}(\hat{u}(t;\mu))$$

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- results in a Hamiltonian reduced model

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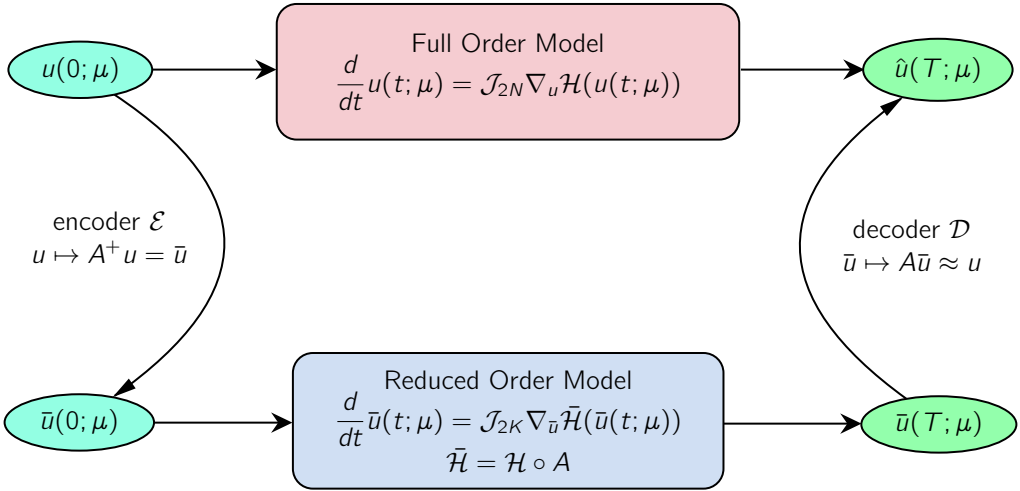
- warning: no complexity improvement in general, need for hyper-reduction techniques (Discrete Empirical Interpolation Method (DEIM), etc., not discussed).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- Solution: from numerical solution snapshots/samples

$$U = \begin{bmatrix} u(t_1;\mu_1) & \dots & u(t_P;\mu_P) \end{bmatrix} \in \mathcal{M}_{2N,P}(\mathbb{R}),$$

- A minimizes the reconstruction error on the snapshots,

$$\min_{A^T \mathcal{J}_{2N} A = \mathcal{J}_{2K}} \left\| U - AA^+ U \right\|_F$$

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- in practice, the **Singular Value Decomposition** (SVD)[2] of U on a modified minimization problem is used.

[2] Lange 2010.

- The SVD of U is a decomposition of the form

$$U = W\Sigma V^*$$

with $W \in \mathcal{U}_{2N}(\mathbb{C})$, $V \in \mathcal{U}_P(\mathbb{C})$ unitary matrices, $\Sigma = (\sigma_i)_{i,i} \in \mathcal{M}_{2N,P}(\mathbb{C})$ a rectangular diagonal matrix, V^* is the conjugate-transpose of V,

- W, V columns are orthonormal bases called left and right singular vectors, respectively, $(\sigma_i)_{i,i}$ are singular values,

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- W, V columns are orthonormal bases called left and right singular vectors, respectively, $(\sigma_i)_{i,i}$ are singular values,
- **best rank** r **approximation** of U:

$$U_r = W_r \Sigma_r V_r^*$$

with $W_r = W[:, : r]$, $V_r = V[:, : r]$, $\Sigma_r = \mathrm{diag}(\sigma_1, \ldots, \sigma_r)$,

- A depends on[3] W_K.

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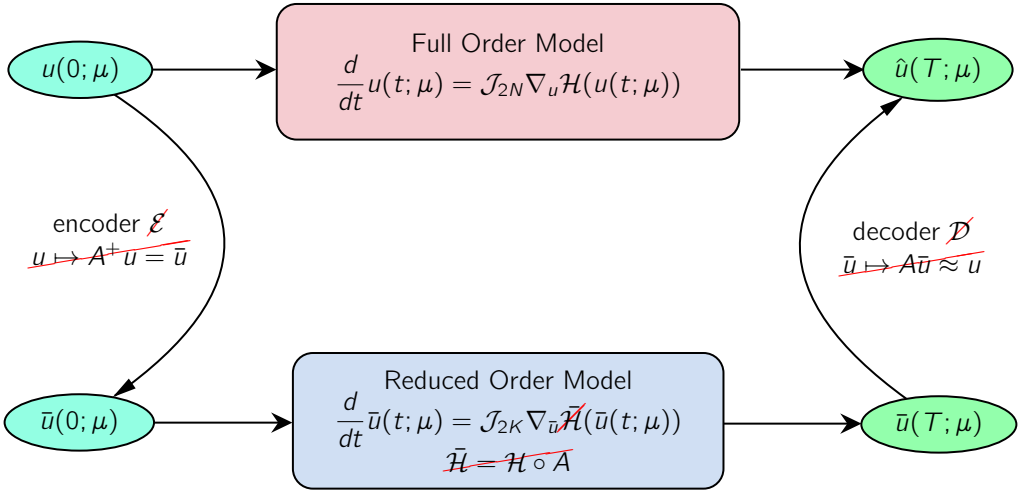
  - **offline stage**: computationally expensive, parametrically independent, performed once (building models, precompute quantities e.g. snapshots, reduced basis A, choose K, etc.),
  - **online stage**: fast computation, done for every new parameter, use offline precomputation to accelerate the reduced simulation.

- Statements on the linear model order reduction:
  - works well in linear and quasi-linear regimes,
  - interpolation/approximation strategies (DEIM, etc.)[4] in nonlinear regimes,
  - struggles in strongly nonlinear regimes,
- idea : replace the encoder, decoder, and eventually the reduced model by neural networks, as presented in Côte, Franck, Navoret, S., and Vigon (2025).

[4] Peng and Mohseni 2016; Hesthaven et al. 2024.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- Neural network = **parametric function** g_θ of parameters $\theta \in \Theta$,
- g_θ = **composition of** c **simple functions** $g_i : \mathbb{R}^{n_i} \to \mathbb{R}^{n_{i+1}}$ = layer,

$$g_\theta = g_c \circ \cdots \circ g_1,$$

- e.g.:
  - dense layer $g_i(x) = \sigma\left(W^{[i]}x + b^{[i]}\right)$ with $W^{[i]} \in \mathcal{M}_{n_{i+1},n_i}(\mathbb{R})$, $b^{[i]} \in \mathbb{R}^{n_{i+1}}$,
  - convolutional layer $g_i(x) = \sigma\left(W^{[i]} * x + b^{[i]}\right)$ with $*$ a convolution with a kernel $W^{[i]}$,
- σ non-linear function, $\theta = \left\{W^{[i]}, b^{[i]}, i \in \{1, \cdots, c\}\right\}$.

- Neural network = **parametric function** g_θ of parameters $\theta \in \Theta$,
- g_θ **fitted to a target function** g : $g_\theta \sim g$,
- on snapshots U, according to a cost function / loss $\mathcal{L}$,

$$\theta^* = \text{argmin}_{\theta\in\Theta}\, \mathcal{L}(g, g_\theta),$$

  e.g. $\mathcal{L}(g, g_\theta) = \sum_{u\in U} \|g(u) - g_\theta(u)\|_2^2$,
- with a gradient descent (*Adam* algorithm...),

$$\theta^{[k+1]} = \theta^{[k]} - \eta^{[k]} \nabla_\theta \mathcal{L}(g, g_{\theta^{[k]}}),$$

  with the learning rate $\eta^{[k]}$,
- called the neural network training.

- Compression/decompression managed by a (convolutional) AutoEncoder[5] (AE) = pair of neural networks $\mathcal{E}_\theta : \mathbb{R}^{2N} \to \mathbb{R}^{2K}, \mathcal{D}_\theta : \mathbb{R}^{2K} \to \mathbb{R}^{2N}$ such that $\mathcal{D}_\theta \circ \mathcal{E}_\theta \approx \mathrm{id}$,
- compression $\mathcal{E}_\theta(u) = \bar{u}$ and decompression $\mathcal{D}_\theta(\bar{u}) \approx u$,
- fitted with the loss $\mathcal{L}_{\mathrm{AE}}$

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

- **no direct symplecticity constraint** in the architecture or the loss.

[5] Goodfellow et al. 2016.

- What happens to the reduced model ?

$$\frac{d}{dt}\bar{u} = \mathcal{J}_{2K}\left[D_{\mathcal{D}_\theta}(\bar{u})\right]^T \nabla_{\mathcal{D}_\theta(\bar{u})}\mathcal{H}\left[\mathcal{D}_\theta(\bar{u})\right] \stackrel{?}{=} \mathcal{J}_{2K}\nabla_{\bar{u}}\bar{\mathcal{H}}(\bar{u})$$

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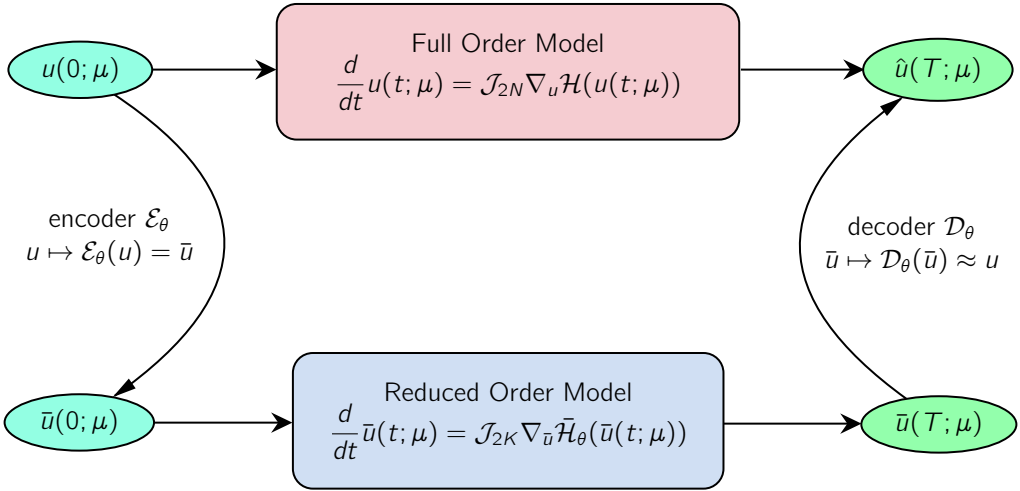
- supplant it with a Hamiltonian Neural Network (HNN) $\bar{\mathcal{H}}_\theta : \mathbb{R}^{2K} \to \mathbb{R}$ from Greydanus, Dzamba, and Yosinski (2019),

$$\begin{cases} \frac{d}{dt}\bar{u}(t;\mu) = \mathcal{J}_{2K}\nabla_{\bar{u}}\bar{\mathcal{H}}_\theta(\bar{u}(t;\mu)) \\ \bar{u}(0;\mu) = \mathcal{E}_\theta(u_{\text{init}}(\mu)), \end{cases}$$

- reduced model is Hamiltonian **by design**.


$u(0;\mu)$
Full Order Model
$\frac{d}{dt}u(t;\mu) = \mathcal{J}_{2N}\nabla_u \mathcal{H}(u(t;\mu))$
$\hat{u}(T;\mu)$
encoder $\mathcal{E}_\theta$
$u \mapsto \mathcal{E}_\theta(u) = \bar{u}$
decoder $\mathcal{D}_\theta$
$\bar{u} \mapsto \mathcal{D}_\theta(\bar{u}) \approx u$
$\bar{u}(0;\mu)$
Reduced Order Model
$\frac{d}{dt}\bar{u}(t;\mu) = \mathcal{J}_{2K}\nabla_{\bar{u}} \bar{\mathcal{H}}_\theta(\bar{u}(t;\mu))$
$\bar{u}(T;\mu)$

- How to learn the reduced dynamics ?

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

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- we add 3 losses:

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

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

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- remark : losses linked to AE inputs/outputs $\rightarrow$ constrain AE-HNN.

- Reduced variables and reduced dynamics constructed separately ($\neq$ PSD) + lack of a symplectic AE,

- solution: **joint training of AE and HNN**,

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- solution: **joint training of AE and HNN**,
- the 4 losses are weighted and coupled during training

$$\min_{\theta} \quad \omega_{\mathrm{AE}}\, \mathcal{L}_{\mathrm{AE}}(\theta) + \omega_{\overline{\mathrm{pred}}}\, \mathcal{L}_{\overline{\mathrm{pred}}}(\theta) + \omega_{\overline{\mathrm{stab}}}\, \mathcal{L}_{\overline{\mathrm{stab}}}(\theta) + \omega_{\mathrm{pred}}\, \mathcal{L}_{\mathrm{pred}}(\theta),$$

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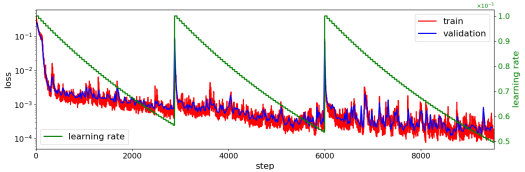
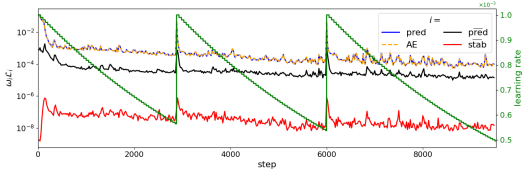
- e.g. $\omega_{\mathrm{AE}} = 1, \quad \omega_{\overline{\mathrm{pred}}} = 10, \quad \omega_{\overline{\mathrm{stab}}} = 1\times10^{-4}, \quad \omega_{\mathrm{pred}} = 1$



(a) Training loss function (blue) and validation loss function (red) history.



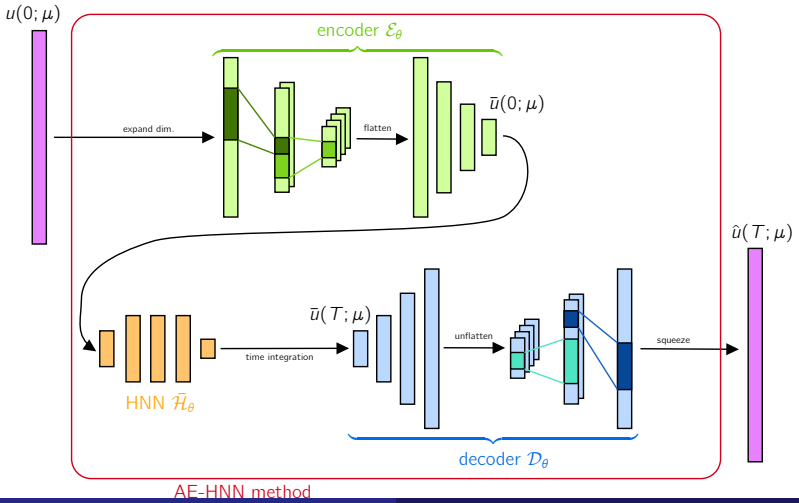
(b) All the weighted loss functions as functions of the training step.

Figure: Example of loss history during a training, overlaid with the evolution of the learning rate (green).

- Key elements on neural networks construction
  - large set of hyperparameters (architecture, layer number, layer size, activation function, Newton solver, etc.)
  - chosen from experience, grid search or random search,
- and training
  - scheduled learning rate, warm restart,
  - AE pretraining, variable loss weights.

- Updated offline stage:
  - build full order model, reduced model, select hyperparameters and a minimal reduced dimension K for correct accuracy,
  - train the AE and HNN together with full order snapshots as dataset.

AE-HNN online stage



- Evolution of a free surface of water on a flat bottom,
- $\chi, \phi : \mathbb{R}^2/(L\mathbb{Z}^2) \times [0, T] \times \Gamma \to \mathbb{R}$ are the perturbation from the equilibrium and the scalar velocity potential, Ω is a periodic square domain on size L,
- $u(x, t; \mu) = (\chi, \phi)^T(x, t; \mu)$

$$\begin{cases} \partial_t \chi + \nabla \cdot ((1 + \chi) \nabla \phi) = 0, \\ \partial_t \phi + \frac{1}{2} |\nabla \phi|^2 + \chi = 0, \end{cases}$$

- with the Hamiltonian

$$\mathcal{H}[\chi, \phi] = \frac{1}{2} \int_{\mathbb{R}^2/(L\mathbb{Z}^2)} \left((1 + \chi) |\nabla \phi|^2 + \chi^2 \right) \, dx.$$

- Domain $\Omega = \mathbb{R}^2/(L\mathbb{Z}^2)$ discretized with a mesh $(x_i, y_j)_{i,j}$ of N nodes,
- discretized state $\chi_h(t;\mu), \phi_h(t;\mu) \in \mathbb{R}^N$, $(\chi_h)_m(t;\mu) = \chi_{i,j}(t;\mu) \approx \chi(x_i, y_j, t;\mu)$

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- with finite differences $\rightarrow$ high dimensional Hamiltonian ODE of solution $u_h = (\chi_h, \phi_h)$

$$\mathcal{H}(\chi_h, \phi_h) = \frac{1}{2}\sum_{i,j=0}^{M-1}\left((1+\chi_{i,j})\left[\left(\frac{\phi_{i+1,j}-\phi_{i-1,j}}{2\Delta x}\right)^2 + \left(\frac{\phi_{i,j+1}-\phi_{i,j-1}}{2\Delta y}\right)^2\right] + \chi_{i,j}^2\right),$$

$$\begin{cases} \dfrac{d}{dt}\chi_h = -D_x\left([1+\chi_h]\odot D_x\phi_h\right) - D_y\left([1+\chi_h]\odot D_y\phi_h\right), \\ \dfrac{d}{dt}\phi_h = -\dfrac{1}{2}\left[(D_x\phi_h)^2 + (D_y\phi_h)^2\right] - \chi_h, \end{cases}$$

with $D_x, D_y \in \mathcal{M}_{2N}(\mathbb{R})$ finite difference matrices,

- cost of $\mathcal{O}(N^2)$ for each $(t,\mu) \in \mathcal{T}\times\Gamma$.

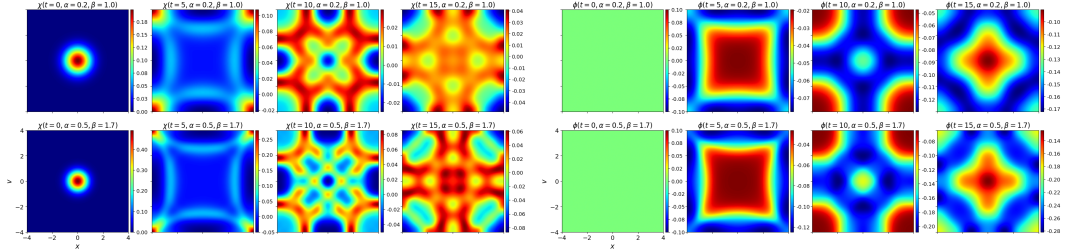
- Discretization with $M = 64$ cells per direction, final time $T = 15$, time step $\Delta t = 1 \times 10^{-3}$, implicit midpoint numerical scheme,

- **parametrized initial condition** with two parameters $\mu = (\alpha, \beta) \in \Gamma = [0.2, 0.5] \times [1, 1.7]$

$$\chi_{\text{init}}(x; \mu) = \alpha \exp\left(-\beta\, x^T x\right), \quad \phi_{\text{init}}(x; \mu) = 0.$$

- Numerical solution with a symplectic scheme

- With a non symplectic scheme



(a) $\chi(t;\mu)$ (b) $\phi(t;\mu)$

Figure: Solutions (χ, ϕ) at different times $t \in \{0, 5, 10, 15\}$ for various parameters $(\alpha, \beta) \in \{(0.2, 1), (0.5, 1.8)\}$.

- $\Gamma = [0.2, 0.5] \times [1, 1.7]$ sampled with 20 snapshots regularly spaced in the segment $[(0.2, 1), (0.5, 1.7)]$,

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- $K = 4$ (from $N = 64^2 = 4096$), chosen minimal while preserving sufficient accuracy,
- inputs $u(t; \mu) = (\chi, \phi)^T(t; \mu) \in \mathbb{R}^{2N}$ are structured $\rightarrow$ **convolutional** autoencoder, $\sim 10^6$ parameters, used once,
- HNN = small dense neural network $\sim 10^4$ parameters / PSD $\sim 10^4$ parameters.

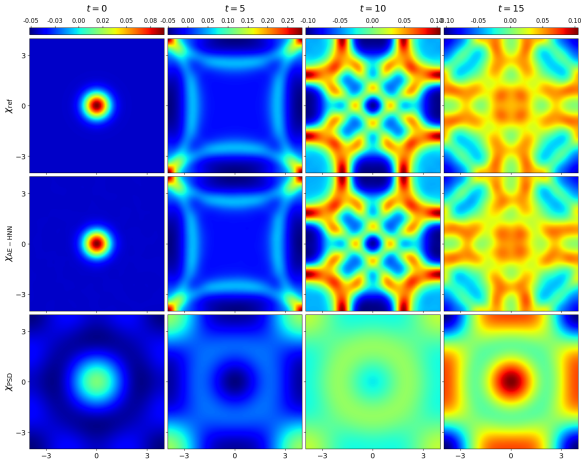

Figure: Solutions $\chi(t;\mu)$ at different times $t \in \{0, 5, 10, 15\}$ on $\mu = (0.51, 1.72) \notin \Gamma$ with $K = 4$, reference solution (top line), AE-HNN solution (middle line) and PSD solution (bottom line).

- Offline time : AE-HNN training $\sim$ 1h / PSD $\sim$ 2-3min (+ snapshots $\sim$ 30min),

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- Limited performance and explainability: different hardware CPU/GPU, different libraries Numpy/Tensorflow, developer expertise.

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- HNN based reduced model : Hamiltonian by design,
- joint AE-HNN training: compensates for the absence of a symplectic AE,

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- weaknesses:
  - increasing K is not enough to systematically improve precision,
  - lack of errors bounds, no clear guarantees of global convergence.

- 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 $\mu \in \Gamma \subset \mathbb{R}^p$, $p > 0$, charge q and mass m,

$$\begin{cases} \partial_t f(t, x, v; \mu) + v\partial_x f(t, x, v; \mu) + \dfrac{q}{m} E(t, x; \mu)\partial_v f(t, x, v; \mu) = 0, \\ \partial_x E(t, x; \mu) = \rho(t, x; \mu), \end{cases}$$

  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 (self-induced) electric field, derives from electric potential $\phi(t, x; \mu)$: $-\partial_x \phi = E$,
- the Poisson equation rewrites

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

- admits an Hamiltonian structure with a Lie-Poisson bracket[6] (not detailed).

[6] Casas et al. 2017.

- 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

$$\begin{cases} \dfrac{d}{dt} x_h(t; \mu) = v_h(t; \mu), \\ \dfrac{d}{dt} v_h(t; \mu) = \dfrac{q}{m} E(x_h(t; \mu); \mu), \end{cases}$$

  where $(x_h)_k = x_k, (v_h)_k = v_k$,

- electric field computed with a mesh : (Hamiltonian) **Particle-In-Cell (PIC) method** from Kraus, Kormann, Morrison, and Sonnendrücker (2017).

- 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.

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- We cannot apply our AE-HNN framework with inputs $u(t;\mu) \in \mathbb{R}^{2N}$: particles are not structured and N too large,

- idea : preprocess $u(t;\mu) \mapsto \tilde{u}(t;\mu) \in \mathbb{R}^{2M}$, $M \ll N$ while keeping the symplectic structure,

- solution: use the **PSD coupled with the AE-HNN method** for a two steps encoder/decoder, Franck, Navoret, Vigon, Côte, and S. (2025).

- Two steps projection

$$\begin{array}{ccccc} \mathbb{R}^{2N} & \longrightarrow & \mathbb{R}^{2M} & \longrightarrow & \mathbb{R}^{2K} \\ u(t;\mu) & \xmapsto{A^+ \cdot} & \tilde{u}(t;\mu) & \xmapsto{\mathcal{E}_\theta} & \bar{u}(t;\mu) \end{array}$$

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

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- first projection = linear operator $A \in \mathcal{M}_{2N,2M}(\mathbb{R})$ from the PSD such that

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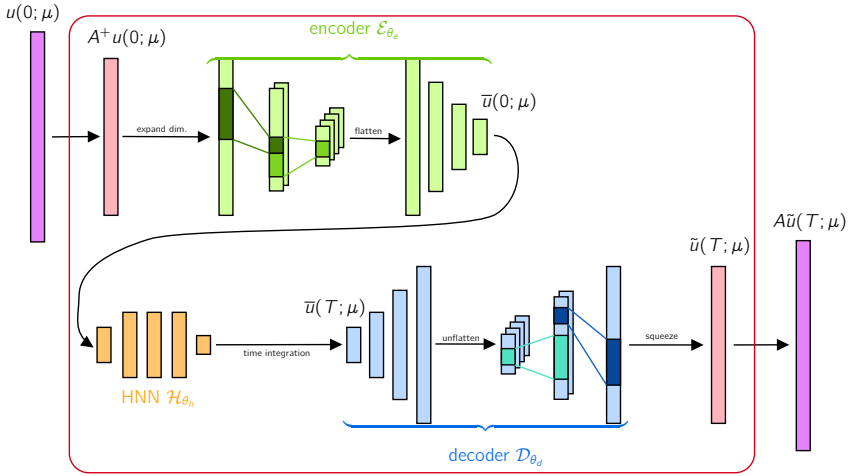
- reduced model captured with a HNN $\bar{\mathcal{H}}_\theta$,
- offline stage: first PSD then AE-HNN training.

PSD-AE-HNN online stage



- Landau damping : parametrized initial condition $\mu = (\alpha, \sigma)^T \in \Gamma \subset \mathbb{R}^2$

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

- $(\alpha, \sigma) \in \Gamma = [0.03, 0.06] \times [0.8, 1]$,
- quantity of interest : damping rate of the electric energy $\frac{1}{2}\|E(x)\|_{L^2}$,
- $N = 10^5$ and $T = 20, \Delta t = 2.5 \times 10^{-3}$,
- $\Gamma = [0.03, 0.06] \times [0.8, 1]$ is sampled over a regular grid of size $8 \times 8 = 64$.

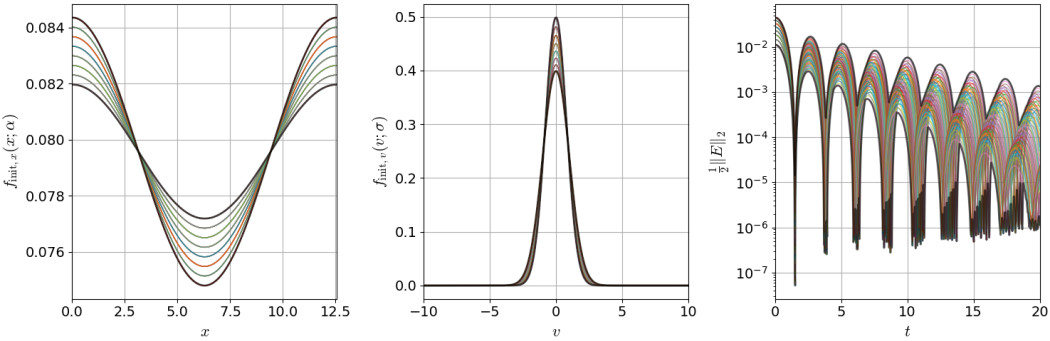


Figure: Initial distribution $f_{\text{init},x}(x;\alpha)$ (left), $f_{\text{init},v}(x;\sigma)$ (middle) and evolution of the electric energy $\frac{1}{2}\|E\|_2\left(x(t;\mu);\mu\right)$ (right) for every $\mu \in \Gamma^{\text{train}}$.

- How to choose $M(= 121)$?
- For example, according to the decay of the snapshots matrix singular values

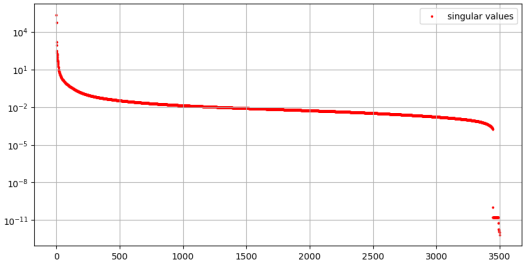


Figure: Singular values $(\sigma_i)_i$ decay.

- in practice:
  - sufficiently small to ensure a fast projection,
  - sufficiently large to provide an intermediate space rich enough for the AE-HNN method.

- How to choose $K(=3=\dim(\Gamma)+1)$? Smallest possible with a sufficient precision,

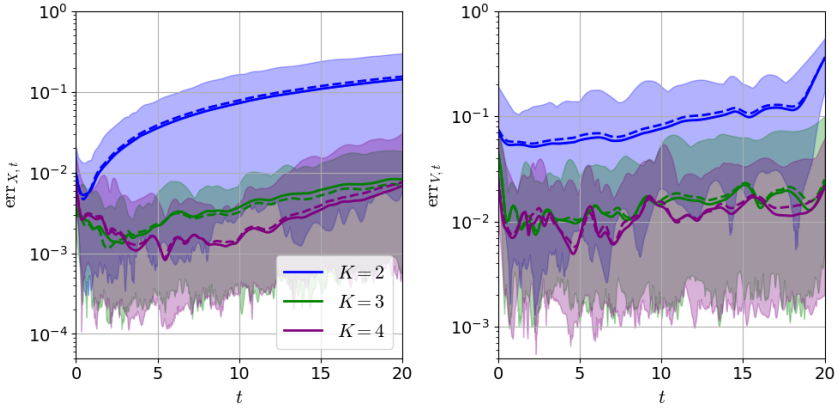


Figure: Mean relative error as a function of time (solid line) for x (left) and v (right), envelopes represents minimum and maximum errors.

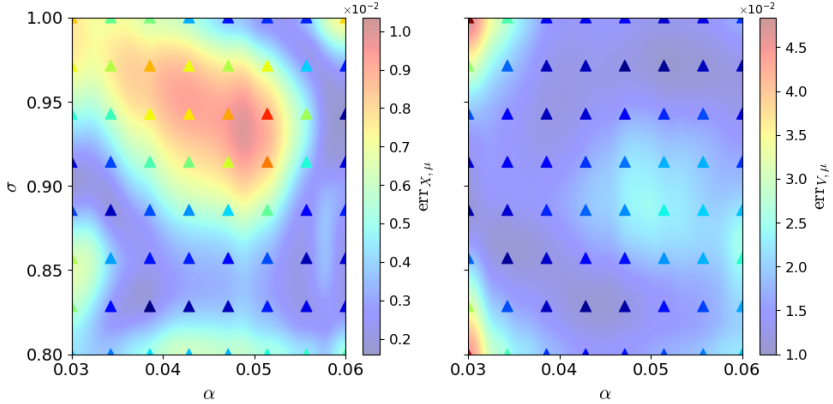


Figure: Errors as a function of the reduction parameters for x (left) and v (right).

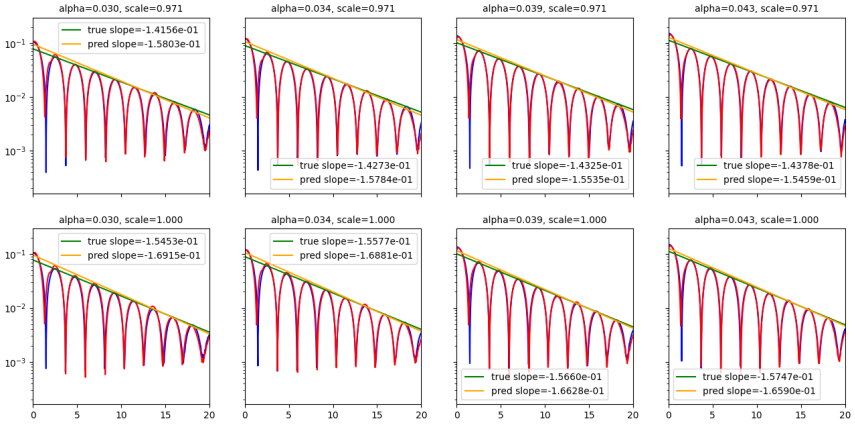


Figure: Some damping rates predictions for various $\mu \in \Gamma$, $K = 3$.

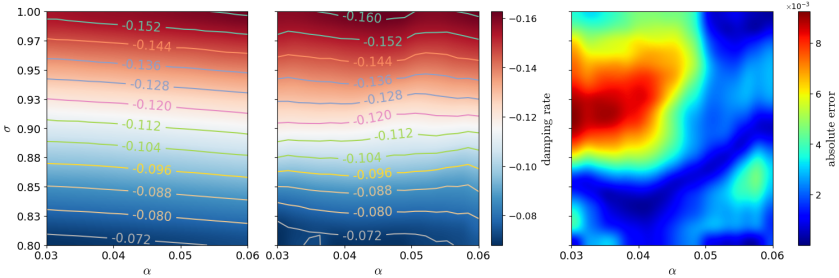


Figure: Electric energy $\frac{1}{2}\|E\|_2\left(x(t;\mu);\mu\right), \mu \in \Gamma$ exponential damping rates of the FOM (left), the ROM (center) and absolute error (right), $K = 3$.

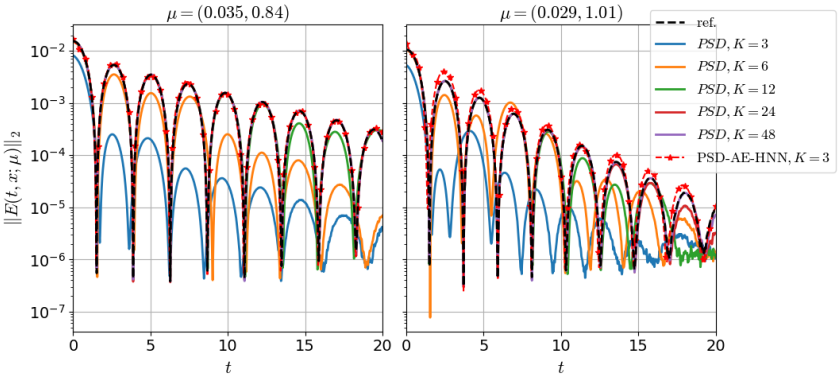


Figure: Electric energies $\frac{1}{2}\|E\|_2\,(x(t;\mu)))$ of the PSD reduced model against our method for $\mu = (0.035, 0.84) \in \Gamma$ (left) and $\mu = (0.029, 1.01) \notin \Gamma$ (right), $K = 3$.

- equivalent precision with $K = 30$ PSD modes.

- small HNN $\sim 10^3$ parameters : competitive,
- offline time :
  - full order PIC : 25s,
  - PIC with comparable accuracy ($N = 7 \times 10^4$) : 11s,
  - PSD-AE-HNN reduced model : 2s,
- Difficult to quantify acceleration: hardware, software, noise, developper expertise.

- What happens if we ignore the Hamiltonian structure ?

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- Learn directly the vector field of the reduced dynamics

$$\frac{d}{dt}\bar{u}(t;\mu) = \bar{\mathcal{F}}_\theta(\bar{u}(t;\mu))$$

- test on the (nonlinear) Landau damping :
  $T = 20 \to 40, \Gamma = [0.46, 0.5] \times [0.96, 1], K = 4$, other parameters unchanged.

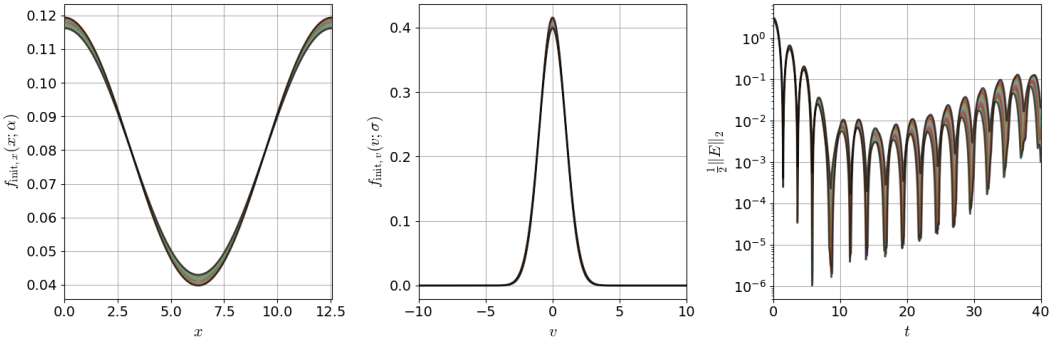

Figure: Initial distribution $f_{\text{init},x}(x;\alpha)$ (left), $f_{\text{init},v}(x;\sigma)$ (middle) and evolution of the electric energy $\frac{1}{2}\|E\|_2\left(x(t;\mu);\mu\right)$ (right) for every $\mu \in \Gamma^{\text{train}}$.

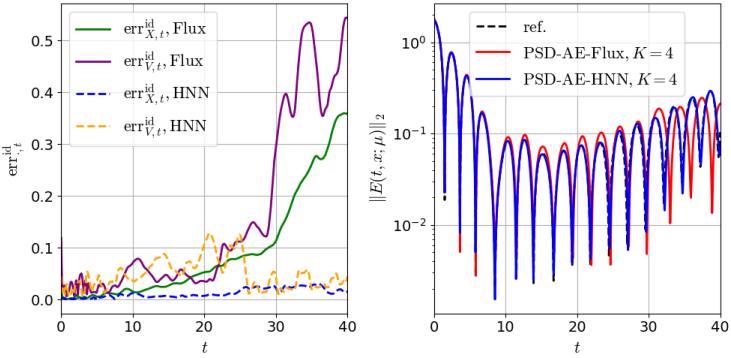

Figure: PSD-AE-Flux prediction for a single test parameter μ compared to the PSD-AE-HNN method. Errors as a function of time (left) and predicted electric energy $\frac{1}{2}\|E\|_2\left(x(t;\mu)\right)$).

- its prediction quickly drifts from the reference.

- Reduction **in the number of particles** of a PIC discretization of the Vlasov Poisson equation,

- two-step mapping combining the PSD and the CAE for an efficient nonlinear compression,

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- two-step mapping combining the PSD and the CAE for an efficient nonlinear compression,
- strong performance in each test case and good computational efficiency,
- same strengths/limitations as the AE-HNN.

Conclusion & perspectives

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[7] Brivio et al. 2024.

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  - no systematic way to improve accuracy, few available results on errors bounds[7].

[7] Brivio et al. 2024.

- Main improvement : systematically enhance the accuracy of the reduced model (currently: manual hyperparameter tuning) with automation, Bayesian optimization, genetic algorithm, sensitivity analysis on hyperparameters ?

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- As of now, we learned canonical Hamiltonian systems: possible extensions to non-canonical Hamiltonian systems[8] or even dissipative systems with port-Hamiltonian[9] or GFINNs[10] frameworks.

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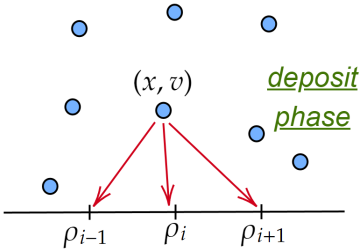
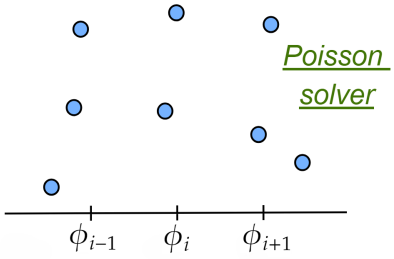


- Compute electric density on the grid

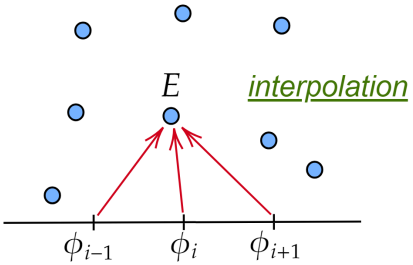
$$\rho^n_{\text{grid}} = \Lambda^0(x(t;\mu))^T \mathbb{1}_N.$$



- Solve Poisson equation

$$\phi^n_{\text{grid}} = L^{-1}\rho^n_{\text{grid}} = L^{-1}\Lambda^0(x(t;\mu))^T \mathbb{1}_N$$

- $L \in \mathcal{M}_{n_x}(\mathbb{R})$ is a discrete Laplace operator.



- Interpolate electric field at particles position

$$E^n = \nabla\Lambda^0(x)\phi^n_{\text{grid}} = \nabla\Lambda^0(x)L^{-1}\Lambda^0(x(t;\mu))^T\mathbb{1}_N.$$