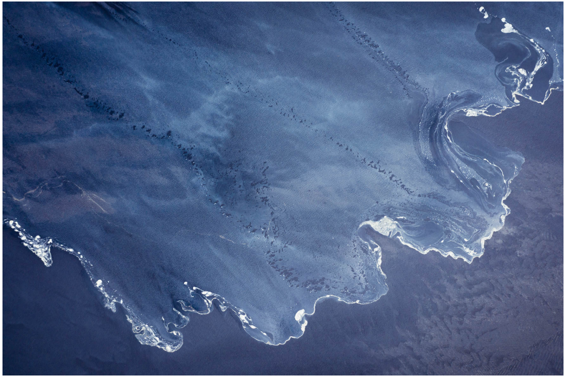
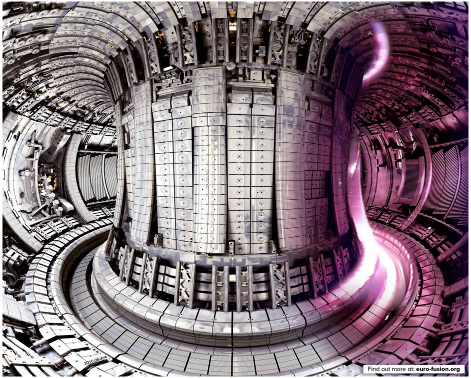
Model order reduction method for Hamiltonian dynamics using deep learning

Raphaël Côte, Emmanuel Franck, Laurent Navoret, Guillaume Steimer and Vincent Vigon

October 21, 2025

Motivation





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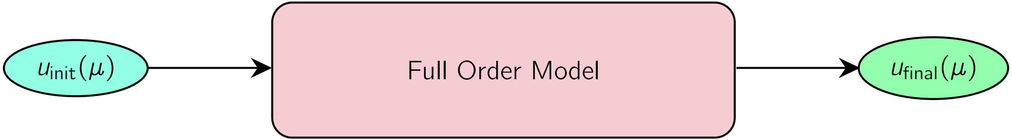
- In many-query or real-time settings, solvers often fail to scale for fast resolution or repeated evaluations across multiple parameters,
- a solution: build a **Hamiltonian** Reduced Order Model (ROM) trading accuracy for computational efficiency, with neural networks,
- efficient over a given time and parameter domain.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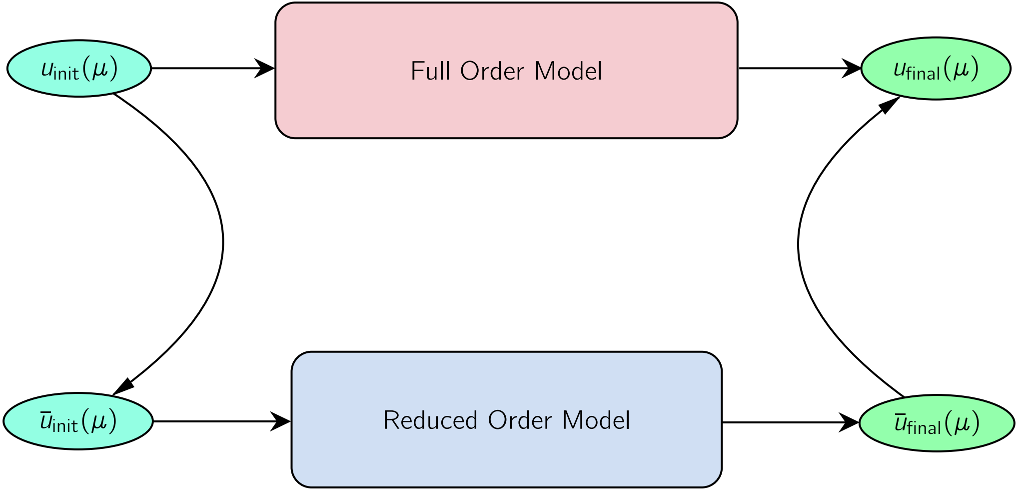
Full Order Model
$u_{\text{final}}(\mu)$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Reduced Order Model
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- Evolution of a field $u(x, t; \mu) \in V$ depending on space $x \in \Omega \subset \mathbb{R}^d$, time $t \in \mathcal{T} = [0, T]$ and 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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- 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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- 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 $\mathcal{H} : \mathbb{R}^{2N} \to \mathbb{R}$

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

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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    with $D\phi_t$ the Jacobian of the flow ϕ_t,
  - time reversibility, volume preservation,
  - etc.,
- provide guarantees for long-time stability, physical relevance.

- Last step : deriving numerical solutions,

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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.

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- We consider the symplectic solution manifold

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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

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

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

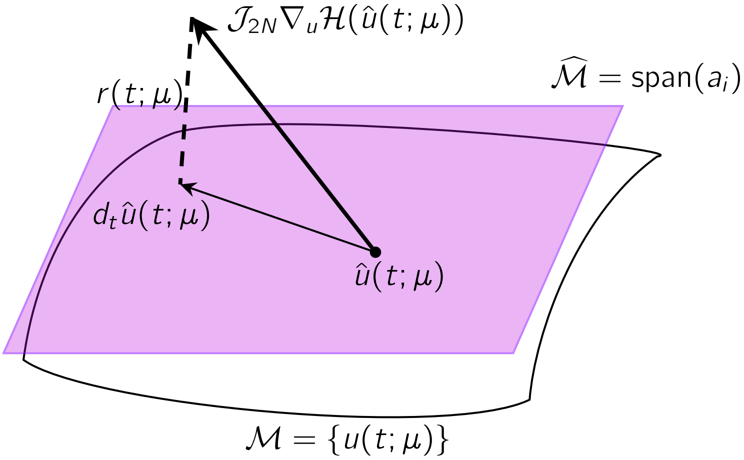
$$A^T \mathcal{J}_{2N} A = \mathcal{J}_{2K}$$

- 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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$r(t;\mu)$
$d_t\hat{u}(t;\mu)$
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$\mathcal{M} = \{u(t;\mu)\}$

- 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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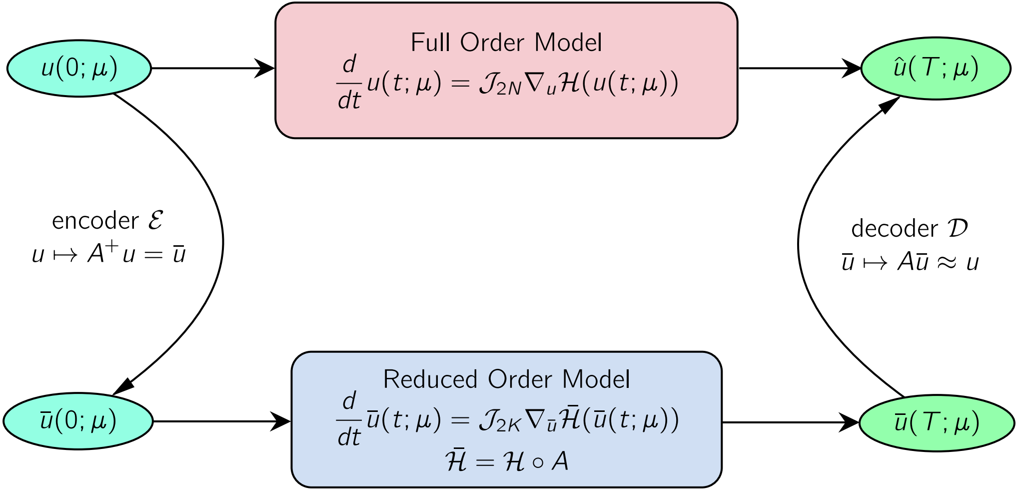
- PSD = symplectic variant of the Proper Orthogonal Decomposition (POD),
- warning: no complexity improvement in general, need for hyper-reduction techniques (Discrete Empirical Interpolation Method (DEIM), etc., not discussed).

Proper Symplectic Decomposition (PSD)



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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.

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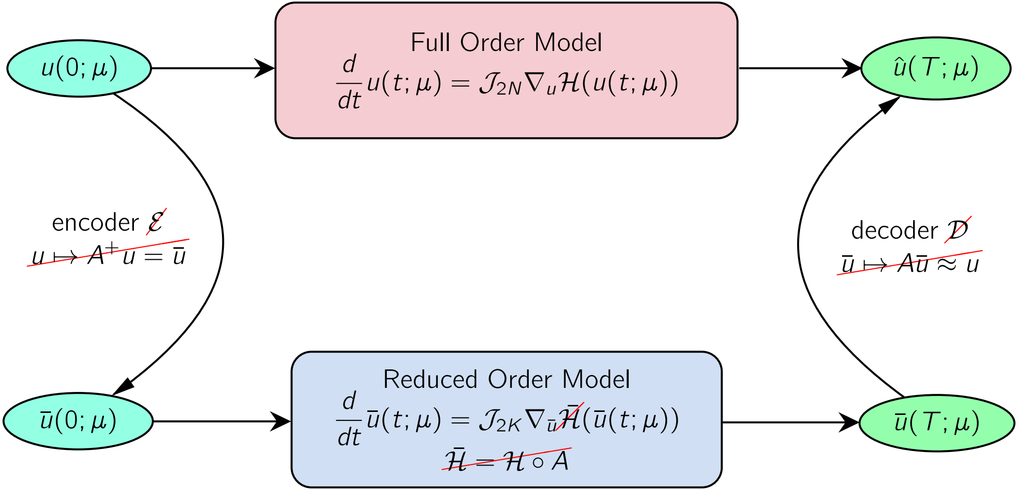
- Offline/online decomposition:
    - **offline stage**: computationally expensive, parametrically independent, performed once (building models, precompute quantities e.g. snapshots, reduced basis A, choose K, etc.),
    - **online stage**: fast computation, done for every new parameter, use offline 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.)[3] 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).

[3] 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 $\mathcal{L}$,

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

  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[4] (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.

[4] Goodfellow et al. 2016.

- What happens to the reduced model ?

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

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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),

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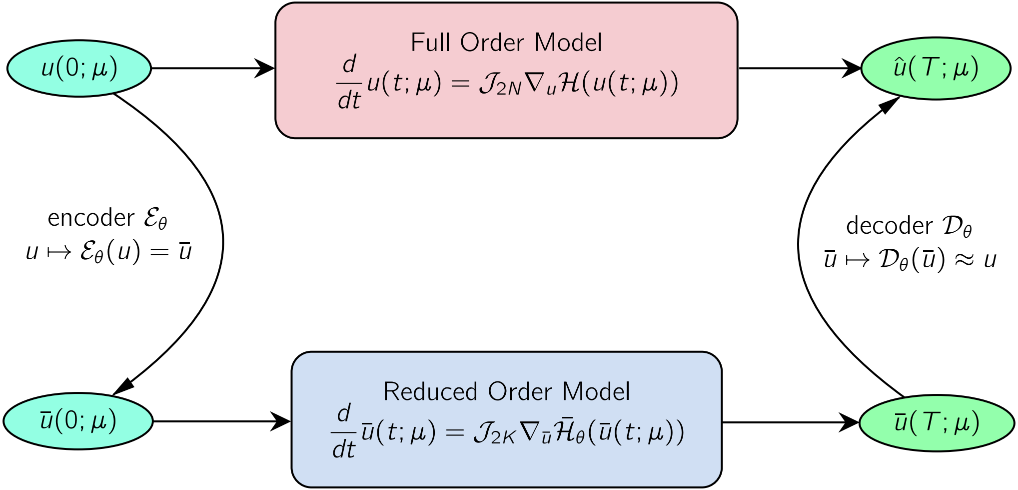
- reduced model is Hamiltonian **by design**.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- prediction operator $\mathcal{P}$ = a step from a symplectic scheme (e.g. midpoint):

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

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

- we add 3 losses:

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

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

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

- How to learn the reduced dynamics ?

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

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- remark : losses linked to AE inputs/outputs $\longrightarrow$ 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

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

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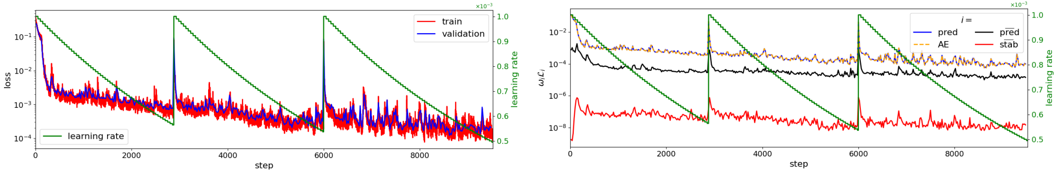
- e.g. $\omega_{\mathrm{AE}} = 1, \quad \omega_{\overline{\mathrm{pred}}} = 10, \quad \omega_{\overline{\mathrm{stab}}} = 1 \times 10^{-4}, \quad \omega_{\mathrm{pred}} = 1$



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

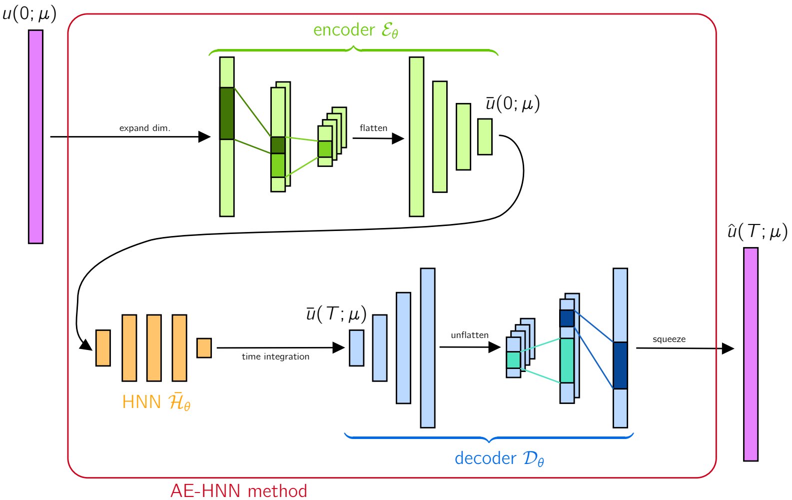
(b) All the weighted loss functions as functions of the training step.

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,
- $u(x, t; \mu) = (\chi, \phi)^T(x, t; \mu)$

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

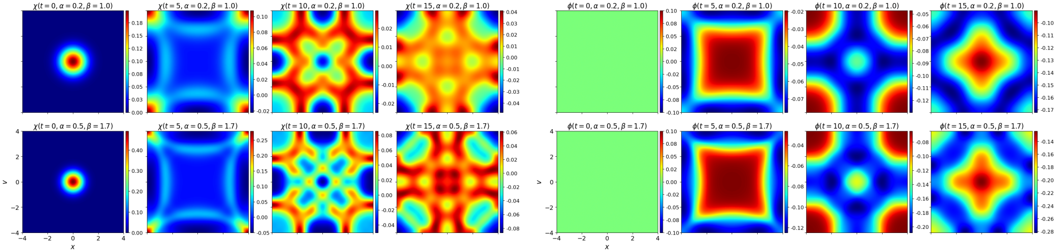
- with the Hamiltonian

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

- Finite differences 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 $\mu = (\alpha, \beta) \in \Gamma = [0.2, 0.5] \times [1, 1.7]$

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



(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.

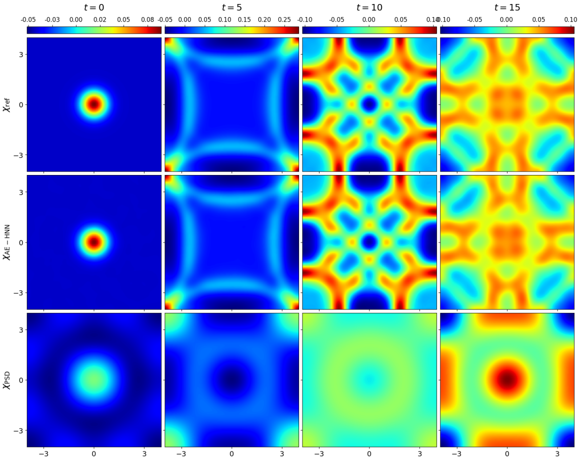

Figure: Solutions $\chi(t; \mu)$ at different times $t \in \{0, 5, 10, 15\}$ on $\mu = (0.51, 1.72) \notin \Gamma$ with $K = 4$, reference solution (top line), AE-HNN solution (middle line) and PSD solution (bottom line).

- 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[5] (not detailed).

[5] 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)

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

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

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

- 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. $K = 4, M = 121$,

- Two steps projection

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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 $A \in \mathcal{M}_{2N,2M}(\mathbb{R})$ from the PSD such that

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

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

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

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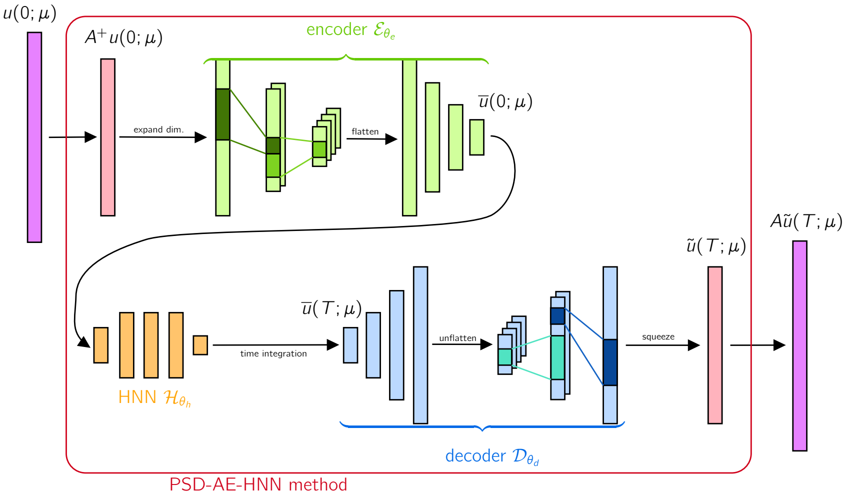
- reduced model captured with a HNN $\bar{\mathcal{H}}_\theta$,
- offline stage: first PSD then AE-HNN training.

PSD-AE-HNN online stage



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

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

- linear case $(\alpha, \sigma) \in \Gamma = [0.03, 0.06] \times [0.8, 1]$,
- 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 $8 \times 8 = 64$.

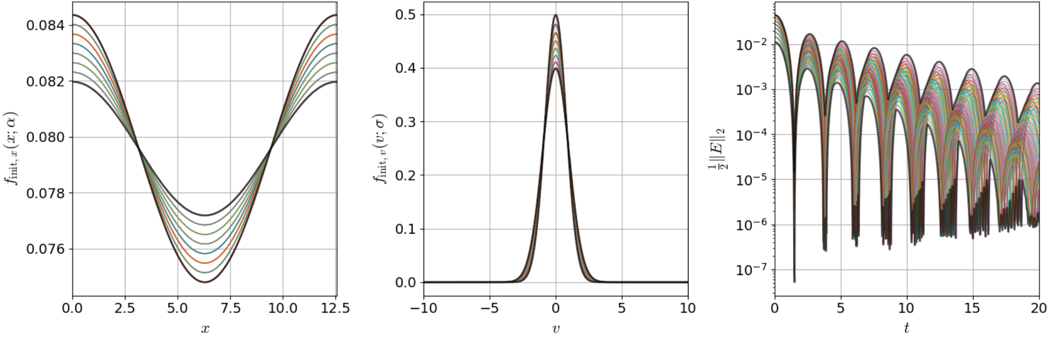


Figure: Initial distribution $f_{\mathrm{init},x}(x;\alpha)$ (left), $f_{\mathrm{init},v}(x;\sigma)$ (middle) and evolution of the electric energy $\frac{1}{2}\|E\|_2\,(x(t;\mu);\mu))$ (right) for every $\mu \in \Gamma^{\mathrm{train}}$.

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

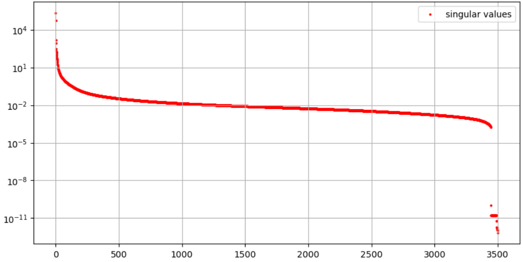


Figure: Singular values $(\sigma_i)_i$ decay.

- 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,

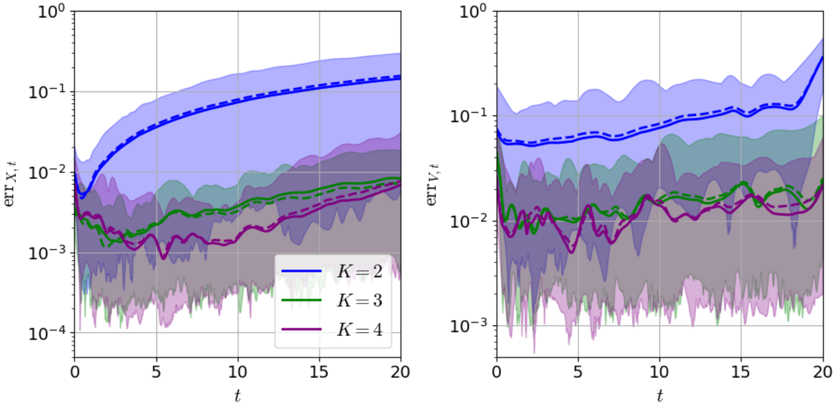


Figure: Mean relative error as a function of time (solid line) for x (left) and v (right), envelopes represents minimum and maximum errors.

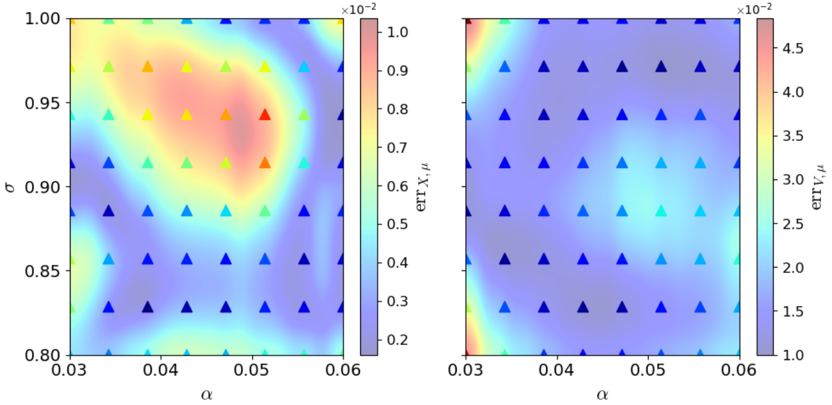


Figure: Errors as a function of the reduction parameters for x (left) and v (right).

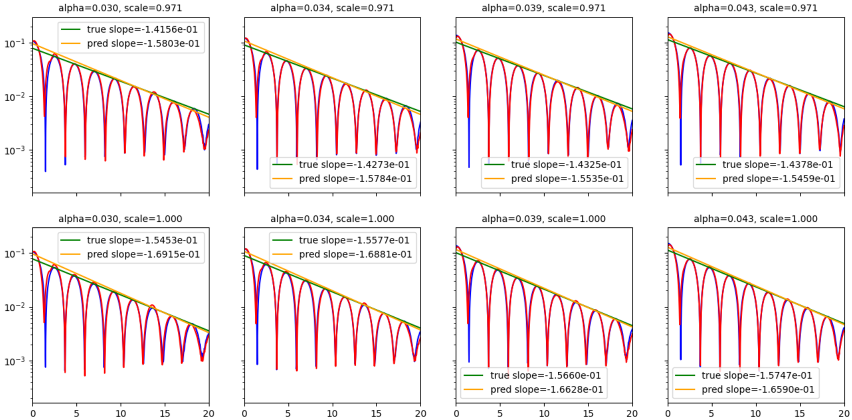


Figure: Some damping rates predictions for various $\mu \in \Gamma$, $K = 3$.

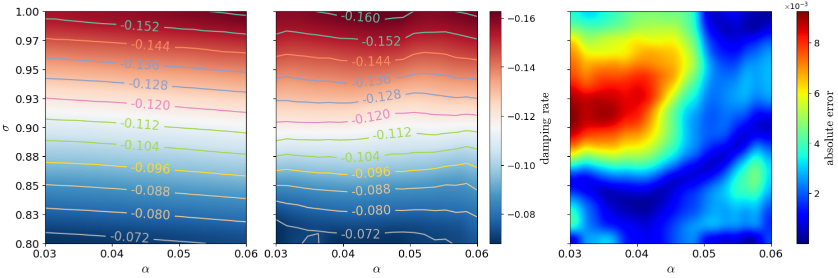


Figure: Electric energy $\frac{1}{2}\|E\|_2\,(x(t;\mu);\mu)\,,\mu\in\Gamma$ exponential damping rates of the FOM (left), the ROM (center) and absolute error (right), $K=3$.

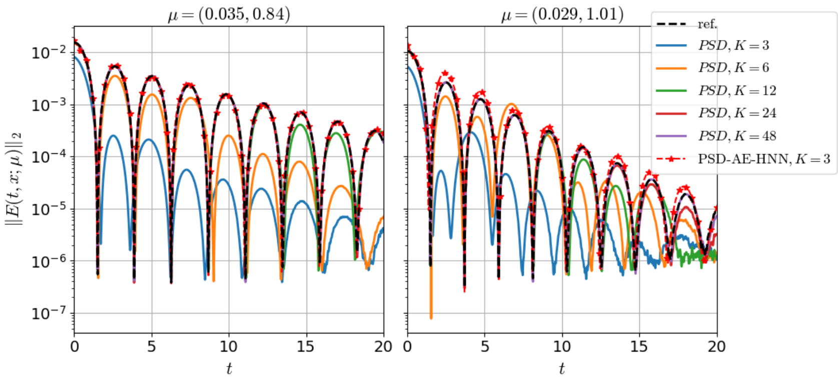
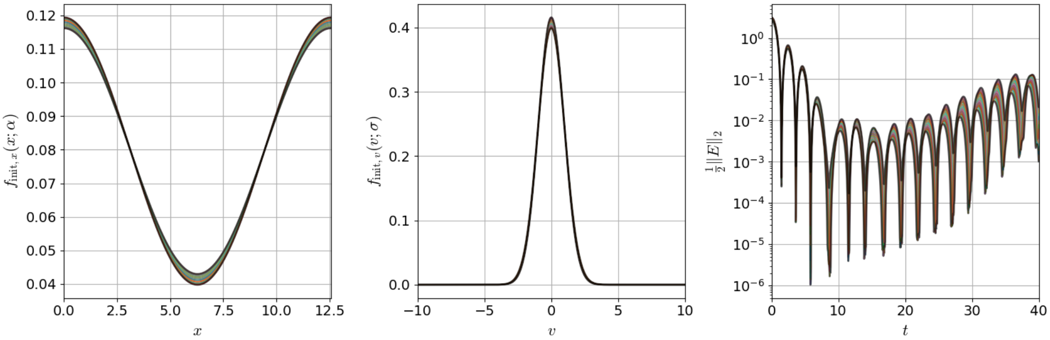


Figure: Electric energies $\frac{1}{2}\|E\|_2\left(x(t;\mu)\right)$ of the PSD reduced model against our method for $\mu = (0.035, 0.84) \in \Gamma$ (left) and $\mu = (0.029, 1.01) \notin \Gamma$ (right), $K = 3$.

- 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.

- Nonlinear case $T = 40, \Gamma = [0.46, 0.5] \times [0.96, 1], K = 4,,$



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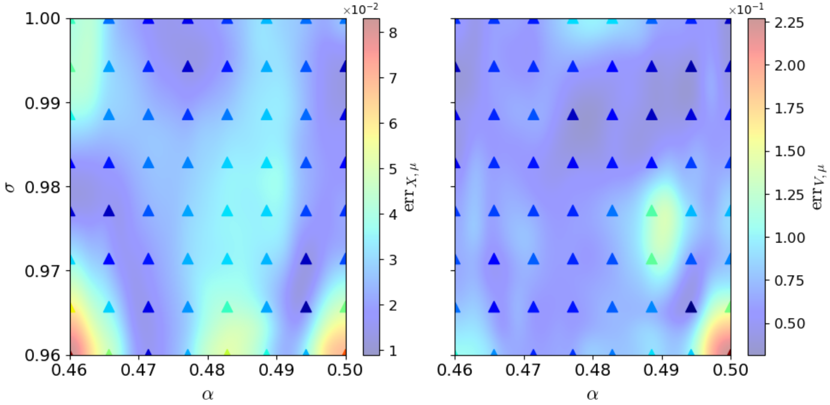
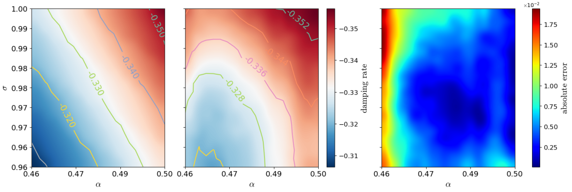
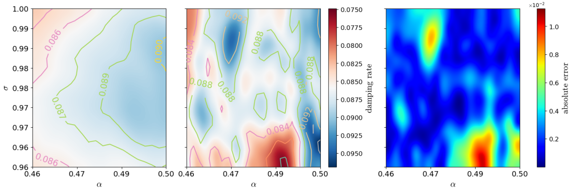


Figure: Errors as a function of the reduction parameters for x (left) and v (right).



(a) Damping rate.



(b) Growth rate.

Figure: Electric energy $\frac{1}{2}\|E\|_2\left(x(t;\mu);\mu\right), \mu \in \Gamma$ exponential damping and growth rates of the FOM (left), the ROM (center) and absolute error (right), $K = 4$.

- What happens if we ignore the Hamiltonian structure ?

- What happens if we ignore the Hamiltonian structure ?

- Learn directly the vector field of the reduced dynamics

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

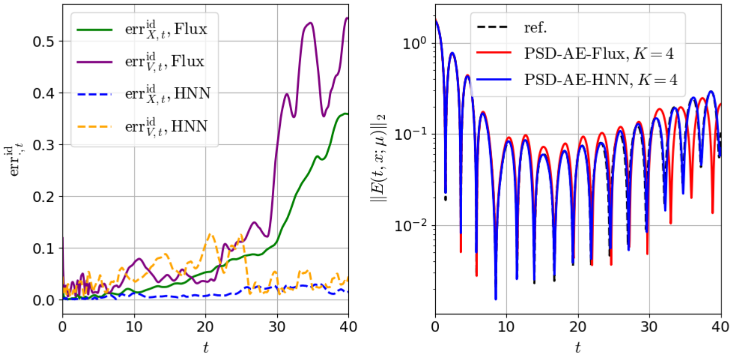


Figure: PSD-AE-Flux prediction for a single test parameter μ compared to the PSD-AE-HNN method. Errors as a function of time (left) and predicted electric energy $\frac{1}{2}\|E\|_2\,(x(t;\mu))$.

- its prediction quickly drifts from the reference.

Conclusion & perspectives

- Generic, non-intrusive and data-driven method
  - PSD preprocess with a symplectic intermediate space,
  - convolutional AE: nonlinear projection, take into account spatial structure,
  - 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.

Conclusion & perspectives

- New test cases, two-dimensional cases,

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

- primary limitation : AE and HNN have potentially competing objectives, design a symplectic AE[6] ?

[6] Brantner and Kraus 2023.

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