Model order reduction of Hamiltonian systems

G. Steimer[1][2]

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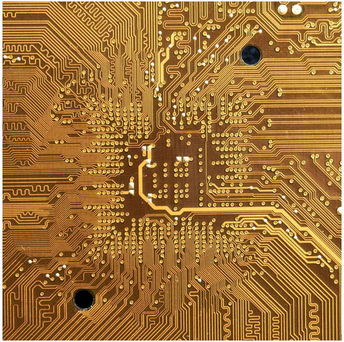
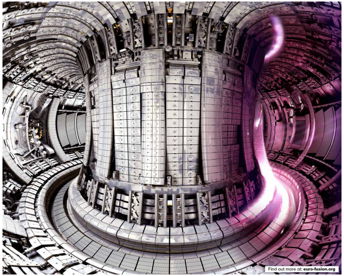
[1] University of Strasbourg, CNRS, Inria, IRMA, F-67000 Strasbourg, France

[2] IRMA, University of Strasbourg, CNRS UMR 7501, 7 rue René Descartes, 67084 Strasbourg, France

Introduction





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  - structure-preserving methods $\to$ implicit solvers,
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  - retains the Hamiltonian structure,
- Shallow-water system as an example throughout the presentation.

- System described by generalized coordinates $q(t;\mu) \in \mathbb{R}^N$, $N \gg 1$ and generalized momenta $p(t;\mu) \in \mathbb{R}^N$ with time $t \in [0, T]$ and some parameters $\mu \in \Xi \subset \mathbb{R}^p$,
- $\mathcal{H} : \mathbb{R}^{2N} \to \mathbb{R}$ is the Hamiltonian, often the total energy of the system,
- q and p are braided together such that

$$\begin{cases} \dfrac{dq(t;\mu)}{dt} = \nabla_p \mathcal{H}(q(t;\mu), p(t;\mu)), \\ \dfrac{dp(t;\mu)}{dt} = -\nabla_q \mathcal{H}(q(t;\mu), p(t;\mu)), \\ q(0;\mu) = q_{\text{init}}(\mu), \\ p(0;\mu) = p_{\text{init}}(\mu), \end{cases}$$

- e.g. $\dot{q} = p, \dot{p} = V(q)$ with V a potential.

- Or equivalently described by the state $u(t;\mu) = (q(t;\mu)\ p(t;\mu))^T \in \mathbb{R}^{2N}$ such that

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

with $\mathcal{J}_{2N} = \begin{pmatrix} 0_N & I_N \\ -I_N & 0_N \end{pmatrix} \in \mathcal{M}_{2N}(\mathbb{R})$ the canonical symplectic matrix.

- Hamiltonian preserved along trajectories by design

$$\begin{aligned}\frac{d\mathcal{H}(q,p)}{dt} &= \nabla_q \mathcal{H}(q,p)\cdot\frac{dq}{dt} + \nabla_p \mathcal{H}(q,p)\cdot\frac{dp}{dt}\\ &= \nabla_q \mathcal{H}(q,p)\cdot\nabla_p \mathcal{H}(q,p) - \nabla_p \mathcal{H}(q,p)\cdot\nabla_q \mathcal{H}(q,p) = 0,\end{aligned}$$

- and many other properties : volume preservation, time reversibility, symplectic flow, etc.,

[1] Hairer, Lubich, and Wanner 2006; Lochak 1995; Michel-Dansac 2023; Franck 2024.

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$$= \nabla_q \mathcal{H}(q,p) \cdot \nabla_p \mathcal{H}(q,p) - \nabla_p \mathcal{H}(q,p) \cdot \nabla_q \mathcal{H}(q,p) = 0,$$

- and many other properties : volume preservation, time reversibility, symplectic flow, etc.,
- This structure has to be preserved during time integration to guarantee long-time stability and physical solutions[1] (not covered) !

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

with $t^n = n\Delta t$.

[1] Hairer, Lubich, and Wanner 2006; Lochak 1995; Michel-Dansac 2023; Franck 2024.

- Some Hamiltonian ODEs come from (Hamiltonian) PDEs of solution a field $u(t, x; \mu)$ on a domain $x \in \Omega$

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

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

- they possess comparable properties[2] (not covered),
- example : the shallow-water system.

[2] Arnold 1978; Marsden and Ratiu 1999.

- Evolution of a free surface of water on a flat bottom,
- $\chi, \phi : \mathbb{R}^2/(L\mathbb{Z}^2) \times [0, T] \times \Xi \to \mathbb{R}$ 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

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

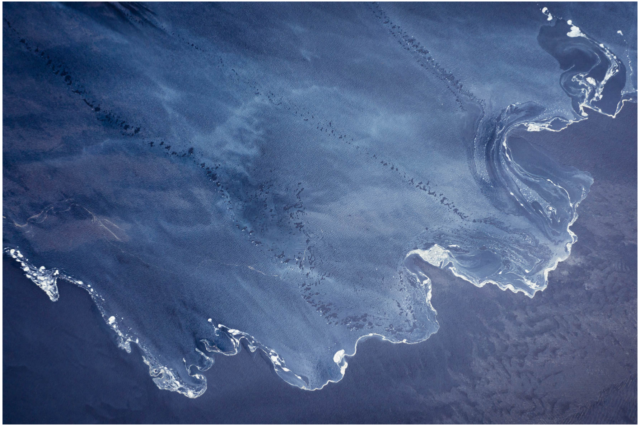

Figure: Tidal flow in Iceland (©Jan Erik Waider)

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

$$\partial_x \phi(x_i, y_j, \dots) \approx \frac{1}{2\Delta x}\left[\phi(x_{i+1}, y_j, \dots) - \phi(x_{i-1}, y_j, \dots)\right], \text{ etc.},$$

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- we obtain a 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,

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with $D_x, D_y \in \mathcal{M}_{2N}(\mathbb{R})$ finite difference matrices,
- cost of $\mathcal{O}(N^2)$ for each $(t,\mu) \in \mathcal{T} \times \Xi$.

Example 1

1 Canonical Hamiltonian ODEs
- Definition & properties
- Our example : Shallow-water system

2 Model Order Reduction (MOR)
- Proper Symplectic Decomposition (PSD)
- Symplectic Discrete Empirical Interpolation Method (SDEIM)

3 Conclusion & perspectives

- Consider the solution manifold

$$\mathcal{M} := \{u(t;\mu) \,|\, (t,\mu) \in [0,T] \times \Xi\} \subset \mathbb{R}^{2N},$$

- is well approximated by a vector subspace $\mathrm{span}(a_i, i \in \{1, \dots, 2K\})$, $K \ll N$

$$\widehat{\mathcal{M}} = \{A\bar{u}(t;\mu) \,|\, (t,\mu) \in [0,T] \times \Xi\}$$

with $A = [a_1|\dots|a_{2K}] \in \mathcal{M}_{2N,2K}(\mathbb{R})$,

- $\bar{u}(t;\mu)$ is the reduced state such that $u(t;\mu) \approx A\bar{u}(t;\mu)$.

- We constraint $\bar{u} \to A\bar{u}\,(\approx u)$ to be a symplectic map

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

- bonus : symplectic inverse A^+ such that $A^+ A = I_{2K}$

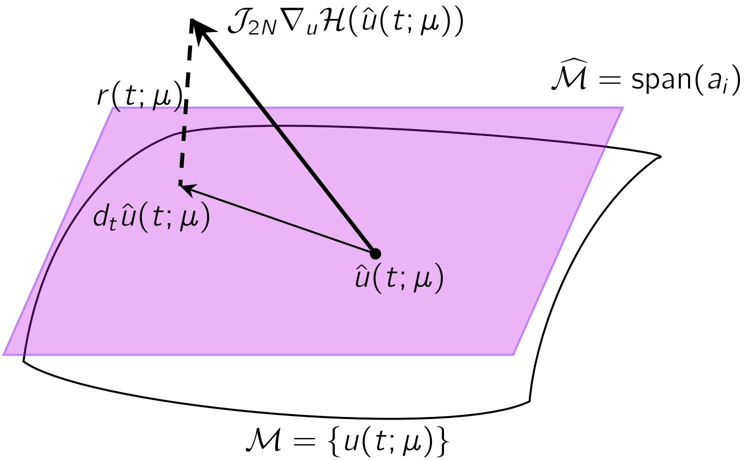
$$A^+ := \mathcal{J}_{2K}^T A^T \mathcal{J}_{2N}$$

- compression/decompress pattern

$$\begin{array}{ccccc} \mathbb{R}^{2N} & \longrightarrow & \mathbb{R}^{2K} & \longrightarrow & \mathbb{R}^{2N} \\ u(t;\mu) & \longmapsto & \bar{u}(t;\mu) := A^+ u(t;\mu) & \longmapsto & A\bar{u}(t;\mu) = \hat{u}(t;\mu) \end{array}$$

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

Symplectic Galerkin projection



- Consider the residual $r(t;\mu)$ of the reconstructed solution

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

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- it vanishes on the reduced subspace $\mathrm{span}(a_i, i \in \{1,\dots,2K\})$ = symplectic Galerkin projection

$$\begin{aligned} 0 &= A^{+} r(t;\mu), \\ &= A^{+}A\frac{d\bar{u}(t;\mu)}{dt} - A^{+}\mathcal{J}_{2N}\nabla_u \mathcal{H}(\hat{u}(t;\mu)), \\ &= \frac{d\bar{u}(t;\mu)}{t} - \mathcal{J}_{2K}\nabla_{\bar{u}} \mathcal{H}(A\bar{u}(t;\mu)), \end{aligned}$$

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$$\begin{aligned} 0 &= A^+ r(t;\mu), \\ &= A^+ A\frac{d\bar{u}(t;\mu)}{dt} - A^+\mathcal{J}_{2N}\nabla_u\mathcal{H}(\hat{u}(t;\mu)), \\ &= \frac{d\bar{u}(t;\mu)}{t} - \mathcal{J}_{2K}\nabla_{\bar{u}}\mathcal{H}(A\bar{u}(t;\mu)), \end{aligned}$$

- so that the reduced dynamics is still Hamiltonian

$$\frac{d\bar{u}(t;\mu)}{dt} = \mathcal{J}_{2K}\nabla_{\bar{u}}\bar{\mathcal{H}}(\bar{u}(t;\mu)) \text{ with } \bar{\mathcal{H}} := \mathcal{H}\circ A.$$

- How to build $A \approx \text{span}(a_i, i \in \{1, \dots, 2K\})$? The solution manifold $\mathcal{M}$ is often unknown !

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- On snapshots U of full order solution

$$U = \left[u(t_1; \mu_1) \quad \dots \quad u(t_s; \mu_s) \right] \in \mathcal{M}_{2N,s}(\mathbb{R}),$$

we minimize the reconstruction error

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

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- approached solution computed via Singular Value Decomposition (SVD) = Proper Symplectic Decomposition (PSD)[3].

[3] Peng and Mohseni 2016.

- In practice, offline/online decomposition for efficient computation,
    - offline : build full model and reduced model, precompute quantities (snapshots, matrix A, etc.), parameter independent, done once,
    - online : quickly solve the reduced model with new parameters, using precomputed quantities, done for every new parameter,
- K chosen as a tradeoff between speed and precision.

- We set $T = 20$ and parametrize the initial condition with $\mu = (\alpha\ \beta)^T = [0.2, 0.5] \times [1, 1.7]$ given by

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

- we sample $p = 20$ snapshots and we build A offline,

- we test on a new parameter $\mu = (0.51\ 1.72)^T$.

Example 2

- The reduced model is

$$\frac{d\bar{u}(t;\mu)}{dt} = \mathcal{J}_{2K}\nabla_{\bar{u}}\bar{\mathcal{H}}(\bar{u}(t;\mu)) \text{ with } \bar{\mathcal{H}} := \mathcal{H} \circ A.$$

[4] Peng and Mohseni 2016.

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- the field $\nabla_{\bar{u}} \bar{\mathcal{H}}$ depends on $\nabla_u \mathcal{H} \rightarrow$ no numerical cost improvement !

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- the field $\nabla_{\bar{u}}\bar{\mathcal{H}}$ depends on $\nabla_{u}\mathcal{H}$ $\rightarrow$ no numerical cost improvement !

- idea : approximate $\nabla_{u}\mathcal{H}$ with a PSD-like method = Symplectic Discrete Empirical Interpolation Method (SDEIM)[4].

[4] Peng and Mohseni 2016.

- split $\nabla_u \mathcal{H}$ into a linear part $D \in \mathcal{M}_{2N}(\mathbb{R})$ and a non-linear part $h_N : \mathbb{R}^{2N} \to \mathbb{R}^{2N}$

$$\nabla_u \mathcal{H}(u) = Du + h_N(u)$$

- the reduced model is

$$\frac{d}{dt}\bar{u} = J_{2K} A^T \nabla_{A\bar{u}} \mathcal{H}(A\bar{u}) = J_{2K} (A^T DA)\bar{u} + J_{2K} A^T h_N(A\bar{u})$$

- linear part : $\bar{D} = A^T DA$ is computed offline $\to$ online cost of $\mathcal{O}(K)$,

- non-linear part : $\psi_N = A^T \circ h_N \circ A$ of cost $\mathcal{O}(N^2)$.

- We form a snapshot matrix of ψ_N

$$U_\psi = \left(\psi_N \left[u(t_1; \mu_1) \right] \quad \dots \quad \psi_N \left[u(t_s; \mu_s) \right] \right) \in \mathcal{M}_{2N,s}(\mathbb{R}),$$

- and build an SVD approximation

$$\psi_N(u) \approx A_\psi \widehat{\psi}(u),$$

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$$\psi_N(u) \approx A_\psi \widehat{\psi}(u),$$

- this system is over-determined : unique solution $\widehat{\psi}(u)$ on $m \ll N$ spatial indices $\{i_1, \dots, i_m\}$ (computed via an algorithm, not discussed),

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- $\widehat{\psi}(u)$ uniquely determined with

$$P^T \psi_N(u) = \left(P^T A_\psi\right) \widehat{\psi}(u)$$

with the selection matrix $P = \begin{pmatrix} e_{i_1} & \dots & e_{i_m} \end{pmatrix}$, e_i is the i-th column of the identity matrix.

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$$\psi_N(u) \approx A_\psi \widehat{\psi}(u) = \underbrace{A_\psi \left(P^T A_\psi\right)^{-1}}_{W} P^T \psi_N(u),$$

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- and the reduced model is

$$\frac{d}{dt}\bar{u} = J_{2K} A^T \nabla_{A\bar{u}} \mathcal{H}(A\bar{u}) = J_{2K} \bar{D}\bar{u} + J_{2K} W h_m(A\bar{u})$$

  with W computed offline,

- $h_m = P^T \circ h_N \circ A$ = nonlinear part of the Hamiltonian gradient evaluated on $m \ll N$ points : the cost does not depend on N anymore !

- On the shallow-water system

$$\nabla_u \mathcal{H}(u) = \begin{pmatrix} \frac{1}{2}\left[(D_x\phi)^2 + (D_y\phi)^2\right] + \chi \\ -D_x\left([1+\chi]\odot D_x\phi\right) - D_y\left([1+\chi]\odot D_y\phi\right) \end{pmatrix},$$

$$= \begin{pmatrix} 0 & -D_x^2 - D_y^2 \\ -I & 0 \end{pmatrix} u + J_{2N} \underbrace{\begin{pmatrix} \frac{1}{2}\left[(D_x\phi)^2 + (D_y\phi)^2\right] \\ -D_x\left(\chi\odot D_x\phi\right) - D_y\left(\chi\odot D_x\phi\right) \end{pmatrix}}_{h_N},$$

- $h_m = h_m = P^T \circ h_N \circ A$ is essentially to find an effective way to compute

$$P^T D_x A\, u$$

can be difficult in practice !

- We set $K = 20$ and $m = 60$.

Example 3

- The Proper Symplectic Decomposition (PSD) is a data-driven projection-based model order reduction technique,
- efficiency guaranteed by offline/online decomposition,
- limited to linear and quasi-linear regimes (SDEIM strategy),
- not competitive in strongly nonlinear regimes : alternative strategies based on neural networks[5] ?

[5] Côte et al. 2025; Franck et al. 2025.

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