Data Assimilation of Hamiltonian Dynamics

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Workshop on Reduced Order and Surrogate Modelling

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Joint work with

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- **Dynamical Approximation and Sensor Placement for Filtering Problems**, SISC 2025. [MPV25]
- **Data Assimilation of Hamiltonian Flows**, In Progress.

Agenda

1. **Hamiltonian Dynamics**
2. Data Assimilation
3. Reconstruction Algorithm and Error
4. Dynamical Sensor Placement
5. Numerical Tests

Hamiltonian Dynamics on a Hilbert Space

- **Hamiltonian system** $(M, \mathcal{H}, \Omega)$:
  - $M = (V, \langle \cdot, \cdot \rangle_V)$ Hilbert space. Variable: $v = (v_1, v_2) \in V$.
  - $\Omega(u, v) \coloneqq \langle u, \mathcal{J}(v) \rangle_V$ for any $u, v \in V$ and $\mathcal{J}((v_1, v_2)) = (v_2, -v_1)$.
  - $\mathcal{H} : V \to \mathbb{R}$ Hamiltonian

- **Dynamics:**

$$\begin{cases} \dot{u}(t) & = \mathcal{J}(\mathrm{grad}_V \, \mathcal{H}(u(t))) \in V, \quad \forall\, t > 0 \\ u(0) & = u_0 \end{cases}$$

where

$$\mathrm{grad}_V \, \mathcal{H}(u) \in V \quad \xleftrightarrow{\text{Riesz}} \quad (D\mathcal{H})_u \in V'$$

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where

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- **Parametric Hamiltonian:** $\mathcal{H} = \mathcal{H}_\theta \rightsquigarrow u(\theta)$ for $\theta \in \Theta$ and

$$\begin{aligned} \mathcal{M} &= \{u(\theta) \,:\, \theta \in \Theta\} & \subset \mathcal{C}(\mathbb{R}_+; V) \\ \mathcal{M}(t) &= \{u(\theta)(t, \cdot) \,:\, \theta \in \Theta\} & \subset V \end{aligned}$$

- Preservation of the Hamiltonian along trajectories:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(u(\theta)(t,\cdot),\theta) = 0, \quad \forall\, t > 0,\ \forall\, \theta \in \Theta.$$

- The flow map $F_t(u_0) = u(t)$ is a symplectic transformation:

$$(F_t)^*\Omega = \Omega$$

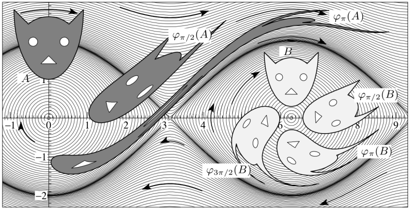

Figure: Volume preservation of the flow [HWL10].

Example: Schrödinger Equation in $\mathbb{R}^d$

$V = L^2(\mathbb{R}^d) \times L^2(\mathbb{R}^d)$

$$\mathcal{H}(u) = \begin{cases} \frac{1}{2}\left(\sum_{i=1}^{d} \|\partial_{x_i} u\|_V^2\right) - \frac{\varepsilon}{4}\|u\|_V^4, & \forall\, u \in \mathrm{dom}(\mathcal{H}) := H_0^1(\mathbb{R}^d)^2 \cap L^2(\mathbb{R}^d)^2, \\ +\infty & \forall\, u \in V \setminus \mathrm{dom}(\mathcal{H}). \end{cases}$$

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For all $u \in H^2(\mathbb{R}^d)^2 \cap L^4(\mathbb{R}^d)^2 \cap \mathrm{dom}(\mathcal{H})$,

$$\begin{aligned} (D\mathcal{H})_u(v) &= \int_D \left(-\Delta u_1 - \varepsilon u_1(u_1^2 + u_2^2)\right) v_1 + \left(-\Delta u_2 - \varepsilon u_2(u_2^2 + u_1^2)\right) v_2, \quad \forall\, v \in V, \\ &= \langle \mathrm{grad}_V\, \mathcal{H}(u), v\rangle_V \end{aligned}$$

so

$$\mathrm{grad}_V\, \mathcal{H}(u) = \begin{pmatrix} -\Delta u_1 - \varepsilon u_1(u_1^2 + u_2^2) \\ -\Delta u_2 - \varepsilon u_2(u_2^2 + u_1^2) \end{pmatrix}$$

The associated Hamiltonian flow is thus: Find $u(t) = (u_1, u_2)(t)$ s.t.

$$\begin{cases} \dot{u}_1 &= -\Delta u_2 - \varepsilon(u_1^2 + u_2^2)u_2, \\ \dot{u}_2 &= +\Delta u_1 + \varepsilon(u_1^2 + u_2^2)u_1. \end{cases}$$

Agenda

The Filtering Problem

- **Task:** For an **unknown** $\theta^\dagger \in \Theta$, reconstruct

$$u^\dagger = u(\theta^\dagger) \in \mathcal{C}(\mathbb{R}_+, V)$$

given observations of the velocity $\dot{u}^\dagger$.

- **Velocity Observations:** For every $t \in \mathbb{R}_+$,

$$\dot{z}_i(\tau) = \ell_i(\dot{u}^\dagger(\tau)) = \langle \omega_i, \dot{u}^\dagger(\tau) \rangle_V, \quad 0 \le \tau \le t, \; i = 1, \dots, m,$$

$$\Leftrightarrow \quad \dot{\omega}(\tau) = P_{\mathrm{W}_m} \dot{u}^\dagger(\tau)$$

where

  - $\ell_i \in V'$ indep. linear functionals (model sensor response)
  - $\omega_i \in V$ Riesz representers.
  - $\mathrm{W}_m := \mathrm{span}\{\omega_1, \dots, \omega_m\} \subset V$ observation space.

- **Example:** $V = L^2(\mathbb{R}^d)$,

$$\ell_i(v) = \int_{\mathbb{R}^d} \underbrace{\frac{1}{(2\pi)^{d/2}\sigma} e^{-\frac{||x-x_i||^2}{\sigma^2}}}_{=\omega_i = g(x_i,\sigma)} v(x)\mathrm{d}x = g(x_i, \sigma) * v$$

Agenda

Symplectic Dynamical Approximation

For every $t > 0$, we want to approximate:

- the true state:

$$u^\dagger(t) \approx \sum_{i=1}^{2n} a_i v_i \ \in \ V_{2n}$$

- the family of parametric solutions:

$$u(\theta)(t,\cdot) \approx \sum_{i=1}^{2n} c_i(\theta) v_i \ \in \ V_{2n}.$$

We search for:

1. $V_{2n} = \mathrm{span}\{v_1, \dots, v_{2n}\} \ \subset \ V$,
2. $a \in \mathbb{R}^{2n}$
3. $c(\theta) \in \mathbb{R}^{2n} \ \to \ c \in L^2(\Theta, \mathbb{R}^{2n})$

Symplectic Dynamical Approximation

For every $t > 0$, we want to dynamically approximate:

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$$u^\dagger(t) \approx \sum_{i=1}^{2n} a_i(t) v_i(t) \ \in \ V_{2n}(t)$$

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3. $c(t)(\theta) \in \mathbb{R}^{2n} \ \to \ c(t) \in L^2(\Theta, \mathbb{R}^{2n})$

Symplectic Dynamical Approximation

We re-write the approximation in terms of a decoder mapping

$$\begin{aligned} \varphi : \Gamma &\to V \times L^2(\Theta; V) \\ \gamma &\mapsto \varphi(\gamma) = (\varphi_1(\gamma), \varphi_2(\gamma)) \end{aligned}$$

with:

- Input parameters:

$$\gamma = (a, c, \mathcal{V}) \in \Gamma := \mathbb{R}^{2n} \times L^2(\Theta; \mathbb{R}^{2n}) \times \mathcal{S}_{2n}$$

  where $\mathcal{V} = \{v_1, \dots, v_{2n}\}$

- Output: For every $\gamma = (a, c, \mathcal{V}) \in \Gamma$,

$$\varphi(\gamma) := (\varphi_1(\gamma), \varphi_2(\gamma)), \quad \text{where} \begin{cases} \varphi_1(\gamma) & = \sum_{i=1}^{2n} a_i v_i \ \in V, \\ \varphi_2(\gamma) & = \sum_{i=1}^{2n} c_i v_i \ \in L^2(\Theta; V). \end{cases}$$

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  where $\mathcal{V} = \{v_1, \dots, v_{2n}\}$ and

$$\mathcal{S}_{2n} := \{\mathcal{V} = \{v_i\}_{i=1}^{2n} \in V^{2n} \, : \, \langle v_i, v_j \rangle_V = \delta_{i,j} \;\text{ and }\; \Omega(v_i, v_j) = (J_{2n})_{i,j}\}$$

  is the set of all $2n$-tuple of orthosymplectic functions where

$$J_{2n} := \begin{bmatrix} 0_n & I_n \\ -I_n & 0_n \end{bmatrix}.$$

- Output: For every $\gamma = (a, c, \mathcal{V}) \in \Gamma$,

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Symplectic Dynamical Approximation

The differential of φ at a point $\gamma = (a, c, \mathcal{V}) \in \Gamma$ reads

$$(D\varphi)_\gamma : \mathrm{T}_\gamma\Gamma \to V \times L^2(\Theta, V)$$

$$\delta\gamma = (\delta a, \delta c, \delta\mathcal{V}) \mapsto \left(\sum_{i=1}^{2n} \left(\delta a_i v_i + a_i \delta v_i\right), \sum_{i=1}^{2n} \left(\delta c_i v_i + c_i \delta v_i\right) \right)$$

where

$$\mathrm{T}_\gamma\Gamma = \mathbb{R}^{2n} \times L^2(\Theta, \mathbb{R}^{2n}) \times \mathrm{T}_\mathcal{V}\mathcal{S}_{2n}.$$

and

$$\mathrm{T}_\mathcal{V}\mathcal{S}_{2n} = \{\delta\mathcal{V} = (\delta v_i)_{i=1}^{2n} \in V^{2n} \ : \langle \delta v_i, v_j\rangle_V + \langle v_i, \delta v_j\rangle_V = 0 \ \text{ and } \ \Omega(\delta v_i, v_j) + \Omega(v_i, \delta v_j) = 0\}.$$

Theorem 1

There are "convenient" subsets $\widetilde{\Gamma} \subset \Gamma$ and $\widetilde{\mathrm{T}_\gamma\Gamma} \subset \mathrm{T}_\gamma\Gamma$ for which

$$(D\varphi)_\gamma : \widetilde{\mathrm{T}_\gamma\Gamma} \to V \times L^2(\Theta, V)$$

is injective.

Filtering Scheme

Given the observations

$$\dot{z}(t) = \ell(\dot{u}^\dagger(t)) \ \in \mathbb{R}^m,$$

we search for a curve $\gamma : \mathbb{R}_+ \to \Gamma$ such that

$$\dot{u}^\dagger(t) \approx \frac{\mathrm{d}}{\mathrm{d}t}\varphi_1(\gamma(t)) = (D\varphi_1)_{\gamma(t)}(\dot{\gamma}(t))$$
$$\dot{u}(\theta)(t,\cdot) \approx \frac{\mathrm{d}}{\mathrm{d}t}\varphi_2(\gamma(t))(\theta) = (D\varphi_2)_{\gamma(t)}(\dot{\gamma}(t))(\theta), \quad \forall\,\theta \in \Theta.$$

Filtering Scheme

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For this, we solve for every $t > 0$,

$$\dot{\gamma}(t) \in \operatorname*{arg\,min}_{\delta\gamma \in \mathrm{T}_{\gamma(t)}\Gamma} \frac{1}{2}\left| \dot{z}(t) - \ell\left(\frac{\mathrm{d}}{\mathrm{d}t}\varphi_1(\gamma(t)) \right) \right|_Z^2 + \frac{\lambda}{2}\int_\Theta \left\| \underbrace{\mathcal{J}(\mathrm{grad}_\Omega\, \mathcal{H}_\theta(f_2(\theta))}_{=\dot{u}(\theta)(t,\cdot)} - \frac{\mathrm{d}}{\mathrm{d}t}\varphi_2(\gamma(t))(\theta) \right\|_V^2 \mu(\mathrm{d}\theta).$$

Remark: $\mu \in \mathcal{P}_2(\Theta)$ is an extra degree of freedom.

Filtering Scheme

Necessary optimality conditions lead to an ODE of the form

$$\dot{\gamma}(t) = f(\gamma(t))$$

which we then integrate in time (using symplectic schemes) $\rightsquigarrow \gamma(t) \rightsquigarrow \varphi(\gamma(t))$.

Theorem 2

- *The ODE is well-posed*
  (when working on the "convenient" subsets $\widetilde{\Gamma} \subset \Gamma$ and $\widetilde{\mathrm{T}_\gamma \Gamma} \subset \mathrm{T}_\gamma \Gamma$).
- $F_t(u_0) = \varphi(\gamma(t))$ *is a symplectic flow map.*

Remark: We reconstruct $u^\dagger = u(\theta^\dagger)$ without estimating $\theta^\dagger$. We can estimate it a posteriori by residual minimization.

Error Analysis (with optimal $|\cdot|_Z$)

Theorem 3

Let

$$e(t) := \|u^\dagger(t) - \varphi_1(\theta(t))\|_V$$

It holds that

$$e(t) \lesssim$$

$$e(0)\exp\left(\frac{L}{2}t\right) + \frac{1}{2}\int_0^t \exp\left(\frac{L}{2}(t-s)\right)\beta^{-1}(s) \inf_{\dot{v}\in T_{\mathcal{V}(t)}\mathcal{S}_{2n}} \|\dot{v} - \mathcal{J}\,\mathrm{grad}_V\,\mathcal{H}(\varphi_1(\gamma(s)))\|_V \mathrm{d}s.$$

where

$$L = \mathrm{Lip}_V(\mathcal{H}),$$

$$\beta(t) := \inf_{\dot{v}\in T_{\mathcal{V}(t)}\mathcal{S}_{2n}} \frac{\|P_{\mathrm{W}_m(t)}v\|_V}{\|v\|_V} \in [0,1].$$

Error Analysis (with optimal $|\cdot|_Z$)

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Let

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It holds that

$$e(0) + \int_0^t \inf_{\dot v \in T_{\mathcal{V}(t)}\mathcal{S}_{2n}} \|\dot v - \mathcal{J}\,\mathrm{grad}_V\,\mathcal{H}(\varphi_1(\gamma(s)))\|_V \mathrm{d}s$$

$$\leq e(t) \lesssim$$

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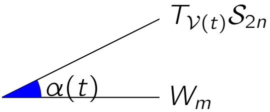
$$\beta(t) := \inf_{\dot v \in T_{\mathcal{V}(t)}\mathcal{S}_{2n}} \frac{\|P_{\mathrm{W}_m(t)} v\|_V}{\|v\|_V} \in [0,1].$$

β is a stability factor



$$\beta(t) = \beta(T_{\mathcal{V}(t)}\mathcal{S}_{2n}, W_m) = \min_{v \in T_{\mathcal{V}(t)}\mathcal{S}_{2n}} \frac{\|P_{W_m} v\|_V}{\|v\|_V} = \cos(\alpha(t)) \ \in \ [0,1]$$

Agenda

1. Hamiltonian Dynamics
2. Data Assimilation
3. Reconstruction Algorithm and Error
4. **Dynamical Sensor Placement**
5. Numerical Tests

Dynamical sensor placement

Suppose $V = L^2(\Omega)$. For a given t,

$$\ell_i(v) = \int_{\mathbb{R}^d} \underbrace{\frac{1}{(2\pi)^{d/2}\sigma_i} e^{-\frac{||x - x_i(t)||^2}{\sigma_i^2}}}_{=\omega_i = g(x_i(t), \sigma_i)} v(x)\mathrm{d}x = g(x_i, \sigma) * v$$

Gathering the sensors' locations in

$$x(t) = \{x_i(t)\}_{i=1}^m \in \left(\mathbb{R}^d\right)^m,$$

we thus have

$$\mathrm{W}_m(x(t)) := \{\omega_i(x_i(t))\}_{i=1}^m$$

with

$$\omega_i(x_i(t)) = g(x_i(t), \sigma_i).$$

Dynamical sensor placement

We search for the sensors' optimal path that maximizes stability

$$\max_{\substack{x\in\mathcal{C}([0,t],\mathbb{R}^m)\\ x(0)=a\\ \dot{x}(0)=b}} \int_0^t \left(\beta(V_n(t),\mathrm{W}_m(x(t))) - \frac{\kappa}{2}\|\dot{x}(t)\|^2\right)\mathrm{d}\tau,$$

where $\kappa > 0$ penalizes unphysically large velocities.

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where $\kappa > 0$ penalizes unphysically large velocities.

The Euler-Lagrange equations yield:

$$\begin{cases} \kappa \ddot{x} = \nabla_x \beta^2(V_n(t), \mathrm{W}_m(x(t))), \\ x(0) = a, \quad \dot{x}(0) = b. \end{cases}$$

and a time integration scheme yields the evolution of the sensors' locations.

Any scheme requires knowing how to compute $\nabla_x \beta^2(x)$.

We could also optimize over covariances $\Sigma_i(t)$.

Agenda

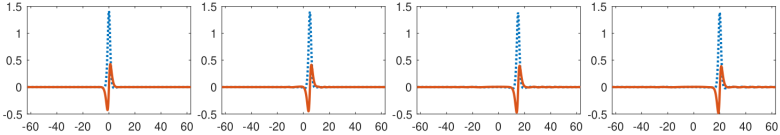
1D Nonlinear Schrödinger Equation

Here $u = (q, p)$ satisfies

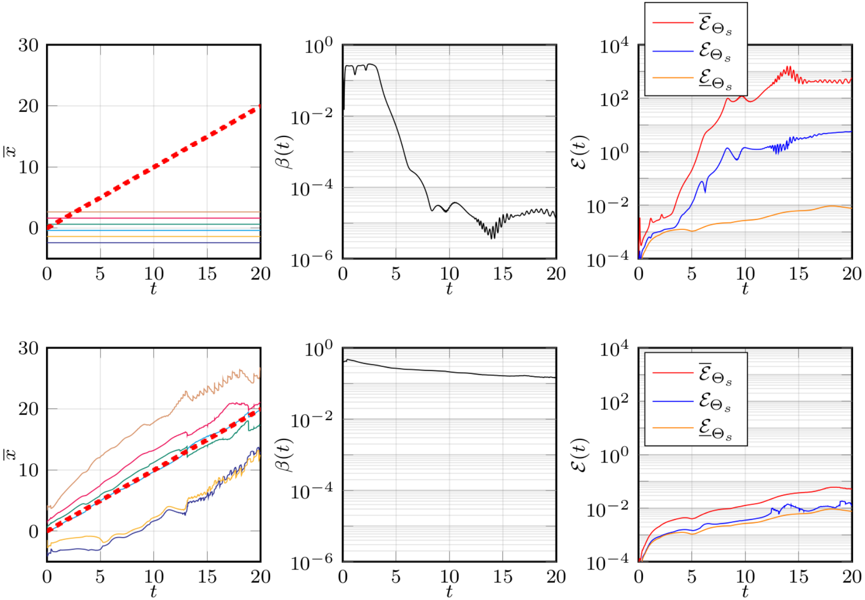
$$\begin{cases} q_t = -p_{xx} - \epsilon(q^2 + p^2)p, \\ p_t = q_{xx} + \epsilon(q^2 + p^2)q. \end{cases}$$

and

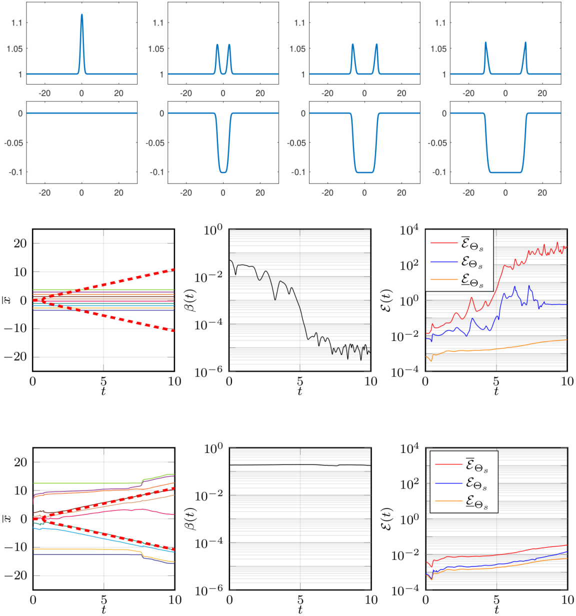
$$\theta = (\epsilon, \alpha) \in \Theta := [0.98, 1.1]^2, \qquad V = L^2([-L, L]).$$



Static VS dynamic sensor placement



1D Shallow Water



2D Shallow Water

$$\begin{cases} h_t + \nabla \cdot (h\nabla\Phi) = 0 & x \in D \quad t \in [0, T] \\ \Phi_t + \frac{1}{2}|\nabla\Phi|^2 + h = 0 & x \in D \quad t \in [0, T] \end{cases}$$

with periodic boundary conditions. Initial condition for h: Gaussian with 2 parameters.

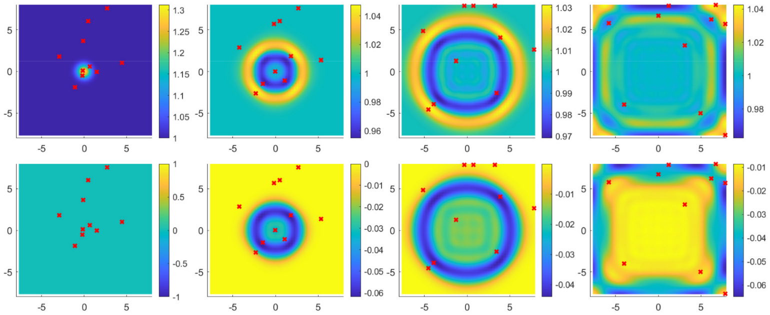


Figure: We use $V_n(t)$, and $m = 10$.

Conclusions

- Reconstruction with dynamical symplectic spaces and dynamical sensor placement.
- Rules for dynamical sensor placement based on stability.
- Error and stability estimates.
- Plenty of future work to derive a general formulation:
  - Fully nonlinear spaces.
  - Learn $\mu(t)$.
  - Deal with other dynamics (gradient flows, GENERIC).
  - How optimal is our algorithm? (extension of [CDMN22])

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