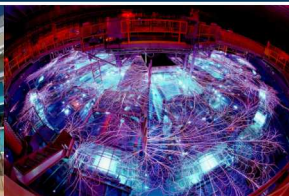


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Mass-Conserving, Hamiltonian-Structure-Preserving Reduced Order Modeling for the Rotating Shallow Water Equations

K. Chad Sockwell¹, Konstantin Pieper², Max Gunzburger³

¹ Center for Computing Research, Sandia National Laboratories, ² Oak Ridge National Laboratory, ³ Florida State University

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- Data-driven, physically constrained model: Fast-Model, Reduced Fidelity?
- Future exascale machines \Rightarrow More physics and resolution. Not necessarily faster
- Applications that suffer
 - Many Query: UQ, Data assimilation, Optimization
 - Real time simulations: Trajectory correction
 - Coupled multi-physics: High fidelity may not pay off
- Emerging Need for Climate models

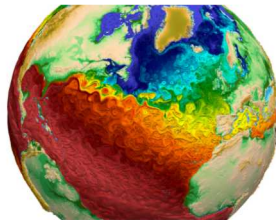


Figure: Temperature from E3SM simulation



- Data-driven alone may not cut it
- Leverage Physics to improve solution of surrogate model. Restrict solution space to physical solutions.

Modifying the basis \Rightarrow Mimetic FEM, Non-standard POD

Modifying the ROM \Rightarrow HSP-ROM

- Physics known & Low data: Physics or structure preserving surrogate models.
Key physical structure: Hamiltonian structure
- Derive Reduced Order Model (ROM) that preserves Hamiltonian Structure:
Mass and Energy Conservation

■ Lagrangian Structure

- Kevin Carlberg, Ray Tuminaro, Paul Boggs, *Preserving Lagrangian structure in nonlinear model reduction with application to structural dynamics* (2015)

■ Hamiltonian Structure

- Liqian Peng and Kamran Mohseni, *Symplectic model reduction of Hamiltonian systems* (2016)
- Yuezhen Gong, Qi Wang, Zhu Wang, *Structure-preserving Galerkin POD reduced-order modeling of Hamiltonian systems* (2016)
- Babak Afkham, Jan Hesthaven *Structure preserving model reduction of parametric Hamiltonian systems* (2017)
- Jan Hesthaven, Cecilia Pagliantini *Structure-Preserving Reduced Basis Methods for Hamiltonian Systems with a Nonlinear Poisson Structure* (2018)
- Bulent Karasozen, Suleyman Yildiz, Murat Uzunca *Structure Preserving Model Order Reduction of Shallow Water Equations* (2019)

■ Conservative Structure

- Kevin Carlberg, Youngsoo Choi, Syuzanna Sargsyan *Conservative model reduction for finite-volume models* (2018)

■ Contributions:

- Extend (Gong et al. 2016) to weighted Hilbert space and Mass Conservation.

Rotating Shallow Water Equations (RSWE)

Serves as proxy to ocean model (primitive equations)

Variables: fluid thickness h and velocity \vec{v} . Domain $\Omega \subset S^2$

$$\begin{aligned}\frac{\partial h}{\partial t} &= -\nabla \cdot (h\vec{v}) \text{ in } \Omega, \\ \frac{\partial \vec{v}}{\partial t} &= -qh(\hat{k} \times \vec{v}) - g\nabla(h+b) - \nabla K + \mathcal{G}[h, \vec{v}] \text{ in } \Omega, \\ \vec{v} \cdot n &= 0 \text{ on } \partial\Omega,\end{aligned}$$

- Kinetic energy: $K[\vec{v}] = |\vec{v}|^2/2$
- Potential vorticity: $q[h, \vec{v}] = (\hat{k} \cdot \nabla \times \vec{u} + f)/h$
- Forcing: $\mathcal{G}[h, \vec{v}]$ - wind, drag, diffusion,...
- Gravitational acceleration g , coriolis force parameter f , bottom topography $b < 0$, unit vector normal to sphere \hat{k}
- **Mimetic TRiSK scheme is used in space discretization**

Notation and Setting

- Discretized in space, continuous in time
- Consider discrete L^2 space $H = (\mathbb{R}^n, (\cdot, \cdot)_H)$ and monolithic variable $\mathbf{u}(t) = (\mathbf{h}(t), \mathbf{v}(t))$, $\mathbf{u} \in H$

$$(\mathbf{u}, \mathbf{u})_H = \mathbf{u}^\top \mathbf{M} \mathbf{u}$$
- Consider the solution space $\mathcal{V} \subset H$
- Reduced solution space $\mathcal{V}_r \subset \mathcal{V}$, spanned by r orthogonal basis functions in $\Phi \in \mathbb{R}^{n \times r}$
- Map to reduced Hilbert space $H_r = (\mathbb{R}^r, (\cdot, \cdot)_{H_r})$ of coefficients (inner product is Euclidean)

$$\Phi: H_r \rightarrow H$$

$$\Phi^*: H \rightarrow H_r$$

- POD in Hilbert space for orthogonality
- Discrete functions \mathbf{u} and operators Φ are bold, functionals $\mathbf{F}: H \rightarrow \mathbb{R}$ are bold-italic

- Two ingredients required: Skew-adjoint operator, in H , $\mathbf{J}[\mathbf{u}] \in \mathbb{R}^{n \times n}$ and Hamiltonian $\mathbf{H}[\mathbf{u}]: H \rightarrow \mathbb{R}$ (total energy)

$$\mathbf{J}[\mathbf{u}] = \begin{pmatrix} 0 & -\widetilde{\nabla} \cdot \\ -\widetilde{\nabla} & \mathbf{q} \widehat{k} \times \end{pmatrix}, \quad \mathbf{H}[\mathbf{u}] = \frac{1}{2}(\mathbf{h}\mathbf{v}, \mathbf{v})_{H_1} + \frac{1}{2}g(\mathbf{h}, \mathbf{h} + 2\mathbf{b})_{H_2}$$

- RSWE are non-canonical Hamiltonian system + **Extraneous terms**:

$$\frac{d\mathbf{u}}{dt} = \mathbf{J}[\mathbf{u}]\nabla\mathbf{H}[\mathbf{u}] + \mathbf{G}[\mathbf{u}]$$

- RSWE have *Hamiltonian Structure* which we wish to preserve in the ROM.
- Conservation of energy by Skew-adjoint operator $\mathbf{J}[\mathbf{u}]$

$$\frac{d\mathbf{H}[\mathbf{u}]}{dt} = \left(\nabla\mathbf{H}[\mathbf{u}], \frac{d\mathbf{u}}{dt} \right)_H = (\nabla\mathbf{H}[\mathbf{u}], \mathbf{J}[\mathbf{u}]\nabla\mathbf{H}[\mathbf{u}])_H = 0$$

Previous Method

- Consider Hamiltonian system

$$\frac{d\mathbf{u}}{dt} = \mathbf{J}[\mathbf{u}] \nabla \mathbf{H}[\mathbf{u}]$$

- Conventional: Test by basis $\Phi \mathbf{w} \in V_r$, $\mathbf{w} \in X_r$, and ansatz $\mathbf{u} = \Phi \mathbf{a}$, where $\text{DOF}(\mathbf{a}) \ll \text{DOF}(\mathbf{u})$

$$\left(\Phi \mathbf{w}, \Phi \frac{d\mathbf{a}}{dt} \right)_H = (\Phi \mathbf{w}, \mathbf{J}[\Phi \mathbf{a}] \nabla \mathbf{H}[\Phi \mathbf{a}])_H \Leftrightarrow \left(\mathbf{w}, \frac{d\mathbf{a}}{dt} \right)_{H_r} = (\mathbf{w}, \Phi^* \mathbf{J}[\Phi \mathbf{a}] \nabla \mathbf{H}[\Phi \mathbf{a}])_{H_r}$$

- Issue: $\Phi^* \mathbf{J}[\mathbf{u}]$ is not skew-symmetric or skew-adjoint in general.
- Additional ansatz: $\exists J_r[\mathbf{u}] \in \mathbb{R}^{r \times r}$ that is skew-symmetric, such that

$$\Phi^* \mathbf{J}[\mathbf{u}] = J_r \Phi^* \Rightarrow J_r = \Phi^* \mathbf{J} \Phi$$

- New Approximation: Hamiltonian–Structure–Preserving ROM (HSP–ROM)

$$\frac{d\mathbf{a}}{dt} = \Phi^* \mathbf{J}[\Phi \mathbf{a}] \Phi \Phi^* \nabla \mathbf{H}[\Phi \mathbf{a}] = \Phi^* \mathbf{J}[\Phi \mathbf{a}] \Phi \nabla \bar{H}[\mathbf{a}] = J_r[\mathbf{a}] \nabla \bar{H}[\mathbf{a}]$$

- "Reduced" functional

$$F[\Phi \mathbf{a}] = \bar{F}[\mathbf{a}], \quad \nabla \bar{F}[\mathbf{a}] = \Phi^* \nabla F[\Phi \mathbf{a}] \in \mathbb{R}^r$$

Error Estimate

- Assume continuity in time:

Theorem

Let $\mathbf{u}(t)$ be the solution of the time-continuous full model and let $\mathbf{a}(t)$ be the solution of the time-continuous HSP-ROM, and with the initial condition $\mathbf{a}(0) = \Phi^* \mathbf{u}(0)$, then the following error estimate is satisfied

$$\int_0^T \|\mathbf{u}(t) - \Phi \mathbf{a}(t)\|_H^2 dt \leq C(T) \left(\int_0^T \|\mathbf{u}(t) - \Phi \Phi^* \mathbf{u}(t)\|_H^2 dt + \int_0^T \|\nabla \mathbf{H}[\mathbf{u}(t)] - \Phi \Phi^* \nabla \mathbf{H}[\mathbf{u}(t)]\|_H^2 dt \right),$$

where $C(T) = \max\{1 + C_2^2 \alpha(T) T, C_3^2 \alpha(T) T\}$, and $\alpha(T) = 2 \int_0^T e^{2C_1(T-\tau)} d\tau$.

- $\Phi \Phi^* \nabla^X \mathbf{H}[\Phi \mathbf{a}] \rightarrow$ Enriched snapshot matrix

$$\mathbf{Y} = (\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_m, \nabla \mathbf{H}[\mathbf{u}_1], \nabla \mathbf{H}[\mathbf{u}_2], \dots, \nabla \mathbf{H}[\mathbf{u}_m]),$$

A Blessing and a Curse

- New snapshots give typical error estimate and convergence

$$\int_0^T \|\mathbf{u}(t) - \Phi \mathbf{a}(t)\|_H^2 dt \leq C(T) \left(\int_0^T \|\mathbf{u}(t) - \Phi \Phi^* \mathbf{u}(t)\|_H^2 dt + \int_0^T \|\nabla \mathbf{H}[\mathbf{u}(t)] - \Phi \Phi^* \nabla \mathbf{H}[\mathbf{u}(t)]\|_H^2 dt \right) = C(T) \sum_{k=r+1}^d \sigma_k^2,$$

where d is number of singular values in SVD.

- $\nabla^X \mathbf{H}$ possess no mass conservation principle.
- Resulting reduced model does not conserve mass

Solution

- Generalize Hilbert space
- 1 Modify to reduce additional error term
 - 2 Modify to construct model with mass-free gradients of functionals

Hamiltonian Model in a weighted Hilbert Space

- Consider weighted discrete L^2 space, X

$$(\mathbf{u}, \mathbf{v})_X = \mathbf{u}^\top \mathbf{X} \mathbf{v} = \mathbf{u}^\top \mathbf{M} \Omega \mathbf{v},$$

where \mathbf{M} is mass matrix and Ω is weighting.

- Adjoint:

$$\begin{aligned} \Phi^\dagger &= \mathbf{X}^{-1} \Phi \mathbf{X} & \Phi^\dagger : X &\rightarrow X_r \\ \Phi^* &= \mathbf{M}^{-1} \Phi \mathbf{M} & \Phi^* : H &\rightarrow H_r \end{aligned}$$

- Ingredients: ∇^X and \mathbf{J}_X

$$H' = (\nabla H[\mathbf{u}], \mathbf{z})_H = (\nabla^X H[\mathbf{u}], \mathbf{z})_X \Rightarrow \nabla^X H[\mathbf{u}] = \Omega^{-1} \nabla H[\mathbf{u}]$$

$$\frac{d\mathbf{u}}{dt} = \mathbf{J}[\mathbf{u}] \nabla H[\mathbf{u}] = \mathbf{J}_X[\mathbf{u}] \nabla^X H[\mathbf{u}] \Rightarrow \mathbf{J}_X[\mathbf{u}] = \mathbf{J}[\mathbf{u}] \Omega$$

- Weighting is trivial in full model but not in reduced model
- Alternative approach to weighting: Petrov–Galerkin

Galerkin Projection: POD-ROM, don't need, group with zhu

- Test with $\Phi \mathbf{w}$, $\mathbf{w} \in X_r$ and project to X_r , $r < n$ undetermined system

$$\left(\Phi \mathbf{w}, \frac{d\mathbf{u}}{dt} \right)_X = (\Phi \mathbf{w}, \mathbf{J}_X[\mathbf{u}] \nabla^X H[\mathbf{u}])_X \Leftrightarrow \left(\mathbf{w}, \Phi^* \frac{d\mathbf{u}}{dt} \right)_{X_r} = (\mathbf{w}, \Phi^* \mathbf{J}_X[\mathbf{u}] \nabla^X H[\mathbf{u}])_{X_r}$$

- Ansatz: $\mathbf{u}(t) = \Phi \mathbf{a}(t) + \mathbf{u}_s$, $\mathbf{a} \in X_r$

$$\left(\mathbf{w}, \frac{d\mathbf{a}}{dt} \right)_{X_r} = (\mathbf{w}, \Phi^* \mathbf{J}_X[\Phi \mathbf{a} + \mathbf{u}_s] \nabla^X H[\Phi \mathbf{a} + \mathbf{u}_s])_{X_r}$$

- Strong Form

$$\frac{d\mathbf{a}}{dt} = \Phi^* \mathbf{J}_X[\Phi \mathbf{a} + \mathbf{u}_s] \nabla^X H[\Phi \mathbf{a} + \mathbf{u}_s]$$

- $\Phi^* \mathbf{J}_X[\Phi \mathbf{a} + \mathbf{u}_s]$ is not skew-symmetric in general.

- Consider Hamiltonian System

$$\frac{d\mathbf{u}}{dt} = \mathbf{J}_X[\mathbf{u}] \nabla^X H[\mathbf{u}]$$

- Following (Gong et al. 2016): Additional ansatz: $\exists \mathbf{J}_{X_r} \in \mathbb{R}^{r \times r}$

$$\mathbf{J}_{X_r}[\mathbf{a}] \Phi^* = \Phi^* \mathbf{J}_X[\Phi \mathbf{a} + \mathbf{u}_s] \Rightarrow \mathbf{J}_{X_r}[\mathbf{a}] = \Phi^* \mathbf{J}_X[\Phi \mathbf{a} + \mathbf{u}_s] \Phi$$

- Insert into reduced model.

$$\frac{d\mathbf{a}}{dt} = \mathbf{J}_{X_r}[\mathbf{a}] \nabla^X \bar{H}[\mathbf{a}]$$

- Compare reduced models in H and X

$$X: \quad \frac{d\mathbf{a}}{dt} = \Phi^T \Omega^T M \mathbf{J}[\Phi \mathbf{a}] \Omega \Phi \Phi^T M \nabla H[\Phi \mathbf{a}]$$

$$H: \quad \frac{d\mathbf{a}}{dt} = \Phi^T M \mathbf{J}[\Phi \mathbf{a}] \Phi \Phi^T M \nabla H[\Phi \mathbf{a}]$$

Note that bases are orthogonal in corresponding space and thus different.

Mass Conservation

- Define space of mass free functions X_c : $\mathbf{u} = \tilde{\mathbf{u}} + \mathbf{u}_s$, $\tilde{\mathbf{u}} \in X_c$
- Mass Conservation:

$$(\mathbf{1}, \mathbf{u})_H = (\mathbf{1}_X, \mathbf{u})_X = (\mathbf{1}_X, \mathbf{u}_s)_X + (\mathbf{1}_X, \tilde{\mathbf{u}})_X = (\mathbf{1}_X, \mathbf{u}_s)_X$$

$$\left(\mathbf{1}_X, \frac{d\mathbf{u}}{dt} \right) = (\mathbf{1}_X, \mathbf{J}_X \nabla^X \mathbf{H}[\mathbf{u}])_X = 0 \Leftrightarrow \mathbf{1}_X \in \ker(\mathbf{J}_X)$$

- Gradient in X_c , $\nabla^{X_c} \mathbf{H} \in X_c$

$$\begin{aligned} \mathbf{H}' &= (\nabla^{X_c} \mathbf{H}, \psi)_X = (\nabla^X \mathbf{H}, \psi)_X, \forall \psi \in X_c, \\ (\mathbf{1}_X, \nabla^{X_c} \mathbf{H}) &= 0 \end{aligned}$$

- Satisfied by adding Lagrange multiplier

$$\begin{aligned} \nabla^{X_c} \mathbf{H}[\mathbf{u}] &= \nabla^X \mathbf{H}[\mathbf{u}] + \lambda \mathbf{1}_X \\ (\nabla^{X_c} \mathbf{H}, \psi)_X &= (\nabla^X \mathbf{H}, \psi)_X + \lambda (\mathbf{1}_X, \psi) = (\nabla^X \mathbf{H}, \psi)_X, \forall \psi \in X_c \end{aligned}$$

- Second condition leads to

$$\lambda = \frac{(\mathbf{1}_X, \nabla^X \mathbf{H}[\mathbf{u}])_X}{(\mathbf{1}_X, \mathbf{1}_X)_X}$$

- New snapshot matrix is mass-free: Leads to mass conserving model

$$\mathbf{Y} = (\tilde{\mathbf{u}}_1, \tilde{\mathbf{u}}_2, \dots, \tilde{\mathbf{u}}_m, \nabla^{X_c} \mathbf{H}[\mathbf{u}_1], \nabla^{X_c} \mathbf{H}[\mathbf{u}_2], \dots, \nabla^{X_c} \mathbf{H}[\mathbf{u}_m]),$$

- How full is model changed?

$$\frac{d\mathbf{u}}{dt} = \mathbf{J}_X[\mathbf{u}] \nabla^{X_c} \mathbf{H}[\mathbf{u}] = \mathbf{J}_X[\mathbf{u}] \nabla^X \mathbf{H}[\mathbf{u}] + \lambda \mathbf{J}_X \mathbf{1}_X = \mathbf{J}_X[\mathbf{u}] \nabla^X \mathbf{H}[\mathbf{u}]$$

- Model not effected. What about the reduced model

$$\begin{aligned} \frac{d\mathbf{a}}{dt} &= \Phi^* \mathbf{J}_X[\Phi \mathbf{a} + \mathbf{u}_s] \Phi \Phi^* \nabla^{X_c} \mathbf{H}[\Phi \mathbf{a} + \mathbf{u}_s] \\ &= \Phi^* \mathbf{J}_X[\Phi \mathbf{a} + \mathbf{u}_s] \Phi \Phi^* \nabla^X \mathbf{H}[\Phi \mathbf{a} + \mathbf{u}_s] + \lambda \Phi^* \mathbf{J}_X[\Phi \mathbf{a} + \mathbf{u}_s] \Phi \Phi^* \mathbf{1}_X \\ &= \Phi^* \mathbf{J}_X[\Phi \mathbf{a} + \mathbf{u}_s] \Phi \Phi^* \nabla^X \mathbf{H}[\Phi \mathbf{a} + \mathbf{u}_s] \end{aligned}$$

- We have not specified weighting Ω
- Claim: An optimal Ω exists for Quadratic Hamiltonian systems
- Let $\Omega = \nabla^2 H$, $\nabla^2 H$ is SPD in H , X is now "approximate energy inner product space"

$$(\mathbf{y}, \nabla^2 H[\mathbf{u}] \mathbf{z})_H = (\nabla^2 H[\mathbf{u}] \mathbf{y}, \mathbf{z})_H \Leftrightarrow \mathbf{M} \nabla^2 H[\mathbf{u}] = \nabla^2 H[\mathbf{u}]^T \mathbf{M}$$

- For H_q given by quadratic form

$$H_q[\mathbf{u}] = (\mathbf{u}, \mathbf{u})_X$$

Quadratic Hamiltonians and Approximate Energy Space

- $\nabla^X H = \Phi\Phi^* \nabla^X H$ under certain conditions.

Theorem

If the Hamiltonian $H[\mathbf{u}]$ is at most quadratic in \mathbf{u} , \mathbf{u}_{eq} is chosen to be the equilibrium state, such that $\nabla H[\mathbf{u}_{eq}] = 0$, and the snapshot matrix is given by

$$\mathbf{Y} = (\mathbf{u}_1 - \mathbf{u}_s, \mathbf{u}_2 - \mathbf{u}_s, \dots, \mathbf{u}_m - \mathbf{u}_s)$$

$$= (\mathbf{u}_1 - \mathbf{u}_{eq} - (\mathbf{u}_s - \mathbf{u}_{eq}), \mathbf{u}_2 - \mathbf{u}_{eq} - (\mathbf{u}_s - \mathbf{u}_{eq}), \dots, \mathbf{u}_m - \mathbf{u}_{eq} - (\mathbf{u}_s - \mathbf{u}_{eq})),$$

where \mathbf{u}_s is some appropriate shift. Furthermore, also let the basis Φ , constructed from \mathbf{Y} , be enriched with the following basis function

$$\psi = \frac{(I - \Phi\Phi^*)\hat{\mathbf{u}}}{\|(I - \Phi\Phi^*)\hat{\mathbf{u}}\|_X},$$

to give the enriched basis $\hat{\Phi} = [\Phi, \psi]$, and $\hat{\mathbf{u}} = \mathbf{u}_s - \mathbf{u}_{eq}$. Then the projection $\hat{\Phi}\hat{\Phi}^* \nabla^X H[\mathbf{u}_s + \Phi\mathbf{a}]$ is exact

$$\nabla^X H[\mathbf{u}_s + \Phi\mathbf{a}] = \hat{\Phi}\hat{\Phi}^* \nabla^X H[\mathbf{u}_s + \Phi\mathbf{a}].$$

Theorem

The HSP-ROM model in X for a Hamiltonian system with a quadratic Hamiltonian is equivalent to the POD-ROM derived in the space X . This means that

$$\frac{d\mathbf{a}(t)}{dt} = \mathbf{J}_{X_r}[\mathbf{a}(t) + \mathbf{u}_s] \nabla^{X_r} \mathbf{H}[\mathbf{a}(t)] = \hat{\Phi}^* \mathbf{J}[\Phi\mathbf{a}(t)] \nabla \mathbf{H}[\Phi\mathbf{a}(t) + \mathbf{u}_s] .$$

This means that the POD-ROM model in the space X also conserves energy for systems with Quadratic Hamiltonians. Furthermore, in the more general case where the system is shifted by \mathbf{u}_s , by using the enriched basis $\hat{\Phi}$, this result also holds true.

Error Estimate Quadratic Hamiltonian

Theorem

Let \mathbf{u} be the solution of the time-continuous full model and let \mathbf{a} be the solution of linear Casimir preserving, time-continuous HSP-ROM in X for a system with a quadratic Hamiltonian using a basis Φ be constructed from the following snapshot matrix

$$\mathbf{Y} = (\tilde{\mathbf{u}}_1, \tilde{\mathbf{u}}_2, \dots, \tilde{\mathbf{u}}_m),$$

and enriched to become using $\hat{\Phi}$ for a shifted system. The error becomes

$$\begin{aligned} \int_0^T \|\mathbf{u}(t) - (\mathbf{u}_s + \hat{\Phi}\mathbf{a}(t))\|_X^2 dt &= \int_0^T \|\tilde{\mathbf{u}}(t) - \hat{\Phi}\mathbf{a}(t)\|_X^2 dt \\ &\leq \tilde{C}(T) \int_0^T \|\mathbf{u}(t) - \hat{\Phi}\hat{\Phi}^*\mathbf{u}(t)\|_X dt = \tilde{C}(T) \sum_{k=r+1}^d \lambda_k, \end{aligned}$$

where for a solution independent \mathbf{J} we have, $\tilde{C}(T) = 1 + \hat{C}_2^2 T$, and for a solution dependent \mathbf{J} we have where $\tilde{C}(T) = 1 + \hat{C}_2^2 \beta(T) T$, and $\beta(T) = \int_0^T e^{(2\hat{C}_1(T-\tau))} d\tau$,

What Does This Mean?

- X space + enriched basis means POD-ROM conserves energy
- POD-ROM also has vastly improved error estimate
- In more general Hamiltonian system, quadratic and lower order contributions to error benefit from this. If H.O.T are small, improved error is seen.

- RSWE has cubic Hamiltonian, 3rd order term is small in magnitude
- Energy conservation to time-truncation error
- $\mathbf{u}_{eq} = \mathbf{u}_{ref} = (\mathbf{b}, 0)$ the resting state. Recall $\mathbf{\Omega} = \nabla^2 \mathbf{H}[\mathbf{u}_{ref}]$
- ROM can use larger time-steps than full model
- Efficient treatment of nonlinearities: Lifting and tensorial POD

Energy Conserving Test Case

- Demonstrate energy conservation to truncation error for HSP-ROM
- Ocean basin of 3000 km wide , 16km resolution ($\approx 30,000$ cells)
- 10 day, geostrophic initial condition
- RK4 time integrator with 75% of CFL constrained time-step in full model (approximately 80 seconds)
- Reproductive run

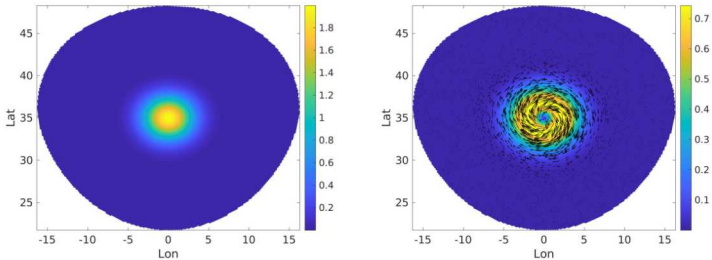


Figure: The geostrophic initial condition for h (left) and v (right).

Method	Space	Error $_{t_{\text{final}}, X}$	Error $_{\text{Energy, rel}}$
HSP-ROM	X	2.45e-2	6.82e-7
HSP-ROM	H	1.79	1.06e-6
POD-ROM	X	2.54e-2	3.83e-4
POD-ROM	H	1.06	5.34e-2

Table: 15 basis functions and 10 times full model's time step

Method	Space	Error $_{t_{\text{final}}, X}$	Error $_{\text{Energy, rel}}$
HSP-ROM	X	2.45e-2	1.04e-11
HSP-ROM	H	1.79	1.79e-11
POD-ROM	X	2.52e-2	3.72e-4
POD-ROM	H	1.06	5.34e-2

Table: 15 basis functions and same as full model's time step

Method	Space	Error $_{t_{final}, X}$	Error $_{Energy, rel}$
HSP-ROM	X	2.65e-2	1.47e-6
HSP-ROM	H	1.58	2.59e-6
POD-ROM	X	2.59e-2	7.65e-5
POD-ROM	H	—	—

Table: 25 basis functions and 10 times full model's time step

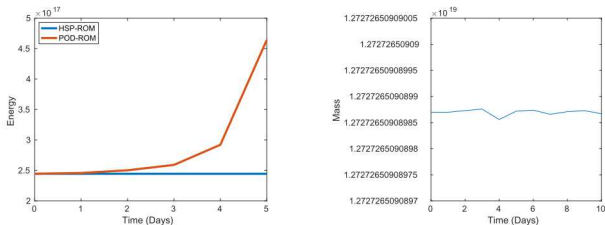


Figure: Energy of HSP-ROM and POD-ROM in H (left). Mass of HSP-ROM method (right).

Conclusions and Future Research

Conclusions

- Method in Gong 2016 extended to weighted Hilbert space
- Convergent method with mass conservation
- Approximate energy space gives vast advantages
- Poisson Bracket interpretation is natural
- Optimal weight equivalent to optimal test basis in Petrov-Galerkin method

Future Research

- Preserving more quantities (nonlinear Casimirs)
- Including hyper-reduction methods for nonlinear terms
- Real applications

Petrov-Galerkin Interpretation

- Using Φ as basis for \mathbf{u} and $\nabla \mathbf{H}$ seems odd
- We can reason from the directional derivative that $\nabla \mathbf{H}$ are in a dual space
- Assume second basis Ψ , a cobasis and projection $\Psi\Phi^*$ such that $\Phi^*\Psi = I$
- Petrov-Galerkin Projection

$$\left(\Psi \mathbf{w}, \Phi \frac{d\mathbf{a}}{dt} \right)_X = (\Psi \mathbf{w}, J_X[\Phi \mathbf{a}] \nabla^X \mathbf{H}[\Phi \mathbf{a}])$$

- New ansatz

$$\mathbf{J}_{X_r} \Phi^* = \Psi^* \mathbf{J}_X \Rightarrow \mathbf{J}_{X_r} = \Psi^* \mathbf{J}_X \Psi$$

- Reduced Model

$$\frac{d\mathbf{a}}{dt} = \Psi^* \mathbf{J}_X \Psi \Phi^* \nabla^X \mathbf{H}[\Phi \mathbf{a}]$$

Backup Slides Petrov-Galerkin Interpretation

- In some case Petrov-Galerkin and Galerkin are the same

Theorem

If $\Psi \in \mathbb{R}^{N \times r}$ and $\Phi^* \Psi = \Psi^* \Phi = I$, then there exists an SPD operator $\mathbf{T} : X \rightarrow X$ such that

$$\Psi = \mathbf{T}\Phi$$

- If we choose X with trivial weighting and $\mathbf{T} = \Omega$, we arrive at previous model.
- Thus for quadratic Hamiltonians, $\Psi = \nabla^2 \mathbf{H}\Phi$ is optimal basis for $\nabla^X \mathbf{H}[\mathbf{u}]$

$$\Psi \Phi^* \nabla^X \mathbf{H}[\mathbf{u}] = \nabla^X \mathbf{H}[\mathbf{u}]_X$$

The Poisson Bracket

- Time evolution of a functional of the solution \mathbf{u} , $F[\mathbf{u}]$, $F : H \rightarrow \mathbb{R}$

$$\frac{dF[\mathbf{u}]}{dt} = \left(\frac{\partial F[\mathbf{u}]}{\partial \mathbf{u}}, \frac{d\mathbf{u}}{dt} \right)_H$$

- Insert $\frac{d\mathbf{u}}{dt}$

$$\frac{dF[\mathbf{u}]}{dt} = (\nabla F[\mathbf{u}], \mathbf{J}[\mathbf{u}] \nabla H[\mathbf{u}])_H$$

- Skew-symmetric bilinear form \rightarrow Poisson bracket

$$\mathcal{J}[\mathbf{u}](F[\mathbf{u}], H[\mathbf{u}]) = (\nabla F[\mathbf{u}], \mathbf{J}[\mathbf{u}] \nabla H[\mathbf{u}])_H$$

- Invariant under of choice Hilbert space

$$\frac{dF[\mathbf{u}]}{dt} = \{F[\mathbf{u}], H[\mathbf{u}]\}[\mathbf{u}]$$

Weak Formulation of Hamiltonian Systems

- Weak formulation for Hamiltonian system

seek $\mathbf{u} \in H$, such that ,

$$\left(\mathbf{z}, \frac{d\mathbf{u}}{dt} \right)_H = (\mathbf{z}, \mathbf{J}[\mathbf{u}] \nabla H[\mathbf{u}])_H, \quad \forall \mathbf{z} \in H.$$

- Time evolution of functional $\mathbf{F}_z[\mathbf{u}] = (\mathbf{z}, \mathbf{u}(t))_H$

$$\frac{d\mathbf{F}_z[\mathbf{u}]}{dt} = \{ \mathbf{F}_z[\mathbf{u}], H[\mathbf{u}] \}[\mathbf{u}],$$

specified in the space H

$$\left(\mathbf{z}, \frac{d\mathbf{u}}{dt} \right)_H = (\mathbf{z}, \mathbf{J}[\mathbf{u}] \nabla H[\mathbf{u}])_H$$

where $\nabla \mathbf{F}_z[\mathbf{u}] = \mathbf{z}$

Conserved Quantities and Casimirs

- Quantities conserved by symmetry: Energy, momentum, angular momentum, etc.
- Energy conservation:

$$\frac{dH[\mathbf{u}]}{dt} = H[\mathbf{u}], H[\mathbf{u}][\mathbf{u}] = 0;$$

- Casimirs: Conserved quantities for non-canonical systems (degenerate $\mathbf{J}[\mathbf{u}]$, $\ker(\mathbf{J}[\mathbf{u}])$ is non trivial)
- Consider Casimir $\mathbf{C}[\mathbf{u}]$, defined by

$$\{\mathbf{C}[\mathbf{u}], \mathbf{F}[\mathbf{u}]\}[\mathbf{u}] = 0 \Leftrightarrow \nabla \mathbf{C}[\mathbf{u}] \in \ker(\mathbf{M}\mathbf{J}[\mathbf{u}])$$

which implies

$$\frac{d\mathbf{C}[\mathbf{u}]}{dt} = \{\mathbf{C}[\mathbf{u}], \mathbf{H}[\mathbf{u}]\}[\mathbf{u}] = 0;$$

$$\mathbf{C}[\mathbf{u}(t)] = c, \forall t$$

- Mass is Casimir and linear-invariant in RSWE

$$(\mathbf{1}, \mathbf{h})_I = c_{\text{mass}}$$

- Casimir is

$$\mathbf{C}_{\text{mass}}[\mathbf{u}] = (\mathcal{L}, \mathbf{u})_H, \mathcal{L} = \begin{pmatrix} \mathbf{1} \\ 0 \end{pmatrix} \in H$$

- Add λ times linear Casimir to Hamiltonian, define mass-free ∇^{H_c}

$$\nabla^{H_c} \mathbf{H}[\mathbf{u}] = \nabla \mathbf{H}[\mathbf{u}] + \lambda \nabla \mathbf{C}[\mathbf{u}]$$

- Linear Casimirs make finding λ easy
- Insert into Poisson Bracket

$$\begin{aligned} \frac{d\mathbf{F}[\mathbf{u}]}{dt} &= \{\mathbf{F}[\mathbf{u}], \mathbf{H}[\mathbf{u}]\}[\mathbf{u}] = (\nabla^{H_c} \mathbf{F}, \mathbf{J} \nabla^{H_c} \mathbf{H})_H \\ &= (\nabla \mathbf{F}, \mathbf{J} \nabla \mathbf{H})_H \end{aligned}$$

because $\nabla \mathbf{C} \in \ker \mathbf{J}$.

HSP-ROM from the Poisson bracket

- Time evolution of functional $\mathbf{F}_z[\mathbf{u}] = (\mathbf{z}, \mathbf{u}(t))_H$

$$\frac{d\mathbf{F}_z[\mathbf{u}]}{dt} = \{\mathbf{F}_z[\mathbf{u}], \nabla H[\mathbf{u}]\}[\mathbf{u}] ,$$

- Ansatz

$$\begin{aligned} \mathbf{u} &= \Phi \mathbf{a} \\ \nabla \mathbf{F} &= \Psi \Phi^* \nabla \mathbf{F} \end{aligned}$$

- Insert in Poisson Bracket, and let $\mathbf{z} = \Psi \mathbf{w}$

$$\begin{aligned} \frac{d\mathbf{F}_z[\mathbf{u}]}{dt} &= (\Psi \Phi^* \nabla \mathbf{F}_z[\Phi \mathbf{a}], \mathbf{J}[\Phi \mathbf{a}] \Psi \Phi^* \nabla H[\Phi \mathbf{a}]) = (\Psi \mathbf{w})^* \Phi \Psi^* \mathbf{J}[\Phi \mathbf{a}] \Psi \Phi^* \nabla H[\Phi \mathbf{a}] = \\ &= \{\nabla \mathbf{F}_z[\mathbf{u}], \nabla H[\mathbf{u}]\}_r[\mathbf{a}] , \end{aligned}$$

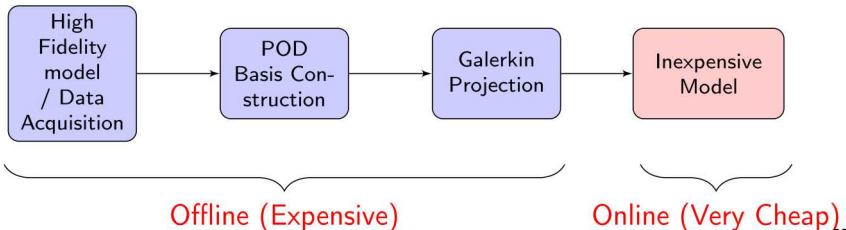
where

$$\{\cdot, \cdot\}_r[\cdot] = (\nabla[\cdot], (\Phi \Psi^* \mathbf{J}[\cdot] \Psi \Phi^*) \nabla[\cdot])_H$$

- Thus we have a new Poisson bracket on reduced space

Reduced Order Modeling (ROM)

- Physically constrained, data-driven method
- Ansatz: Solution lives on reduced manifold
- Build basis from data
- Galerkin Projection onto basis



Novel Contributions

- Hamiltonian-structure-preserving reduced order model for non-canonical Hamiltonian system
- Reduction through the Poisson Bracket
- Use of novel inner product which improves accuracy
- Mass conservation derived for model: Any linear invariant - Casimir can be preserved

Coupled and Decoupled Basis

- Consider systems of equations where $\mathbf{y}_i = (\mathbf{x}_i, \mathbf{z}_i)^\top$
- Monolithic SVD over \mathbf{Y} . Basis:

$$\Phi = \begin{pmatrix} \Phi_x \\ \Phi_z \end{pmatrix} .$$

- Does not preserve block structure of problem. One variable \mathbf{a}
- SVD on each variable: Basis

$$\Phi = \begin{pmatrix} \Phi_x & 0 \\ 0 & \Phi_z \end{pmatrix} ,$$

- Preserves block structure, variable number of basis functions. Two variables $\mathbf{a} = (\mathbf{a}_x, \mathbf{a}_z)$

Galerkin Projection: POD-ROM

- Consider Hamiltonian System

$$\frac{d\mathbf{u}}{dt} = \mathbf{J}[\mathbf{u}] \nabla H[\mathbf{u}]$$

- Test with $\Phi \mathbf{w}$, $\mathbf{w} \in X_r$

$$\left(\Phi \mathbf{w}, \frac{d\mathbf{u}}{dt} \right)_X = (\Phi \mathbf{w}, \mathbf{J}[\mathbf{u}] \nabla H[\mathbf{u}])_X$$

- Project to X_r , $r < n$ undetermined system

$$\left(\mathbf{w}, \Phi^* \frac{d\mathbf{u}}{dt} \right)_{X_r} = (\mathbf{w}, \Phi^* \mathbf{J}[\mathbf{u}] \nabla H[\mathbf{u}])_{X_r}$$

- Ansatz: $\mathbf{u}(t) = \Phi \mathbf{a}(t)$, $\mathbf{a} \in X_r$

$$\left(\mathbf{w}, \frac{d\mathbf{a}}{dt} \right)_{X_r} = (\mathbf{w}, \Phi^* \mathbf{J}[\Phi \mathbf{a}] \nabla H[\Phi \mathbf{a}])_{X_r}$$

- Strong Form

$$\frac{d\mathbf{a}}{dt} = \Phi^* \mathbf{J}[\Phi \mathbf{a}] \nabla H[\Phi \mathbf{a}]$$

- Wind forcing, bottom drag, bi-harmonic smoothing
- Ten year spin-up initial condition
- 1 year test case with model in X
- Reproductive run
- In this case statistics will be compared, the RMSSSHA (square root of the variance in \mathbf{h})

- POD-ROM and HSP-ROM methods tested for 1 year with coupled and decoupled basis in X

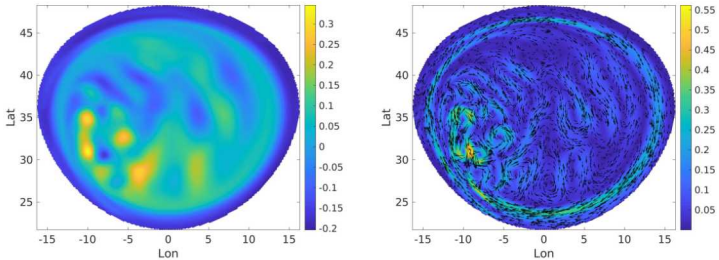
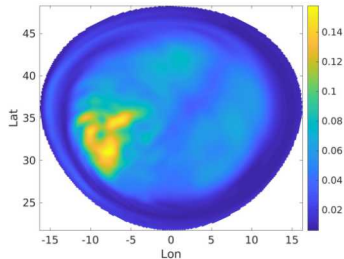


Figure: The spin-up initial condition in the SOMA test case for h (left) and v (right).

Coupled Versus Decoupled Basis

Method	Basis Type	r	SYPD	Error _{t_{final}}	Error _{RMSSSHA,H,rel}
Full		—	2.09	—	—
HSP-ROM	Decoupled	45	1157	1.03	3.3685
HSP-ROM	Decoupled	125	105.7	3.82e-2	4.94e-2
HSP-ROM	Coupled	45	1153	1.07	2.49e-1
HSP-ROM	Coupled	125	104.1	1.38e-2	5.01e-3
POD-ROM	Decoupled	45	—	9.69e-1	3.63e-1
POD-ROM	Decoupled	125	—	1.79e-2	1.16e-2
POD-ROM	Coupled	45	—	9.65e-1	6.78e-2
POD-ROM	Coupled	125	—	1.02e-2	2.50e-3

Table: Errors in final solution and RMSSSHA



Coupled Versus Decoupled Basis: HSP-ROM

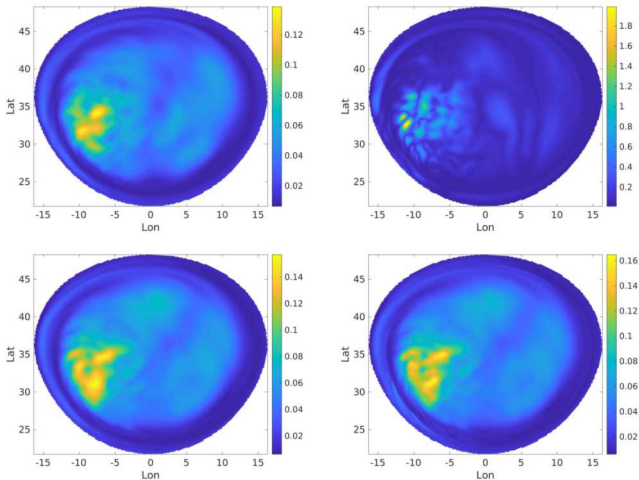


Figure: The RMSSSHA for the coupled basis with 45 basis functions (top left), for the decoupled basis with 45 basis functions (top right), for the coupled basis with 125 basis functions (bottom left), and for the decoupled basis with 125 basis functions (bottom right) using the HSP-ROM method

Coupled Versus Decoupled Basis: POD-ROM

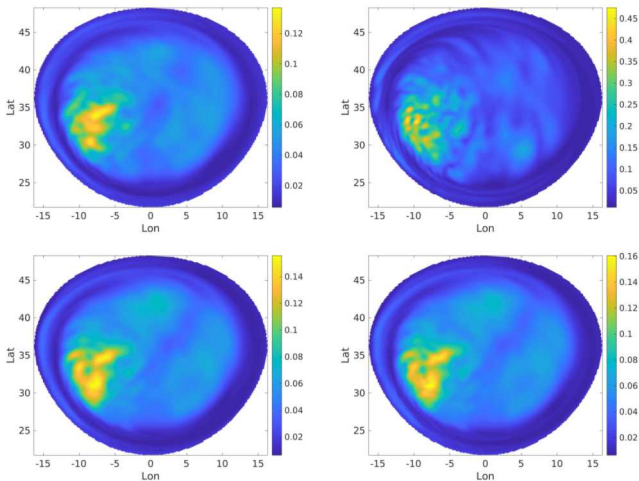


Figure: The RMSSSHA for the coupled basis with 45 basis functions (top left), for the decoupled basis with 45 basis functions (top right), for the coupled basis with 125 basis functions (bottom left), and for the decoupled basis with 125 basis functions (bottom right) using the POD-ROM method

- 10 year reproductive test case to build basis, 2 year prediction
- Coupled basis in X , 125 basis functions
- RK4 for reduced model with 100 times full model's RK4 time-step
- Dynamics behavior makes only statistics reliable

Method	Sim.	SYPD	Error _{RMSSSHA, H, rel}
HSP-ROM	10 yr. Rep.	103.2	4.79e-2
HSP-ROM	2 yr. Pred.	103.4	6.81e-2
POD-ROM	10 yr. Rep	—	5.18e-2
POD-ROM	2 yr. Pred.	—	5.082-2

Table: The performance in SYPD and relative error of the RMSSSHA in the H norm, compared to the full model, for both the ten year reproductive run (10 yr. Rep) and the two year predictive run (2 yr. Pred).

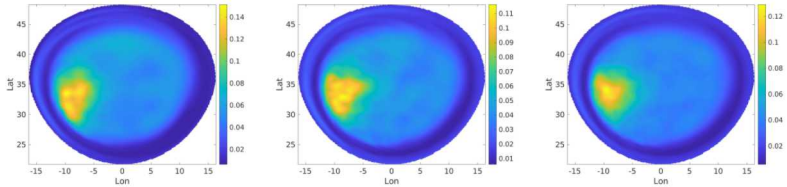


Figure: The RMSSSHA over ten years for the full model (left), for the HSP-ROM model (center), and the POD-ROM model (right).

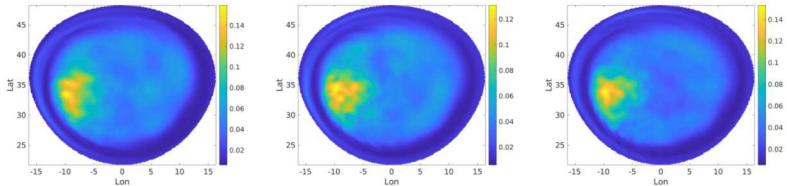


Figure: The RMSSSHA over the additional two years for full model (left), for the HSP-ROM model prediction (center), and the POD-ROM model prediction (right).

- Prediction, no validation, over a century
- Demonstrates stability
- Previous 10 year basis is used

Century Predictions

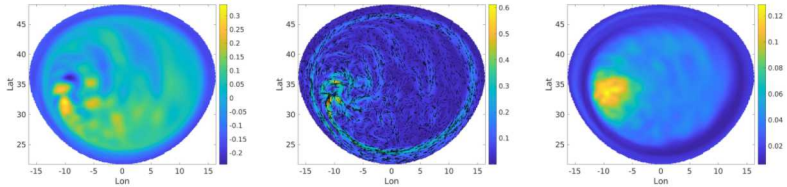


Figure: The solution, h and v , at the end of the century time-horizon and the RMSSSHA over the century time-horizon for the HSP-ROM method.

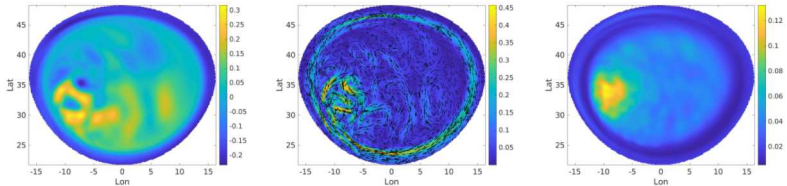


Figure: The solution, h and v , at the end of the century time-horizon and the RMSSSHA over the century time-horizon for the HSP-ROM method.

Century Predictions: Mass and Energy

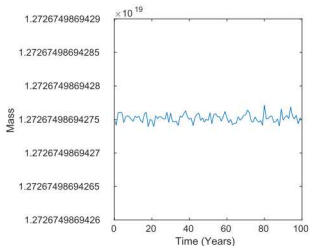
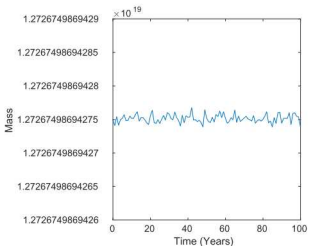
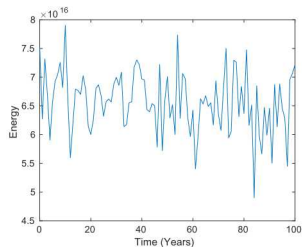
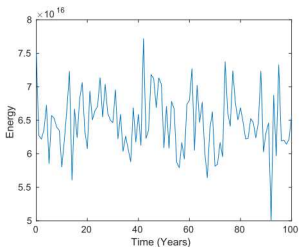


Figure: The energy (top-left) and mass (bottom-left) for the HSP-ROM method, and the energy (top-right) and mass (bottom-right) for the POD-ROM method over the century time horizon

Conclusions and Future Research

Conclusions

- HSP-ROM method conserves energy and mass is conserved
- Either model in derived in the space X has much better accuracy
- Large speedups can be attained with the HSP-ROM method
- Coupled basis is better than decoupled for small basis
- Both methods are stable in the forced test-case over a century

Future Research

- Primitive equations
- Non-intrusive physics preserving method
- Conserving more general Casimirs
- Hyper-reduction techniques for nonlinearities.
- Applications: uncertainty quantification, data assimilation, spin-up