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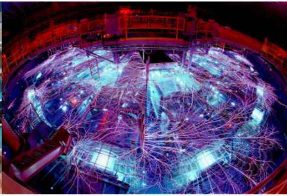

# Mass–Conserving, Hamiltonian–Structure-Preserving Reduced Order Modeling for the Rotating Shallow Water Equations

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# Motivation: Surrogate Models

- Fast-Model, Reduced Fidelity?
- Future exascale machines ⇒ 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: Ocean Spin-up, UQ

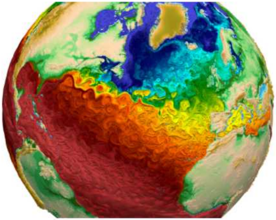


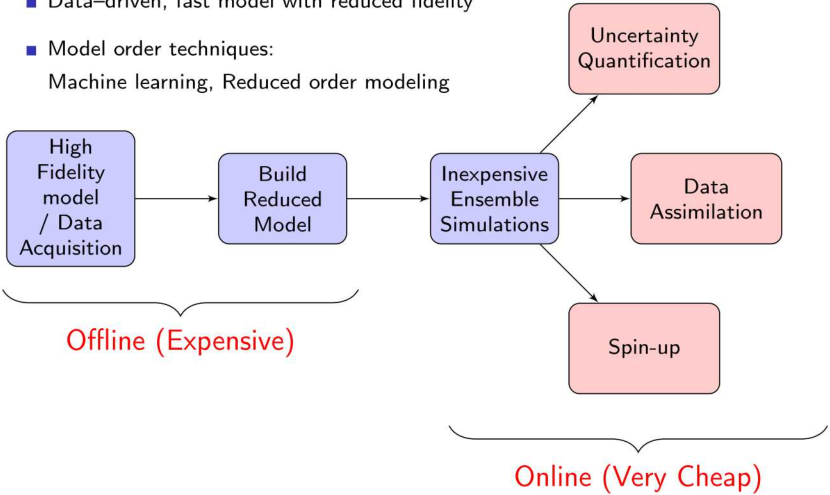
Figure: Temperature from E3SM simulation

E3SM Energy Exascale Earth System Model

MPAS-O Model for Prediction Across Scales

# Surrogate Model Quick Course

- Data–driven, fast model with reduced fidelity
- Model order techniques:
  Machine learning, Reduced order modeling



# Surrogate Model Quick Course

- Data–driven alone may not cut it
- Physics known & Low data: Physics or structure preserving surrogate models
- Leverage Physics to improve solution of surrogate model

Data $\Rightarrow$ Machine Learning $\Rightarrow$ Physics Constaints

PDE $\Rightarrow$ Galerkin Project to Data Space $\Rightarrow$ Modify ROM

- Reduced order Model (ROM) which preserves Hamiltonian Structure

# Previous Work

- Kevin Carlberg, Ray Tuminaro, Paul Boggs, Preserving Lagrangian structure in nonlinear model reduction with application to structural dynamics (2015)
- Liqian Peng and Kamran Mohseni,*Symplectic model reduction of Hamiltonian systems* (2016)
- Yuezheng 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)
- Kevin Carlberg, Youngsoo Choi, Syuzanna Sargsyan *Conservative model reduction for finite-volume models* (2018)
- 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)

# Rotating Shallow Water Equations (RSWE)

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Serves as proxy to ocean model (primitive equations)

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

$$\frac{\partial h}{\partial t} = -\nabla \cdot (h\vec{v}) \text{ in } \Omega,$$

$$\frac{\partial \vec{v}}{\partial t} = -qh(\hat{k} \times \vec{v}) - g\nabla(h+b) - \nabla K + \mathcal{G}[h, \vec{v}] \text{ in } \Omega,$$

$$\vec{v} \cdot n = 0 \text{ on } \partial\Omega,$$

- 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

# Hamiltonian Framework

- Define monolithic variable $\mathbf{u}(t) = (\mathbf{h}(t), \mathbf{v}(t))$, $\mathbf{u} \in H = (\mathbb{R}^n, (\cdot,\cdot)_H)$, $\mathbf{u}\colon \mathbb{R} \to H$

$$(\mathbf{u}, \mathbf{u})_H = \mathbf{u}^\top \mathbf{M}\mathbf{u}$$

- Energy conservation at abstract level: Two ingredients required
- Skew-adjoint operator $\mathbf{J}[\mathbf{u}]$ and Hamiltonian (total energy)

$$\mathbf{J}[\mathbf{u}] = \begin{pmatrix} 0 & -\widetilde{\boldsymbol{\nabla}\cdot} \\ -\widetilde{\boldsymbol{\nabla}} & \widetilde{\mathbf{q}\hat{k}\times} \end{pmatrix}, \quad \boldsymbol{H}[\mathbf{u}] = (\mathbf{hv}, \mathbf{v})_H + g(\mathbf{h}, \mathbf{h} + 2\mathbf{b})_H$$

- Gradient of Hamiltonian

$$\nabla \boldsymbol{H}[\mathbf{u}] = \begin{pmatrix} \mathbf{v}^2 + g(\mathbf{h} + \mathbf{b}) \\ \mathbf{hv} \end{pmatrix}$$

- RSWE are non-canonical Hamiltonian system:

$$\mathbf{u}_t = \mathbf{J}[\mathbf{u}]\nabla \boldsymbol{H}[\mathbf{u}] + \mathbf{G}[\mathbf{u}]$$

- **G[u]** is extraneous to the framework

# Symmetries

- $\mathbf{J}[\mathbf{u}]$ is skew-adjoint in $H$

$$(\mathbf{y}, \mathbf{J}[\mathbf{u}]\,\mathbf{z})_H = -(\mathbf{J}[\mathbf{u}]\,\mathbf{y}, \mathbf{z})_H \Leftrightarrow \mathbf{M}\mathbf{J} = -\mathbf{J}^\top \mathbf{M}$$

- Hessian of Hamiltonian $\nabla^2 \boldsymbol{H}[\mathbf{u}]$ is self-adjoint in $H$

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

- If the Hamiltonian is given by a quadratic form $\boldsymbol{H}_{\mathrm{qf}}[\mathbf{u}]$, then

$$\boldsymbol{H}_{\mathrm{qf}}[\mathbf{u}] = (\mathbf{u}, \nabla^2 \boldsymbol{H}_{\mathrm{qf}}\,\mathbf{u})_H$$

- Conservation of Energy

$$\frac{\mathrm{d}\boldsymbol{H}[\mathbf{u}]}{\mathrm{d}t} = (\nabla \boldsymbol{H}[\mathbf{u}], \mathbf{u})_H = (\nabla \boldsymbol{H}[\mathbf{u}], \mathbf{J}[\mathbf{u}]\nabla \boldsymbol{H}[\mathbf{u}])_H = 0$$

# Hamiltonian Model in a Hilbert Space

- Consider weighted discrete $L^2$ space $X$

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

  where $M$ is mass matrix and $\boldsymbol{\Omega}$ is weighting.

- Ingredients: $\nabla^X$ and $\mathbf{J}_X$

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

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

- Weighting is trivial in full model but not in reduced model

- Alternative approach to weighting: Petrov–Galerkin

# Proper Orthogonal Decomposition (POD): Construct A Basis

- Consider set of snapshots (in time) in matrix $\mathbf{Y}$.

$$\mathbf{Y} = (\mathbf{y}_1, \mathbf{y}_2, \cdots, \mathbf{y}_m)$$

$$\text{Typical}: \mathbf{Y} = (\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_m)$$
$$\text{Mass–Free}: \mathbf{Y} = (\mathbf{u}_1 - \mathbf{u}_s, \mathbf{u}_2 - \mathbf{u}_s, \cdots, \mathbf{u}_m - \mathbf{u}_s)$$

- Basis $\Phi \in \mathbb{R}^{n \times r}$ which solves minimization problem in weighted $L^2$ space such as $X$

$$\min_{\text{Rank}(\Phi)=r} \sum_{i=1}^{m} ||\mathbf{y}_i - \Phi\Phi^* \mathbf{y}_i||_X^2$$
$$\text{subject to } \Phi^*\Phi = \mathbf{I}_r$$

- Solve eigenvalue problem / SVD for most dominant $r$ modes in $X$ space
- Reduced space $X_r = (\mathbb{R}^r, (\cdot,\cdot)_{X_r})$, Euclidean inner product

$$\Phi : X_r \to X$$
$$\Phi^* : X \to X_r$$

# Galerkin Projection: POD-ROM

- Consider Hamiltonian System

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

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

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

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

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

- Strong Form

$$\frac{\mathrm{d}\mathbf{a}}{\mathrm{d}t} = \Phi^* \mathbf{J}_X[\Phi\mathbf{a} + \mathbf{u}_\mathrm{s}]\boldsymbol{\nabla}^X \boldsymbol{H}[\Phi\mathbf{a} + \mathbf{u}_\mathrm{s}]$$

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

# Structure-Preserving Reduced Order Model

- How to retain Hamiltonian structure?
- Following Gong, Wang, Wang 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

$$\frac{\mathrm{d}\mathbf{a}}{\mathrm{d}t} = \Phi^* \mathbf{J}_X[\Phi\mathbf{a} + \mathbf{u_s}]\boldsymbol{\nabla}^X \boldsymbol{H}[\Phi\mathbf{a} + \mathbf{u_s}] \approx \mathbf{J}_{X_r}[\mathbf{a}]\Phi^* \boldsymbol{\nabla}^X \boldsymbol{H}[\Phi\mathbf{a} + \mathbf{u_s}]$$

$$= \Phi^* \mathbf{J}_X[\Phi\mathbf{a} + \mathbf{u_s}]\Phi\Phi^* \boldsymbol{\nabla}^X \boldsymbol{H}[\Phi\mathbf{a} + \mathbf{u_s}]$$

- Define $\bar{\boldsymbol{H}}[\mathbf{a}] = \boldsymbol{H}[\Phi\mathbf{a} + \mathbf{u_s}]$

$$\Phi^* \boldsymbol{\nabla}^X \boldsymbol{H}[\Phi\mathbf{a} + \mathbf{u_s}] = \nabla^{X_r} \bar{\boldsymbol{H}}[\mathbf{a}]$$

- Hamiltonian reduced model: Conserves Energy

$$\frac{\mathrm{d}\mathbf{a}}{\mathrm{d}t} = \mathbf{J}_{X_r}[\mathbf{a}]\Phi^* \boldsymbol{\nabla}^{X_r} \bar{\boldsymbol{H}}[\mathbf{a}]$$

# 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*

$$\int_0^T ||\mathbf{u}(t) - (\Phi\mathbf{a}(t) + \mathbf{u_s})||_X^2 \, \mathrm{d}t \leq C(T) \left( \int_0^T ||\mathbf{u}(t) - \Phi\Phi^*\mathbf{u}(t)||_X^2 \, \mathrm{d}t + \int_0^T ||\nabla^X \boldsymbol{H}[\mathbf{u}(t)] - \Phi\Phi^*\nabla^X \boldsymbol{H}[\mathbf{u}(t)]||_X^2 \, \mathrm{d}t \right) ,$$

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

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

$$\mathbf{Y} = (\mathbf{u}_1 - \mathbf{u_s}, \mathbf{u}_2 - \mathbf{u_s}, \ldots, \mathbf{u}_m - \mathbf{u_s}, \nabla^X \boldsymbol{H}[\mathbf{u}_1], \nabla^X \boldsymbol{H}[\mathbf{u}_2], \ldots, \nabla^X \boldsymbol{H}[\mathbf{u}_m]) ,$$

# A Blessing and a Curse

- New snapshots give typically error estimate and convergence

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

where $d$ is number of singular values in SVD.

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

# Mass Conservation

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

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

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

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

$$\boldsymbol{H}' = (\nabla^{X_c} \boldsymbol{H}, \psi)_X = (\nabla^X \boldsymbol{H}, \psi)_X \ , \forall \psi \in X_c \ ,$$

$$(1_X, \nabla^{X_c} \boldsymbol{H}) = 0$$

- Satisfied by adding Lagrange multiplier

$$\nabla^{X_c} \boldsymbol{H}[\mathbf{u}] = \nabla^X \boldsymbol{H}[\mathbf{u}] + \lambda \mathbf{1}_X$$

$$(\nabla^{X_c} \boldsymbol{H}, \psi)_X = (\nabla^X \boldsymbol{H}, \psi)_X + \lambda(\mathbf{1}_X, \psi) = (\nabla^X \boldsymbol{H}, \psi)_X \ , \forall \psi \in X_c$$

- Second condition leads to

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

# Mass–Conserving HSP–ROM

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

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

- How full is model changed?

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

- Model not effected. What about the reduced model

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

# Quadratic Hamiltonians and Approximate Energy Space

- We have not specified weighting $\boldsymbol{\Omega}$
- Claim: An optimal $\boldsymbol{\Omega}$ exists for Quadratic Hamiltonian systems
- Let $\boldsymbol{\Omega} = \nabla^2 \boldsymbol{H}$, $\nabla^2 \boldsymbol{H}$ is SPD, $X$ is now "approximate energy inner product space"
- For $\boldsymbol{H}_q$ given by quadratic form

$$\boldsymbol{H}_q[\mathbf{u}] = (\mathbf{u}, \mathbf{u})_X$$

## Theorem

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

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

*which means that $\mathbf{u}_s = \mathbf{u}_{eq}$, then the projection of $\nabla^X \boldsymbol{H}[\Phi\mathbf{a} + \mathbf{u}_{eq}]$ in the space $X$, $\Phi\Phi^* \nabla^X \boldsymbol{H}[\Phi\mathbf{a} + \mathbf{u}_{eq}]$, is exact*

$$\nabla^X \boldsymbol{H}[\mathbf{u}_{eq} + \Phi\mathbf{a}] - \Phi\Phi^* \nabla^X \boldsymbol{H}[\mathbf{u}_{eq} + \Phi\mathbf{a}] = 0 \ .$$

# Quadratic Hamiltonians and Approximate Energy Space

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### Theorem

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

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

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

*where $\mathbf{u}_s$ is some appropriate shift. Furthermore, also let the basis $\Phi$, 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 $\hat{\Phi}\hat{\Phi}^* \nabla^X \boldsymbol{H}[\mathbf{u}_s + \Phi \mathbf{a}]$ is exact*

$$\nabla^X \boldsymbol{H}[\mathbf{u}_s + \Phi \mathbf{a}] = \hat{\Phi}\hat{\Phi}^* \nabla^X \boldsymbol{H}[\mathbf{u}_s + \Phi \mathbf{a}] \ . \qquad (1)$$

# Equivalence of POD-ROM and HSP-ROM

## Theorem

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

$$\frac{\mathrm{d}\mathbf{a}(t)}{\mathrm{d}t} = \mathbf{J}_{X_r}[\mathbf{a}(t) + \mathbf{u_s}]\nabla^{X_r}\boldsymbol{H}[\mathbf{a}(t)] = \Phi^*\mathbf{J}[\Phi\mathbf{a}(t)]\nabla\boldsymbol{H}[\Phi\mathbf{a}(t) + \mathbf{u_s}] \ . \tag{2}$$

*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 Esitmate Quadratic Hamiltonian

## Theorem

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

$$\mathbf{Y} = (\widetilde{\mathbf{u}}_1, \widetilde{\mathbf{u}}_2, \ldots, \widetilde{\mathbf{u}}_m) ,$$

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

$$\int_0^T \|\mathbf{u}(t) - (\mathbf{u}_s + \hat{\Phi}\mathbf{a}(t))\|_X^2 \, \mathrm{d}t = \int_0^T \|\widetilde{\mathbf{u}}(t) - \hat{\Phi}\mathbf{a}(t)\|_X^2 \, \mathrm{d}t$$

$$\leq \widetilde{C}(T) \int_0^T ||\mathbf{u}(t) - \hat{\Phi}\hat{\Phi}^* \mathbf{u}(t)||_X \, \mathrm{d}t = \widetilde{C}(T) \sum_{k=r+1}^{d} \lambda_k ,$$

*where for a solution independent* **J** *we have,* $\widetilde{C}(T) = 1 + \widetilde{C}_2^2 T$ *, and for a solution dependent* **J** *we have where* $\widetilde{C}(T) = 1 + \hat{C}_2^2 \beta(T) T$ *, 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 conserves energy
- POD 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.

# Application to the RSWE

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

# Energy Conserving Test Case

- Demonstrate energy conservation to truncation error for HSP-ROM
- Ocean basis 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

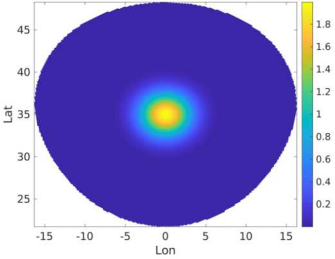



Figure: The geostrophic initial condition for **h** (left) and **v** (right).

# Numerical Results

| Method | Space | $\text{Error}_{t_{\text{final}}, X}$ | $\text{Error}_{\textbf{Energy, rel}}$ |
|---|---|---|---|
| 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

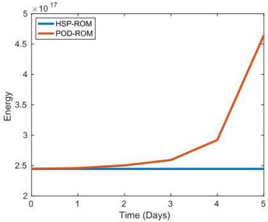
| Method | Space | $\text{Error}_{t_{\text{final}}, X}$ | $\text{Error}_{\textbf{Energy, rel}}$ |
|---|---|---|---|
| HSP-ROM | $X$ | 2.45e-2 | 1.04e-11 |
| HSP-ROM | $H$ | 1.79 | 1.79e-11 |
| POD-ROM | $X$ | 2.52e-2 | 3.72e-4 |
| POD-ROM | $H$ | 1.06 | 5.34e-2 |

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

# Numerical Results: 25 Basis Function

| Method | Space | $\text{Error}_{t_{\textbf{final}}, X}$ | $\text{Error}_{\textbf{Energy, rel}}$ |
|---|---|---|---|
| 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



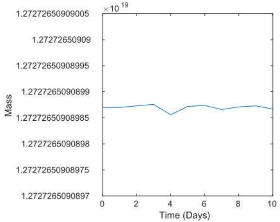




Figure: Energy of HSP-ROM and POD-ROM with a decoupled basis in $H$ (left). Mass of HSP-ROM method (right).

# Conclusions and Future Research

## Conclusions

- Method in Gong 2017 extended to weighted Hilbert space
- Convergent method with mass conservation
- Approximate energy space gives vast advantages
- Poisson Bracket interpretation is natural

## Future Research

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

# Petrov-Galerkin Interpretation

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

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

- New ansatz

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

- Reduced Model

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

# 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 $\mathbf{T} : X \to X$ such that*

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

- If we choose $X$ with trivial weighting and $\mathbf{T} = \boldsymbol{\Omega}$, we arrive at previous model.

- Thus for quadratic Hamiltonians, $\Psi = \nabla^2 \boldsymbol{H}\Phi$ is optimal basis for $\nabla^X \boldsymbol{H}[\mathbf{u}]$

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

# The Poisson Bracket

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

$$\frac{\mathrm{d}\boldsymbol{F}[\mathbf{u}]}{\mathrm{d}t} = \left(\frac{\partial \boldsymbol{F}[\mathbf{u}]}{\partial \mathbf{u}}, \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t}\right)_H$$

- Insert $\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t}$

$$\frac{\mathrm{d}\boldsymbol{F}[\mathbf{u}]}{\mathrm{d}t} = (\nabla \boldsymbol{F}[\mathbf{u}], \mathbf{J}[\mathbf{u}]\nabla \boldsymbol{H}[\mathbf{u}])_H$$

- Skew-symmetric bilinear form $\to$ Poisson bracket

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

- Invariant under of choice Hilbert space

$$\frac{\mathrm{d}\boldsymbol{F}[\mathbf{u}]}{\mathrm{d}t} = \{\boldsymbol{F}[\mathbf{u}], \boldsymbol{H}[\mathbf{u}]\}[\mathbf{u}]$$

# Weak Formulation of Hamiltonian Systems

- Weak formulation for Hamiltonian system

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

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

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

$$\frac{\mathrm{d}\boldsymbol{F}_{\mathbf{z}}[\mathbf{u}]}{\mathrm{d}t} = \{\boldsymbol{F}_{\mathbf{z}}[\mathbf{u}], \boldsymbol{H}[\mathbf{u}]\}[\mathbf{u}] \ ,$$

specified in the space $H$

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

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

# Conserved Quantities and Casimirs

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

$$\frac{\mathrm{d}\boldsymbol{H}[\mathbf{u}]}{\mathrm{d}t} = \boldsymbol{H}[\mathbf{u}], \boldsymbol{H}[\mathbf{u}][\mathbf{u}] = 0;$$

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

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

which implies

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

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

- Mass is Casimir and linear-invariant in RSWE

$$(\mathbf{1}, \mathbf{h})_{\mathsf{l}} = c_{\mathsf{mass}}$$

- Casimir is

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

# Mass-Free Model

- Add $\lambda$ times linear Casimir to Hamiltonian, define mass–free $\nabla^{H_c}$

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

- Linear Casimirs make finding $\lambda$ easy
- Insert into Poisson Bracket

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

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

# HSP-ROM from the Poisson bracket

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

$$\frac{\mathrm{d}\boldsymbol{F}_{\mathbf{z}}[\mathbf{u}]}{\mathrm{d}t} = \{\boldsymbol{F}_{\mathbf{z}}[\mathbf{u}], \nabla \boldsymbol{H}[\mathbf{u}]\}[\mathbf{u}] \ ,$$

- Ansatz

$$\mathbf{u} = \Phi \mathbf{a}$$

$$\nabla \mathbf{F} = \Psi \Phi^* \nabla \mathbf{F}$$

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

$$\frac{\mathrm{d}\boldsymbol{F}_{\mathbf{z}}[\mathbf{u}]}{\mathrm{d}t} = (\Psi\Phi^* \nabla \boldsymbol{F}_{\mathbf{z}}[\Phi\mathbf{a}], \mathbf{J}[\Phi\mathbf{a}]\Psi\Phi^*\nabla \boldsymbol{H}[\Phi\mathbf{a}]) = (\Psi\mathbf{w})^*\Phi\Psi^*\mathbf{J}[\Phi\mathbf{a}]\Psi\Phi^*\nabla \boldsymbol{H}[\Phi\mathbf{a}] =$$

$$= \{\nabla \boldsymbol{F}_{\mathbf{z}}[\mathbf{u}], \nabla \boldsymbol{H}[\mathbf{u}]\}_r[\mathbf{a}] \ ,$$

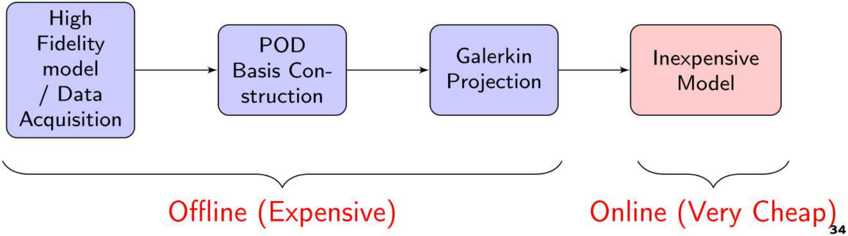
where

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

- 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:

$$\Phi = \begin{pmatrix} \Phi_\mathsf{x} \\ \Phi_\mathsf{z} \end{pmatrix} .$$

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

$$\Phi = \begin{pmatrix} \Phi_\mathsf{x} & 0 \\ 0 & \Phi_\mathsf{z} \end{pmatrix} ,$$

- Preserves block structure, variable number of basis functions. Two variables $\mathbf{a} = (\mathbf{a}_\mathsf{x}, \mathbf{a}_\mathsf{z})$

# Galerkin Projection: POD-ROM



- Consider Hamiltonian System

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{J}[\mathbf{u}]\nabla \boldsymbol{H}[\mathbf{u}]$$

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

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

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

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

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

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

- Strong Form

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

- $\Phi^* \mathbf{J}[\Phi\mathbf{a}]$ is not skew symmetric in general! No Poisson bracket!

# SOMA Inspired Test Case

- 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 $\mathbf{h}$)

# Coupled Versus Decoupled basis

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

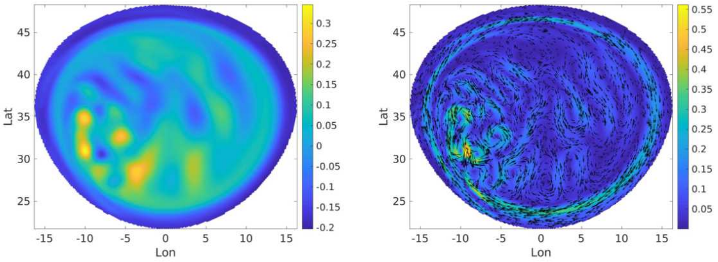



Figure: The spin-up initial condition in the SOMA test case for **h** (left) and **v** (right).

# Coupled Versus Decoupled Basis

| Method | Basis Type | r | SYPD | $\text{Error}_{t_{\text{final}}}$ | $\text{Error}_{\text{RMSSSHA},H,\text{rel}}$ |
|---|---|---|---|---|---|
| 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

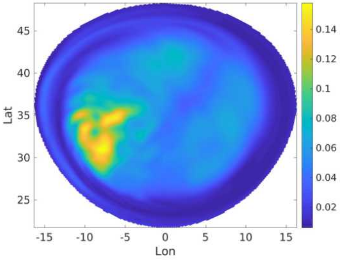



Figure: (Example 3) The RMSSSHA for the full model over one year

# Coupled Versus Decoupled Basis: HSP-ROM

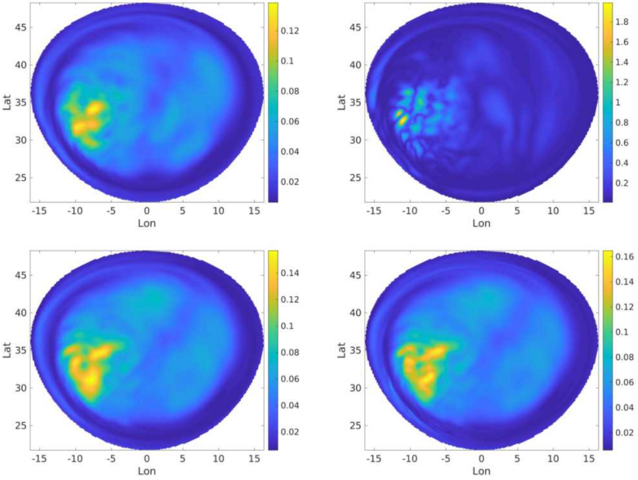



Figure: The RMSSSHA for the coupled basis with 45 basis functions (top left), for the decoupled basis with 45 basis functions(top right), for the coupled basis with 125 basis functions (bottom left), and for the decoupled basis with 125 basis functions(bottom right) using the HSP-ROM method

# Coupled Versus Decoupled Basis: POD-ROM



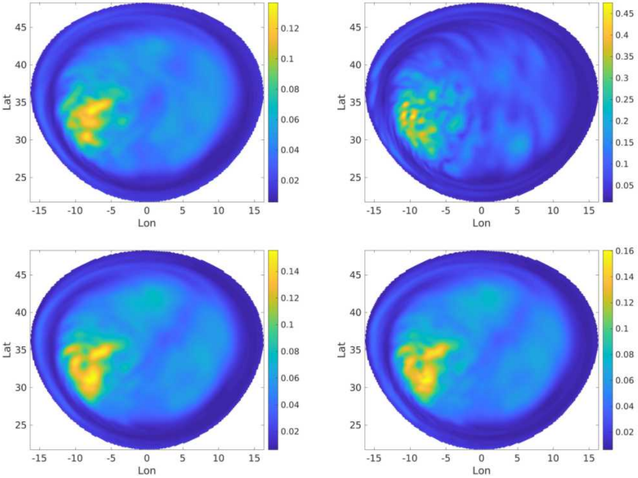



Figure: The RMSSSHA for the coupled basis with 45 basis functions (top left), for the decoupled basis with 45 basis functions(top right), for the coupled basis with 125 basis functions (bottom left), and for the decoupled basis with 125 basis functions(bottom right) using the POD-ROM method

# Prediction and Validation

- 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 | $\text{Error}_{\text{RMSSSHA},H,\text{rel}}$ |
|---|---|---|---|
| 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).

# Prediction and Validation



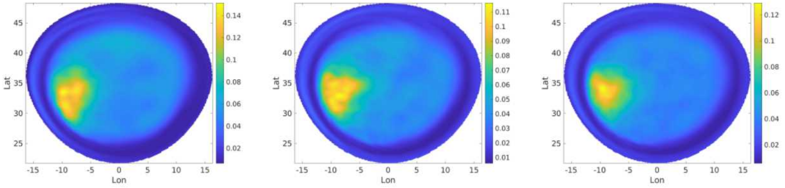



Figure: The RMSSSHA over ten years for the full model (left), for the HSP-ROM model (center), and the POD-ROM model (right).

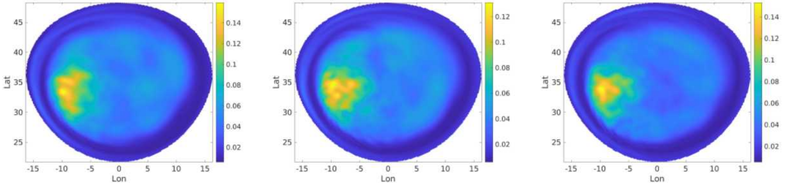



Figure: The RMSSSHA over the additional two years for full model (left), for the HSP-ROM model prediction (center), and the POD-ROM model prediction (right).

# Century Predictions

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

# Century Predictions

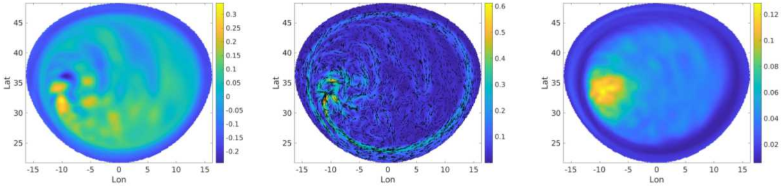



Figure: The solution, **h** and **v**, at the end of the century time-horizon and the RMSSSHA over the century time-horizon for the HSP-ROM method.

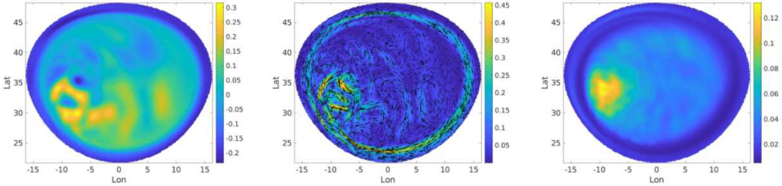



Figure: The solution, **h** and **v**, at the end of the century time-horizon and the RMSSSHA over the century time-horizon for the HSP-ROM method.

# Century Predictions: Mass and Energy

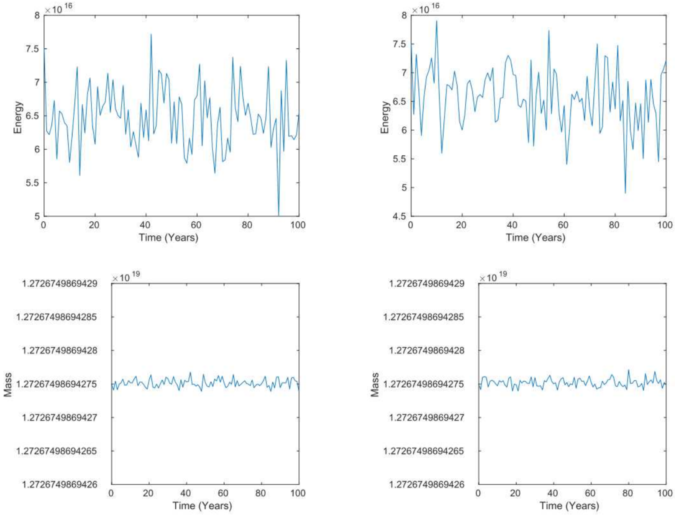



Figure: The energy (top-left) and mass (bottom-left) for the HSP-ROM method, and the energy (top-right) and mass (bottom-right) for the POD-ROM method over the century time horizon

# Conclusions and Future Research

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## 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