Mass Conserving Hamiltonian-Structure-P SAND2019-9513PE Modeling for the Rotating Shallow Water Equations Discretized by a Mimetic Spatial Scheme

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Motivation: Ocean-Climate Modeling

- High-Resolution ocean-climate modeling
- Future exascale machines
- Adding more physics and resolution

MPAS-O
Model for Prediction Across Scales

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EST.1943

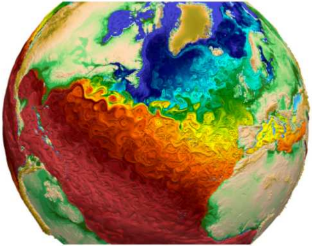


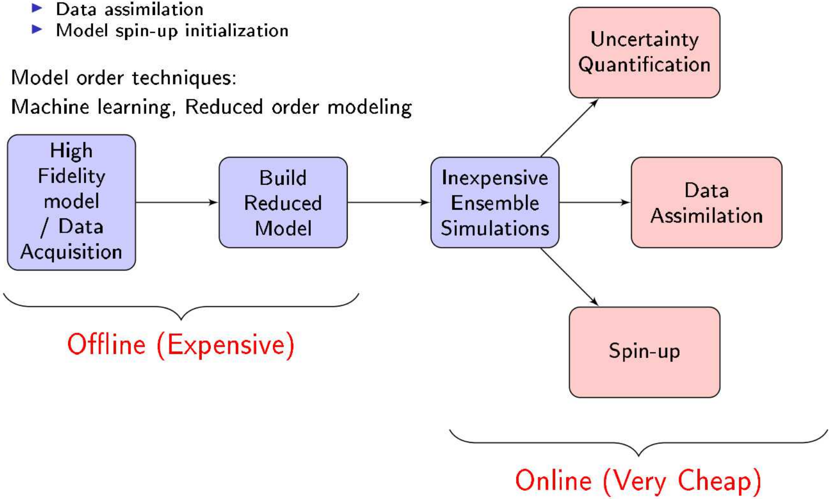
Figure: Temperature from E3SM simulation

E3SM
Energy Exascale
Earth System Model

DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA

Motivation: Ocean-Climate Modeling

- Models are more complicated not faster
- Biases and uncertainty still exist
- Infeasible applications
  - Uncertainty quantification
  - Data assimilation
  - Model spin-up initialization
- Model order techniques:
  Machine learning, Reduced order modeling



Model Order Reduction: Challenges for the Ocean

Challenges

- Long time-horizons
- Hyperbolic PDE's: waves and transport
- Multiple time-scales
- Highly nonlinear behavior
- Transient effects
- Conservation properties: mass and energy

Novel Contributions

- Hamiltonian-structure-preserving reduced order model in Hilbert space from Poisson bracket
- Use of novel inner product which improves accuracy
- Mass conservation derived for model: Any linear invariant - Casimir can be preserved
- Error analysis
- Lifting technique for potential vorticity
- Simulations

Rotating Shallow Water Equations (RSWE)

Serves as proxy to ocean model (primitive equations)

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

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

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

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

- 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

Mimetic TRiSK Spatial Discretization Scheme

- Spherical Centroidal Voronoi tessellation - Delaunay triangulation dual mesh: Covolume scheme

- Normal velocity with respect to cell $\mathbf{v}$

- Discrete quantities:

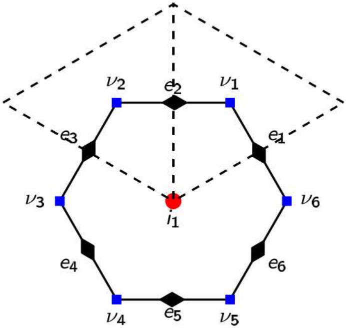
$$\mathbf{h} \in H_{\mathsf{I}} = (\mathbb{R}^{N_{\mathsf{I}}}, (\cdot,\cdot)_{\mathsf{I}}) \ , \quad (\mathbf{h},\mathbf{h})_{\mathsf{I}} = \mathbf{h}^\top \mathbf{M}_i \mathbf{h} \ ,$$
$$\mathbf{v} \in H_{\mathsf{E}} = (\mathbb{R}^{N_{\mathsf{E}}}, (\cdot,\cdot)_{\mathsf{E}}) \ , \quad (\mathbf{v},\mathbf{v})_{\mathsf{E}} = \mathbf{v}^\top \mathbf{M}_e \mathbf{v} \ ,$$
$$\mathbf{q} \in H_{\mathsf{V}} = (\mathbb{R}^{N_{\mathsf{V}}}, (\cdot,\cdot)_{\mathsf{V}}) \ , \quad (\mathbf{q},\mathbf{q})_{\mathsf{V}} = \mathbf{q}^\top \mathbf{M}_\nu \mathbf{q}$$

  - $\mathbf{M}_i$: Cell areas
  - $\mathbf{M}_v$: Triangle areas
  - $\mathbf{M}_e$: "Edge" areas

- Discrete operator mimic properties of continuous operators

$$(\widetilde{\boldsymbol{\nabla}}\mathbf{h},\mathbf{v})_{\mathsf{E}} = -(\mathbf{h},\widetilde{\boldsymbol{\nabla}\cdot}\mathbf{v})_{\mathsf{I}}$$

$$(\widetilde{\hat{k}\times}\mathbf{v},\mathbf{z})_{\mathsf{E}} = -(\mathbf{v},\widetilde{\hat{k}\times}\mathbf{z})_{\mathsf{E}}$$



Cell centers: $\mathsf{I} = \{i_1, i_2, \ldots, i_{N_{\mathsf{I}}}\}$

Cell vertices: $\mathsf{V} = \{\nu_1, \nu_2, \ldots, \nu_{N_{\mathsf{V}}}\}$

Edge centers: $\mathsf{E} = \{e_1, e_2, \ldots, e_{N_{\mathsf{E}}}\}$

Hamiltonian Framework

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

$$(\mathbf{u}, \mathbf{u})_H = \mathbf{u}^\top \mathbf{M} \mathbf{u} = (\mathbf{h}, \mathbf{h})_\mathsf{I} + (\mathbf{v}, \mathbf{v})_\mathsf{E}$$

- Energy conservation at abstract level: Two ingredients required
- Skew-adjoint operator $\mathbf{J}[\mathbf{u}]$

$$\mathbf{J}[\mathbf{u}] = \begin{pmatrix} 0 & -\widetilde{\boldsymbol{\nabla}\cdot} \\ -\widetilde{\boldsymbol{\nabla}} & \mathbf{q}\widetilde{\hat{k}\times} \end{pmatrix}.$$

- Hamiltonian (total energy), $\{\cdot\}$ denotes interpolation operator

$$H[\mathbf{u}] = (\{\mathbf{h}\}_\mathsf{E} * \mathbf{v}, \mathbf{v})_\mathsf{E} + g(\mathbf{h}, \mathbf{h} + 2\mathbf{b})_\mathsf{I}$$

- Gradient of Hamiltonian

$$\nabla H[\mathbf{u}] = \begin{pmatrix} \{\mathbf{v}^2\}_\mathsf{I} + g(\mathbf{h} + \mathbf{b}) \\ \{\mathbf{h}\}_\mathsf{E}\mathbf{v} \end{pmatrix}$$

- RSWE are non-canonical Hamiltonian system:

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

- $\mathbf{G}[\mathbf{u}]$ 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 $\boldsymbol{H}_{\mathbf{qf}}[\mathbf{u}]$, then

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

- Approximate energy space $X = (\mathbb{R}^n, (\cdot,\cdot)_X)$; Let $\boldsymbol{\Omega} = \nabla^2 \boldsymbol{H}[\mathbf{u}_{\mathbf{ref}}]$

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

The Poisson Bracket

- Time evolution of a functional of the solution $\mathbf{u}$, $\boldsymbol{F}[\mathbf{u}]$

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

- 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

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

Conserved Quantities and Casimirs

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

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

- 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

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

  which implies

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

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

- Mass is Casimir and linear-invariant in RSWE

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

- Casimir is

$$\boldsymbol{C}_{\mathsf{mass}}[\mathbf{u}] = (\mathfrak{L}, \mathbf{u})_H$$

$$\mathfrak{L} = \begin{pmatrix} \mathbf{1} \\ 0 \end{pmatrix} \in H$$

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 $\boldsymbol{F}_{\mathbf{z}}[\mathbf{u}] = (\mathbf{z}, \mathbf{u})_H$

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

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

Weak Formulation of Hamiltonian Systems

- Utilize the invariance of the Poisson Bracket

- Consider discrete, weighted L^2 space such as X
$$\mathcal{J}[\mathbf{u}](\cdot,\cdot) = (\nabla, \mathbf{J}[\mathbf{u}]\nabla)_H = (\nabla^X, \mathbf{J}_X[\mathbf{u}]\nabla^X)_X$$

- The gradient in X
$$\boldsymbol{H}'[\mathbf{u};\mathbf{z}] = (\nabla \boldsymbol{H}[\mathbf{u}], \mathbf{z})_H = (\nabla^X \boldsymbol{H}[\mathbf{u}], \mathbf{z})_X \Leftrightarrow \nabla^X \boldsymbol{H}[\mathbf{u}] = \boldsymbol{\Omega}^{-1}\nabla \boldsymbol{H}[\mathbf{u}]$$

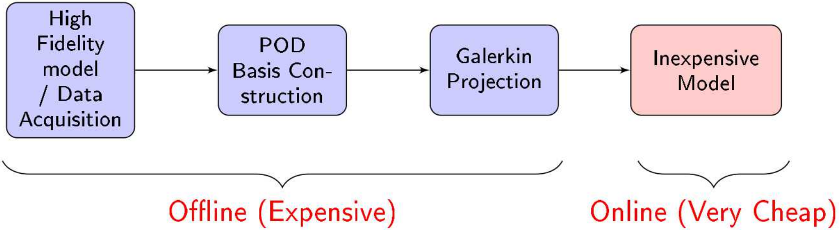
- The skew-adjoint operator in X
$$\mathcal{J}[\mathbf{u}](\cdot,\cdot) = (\nabla, \mathbf{J}[\mathbf{u}]\nabla)_H = (\nabla^X, \mathbf{J}_X[\mathbf{u}]\nabla^X)_X = (\boldsymbol{\Omega}^{-1}\nabla, \mathbf{J}_X[\mathbf{u}]\boldsymbol{\Omega}^{-1}\nabla)_X = (\nabla, \mathbf{J}_X[\mathbf{u}]\boldsymbol{\Omega}^{-1}\nabla)_H$$
implies that $\mathbf{J}_X[\mathbf{u}] = \mathbf{J}[\mathbf{u}]\boldsymbol{\Omega}$

- Consider $\boldsymbol{F}_{\mathbf{x}}[\mathbf{u}] = (\mathbf{x}, \mathbf{u})_X$
$$\frac{\mathrm{d}\boldsymbol{F}_{\mathbf{x}}[\mathbf{u}]}{\mathrm{d}t} = \left(\mathbf{x}, \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t}\right)_X = \mathcal{J}[\mathbf{u}](\boldsymbol{F}_{\mathbf{x}}[\mathbf{u}], \boldsymbol{H}[\mathbf{u}]) = (\mathbf{x}, \mathbf{J}_X[\mathbf{u}]\nabla^X \boldsymbol{H}[\mathbf{u}])_X$$

- Strong form doesn't change
$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{J}[\mathbf{u}]\nabla \boldsymbol{H}[\mathbf{u}]$$

Reduced Order Modeling (ROM)

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



Proper Orthogonal Decomposition (POD)

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

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

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

$$\min_{\text{Rank}(\Phi)=r} ||\mathbf{Y} - \Phi\Phi^*\mathbf{Y}||_X^2$$
$$\text{subject to } \Phi^*\Phi = \mathbf{I}_r$$

- Solve eigenvalue problem / SVD for most dominant r modes

$$\mathbf{Y}^\top \mathbf{M}_X \mathbf{Y} = \mathbf{V}\boldsymbol{\Lambda} \leftrightarrow \mathbf{M}_X^{1/2}\mathbf{Y} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^\top$$

- The reduced basis Φ=$\mathbf{M}_X^{-1/2}\mathbf{U}$; Adjoint: $\rightarrow \Phi^* = \Phi^\top \mathbf{M}_X$, Projection:$\Phi\Phi^*$

- Reduced space $X_r = (\mathbb{R}^r, (\cdot,\cdot)_{X_r})$, Euclidean inner product

$$\Phi : \; X_r \rightarrow X$$
$$\Phi^* : \; X \rightarrow X_r$$

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:
$$\Phi = \begin{pmatrix} \Phi_\mathbf{x} \\ \Phi_\mathbf{z} \end{pmatrix} .$$
- Does not preserve block structure of problem. One variable $\mathbf{a}$
- SVD on each variable: Basis
$$\Phi = \begin{pmatrix} \Phi_\mathbf{x} & 0 \\ 0 & \Phi_\mathbf{z} \end{pmatrix} ,$$
- Preserves block structure, variable number of basis functions. Two variables $\mathbf{a} = (\mathbf{a}_\mathbf{x}, \mathbf{a}_\mathbf{z})$

Galerkin Projection: POD-ROM

- Consider Hamiltonian System

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

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

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

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

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

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

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

- Strong Form

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

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

Hamiltonian-Structure-Preserving ROM (HSP-ROM)

- Idea: Build Hamiltonian reduced order model
- Start with Poisson bracket. Ansatz that dynamics are in reduced space.

$$\mathcal{J}[\mathbf{a}](\cdot,\cdot) = (\nabla^X, \mathbf{J}_X[\Phi\mathbf{a}]\nabla^X)_X = (\nabla^{X_r}, \mathbf{J}_{X_r}[\mathbf{a}]\nabla^{X_r})_{X_r}$$

- Let $\bar{H}[\mathbf{a}] = H[\Phi\mathbf{a}]$. Gradient in X_r

$$H'[\Phi\mathbf{a};\Phi\mathbf{w}] = (\nabla^X H[\Phi\mathbf{a}], \Phi\mathbf{w})_X = (\nabla^{X_r}\bar{H}[\mathbf{a}], \mathbf{w})_{X_r}$$
$$\Leftrightarrow \nabla^{X_r}\bar{H}[\mathbf{a}] = \Phi^*\nabla^X H[\Phi\mathbf{a}] = \Phi^*\Omega^{-1}\nabla H[\Phi\mathbf{a}]$$

- Ansatz leads to $\nabla^X = \Phi\Phi^*\nabla^X$

$$\mathcal{J}[\mathbf{a}](\cdot,\cdot) = (\Phi\Phi^*\nabla^X, \mathbf{J}_X[\Phi\mathbf{a}]\Phi\Phi^*\nabla^X)_X = (\Phi^*\nabla^X, \Phi^*\mathbf{J}_X[\mathbf{a}]\Phi\Phi^*\nabla^X)_{X_r} = (\nabla^{X_r}, \mathbf{J}_{X_r}[\mathbf{a}]\nabla^{X_r})_{X_r}$$

- Implies that $\mathbf{J}_{X_r}[\Phi\mathbf{a}] = \Phi^*\mathbf{J}_X[\mathbf{a}]\Phi$

Hamiltonian-Structure-Preserving ROM (HSP-ROM)

- Functional $\boldsymbol{F}_{\mathbf{w}}[\mathbf{a}] = (\mathbf{w}, \mathbf{a})_{X_r}$

$$\frac{\mathrm{d}\boldsymbol{F}_{\mathbf{w}}[\mathbf{a}]}{\mathrm{d}t} = \mathcal{J}[\mathbf{a}](\boldsymbol{F}_{\mathbf{w}}[\mathbf{a}], \bar{\boldsymbol{H}}[\mathbf{a}])$$

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

- Strong form

$$\frac{\mathrm{d}\mathbf{a}}{\mathrm{d}t} = \mathbf{J}_{X_r}[\mathbf{a}]\nabla^{X_r}\bar{\boldsymbol{H}}[\mathbf{a}] = \Phi^*\mathbf{J}[\Phi\mathbf{a}]\boldsymbol{\Omega}\Phi\Phi^*\boldsymbol{\Omega}^{-1}\nabla\boldsymbol{H}[\Phi\mathbf{a}]$$

- Conservation of energy

$$\frac{\mathrm{d}\bar{\boldsymbol{H}}[\mathbf{a}]}{\mathrm{d}t} = \mathcal{J}[\mathbf{a}](\bar{\boldsymbol{H}}[\mathbf{a}], \bar{\boldsymbol{H}}[\mathbf{a}]) = 0$$

Hamiltonian-Structure-Preserving ROM (HSP-ROM)

- 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*

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

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

- $\Phi\Phi^*\nabla^X \boldsymbol{H}[\Phi\mathbf{a}] \rightarrow$ new snapshots

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

Preserving Linear Casimirs: Mass Conservation

- In POD-ROM mass conservation is trivial

$$\mathbf{u}(t) = \Phi \mathbf{a}(t) + \mathbf{u}_s$$

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

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

- $\mathbf{u}_s$ has correct mass. Initial condition or mean-flow
- Problem: $\nabla^X \boldsymbol{H}[\mathbf{u}]$ has no conserved first integral (mass)
- Solution: Build "mass free" model
- Mass is linear invariant and Casimir in RSWE

Mass Conserving Reduced Model

- Split solution $\mathbf{u}(t) = \widetilde{\mathbf{u}}(t) + \mathbf{u}_\mathrm{s}$, $\widetilde{\mathbf{u}} \in X_{\mathfrak{L}}$, such that

$$\boldsymbol{C}_{\mathrm{mass}}[\widetilde{\mathbf{u}} + \mathbf{u}_\mathrm{s}] = (\mathfrak{L}_X, \widetilde{\mathbf{u}})_X + (\mathfrak{L}_X, \mathbf{u}_\mathrm{s})_X = (\mathfrak{L}_X, \mathbf{u}_\mathrm{s})_X$$

- "Mass free" gradient

$$(\mathfrak{L}_X, \nabla^{X_{\mathfrak{L}}} \boldsymbol{H}[\mathbf{u}])_X = (\mathfrak{L}_X, \nabla^X \boldsymbol{H}[\mathbf{u}] + \mu \mathfrak{L}_X)_X = 0$$

$$\mu = -\frac{(\mathfrak{L}_X, \nabla^X \boldsymbol{H}[\mathbf{u}])_X}{(\mathfrak{L}_X, \mathfrak{L}_X)_X}$$

- Modify $\nabla^X \boldsymbol{H}$ snapshots

$$\mathbf{Y} = (\mathbf{u}_1 - \mathbf{u}_\mathrm{s}, \mathbf{u}_2 - \mathbf{u}_\mathrm{s}, \ldots, \mathbf{u}_m - \mathbf{u}_\mathrm{s}, \nabla^{X_{\mathfrak{L}}} \boldsymbol{H}[\mathbf{u}_1], \nabla^{X_{\mathfrak{L}}} \boldsymbol{H}[\mathbf{u}_2], \ldots, \nabla^{X_{\mathfrak{L}}} \boldsymbol{H}[\mathbf{u}_m]) \ ,$$

- Reduced Model: Modification to gradient is zero in Poisson bracket

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

Error Estimate

- Snapshots matrix

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

Theorem

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

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

$$= C(T) \sum_{i=r+1}^{d} \lambda_i \qquad (1)$$

where $C(T) = max\{1 + C_2^2 \alpha(T) T \ , \ C_3^2 \alpha(T) T\}$, and $\alpha(T) = 2 \int_0^T e^{(2C_1(T-\tau))} \, \mathrm{d}\tau$. $d = \dim(\mathbf{Y})$ and λ_i , $i = r+1, \ldots, d$ are the eigenvalues discarded in the POD process.

Quadratic Hamiltonians and Approximate Energy Space

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*

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

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

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

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

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

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 $\hat{\Phi}\hat{\Phi}^* \nabla^X \boldsymbol{H}[\mathbf{u}_s + \Phi\mathbf{a}]$ is exact

$$\nabla^X \boldsymbol{H}[\mathbf{u}_s + \Phi\mathbf{a}] = \hat{\Phi}\hat{\Phi}^* \nabla^X \boldsymbol{H}[\mathbf{u}_s + \Phi\mathbf{a}] \ . \tag{2}$$

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

$$\frac{\mathrm{d}\mathbf{a}(t)}{\mathrm{d}t} = \mathbf{J}_{X_r}[\mathbf{a}(t)]\nabla^{X_r}\boldsymbol{H}[\mathbf{a}(t)] = \Phi^*\mathbf{J}[\Phi\mathbf{a}(t)]\nabla\boldsymbol{H}[\Phi\mathbf{a}(t)]\ . \tag{3}$$

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 $\mathbf{u}$ *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*

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

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

Application to the RSWE

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

Treatment of Extraneous Terms

- Extraneous term $\mathbf{G}[\mathbf{u}]$ has the form

$$\mathbf{G}[\mathbf{u}] = \mathbf{S}[\mathbf{u}]\mathbf{u} + \mathbf{G}_{\text{wind}}$$

- $\mathbf{G}_{\text{wind}}$ contains prescribed wind forcing

$$\mathbf{G}_{\text{wind}} = \begin{pmatrix} 0 \\ \mathbf{g}_{\text{wind}} \end{pmatrix}$$

- $\mathbf{S}[\mathbf{u}]$ contains dissipative terms: Smoothing and dissipation (bottom drag) in $\mathbf{v}$ equation

- HSP-ROM can maintain dissipative behavior if

$$\mathbf{S}[\mathbf{u}]\mathbf{u} = \widetilde{\mathbf{S}}[\mathbf{u}]\nabla\mathbf{H}[\mathbf{u}]$$

- Then system is

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{J}_{\mathbf{S}}[\mathbf{u}]\nabla H[\mathbf{u}] + \mathbf{G}_{\text{wind}}$$

where

$$\mathbf{J}_{\mathbf{S}}[\mathbf{u}] = \mathbf{J}[\mathbf{u}] + \widetilde{\mathbf{S}}[\mathbf{u}]$$

Nonlinearities: Lifting and Tensor Methods

- Defining reduced model independently of fulls model's DOF
- Polynomial nonlinearities: tensor methods

$$\Phi^*(\Phi\mathbf{a} * \Phi\mathbf{a}) = \mathcal{T}_{ijk}\mathbf{a}_j\mathbf{a}_k$$

- $\mathbf{q} = (\widetilde{\nabla\times}\mathbf{u} + \mathbf{f})/\{\mathbf{h}\}_\mathsf{V}$ presents another challenge
- Lifting technique:

$$\{\mathbf{h}\}_\mathsf{V} * \mathbf{q} = (\widetilde{\nabla\times}\mathbf{u} + \mathbf{f})$$

- Basis for $\mathbf{q}$, $\boldsymbol{\Xi}$, in H space ($\boldsymbol{\Xi}^\dagger$ is adjoint in H)

$$\boldsymbol{\Xi}^\dagger(\{(\Phi_\mathbf{h}\mathbf{a}_\mathbf{h})\}\}_\mathsf{V} * (\boldsymbol{\Xi}\mathbf{a}_\mathbf{q})) = \boldsymbol{\Xi}^\dagger(\widetilde{\nabla\times}\Phi_\mathbf{u}\mathbf{a}_\mathbf{u} + \mathbf{f})$$

$$\mathbf{T}[\mathbf{a}_\mathbf{h}]\mathbf{a}_\mathbf{q} = \boldsymbol{\Xi}^\dagger(\widetilde{\nabla\times}\Phi_\mathbf{u}\mathbf{a}_\mathbf{u} + \mathbf{f})$$

- For coupled basis, $\mathbf{q}$ still has own reduced variable

Energy Conserving Test Case

- Demonstrate energy conservation to truncation error for HSP-ROM
- $\mathbf{G}[\mathbf{u}] = 0$ for this case
- 10 day, geostrophic initial condition
- RK4 time integrator with 75% of CFL constrained time-step in full model (approximately 80 seconds)
- Reproductive run

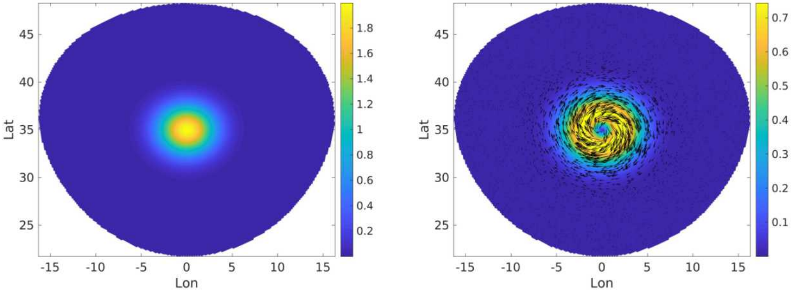


Figure: The geostrophic initial condition for **h** (left) and **v** (right).

Numerical Results

Method	Space	Basis	$\text{Error}_{t_{\text{final}},X}$	$\text{Error}_{\text{Energy, rel}}$
HSP-ROM	X	CP	2.90e-2	4.20e-8
HSP-ROM	X	DP	2.45e-2	6.82e-7
HSP-ROM	H	CP	6.77e-1	8.86e-8
HSP-ROM	H	DP	1.79	1.06e-6
POD-ROM	X	CP	2.13e-2	8.70e-3
POD-ROM	X	DP	2.54e-2	3.83e-4
POD-ROM	H	CP	7.45e-1	5.32e-1
POD-ROM	H	DP	1.06	5.34e-2

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

Method	Space	Basis	$\text{Error}_{t_{\text{final}},X}$	$\text{Error}_{\text{Energy, rel}}$
HSP-ROM	X	CP	2.90e-2	4.14e-13
HSP-ROM	X	DP	2.45e-2	1.04e-11
HSP-ROM	H	CP	6.77e-1	9.14e-13
HSP-ROM	H	DP	1.79	1.79e-11
POD-ROM	X	CP	2.13e-2	8.71e-3
POD-ROM	X	DP	2.52e-2	3.72e-4
POD-ROM	H	CP	7.45e-1	5.32e-1
POD-ROM	H	DP	1.06	5.34e-2

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

Numerical Results: 25 Basis Function

Method	Space	Basis	$\text{Error}_{t_{\text{final}},X}$	$\text{Error}_{\text{Energy, rel}}$
HSP-ROM	X	CP	2.82e-2	7.26e-7
HSP-ROM	X	DP	2.65e-2	1.47e-6
HSP-ROM	H	CP	4.84e-2	2.08e-6
HSP-ROM	H	DP	1.58	2.59e-6
POD-ROM	X	CP	2.16e-2	8.44e-3
POD-ROM	X	DP	2.59e-2	7.65e-5
POD-ROM	H	CP	5.13e-1	1.26e-1
POD-ROM	H	DP	—	—

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

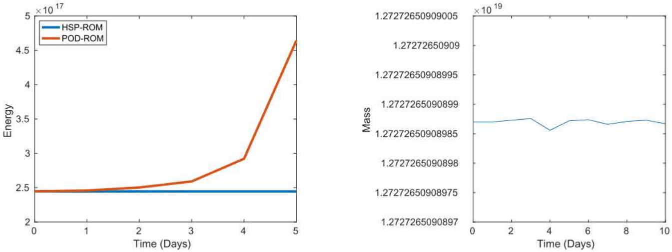


Figure: Energy of HSP-ROM and POD-ROM with a decoupled basis in H (left). Mass of HSP-ROM method (right).

SOMA Inspired Test Case

- Wind forcing, bottom drag, bi-harmonic smoothing
- Ten year spin-up initial condition
- Performance Test for HSP-ROM: ten times larger viscosity$\rightarrow$ smaller basis
- 1 year test case with model in X with decoupled basis
- Reproductive run

Method	r	$\Delta t / \Delta t_{\textbf{Full}}$	SYPD	$\text{Error}_{t_{\textbf{final}}}$
Full	—	1	2.09	—
HSP-ROM	15	10	576	2.85e-1
HSP-ROM	15	100	5743	2.85e-1
HSP-ROM	25	10	321	5.58e-2
HSP-ROM	25	100	3206	5.59e-2
HSP-ROM	45	10	103	1.14e-2
HSP-ROM	45	100	1026	1.15e-2

Table: Performance and errors for different basis sizes and time-step sizes

Coupled Versus Decoupled basis

- Prescribed bi-harmonic smoothing: harder test case
- In this case statistics will be compared, the RMSSSHA (square root of the variance in **h**)
- POD-ROM and HSP-ROM methods tested for 1 year with coupled and decoupled basis in X

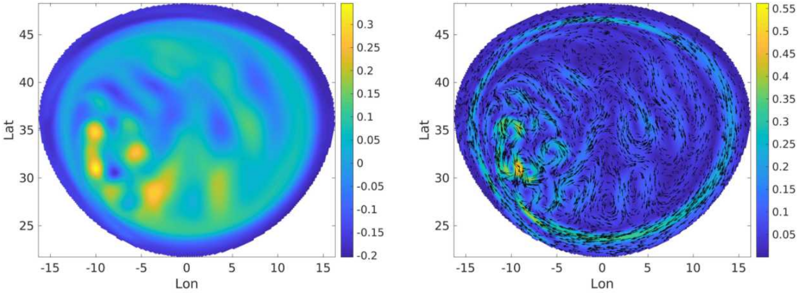


Figure: The spin-up initial condition in the SOMA test case for **h** (left) and **v** (right).

Coupled Versus Decoupled Basis

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

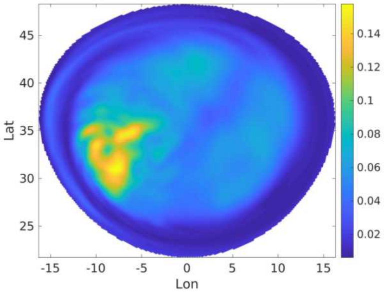


Figure: (Example 3) The RMSSSHA for the full model over one year

Coupled Versus Decoupled Basis: HSP-ROM

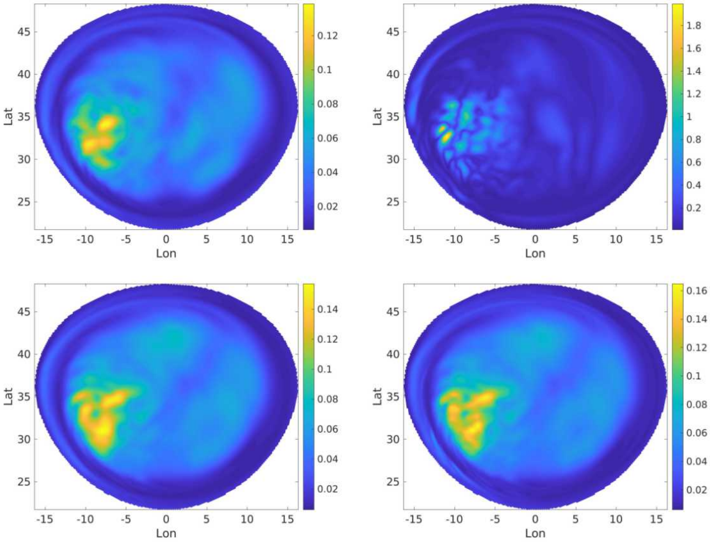


Figure: The RMSSSHA for the coupled basis with 45 basis functions (top left), for the decoupled basis with 45 basis functions(top right), for the coupled basis with 125 basis functions (bottom left), and for the decoupled basis with 125 basis functions(bottom right) using the HSP-ROM method

Coupled Versus Decoupled Basis: POD-ROM

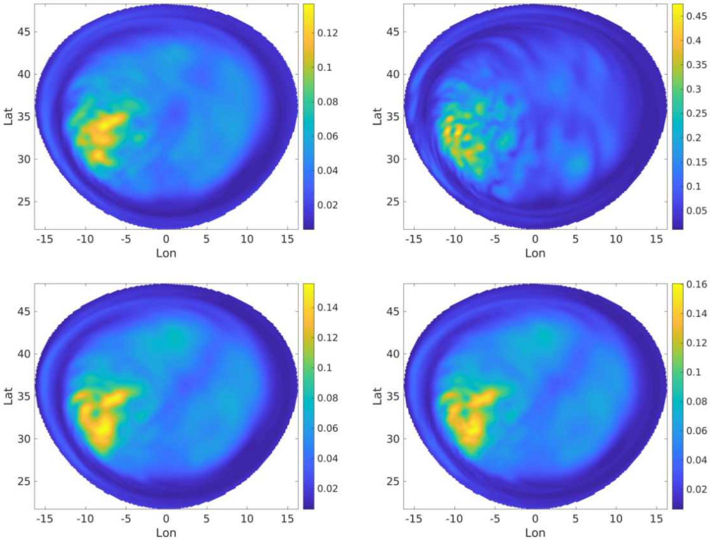


Figure: The RMSSSHA for the coupled basis with 45 basis functions (top left), for the decoupled basis with 45 basis functions(top right), for the coupled basis with 125 basis functions (bottom left), and for the decoupled basis with 125 basis functions(bottom right) using the POD-ROM method

Prediction and Validation

- 10 year reproductive test case to build basis, 2 year prediction
- Coupled basis in X
- 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

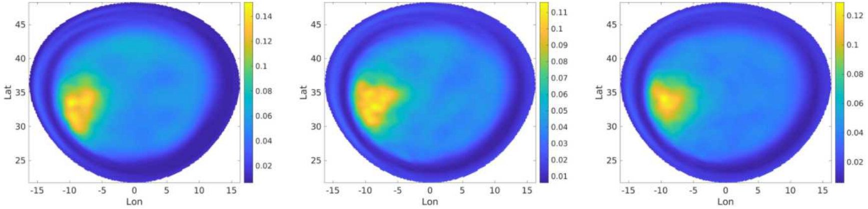


Figure: The RMSSSHA over ten years for the full model (left), for the HSP-ROM model (center), and the POD-ROM model (right).

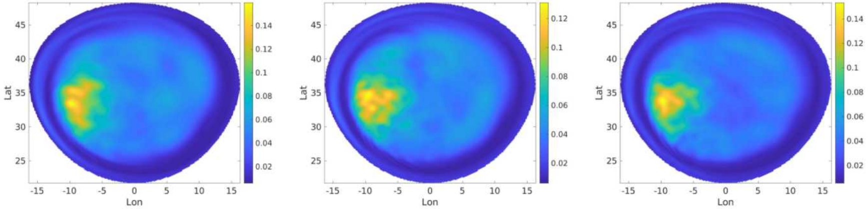


Figure: The RMSSSHA over the additional two years for full model (left), for the HSP-ROM model prediction (center), and the POD-ROM model prediction (right).

Century Predictions

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

Century Predictions

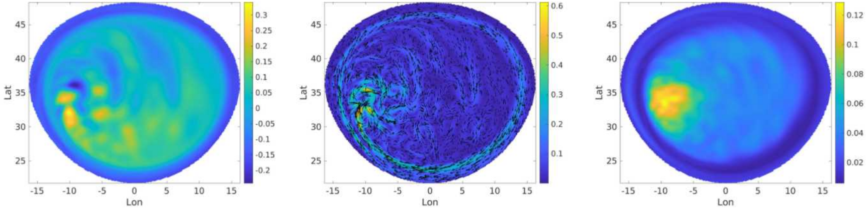


Figure: The solution, **h** and **v**, at the end of the century time-horizon and the RMSSSHA over the century time-horizon for the HSP-ROM method.

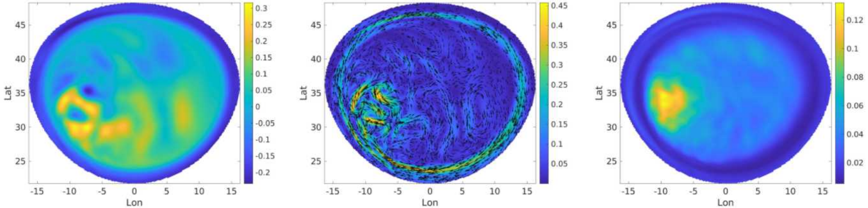


Figure: The solution, **h** and **v**, at the end of the century time-horizon and the RMSSSHA over the century time-horizon for the HSP-ROM method.

Century Predictions: Mass and Energy

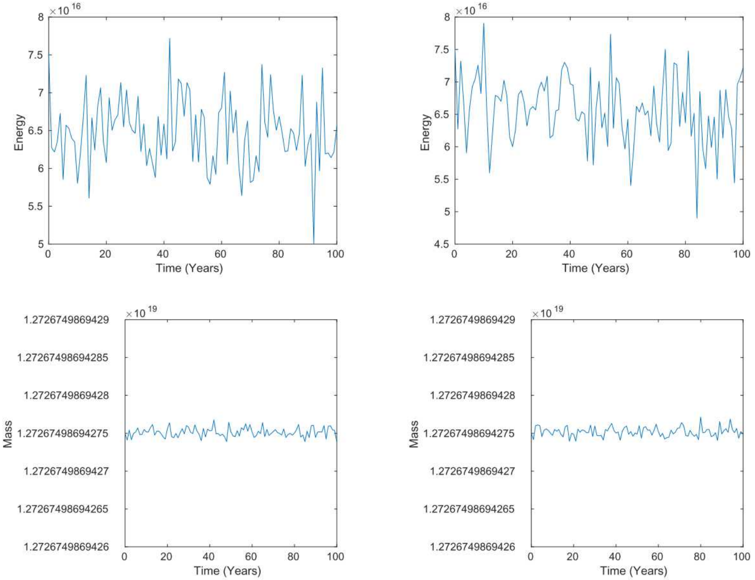


Figure: The energy (top-left) and mass (bottom-left) for the HSP-ROM method, and the energy (top-right) and mass (bottom-right) for the POD-ROM method over the century time-horizon.

Conclusions and Future Research

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
- Applications: uncertainty quantification, data assimilation, spin-up
- Potential vorticity dynamics and error
- Conserving more general Casimirs
- Hyper-reduction techniques for nonlinearities.