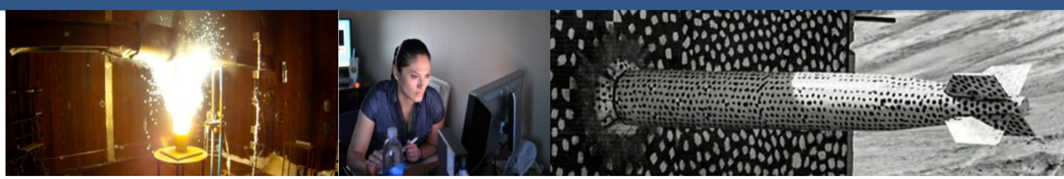
Progress towards a new CRM for E3SM-MMF



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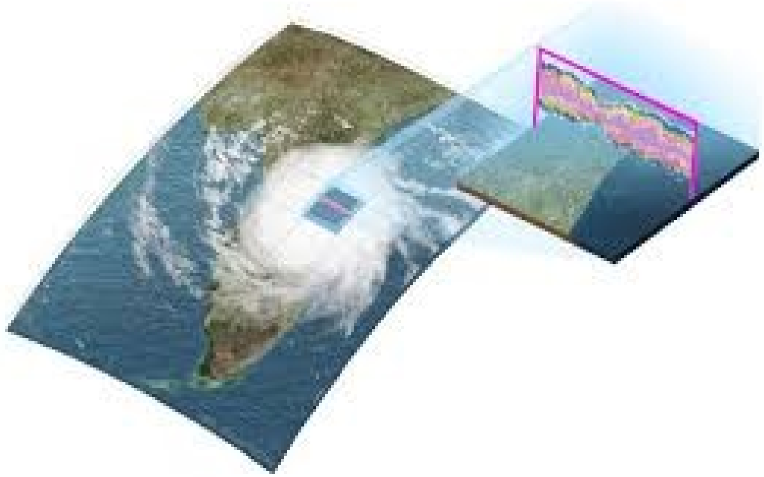
What is E3SM-MMF and why are we doing it?

- Major source of uncertainty in (the atmospheric component of) climate models is clouds and other small-scale processes
- Two approaches pursed by E3SM to improve this:
  - **SCREAM**: High-resolution (1-3km) global cloud resolving model
  - **E3SM-MMF**: Multiscale modelling framework/superparameterization → Embed a Cloud Resolving Model (CRM) inside each coarse global grid cell
- Only MMF approach seems likely to achieve throughput (~5 SYPD) needed for IPCC-type climate simulations
- Large number of independent, computationally intensive CRMs maps (very) well onto current and future accelerator-focused supercomputing hardware



Current CRM and motivation for a new one

- Currently using System for Atmospheric Modeling (SAM) as the CRM
  - Would like to replace this, to improve both computational and scientific performance
- Main desired features for new CRM are:
  - Better computational performance and performance portability, focusing on accelerators (done via C++ using YAKL/Kokkos)
  - Improved temporal numerics (ADER-DT, Multiderivative RK)
  - **Improved spatial numerics: WENO, FCT, Structure-Preservation**

I will talk today about the work I have been doing towards improved spatial numerics, in particular the combination of WENO/FCT with Structure-Preservation.

What (numerical) properties are desired?

- **Reversible dynamics** of fluids are composed of transport equations (**Lie derivative**) for transported quantities plus associated dual terms (**diamond operator)** in the velocity/ momentum equation
- This is encoded in a **geometric structure**: the **Hamiltonian formulation**
- Ideally numerical transport is:
  - No spurious numerical oscillation (oscillation-limited)
  - Possibly monotonic or positive-definite
  - High effective resolution ↔ high-order accuracy
  - Energy-conserving / structure-preserving (preserve key elements of geometric structure)
- The first 3 goals are often in conflict with the last
  - sophisticated transport schemes such as weighted essentially non-oscillatory (WENO) are not energy-conserving
  - structure-preserving schemes such as centered finite-volume (CFV) usually make poor transport operators

How did we remedy this?

- Developed a new **structure-preserving WENO** approach
- **Approach**: discretize **Hamiltonian formulation** in a way that preserves key properties, by using **mimetic discretization** and **WENO reconstructions**
- **Mimetic discretization:** discrete analogue of key **vector calculus identities** (such as):

$$\nabla^T \cdot \mathbf{x}^T = \nabla \cdot \mathbf{x} \qquad \nabla \times \nabla = 0, \ \nabla \cdot \nabla \times = 0$$

$$\times \text{ is self-(skew)adjoint} \qquad \nabla \text{ and } \nabla \cdot \text{ are adjoints}$$

- Hamiltonian formulation: write equations of motion using symplectic operator and Hamiltonian:

$$\frac{\partial \mathbf{x}}{\partial t} = \mathbb{J}(\mathbf{x}) \frac{\delta \mathcal{H}}{\delta \mathbf{x}}(\mathbf{x}) \qquad \mathbb{J} = -\mathbb{J}^T \qquad \mathbb{J} \frac{\delta \mathcal{C}}{\delta \mathbf{x}} = 0$$

$$\frac{d\mathcal{H}}{dt} = \left(\frac{\delta \mathcal{H}}{\delta \mathbf{x}}\right)^T \mathbb{J} \frac{\delta \mathcal{H}}{\delta \mathbf{x}} = -\left(\frac{\delta \mathcal{H}}{\delta \mathbf{x}}\right)^T \mathbb{J} \frac{\delta \mathcal{H}}{\delta \mathbf{x}} = 0 \qquad \frac{d\mathcal{C}}{dt} = \left(\frac{\delta \mathcal{C}}{\delta \mathbf{x}}\right)^T \mathbb{J} \frac{\delta \mathcal{H}}{\delta \mathbf{x}} = 0$$

Thermal Shallow Water in Hamiltonian Form

Hamiltonian and Functional Derivatives

$$\mathcal{H}[\mathbf{v}, h, S] = \int \frac{Sh}{2} + Sh_s + h\frac{\mathbf{v}\cdot\mathbf{v}}{2}$$

$$B = \frac{\delta\mathcal{H}}{\delta h} = \frac{S}{2} + \frac{\mathbf{v}\cdot\mathbf{v}}{2} \qquad \mathbf{F} = \frac{\delta\mathcal{H}}{\delta\mathbf{v}} = h\mathbf{v} \qquad T = \frac{\delta\mathcal{H}}{\delta S} = \frac{h}{2} + h_s$$

Symplectic Operator

$$\mathbb{J}(\mathbf{x}) = \begin{bmatrix} q\square^T & \nabla\square & s\nabla\square \\ \nabla\cdot(\square) & 0 & 0 \\ \nabla\cdot(s\square) & 0 & 0 \end{bmatrix}$$

Equations of Motion

$$\frac{\partial\mathbf{v}}{\partial t} + q\mathbf{F}^T + \nabla B + s\nabla T = 0 \qquad \frac{\partial S}{\partial t} + \nabla\cdot(s\mathbf{F}) = 0$$

$$\frac{\partial h}{\partial t} + \nabla\cdot\mathbf{F} = 0$$

Structure-Preserving (C-Grid) Numerics Part 1

- Based on **discrete exterior calculus** plus **mimetic finite differences**
- Predicted variables

$$h^c \quad v^e \quad S^c$$

- Functional derivatives

$$T^c \quad F^e \quad B^c$$

- WENO or CFV Reconstructions

$$q^e \quad S^e \quad f^e \quad h^e$$

- Exterior derivatives (gradient, curl, skew-gradient, divergence)

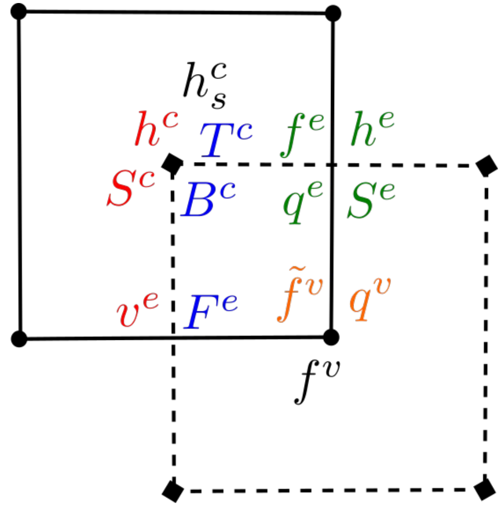
$$\mathbf{D}_1 \quad \mathbf{D}_2 \quad \bar{\mathbf{D}}_1 \quad \bar{\mathbf{D}}_2$$

- Wedge products (dot/scalar/cross product)

$$\mathbf{R} \quad \mathbf{W} \quad \mathbf{Q} \quad \mathbf{C} \quad \mathbf{\Phi} \quad \mathbf{\Phi}^T$$

- Hodge stars

$$\mathbf{H} \quad \mathbf{I}$$



Structure-Preserving (C-Grid) Numerics Part 2

Hamiltonian and Functional Derivatives

$$\mathcal{H} = \frac{1}{2}(S^c)^T \mathbf{I} h^c + (S^c)^T \mathbf{I} h_s^c + \frac{1}{2}(h^c)^T \mathbf{I} \boldsymbol{\phi}^{\boldsymbol{T}}(v^e, U^e)$$

$$F^e = \bar{h}^e U^e \qquad B^c = \frac{1}{2}\mathbf{I}(S^c + \boldsymbol{\phi}^{\boldsymbol{T}}(v^e, U^e)) \qquad T^c = \mathbf{I}(\frac{h^c}{2} + h_s^c)$$

Equations of Motion

$$\frac{\partial h^c}{\partial t} + \bar{\mathbf{D}}_{\mathbf{2}}(h^e U^e) = 0 \qquad \frac{\partial S^c}{\partial t} + \bar{\mathbf{D}}_{\mathbf{2}}(S^e U^e) = 0$$

$$\frac{\partial v^e}{\partial t} + \mathbf{Q} F^e + \mathbf{C} F^e + \frac{h^e}{\bar{h}^e}\mathbf{D_1} B^c + \frac{S^e}{\bar{h}^e}\mathbf{D_1} T^c = 0$$

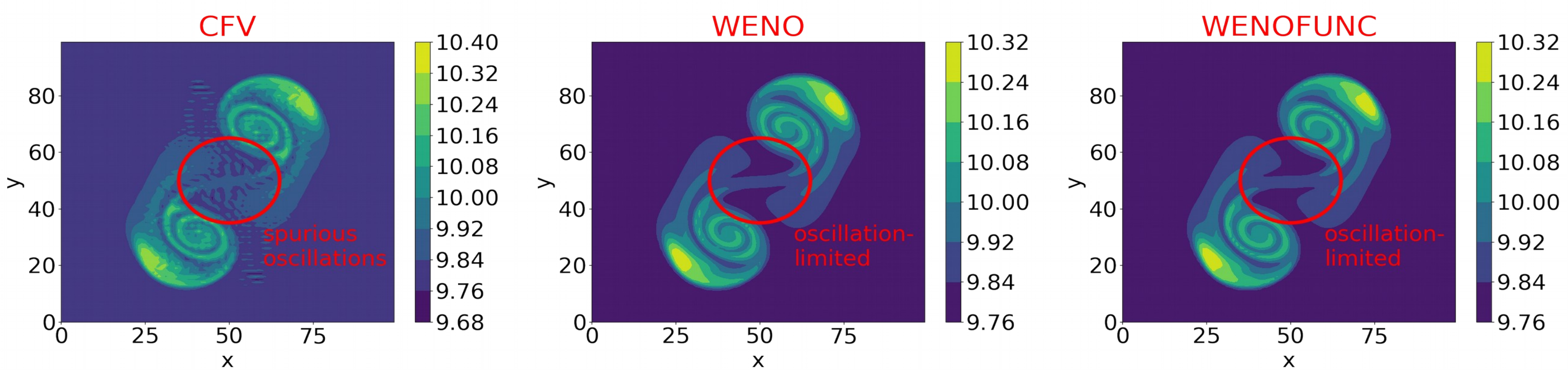
Auxiliary Quantities and Definitions

$$q^v = \frac{\mathbf{D_2} v^e}{\mathbf{R} h^c} \qquad \tilde{f}^v = \frac{f^v}{\mathbf{R} h^c} \qquad U^e = \mathbf{H} v^e \qquad \bar{h}^e = \boldsymbol{\phi} \mathbf{I} h^c$$

$$\mathbf{Q} = \frac{1}{2}(q^e \mathbf{W} + \mathbf{W} q^e) \qquad \mathbf{C} = \frac{1}{2}(f^e \mathbf{W} + \mathbf{W} f^e)$$

Results

- Thermal shallow water equations in doubly-periodic f-plane
- Double vortex test case
  - 100x100 mesh, CFL ~0.5, KG42 RK time integrator
- Operator choices are:
- Combinatorical exterior derivatives and wedge products
- 6th order Hodge stars from mimetic finite difference (MFD) literature
- 2nd order CFV for Coriolis reconstruction
- 9th order WENO (pointwise and function-based) vs. 10th order CFV for other reconstructions
- Showing specific bouyancy s



All versions conserve energy to time-truncation error

Conclusions and Future Directions

- Obtained structure-preserving scheme by combining **discrete exterior calculus** with **WENO/FCT reconstructions**
  - **Explicit**, **high-order**, **structure-preserving** numerics that are **oscillation-limited**, (optionally) **monotonic/positive-definite** and have **high effective resolution**
  - Key feature is split between **topological** operators (**exterior derivative** and **wedge product**) and **metric** operators (**Hodge star** and **reconstructions**)
  - **(Most) of the scheme properties depend only on the topological operators**
  - Currently limited to **doubly-periodic**, **rectangular** grids
- Current work: extension to **bounded** rectangular grids → **anelastic/fully-compressible** equations for **CRM**
- **Possibly future work:** extension to **deformed/arbitrary geometries** and **arbitrary topologies w/ and w/o boundaries** → **cubed-sphere** grids, **icosahedral** grids, **unstructured** grids → **global** models
- What about structure-preserving discretizations for **irreversible** and **subgrid dynamics** (physics parameterizations)?