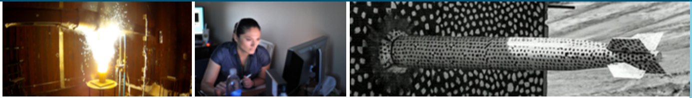
National Laboratories

A multiscale modeling framework (MMF) for the E3SM climate model



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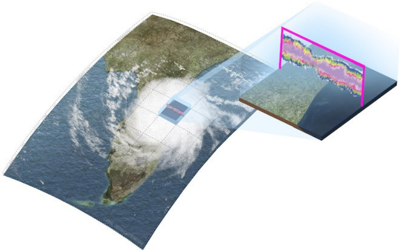
E3SM-MMF

- Clouds are a dominant source of uncertainty in climate predictions → how can we improve their representation?
- Superparameterization (=multiscale modeling framework): embed a cloud resolving model (CRM) inside each grid box of a coarse global
- On modern GPU machines can obtain 5 simulated years per day (SYPD) = enough for many climate simulations



The Portable Atmospheric Model (PAM)

- Developing a new CRM for E3SM-MMF: the Portable Atmospheric Model (PAM)
  - Uses SCREAM physics: two-moment microphysics (P3), turbulence (SHOC) and radiation (RRTGMP)
  - New dynamical core: SPAM++ (the Structure Preserving Atmospheric Model in C++)
  - Written in C++ using YAKL (Yet Another Kernel Launcher) and Kokkos for portability
- PAM is based on a curl-form Hamiltonian formulation (advected densities model)
- PAM is designed around new structure-preserving spatial (discrete exterior calculus) and temporal (energy-conserving Poisson integrator) numerics

Advected Densities Model underlying PAM

- General *advected densities model* in *height coordinates* with *n densities* D_k ($k=1,\ldots,n$, ex. mass density ρ, water vapor density ρ_v and entropy density $S=\rho\eta$) and *velocity* $\mathbf{v}$ written in *Hamiltonian curl form* for an arbitrary *Hamiltonian* $\mathscr{H}[\mathbf{v},D_k]$:

$$\frac{\partial \mathbf{v}}{\partial t}+\mathbf{Q}\times\mathbf{F}+\sum_k d_k\nabla B_k = 0 \qquad (1)$$

$$\frac{\partial D_k}{\partial t}+\nabla\cdot(d_k\mathbf{F}) = 0 \qquad (2)$$

  where $\mathbf{Q}=\frac{\nabla\times\mathbf{v}}{D}$, $d_k=\frac{D_k}{D}$, D is total density (a linear combination of D_k's), $\mathbf{F}=\frac{\delta\mathscr{H}}{\delta\mathbf{v}}$ and $B_k=\frac{\delta\mathscr{H}}{\delta D_k}$.
- With appropriate choices of $\mathscr{H}$ and densities D_k can get many different GFD models: ex. (thermal) shallow water, (multicomponent) compressible Euler and anelastic with arbitrary thermodynamic potentials

Spatial Numerics: Discrete Exterior Calculus

Spatially discretize Hamiltonian formulation (1) - (2) using a (structure-preserving) *discrete exterior calculus* (DEC) scheme (shown in 2D):

$$\frac{\partial v^1}{\partial t} + \mathbf{Q}\tilde{F}^{n-1} + \sum_k \tilde{D}^e_k \mathbf{D}_1 {B_k}^0 = 0 \qquad (3)$$

$$\frac{\partial \tilde{D}^n_k}{\partial t} + \tilde{\mathbf{D}}_n(\tilde{D}^e_k \tilde{F}^{n-1}) = 0 \qquad (4)$$

where $\mathbf{Q} = \frac{1}{2}[\tilde{q}^e \mathbf{W} + \mathbf{W}\tilde{q}^e]$, $\tilde{F}^{n-1} = \frac{\delta \mathscr{H}}{\delta v^1}$ and ${B_k}^0 = \frac{\delta \mathscr{H}}{\delta \tilde{D}^n_k}$ for (discrete) Hamiltonian $\mathscr{H}[v^1, \tilde{D}^n_k]$. Uses new DEC features developed at SNL:

- Treatment of arbitrary boundary conditions
- Higher-order Hodge stars
- Structure-preserving, high-order, oscillation-limiting transport operators with optional positivity-preservation (SPHOOL-PD)

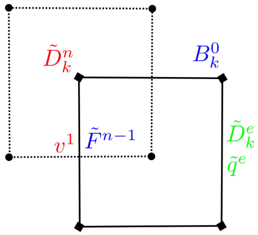


Figure: Discrete variables and C-grid staggering used in the general scheme in 2D, with solid lines for the *primal* grid and dashed lines for the *dual* grid.

Properties of Spatial Discretization

- **Conservation laws**: mass, entropy, energy
- **Mimetic**: no spurious vorticity production, freedom from spurious computational modes, good representation of linear modes
- **Accuracy**: 2nd order accurate
- **Realistic transport**: transport is oscillation-limiting and positive-definite (could be made global or local bounds preserving as well)

Temporal Numerics: Energy Conserving Poisson Integrator

Temporally discretize (3) - (4) in a way that preserves the invariants (Hamiltonian and Casimirs), by using a *fully implicit energy-conserving Poisson integrator* (EC2, a type of discrete gradient method):

$$\frac{\mathbf{x}^{n+1} - \mathbf{x}^n}{\Delta t} = \mathbb{J}(\mathbf{x}^*) \widetilde{\frac{\delta \mathscr{H}}{\delta \mathbf{x}}} \tag{5}$$

where $\widetilde{\frac{\delta \mathscr{H}}{\delta \mathbf{x}}} = \int_0^1 \frac{\delta \mathscr{H}}{\delta \mathbf{x}}(\mathbf{x}^n + \tau(\mathbf{x}^{n+1} - \mathbf{x}^n))d\tau \approx \sum_i w_i \frac{\delta \mathscr{H}}{\delta \mathbf{x}}(\mathbf{x}^i)$ with $\mathbf{x}^i = \mathbf{x}^n + \tau^i(\mathbf{x}^{n+1} - \mathbf{x}^n)$ (discrete gradient) and $\mathbf{x}^* = \frac{\mathbf{x}^{n+1}+\mathbf{x}^n}{2}$. Conserves linear/quadratic Casimirs and arbitrary Hamiltonians to machine-precision (with enough quadrature points i, $\approx$4 in practice for compressible Euler and anelastic)

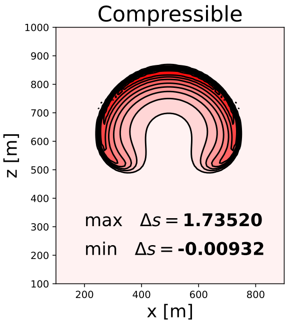
Lacks positive-definiteness, but we are working on this

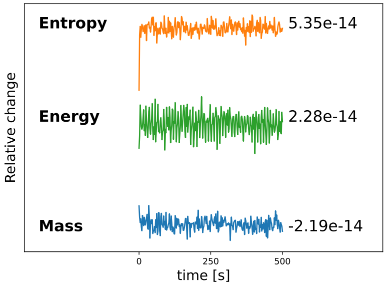
Implementation Details of Time Integrator:

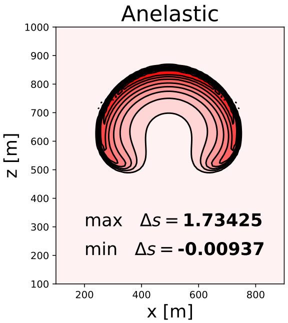
- Solve (5) using a quasi-Newton method (simplified Jacobian, from the linearized equations) for compressible Euler; and fixed point for anelastic
- Simplify resulting linear system to a single positive-definite Helmholtz (fully compressible and thermal shallow water) or Poisson problem (anelastic) using static condensation.
- Solve this problem using a direct solve (FFT + banded diagonal solvers).
  - This step is specific to CRM configuration (no topography, uniform horizontal grids)
  - For non-uniforms grids and topography, could use multigrid-based preconditioners + an iterative solver.
- Resulting nonlinear system requires $\approx$5 (anelastic) or $\approx$7 (compressible) iterations = comparable to # of stages in an explicit Runge-Kutta scheme; takes around 15% of total runtime

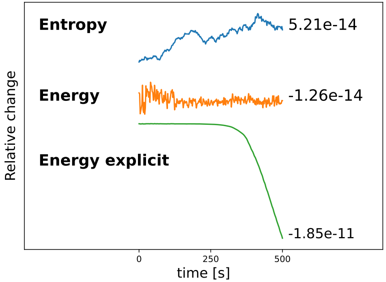
Rising Bubble

- maximum advective CFL ≈ 0.6
- 3 quadrature points
- Compressible iterations average 7.3
- Anelastic iterations average 5.3

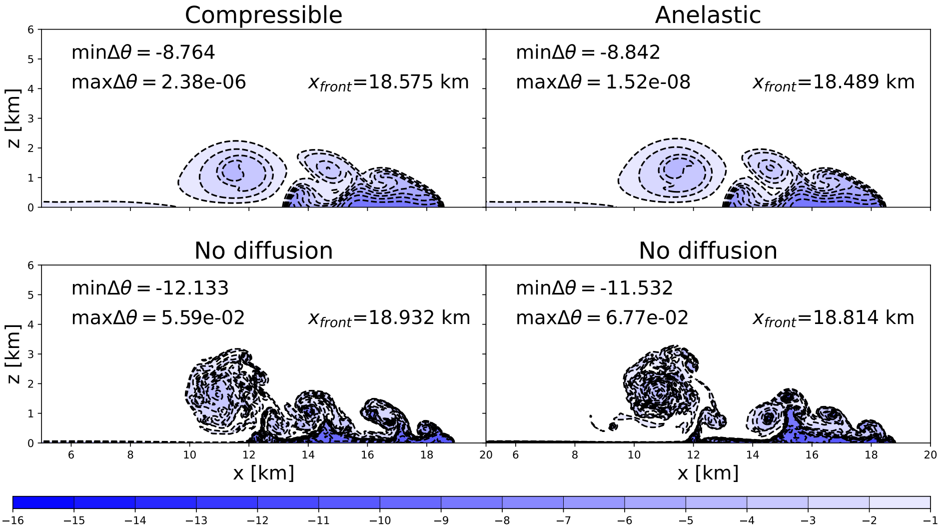






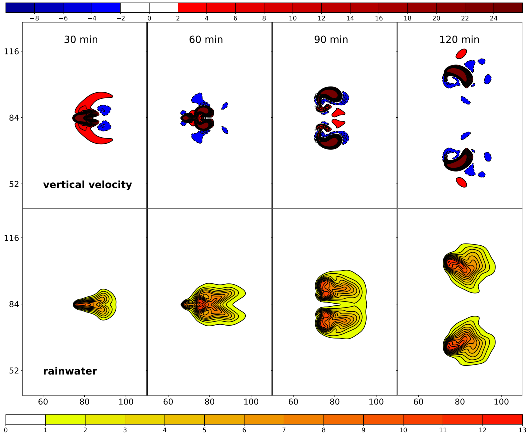


Density Current

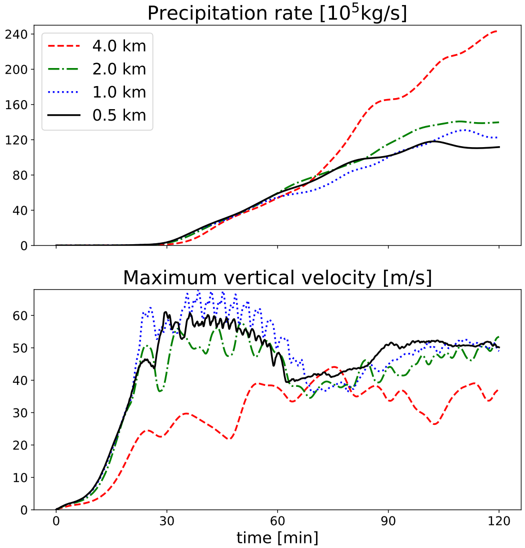


Splitting Supercell Storm

- Benchmark with simplified moist physics (Kessler microphysics)



Supercell Statistics



Conclusions

- New CRM in E3SM-MMF: PAM (SPAM++ dycore + SCREAM physics)
- Based on curl-form Hamiltonian formulations and structure-preserving spatial (discrete exterior calculus) and temporal (energy conserving poisson integrator) numerics
- Provides exact conservation of invariants (mass, energy, entropy) to machine precision along with SPHOOL-PD transport
- Does well on standard dynamical core test cases

$$\frac{\partial v^1}{\partial t} + \mathbf{Q}\tilde{F}^{n-1} + \sum_k \tilde{D}_k^e \mathbf{D}_1 {B_k}^0 = 0$$

$$\frac{\partial \tilde{D}_k^n}{\partial t} + \tilde{\mathbf{D}}_n(\tilde{D}_k^e \tilde{F}^{n-1}) = 0$$

$$\frac{\mathbf{x}^{n+1} - \mathbf{x}^n}{\Delta t} = \mathbb{J}(\mathbf{x}^*)\widetilde{\frac{\delta \mathscr{H}}{\delta \mathbf{x}}}$$

Future Work

- Improved vertical spatial numerics (summer student, ongoing): high-order Hodge stars for variable grids, CFV/WENO recons
- Improve Newton solver convergence to fix exact energy conservation for some tests (solutions are fine even with convergence stalls)
- Positivity-preserving version of time integrator to fix exact positivity-definiteness
- More sophisticated treatment of moist thermodynamics and moist parameterizations:
  - non-equilibrium thermodynamics + better thermodynamic potentials
  - bring (some) microphysics into the dycore
  - single set of equations for dynamics + physics? ie true multiscale formulations?

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