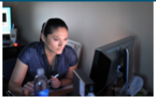
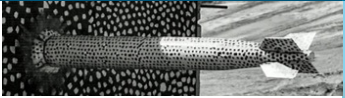
National Laboratories

Energy-conserving time integration in a cloud-resolving atmospheric model





Presented by:

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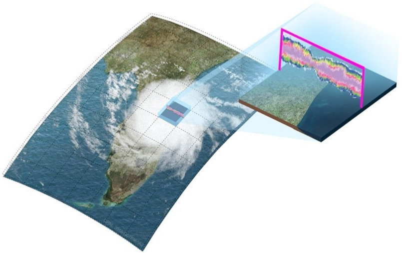
Background

- Exascale Computing Project (ECP)
- Representation of clouds is a major of source of uncertainty in climate predictions – how to use exascale resources to improve cloud representation in climate models ?
- Two subprojects related to Energy Exascale Earth System Model (E3SM)
  - Simple Cloud Resolving E3SM Atmosphere Model (SCREAM) - 3 km global atmosphere model
  - **Multiscale Modeling Framework (MMF) - superparametrized E3SM climate model**

Superparametrization

- Cloud-resolving model (CRM) embedded inside each global climate model (GCM) column
- Can be fast enough ($\approx$ 5 SYPD) to enable multi-decadal runs with some aspects of cloud resolving simulations
- CRMs typically 2d with horizontal resolution 1km
- All physics (microphysics, turbulence scheme, radiation) contained in the CRM



Portable Atmosphere Model (PAM)

- New CRM for E3SM
- More flexibility and better numerics compared to the old CRM – SAM
- New physics: two-moment microphysics (P3) and turbulence (SHOC)
- Designed from the start for exascale machines (i.e. GPUs)
- Written in C++ using YAKL (Yet Another Kernel Launcher) for portability

Superparametrization - considerations for choice of numerics

- Cartesian box domain
- Periodic in the horizontal
- No topography
- Hydrostatically balanced reference profile available from the GCM
- **Needs to robustly handle various cloud regimes**

PAM continuous formulation

- Hamiltonian formulation of moist Euler equations

$$\frac{dx}{dt} = \mathbb{J}\frac{\delta \mathscr{H}}{\delta x}$$

- Fully compressible or anelastic
- Prognostic variables: velocity and arbitrary number of densities
- Thermodynamics variable is generic entropic density (entropy density, (virtual) potential temperature density, ...)
- Thermodynamics formulated in terms of potentials (energy, enthalpy, ...)
- Choice of "unapproximated" moist thermodynamics or constant kappa approximation

PAM continuous formulation - concrete example

$$\mathscr{H}(\mathbf{v}, \rho\theta, \rho, \rho_s) = \int \rho \left(\frac{\mathbf{v}^2}{2} + U(\alpha, \theta, q_s) + \Phi \right)$$

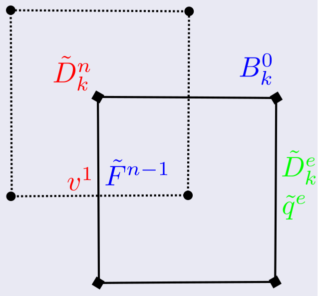
$$\frac{\delta \mathscr{H}}{\delta \mathbf{v}} = \mathbf{F} = \rho \mathbf{v} \qquad \frac{\delta \mathscr{H}}{\delta \rho\theta} = \Pi$$

$$\frac{\delta \mathscr{H}}{\delta \rho} = \frac{\mathbf{v}^2}{2} + \Phi + U + p\alpha - \theta\Pi + \sum_s (\Xi_d - \Xi_s) \qquad \frac{\delta \mathscr{H}}{\delta \rho_s} = Xi_s - \Xi_d$$

$$\mathbb{J} = \begin{pmatrix} -\mathbf{Q} \times (\cdot) & -\theta\nabla(\cdot) & -\nabla(\cdot) & -q_s\nabla(\cdot) \\ -\nabla\cdot(\theta\cdot) & 0 & 0 & 0 \\ -\nabla\cdot(\cdot) & 0 & 0 & 0 \\ -\nabla\cdot(q_s\cdot) & 0 & 0 & 0 \end{pmatrix}$$

PAM spatial discretization

- Primal/dual grid staggered discretization based on discrete exterior calculus (DEC) that ensures good linear modes and various mimetic properties
- DEC enhancements developed for PAM:
  - Nonoscillatory (WENO) and positivity-preserving transport
  - Treatment of arbitrary boundary conditions
  - High-order Hodge stars
- See Chris Eldred's talk on Friday



PAM temporal discretizations

- Various explicit Runge-Kutta (RK) schemes
  - Strong Stability Preserving RK
  - Kinnmark-Gray RK
  - Low-storage RK
- **Fully implicit energy-conserving Poisson integrator (EC2)**

To achieve reasonable time-to-solution:

- Anelastic model can use explicit integrators since it filters out acoustic waves
- Fully compressible needs (semi-)implicit scheme to step over acoustic waves

EC2 time integrator

$$\frac{x^{n+1} - x^n}{\Delta t} = \mathbb{J}\left(\frac{x^n + x^{n+1}}{2}\right)\widetilde{\frac{\delta \mathscr{H}}{\delta x}}$$

where

$$\widetilde{\frac{\delta \mathscr{H}}{\delta x}} = \int_0^1 \left((1-\tau)x^n + \tau x^{n+1}\right) d\tau$$

is called the discrete gradient and is usually evaluated using quadrature

- Also know as the average vector field method
- Quadrature order to achieve exact energy conservation depends on the nonlinearity of $\mathscr{H}$ (4 points is usually sufficient)

Solution strategy for nonlinear problem

$$F(x^{n+1}) = x^{n+1} - x^n - \Delta t \mathbb{J} \left(\frac{x^n + x^{n+1}}{2} \right) \sum_{m=1}^{n_q} \omega_m \frac{\delta \mathscr{H}}{\delta x} \left((1 - \tau_m) x^n + \tau_m x^{n+1} \right) = 0$$

- Anelastic: fixed-point iteration
- Compressible: quasi-Newton method

$$J_{\text{linear}} \delta x^k = -F(x^k)$$

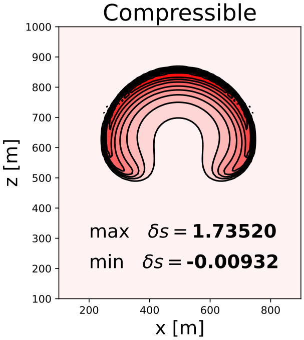
where the approximate Jacobian J_{linear} comes from linearization about a reference state

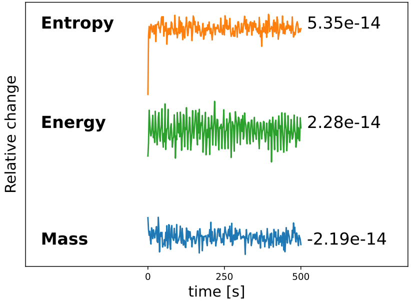
Solution strategy for linear systems

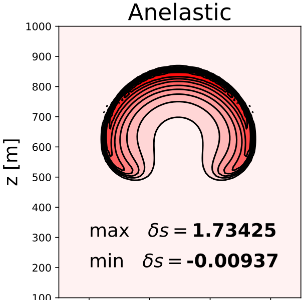
- Both anelastic and compressible schemes require solving one linear system per nonlinear iteration
- Both can be reduced (Schur complement) to solving for a single variable (pressure or vertical velocity)
- **Direct solve** based on
  - FFT in the horizontal directions
  - Banded solve in the vertical (tridiagonal for the lowest order case)
- This is very efficient on GPUs (linear solve usually less than 15% of the total runtime)

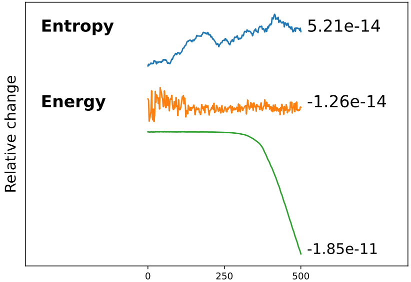
Rising bubble

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

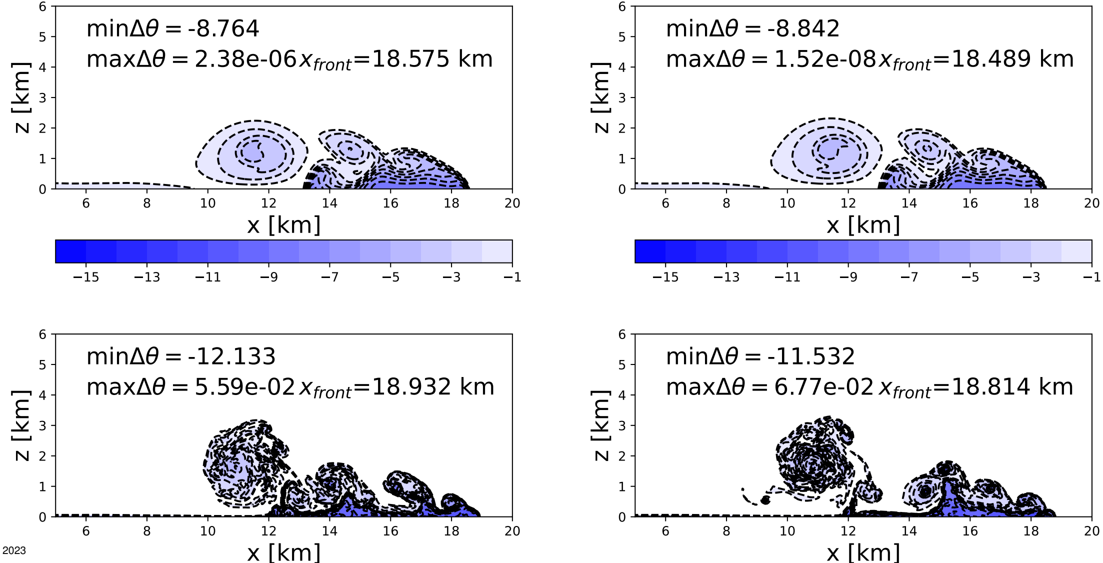






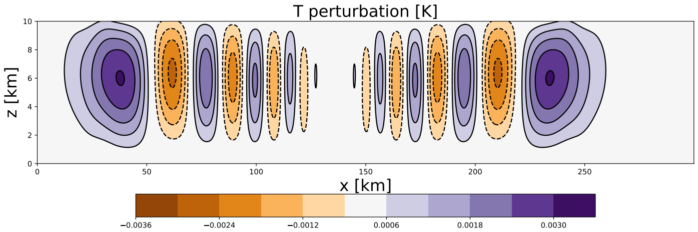


Density current



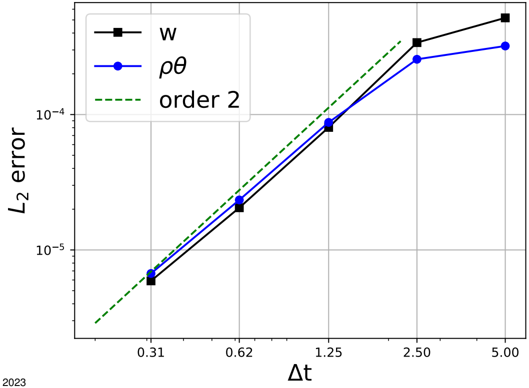
Gravity waves

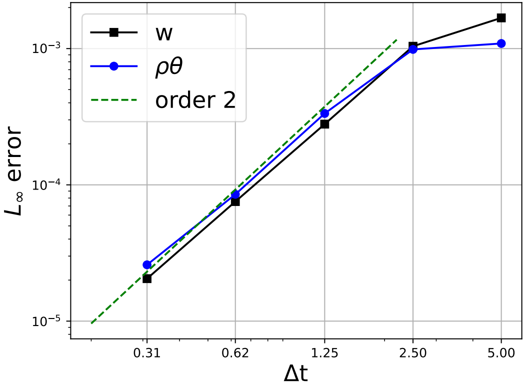
- Gravity waves in a channel from Baldauf & Brdar (QJR, 2013)
- Exact solution of linearized Euler equations with gravity
- For small initial perturbations can be used to test convergence of nonlinear models



Gravity waves: convergence

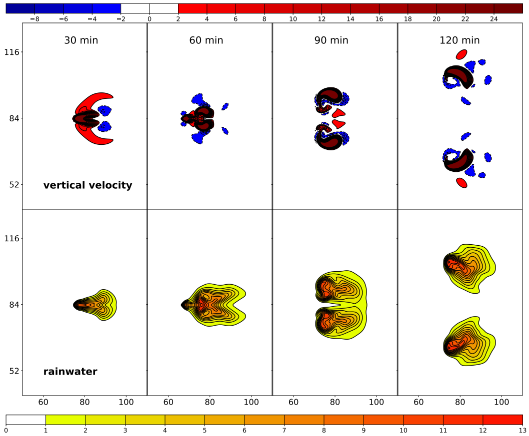
- Fixed high spatial resolution 2400×161
- Changing Δt to look at temporal convergence



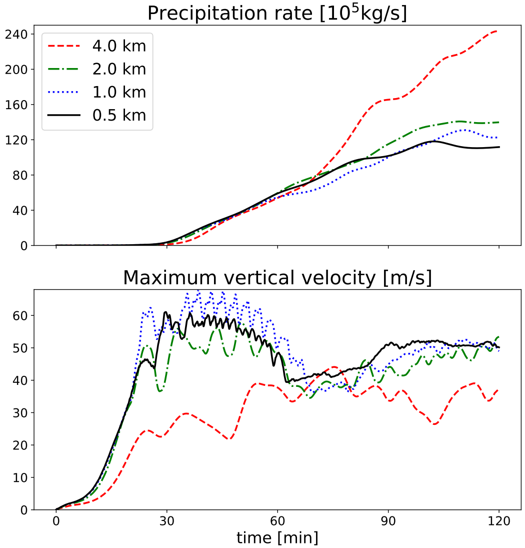


Supercell

- Splitting supercell storm test based on DCMIP but in planar geometry
- Kessler physics



Supercell statistics



Summary and future work

Summary:

- New CRM for E3SM based on structure-preserving numerics
- Implicit second-order energy-conserving time integrator
- Verified energy-conservation, convergence, and obtained good results on standard test cases
- Not overly expensive compared to more standard approaches

Future work:

- Improve convergence (nonlinear solvers can sometimes stall)
- Positivity preservation without SSP property
- Fully compressible model in 3d based on pressure solve