Multiscale methods for enabling scale-aware capability in CESM: A SciDAC Climate Application

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Drivers for the project

• Many phenomena we want to simulate occur at the very small scales of clouds and ocean eddies.

• Two-way interactions are important for the organization and variability of the climate.

• Given cost of uniform ultra-high resolution, \textit{statically or dynamically refinable models} could be a key experimental platform.
Goals of the project

• Develop, validate, and apply multiscale models of the climate system based upon atmospheric and oceanic components with variable resolution.

• Exploit new variable resolution unstructured grids based on finite element and finite volume formulations developed by DOE.

• Integrate advances in time-stepping methods, grid generation, and automated optimization methods for next-generation computer architectures.
Clouds scales and model resolution

Median cloud size (km)

Cloud coverage (%)
Requirements for next generation physics

• Fidelity down to scales of key features of interest: cloud systems and ocean eddies

• Relaxation of usual parameterization assumptions:
  - *Ensembles:* Grid box may contain ~1 system, not >>1
  - *Scale separation:* Time steps and grid resolutions comparable to characteristic time and length scales of systems
  - *Equilibrium:* Due to scale “entanglement”, sub-grid physics are not in equilibrium with boundary conditions imposed by resolved fields
  - *No memory:* Sub-grid systems will retain state across steps
  - *Scale awareness:* Physics needs to quasi-invariant to resolution
  - *Determinism:* Physics evolution is inherently stochastic.
Needs for scale aware parameterization

CAM-SE with resolutions: 2.7° 1.9° 1.0° 0.5° 0.25°

• Monotonic decrease in LWCF also seen in CAM 3.1 Aqua Planet Experiments (Williamson, Tellus 2008)
• Cloud Fraction monotonically decreases with resolution
• CAM-SE simulations (shown) are similar.

Taylor, 2011
Reverse Resolution Dependence in CAM

Expected Resolution Dependence

Actual Resolution Dependence

O’Brien et al, 2013
Project Elements

Variable Mesh Dycores

Model for Prediction Across Scales (MPAS)

Convection

Microphysics

Process Integration

Multiscale UQ

Atmosphere

Ocean

Spectral Element Dycore

Physics-Dynamics Interface

Mesoscale Eddy Treatments

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Ocean: MPAS-O Optimization

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Spectral Element Method

- Spectral Elements: A Continuous Galerkin Finite Element Method
- All inter-element communication is isolated to one step in method, providing a clean decoupling of computation & communication
- High-order (4th) discretization
- Excellent local conservation: mass, energy, potential temperature, 2D PV
- All properties preserved on fully unstructured grids

Taylor, 2011
• Excellent scaling to near full machine on both LCFs:

• **Intrepid**: Excellent scalability, peak performance at 115K cores, 2.8 SYPD.
• **JaguarPF**: Good scalability, peak performance at 173K cores, 6.8 SYPD.
Development of fully implicit solver for SE

**Goal:** Maintain time step size with spatial refinement

Application of solver to a refined grid (2° refined to 1°) near a mountain feature

**Implementation:** Extend implicit solver to hydrostatic dycore

Coarse baroclinic test case: Implicit backward Euler solves for a 1800s time step

SW Test: Implicit 1200s time step converged successfully with an $L_2$ norm of $3.1 \times 10^{-4}$ for 1 day compared to explicit CFL limited 120s time step

Preconditioning to accelerate implicit solves

Efficiency gains from implicit methods are not fully realized without an effective preconditioner:

1. Cast in vector formulation

\[
\frac{dy}{dt} = f(y_{n+1}) \approx \frac{y_{n+1} - y^n}{\Delta t}
\]

2. Apply Newton-Krylov method w/ preconditioner \( P \):

\[
F(y_{k+1}) \approx F(y_k) + F'(y_k)[y_{k+1} - y_k]
\Rightarrow F'(y_k)P^{-1}P[y_{k+1} - y_k] = -F(y_k)
\]

P should be invertible and make the linear solve easier

We have developed a block preconditioner based on the shallow water equation

- Blocks based on velocities and height, coupling between is relaxed
- FastMath’s CAM-SE-Trilinos interface is used for this work
- Formulations should carry over to variable resolution grids

Fig: scalings from Evans et al. (2009)
Optimization of implicit preconditioner

Accomplishments:
- Code optimizations for preconditioner
- Interfaced Helmholtz Solver with Trilinos
- Performed initial run on variable res grid
- Tested preconditioner with Piro interface

Current Focus:
- Implementing a multilevel solver for S solves
- Building matrices for multilevel solvers in Trilinos
- Testing on variable resolution grids
- Extending preconditioner to 3D

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Jablonowski-Williamson Test case 5;
1 sim. day; Implicit method with Crank-Nicholson Time Stepping & 720s step size

Code optimizations produced some speedup in runtime

Main Cost: Schur Complement Solve -Developing Multilevel Solver

A. Lott, C. Woodward, K. Evans, A. Salinger, M. Taylor
Goal: Develop CAM-SE kernels providing GPU acceleration on next generation architecture

Accomplishments:

- Common build system that links Trilinos to CAM-SE and the GPU kernel development.
- Profile analysis to identify data and computation bottlenecks limiting performance of the CAM-SE/GPU implicit solve

Still to do:

- Provide algorithmic/code optimization to minimize data transfer through TITAN’s hierarchy and computation for CAM-SE/GPU implicit solve
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Mesoscale Eddy Treatments
1. MPAS is an unstructured-grid approach to climate system modeling.

2. MPAS supports both quasi-uniform and variable resolution meshing of the sphere using quadrilaterals, triangles or Voronoi tessellations.

3. MPAS is a software framework for the rapid prototyping of single-components of climate system models (atmosphere, ocean, land ice, etc.).

4. MPAS offers the potential to explore regional-scale climate change within the context of global climate system modeling. Multiple high-resolution regions are permitted.

snapshot of kinetic energy from a global ocean simulation with 7.5 km resolution in the North Atlantic.

Ringler, 2012
The variable resolution mesh in MPAS

A closer look at the structure of the variable-resolution meshes.

coastline is fit to the mesh

even in mesh transition zone, the grid is smooth and uniform.

Ringler, 2012
We have sufficient evidence in shallow-water, 3D atmosphere and 3D ocean systems to declare this a non-issue as far as the dynamics are concerned.
MPAS-Ocean has scaling limits using MPI only
• Adding OpenMP threading to efficiently leverage multicore systems
• TAU (SciDAC-3 SUPER) was used to evaluate MPI+OpenMP approach, suggest improvements
• Tests performed by Doug Jacobsen (LANL), Kevin Huck and Sameer Shende (U. Oregon)
• Observations, optimizations found:
  1. MPI block decomposition + OpenMP element decomposition reduces total instructions in computational regions (~10% faster) when compared to MPI block decomposition alone
  2. New weighted block decomposition using vertical elements (depth) balances work across processes (~5% faster)
  3. Guided schedule balances work across threads (~6% faster)
  4. Overlapping communication and computation will reduce synchronization delays when exchanging halo regions (underway)
• Evaluation of OpenMP implementation is ongoing coupled with new TAU development. Next steps include porting to MIC platform.
MPAS_O Performance Improvements

1. Increasing thread concurrency with constant resources (64 cores used in all cases).

   Weighted decomposition (2), guided schedule (3) balances workload, reduces synchronization delay

3. Adjusting thread schedule balances workload, reduces computation time
Process Integration: Physics Convergence

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Time Step Sensitivity of CAM

- Global simulations showed strong time step sensitivity, with liquid water path and cloud cover increasing as timestep decreased.
- As a proxy for the full 3D model, we are compiling 10 single column case studies spanning a variety of climate regimes to better explore time step sensitivity and convergence in CAM.
- Initial results with timestep varying from 1 to 20 min show sensitivity similar to global model results.
Importance:

Time-integration issues corrupt physics code and cause $\Delta t$ sensitivity

Progress:

1. Discovered time-stepping issue in PBL scheme (see fig)
   - developing idealized model to isolate the essence of the problem

2. Used a suite of single-column simulations to clarify time-convergence issues in important climate regimes
   - confirmed $q_l$ increase w/ decreased $\Delta t$ found in global simulations

3. Identified a new variant of operator splitting (sequential-tendency splitting) which maintains better process coupling yet allows for long model timesteps

Fig. Global-ave turbulent liquid water tendency as a function of $\Delta t$ in CAM5 (solid) and in a variant with turbulent $\Delta t=1800$ s regardless of model $\Delta t$ (dashed)
UQ: Toward Multi-fidelity Calibration

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Sensitivity to sub-cycle physics parameter variations

Goal: determine the sensitivity of CAM5 to changes in 6 sub-cycle parameters

Challenge: there are 22,500 unique configurations among these 6 parameters

Approach: ran 272 Latin hypercube ensemble simulations and used random forests to calculate sensitivities

Random forests (RFs) are popular in supervised machine learning (Breiman 2001)

RFs use randomized decision trees to partition the input space (see example on right)

RF predictions are based on an ensemble of trees

RFs assess sensitivities via feature selection
UQ: sub-cycle parameter sensitivities

Year 1: define metrics to quantify model development changes, identify scale-dependent physics parameters, and begin sensitivity studies at coarse model resolutions.

**Sensitivity to discrete sub-cycle physics parameters**

Used Latin hypercube to sample discrete values of 6 sub-cycle physics parameters. Calculated model sensitivity to changes in sub-cycling parameters. Demonstrated statistical method to model changes from discrete factors.
UQ: toward multi-fidelity calibration

Year 1: define metrics to quantify model development changes, identify scale-dependent physics parameters, and begin sensitivity studies at coarse model resolutions

Progress toward multi-fidelity calibration

Began design of multi-fidelity UQ studies
Adapted UQ interface to 3-4 uniform resolutions (f45, f19, f09, f05)
Implemented scale-dependent UQ parameters in new release CESM v1.2

Leverage low fidelity simulations to calibrate high fidelity model

\[ Y_{\text{high}}(p) = \widetilde{Y}_{\text{low}} + \delta_{\text{high-med}} + \delta_{\text{med-low}} + \delta_{\text{low}} + \delta_{\text{high-obs}} + \varepsilon_{\text{obs}} \]
UQ: Sub-grid Physics Quadratures

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Physics-Dynamics Interface

Spectra
**Autoconversion** – conversion of cloud droplets to rain droplets (measured as rate of mass transfer).

- Autoconversion depends on the cloud water mixing ratio, $s$, and the cloud droplet concentration $N$.

- In the CLUBB model, it is assumed that $s$ and $N$ take on a joint normal-lognormal probability density function (PDF), which depends on 5 parameters (the means and variances) in $x_j$.

- Currently, at each time step, and every grid box, the normal-lognormal PDF is sampled in each grid box using Latin Hypercube sampling.

- The samples are then used to compute the Autoconversion mean at each grid box and time step.
Better sub-grid physics PDF quadrature

- We can replace Latin Hypercube sampling with a quadrature based approach.

**Latin Hypercube Sampling vs Quadrature**

Using a quadrature approach, we can bypass the random sampling and calculate the Autoconversion mean using far fewer points, with even greater accuracy.
Selected interactions with SciDAC Institutes

- FastMATH: Implicit solver introduction and optimization for variable grids
- SUPER: Performance portability and acceleration of ocean dycore
- QUEST: Acceleration of quadratures for sub-grid integrals over PDFs