Multiscale Methods for Accurate, Efficient, and Scale-Aware Models of the Earth System

Project Leads: Bill Collins, Bert Debusschere, and Steve Ghan

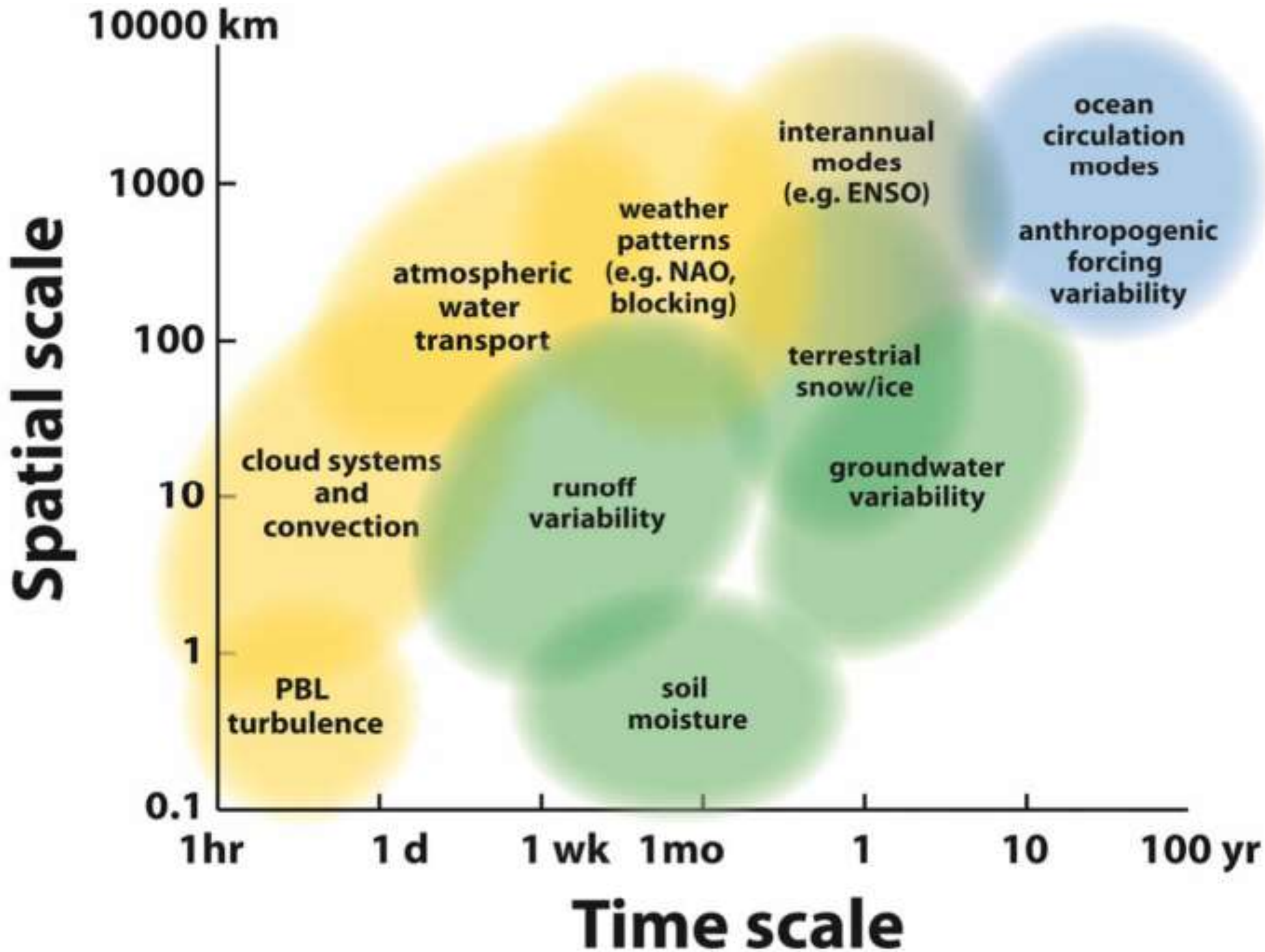
Science Team Leads and Institute Liaisons:

• Atmosphere	Steve Ghan
• Ocean	Todd Ringler
• Computational Science	Carol Woodward
• Multiscale UQ	Don Lucas
• FASTMath Liaison	Carol Woodward
• SUPER Liaisons	Lenny Oliker and Sam Williams
• QUEST Liaison	Bert Debusschere

MULTISCALE

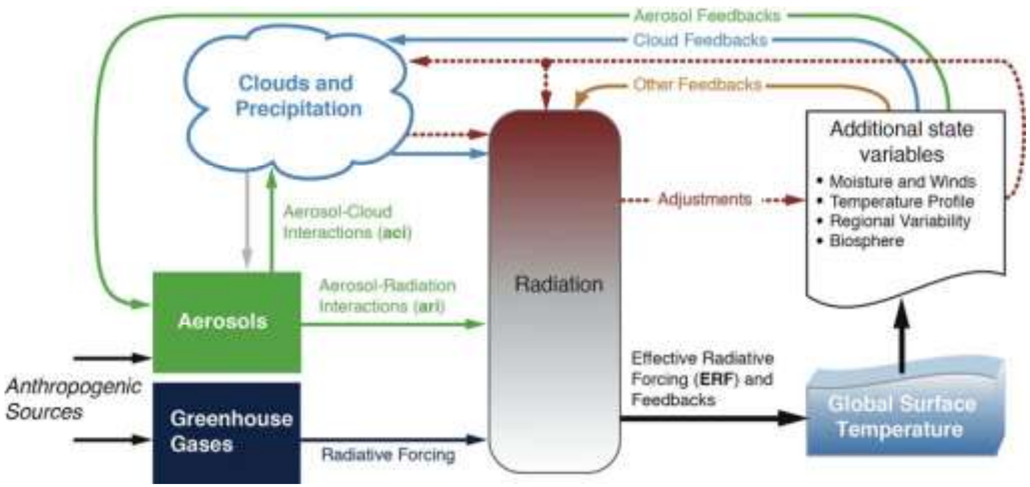
SciDAC
Scientific Discovery through Advanced Computing

Key space and time scales of water cycle

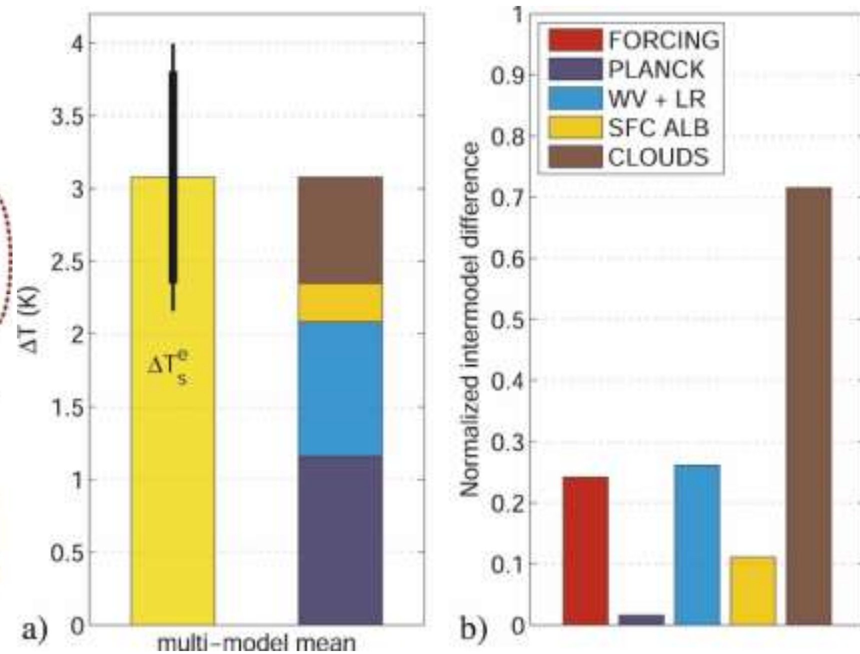


- Range of spatial and temporal scales for predictions is 6 orders of magnitude.
- Scales are strongly coupled via climate processes and climate change.

Clouds in the climate system



IPCC AR5 WG1

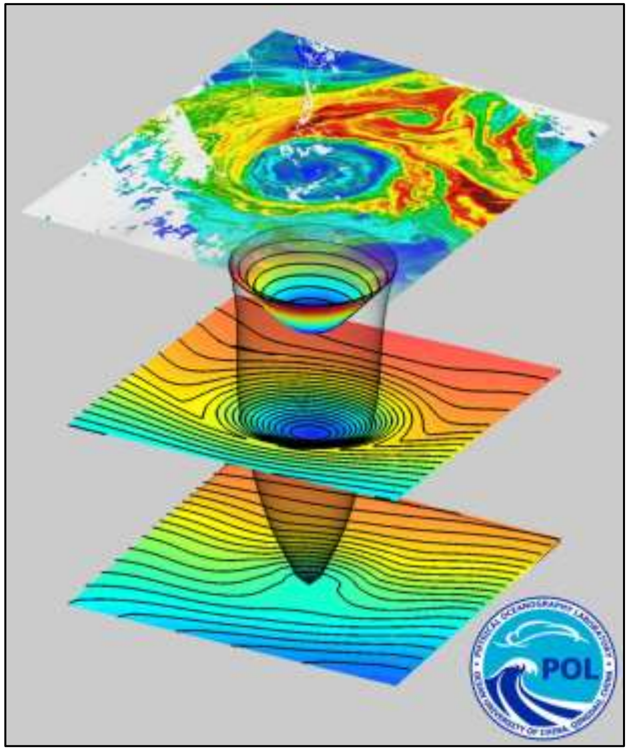


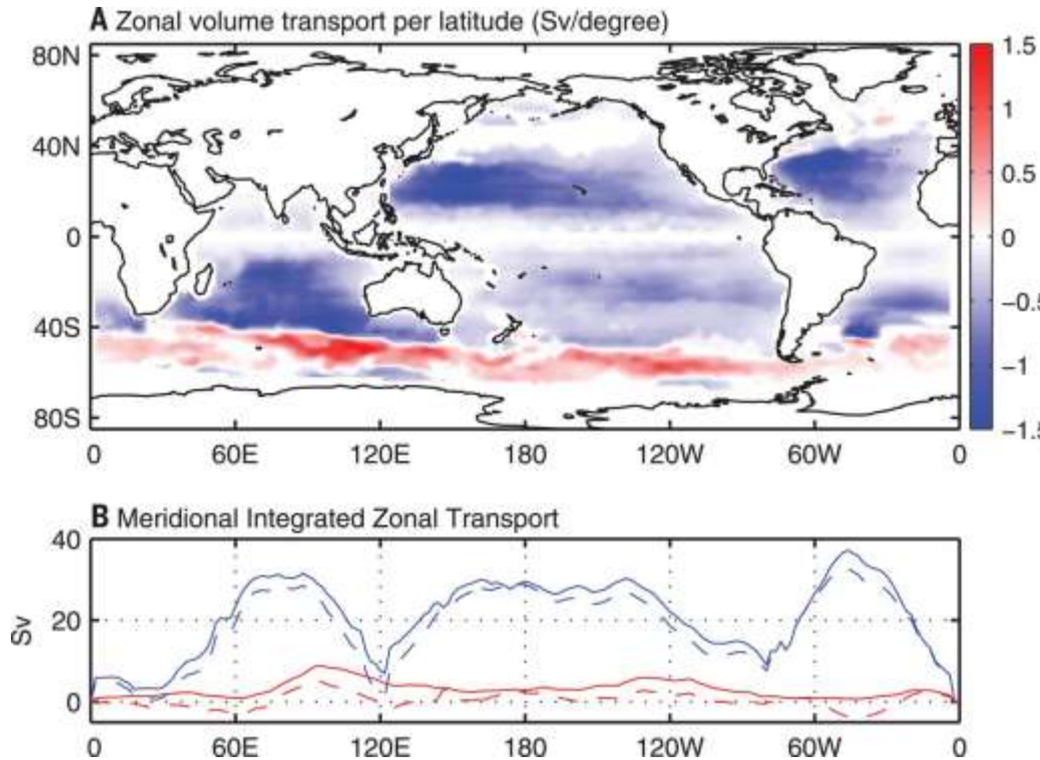
Dufresne et al, 2008

- Clouds are closely coupled to the mean state and feedbacks of climate system.
- Clouds contribute largest source of uncertainty to projections of climate change.

- Most cloud systems are subgrid relative to the meshes of current climate models.
- Small size, combined with lack of 1st principles theory, requires push to explicit modeling.

Significant role of ocean mesoscale eddies



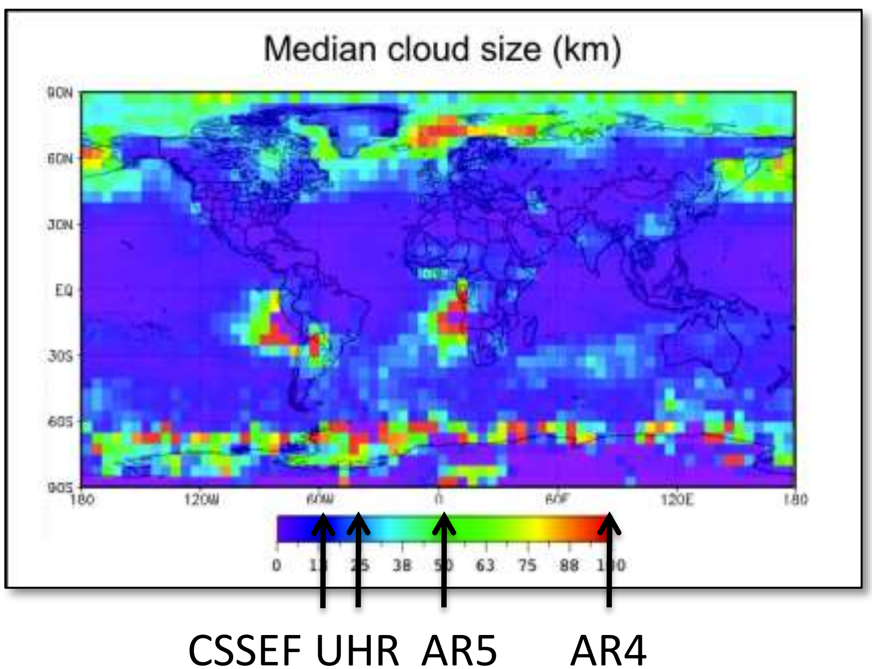


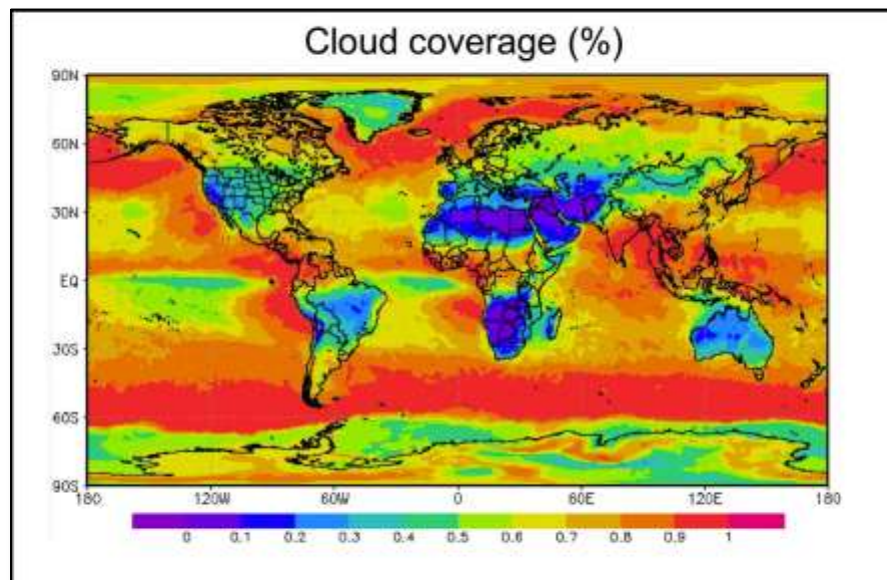
Oceanic mass transport by mesoscale eddies
Science 18 July 2014: vol. 345 no. 6194 322-324

- Mesoscale ocean eddies produce mass transports of same order as wind & circulation .
- The eddies are unresolved by current ocean models, introducing large uncertainties.

Goals of the Multiscale Project

- Develop, and apply multiscale models of the climate system using 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 for next-generation computer systems.

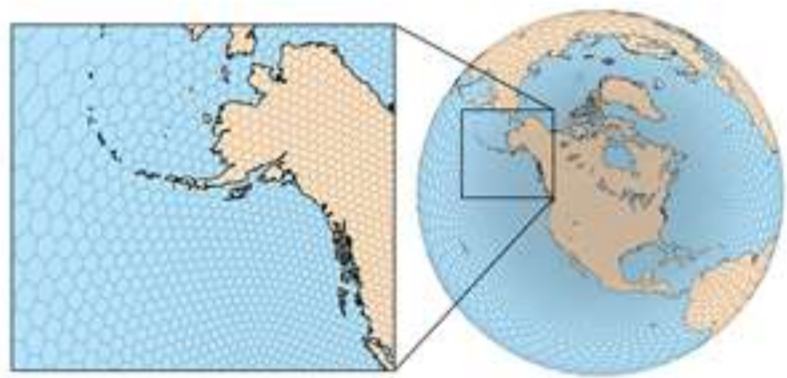




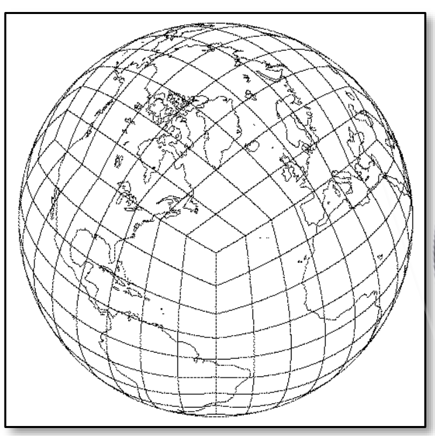
Project Elements

Variable Mesh Dycores

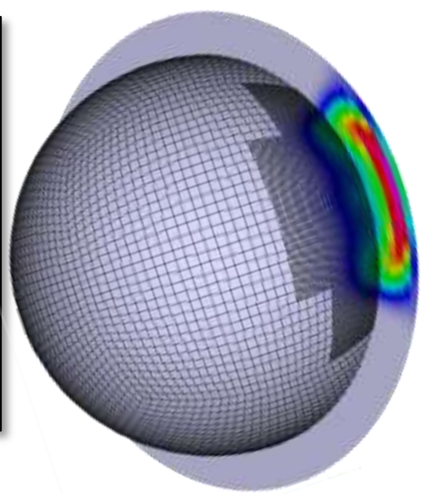
Model for Prediction Across Scales (MPAS)



Spectral Element Dycore



Chombo Dycore



Physics-Dynamics Interface

Convection

Microphysics

Process Integration

Multiscale UQ

Atmosphere

Ocean

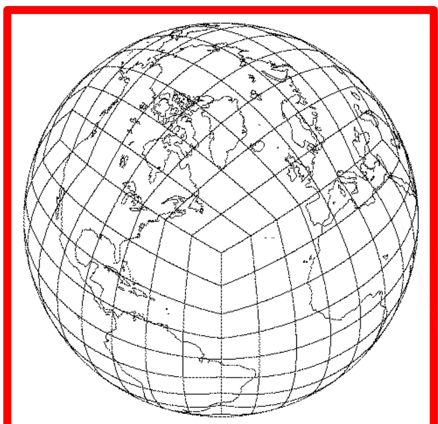
Mesoscale Eddy Treatments

Project Elements

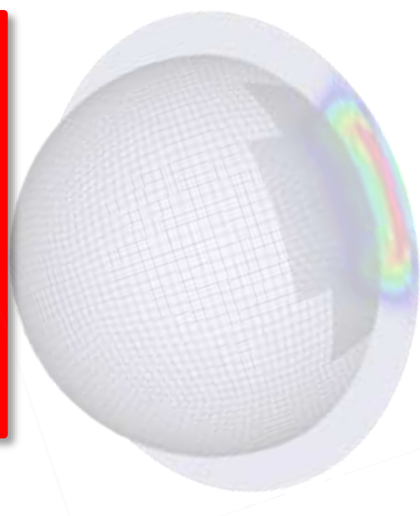
Variable Mesh Dycores

Model for Prediction Across Scales (MPAS)

Spectral Element Dycore



Chombo Dycore



Physics-Dynamics Interface

- Convection
- Microphysics
- Process Integration
- Multiscale UQ

Atmosphere

Ocean

- Mesoscale Eddy Treatments

Arbitrary-Order Conservative and Consistent Remapping and a Theory of Linear Maps

SciDAC Multiscale

Objectives

- Develop a robust arbitrary-order linear remapping scheme between finite volume and finite element meshes that is conservative, consistent, and (optionally) monotone.

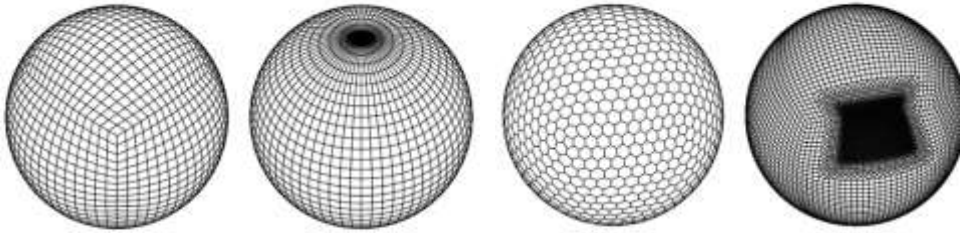
Impact

Linear maps are important for post-processing of model data (generally for mapping unstructured model output to latitude-longitude coordinates), and for coupling model components which can reside in different grid systems.

Accomplishments

- Developed a theory of linear maps necessary for maintaining conservation, consistency and monotonicity.
- Developed the Tempest Remap toolkit for generating linear maps between finite volume and finite element meshes supporting all desired properties.

Ullrich, P.A., M.A. Taylor (2015): "Arbitrary-Order Conservative and Consistent Remapping and a Theory of Linear Maps, Part 1", Mon. Wea. Rev. 143, 2419--2440. doi:10.1175/MWR-D-14-00343.1.



Some of the many structured and unstructured meshes that are supported by the TempestRemap toolkit. Unstructured meshes (far right) and regional area remapping are two key features of the toolkit.

Support provided by the BER SciDAC Multiscale project

Implicit Climate Dynamics with Newton-Krylov Solvers with Spectral Elements

SciDAC Multiscale

Objectives

- Improve nonlinear solver performance with implicit time integration methods which allow for longer time steps within climate dynamics simulations
- Determine the impact of finite difference matrix-vector products on solver speed and robustness

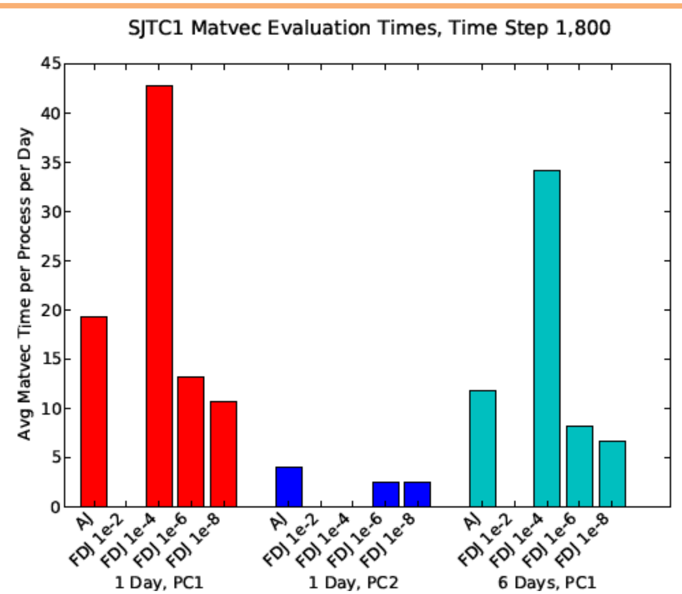
Impact

- Demonstrated that finite difference approximations are efficient within Newton-Krylov solvers for implicit climate dynamics with spectral element methods
- Determined that the default differencing parameter is not optimal and a smaller value of 1e-8 yields faster solve times with lager time step sizes

Accomplishments

- Added the capability to utilize analytic Jacobian-vector products with the Trilinos NOX solver in CAM-SE
- Determined optimal differencing parameter for finite difference approximation
- Identified areas for improving solver and preconditioner efficiency by precomputing Jacobian information

C. S. Woodward, D. J. Gardner, and K. J. Evans, "On the Use of Finite Difference Matrix-Vector Products in Newton-Krylov Solvers for Implicit Climate Dynamics with Spectral Elements," Procedia Computer Science, 51, (2015), pp. 2036-2045. DOI: 10.1016/j.procs.2015.05.468



With a 30 min. time step the smaller differencing parameter of 1e-8 improves run times compared to the default of 1e-6

Support provided by the BER SciDAC Multiscale project

Climate Change Science Institute
AT OAK RIDGE NATIONAL LABORATORY

Effects of a High-Order Vertical Coordinate in a Non-Hydrostatic Global Model

SciDAC Multiscale

Objectives

- Determine how standard low-order staggered finite difference methods can be extended to high-order finite element methods in the vertical column.
- Investigate the effects of a high-order vertical discretization on model accuracy.

Impact

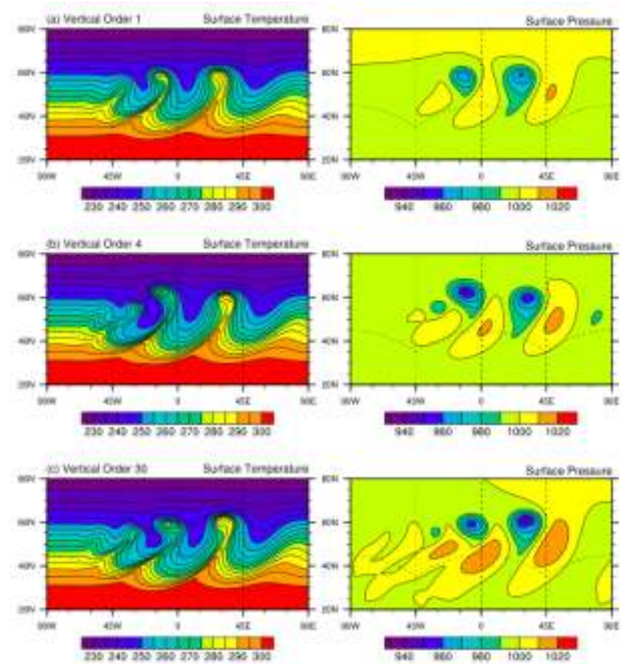
Demonstrated that arbitrary-order finite element can be used in the vertical direction in order to improve model accuracy without substantially improving computational cost.

Accomplishments

- Developed a numerical formulation that extends low-order staggered methods such as Lorenz and Charney-Phillips and enables arbitrary order-of-accuracy in each vertical column.

Ullrich, P., J. Guerra. "Exploring the Effects of a High-Order Vertical Coordinate in a Non-Hydrostatic Global Model." Procedia Computer Science 51:2015, p. 2065-2074.

Increased vertical order-of-accuracy provides greatly improved model accuracy at minimal additional computational cost.



ACME Accelerated Climate Model for Energy

Support provided by the BER SciDAC Multiscale project

Climate Change Science Institute AT OAK RIDGE NATIONAL LABORATORY

Accelerating Time Integration for the Spherical Shallow Water Equations Using GPUs

SciDAC Multiscale

Objectives

- Enable the implicit solver capability within the Community Atmosphere Model (CAM) to use GPU to achieve performance gains
- Leverage the use of data copies already required to use the C++ based Trilinos solver libraries within CAM to transfer data to the GPU "for free"

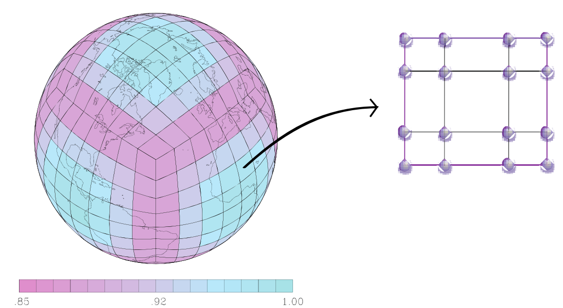
Impact

Demonstrated that some configurations of the implicit solver achieve efficiency gains when using the GPU, and that packing the nodes with more work, like other efforts to enable CAM to use the GPU, determines the degree of speedup

Accomplishments

- Developed the capability for the implicit solver option of CAM to use the GPU on the hybrid Titan system at the Oak Ridge computing facility (OLCF)
- Demonstrated the gains in using the GPU for higher spatial order discretization configurations, which are useful at high-resolution

Archibald, R. K., K. J. Evans, and A. G. Salinger (2015). Accelerating Time Integration for Climate Modeling Using GPUs, *Procedia Computer Science*, 51:2046-2055.



The individual elements within the cubed sphere grid of the CAM model are further decomposed with a spectral representation, and the order of the polynomials determines the density of the matrix solve, and thus the amount of work allocated to a GPU implementation.

Support provided by the BER SciDAC Multiscale project

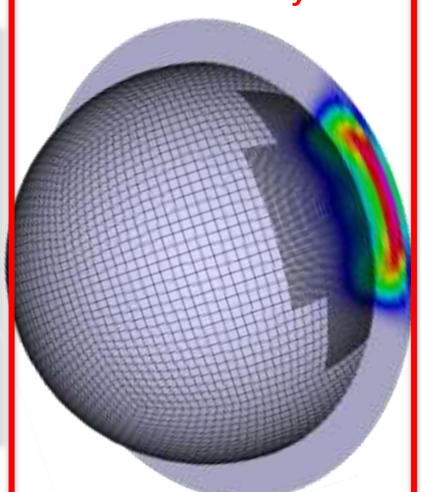
Project Elements

Variable Mesh Dycores

Model for Prediction Across Scales (MPAS)

Spectral Element Dycore

Chombo Dycore



Physics-Dynamics Interface

- Convection
- Microphysics
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Atmosphere

Ocean

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Cubed Sphere AMR for High-accuracy SWE solutions

Objective

We use adaptive refinement in space and time (AMR) and higher-order finite volume discretizations on the cubed sphere, to reduce solution error for typical climate dycore test problems, for tracer advection and the shallow water equations (SWE).

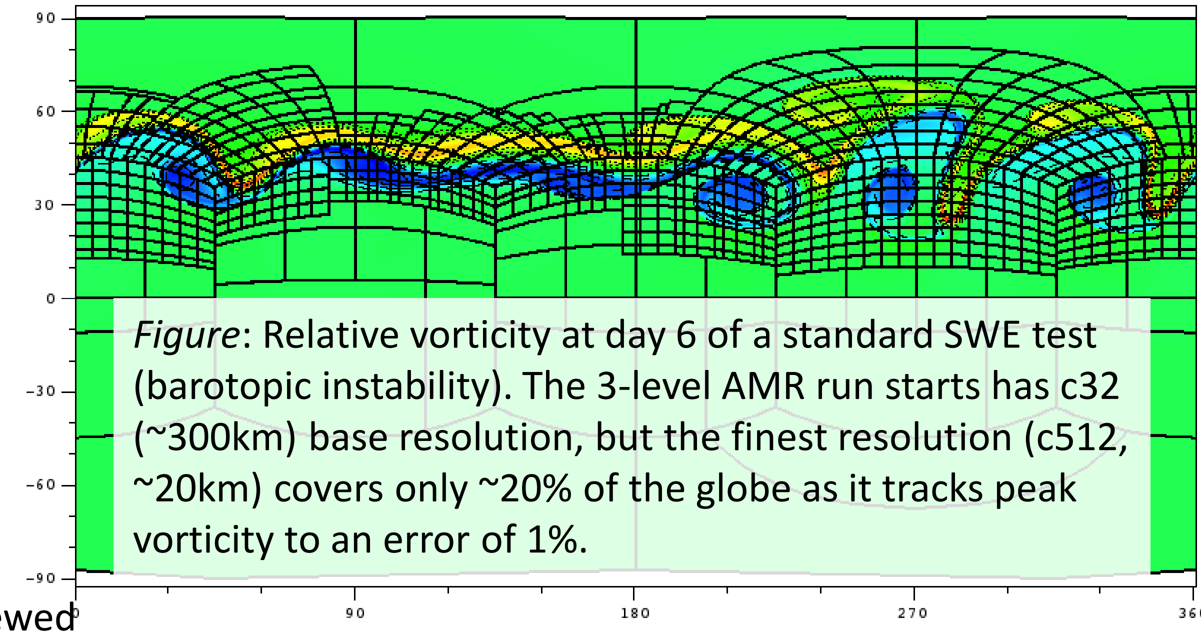


Figure: Relative vorticity at day 6 of a standard SWE test (barotopic instability). The 3-level AMR run starts has c32 (~300km) base resolution, but the finest resolution (c512, ~20km) covers only ~20% of the globe as it tracks peak vorticity to an error of 1%.

Research

- Space-time refinement has been viewed with skepticism both due to its computational complexity and poorly-understood errors.
- Starting with standard suites of tests, we are showing that AMR errors are manageable and that there are benefits for certain classes of climate phenomena.

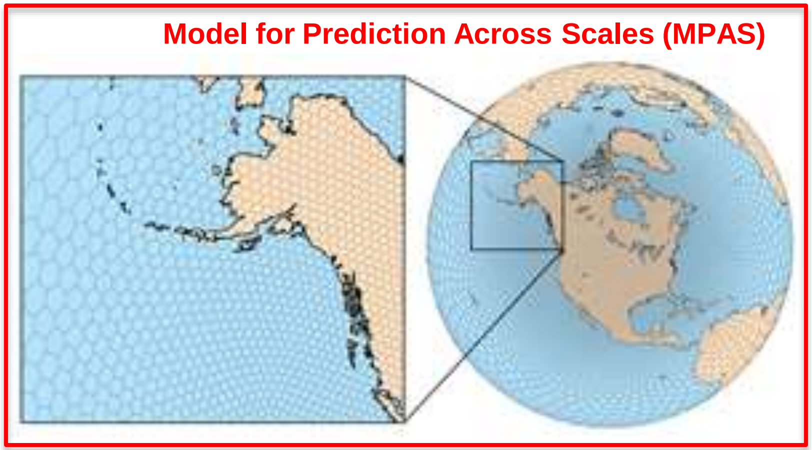
Impact

- AMR techniques compare well against uniform resolution simulations in tracer and SWE tests.
- Future research supports investigations of errors in climate “gray zone” (< 5km / 15s resolution) from interactions with physics parameterizations and dynamic features (e.g., tropical cyclones).

Reference: P. McCorquodale[2], ***P. Ullrich[1], H. Johansen[1]***, P. Colella[2], "An adaptive multiblock high-order finite-volume method for solving the shallow-water equations on the sphere," Communications in Applied Mathematics and Computational Science (CAMCoS), (accepted, http://msp.org/scripts/coming.php?jpath=camcos).
[1] *Funded under DOE SciDAC Multiscale project,* [2] *Funded under DOE SciDAC FASTMath institute*

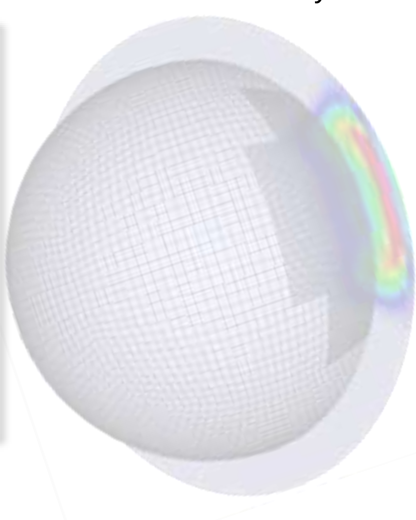
Project Elements

Variable Mesh Dycores

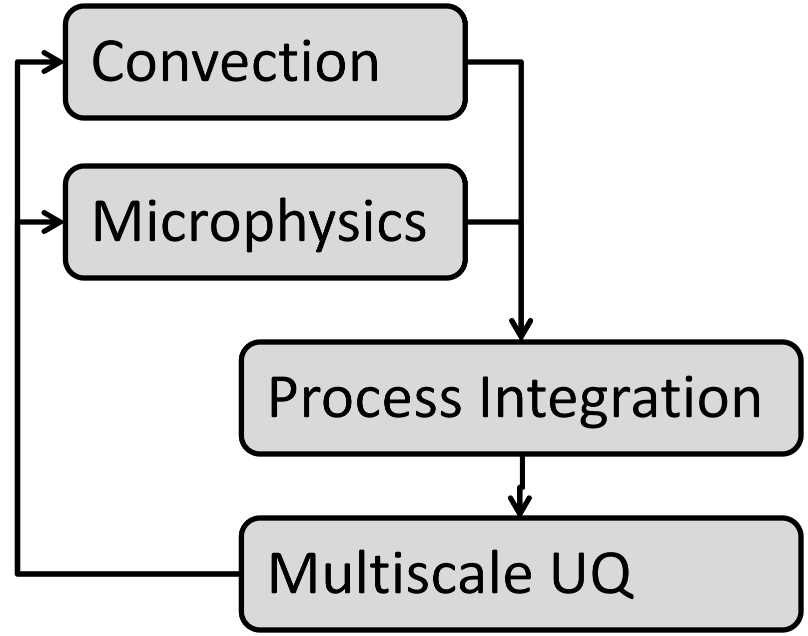


Spectral Element Dycore

Chombo Dycore



Physics-Dynamics Interface



Atmosphere

Ocean

Mesoscale Eddy Treatments

Performance Optimizations for MPAS-Ocean

A. Sarje, S. Williams, L. Oliker (LBNL), D. Jacobsen (LANL)

SciDAC Multiscale

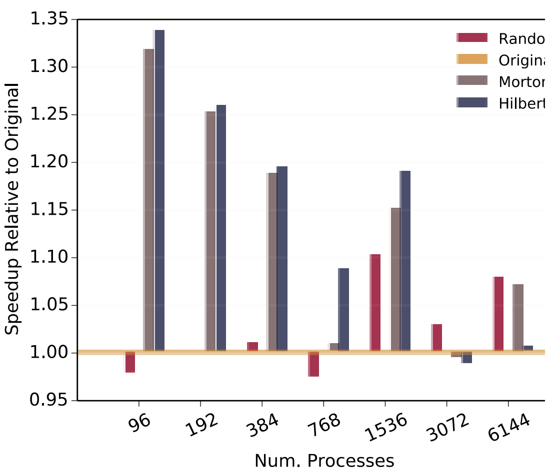
Objectives:

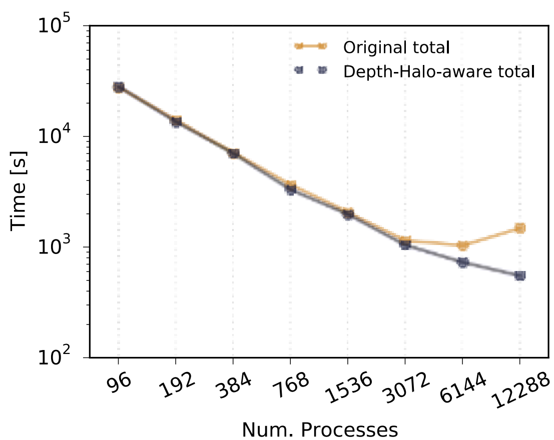
- Accelerate MPAS-Ocean code performance on state-of-the-art supercomputers
- Prepare MPAS-Ocean for transition to next generation highly parallel architectures
- Work collaboratively with SUPER Institute to leverage performance optimization tools and expertise

Impact:

- Demonstrated that space-filling curve based ordering essential for intra-node communication reduction
- Developed partitioning optimization approaches broadly applicable to numerous of unstructured-mesh based computations
- Allow higher Simulated-Years-Per-Day throughput for ocean modeling simulations with MPAS-Ocean.

(Left) Low concurrency speedup via mesh reordering on Edison
(Right) High concurrency speedup via hypergraph partitioning





Progress and Accomplishments:

- **SFC-based mesh data reordering: average 1.25x performance gain**
- **New halo-aware hypergraph partitioning algorithm improves scalability at high concurrency by over 2x.**
- **Combined with SUPER optimizations, including pointer reduction at 12K cores: <u>3-4x MPAS overall speedup</u>**
- **A. Sarje et al. MSESM/ICCS 2015** ***nominated best paper***

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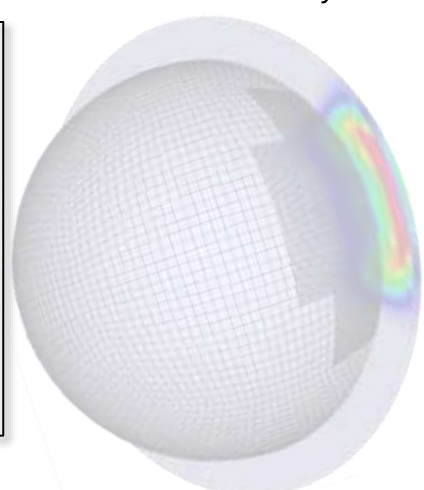
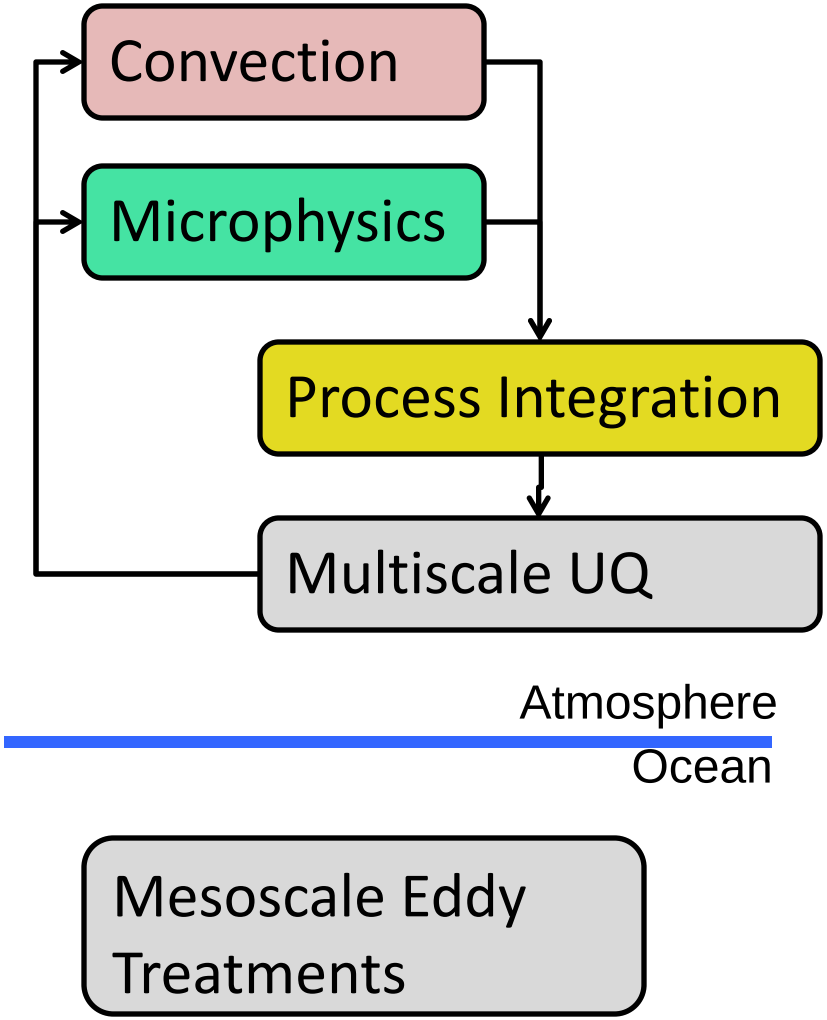


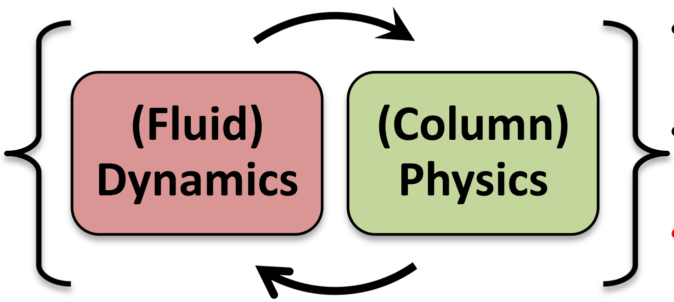
Physics-Dynamics Interface



Challenges in GCM Process Integration, Part 1

Atmospheric climate models have 2 parts:

- **Treats fluid flow**
- **Based on Navier-Stokes eqns**
- **Mathematically rigorous**



- **Treats diabatic processes**
- **Governing eqns often unclear**
- **Numerics less scrutinized**

Questions we are trying to answer:

- Are numerical implementations of physics processes accurate solutions of the intended equations?
- Does coupling between physical processes corrupt the intended model behavior?
- What is the source of resolution/timestep sensitivity?

Challenges in GCM Process Integration, Part 2

- General circulation models such as the Community Atmosphere Model (CAM) typically use a physics time step of ~30 minutes
- Large time step sizes can lead to large numerical errors
- Two important components of the physics are :
  - **Cloud Macrophysics**: condenses or evaporates water (and changes cloud fraction) in order to keep relative humidity ≤ 100%
  - **Cloud Microphysics**: provides tendencies due to precipitation and freezing processes
- Coupling errors between the cloud macro- and microphysics have not been rigorously tested
- We are now characterizing and addressing these issues.

A Simple but Effective Method for Quantifying and Attributing Time-stepping Errors in Climate Models

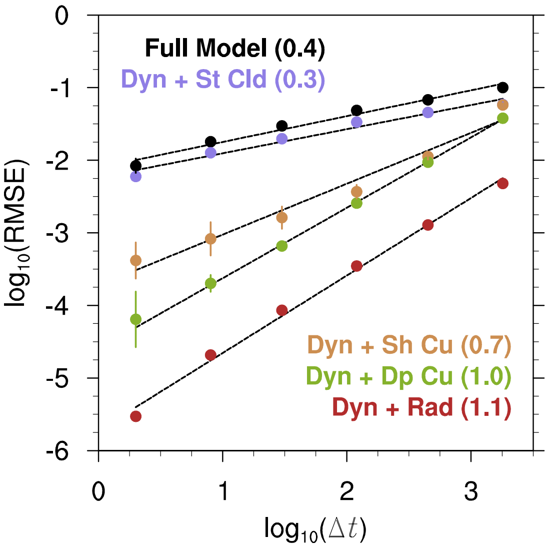
SciDAC Multiscale

Objective

- To characterize time step sensitivities in CAM5 and identify the sources of numerical artifacts

Approach

- Test time step convergence with fixed spatial resolution but reduced time step lengths
- Simulate on a very short period (1-hour) for computational efficiency and to minimize process interaction
- Solution obtained with shortest time step (1 second) regarded as reference
- Evaluate magnitude of temperature root-mean-square error and its dependence on time step
- Test the default model "as is" to assess time-integration error and sensitivity
- Test individual model components in isolation to help attribute error



Test reveals that the time integration error in CAM5 reduces more slowly than expected when the time step is shortened. The representation of stratiform clouds is the primary source of time-stepping error.

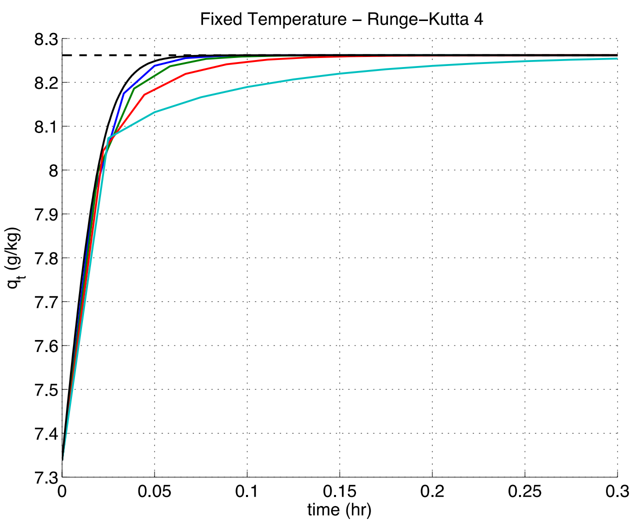
Impact

- The simple, effective, and computationally efficient error quantification method is applicable to all atmospheric general circulation models
- Results provide clear guidelines for subsequent efforts to develop more accurate time-stepping methods.

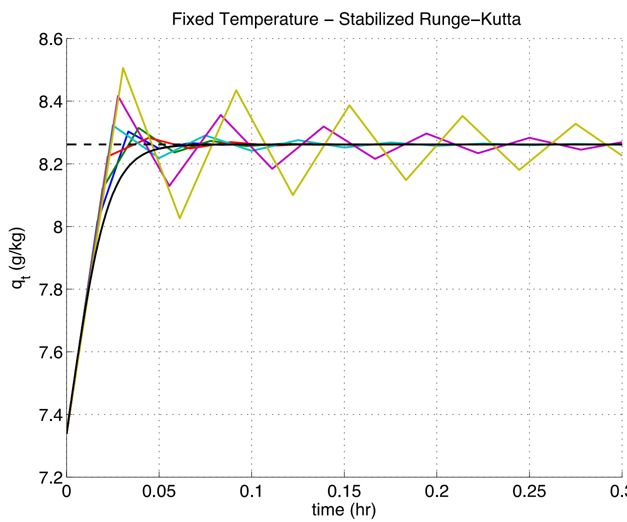
Wan H, PJ Rasch, MA Taylor, and C Jablonowski. 2015. "Short-Term Time Step Convergence in a Climate Model." *Journal of Advances in Modeling Earth Systems* 07. DOI: 10.1002/2014MS000368

Methods for Achieving Larger Time Steps

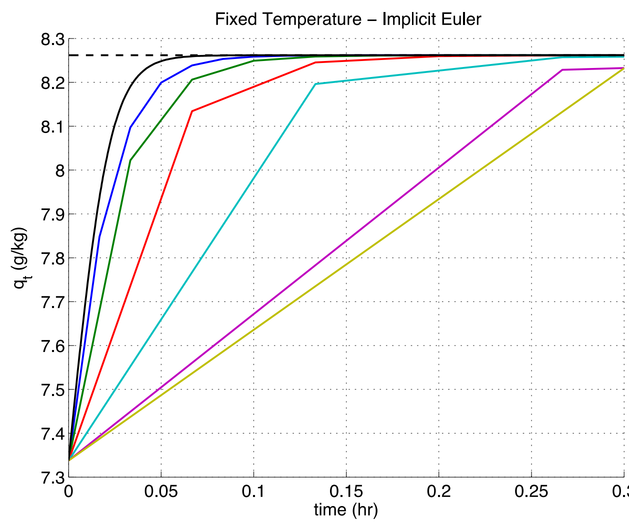
- **Higher order explicit methods (i.e. Runge-Kutta methods)**
  - Larger stability regions; Additional function evaluations
- **Stabilized explicit methods (i.e. Stabilized RK methods)**
  - Expanded stability regions; Increasing function evaluations
- **Implicit methods (i.e. Implicit RK, BDF, Adams-Moulton)**
  - Unconditionally stable methods; Solution to nonlinear system



Runge-Kutta 4
60s, 70s, 80s, 90s



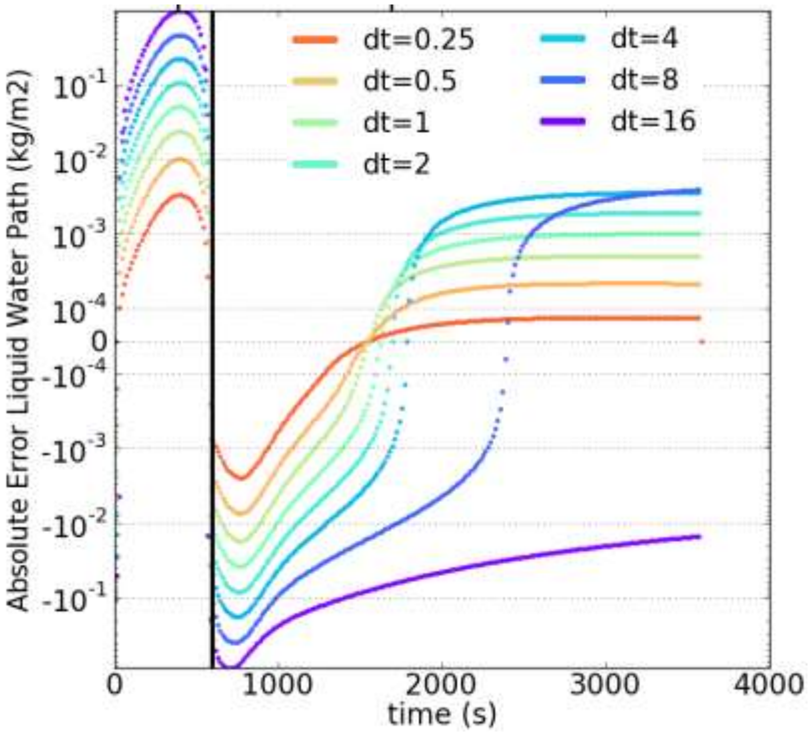
Stabilized RK
60s, 70s, 80s, 90s, 100s, 110s



Implicit Euler
60s, 120s, 240s, 480s, 960s, 1080s

Kinematic Driver (KiD) Model as a Testbed

- The **KiD single column model** is a simplified framework that:
  - Tests the micro- and macrophysics of CAM
  - Idealizes all other aspects of the model
- Simplicity of the KiD model also makes
  - Diagnosing problems easier
  - Testing numerical approaches faster
- This will allow us to explore the coupling and time stepping errors observed with the box model in a more realistic setting



The absolute error in Liquid Water Path for various step sizes compared to a reference solution with Δt = 0.0625s in the Warm1 test case

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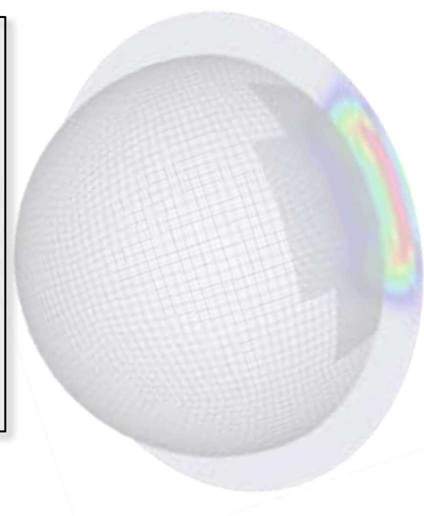
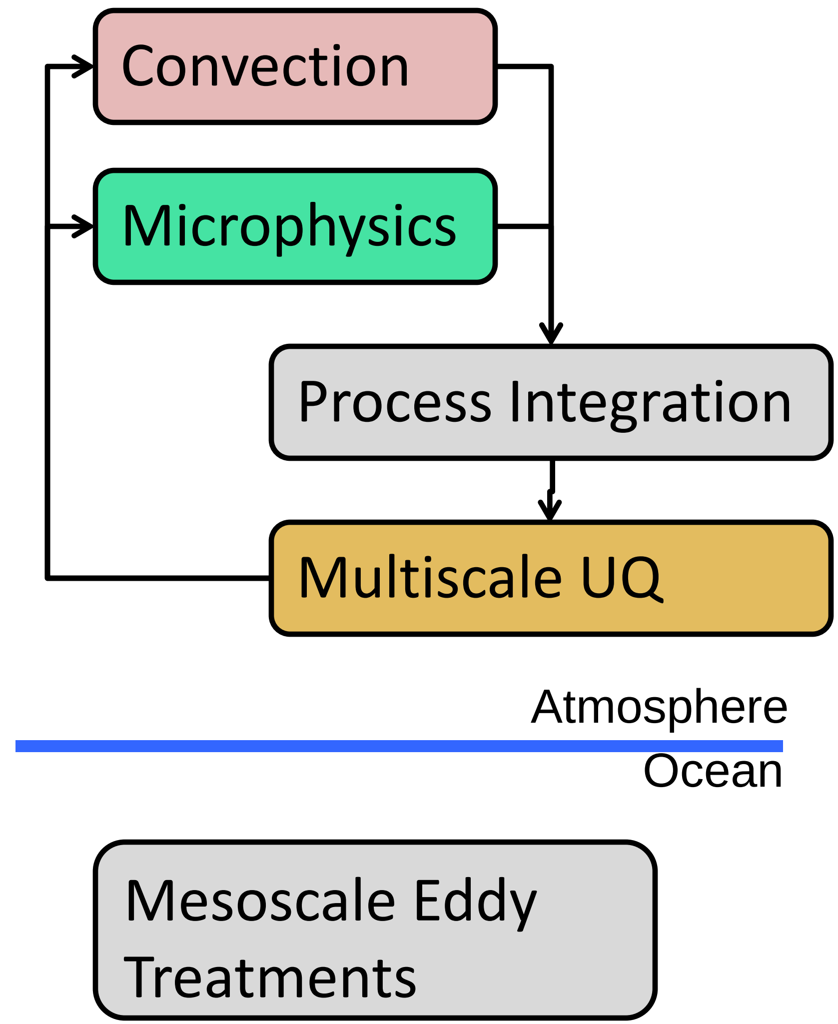


Physics-Dynamics Interface



Quadrature based sampling methods to account for sub-grid microphysics variability

SciDAC Multiscale

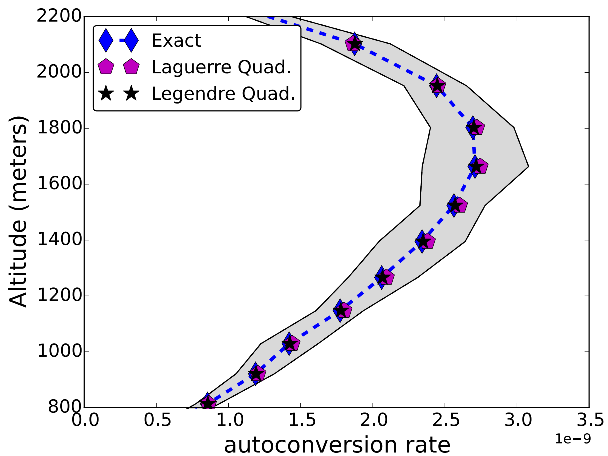
Objectives

- Develop and implement efficient approaches to account for sub-grid variability in microphysics
- More accurately compute grid-box averaged moments of microphysics such as autoconversion and accretion rates
- Utilize quadrature based approaches instead of random sampling to get better convergence at a lower computational cost.

Impact

- Better accounting for microphysics variability in atmospheric modeling
  - More accurate microphysics moments calculations
  - Potential for significant reduction in computational cost
  - Better reproducibility
  - Improved model accuracy and prediction

Accomplishments

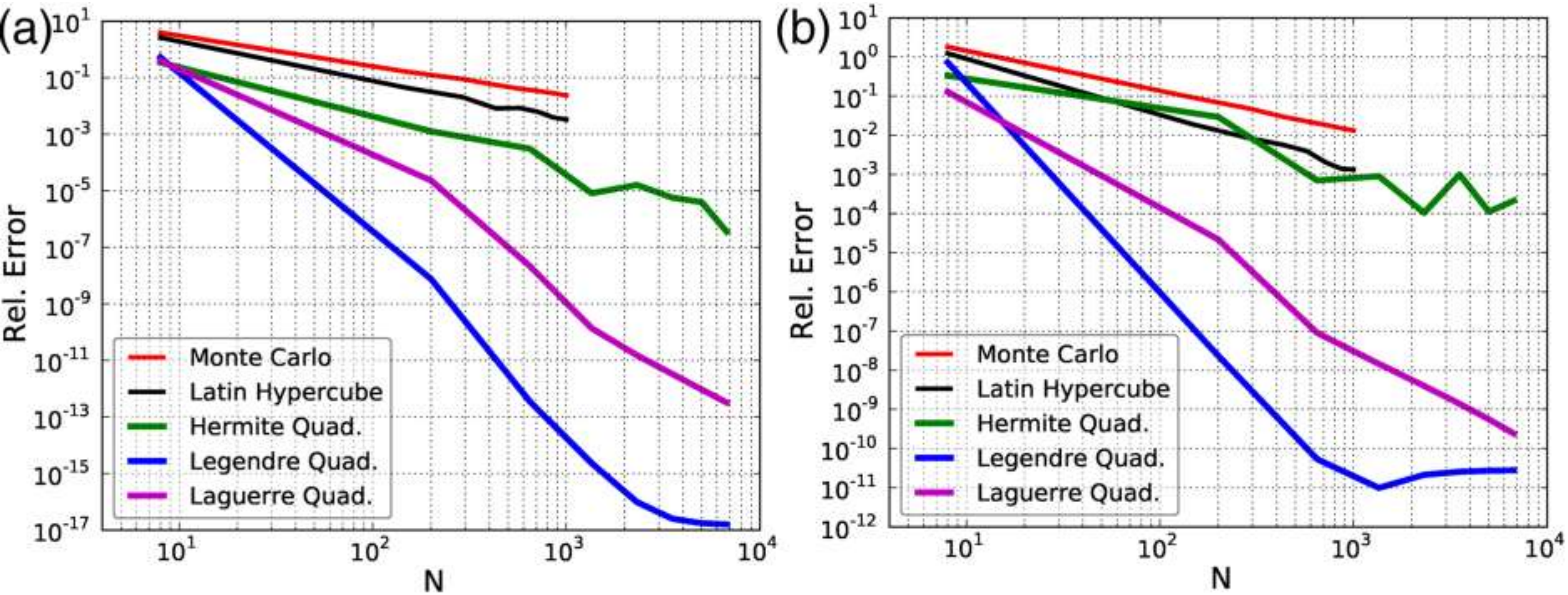


Comparison of mean autoconversion rate at different altitudes using quadrature (purple and black) vs. Latin Hypercube sampling (variance shown in gray shaded region). Blue dashed line is the exact value.

- Quadrature approaches show significant improvement of sub-grid microphysics calculations for autoconversion and accretion averages
  - Figure shows greater accuracy using ten times fewer points than random sampling
- These quadrature approaches will be applied to other microphysics quantities in a similar manner
  - Developed a FORTRAN library, ForQInt v1.0, to integrate with microphysics parameterizations (CLUBB) in CAM.

Chowdhary, K., M. Salloum, B. Debusschere, V. E. Larson. "Quadrature methods for the calculation of subgrid microphysics moments." MWR, Vol. 143, No. 7, July 2015.

Performance and Release of Quadrature Library



- Maher Salloum, Kenny Chowdhary, Bert Debusschere, "ForQint v. 1.0". Fortran library for quadrature integration released as open source under Lesser General Public License (LGPL), 7/31/2014

Vision:

ACME is Earth system modeling, simulation and prediction project that optimizes the use of DOE laboratory resources to meet the science needs of the Nation and the mission needs of DOE
.

10-year science goals:

- A series of **prediction and simulation experiments** addressing scientific questions and mission needs
- A well documented and tested, continuously advancing, evolving and improving **system of model codes that comprise the ACME Earth system model**

SciDAC Multiscale → ACME Collaboration #1: Scale-aware Convective Parameterizations

SciDAC Multiscale

Objective

- Improve the representation of convective transport for scale-aware cumulus parameterization in regional and global climate models

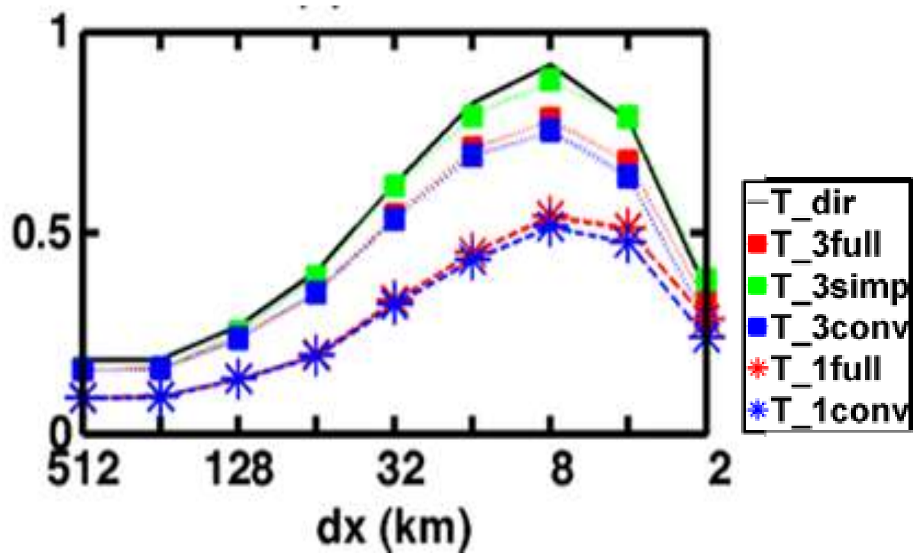
Approach

- Based on the traditional Z-M scheme, analyze cloud resolving model simulation results for different convective cloud systems to develop a better cumulus scheme.

Impact

- Gained clear understanding of scale-dependencies of cloud fraction and convective transport.
- Better representation of convective transport across all grid scales with a new cumulus parameterization, which is an update of the commonly used Zhang-McFarlane (Z-M) scheme for mesoscale to global model to use.

Vertical transport of moisture (g/kg m/s)



Vertical transport of moisture (VTM) calculated from our new formulation (T_3simp) agrees very well with CRM results (T_dir). Others, such as the Arakawa approach (T_1conv) underestimates VTM dramatically.

Liu Y-C, J Fan, G Zhang, K-M Xu, and SJ Ghan. 2015. "Improving Representation of Convective Transport for Scale-Aware Parameterization, Part II: Analysis of Cloud-Resolving Model Simulations." *Journal of Geophysical Research Atmospheres*, Accepted. DOI: 10.1002/2014JD022145.

SciDAC Multiscale ➔ ACME Collaboration #2: Block Preconditioners for Implicit Atmospheric Timestepping

SciDAC Multiscale

Objectives

- Develop robust and efficient numerical solvers for evolving climate simulations
- Build on FASTMath SciDAC Institute technologies and libraries for optimal nonlinear and linear solvers
- Develop custom preconditioner for the spectral element dycore of CAM (CAM-SE) that is scalable and works well with variable resolution grids

Impact

- Algorithm scalability required to contain run time costs by ensuring iteration counts do not increase with problem size
- Robust solvers and larger time steps enable faster throughput and/or more accurate nonlinearly converged solutions
- Constant time steps sizes that are independent of grid spacing

Accomplishments

- Developed and implemented an algorithmically scalable block preconditioner for shallow water equations, in trunk of CAM:

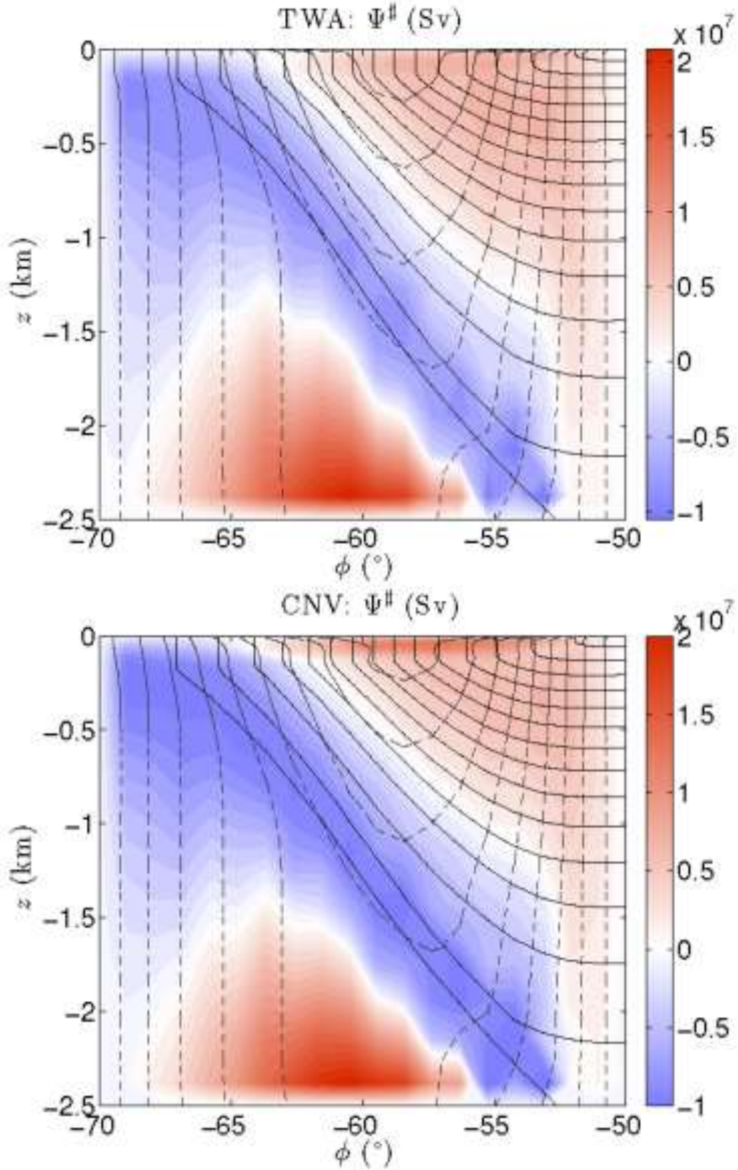
# Procs	# Unknowns	Lin. Its. (no PC)	Lin. Its. (w/ PC)
96	1,916,928	5,105	491
216	4,313,088	7,854	489
384	7,667,712	10,544	484
600	11,980,800	13,490	484

Left table: # linear iterations with implicit solver with and without a preconditioner, using a 720s time step size, Williamson et al. 1992 test case; 1 day;

- Mathematical and Computational advances in:
  - Block preconditioners
  - Impact within operational climate models

P. A. Lott, C.S. Woodward, K.J. Evans (2014). Algorithmically scalable block pre-conditioner for fully implicit shallow water equations in CAM-SE. Comp. Geosci. , 19:49-61, doi: 10.1007/s10596-014-9447-6.

SciDAC Multiscale → ACME Collaboration #3: Scale-aware Ocean Dynamics and Eddy Parameterization



- Theory for a new eddy parameterization has been formulated.
- A hierarchy of parameterizations with increasing accuracy and complexity has been formulated.
- DNS required to calibrate the free parameters in these parameterizations is underway.

- Once calibration and reference calculations are complete, the team will start preparations to introduce the parameterization into ACME.

Saenz, J., Q. Chen, and T. Ringler, 2015: Prognostic residual-mean flow in an ocean general circulation model and its relation to prognostic Eulerian-mean flow. J. Phys. Oceanogr. doi:10.1175/JPO-D-15-0024.1, in press.

Conclusions

- We have developed methods for extending variable mesh atmospheric dycores with implicit time stepping, accurate regridding, extensions to nonhydrostatic domain, and adaptive mesh refinement with significant contributions from FASTMath.
- We have accelerated the performance of ocean dycores through SUPER collaboration.
- We have characterized the accuracy of atmospheric physics under timestep refinement, and we are developing testbeds to remove artifacts preventing convergence.
- We have developed a new parameterization of mesoscale eddies from 1st principles.
- Both the ocean and atmosphere physics are being calibrated and accelerated w/ QUEST.

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