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

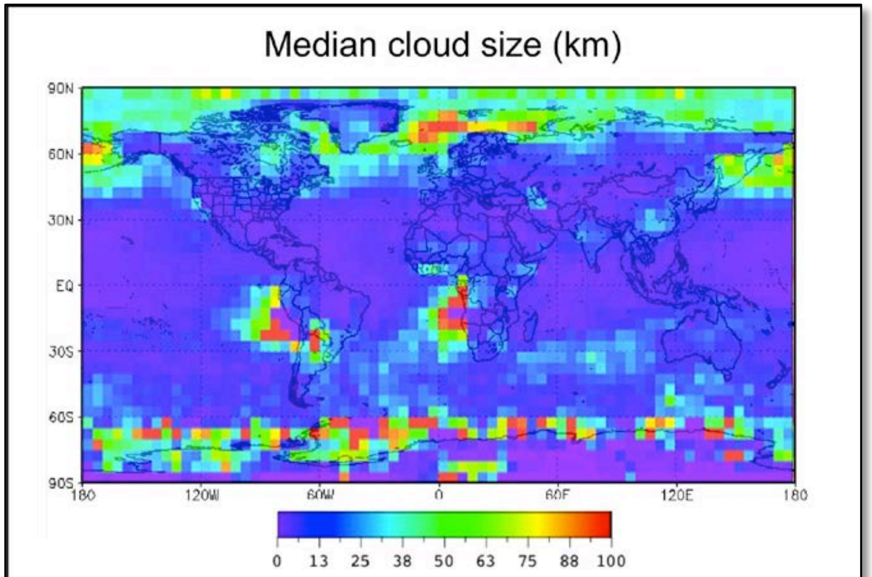
Principal Investigator: Bill Collins

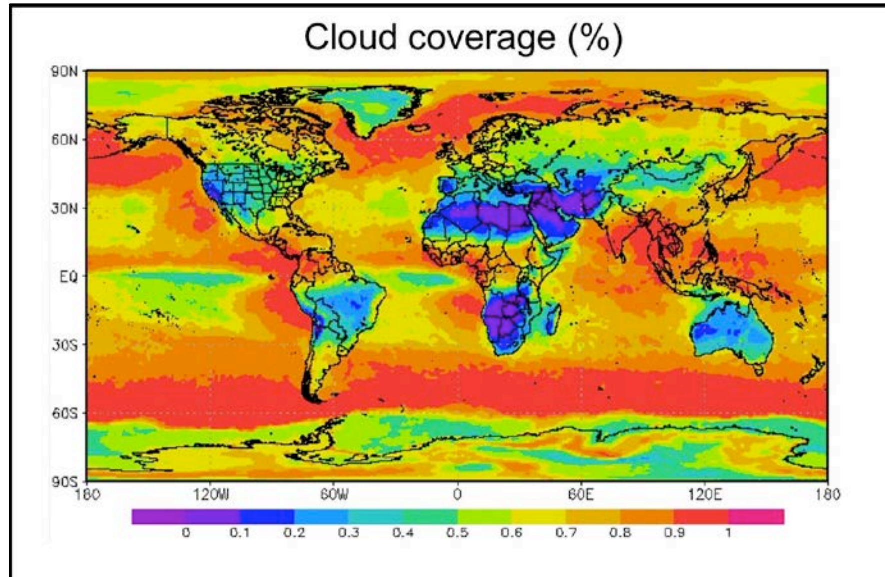
Science Team Leads and Institute Liaisons:

• **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**

Clouds scales beyond current model resolution

SciDAC Multiscale





CSSEF UHR AR5 AR4

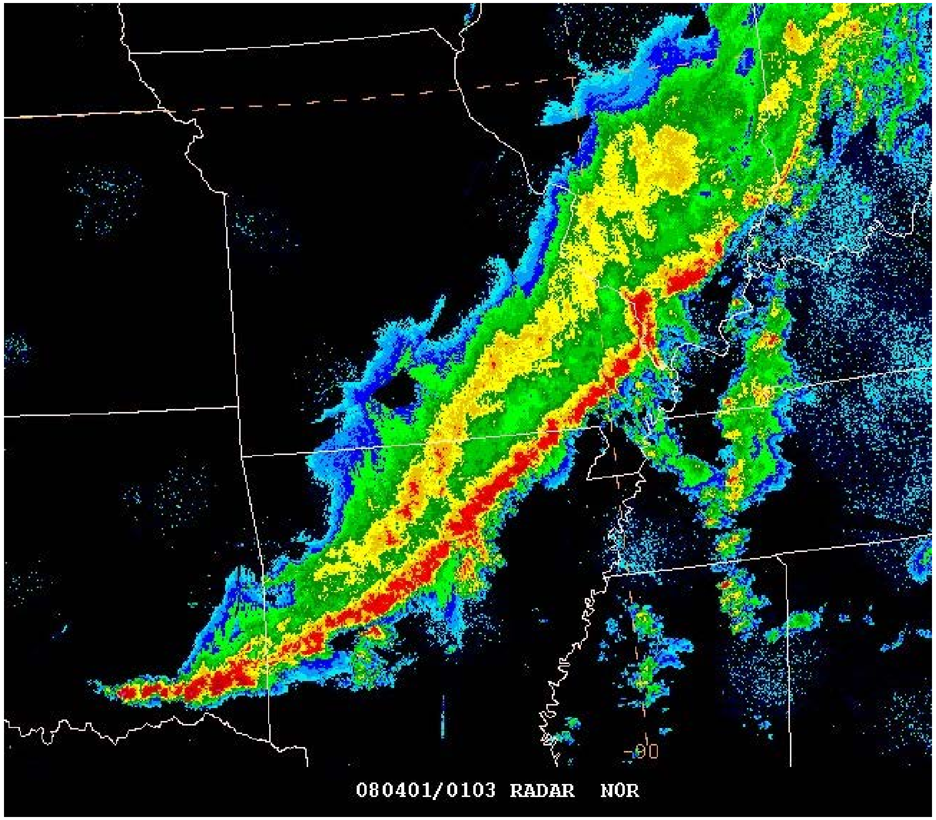
Potential of multiscale climate dynamics

- Many climate-relevant features are localized in space and time
- Features can be: stationary, move at advected speeds, or evolve from wave dynamics
- Refinement can greatly reduce computational resources needed

Examples:

- Tropical cyclones
- Squall lines / storm fronts
- Atmospheric rivers
- Ocean eddies

→ Refine where/when required

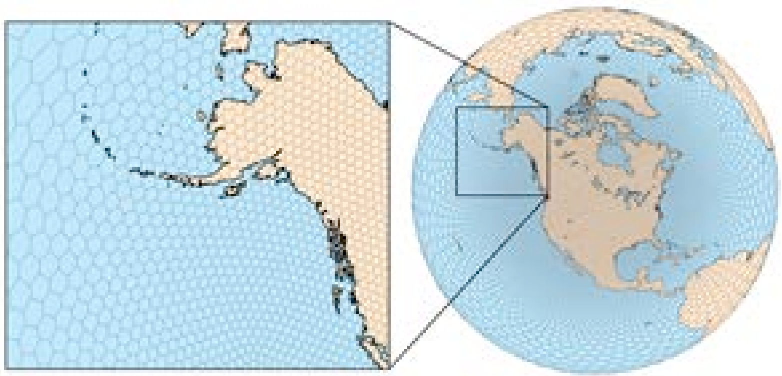


Radar image of a squall line over central US

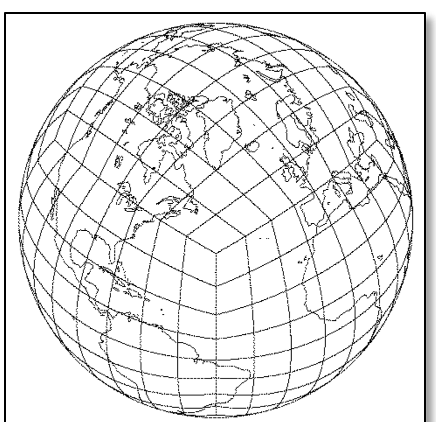
Project Elements

Variable Mesh Dycores

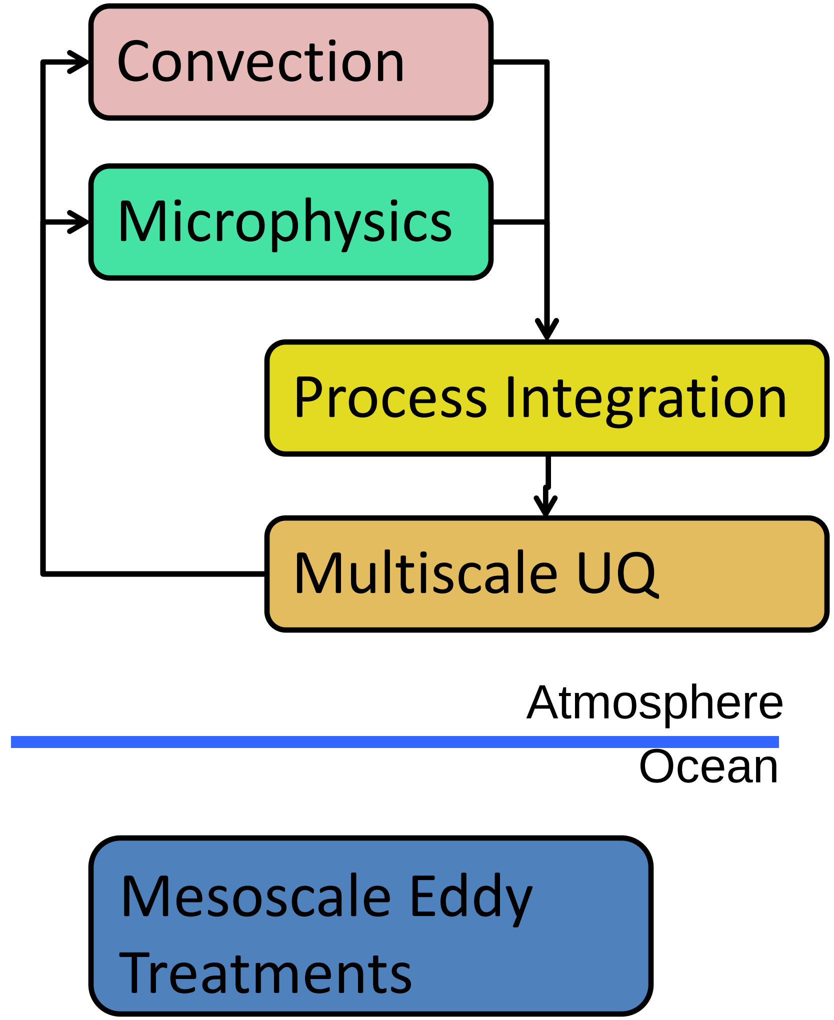
Model for Prediction Across Scales (MPAS)



Spectral Element Dycore



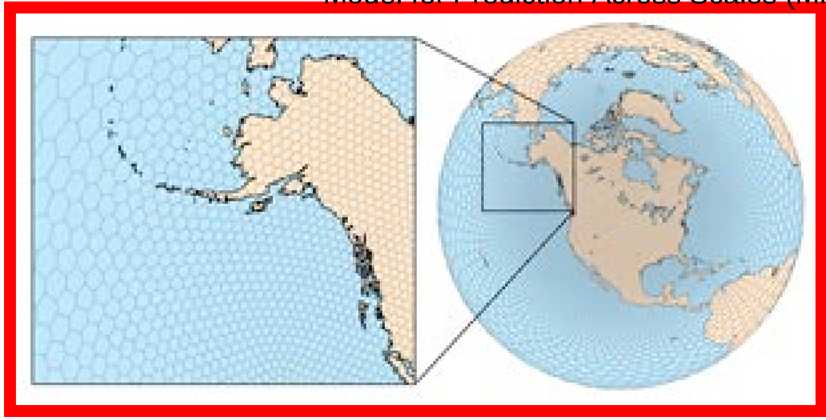
Physics-Dynamics Interface



Optimization of MPAS dycore with SUPER

Variable Mesh Dycores

Model for Prediction Across Scales (MPAS)



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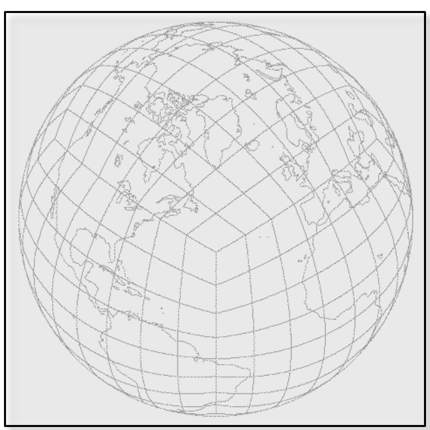

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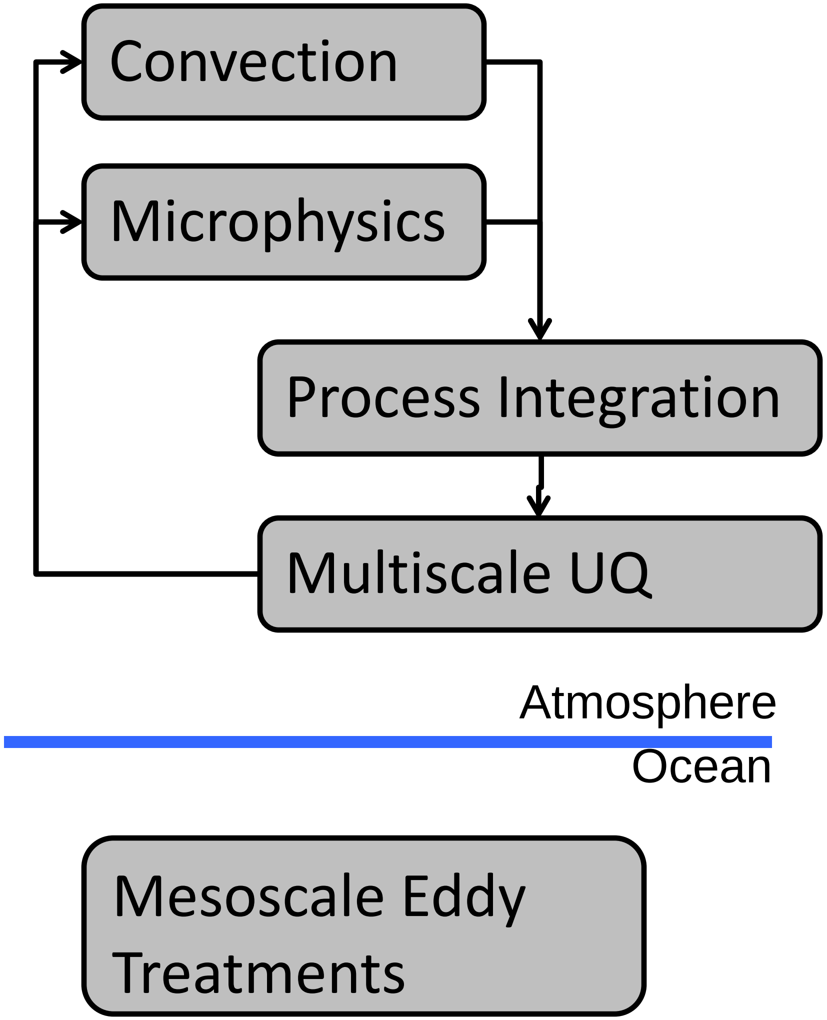
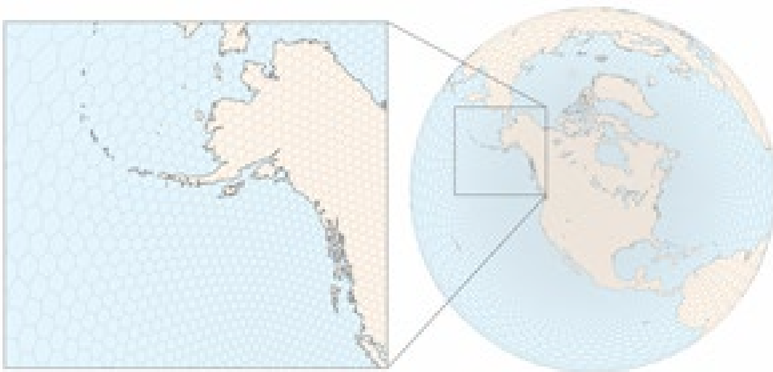


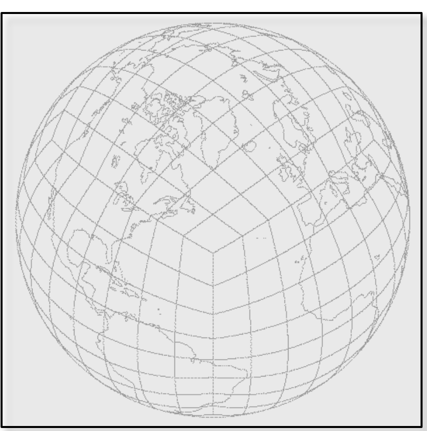
Addition of Chombo dycore with FASTMath

Variable Mesh Dycores

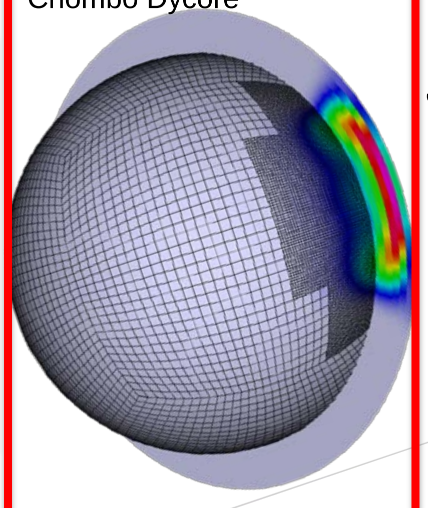
Model for Prediction Across Scales (MPAS)



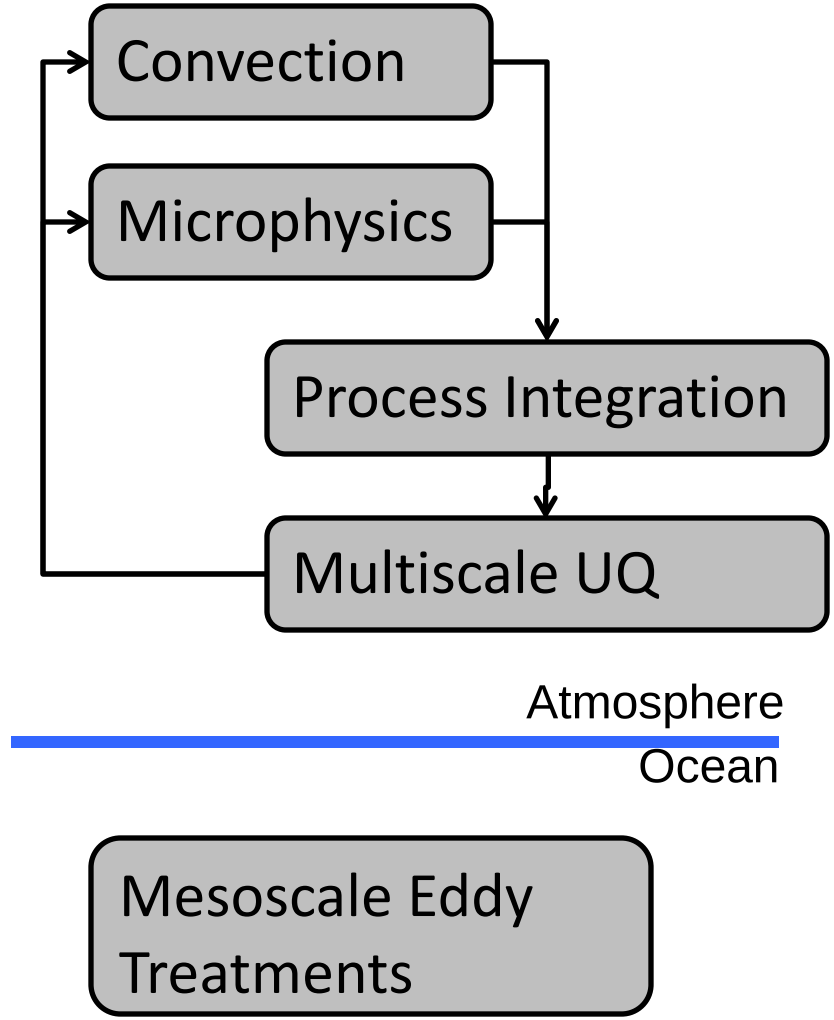
Spectral Element Dycore



Chombo Dycore



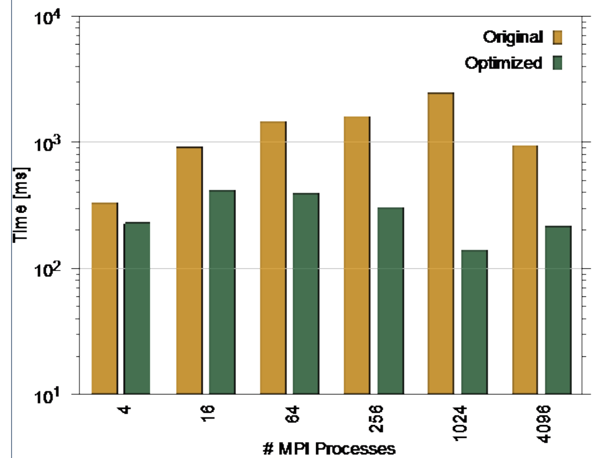
Physics-Dynamics Interface



SUPER / FASTMath / Quest Interactions

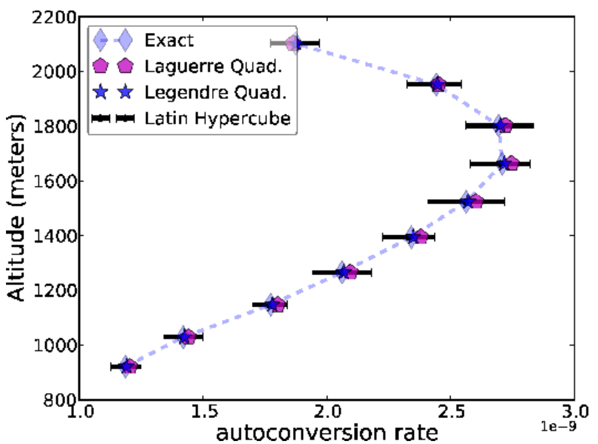
SciDAC Multiscale

- **SUPER:** Investigating intra-node optimization of MPAS-Ocean via Space-Filling-Curve ordering and inter-node optimization via aggregate communication schemes
- **FASTMath:** Developing preconditioners for scalable implicit solves for CAM-SE
  - Journal paper submitted
  - Initiated multilevel solver development
- **FASTMath:** Developing Implicit-Explicit Non-hydrostatic AMR Dycore; Completed tests for SWE, Linearized Gas Dynamics
- **QUEST:** Developed and applied a deterministic quadrature approach for integrating microphysics over subgrid variability
  - To CLUBB autoconversion & accretion
  - Journal paper submitted
- **QUEST:** Applying Bayesian Compressed Sensing for surrogate development and sensitivity analysis in CLUBB (29 input params)



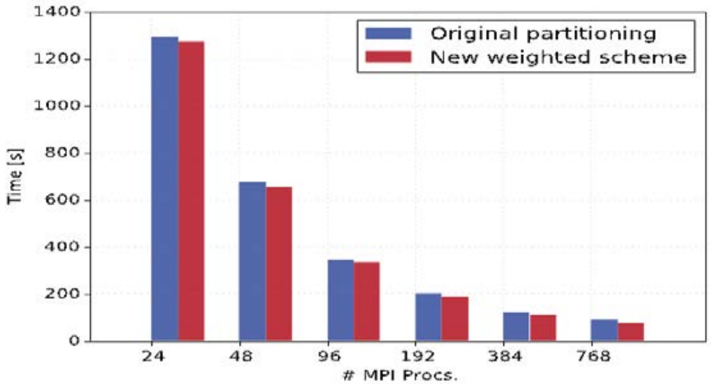
Optimized communication potential via a micro-benchmark developed to capture the MPAS-O halo exchange (Edison)

Autoconversion at 72 hours in the RICO case, showing superior accuracy of quadrature results based on just 16 samples over Latin Hypercube results based on 500 random samples

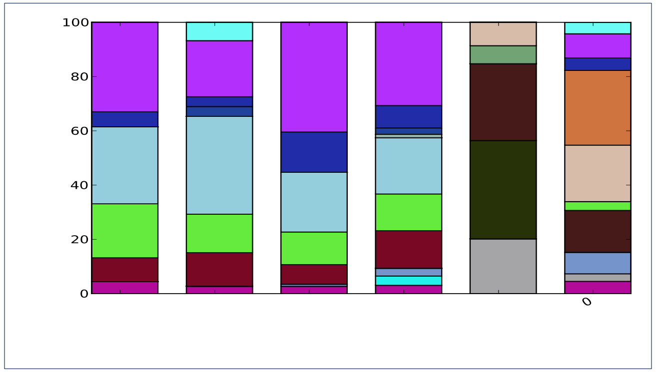


Institute Interactions, continued

- **SUPER:** New MPAS-O partitioning scheme based on hyper-graph with weights taking into account the computations and communication due to local cells as well as halo cells
- **FASTMath:** Initiated project to analyze splitting methods and convergence with time step for microphysics
- **QUEST:** Bayesian Compressed Sensing to perform sensitivity analysis and build liquid cloud fraction models in CLUBB
  - Adaptive approach generates surrogates with fewer terms and reduced over-fitting



Reduction in total MPAS-O run time using hyper-graph partitioning, with 5% speedup at highest concurrency



BCS derived sensitivity: similar to full 1st order basis approximation, with only half as many terms

Numerical Fluid Dynamics

Implicit Time Integrators **(KE, MT, C. Woodward)**

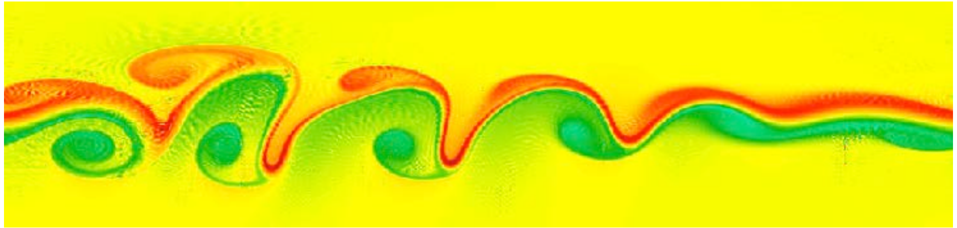
- In the CAM-SE dycore, the hyperviscosity term is now included within the implicit solve of the primitive 3D equations
- Allows a 2nd order accurate implicit solution at the time-scale of tracer advection.
- Optimization is under way; preconditioning options being explored for efficiency.

Adaptive Mesh Refinement Dycore
(HJ, E. English, w/ FASTMath team @ LBNL)

- 2D shallow water complete (1 paper)
- 3D non-hydrostatic dynamics implemented, with 1000:1 aspect ratio (non-linear implicit vertical)
- Running DCMIP tests with space-time AMR

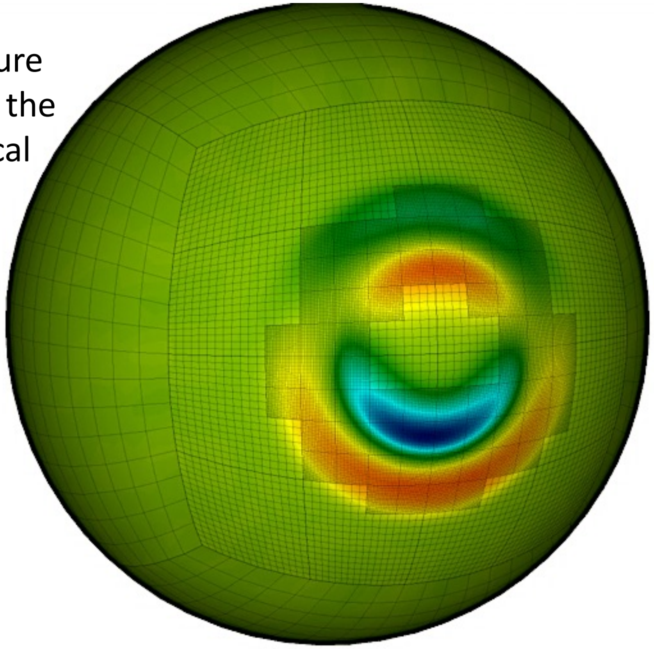
CAM Multi-resolution techniques (MT)

- Paper (in review, GMD), "The spectral element method on variable resolution grids: Evaluating grid sensitivity and resolution-aware numerical viscosity"
- Presentation (MT) at ICOSAHOM, Salt Lake City, June 2014.



Relative vorticity after 6 days of the Galewsky et al. (2004) baroclinic instability test case, using the implicit method.

Potential temperature perturbations from the interaction of vertical structure with Coriolis forces. Test uses 1° mesh with 16x AMR in the new 3D non-hydrostatic dycore.



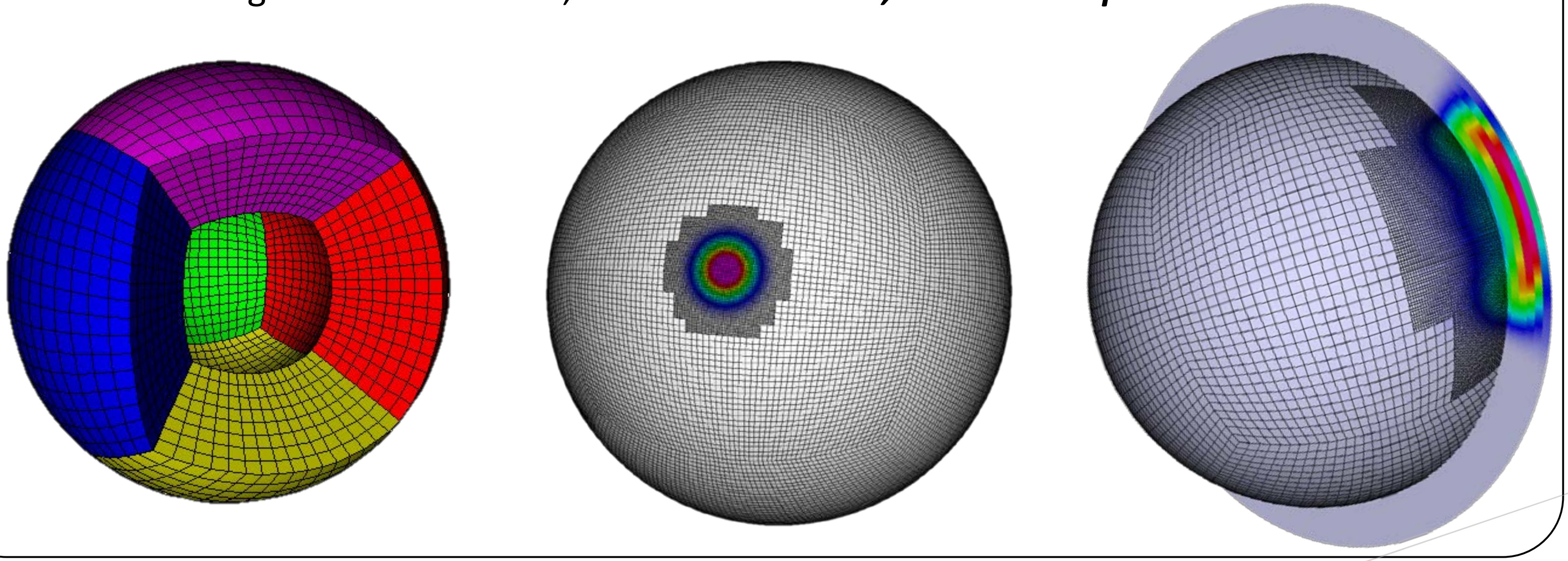
Goals of dynamic AMR atmospheric simulations

Create a high-resolution, high accuracy dycore to *eliminate local numerical errors*

- Fully non-hydrostatic dynamics (4^{th}-order in space and time)
- Excellent scaling (100k+ cores) without vertical explicit acoustic CFL limitation
- Anisotropic adaptive mesh refinement in space, refinement in time

→ 3 levels with 4x refinement produces > ***5 more digits*** of accuracy

→ Starting with 1° base level, ***resolution < 500m, ~2s time steps***



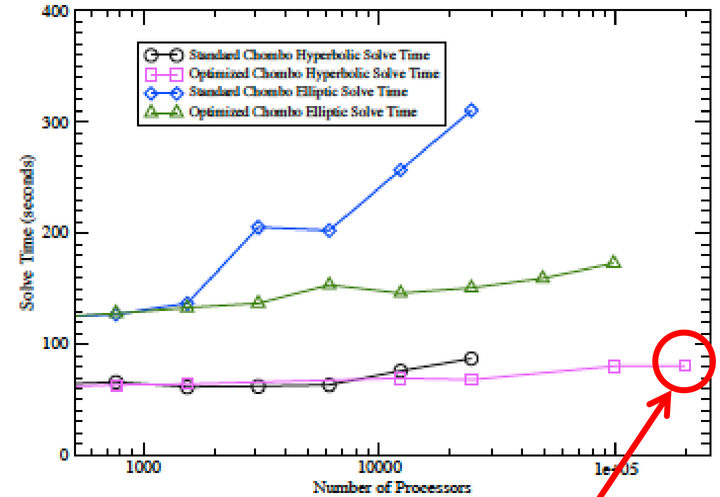
Chombo AMR code is well-established, scalable

Broad set of applications leveraging Chombo framework with complex physics:

- MHD for tokamaks (R. Samtaney, PPPL)
- Cosmology: CFD + particles (Miniati, ETH)
- Space plasmas: compressible CFD   electromagnetic, kinetic effects (G. Zank, UA)
- Astro. MHD turbulence (McKee / Klein, UCB)
- SF Bay Hydrology modelling (CA DWR)
- Microscale fluids (UNC / UCD / LBNL EFRC)
- Heat transfer in nuclear reactors (LBNL)
- Nuclear reactor safety - hydrogen combustion entrainment models (Calhoun, CEA-Saclay)
- Type II Supernovae (Woosley, UCSC, LLNL)
- 4D gyrokinetic tokamak edge plasmas (LLNL) …

Long-term ASCR investment: SciDAC, FastMATH …

→ Target platforms extreme-scale / DoE LCF's



200k processor benchmark, nearly ideal weak scaling
on similar hyperbolic problems!
[EuroPar2011]

BISICLES: Dynamic AMR for Ice Sheets

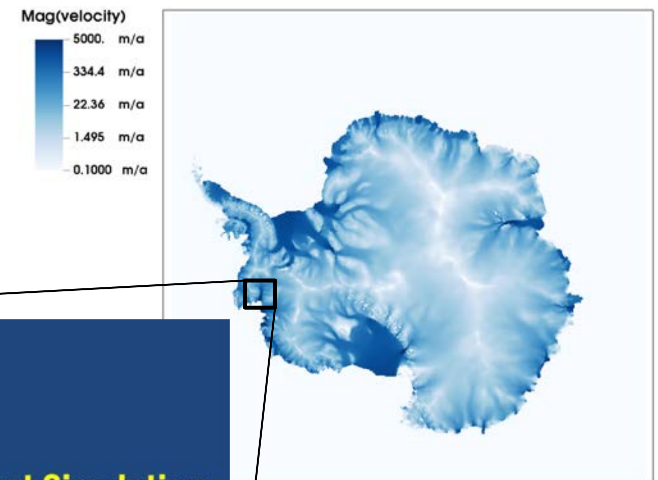
Objectives

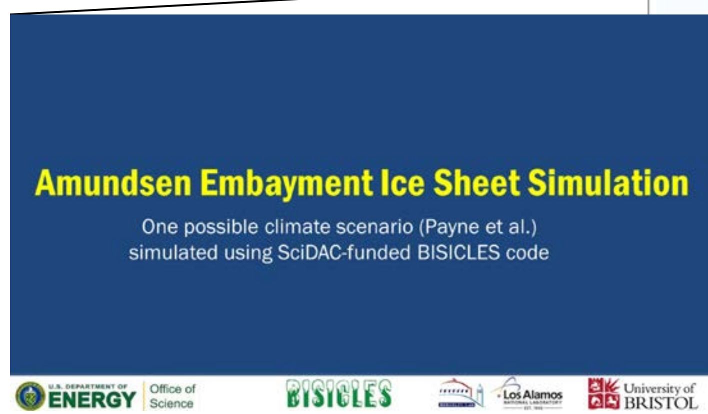
- Understanding ice sheet dynamics is crucial for credible predictions of future sea level rise (SLR)
- Very fine resolution (better than 1 km) needed to resolve dynamics of grounding lines – unfeasible for entire ice sheets
- Dynamic Adaptive Mesh Refinement (AMR) brings fine resolution to bear only where needed to resolve the dynamics.

Impact

- Enables modeling grounding line dynamics of marine ice sheets with sufficient spatial resolution to correctly model advance or retreat.
- AMR models dynamics correctly (vs. lo-res reduced or no mobility)
- Enables continental-scale modeling of ice sheets at the resolution / computational cost for global climate models (GCMs).

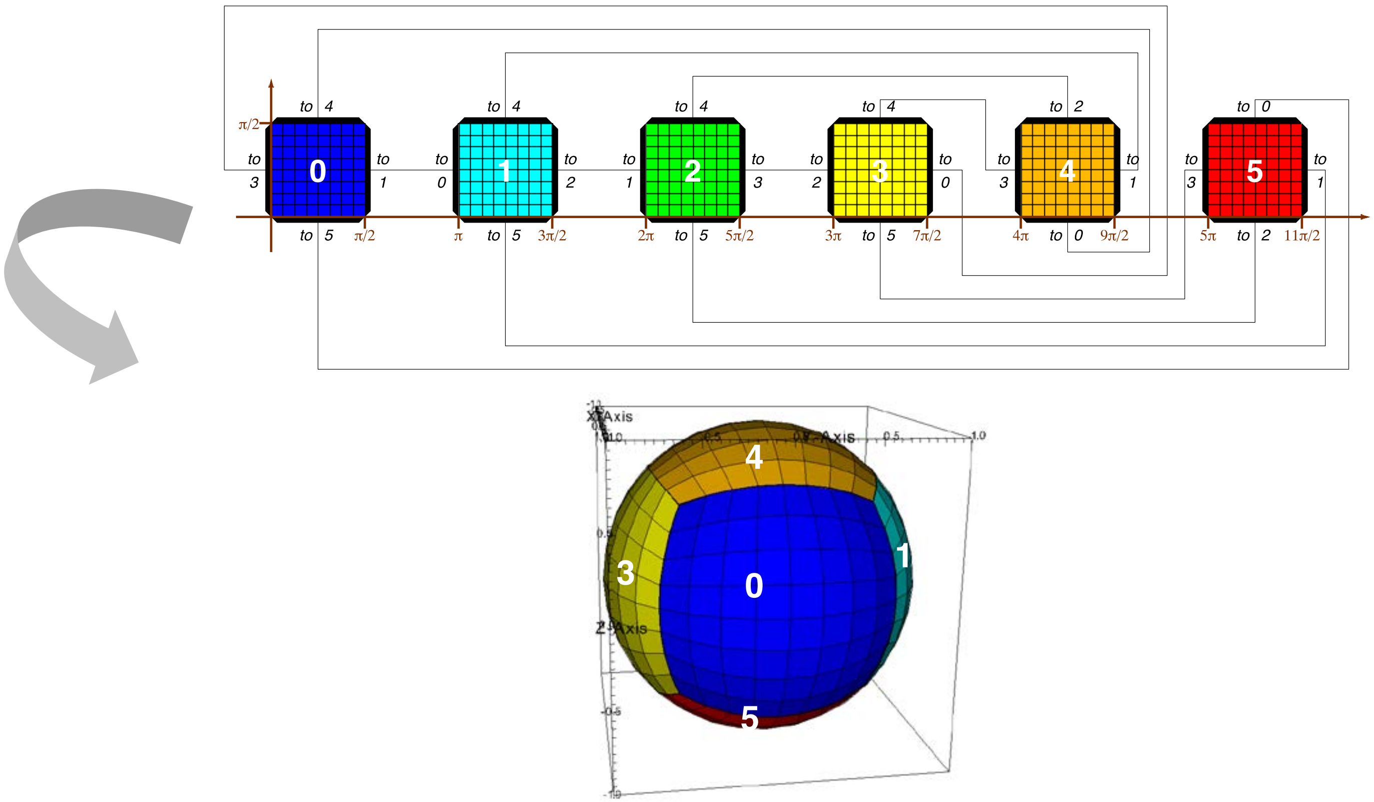
(below) Computed ice velocity for Antarctica, mesh and grounding line for Pine Island Glacier.





Cubed Sphere Formulation

- Use a “multi-block” mapping between rectangular index space and CS panels
- Use an arbitrary stretched grid in the radial direction (pressure coordinate, etc.)



Conservative FV on Cubed Sphere "Shells"

- Riemannian form of compressible Euler [Ullrich Jabl. JCP 2012]
- Conservative, in flux divergence form, with "~" indicating deviation from constant hydrostatic background state

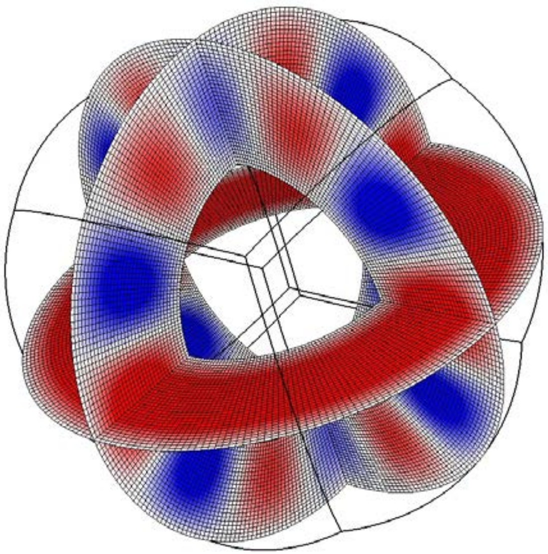
density $$\frac{\partial J\tilde{\rho}}{\partial t} = \dots$$

potential temp. $$\frac{\partial J\tilde{\Theta}}{\partial t} = \dots$$

humidity $$\frac{\partial J\tilde{Q}}{\partial t} = \dots$$

momentum $$\frac{\partial J\rho\mathbf{u}}{\partial t} = \dots$$

- Cubed sphere metrics calculated analytically, mapped to unit sphere
- "Shells" because we neglect the radial metric dependencies



$$\mathbf{u} = u^\alpha \mathbf{g}_\alpha + u^\beta \mathbf{g}_\beta + u^\xi \mathbf{g}_\xi$$

Implicit methods for fast vertical waves

- At 1° resolution, lower atmosphere cells can have ~1000:1 aspect ratio
- Euler has (fast) acoustic waves, (almost as fast) gravity waves
- Sound wave-based CFL for explicit methods → 1000x smaller time step
- Implicit methods used in place of explicit time integration in the vertical direction.

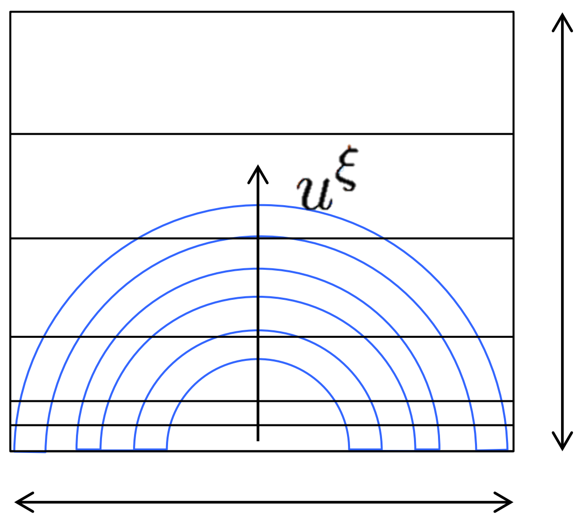
$$\frac{\partial J\tilde{\rho}}{\partial t} + \frac{\partial}{\partial \xi}(J\bar{\rho}u^{\xi}) = \ldots$$

$$\frac{\partial J\tilde{\Theta}}{\partial t} + \frac{\partial}{\partial \xi}(J\bar{\Theta}u^{\xi}) = \ldots$$

$$\frac{\partial J\bar{\rho}u^{\xi}}{\partial t} + \frac{\partial}{\partial \xi}(JG^{\xi\xi}\tilde{p}) = \ldots$$

$$\frac{\partial J\tilde{p}}{\partial t} + \gamma J\bar{p}\frac{\partial u^{\xi}}{\partial \xi} = \ldots$$

$$p = p_0\left(\frac{R_d\rho\theta}{p_0}\right)^{\gamma}$$

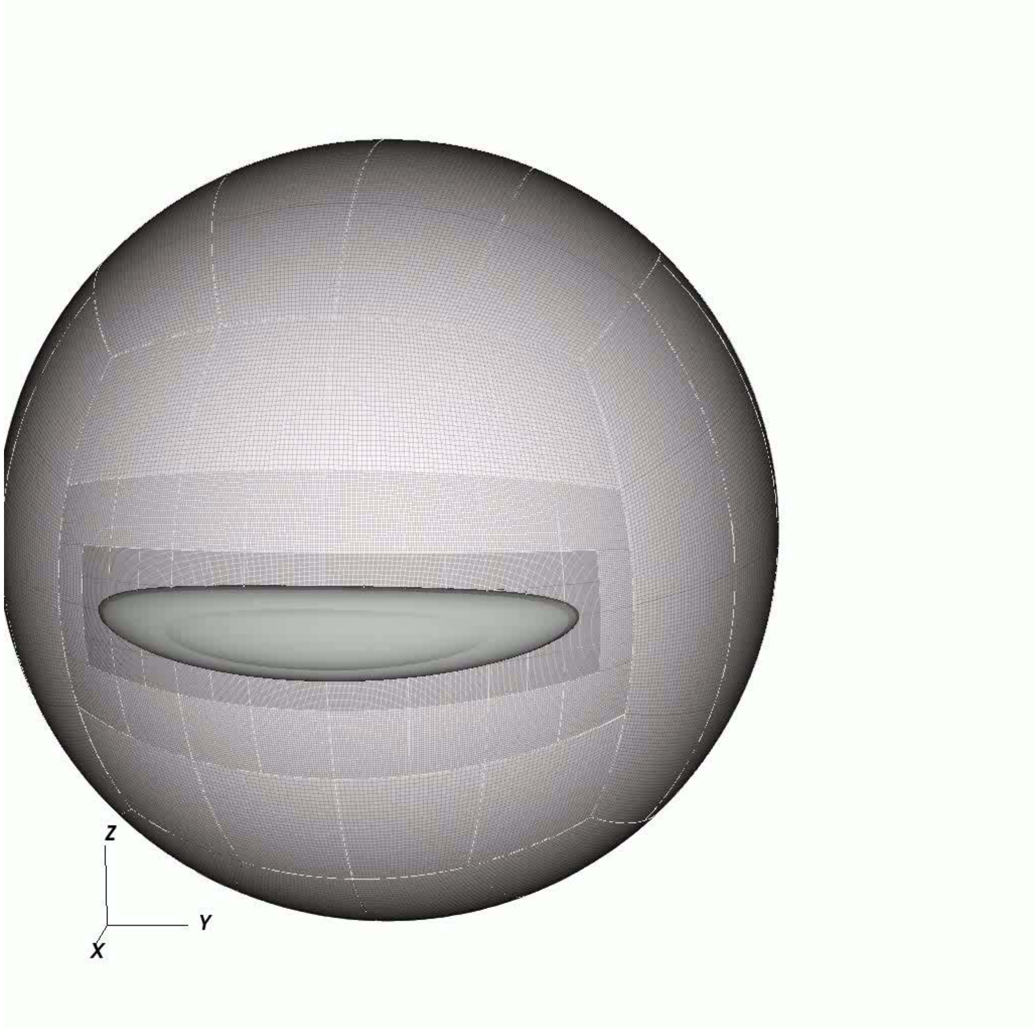


Vertical acoustic waves cross thin cells too quickly for explicit CFL!

Horizontal acoustic waves ok within a wide aspect ratio cell

Demonstration Calculation with Refinement

- **Dynamics:** **Prescribed Hadley circulation**
- **Physics:** **Large-scale condensation**
- **Lower boundary:** **Aquaplanet**
- **H2O processes:** **Advection & condensation**
- **Movie:** **3D vapor and surface rainfall**
- Simulation time: 30 days
- AMR grid: 0.7° resolution, 3 mesh tiers



Near-term Future Plans for AMR

What are we hoping to accomplish?

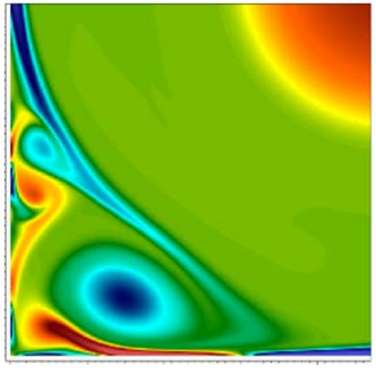
- 4th-order in space and time, without limitation of vertical explicit CFL
- Near-perfect scaling (CHOMBO explicit implementations have gone to 100k+)
- Anisotropic adaptive mesh refinement, 4th-order in space, refinement in time

→ 4 levels of 4x refinement produces almost ***5 more digits*** of accuracy

→ 1° base level, that would be ***< 500m resolution***, not feasible with uniform grid

Future plans:

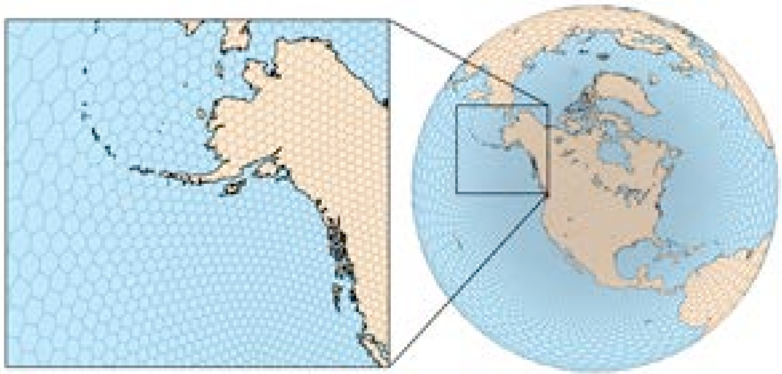
- Finish non-hydrostatic implementation,
- Add orography
- Integrate with various "column physics" to observe refinement behavior
- Support "grid insensitive," time-accurate physics parameterizations



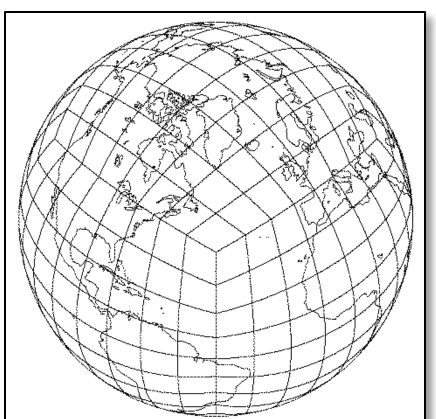
Project Elements

Variable Mesh Dycores

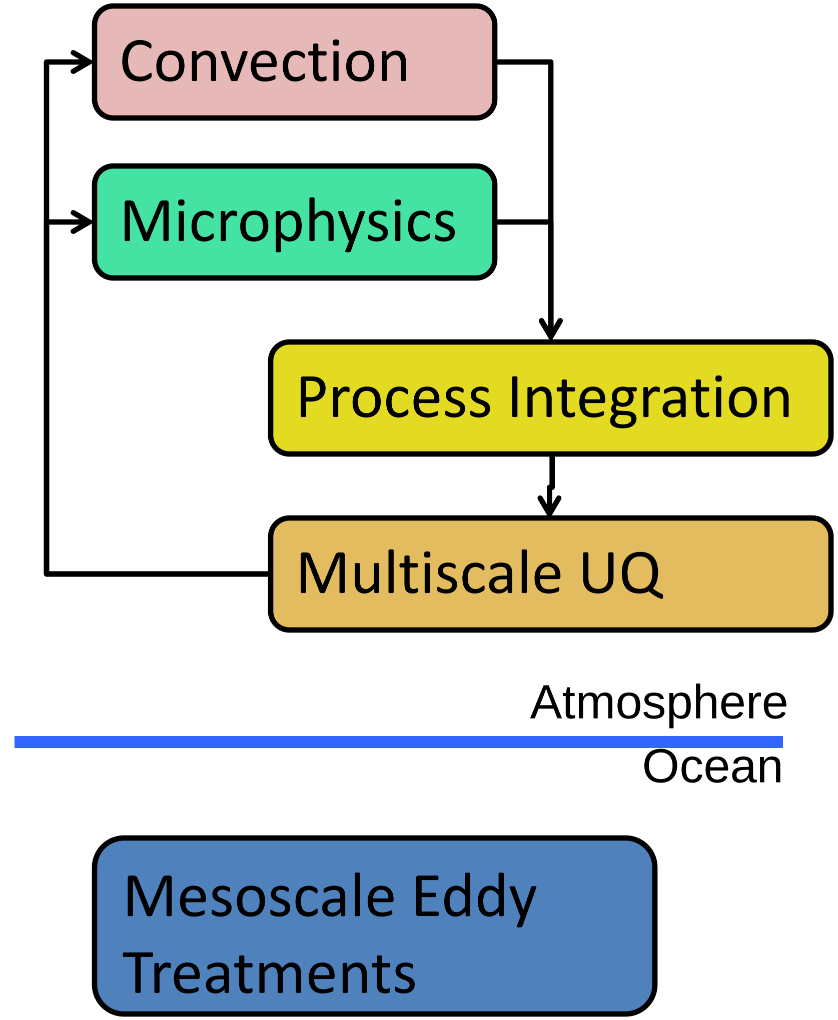
Model for Prediction Across Scales (MPAS)



Spectral Element Dycore

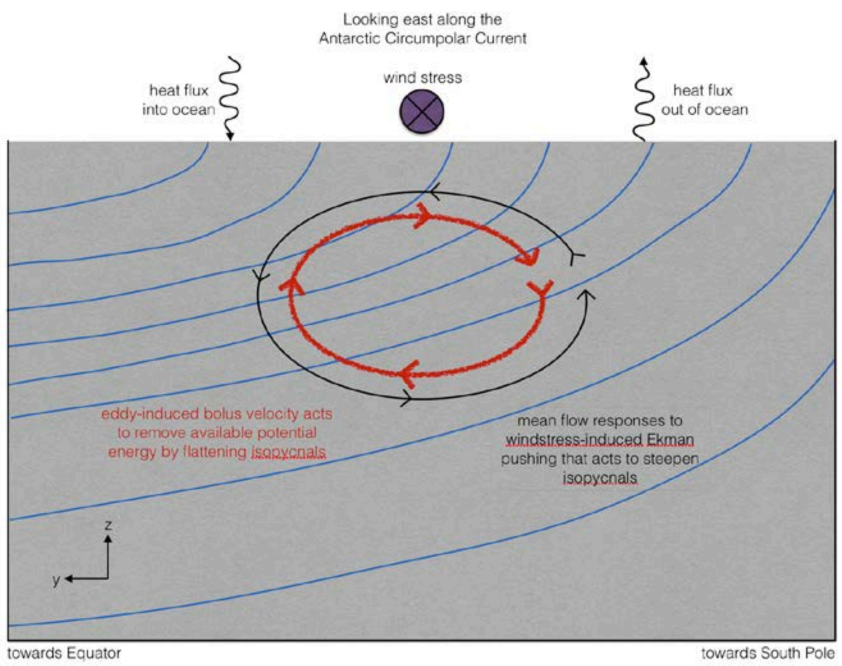


Physics-Dynamics Interface



New multiscale-capable ocean eddy schemes

- Since the seminal work of Gent and McWilliams (GM, 1990), ocean models have used two (typically opposing) velocities: mean and bolus.
- This has caused confusion, ambiguity and inconsistencies in how we characterize the fluid velocity, as well as hinder parameterization development.
- Based on recent theoretical analysis by Young (2012), we have re-expressed the MPAS-O governing equations to solve for the total (residual) velocity.
- A direct comparison to GM is underway.

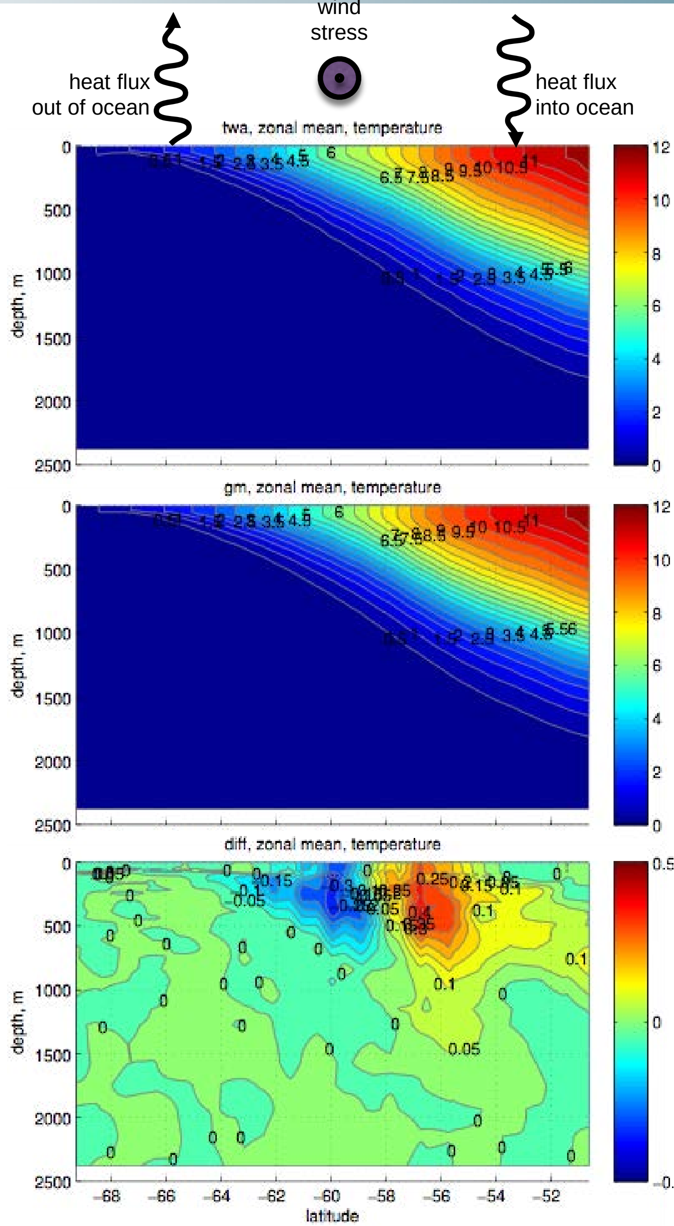


The dynamically-relevant, residual velocity can be solved for directly by recasting the mesoscale eddy parameterization as a force in the momentum equation.

Mesoscale Eddy Treatments

Residual-Mean Scheme for Mesoscale Eddies

- Comparison of the residual-mean solution (TWA - top) to the bolus solution (GM - middle) is underway.
- An idealized configuration of the Antarctic Circumpolar Current is being used to compare/contrast TWA/GM.
- Equilibrated TWA system exhibits a meridional temperature gradient ~10% stronger than the GM system (bottom).
- Tracking down root cause of differences. Likely due to different treatment of potential vorticity.



Mesoscale Eddy Treatments

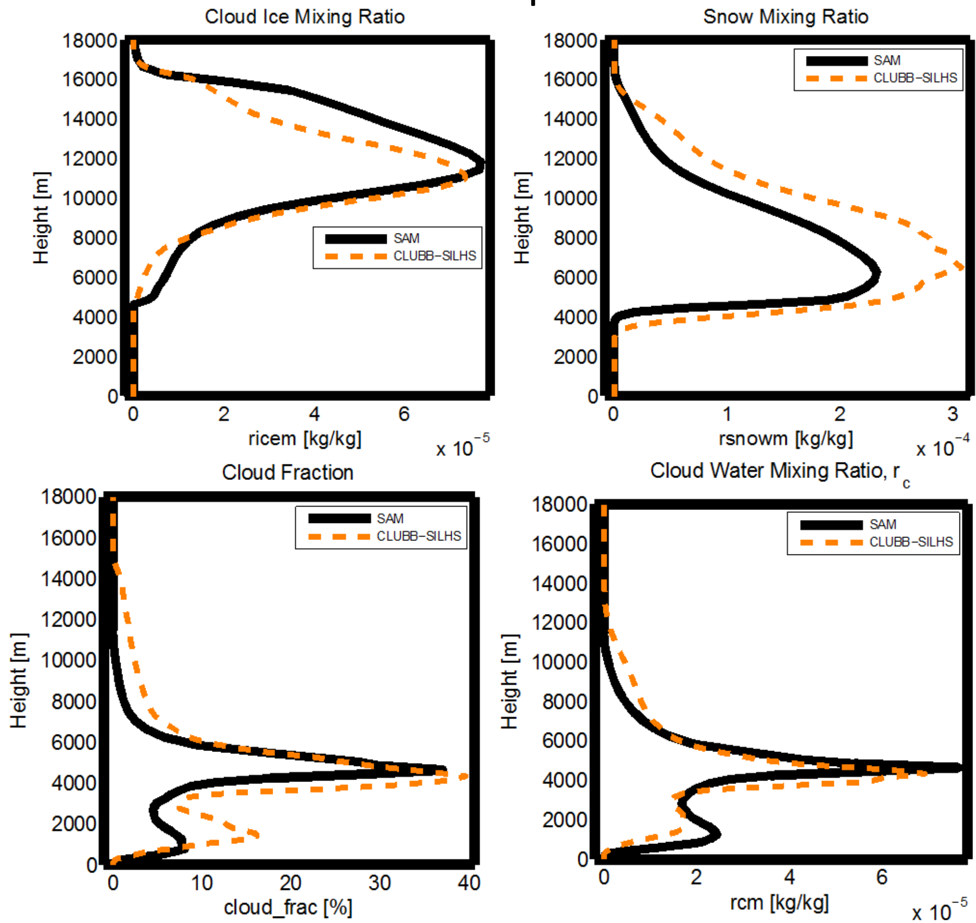
Application of QUEST to convective physics

SciDAC Multiscale

Convection

- CLUBB cloud-turbulence probability density function scheme was designed for shallow clouds
- With two log-normal modes comprising the PDFs, it can represent skewness
- Using Latin hypercube sampling for microphysics, it simulates five deep, shallow and stratiform cloud cases realistically

TWP-ICE Deep Convection

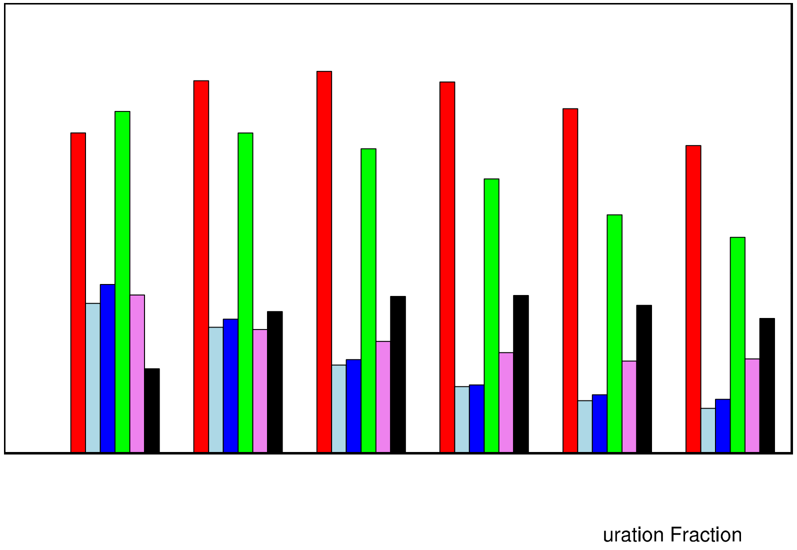


Parametric dependence of convection

Convection

- Used 512 CAM5_CLUBB simulations to determine the sensitivity of low cloud distribution to 18 tunable parameters

- Sensitivity analysis of effects of uncertainty in 11 CAM5 parameters on global mean RESTOM at 3 resolutions finds RESTOM uncertainty dominated by uncertainty in one parameter, with bias largest but variance smallest at finest resolution



- Evaluated six convection closures using cloud-resolving model output. Found that moisture convergence closure performs the best as model resolution increases

Development of scale-aware cumulus scheme

SciDAC Multiscale

Yi-Chin Liu[1], Jiwen Fan[1], Guang J. Zhang[2], Kuan-Man Xu[3], and Steve Ghan[1]
[1] Pacific Northwest National Laboratory; [2] Scripps Institution of Oceanography; [3] NASA Langley Research Center

Objectives

Develop a scale-aware cumulus parameterization based on the traditional Zhang-McFarlane (Z-M) scheme based on cloud resolving model simulations.

Impact

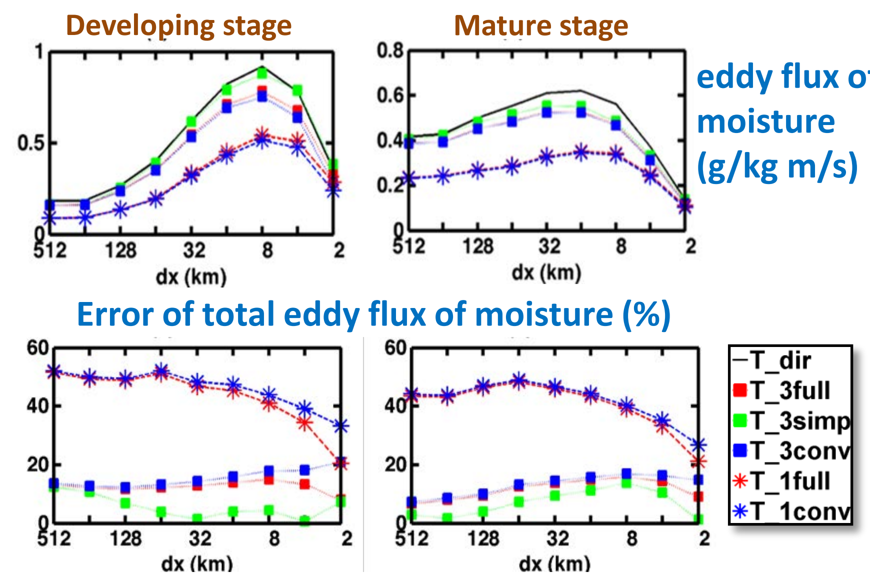
More accurate clouds and water vapor in the upper troposphere at a wide range of model resolutions from mesoscale to global scale .

Accomplishments

- Examine the scale-dependence of eddy transport of moisture at different altitudes, cloud life stages, and different regions.

- Evaluate different eddy transport formulations and propose a simplified formulation with 3-updraft and 1-downdraft, which has the following three advantages:

✓ valid for cloud fraction up to 1
✓ simple formulation
✓ accurate representation of CRM-simulated eddy flux across scales

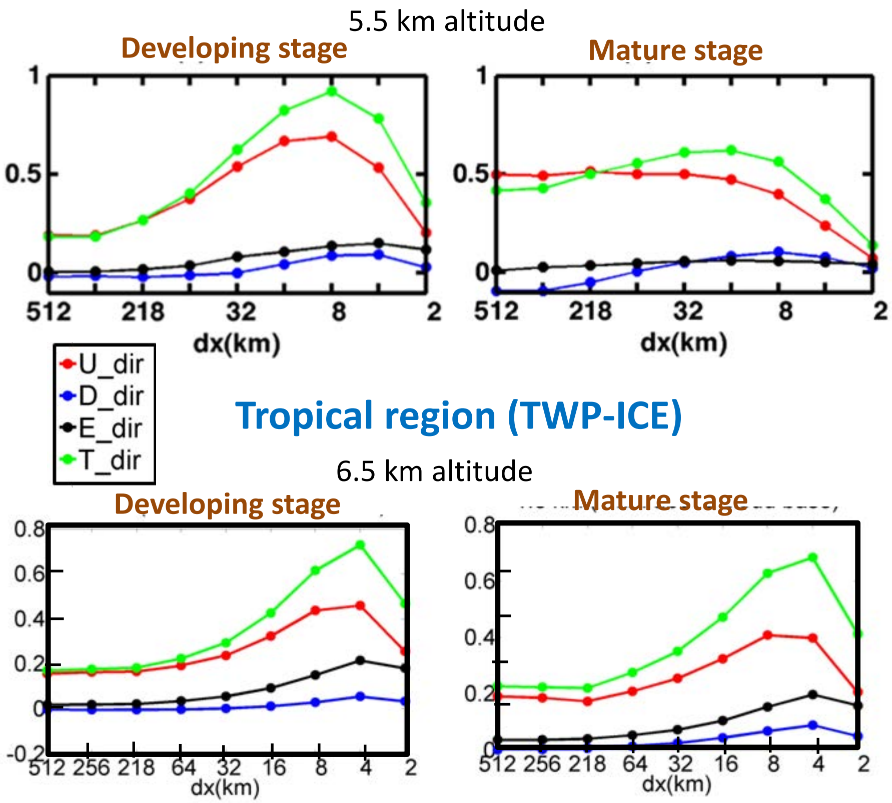


- Our proposed simplified 3-updraft formulation (T_3simp), predicts eddy flux very close to CRM results (T_dir). Single updraft approaches (T_1full, T_1conv) greatly underestimate eddy flux.

Eddy flux of moisture in convection

Vertical eddy flux of moisture (g/kg m/s)

Mid-latitude (MC3E)



Note: ***U***,***D***, ***E***: updraft, downdraft, and environment component
dir: the direct calculation based on the CRM simulations.
The green line is the total eddy flux

- **Updraft eddy flux is the major contributor to total eddy flux**
- **Mid-latitude continental vs. tropical convection**

Mid-latitude convection:

(a) Downdraft eddy transport can be as large as updraft eddy transport below 3-km altitude, especially at the mature stage.

(b) Updraft eddy transport has stronger scale dependency at the developing stage than the mature stage.

Tropical convection:

(a) Downdrafts contribute less to the total transport compared with the mid-latitude cases.

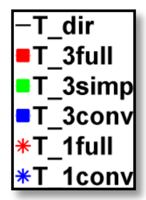
(b) No distinguishable difference in scale dependency between the developing and mature stages.

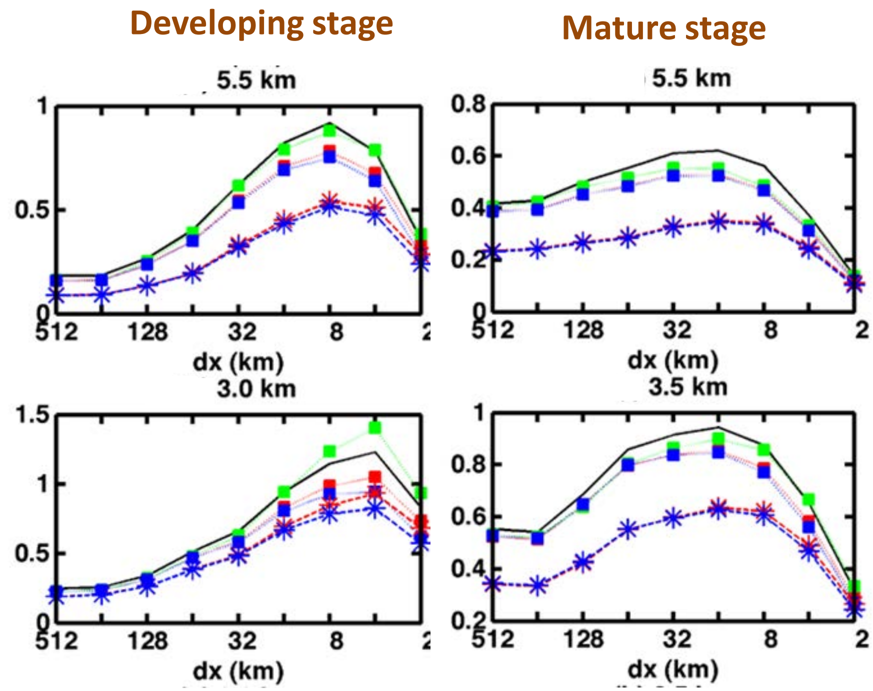
New scale-aware eddy parameterization

SciDAC Multiscale

We propose the simplified 3-updraft and 1-downdraft formulation for total eddy flux of moisture:

$$T\_3simp = \sum_{k=1}^{3} \sigma_{Uk}(1-\sigma_{Uk})(\widehat{w}_{Uk}-\widehat{w}_E)(\hat{q}_{Uk}-\hat{q}_E) + \sigma_D(1-\sigma_D)(\widehat{w}_D-\widehat{w}_E)(\hat{q}_D-\hat{q}_E)$$





Y-axis: eddy flux of moisture (g/kg m/s)

- **The proposed formulation (green line) accounts for the inter-draft variance of updrafts and provides the best approximation to the direct CRM results (black line).**

- **Considering a cloud fractional area as proposed by Arakawa (*T_1full*) does not significantly improve the eddy transport of moisture at any grid-spacing. Accounting for the inter-draft variability of updrafts is the key, especially at the scales of 4-64 km.**

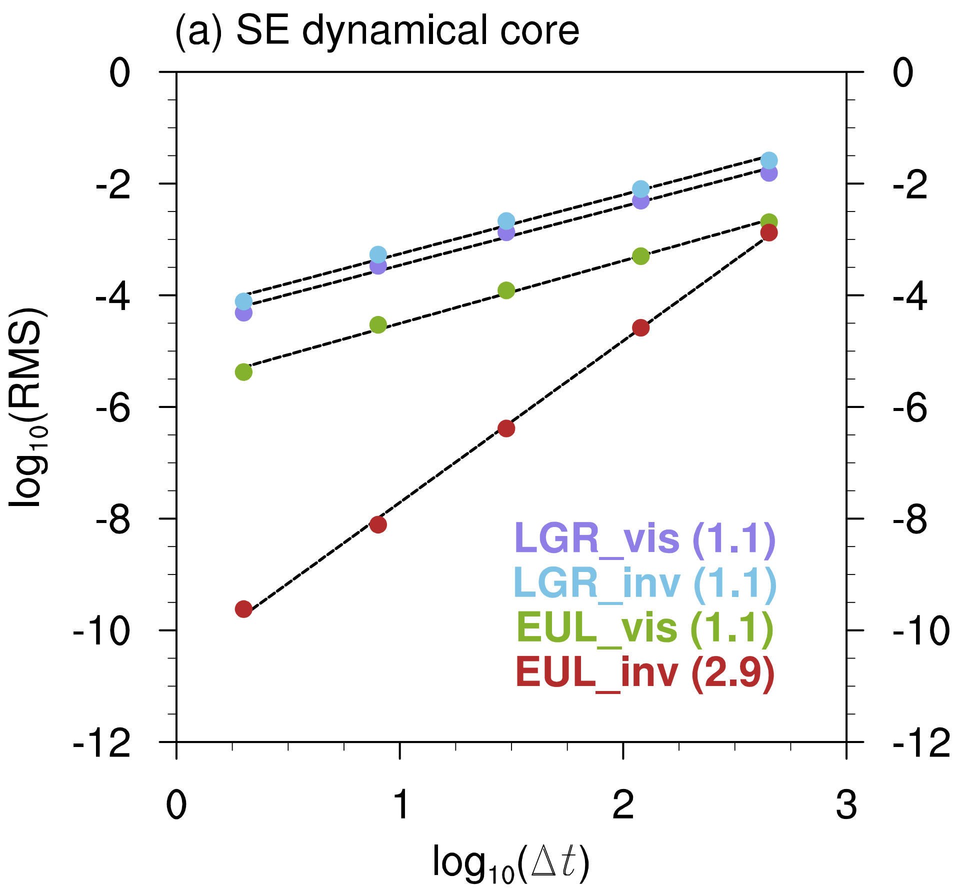
Note:
T_dir: total eddy flux from CRM simulations
1 or 3: 1-draft or 3-draft approach
conv: formulation with assumption of cloud fraction <<1
full: full formulation for a cloud fraction up to 1
simp: simplification of full neglecting interaction terms

Ensuring physics convergence as δt -> 0

- Goal: Test physics convergence as δt -> 0:
  - Convergence rate (1st order as we expect?)
  - Magnitude of time stepping error
- Method: Evaluate physics convergence using:
  - Very short (1 h) simulations with CAM5.3
  - Time step sizes from 30 min down to 1 s
  - Metric: RMS difference of T

Method validation

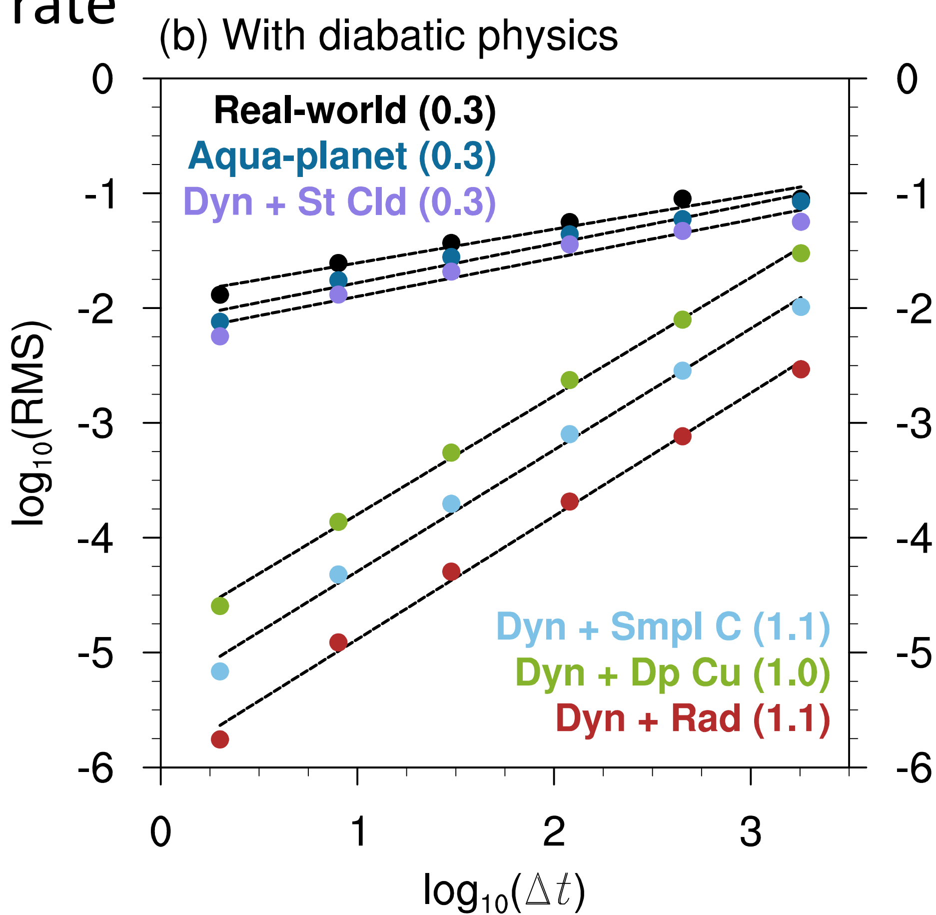
- Using only the dycore



Impact of adding physics on convergence

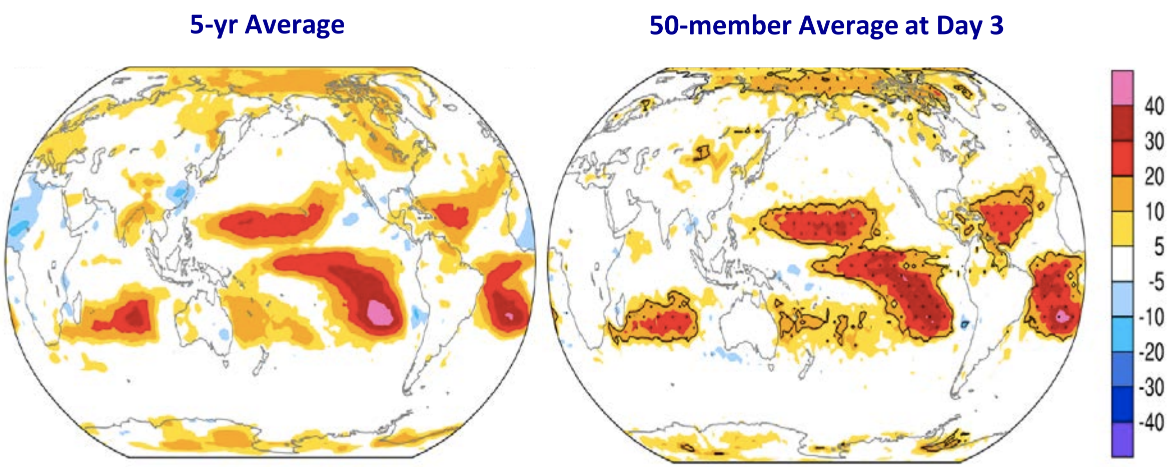
- Full model converges much slower than expected

- Cloud macro and micro are most problematic
- In contrast, the simplified large-scale condensation converges at the expected rate



Fast methods for testing convergence

SciDAC Multiscale



- Multiple simulation years are often required in sensitivity studies to overcome natural variability - inconveniently expensive at high resolutions
- We explored an alternative strategy using ensembles of shorter simulations, exploiting the important role of fast processes in determining model characteristics
- New method can correctly reproduce the main signals of model sensitivities revealed by long-term climate simulations, but at a fraction of total computation time and turnaround time.
- A powerful tool to efficiently use flagship computing facilities (e.g. Titan at Oak Ridge) and to speed up model development

Sensitivity of Total Cloud Cover to Model Time Step (4 minute vs 30 minute)

Factor of 15 reduction in CPU time

Reference:
Wan et al. (2014), Geosci. Model Dev. Discuss., 7, 2173-2216, doi:10.5194/gmdd-7-2173-2014

Multiscale Climate Application

- Progress due to SciDAC Institute interactions:
  - Implicit methods for time evolution at high resolution
  - Acceleration in ocean model performance
  - Addition of Chombo to suite of multiscale dycores
- Advances in the the physics / dynamics coupling:
  - Advances in the eddy formulation in our ocean model
  - Development of scale-aware convection schemes
  - Frameworks for ensuring physics time-step convergence