Assessing and Improving Numerical Treatments of Multiscale Processes in the Atmosphere

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MULTISCALE

Summary: An atmospheric general circulation model solves the mass, momentum and energy conservation equations of the atmosphere with sources and sinks induced by sub-grid scale processes. Solving the adiabatic fluid equations is a relatively well-established numerical problem, for which our work focuses mainly on the improvement of algorithm efficiency. Numerics for the sub-grid scale parameterizations is an under-addressed research topic. The discretization methods are generally diverse and crude. Our work in this area focuses on quantifying error and improving accuracy.

Fluid Dynamics Solvers

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Regional Mesh Refinement and GPU Acceleration

Recent implementation of fully implicit time integration in the 3D dynamical core of CAM with regional mesh refinement provides stable, demonstrable accuracy for a baroclinic instability test case (Figure 1) using a 20 min time step instead of a 10 s time step required by traditional methods for the high-resolution domain. The implementation utilizes solver libraries from FastMATH for optimal efficiency and code design. On-going work include incorporation and optimization of the FastMATH preconditioner libraries, as well as porting of the entire fluid dynamics solver to the GPU to effectively utilize leadership class computers with accelerators.

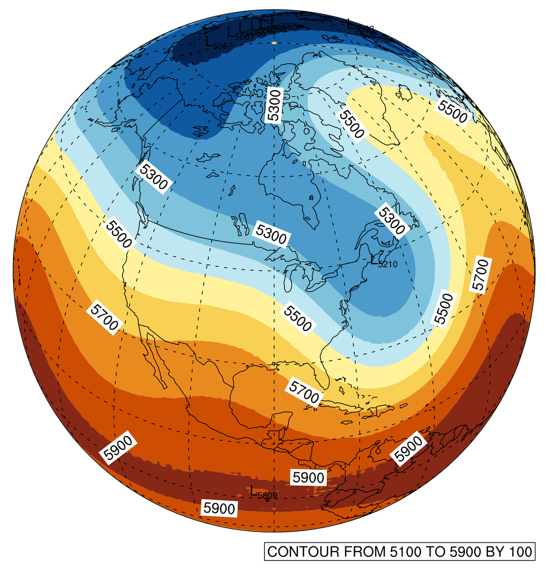


Figure 1. Simulation of a baroclinic wave using fully implicit solver and regionally refined horizontal mesh.

Development of Algorithmically Scalable Block Preconditioner

To improve efficiency of the implicit time integration method used in the spectral-element dynamical core of the Community Atmosphere Model (CAM-SE), a preconditioner is developed based on an approximate block factorization of the linearized shallow-water equations. The implementation uses FastMATH Trilinos libraries, which enables future solver advances. Algorithmic scalability is achieved for a suite of shallow water test cases (Table 1). *Reference: Lott et al. (2015), Comput. Geosciences, DOI: 10.1007/s10596-014-9447-6.*

Number of Processes	Number of Unknowns	Linear Iterations w/o Preconditioner	Linear Iterations with Preconditioner
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

Table 1 . Scalability of implicit solver in test case 5 of Williamson et al. (1992).

A preconditioner for the 3D hydrostatic primitive equations is currently under development using a similar strategy (shown below).

The preconditioner is based on an approximate block factorization of the Jacobian matrix:

$$J = \begin{bmatrix} A & B & C \\ D & E & F \\ G & H & K \end{bmatrix} \approx \begin{bmatrix} I & 0 & 0 \\ DA^{-1} & I & 0 \\ GA^{-1} & \left(H - GA^{-1}B\right)\hat{S}^{-1} & I \end{bmatrix} \begin{bmatrix} A & B & C \\ 0 & \hat{S} & R \\ 0 & 0 & \hat{P} \end{bmatrix} = \hat{J}$$

$\hat{A} = diag(A)$ Approximate A by a diagonal matrix

$\hat{S} = E - D\hat{A}^{-1}B$ Approx. Schur complement 1

$\hat{P} = K - G\hat{A}^{-1}C - \left(H - G\hat{A}^{-1}B\right)\hat{S}^{-1}\left(F - D\hat{A}^{-1}C\right)$ Approx. Schur complement 2

A, B, C : Change in velocity with velocity, surface pressure, and temperature

G, H, K : Change in surface pressure with velocity, surface pressure, and temperature

D, E, F : Change in temperature with velocity, surface pressure, and temperature

Applying the inverse of the preconditioning matrix to a vector requires solving the system $\hat{J}y = b$ in six steps:

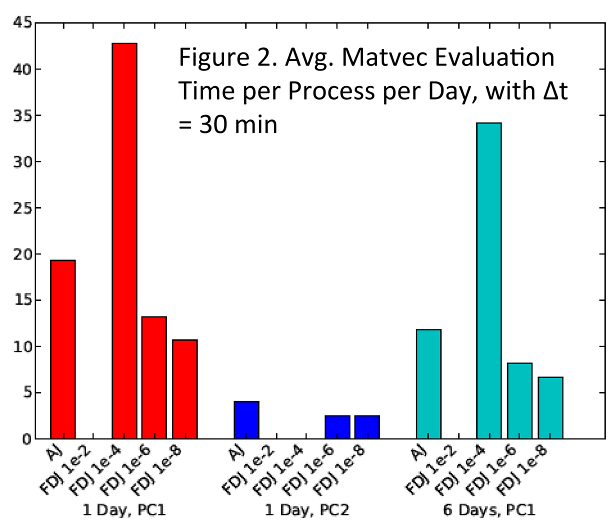
1. $x_1 = b_1$
2. $x_2 = b_2 - DA^{-1}x_1$
3. $x_3 = b_3 - GA^{-1}x_1 - \left(H - GA^{-1}B\right)\hat{S}^{-1}x_2$
4. Solve $\hat{P}y_3 = x_3$
5. Solve $\hat{S}y_2 = x_2 - \left(F - DA^{-1}C\right)y_3$
6. Solve $Ay_1 = x_1 - By_2 - Cy_3$

Summary of the method for extending the 2D shallow-water preconditioner to the 3D primitive equations.

Use of Finite Difference Matrix-Vector Products in Implicit Solvers

The capability to utilize analytic Jacobian-vector products with the Trilinos nonlinear solver NOX is added to the spectral-element shallow water dynamical core of the Community Atmosphere Model (CAM). Finite difference approximations are found to be efficient within Newton-Krylov solvers for implicit time integration methods with spectral element methods. With a 30 min time step, a smaller differencing parameter of 1E-8 improves run times compared to the default of 1E-6 (Figure 2).

Reference: Woodward et al. (2015), Procedia Computer Science, DOI: 10.1016/j.procs.2015.05.468



Sub-grid Scale Parameterizations

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Top-down Error Quantification

Time step convergence tests performed using CAM-SE with sub-grid scale parameterizations provide a quantification of time stepping errors in different components of the model. Root-mean-square temperature difference relative to solution with shortest time step (1 sec) is used as error measure. Test results reveal slow convergence and strong time step sensitivity in the full model. Stratiform cloud parameterizations are identified as the largest source of time stepping error (Figure 3). The test strategy is computationally efficient, and can be easily applied to any other atmosphere models. *Reference: Wan et al. (2015), Geosci. Model Dev., DOI: 10.1002/2014MS000368*

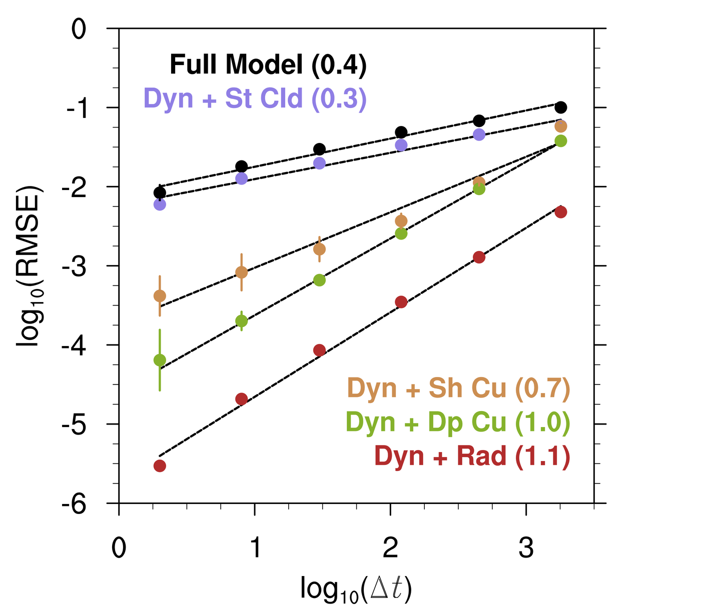

Figure 3. Time stepping errors associated with various parameterized sub-grid scale physical processes in CAM-SE.

Analysis in Problematic Model Components

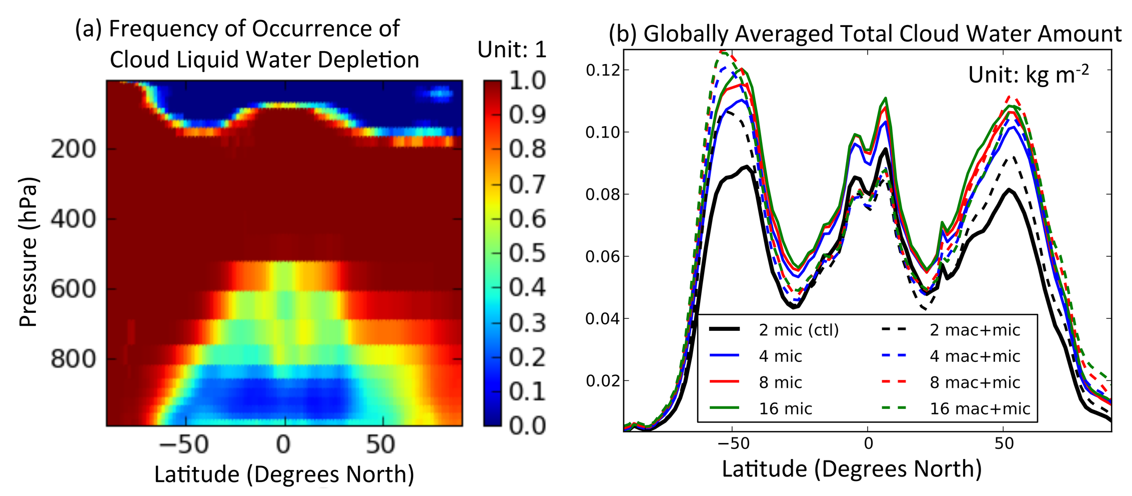

Figure 4: (a) Frequency of occurrence of the case when cloud microphysics starts with significant liquid water content and depletes it within one time step. (b) Sensitivity of the globally averaged total (liquid + ice) water path to the number of sub-steps used in the stratiform cloud macrophysics and/or microphysics. Both panels shows results of multi-year present-day climate simulations.

Stratiform cloud parameterizations in CAM includes macrophysics (condensation of water vapor) and microphysics (conversion of cloud water to rain). Crude numerics leads to many artifacts, e.g., overestimate of the frequency of occurrence of cloud water depletion (Figure 4a). Tests that apply brute-force remedies using sub-stepping indicate that model results are sensitive to both the treatment of individual processes (or process groups) and the numerical coupling between different processes (Figure 4b).

Use of Simpler Models to Obtain Insights and Design Better Numerics

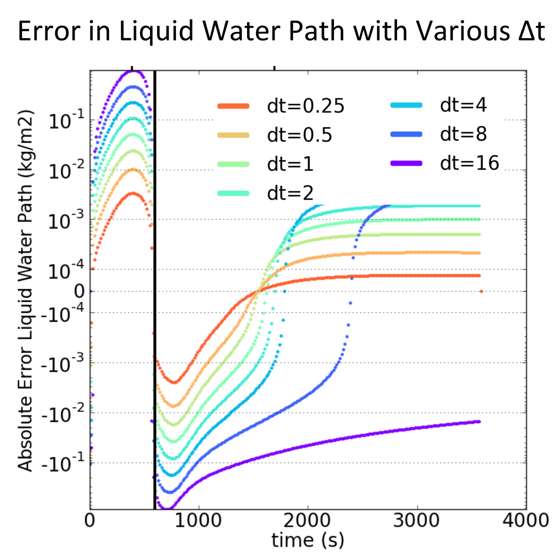

Figure 5: Absolute error in liquid water path for various step sizes compared to a reference solution with Δt = 0.0625 s in the KiD Warm1 test case.

The CAM stratiform cloud macrophysics and microphysics are tested with the Kinematic Driver (KiD) which evaluates these parameterizations while idealizing all other aspects of the model. In the Warm1 test case with fixed temperature and a time dependent updraft for 600 s, the error in liquid water path shows that linear convergence requires a time step size ≤ 4 s (Figure 5). An even simpler box model was built to study the numerical coupling between macrophysics and microphysics (Figure 6a) assuming constant vapor source and a simplified mathematical form for condensation and rain formation. Results show that time step sizes exceeding stability limits lead to oscillation in solution. Limiters can remove negative values but do not help with convergence. Solutions obtained without operator splitting are generally more accurate than those with splitting (Figure 6b,c) . Higher order explicit methods, stabilized explicit methods, and implicit methods are currently being explored to improve the time step size necessary for stability.

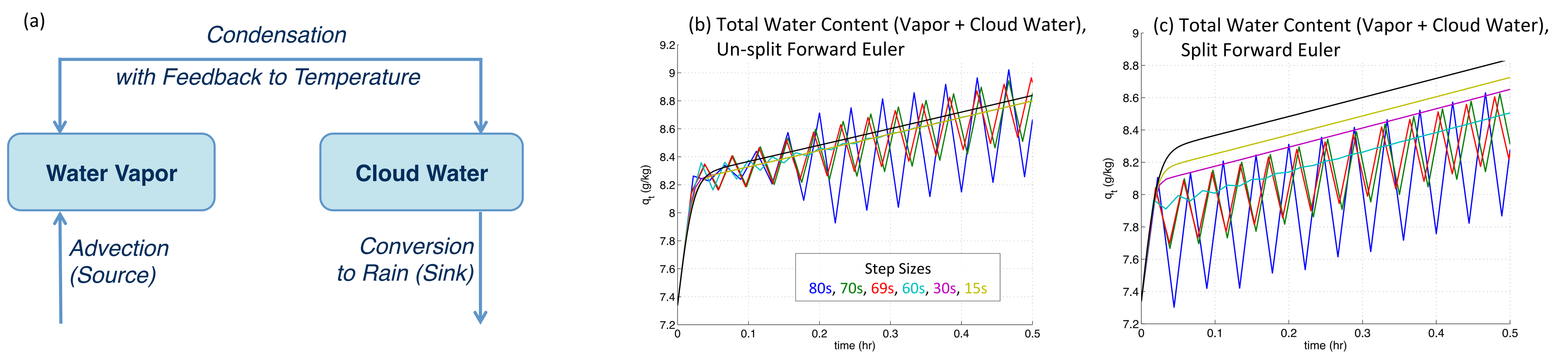

Figure 6: (a) Schematic showing processes described in a toy model for investigating the numerical coupling between macrophysics and microphysics. (b) - (c) Time evolution of total water content (vapor + cloud water) simulated by various time stepping methods using different step sizes.

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