Assessing and Improving the Numerical Solution of Atmospheric Physics in E3SM

E3SM Energy Exascale Earth System Model

SciDAC Scientific Discovery through Advanced Computing

Motivation and Overview

Background: The E3SM atmosphere model comprises a fluid dynamics solver (the dynamical core) and the representation of many sub-grid-scale processes (the parameterizations). The latter typically uses simple time integration methods and long step sizes.

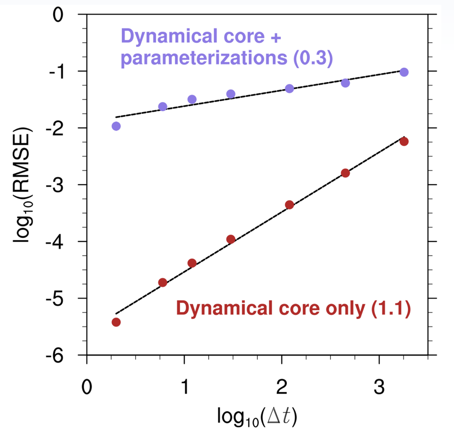


Figure 1: Time-stepping errors and self-convergence rates in E3SMv1 atmosphere model.

The challenge: In E3SMv1 and several of its predecessors, time-step convergence in the parameterizations is significantly slower than the expected 1st-order rate, and the time stepping errors are substantially larger than those in the dynamical core (Figure 1). This issue is also relevant to probably all global and regional atmospheric models.

Project objectives:

- Understand causes of poor convergence
- Improve solution accuracy in E3SM

Strategy:

- Close collaboration among atmospheric scientists, applied mathematicians, and computational scientists
- Efforts are organized as tasks described in the rest of this poster
- New model formulations and time integration methods are first developed in simplified model configurations and then implemented and evaluated in E3SM

Identifying Accuracy Bottlenecks

Goal: Isolate physical processes and code pieces with poor convergence. Provide detailed description of model equations and code implementation for mathematical and numerical analysis

Approach: Conduct convergence tests. Use physical insights to identify pathological behavior and simplify model equations or code to facilitate further investigations

Key Results:

- Identified and fixed a significant bug in the single-column model. Demonstrated self-convergence test as a useful way to detect issues hard to notice in the default model configuration (Figure 2)
- Constructed a simplified large-scale condensation scheme and identified dependence of convergence on model formulation, physics-dynamics coupling, and time stepping within the parameterization. Demonstrated that restoring convergence can lead to substantial changes in model's long-term climate (Figure 3)

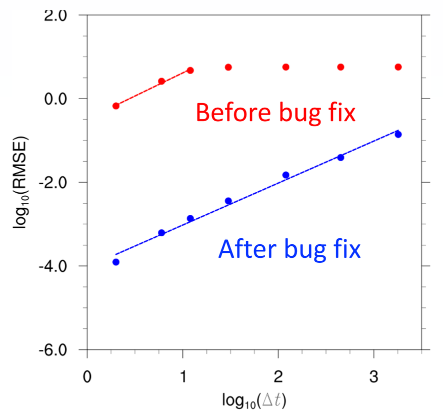


Figure 2: Time stepping error and self-convergence rate in single-column simulations of stratocumulus clouds before and after a bug fix.

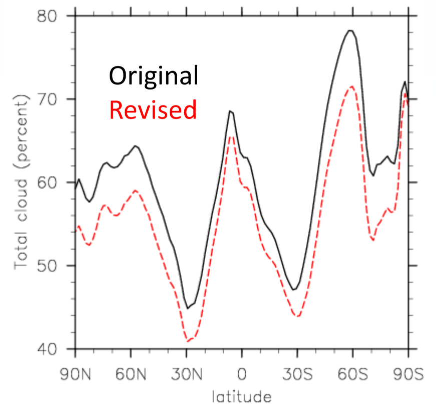


Figure 3: Multi-year zonal mean total cloud fraction in CAM4 using a revised physics-dynamics coupling (red) that helped to restore 1st-order convergence in a simple large-scale condensation model.

Development and Analysis from a Deterministic PDE Perspective

Goal: Improve numerical convergence through identification of mathematical sources of convergence degradation and improved models of sub-grid processes

Approach: Conduct an error analysis of the integration scheme applied in the simple condensation model and identify assumptions for convergence that may not hold. Based on findings, rederive the model parameterization using explicit sub-grid profiles, reconstructed from grid-cell averaged values.

Key Results:

- Completed error analysis of additively split two-process integration scheme with/without sequential splitting and finite difference (FD) approximations

$$|e_n| \le \underbrace{|\tilde{e}_0| e^{(t_f-t_0)K}}_{\text{initial error}} + \underbrace{\frac{e^{(t_f-t_0)K}-1}{2K}}_{\text{truncation error}}\Big[\underbrace{\|y''\|_\infty + \|f''\|_\infty}_{\text{FD error}} + \underbrace{2K_{f_y}\|DF\|_\infty + 2K_D\|f_yF\|_\infty + 2\|D^2 f_{yy}\|_\infty}_{\text{combined splitting and FD error}}\Big]\underbrace{\Delta t}_{\text{1st order}}$$

- Singularities and limited continuity in model terms, in particular the cloud fraction, f, can reduce convergence order
- Derived and implemented a new version of the simple condensation model in E3SM tested on Cori

First results with revised model show good convergence but large errors; 1-partition profile makes assumption on model state but 2-partition does not

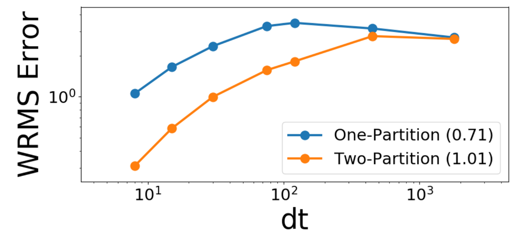


Figure 4: First self convergence results with revised simple condensation model.

Development and Analysis from a Stochastic PDE Perspective

Goal: Improve numerical convergence by accurate stochastic modeling of sub-grid processes

Approach: Introduce a stochastic (Ito) correction term to represent the impact of fast forcing on slower components of the fluid motion.

Key Results:

- Configured an advection-diffusion model with a wide spectrum of state-dependent fast forcing as a test problem
- Demonstrated the use of Ito correction to restore convergence for white forcing spectra
- Generalized Ito correction for red forcing spectra; improved convergence and accuracy (Figure 5)

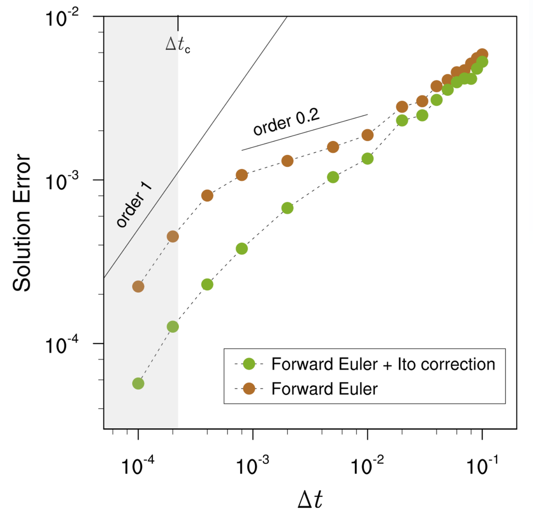


Figure 5: Time stepping error and numerical convergence rate of the advection-diffusion model with and without the Ito correction term.

Advection-diffusion model:

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x} + \mu\frac{\partial^2 u}{\partial x^2} + g(u)n(t)$$

$u(x,t)$ - solution $\quad n(t)$ - fast physical process

With sufficiently small time step sizes, both schemes exhibit first-order convergence. When the fast forcing can not be fully resolved, the Ito correction term improves the numerical convergence rate from $O(\Delta t^{0.2})$ to $O(\Delta t^{0.5})$.

Team-building Tutorials

Goal: Overcome the barriers between two disciplines

Approach: Use informal team tutorials to clarify language, introduce basic concepts and methods. Topics covered to date:

- E3SM code structure
- Time stepping problems in atmospheric models
- CLUBB and the filtering approach
- Introduction to stability and convergence
- Introduction to stochastic differential equations and model reduction

Figure courtesy of Wikimedia Commons

11 tutorials with archived slides and recordings

Analysis and Development Using Process-level Understanding

Key results:

- Quantified time-step sensitivity in E3SMv1 simulations (Figure 6)
- Implemented a closure in deep convection parameterization with improved precipitation over the tropical west Pacific
- Identified process coupling issues related to aerosols and water cycle

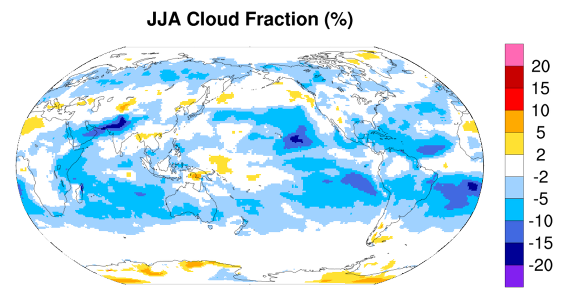


Figure 6: 20-year mean cloud fraction change caused by reduction of model step size from 30 min to 5 min in E3SMv1.

Accuracy Metrics and Testing Methods

Goal: Establish additional metrics for measuring solution accuracy

Key results:

- Found the magnitude of clipping terms to be a good indicator of numerical problem
- Found significant correlation between poor convergence, large time stepping error, and fast growth of rounding error

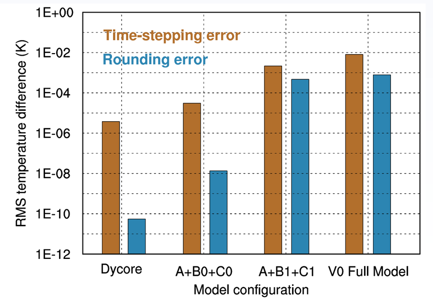


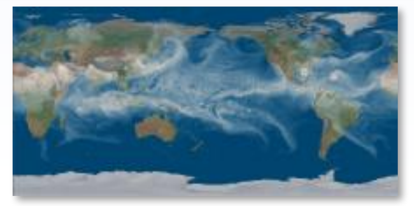
Figure 6: Initial results suggest that fast growth of rounding error can be an indicator of low accuracy in time stepping.

Integration into E3SM

Goal: Ensure project findings are incorporated into E3SM

Key results:

- Provided multiple bug fixes to E3SM
- Currently incorporating a recent version of CLUBB into E3SM as a Git subtree
- Regularly rebasing project's code branches to the E3SM master
- Enabling all (including math) team members to modify and run E3SM



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