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Assessing and Improving the Numerical Solution of Atmospheric Physics in an Earth System Model

Phil Rasch

on behalf of a SciDAC project team:

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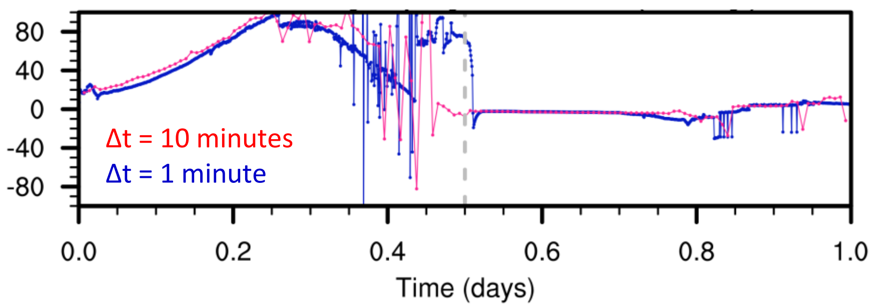
Parameterizations in AGCMs

- Traditional focus on conceptualization of understanding + handling of spatial scales
- Practical motivation to use longest possible time step
- Ubiquitous use of clipping, limiters etc.

1-day time series of T tendency (K/day) at 700 hPa from E3SM v0 physics



- Physics parameterizations
  - are known to be noisy in time (i.e., varying fast compare to dynamics)
  - can be very sensitive to perturbation
- Are these expected for deterministic PDE systems?

The Time-step Convergence Puzzle

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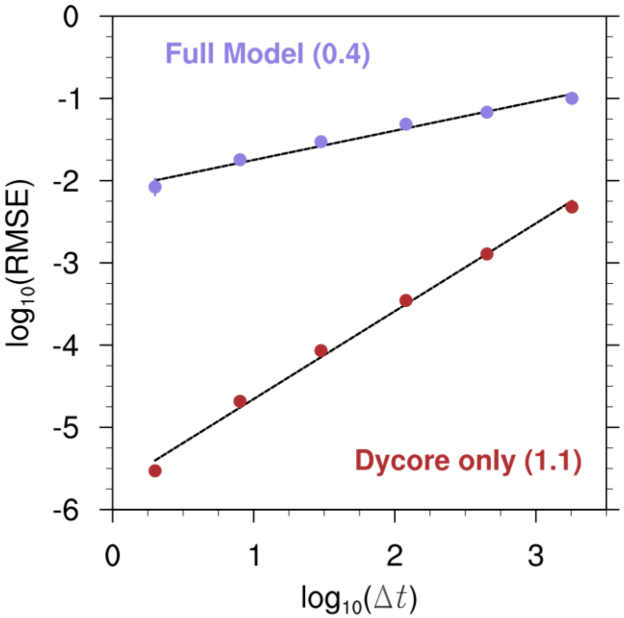
- Experimental design
  - Very short (1-hour) simulations
  - A wide range of time step sizes
  - Solution with shortest step size as reference (i.e. self-convergence)
  - Ensemble runs to take into account possible flow-dependency
- Convergence rate of the full model
  - Expected: 1.0
  - Diagnosed: 0.4
- Contrast between dynamical-core-only and full-model results
- Slower convergence is associated with larger time stepping error

Time Stepping Error and Convergence Rate in CAM5



Value of Convergence Testing

- For a full-fledged model with complex physics, does it make sense to talk about time-step convergence at all?

- **Our opinion**: For very short simulations, if the solutions do not converge or converge to an unexpected state, then the equations, the discretization, and the coding need to be revisited

- The next slides demonstrate that convergence testing can help identify issues in
  - **Model's continuous formulation**
  - **Physics-dynamics coupling (splitting)**
  - **Time stepping in physics**

A Test Problem

- E3SM's dynamical core + a very simple parameterization
- Equations directly affected by parameterizations are:

Temperature: $$\frac{\partial \overline{T}}{\partial t} = \overline{A_T} + \frac{L_v}{C_p}\overline{Q}$$

Water vapor: $$\frac{\partial \overline{q_v}}{\partial t} = \overline{A_v} - \overline{Q}$$

Cloud liquid: $$\frac{\partial \overline{q_l}}{\partial t} = \overline{A_l} + \overline{Q}$$

Physics: bare-bone version of the large-scale condensation scheme in CAM2-CAM4

(Zhang et al., 2003; Rasch and Kristjansson,1998; Sundqvist,1978)

Dynamics (advection): Spectral-element dynamical core on cubed sphere,1-degree, 30 layers

Large-scale Condensation Scheme

- Basic assumptions
  - Instantaneous condensation
  - Fractional cloudiness

- Grid-box mean condensation rate

$$\overline{Q} = \boxed{f\widehat{Q}}\ \boxed{-\left(\overline{A_l} - f\widehat{A_l}\right)} + \boxed{\tilde{q}_l \frac{\partial f}{\partial t}}$$

In-cloud condensation

Clear-sky evaporation

Phase change associated with cloud fraction change

- Closure assumption: $\widetilde{q_l} = \dfrac{\overline{q_l}}{f}$

"When the cloud is growing (df/dt > 0), the new cloud water increases to match that within the cloudy part of the grid box. Conversely, when the cloud is eroding (df/dt < 0), the cloud water goes to zero in that region."

— *Rasch and Kristjansson (1998); Zhang et al. (2003)*

Singularity

- Closure assumption $$\widetilde{q_l} = \frac{\overline{q_l}}{f}$$

- If ql > 0 but f ~ 0, we get "infinitely dense cloud" (singularity)
- The use of a "safeguard parameter" is a common remedy $$\widetilde{q_l} = \frac{\overline{q_l}}{\max(f,\ f_{\min})}$$

- … but it can hide problems
  (will show ona later slide)

- Does such singularity actually occur in the simulations?
  Unfortunately, yes, and it affects convergence

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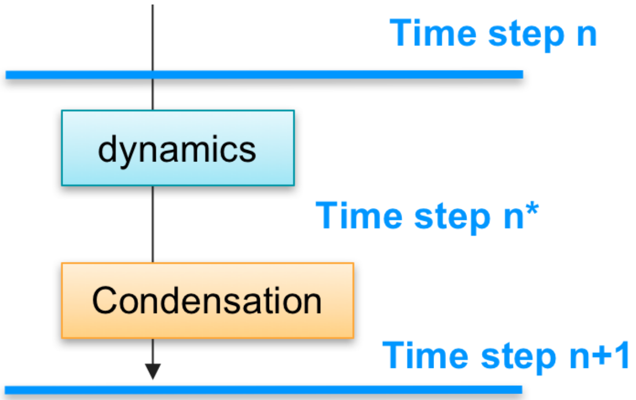
Impact of Physics-Dynamics Coupling (Splitting)

Splitting in CAM4

- Physics and dynamics are sequentially split



- At the intermediate step n*
  - Model state is out of saturation equilibrium
  - Condensation scheme is expected to bring the state back to equilibrium
  - *This is **totally legitimate** (i.e., this is how the parameterization was designed to work)*

- **But** consider this scenario:
  - Advection brings liquid to a very dry cell
  - Condensation scheme evaporates liquid and brings cell back to cloud-free at step n+1
  - The intermediate step n* has ql > 0 and f = 0!

Revised Splitting for the Closure

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- Original implementation in e.g., CAM4:

$$\widetilde{q_l} = \frac{\overline{q_l}^{(n*)}}{\max(f^{(n*)},\ f_{\min})}$$

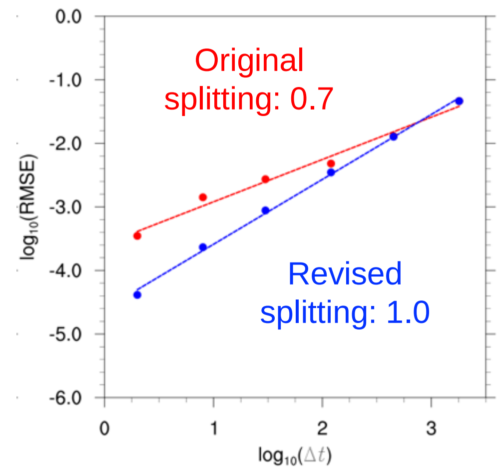
- Revision: use step n (in equilibrium)

$$\widetilde{q_l} = \frac{\overline{q_l}^{(n)}}{\max(f^{(n)},\ f_{\min})}$$

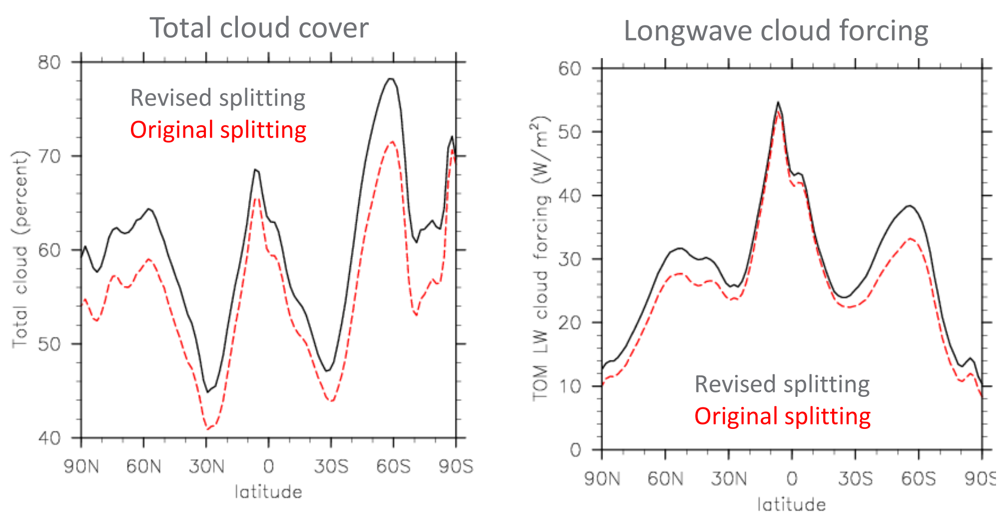
- Helps restore convergence in test problem

- Also has a substantial impact on model climate in CAM4!

Convergence rate in test problem



Mean climate in full-model simulations with CAM4 physics



Formal Error Analysis

$$\frac{dy}{dt} = D(y) + P(y)$$

$$|e_n| \leq |\tilde{e}_0| e^{(t_f - t_0)K} + \frac{e^{(t_f - t_0)K} - 1}{2K} \left[2K_{f_y} \left\| \frac{y}{f} D(D+P) \right\|_\infty + 2K_D \left\| \frac{y}{f} f_y (D+P) \right\|_\infty + \|y''\|_\infty \right.$$
$$\left. +2 \left\| \frac{y}{f} D^2 f_{yy} \right\|_\infty + \left\| \frac{y}{f} f'' \right\|_\infty + 2 \left\| D \frac{f_y f'}{f^2} \right\|_\infty + 2 \left\| D \frac{f'}{f} \right\|_\infty \right] \Delta t$$

- Impact of singularity: f = 0 can lead to unbounded solution error, hence loss of convergence

Impact of Model’s Continuous Formulation

Cause of Singularity

- Disconnect between ql and f in basic model setup
  - Cloud fraction based purely on RH (Slingo-type)
  - Liquid concentration predicted by a separate equation
- Closure assumption $\widetilde{q_l} = \dfrac{\overline{q_l}}{f}$
- Revised splitting helps, but convergence can still be lost
  - Within 1 hour -- if initial condition contains singularity
  - In longer simulations -- because singularity can be generated even when it does not occur in the initial conditions
- Ultimate solution of convergence problem requires revision of model formulation

A Revised Formulation

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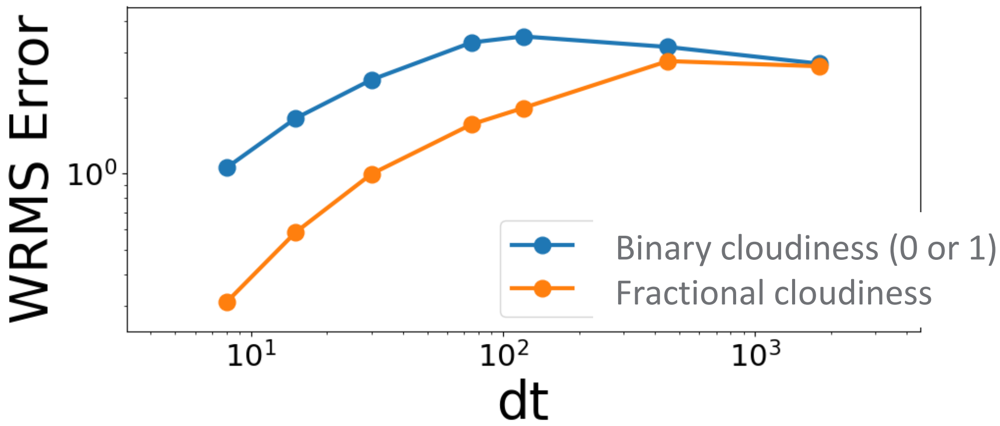
- Keeps the basic setup and assumptions
- Replaced the closure assumption $\widetilde{q_l} = \frac{\overline{q_l}}{f}$



- Preliminary results:
  Closure without assumption of continuity shows better convergence

- Another possibility: change the basic setup, choose different prognostic variables (we are interested in exploring this option, too)

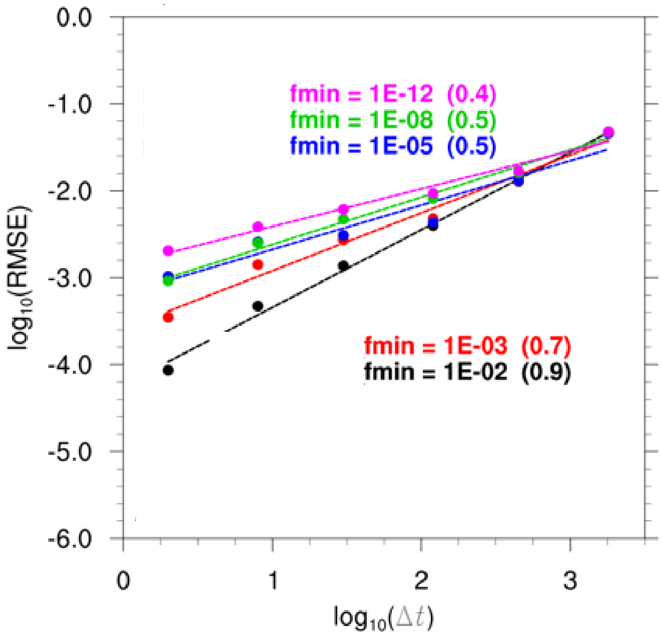
Why Is This Important?

- What we encountered was essentially a “division by zero” problem, commonly encountered in, e.g.
  - In-cloud hydrometeor concentrations
  - In-cloud aerosol concentrations
  - Skewness of sub-grid PDFs in CLUBB

- The use of the “safeguard parameter” seems to simplify life
- … but it can hide problems

- The revised splitting avoids sensitivity to the artificial parameter
- The revised formulation does not need the parameter at all.

Original closure assumption and splitting, poor convergence masked by large fmin



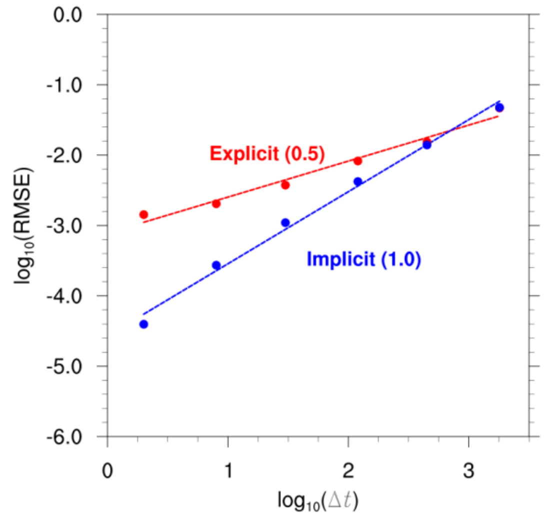
Impact of Time Stepping in Physics

Cloud Fraction Change

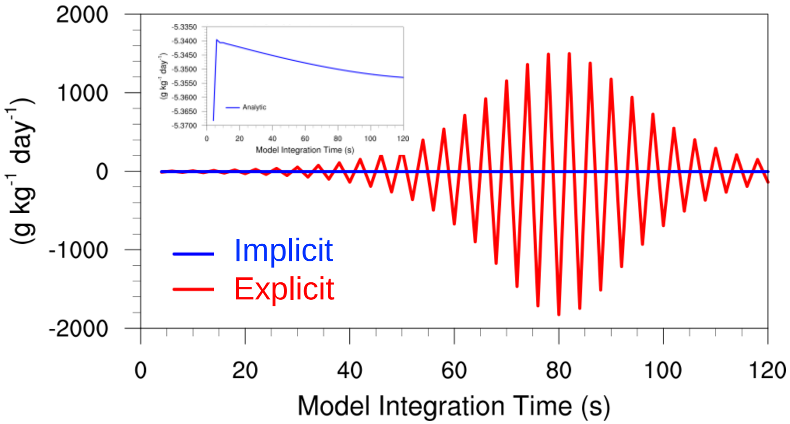
$$\overline{Q} = f\widehat{Q} - \left(\overline{A}_l - f\widehat{A}_l\right) + \tilde{q}_l \frac{\partial f}{\partial t}$$

- Two options based on a semi-analytic method (Zhang et al. 2003): explicit and implicit
- Explicit method converges poorly and produces unphysically large oscillations
- Fast and strongly coupled processes need to be handled with care

Time Stepping Error and Convergence Rate



Time Series of Condensation Rate



Summary

- E3SM model developers have teamed up with applied mathematicians to address the time-step convergence puzzle in the atmosphere model
- First results from a simplified model demonstrate that poor convergence in short-tem simulations can be understood and improved
- Poorly converging and properly converging models can produce different climate
- Insights from convergence testing can help improve not only time integration but also the continuous formulation of a parameterization.
- We are now working on more complex and realistic equations (i.e., parameterizations in E3SM: CLUBB, cloud microphysics, etc.)

E3SM Energy Exascale Earth System Model

SciDAC Scientific Discovery through Advanced Computing

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- Climate dynamics and atmospheric feedbacks
- Terrestrial biogeochemistry
- Arctic amplification and high-latitude processes
- Integrated assessment and multi-sector modeling
- Software engineering to support multi-sector modeling

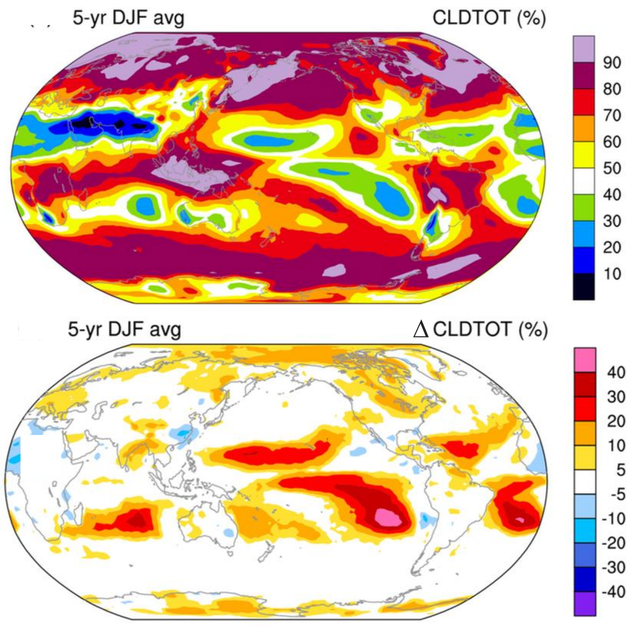
Contact Gary.Worrell@pnnl.gov or visit https://www.pnnl.gov/atmospheric/jobs.asp.

Backup slides

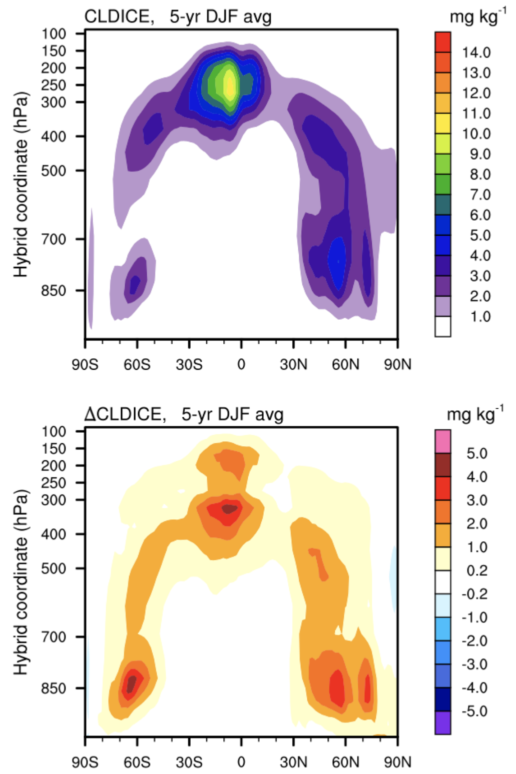
Strong Time-step Sensitivity in E3SM and Its Predecessors

- Present-day climate simulated with CAM5

Total Cloud Cover



Cloud Ice Mass Concentration



Default model (2-degree FV, 30-min step size)

Difference due to reduction of step size to 4 min

Wan, Rasch et al. (2014, GMD)

- E3SM v0 uses a different dynamical core but shows very similar results, indicating the issues are in the physics package

Noisy Physics

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- Our strategy for addressing this challenge
  - Identify and remove pathological noisiness
  - Apply deterministic and stochastic PDE theories to handle physical noisiness
- Initial investigations into prototype problems show promising results

- SDE work inspired by Hodyss et al. (2013, MWR)
- Our first test problem:
  - 1D advection-diffusion equation with a wide spectrum of fast forcing
  - Generalized Ito correction
  - Improved accuracy and convergence

Time-stepping error in advection-diffusion model with colored spectrum of fast forcing