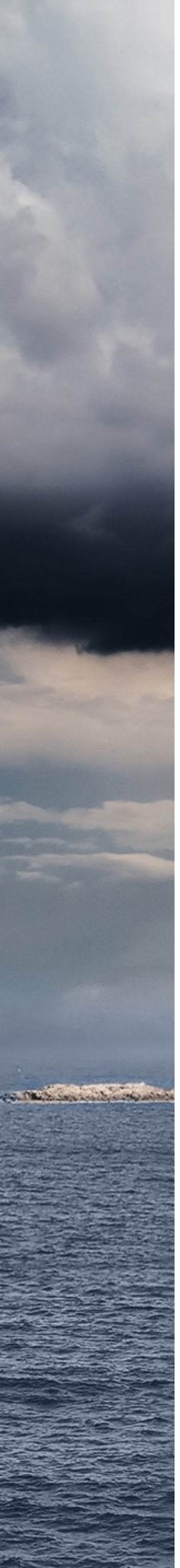
E3SM All-hands Presentation, April 13, 2023

PAESCAL SciDAC5 Project Overview

Hui Wan (PNNL)

On behalf of the PAESCAL team:

Ann Almgren, Michael Brunke, Berk Geveci, Brian Gaudet, Brian Griffin, Vince Larson, Jianfeng Li, Wuyin Lin, Brianna Major, Phil Rasch, Sean Santos, Panos Stinis, Xiaoliang Song, Chris Vogl, Carol Woodward, Heng Xiao, Abhishek Yenpure, Xubin Zeng, Guang Zhang, Tao Zhang



SciDAC: Scientific Discovery through Advance Computing

- DOE Office of Science research program since 2001
- 5th instantiation of the BER-ASCR partnership since Sept. 2022
- Projects are collaborative basic research efforts involving physical scientists, computational scientists, and computer scientists

PAESCAL: Physical, Accurate, and Efficient Atmosphere and Surface Coupling Across Scales

- Collaboration among 4 labs + 3 universities + 1 industry partner
- Scope: develop new algorithms for numerical process coupling in E3SM, especially in EAM
- Goal: contribute to the improvement of numerical accuracy and computational efficiency of E3SM's multi-decadal climate predictions

Pacific Northwest National Laboratory · Lawrence Livermore National Laboratory · Berkeley Lab – Lawrence Berkeley National Laboratory · Brookhaven National Laboratory

The University of Arizona · University of Wisconsin UW Milwaukee · UC San Diego · kitware

This presentation

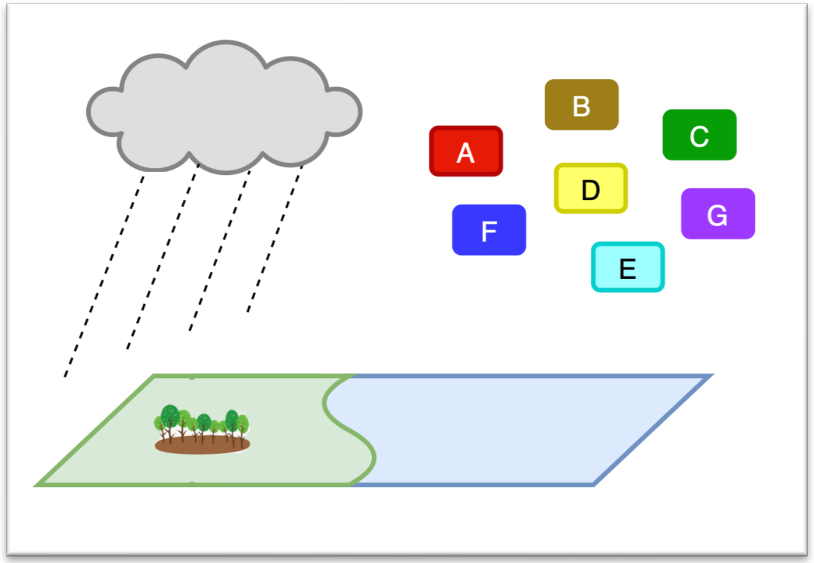
- Describe project objectives and provide an overview of the tasks
- Purpose is to facilitate coordination and collaboration with the E3SM team

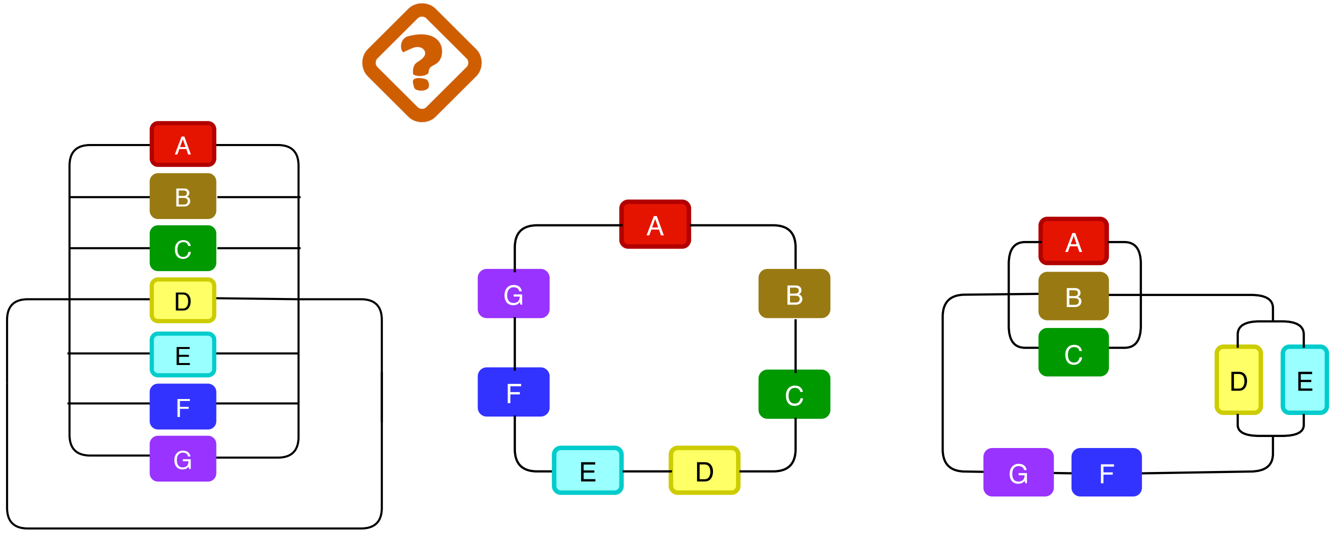
What do we mean by numerical process coupling?

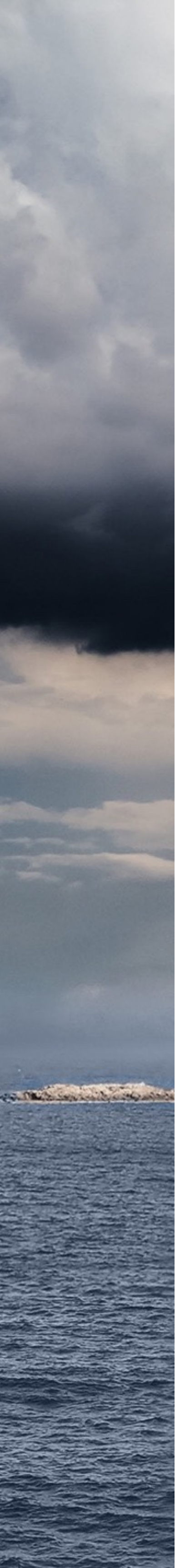
After state-of-the-art representations of individual processes have been developed by the corresponding experts, what numerical algorithms do we use to assemble the different pieces into a full, coherent, and performant model?

- PAESCAL focuses mainly on time integration
- Some tasks unavoidably involve vertical discretization

- Time integration: primary focus is on reducing splitting errors







Splitting errors have caused significant inconvenience in E3SM development

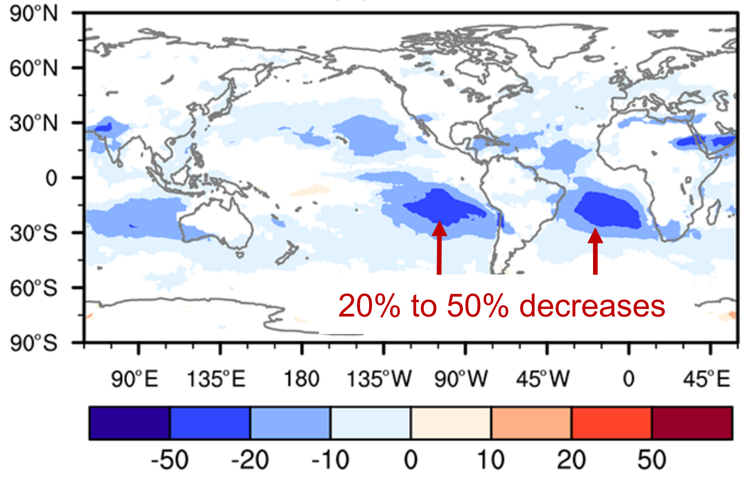
- Strong sensitivities of model results to Δt and Δz
- Both examples shown here have to do with splitting errors

- EAM is expected to be evaluated and used at a wide range of horzonal resolutions
- How to choose Δt or Δz?

- If these sensitivities are not addressed, developers will have to
  - Change Δt or Δz and repeatedly retune model parameters, or
  - Avoid the retuning by living with fixed Δt or Δz
- Both are undesirable scenarios

1

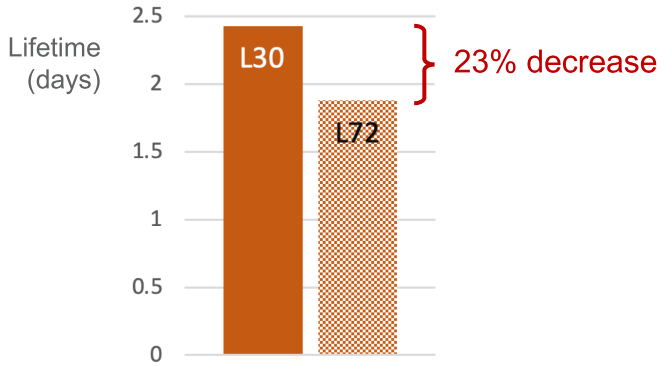
Relative difference in annual mean total cloud cover caused by shortening Δt to 1/6 in EAMv1



See also Wan et al. (2021) and Santos et al. (2021)

2

Global mean dust aerosol lifetimes in EAMv1 using 30 or 72 layers

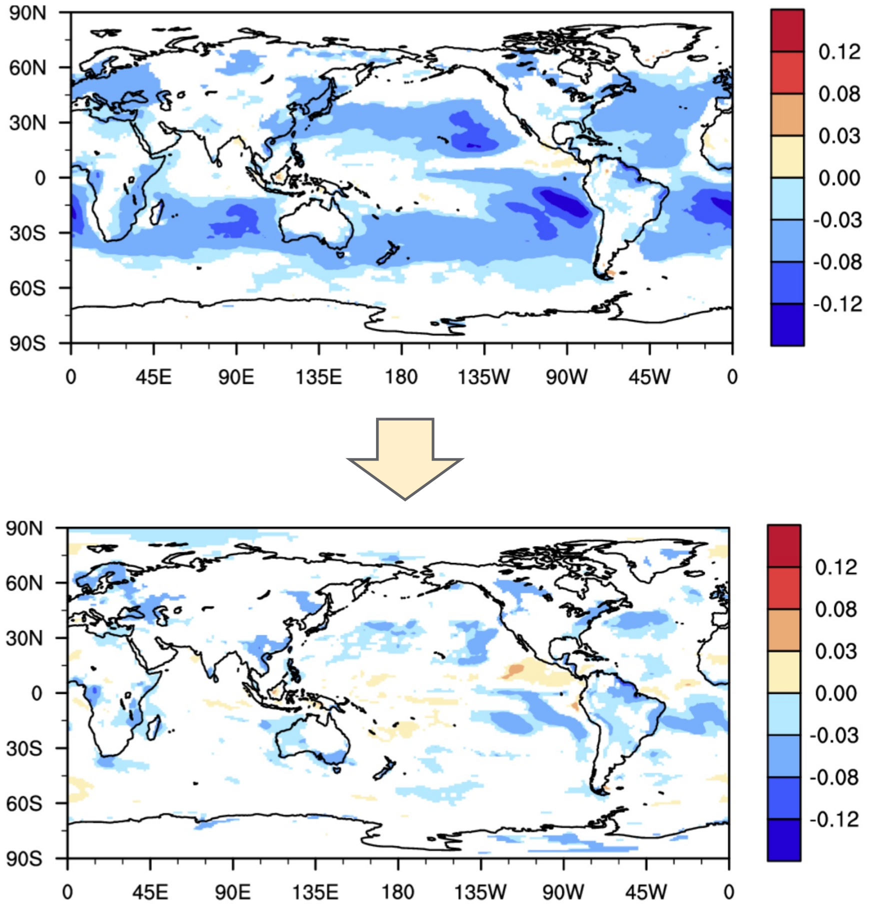


See also Feng et al. (2022)

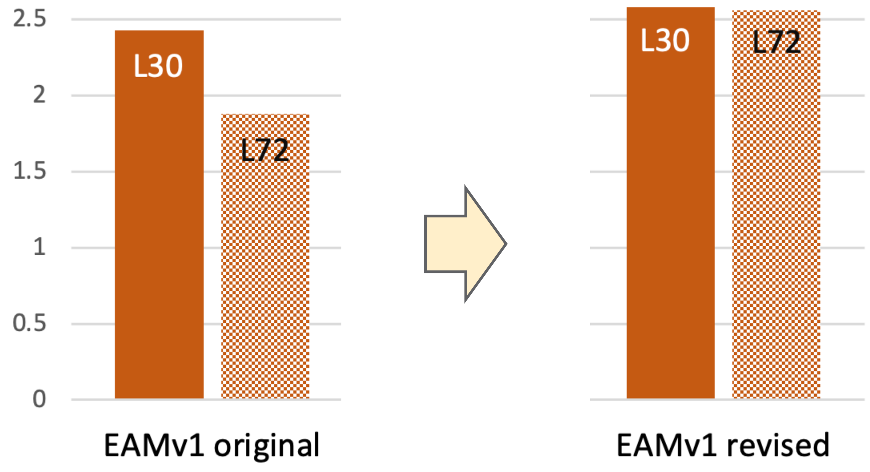
SciDAC4 work showed that splitting errors can be identified, understood, and substantially reduced

... but many sensitivities and coupling problems remain unaddressed

Δt sensitivity in annual mean low-cloud fraction in EAMv1



Δz sensitivity in global annual mean dust lifetime in EAMv1



PAESCAL addresses numerical coupling challenges at multiple levels of E3SM's model hierarchy

Earth system level

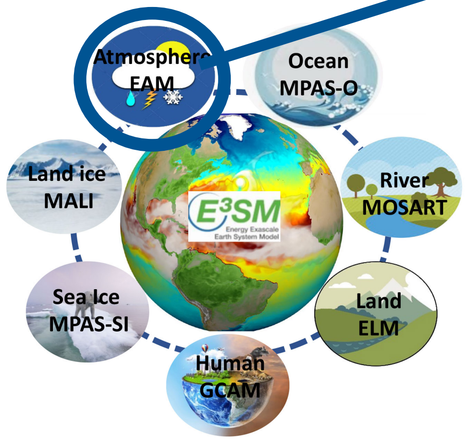
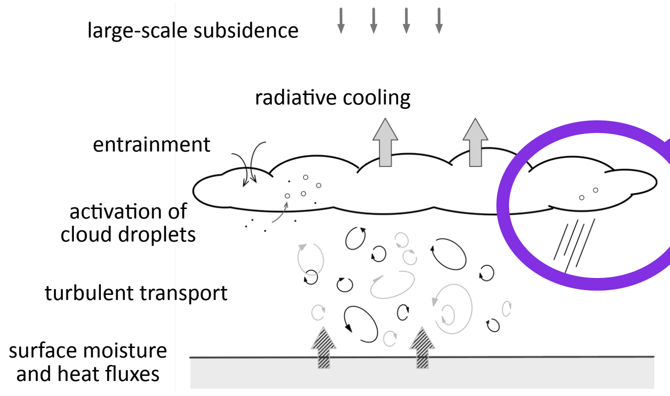


Image credit: E3SM website

"Atmosphere driver" level



Cartoon adapted from Stevens (2005) by Hui Wan

Parameterization level

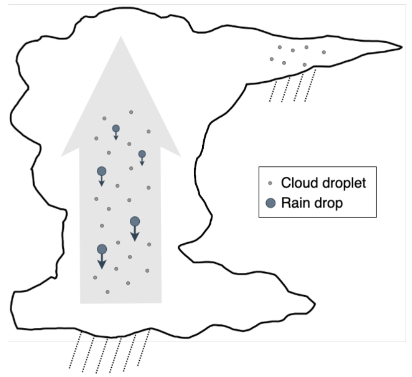


Image credit: PAESCAL proposal (2022)

Task 1.2: Atmosphere-surface coupling

Task 1.1: Process coupling in the atmosphere

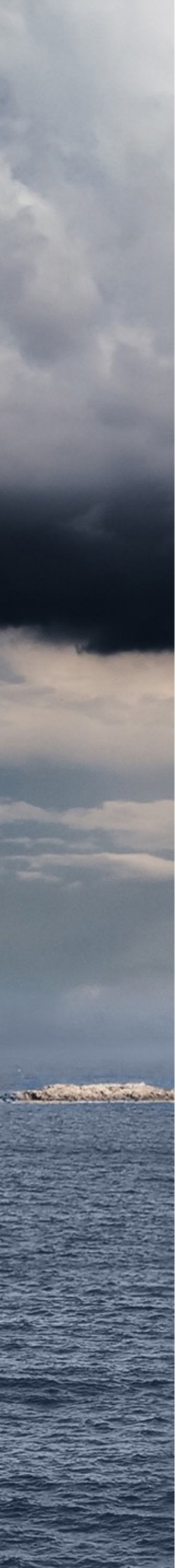
Task 3: Coupling issues in PDE-ML hybrid systems

Task 2.1: Discretization for Cloud Microphysics

Task 2.2: Discretization for boundary layer turbulence

Task 4: New visual analytics tools

Task 5: Integration to E3SM



Project objectives

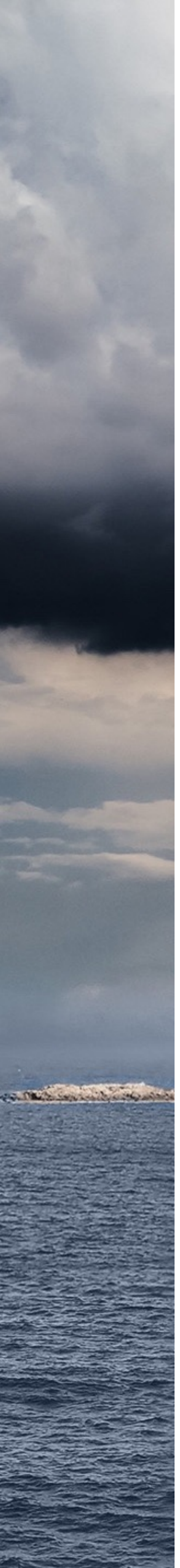
At EAM’s workhorse resolutions

- Reduce time integration errors to a level below the spatial resolution errors and model formulation errors

Anticipating a wide Δx range in EAM’s development and application

- Improve Δt-Δz convergence for EAM’s cloud microphysics and turbulence parameterizations

Deliver a version of EAM that allows the developers and users to choose Δt and Δz consistent with Δx and the underlying physics

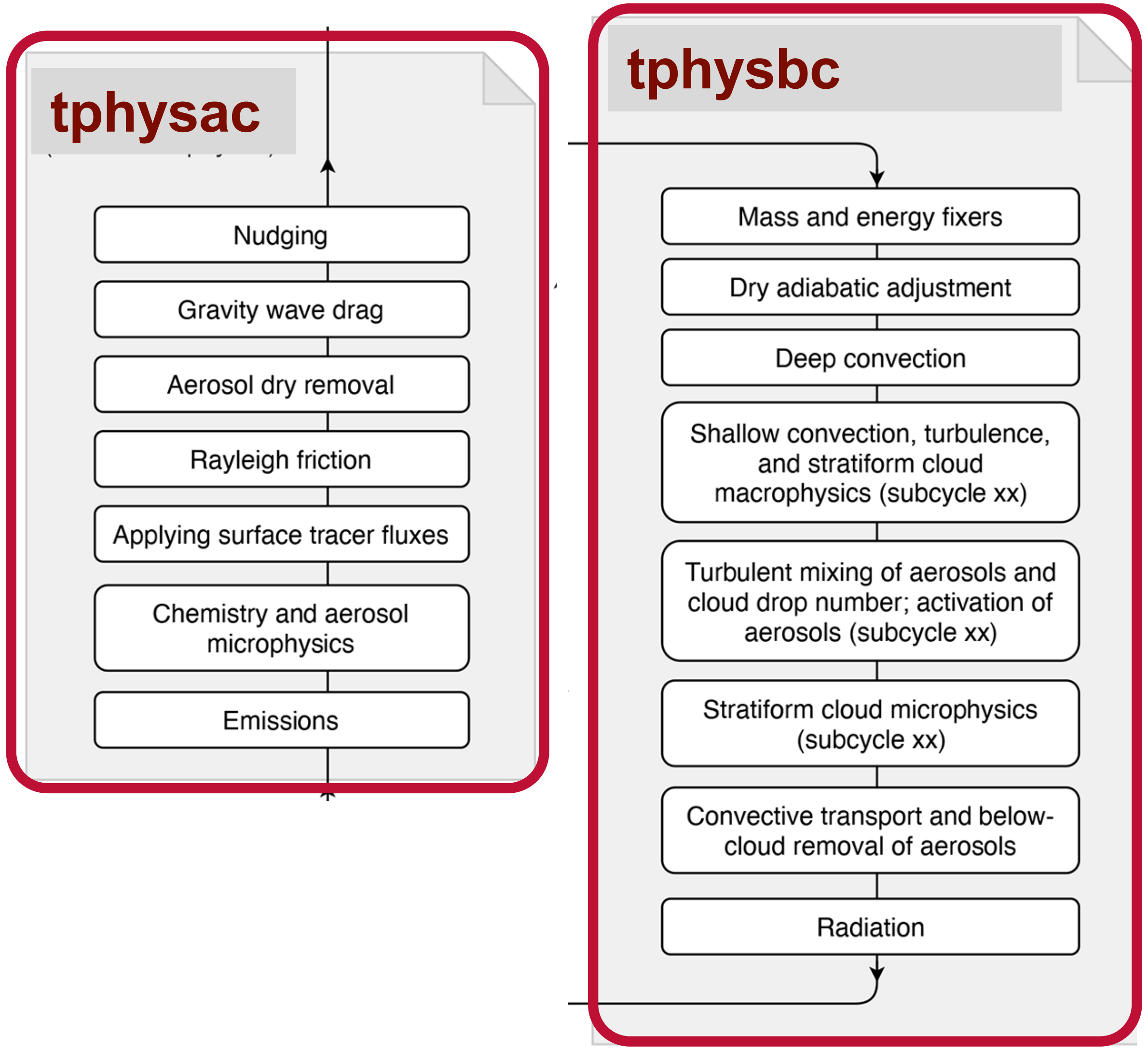


Task Overview and Plans

Task 1.1: Process coupling in the atmosphere

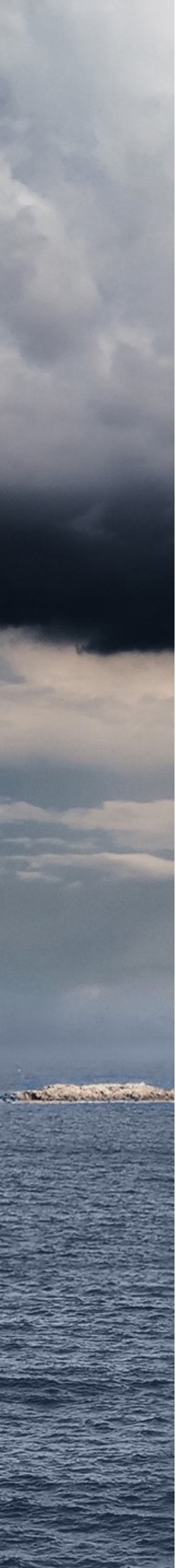
Co-leads: Hui Wan (PNNL), Chris Vogl (LLNL)

Scope: Reorganize process groups and their coupling at the atmosphere driver level



- Details of revision will be guided by
  - The physics: main sources and sinks; their characteristic time scales
  - Model sensitivity to revision; impact
  - Theoretical error analysis (using new framework that supports process-level analysis)
  - FASTMath expertise on time integration
  - Estimated computational cost

- Code changes will be done in EAMv2 (and v3 when released); will be intrusive



Task 1.2: Atmosphere-surface coupling

Co-leads: Xubin Zeng (U. Arizona), Carol Woodward (LLNL)

Scope:

- Investigate and address numerical instabilities in near-surface atmosphere quantities
- Assess and address the surface layer "gray zone" problem

Addressing the nonphysical oscillations

- Identify the root cause
- Revise coupling between the surface and the turbulence parameterization

Investigating the surface layer "gray zone" problem

- Clarify and revisit model assumptions, identify inconsistencies
- Assess impact
- Propose possible solutions

Strong, nonphysical near-surface wind oscillations in EAM

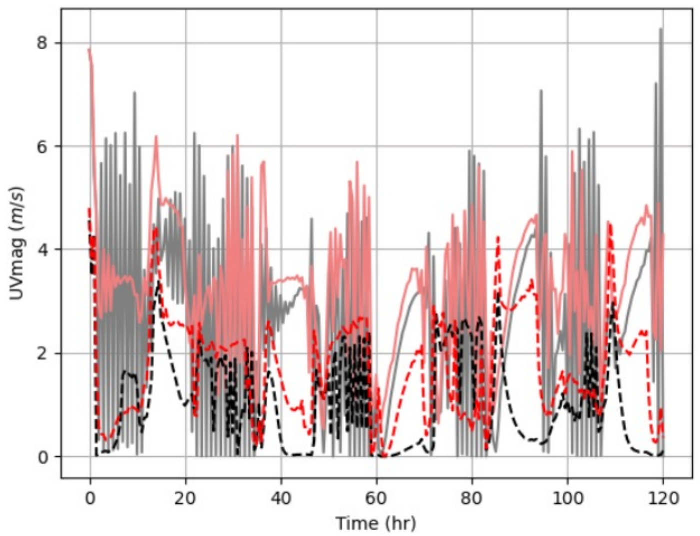


Figure by Sean Santos

Surface layer "gray zone" problem

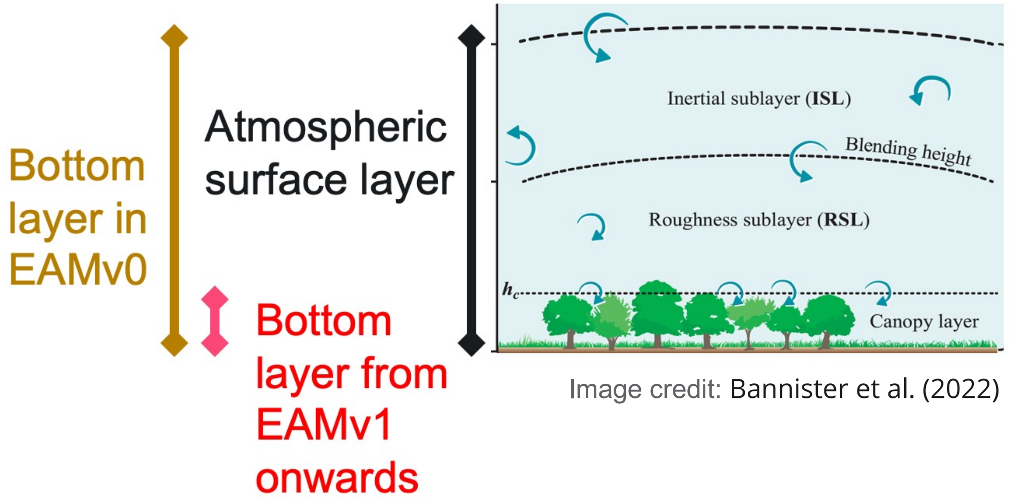
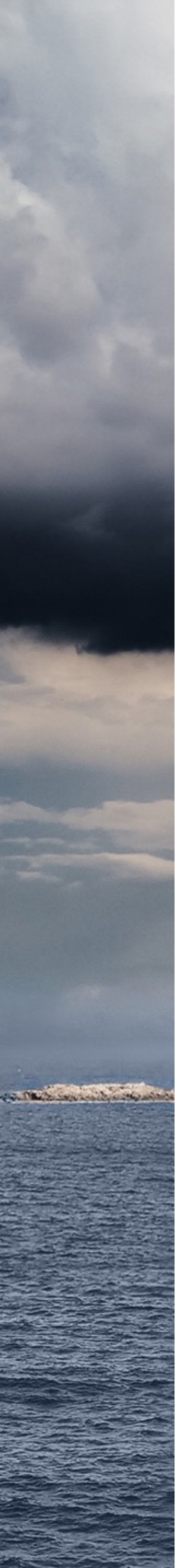


Image credit: Bannister et al. (2022)



Task 2.1: Discretization for cloud microphysics

Co-leads: Sean Santos (PNNL), Carol Woodward (LLNL)

Scope: Develop new spatiotemporal discretization methods for coupling local and nonlocal cloud microphysics processes

Motivation

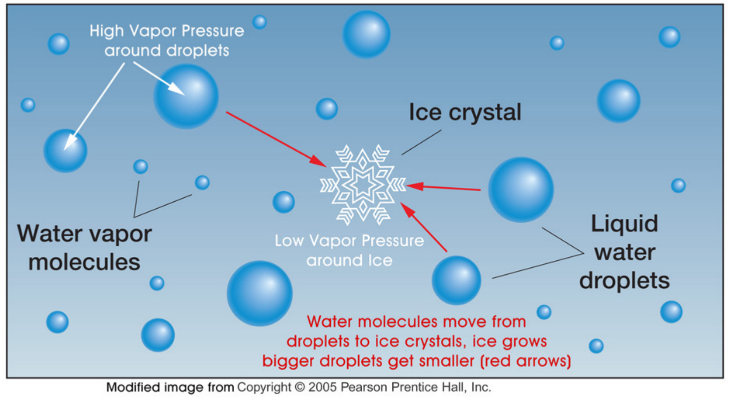
- “Conservation checks” in cloud microphysics code are in fact fixers for negative tracer concentrations
- Rain/snow formation and hydrometeor sedimentation are sequentially split, preventing rain/snow to interact with cloud layers they fall through
- Deep convection has additional challenges associated with strong updraft

Planned work

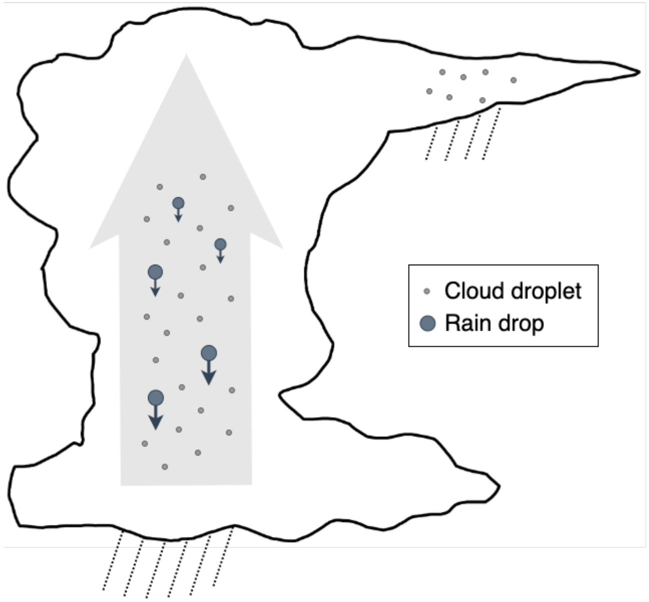
- Write a new cloud microphysics driver for the P3 microphysics
- Implement tighter coupling between local and nonlocal processes
- Explore a range of spatio-temporal discretization method (e.g., multi-rate time integrators, semi-Lagrangian methods)

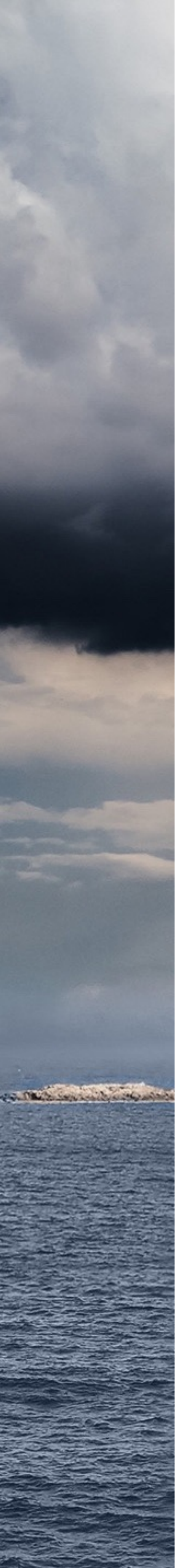
- Code is written in C++

Local processes



Nonlocal processes





Task 2.1: Discretization for boundary layer turbulence

Co-leads: Vince Larson (U. Wisconsin - Milwaukee), Ann Almgren (LBNL)

Scope: Develop new strategy based on finite volume (FV) methods to address challenges associated with sharp vertical gradients in systems of coupled nonlinear equations

Why FV?

- Integral equations are a more fundament representation of the physics
- Equations and discretization methods will not break down at discontinuities
- Encouraging results from SciDAC4

Plans

- Explore FV methods in CLUBB (exploratory due to complexity of the physics)
- Use single-column simulations for a large part of the development

At a given resolution, an FV-based discretization might be more expensive than the current FD methods, but

- Has the chance of providing substantially improved solution quality
- gives a starting point for further optimization

Big jumps of total water and potential temperature at the top of stratocumulus clouds

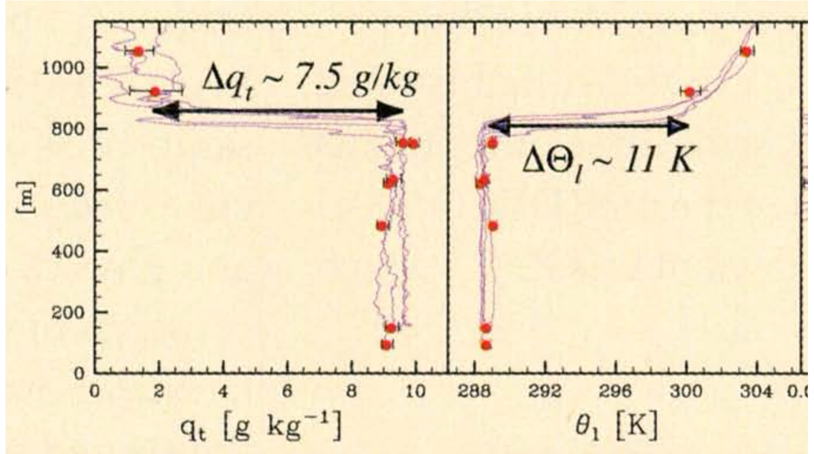


Figure credit: Stevens et al. (2003)

Zonally averaged clipping magnitude of dw'2/dt in EAMv1

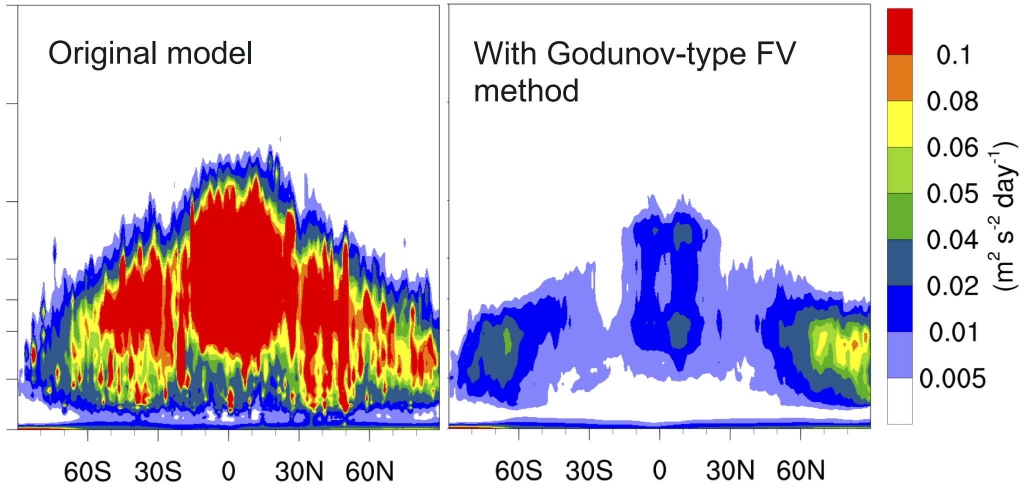


Figure from Shixuan Zhang and Chris Vogl

Task 3: Coupling issues in PDE-ML hybrid systems

Co-leads: Guang Zhang (UCSD), Panos Stinis (PNNL)

Scope: Identify root causes of commonly encountered instabilities problems in PDE-ML hybrid models of the atmosphere; explore possible solutions

Plans

- Use a version of CAM5 with neural-network-based (NN-based) parameterizations
- Compare stable simulations from the PDE-based model with unstable simulations from the PDE-ML hybrid system for their characteristics of process interactions
- Explore revisions in process coupling and the construction of ML-based parameterizations

- The task makes use of tools and insights from the other tasks;
- In return, it is expected to provide additional insights into the interacting physics to help work in the other tasks

Gravity wave propagation causing numerical instability in a PDE-ML hybrid model

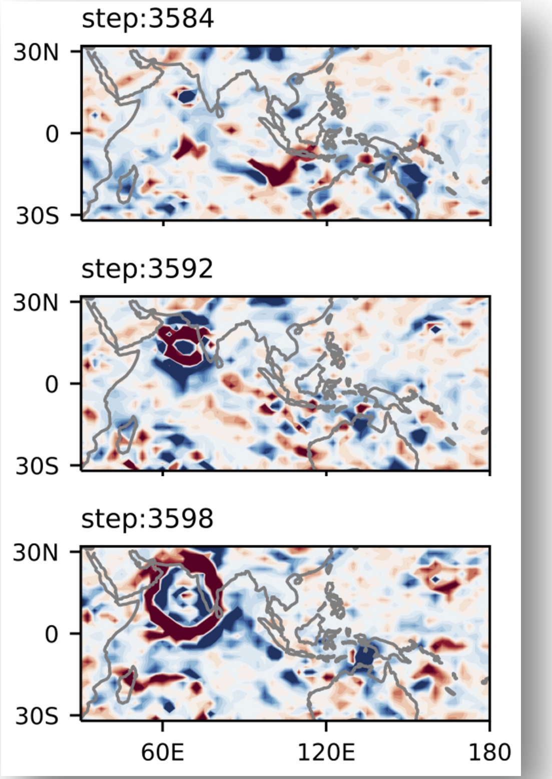


Figure credit: Guang Zhang

Task 4: New visual analytics tools

Co-leads: Berk Geveci (Kitware), Hui Wan(PNNL)

Scope: Develop new visual analytics tools to facilitate analysis of numerical simulations conducted with EAM and its parameterizations

Motivation

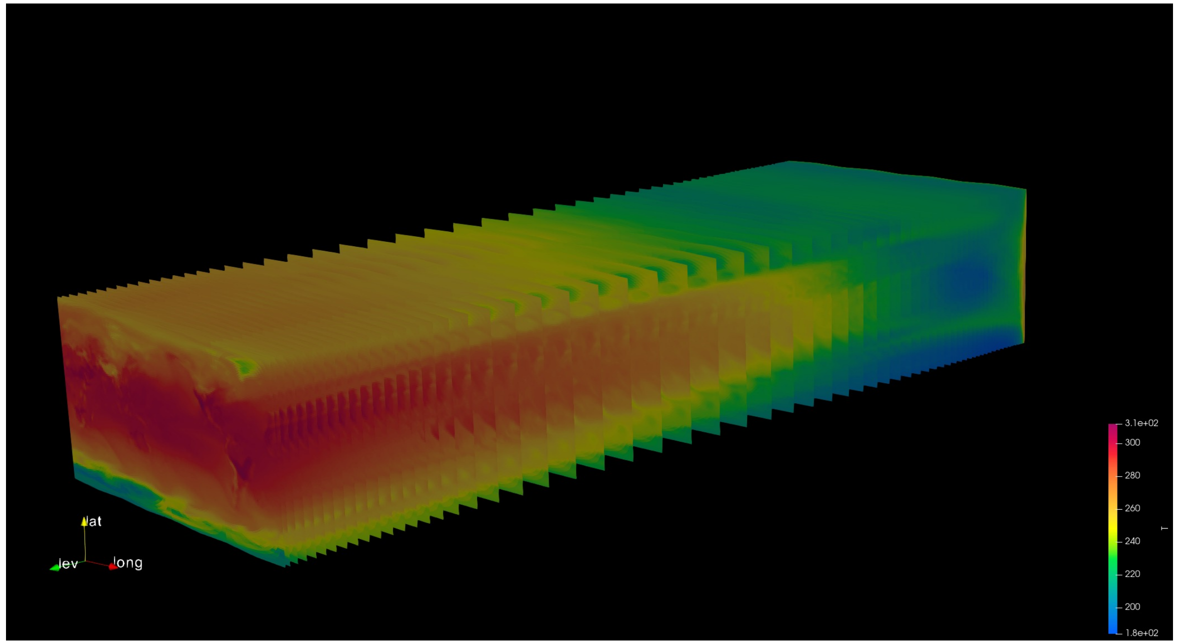
- Process-level evaluation of E3SM simulations can involve tedious scripting during postprocess
- Modern visual analytics frameworks are available across DOE LCFs but not used by atmosphere modelers in daily work

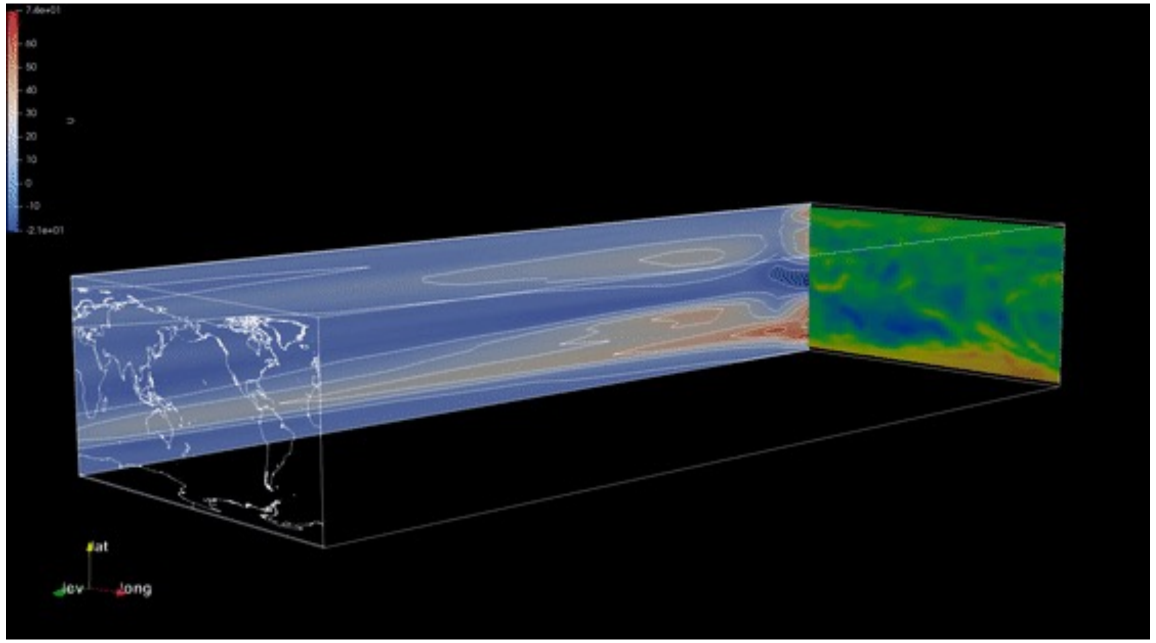
Plans

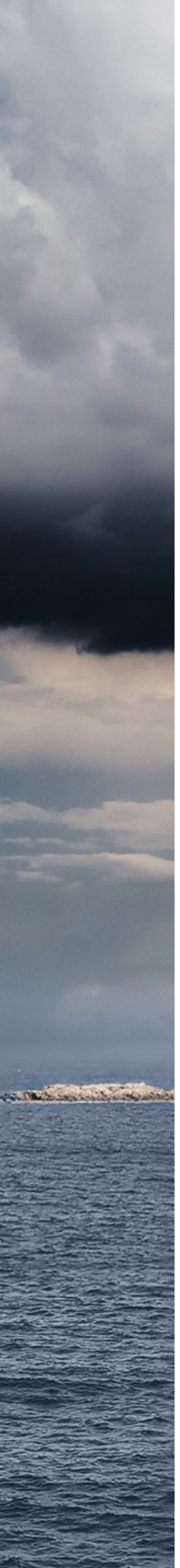
- Use the powerful modern tools as the back end; develop an easy-to-use interface tailored the needs of atmosphere modlers
- Develop visual analytics workflows for both global and single-column simulations

New ParaView Reader supports EAMv2's new mesh and presents model output in intuitive views

Image/video by Abhishek Yenpure and Berk Geveci







Task 5: Integration with E3SM

Co-leads: Wuyin Lin (BNL), Jianfeng Li (PNNL)

Scope

- Ensure code developed in the project is compatible with current and future versions of the E3SM code
- Incorporate code improvements into E3SM's master branch in a timely manner

- Wuyin Lin as liaison with E3SM
- Team members participating in
  - E3SM Phase 3 Atmosphere Group's bi-weekly meetings
  - SCREAM team's weekly meetings
- Jianfeng Li and Wuyin Lin playing key roles in integrating our code changes to E3SM

PAESCAL is all about interactions.

Collaborations are welcome. Please don't hesitate to contact us.