SciDAC
Scientific Discovery through Advanced Computing

U.S. DEPARTMENT OF ENERGY

# Physical, Accurate, and Efficient Atmosphere and Surface Coupling Across Scales (PAESCAL)

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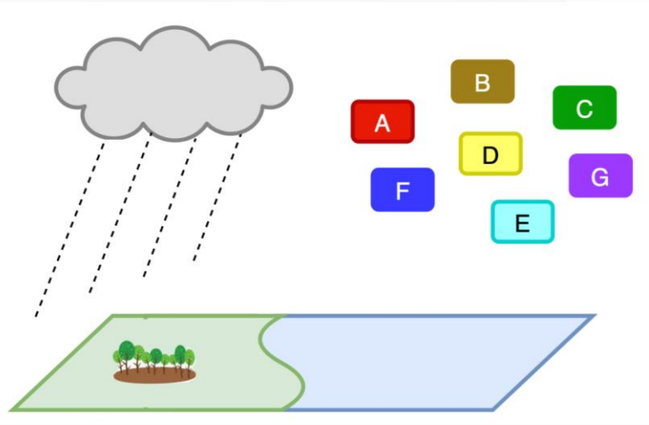
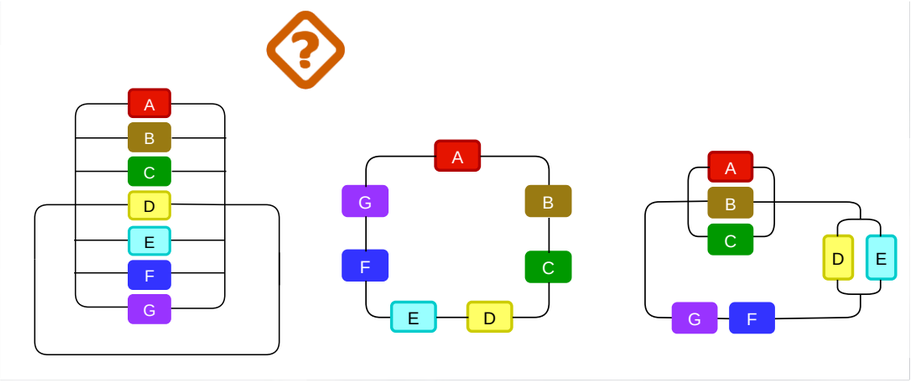
# Project scope: improving numerical process coupling in the E3SM Atmosphere Model (EAM)

*"After the mathematical representations of the individual physical processes have been developed, what **numerical algorithms** should be used to **assemble** those pieces into a coherent and performant model?"*

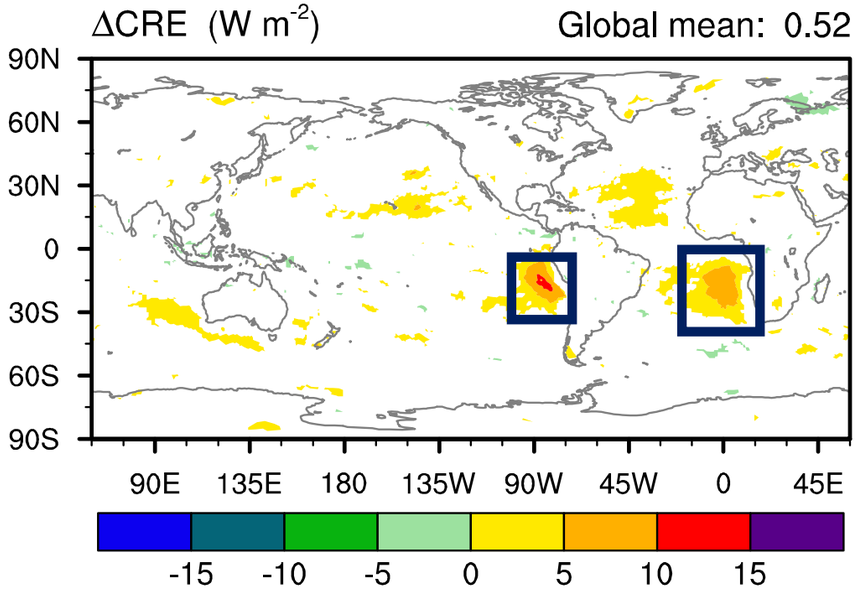



- Primary focus is **time integration**
- Some tasks involve **vertical discretization** and **model formulation**



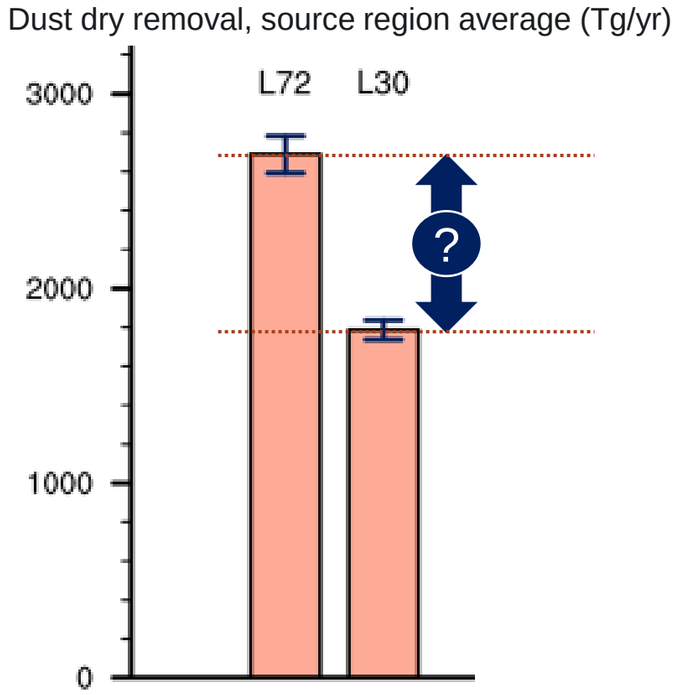
# Why this is important: examples from EAMv1

A small change in cloud process coupling led to significant decreases of cloud radiative forcing in the subtropical marine stratocumulus regions




*Wan et al. (2021)*

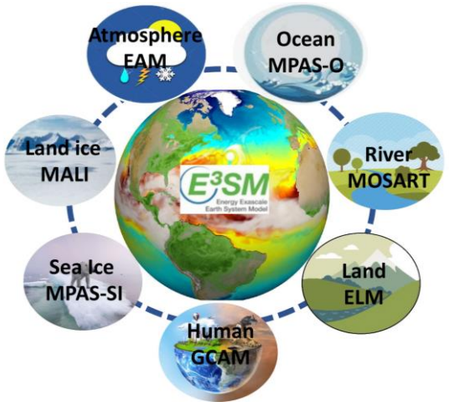
Strong and unphysical sensitivities in dust life cycle to vertical resolution were attributable to process ordering



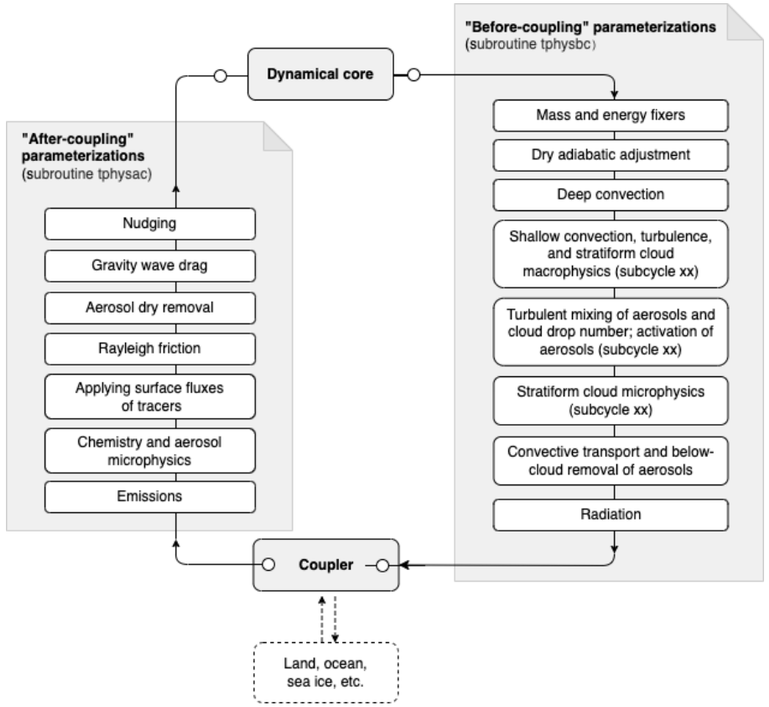

*Wan et al. (2024)*

# PAESCAL addresses process coupling issues at three levels of E3SM's model hierarchy

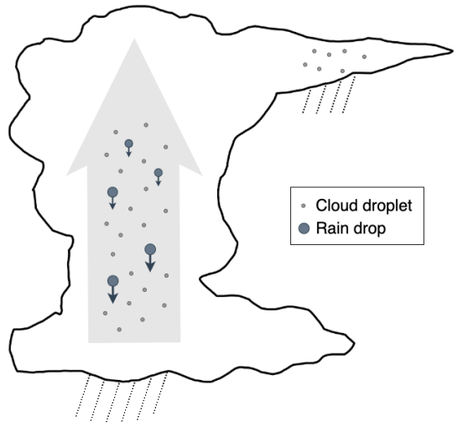
## Earth system level




## Atmosphere driver level




## Parameterization level



# Key challenges

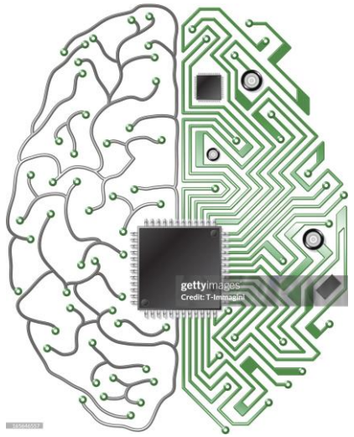
- **MANY processes** and a lot of codes that are **continuously evolving**
- Bridging **physical understanding** and **mathematical rigor**

# Our goal

Move away from overly simplified plug-and-play

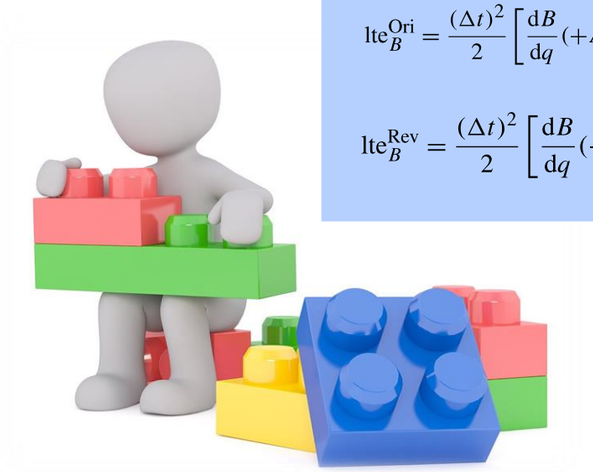
Avoid spaghetti code

Design something sophisticated and elegant



# Addressing coupling issues at the atmosphere driver level

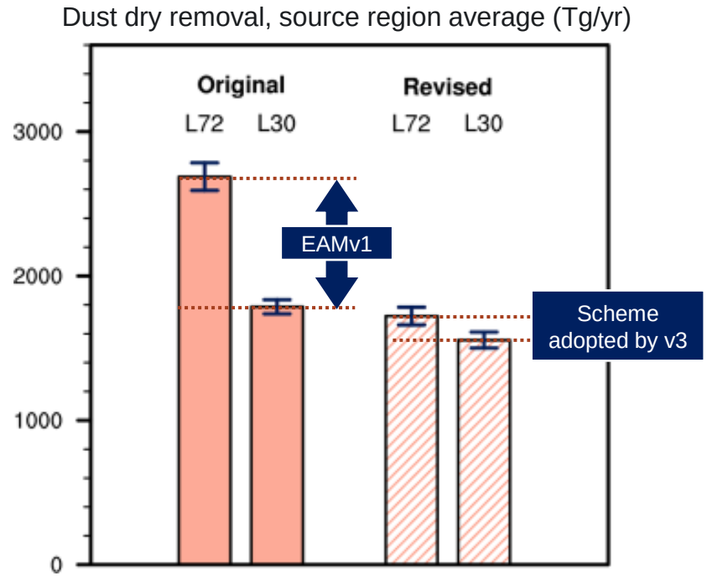
- Performing **process-level analysis** in EAM to understand the intended physics and identify numerical problems
- Developing **idealized (“toy”) models** to cleanly test hypothesis
- Using a general and intuitive **error analysis framework** to guide the design of new coupling options



$$\mathrm{lte}_B^{\mathrm{Ori}} = \frac{(\Delta t)^2}{2}\left[\frac{\mathrm{d}B}{\mathrm{d}q}(+A-C)\right]\Big|_{q=q(t_n)} + \mathcal{O}\left((\Delta t)^3\right)$$

$$\mathrm{lte}_B^{\mathrm{Rev}} = \frac{(\Delta t)^2}{2}\left[\frac{\mathrm{d}B}{\mathrm{d}q}(-A-C)\right]\Big|_{q=q(t_n)} + \mathcal{O}\left((\Delta t)^3\right)$$

*Vogl et al. (2024)*




*Wan et al. (2024)*

*More recent work can be found on poster Thu-157.*

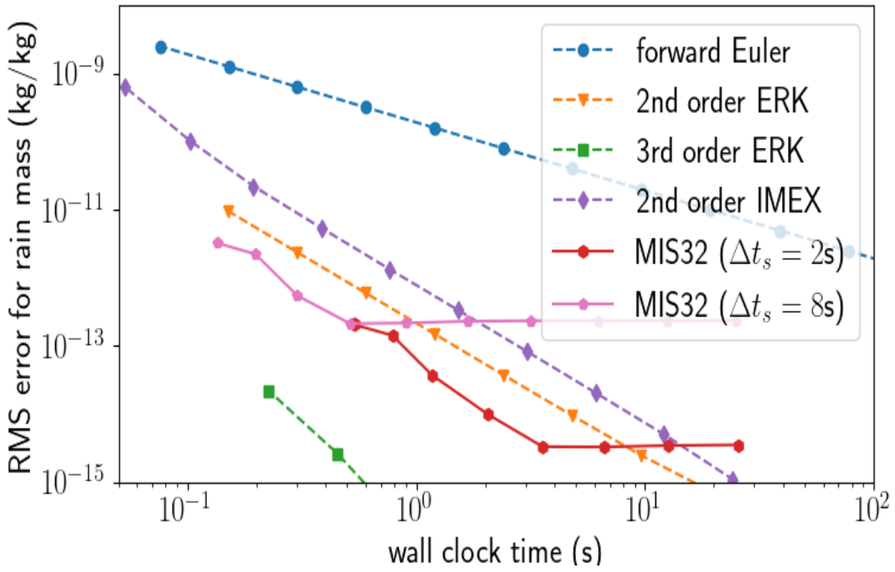
# Addressing coupling challenges at the parameterization level

New cloud microphysics code **SPAECIES**

- Written in C++ and interfaced with ASCR's SUNDIALS time integrator suite
- Designed to be a library (➔ extension beyond clouds)
- Properly convergent(!)
- Work-precision diagrams helps to evaluate different coupling options to balance accuracy and cost

Sean Santos,
lead developer of SPAECIES

Work-precision diagram
for a 4-process warm rain problem

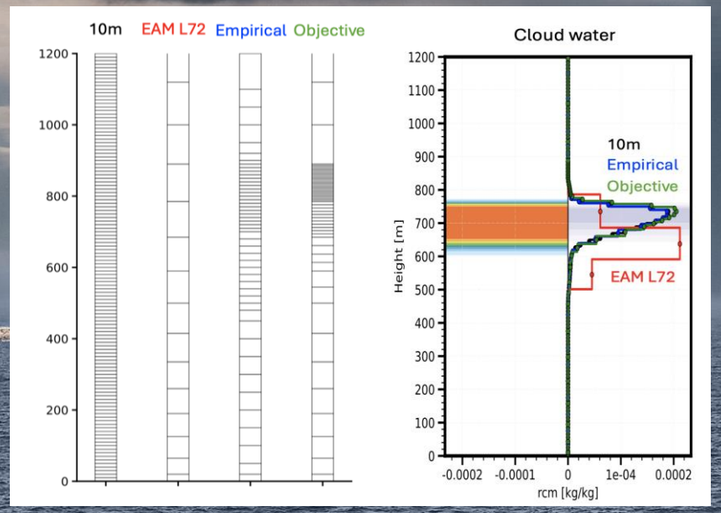



Reference values for rain mass mixing ratio $q_r$:
min: 4.1e-5 kg/kg, mean: 5.6e-5 kg/kg, max 8.9e-5 kg/kg

# Other examples of ongoing work (and team members at this meeting)

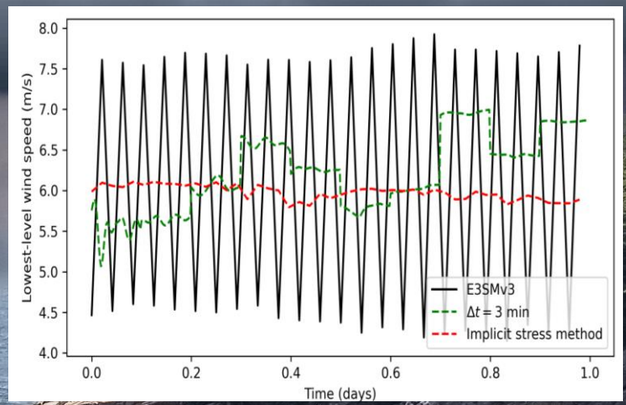
## Addressing vertical resolution challenges

**Ann Almgren, Thu breakout 2**



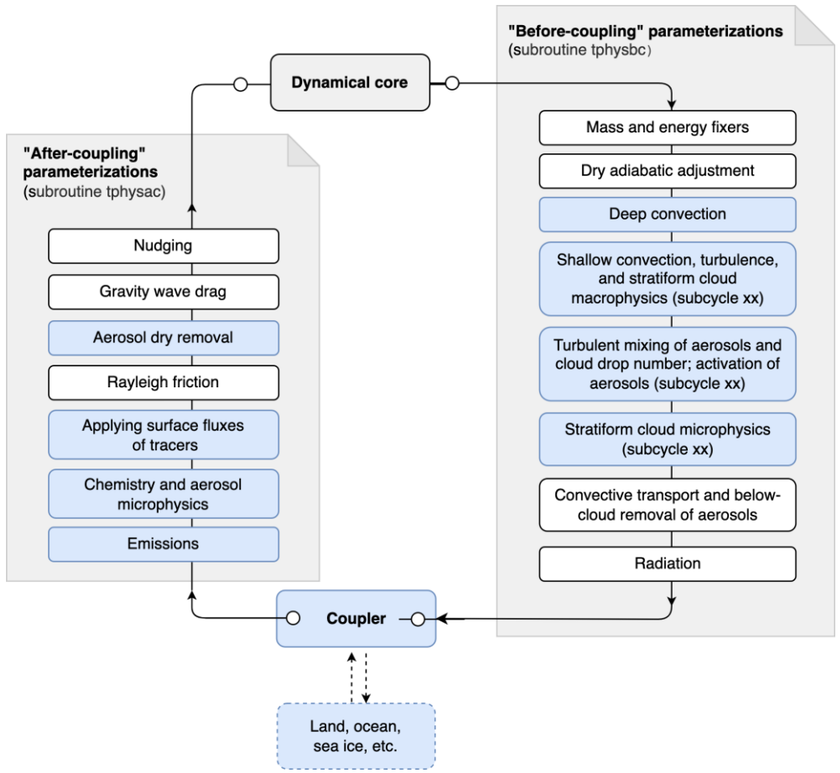

## Improving solution stability at the atmosphere-land interface

**Sean Santos, poster Wed-162**



# PAESCAL is all about interactions

The coupling theme: interactions between processes and between developers




The BER-ASCR collaboration: an example of companion papers

**Numerical coupling of aerosol emissions, dry removal, and turbulent mixing in the E3SM Atmosphere Model version 1 (EAMv1) – Part 1: Dust budget analyses and the impacts of a revised coupling scheme**

Hui Wan[1], Kai Zhang[1], Christopher J. Vogl[2], Carol S. Woodward[2], Richard C. Easter[1], Philip J. Rasch[3], Yan Feng[4], and Hailong Wang[1]

[1]Atmospheric, Climate, and Earth Sciences Division, Pacific Northwest National Laboratory, Richland, Washington, USA
[2]Center for Applied Scientific Computing, Lawrence Livermore National Laboratory, Livermore, California, USA
[3]Department of Atmospheric Sciences, University of Washington, Seattle, Washington, USA
[4]Environmental Science Division, Argonne National Laboratory, Lemont, Illinois, USA

**Numerical coupling of aerosol emissions, dry removal, and turbulent mixing in the E3SM Atmosphere Model version 1 (EAMv1) – Part 2: A semi-discrete error analysis framework for assessing coupling schemes**

Christopher J. Vogl[1], Hui Wan[2], Carol S. Woodward[1], and Quan M. Bui[1,a]

[1]Center for Applied Scientific Computing, Lawrence Livermore National Laboratory, Livermore, California, USA
[2]Atmospheric, Climate, and Earth Sciences Division, Pacific Northwest National Laboratory, Richland, Washington, USA
[a]now at: Blue River Technology, Sunnyvale, California, USA

**We contribute to the ESM community by getting numerical errors out of the way of physics/science-focused research. Collaboration is the key to our path forward.**