



Enabling Aerosol-cloud interactions at G**L**obal convection-permitting scales (E**A**GLES)

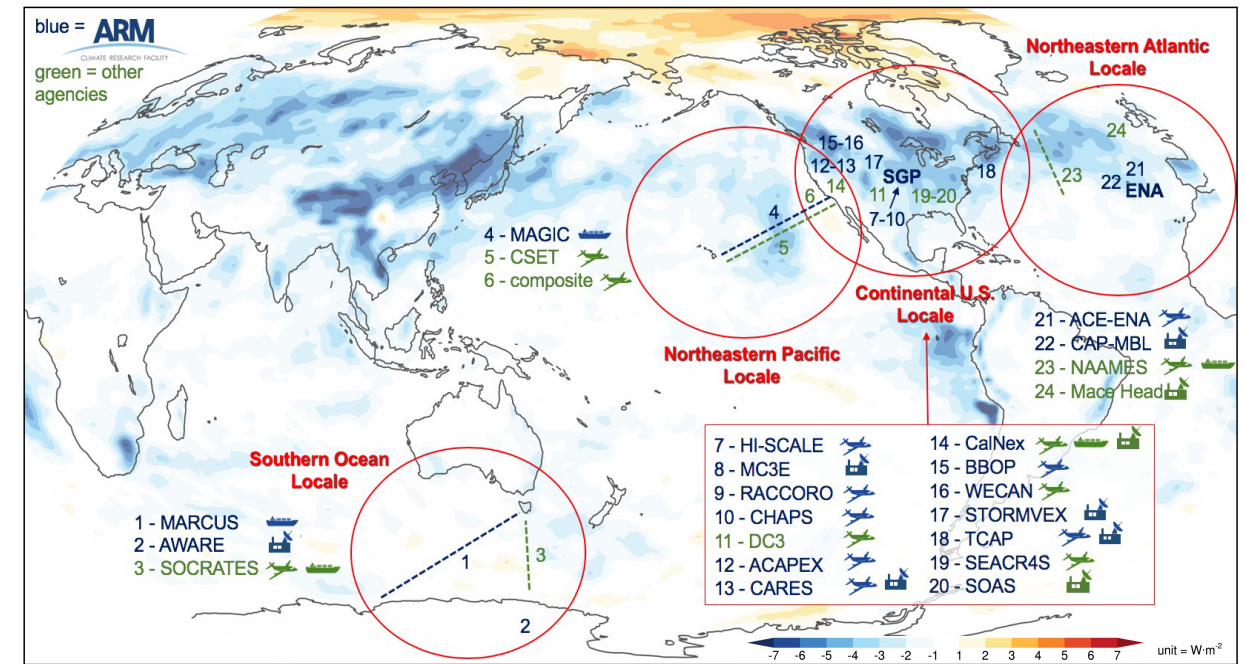
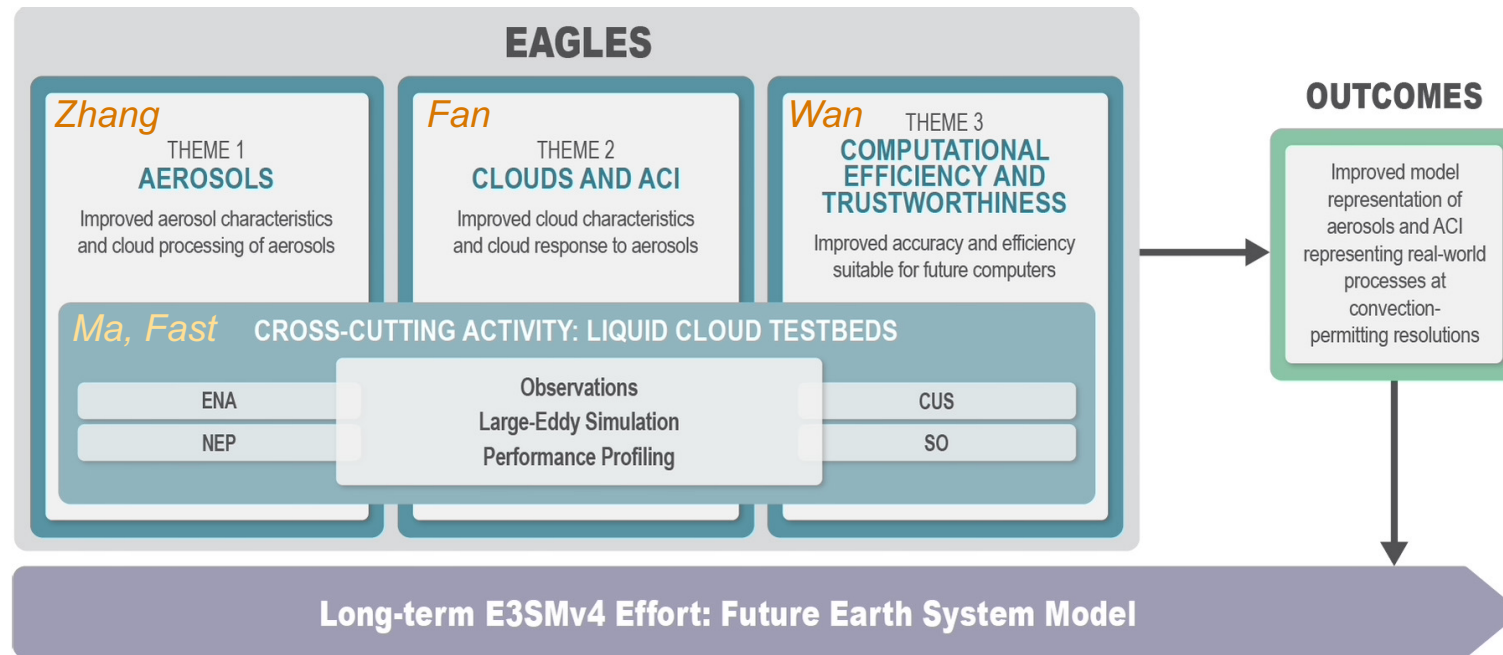
Po-Lun Ma
The EAGLES project team

April 28, 2022

EAGLES

3 model development themes (Aerosol, Clouds, Computation)
 1 cross-cutting activity (Testbeds)
 Deliver improved model representation for E3SMv4

Goal: To increase confidence in, and understanding of, the role of aerosols and aerosol-cloud interactions in the evolution of the Earth system in the **global convection-permitting E3SMv4**

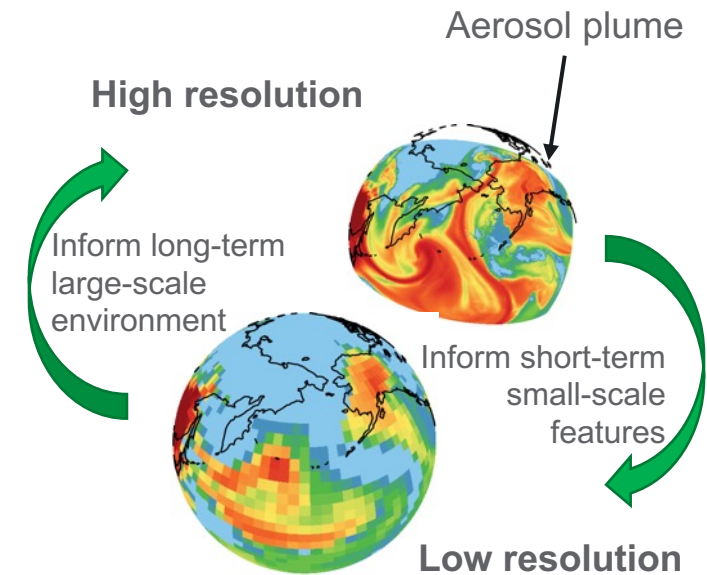
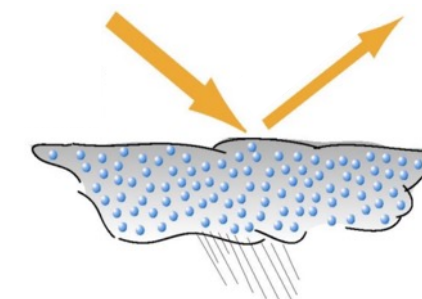
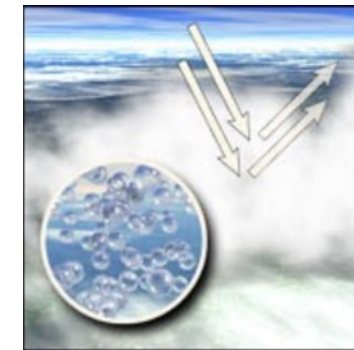
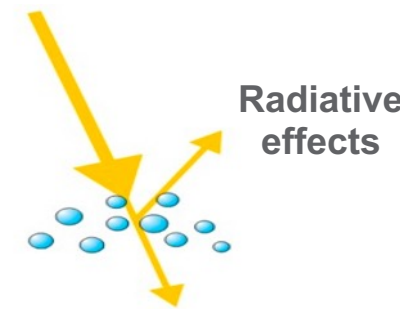
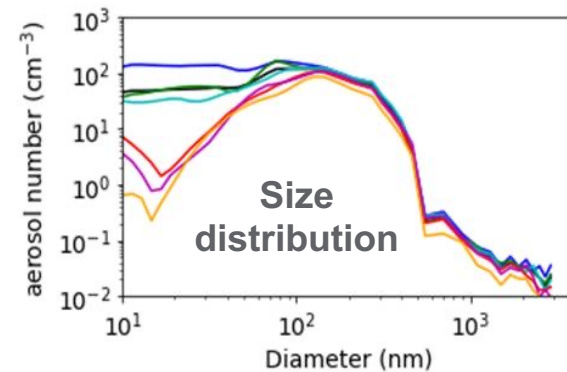
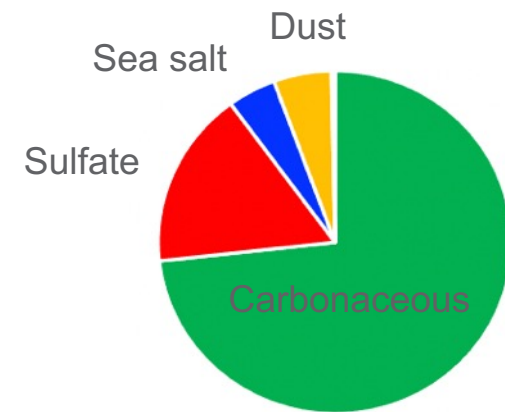
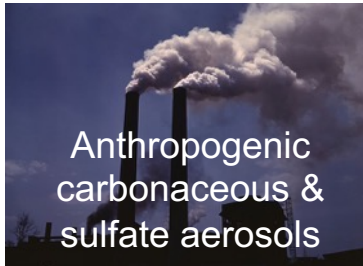


Improve the representations of aerosols and ACI in E3SMv4

Emission, transport, chemical/physical processes predicting aerosol properties, lifecycle, and distribution

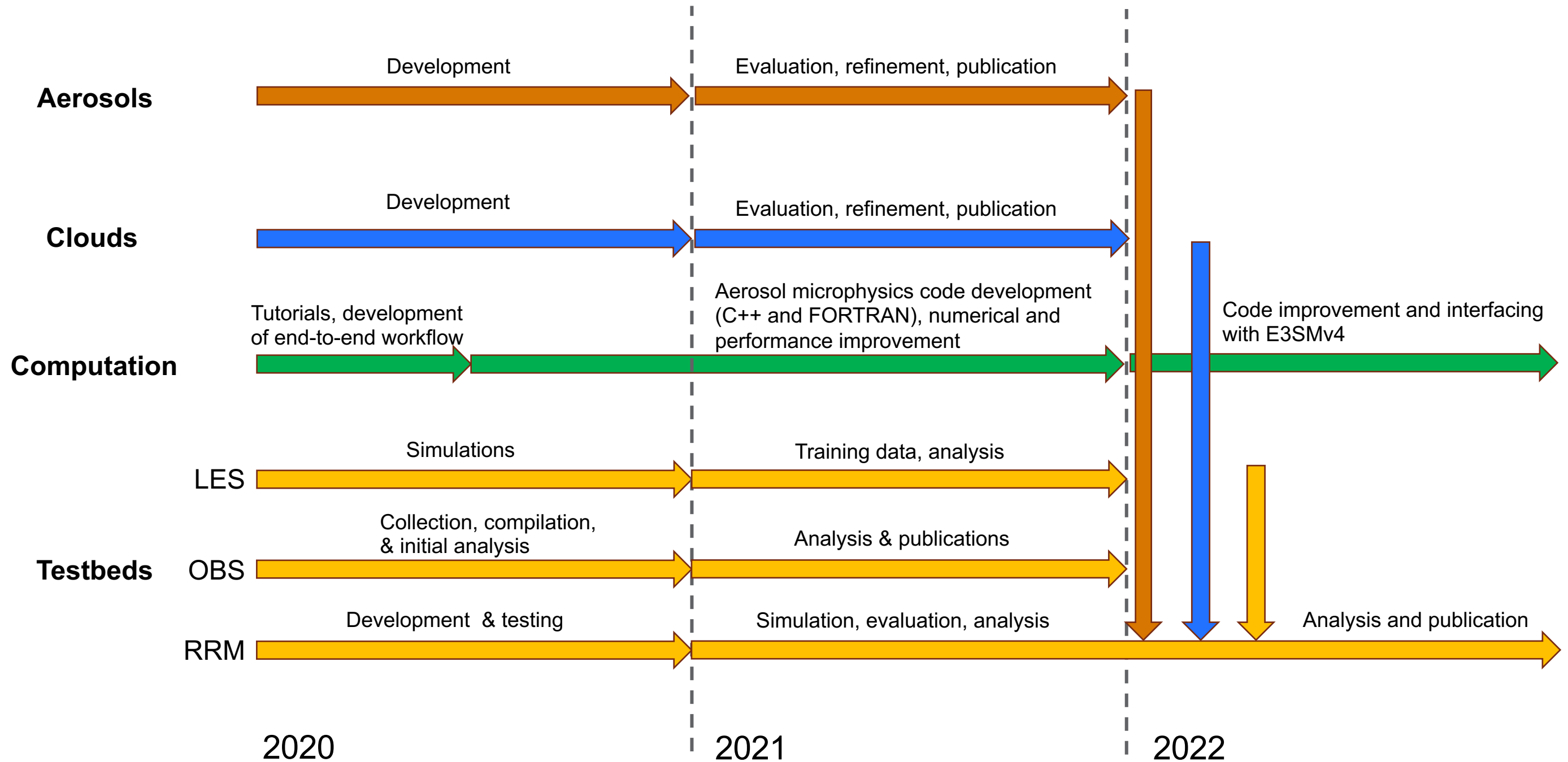
Aerosol-radiation-cloud-precipitation interactions

Modern software for exascale computation

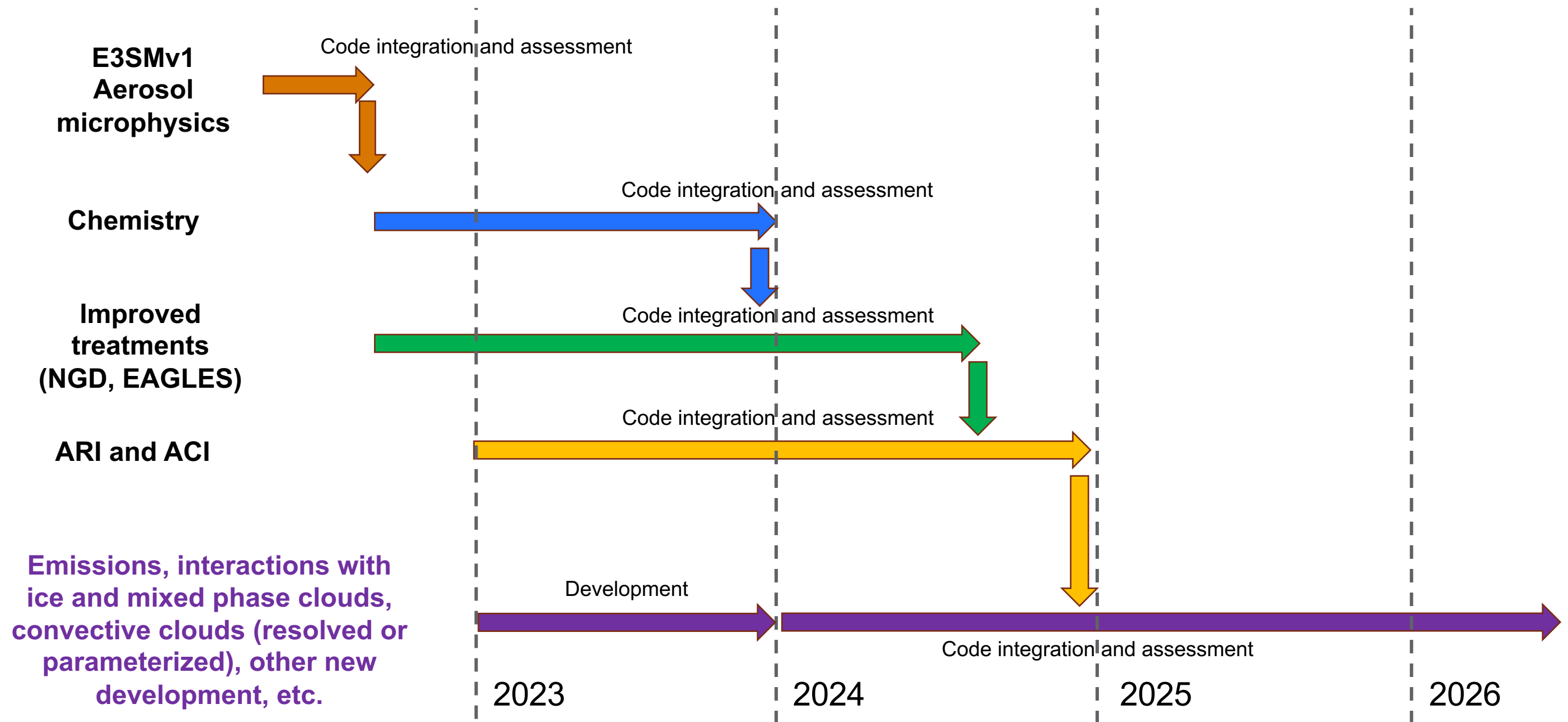


Accurate and fast simulations at various resolutions to address science challenges

Timeline of activities



Integration with E3SMv4



Adjust as needed to meet E3SMv4 timeline



Accomplishments

- **Addressing the structural deficiency by improving aerosol and ACI in E3SM**
 - **New treatments** for ultra-fine and giant aerosols, wildfire aerosols, dust, SOA, aerosol activation, rain characteristics and processes, turbulence, etc., bring aerosol and ACI parameterizations **ready for convection-permitting scales**
- **Streamlining the “machine learning (ML)-to-E3SM” workflow**
 - Use cloud parcel model, Mie code, bin microphysics, and a newly developed computationally performant LES model **PINACLES** to provide aerosol, cloud, precipitation, and meteorological data across regimes
 - Develop new physically regularized **ML-based parameterizations** for aerosol and ACI processes
 - Integrate ML emulators in **E3SM**
- **Integrating observationally based process-oriented constraints for ACI in parameterization development**
 - Develop an **automated aerosol and ACI diagnostics package** based on ARM, satellites, and other observations to evaluate E3SM aerosol and ACI
- **Modernizing software for DOE’s GPU-based computers**
 - Redesign the software infrastructure to **improve efficiency, accuracy, and trustworthiness** using modern modeling techniques, better numerics, and testing and verification tools
 - Solid progress on refactoring and transplanting MAM aerosol microphysics code to **C++/kokkos**

Impact of aerosol nucleation on cloud formation and anthropogenic aerosol forcing

Kai Zhang, Jian Sun, Bin Zhao, Guangxing Lin, Hailong Wang, Balwinder Singh, Po-Lun Ma

Objective

- Investigate the impact of new particle formation on the cloud formation and anthropogenic aerosol forcing using the newly developed E3SM-MAM5 (with nucleation mode)

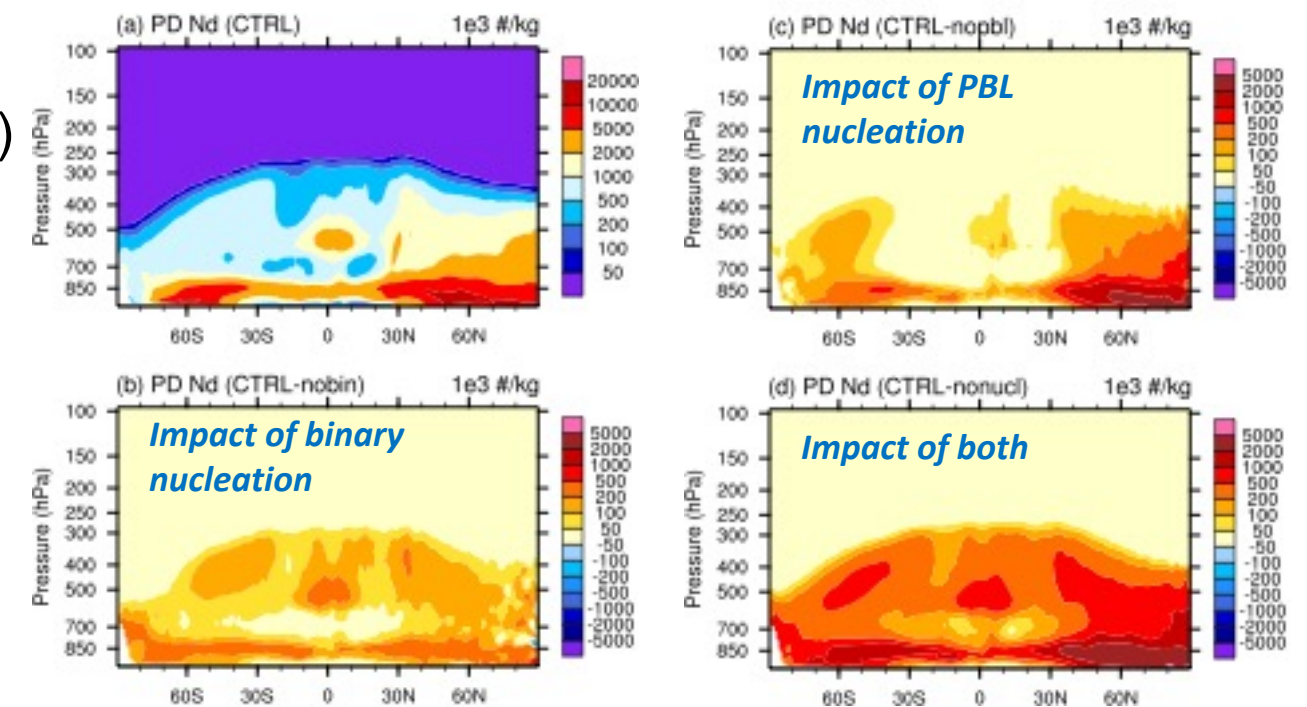
Approach

- Switch off individual nucleation mechanisms in simulations with present-day and pre-industrial emissions
- Evaluate the simulated cloud properties and anthropogenic aerosol forcing

Scientific significance

- Both PBL and binary nucleation processes have significant impacts on the cloud formation (see figure) and anthropogenic aerosol forcing.
- The impacts through different mechanisms are non-linear and both liquid and ice clouds are affected.

Changes in cloud droplet number concentration when individual nucleation mechanisms are switched off



Next Steps

- Evaluate the model at higher resolutions
- Investigate the impact of organics-mediated NPF on the anthropogenic aerosol forcing

Developing interactive fire plume-rise model for E3SM

Zheng Lu, Xiaohong Liu, Ziming Ke, Kai Zhang, Jiwen Fan, and Po-Lun Ma

Objective

- To interactively calculate fire plume injection heights based on fire properties and ambient meteorological conditions in the model.

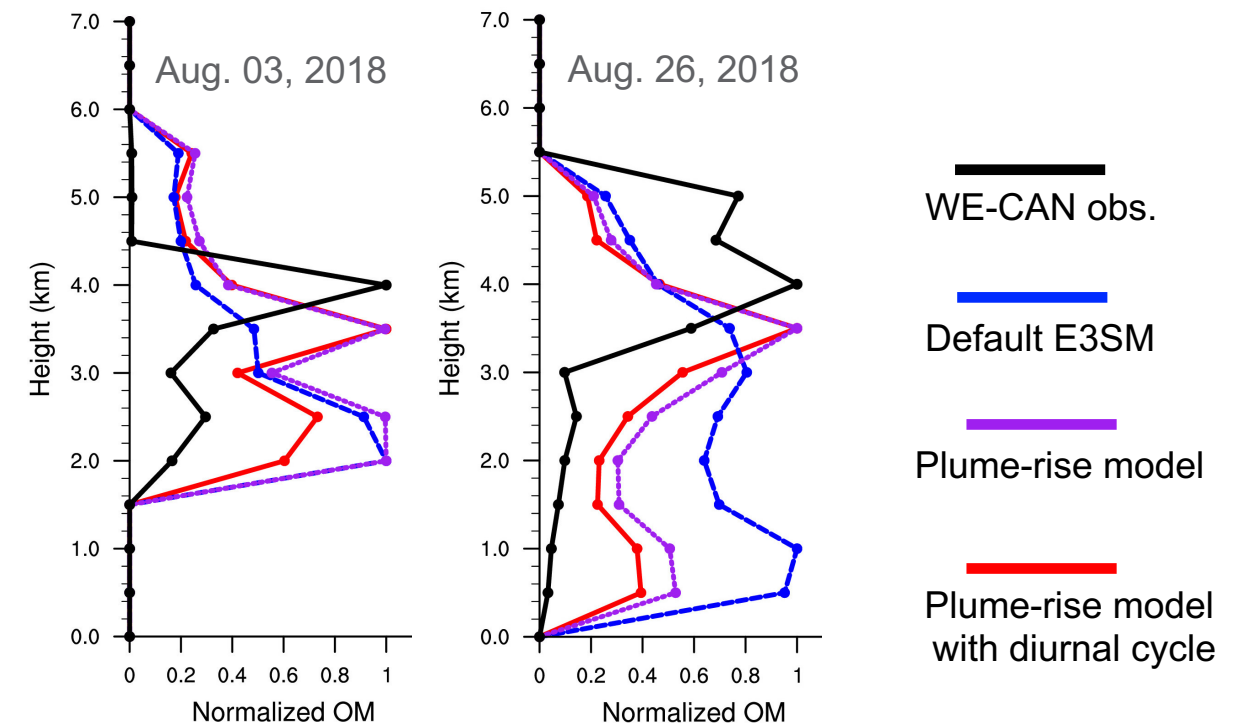
Approach

- Partition total fire emissions into four intensity categories based on fire radiative power (FRP) values.
- Incorporate a 1-D fire plume-rise model (Freitas et al. 2015) in E3SM to calculate vertical distributions for each intensity category.

New capabilities and scientific significance

- The fire plume transport is better simulated. The impacts of biomass burning aerosols on radiation budget and cloud fields can be better represented in E3SM.

Modeled OM aerosol vertical profiles against WE-CAN campaign



Next Steps:

- Finalizing the manuscript.
- Extending the simulation to other years, especially the ones with extreme wildfires.

Anthropogenic dust emission for E3SM

Yang Shi, Xiaohong Liu, Chenglai Wu, Zheng Lu

Objective

- Develop a parameterization for anthropogenic dust (AD) emissions from cropland in E3SMv1

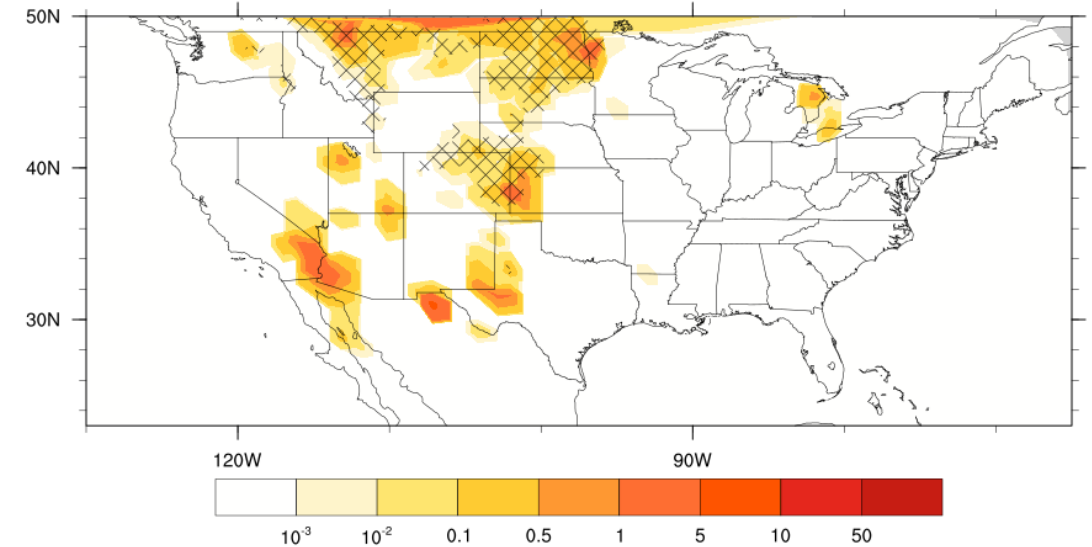
Approach

- Separate the leaf area index on crop PFT from the other PFTs; calculate the AD emission using the separated leaf area index
- Couple the AD parameterization with a dust tagging technique to explicitly track anthropogenic and natural dust emissions

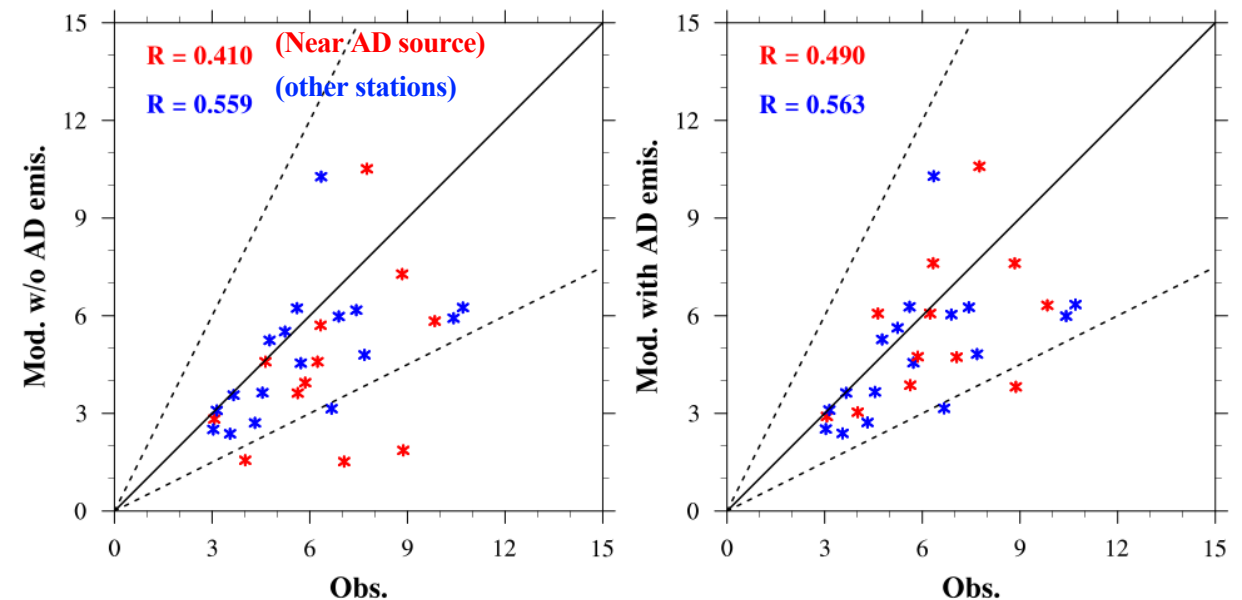
New capabilities and scientific significance

- AD sources in the US, North China, and the Sahel region are well captured by the parameterization.
- The AD emission accounts for $\sim 25\%$ of the global dust emission.

Dust emission in the US (hatch for AD sources)



Comparison of coarse aerosol mass with (left) and w/o AD (right) with IMPROVE data



Next Steps:

- Finish writing and submit the manuscript

Improve the emission data treatment in E3SM

Taufiq Hassan, Kai Zhang, Balwinder Singh, Hailong Wang and Po-Lun Ma

Objective

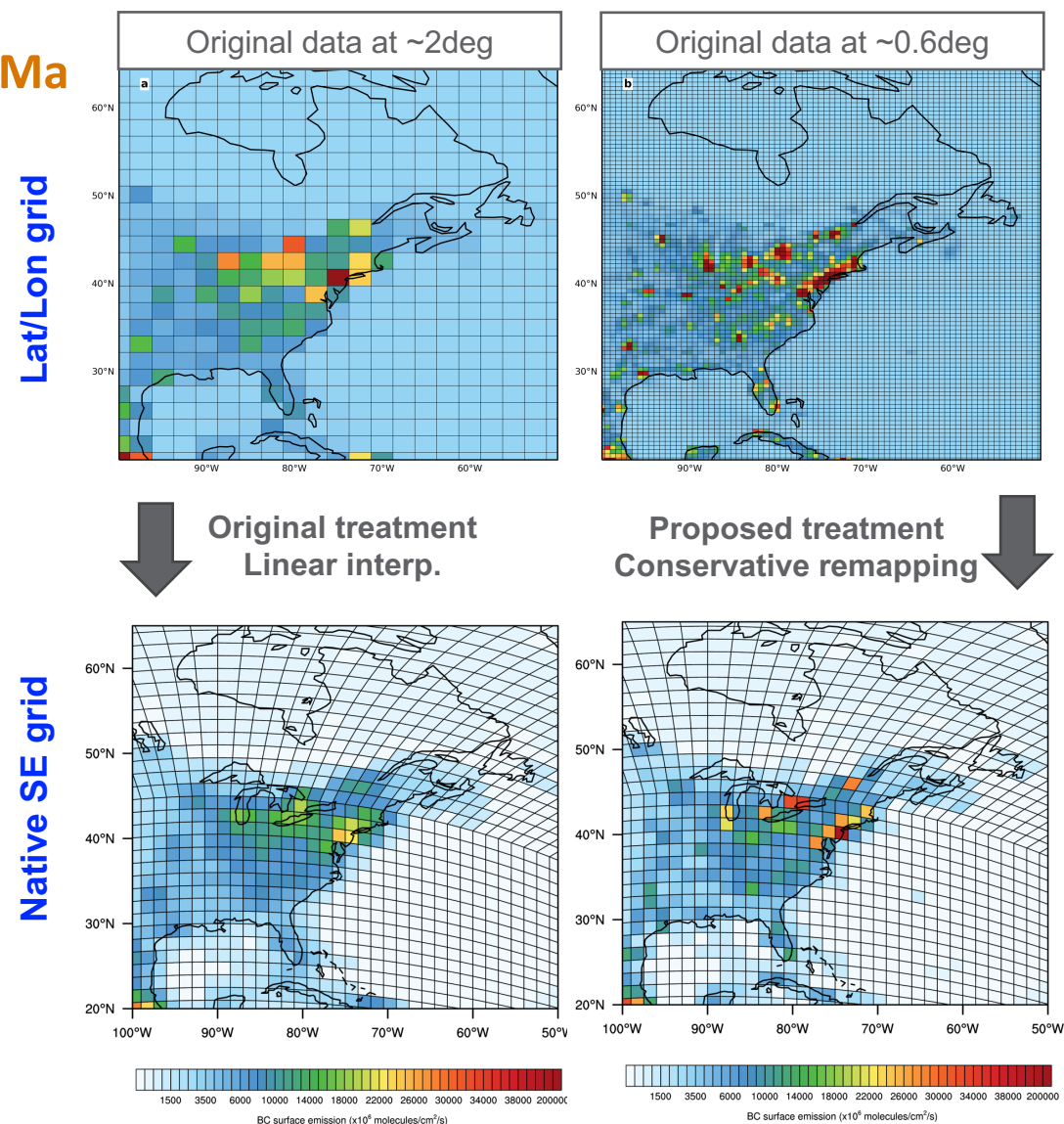
- Improvement of the emission data treatment to reduce the large errors at locations with sharp gradient

Approach

- Conservatively remap high-resolution emission data from rectangular lat-lon grid to E3SM native grid (SE)
- Python wrapper (based on NCO/TempestRemap) developed to automate the grid generation and remapping process for any resolution

Impact

- Avoid large biases caused by linear interpolation from data on coarse grid (2deg in the default model).
- Improve the simulated aerosol concentrations near source regions and better evaluate the model against in-situ measurements (especially for RRM).



Ongoing work

- Directly read the emission data on SE grid
- Conduct E3SMv2 simulations to access the new emission data treatment

A better approximation of updraft speed for aerosol activation

Vincent Larson, Jan Gruenenwald, Brian Griffin

Objective

- To improve the accuracy of the updraft speed that is used in E3SM to drive aerosol activation.

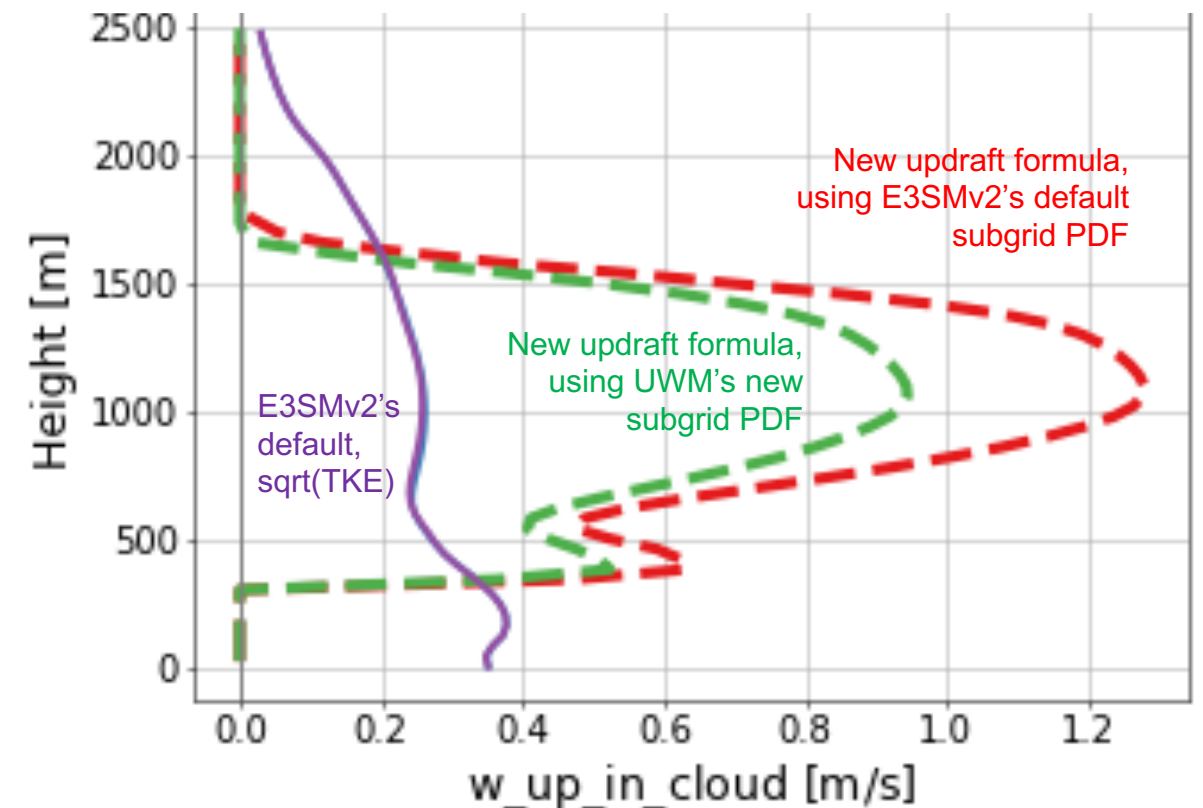
Approach

- We integrate the within-cloud updraft speed over CLUBB's subgrid PDF. This yields a single representative updraft with little computational cost.

Scientific significance

- E3SMv2 underestimates updraft speed in shallow cumuli. This will lead to an underestimate of droplet number and an erroneous aerosol indirect effect. By accounting for the skewed nature of cumulus updrafts, a more accurate (larger) updraft speed is obtained in cumuli, with no degradation in stratocumuli.

Updraft speed, calculated using 3 approximations, for the BOMEX shallow cumulus case:



E3SM's default formula underestimates the updraft speed used to force aerosol activation. New formulas, plotted in red and green, show improvements.

Next Step:

- Test the impact of the revised formulation in a global EAM simulation.

Improving autoconversion parameterization in E3SM

Mikhail Ovchinnikov, Colleen Kaul, Kyle Pressel, Jiwen Fan, Jacob Shpund, Christopher Jones

Objective

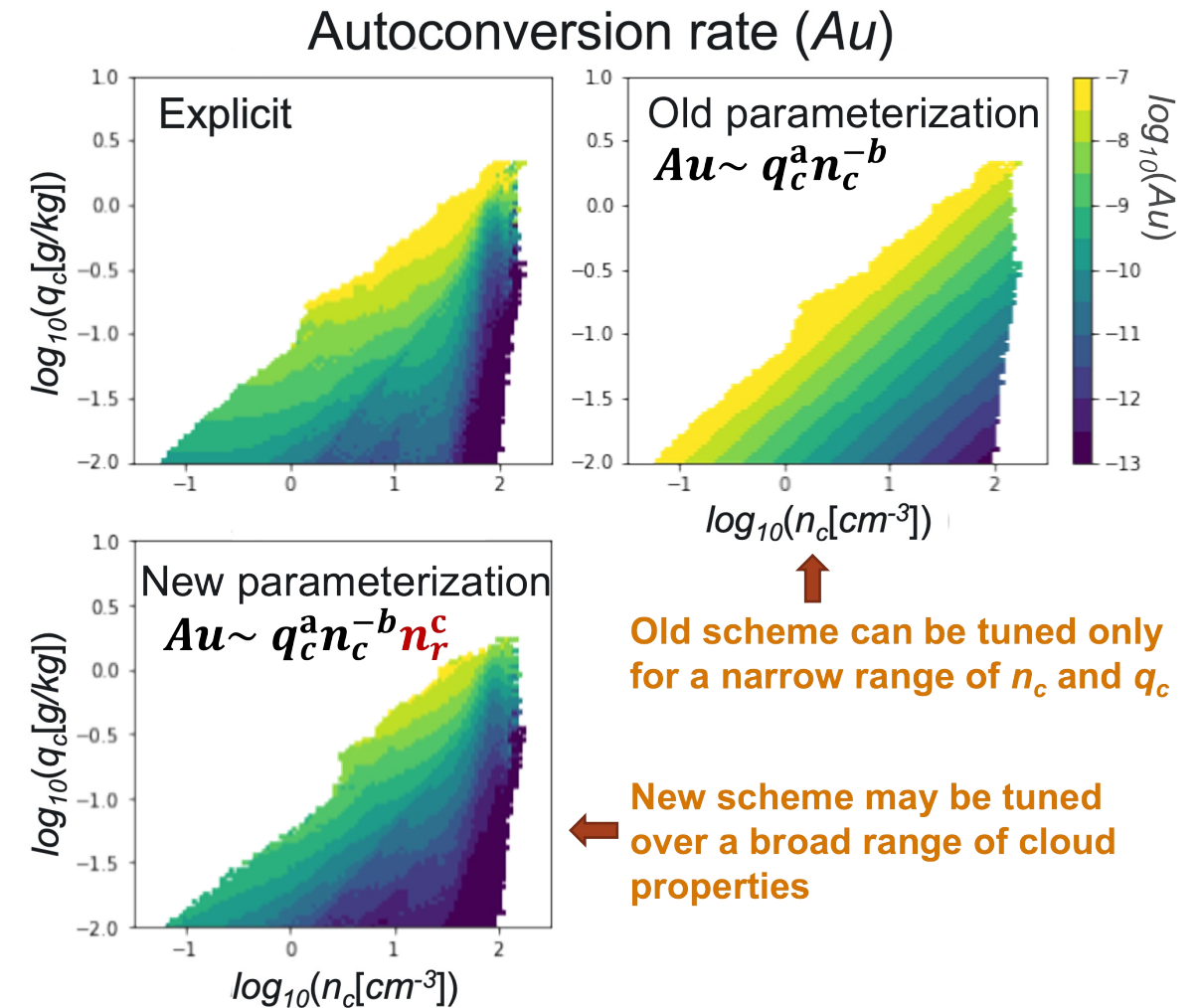
- Improve representation of warm-rain initiation in E3SM

Approach

- Compile and analyze testbed cases of shallow precipitating clouds
- Compute explicit autoconversion rate (Au) from observed and LES-modeled droplet size spectra
- Characterize biases and improve parameterizations of local Au

New capabilities and scientific significance

- Quantified performance of Au parameterizations under diverse cloud and environment conditions
- Adding rain number concentration may drastically improve Au in a wide range of cloud properties



Next Steps:

- Evaluate Au errors for the $q_c - n_c$ parameter space in E3SM
- Quantify the effects of resolution on grid-mean autoconversion rates



Employ AI/ML to integrate data and models to improve aerosols and ACI in E3SM

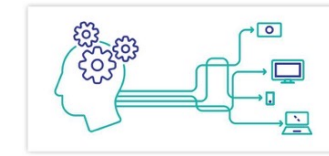
Data hungry, knowledge hungry, or both?



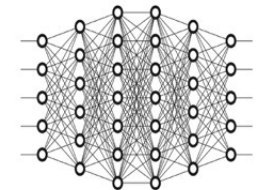
ARM



Measurements of aerosols, clouds, precipitation, and meteorology



AI-assisted analytics to improve the design of parameterizations



Data-driven & physically informed ML emulator

Combine expertise in climate science, data science, software engineering



Big training data: O(100TB)



Software infrastructure incorporating AI/ML in Earth system models



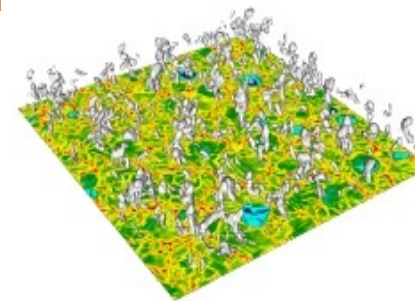
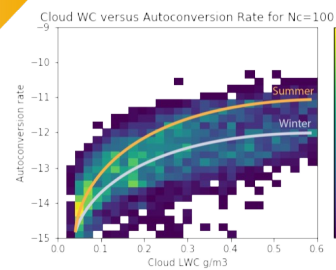
THE UNIVERSITY OF ARIZONA



UNIVERSITY OF WASHINGTON



UNIVERSITY OF WISCONSIN MILWAUKEE



World's largest detailed process model and LES ensemble provides information on aerosols, clouds, precipitation, and meteorology



Next steps:

- More **physically informed ML emulator** for aerosols and aerosol-cloud processes based on **big data**
- **Quantify the uncertainty** associated with the ML approach
- Use **explainable artificial intelligence** (XAI) to improve understanding and trustworthiness of the emulators



unfunded

Integrating Machine Learning Emulators in E3SM

Balwinder Singh, Po-Lun Ma, Mike Prtichard, Sam Silva, Sungduk Yu

Objective

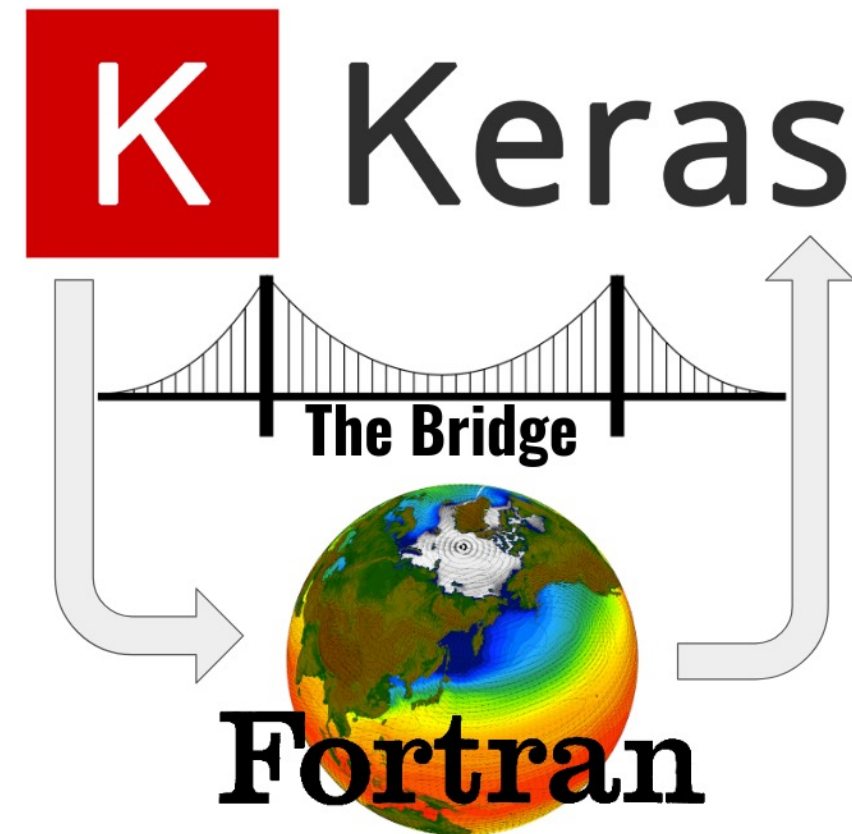
- To develop an end-to-end workflow for integrating machine learning (ML) emulators in E3SM

Approach

- Compile Fortran-Keras-Bridge (FKB) library and link it to E3SM
- Write an interface to invoke ML emulator within free running E3SM simulations

New capabilities and scientific significance

- An end-to-end workflow to invoke ML emulators within E3SM
- Physical parameterizations can be replaced or augmented by data driven ML emulators in E3SM
- E3SM can run successfully multi-year simulations with embedded ML emulators.



Next Steps:

- Investigate into HPC aware methods to invoke ML emulators within E3SMv4 (hybrid Fortran-C++)

Improving aerosol's cloud albedo effect: Emulating aerosol activation using deep neural network

Silva, Ma, Singh, et al

Challenge

- Traditional parameterization neglects kinetic limitations
- Explicit parcel model calculations way too expensive to employ in Earth system models

Objective

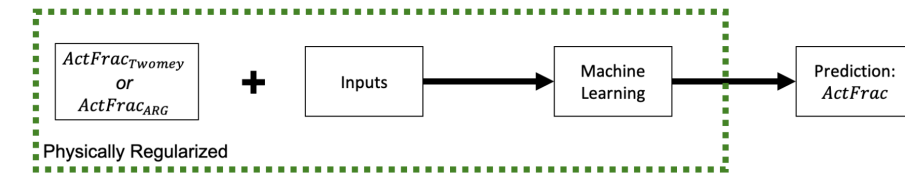
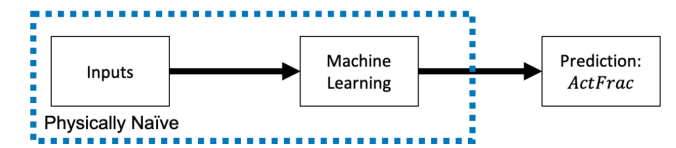
- Improve aerosol activation in E3SM by correcting the E3SM bias introduced by the original parameterization without adding computational cost

Approach

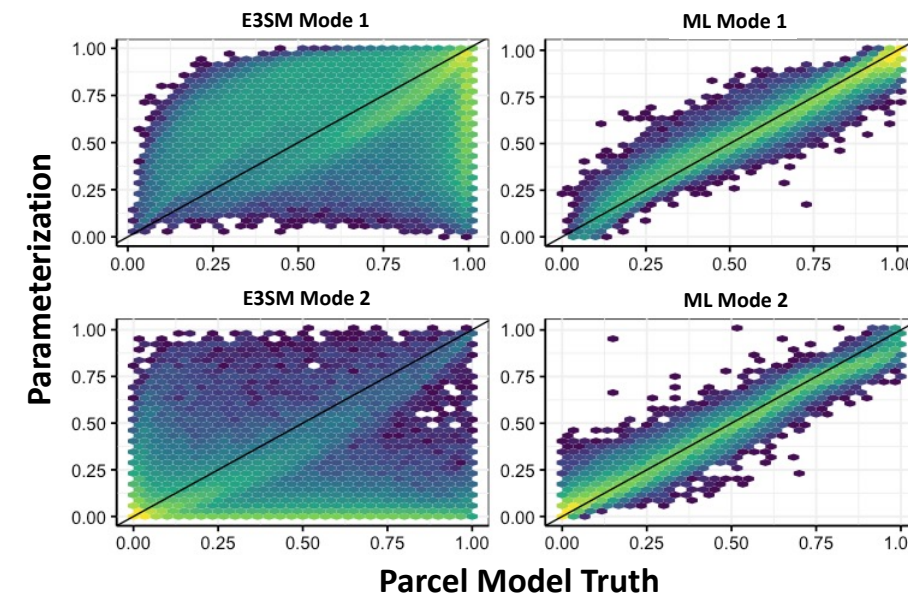
- Build ML emulators based on explicit cloud parcel model results
- Train on big data (1M samples out of 100M)

Results

- Significant improvement on aerosol activation
- Computational cost is negligible
- Stable and more accurate global simulations
- Aerosol-induced radiative effects reduced in both SW and LW



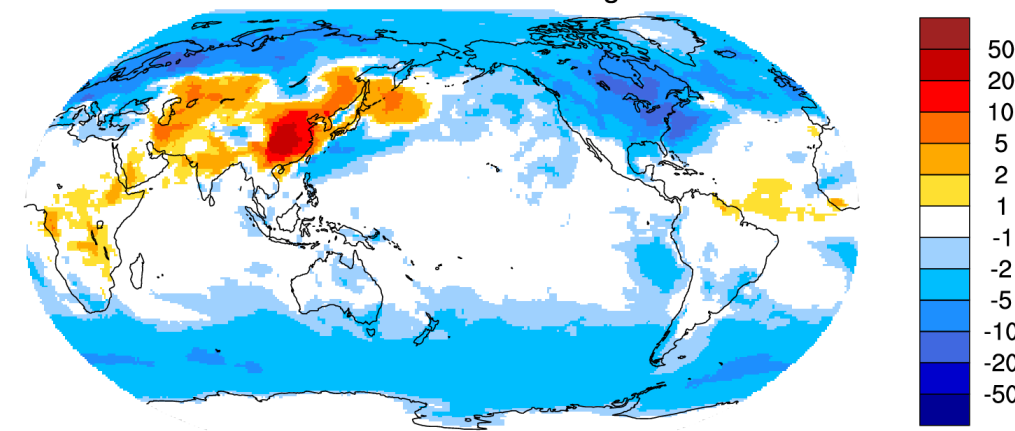
Silva et al (2020), *Geosci Model Dev*



- *New DNN-based aerosol activation significantly improves the accuracy*

Column integrated CDNC

DNN – E3SM difference avg= $-1.26 \times 10^9 \text{ m}^{-2}$



- *Compared to the default E3SM, DNN produces significantly less droplets in most mid- and high latitude regions (reducing the known bias in E3SM)*
- *We are investigating the increased CDNC in Asia.*

Optimizing aerosol activation emulator for E3SM using parallelized industrial scale hyperparameter tuning

Sungduk Yu, Mike Pritchard, Po-Lun Ma, Balwinder Singh

Objective

- To further reduce the errors of aerosol activation calculations by optimizing the hyperparameters of emulators

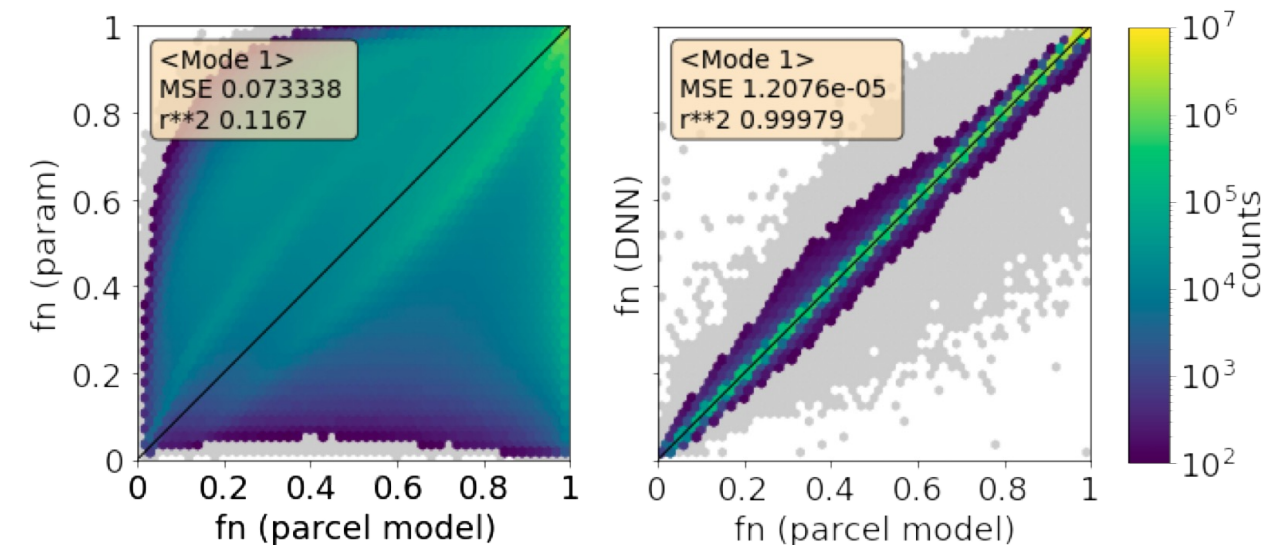
Approach

- Developed a workflow to utilize multiple GPU nodes in a hyperparameter optimization framework
- Optimized hyperparameter for aerosol activation emulators by **searching the best configuration** in parallel (40,000 trials)

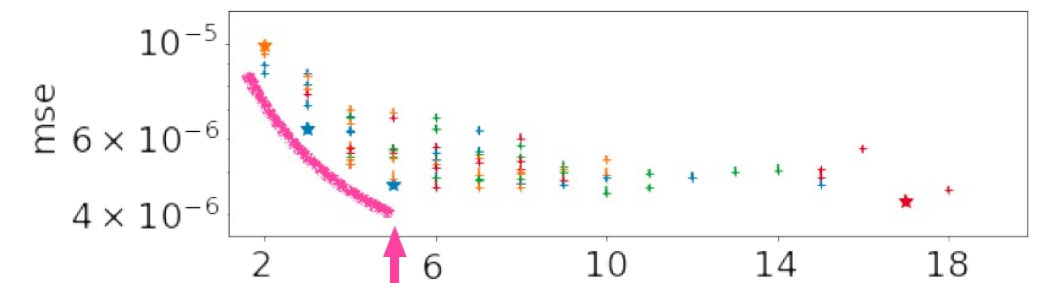
New capabilities and scientific significance

- Further improved the performance of aerosol activation emulator by **two orders of magnitude**, further decreasing errors of the original parameterization in E3SM
- Assessed data volume sensitivities and identified threshold of maximally useful ML training data volume (~1M samples)
- Identified depth-skill relationship and discovered threshold # of layers required for optimal skill (5 layers)

Activated Aerosol Fraction



of Layers vs. Emulator Errors



Next Steps:

- Testing the performance within E3SM to assess the impact to aerosol-cloud interaction
- Applying this technique for building other emulators in E3SM to reduce model errors

Aerosol optics with random neural networks

Andrew Geiss and Po-Lun Ma

Objective:

- Improve the E3SM aerosol optics parameterization using machine learning

Approach:

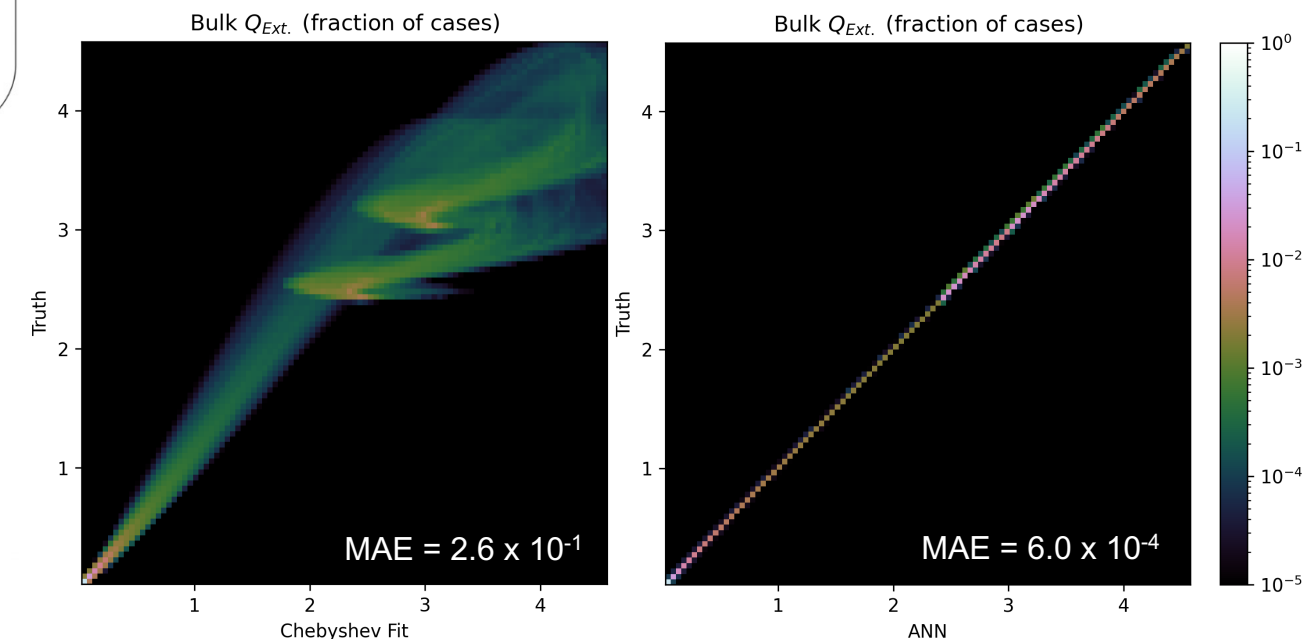
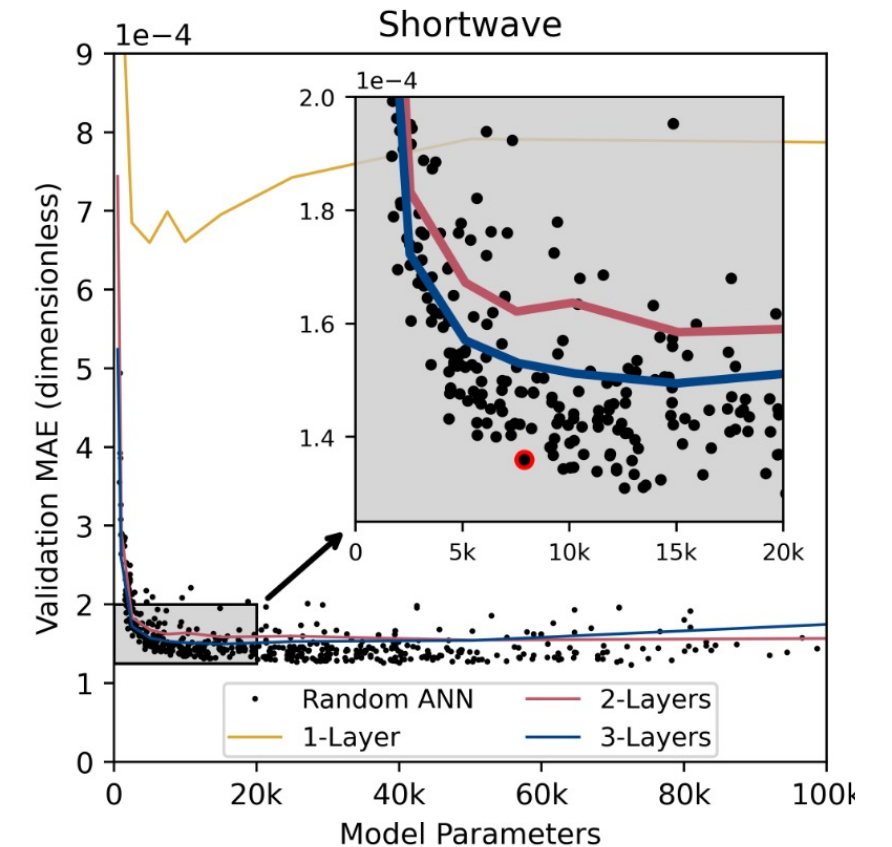
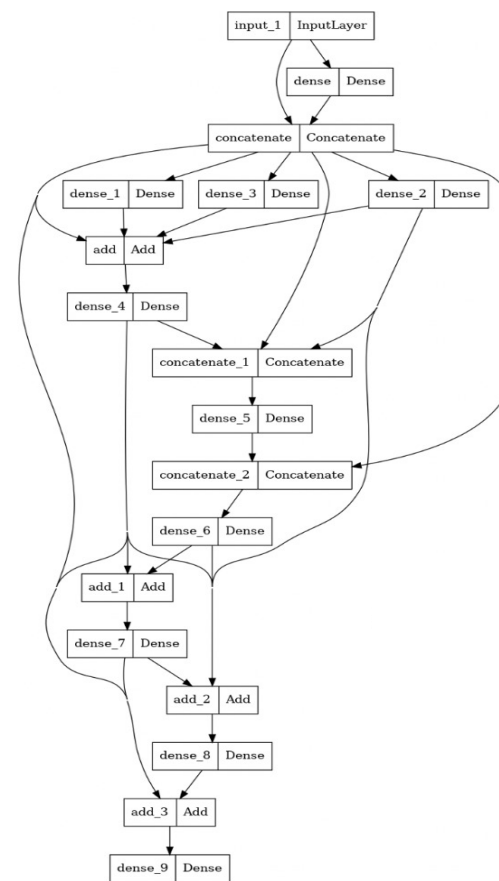
- Replace the Chebyshev interpolation/lookup-table based aerosol optics parameterization with a neural network
- Use **random wiring** to find a network architecture that is small and accurate

Significance:

- Large improvement in accuracy of aerosol optical properties
- Random wiring found architectures much better than a feed-forward perceptron type networks

Future Work:

- Integrate in E3SM
- More sophisticated **shell-core optics**



Improving aerosol's cloud lifetime effects: Emulating warm rain initiation using deep neural network

Ma, Shpund, Jones, Varble, Kaul, Pressel, Pritchard, Yu, Rader, Silva, Fan, Singh, et al.

Challenge

- Traditional parameterization built on single cloud regime, not suitable for global models
- Limited predictability due to limited data and understanding

Objective

- Develop a representation of warm rain initiation to address ACI and drizzling issues in ESMs

Approach

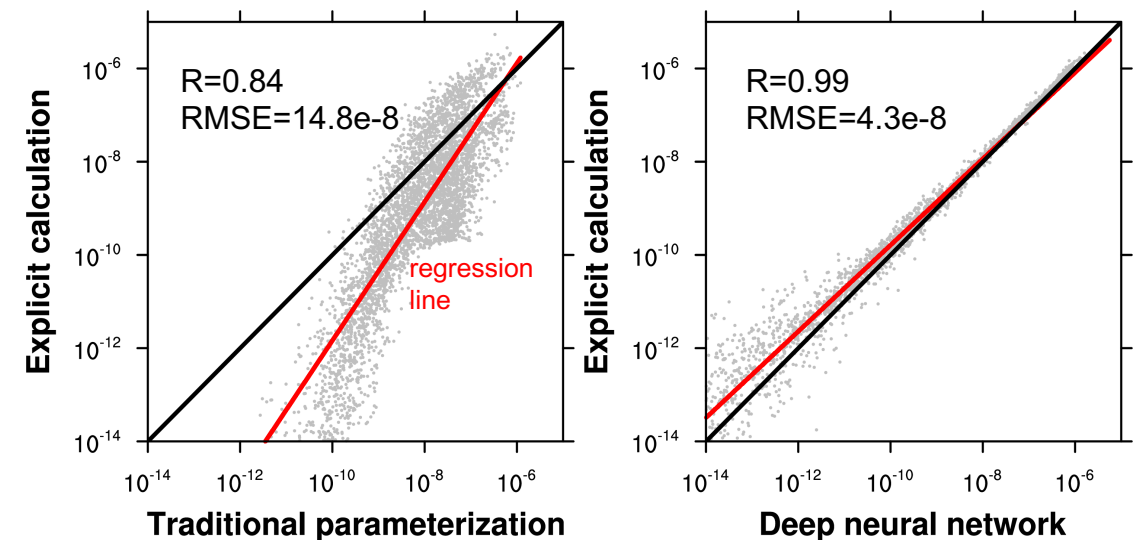
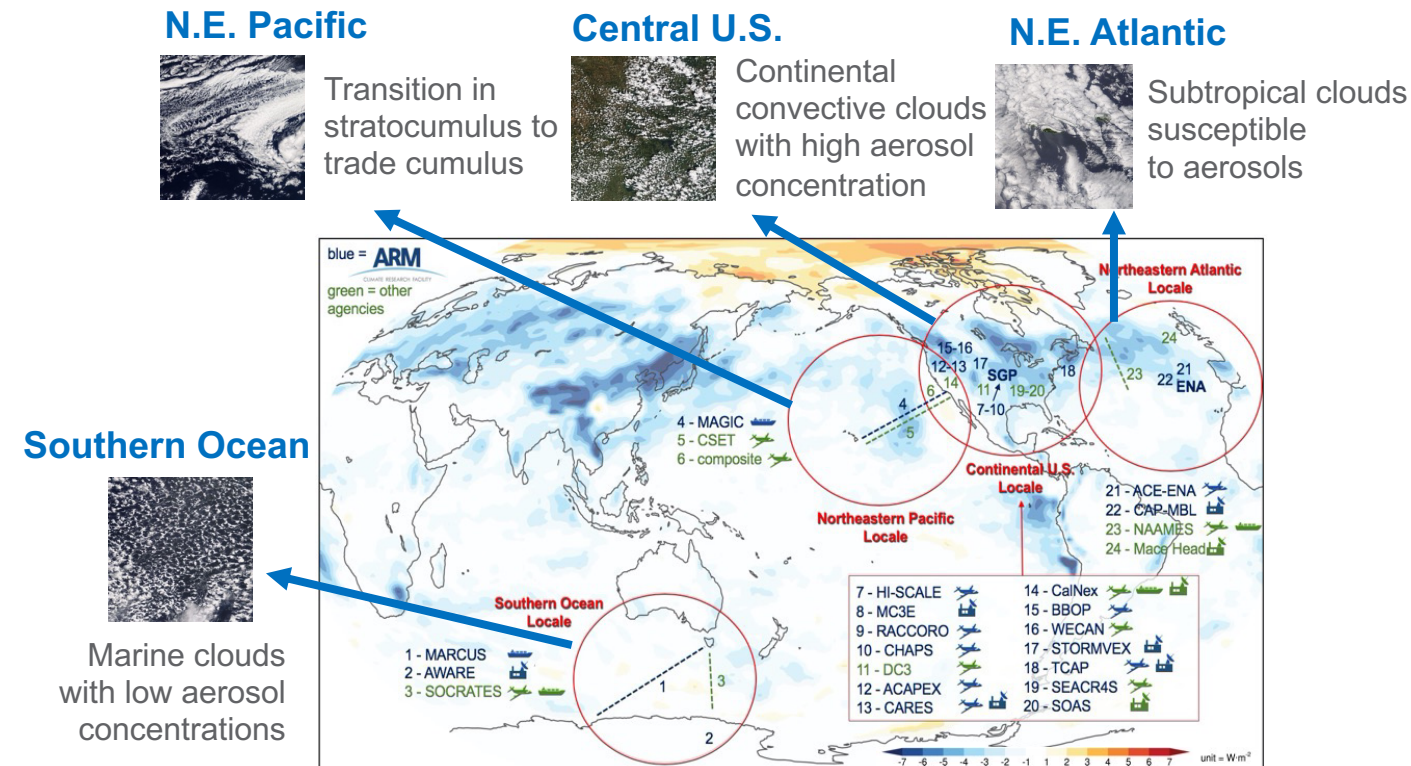
- Build ML emulators based on explicit collision-coalescence calculations and environmental conditions from ARM and LES, covering a wide range of aerosol, cloud, meteorological conditions

Results

- Significant improvement using DNN

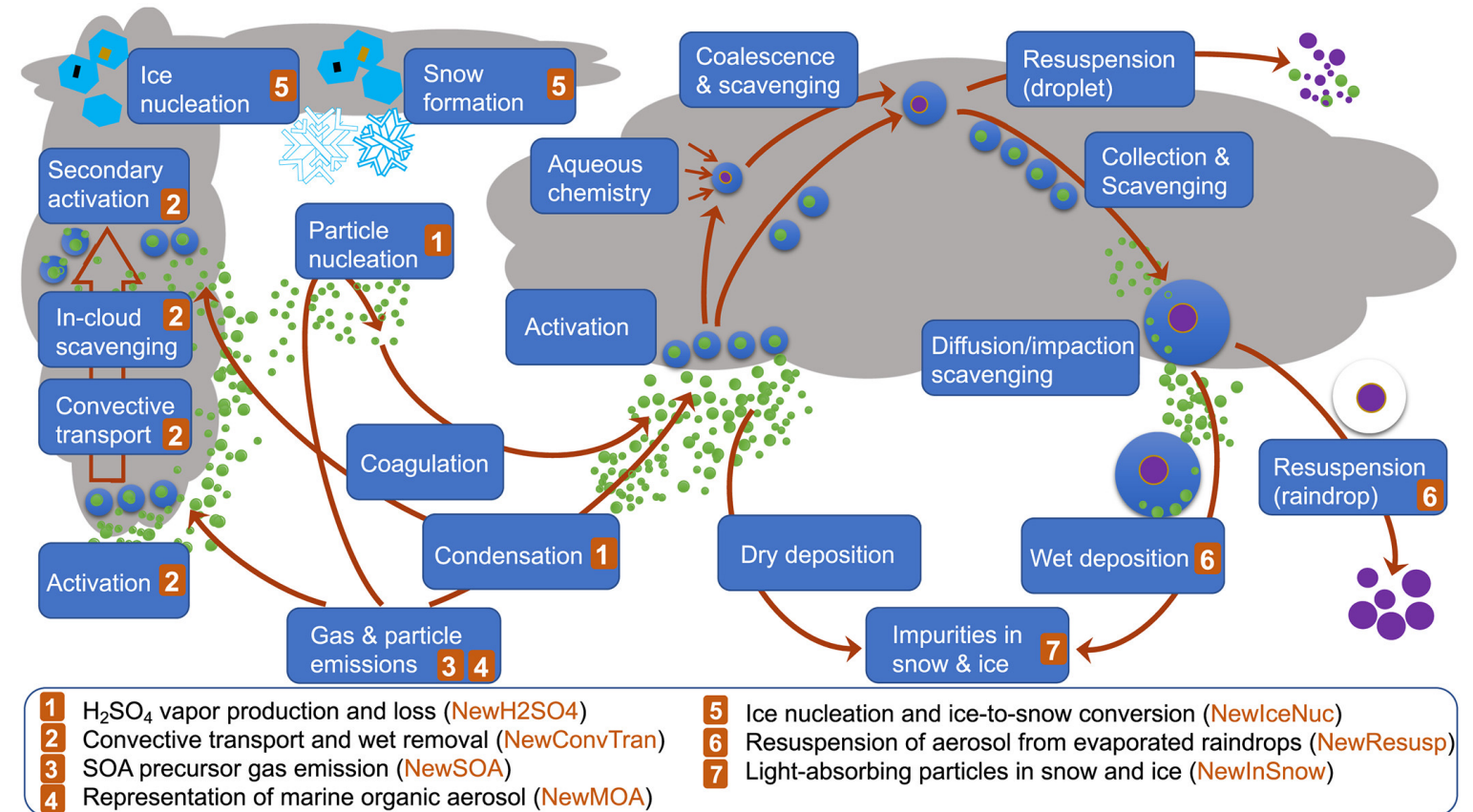
Next Steps

- Co-design the DNN to include physical considerations (multi-scale physics, evolution of DSD, and environmental factors)



Bringing MAM ready for E3SMv4

- Unlike P3 and SHOC, MAM is invoked in several places by EAM
- MAM includes numerous distinct parameterizations, reflecting the complexity of aerosol-climate interactions
- There are many ways to couple these parameterizations that produce different results



Wang et al (2020), JAMES

Reorganizing MAM aerosol microphysics and porting it to C++

Pete Bosler, Jeffrey Johnson, Asher Mancinelli, James Overfelt, Balwinder Singh, Hui Wan, Qiyang Yan

Objectives

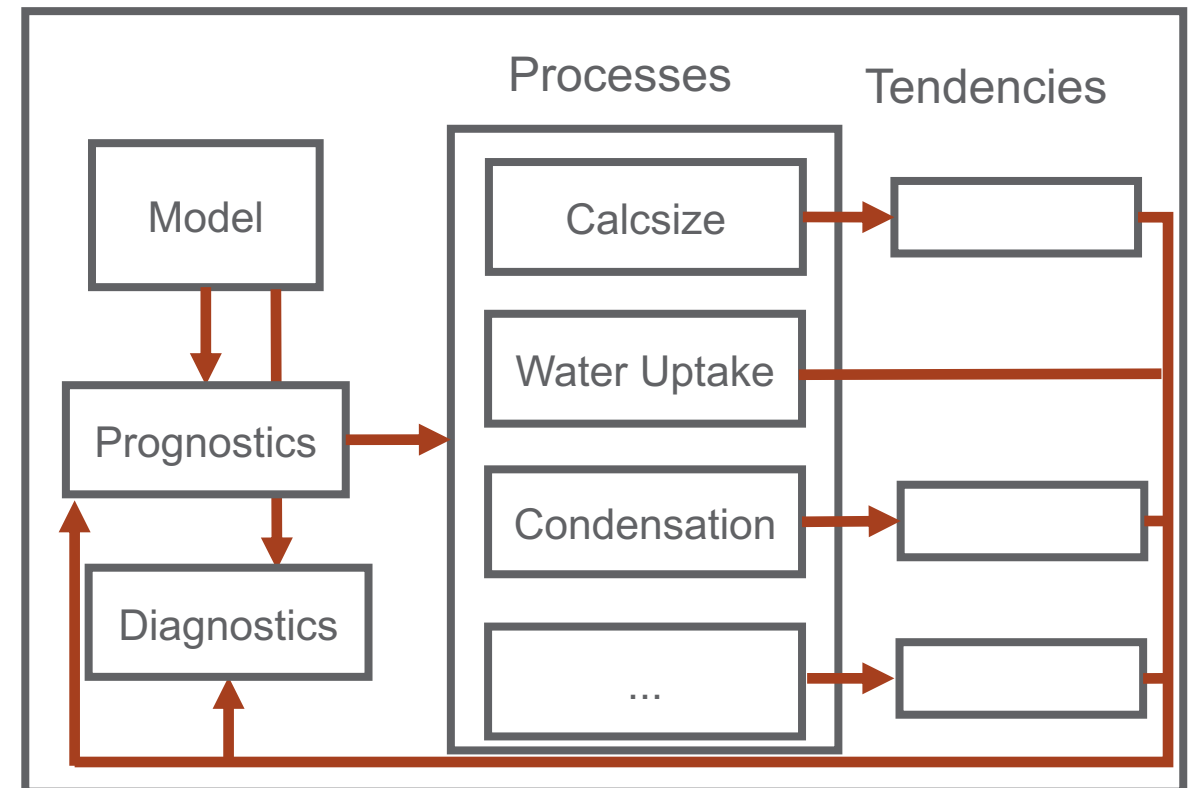
- To address gaps in understanding MAM and mitigate maintenance costs
- To develop a GPU-capable version of MAM for E3SMv4

Approach

- Restructure and simplify the MAM aerosol microphysics
- Implement these parameterizations in a new software infrastructure

New capabilities and scientific significance

- Improved the usability of the box model and the clarity of its approximations/algorithms
- Refactored and ported the MAM aerosol microphysics code



A verification workflow for porting E3SM parameterizations

Balwinder Singh, Asher Mancinelli, Jeffrey Johnson, Pete Bosler

Objective

- To develop a workflow for porting most recent version of MAM4 processes directly from E3SM

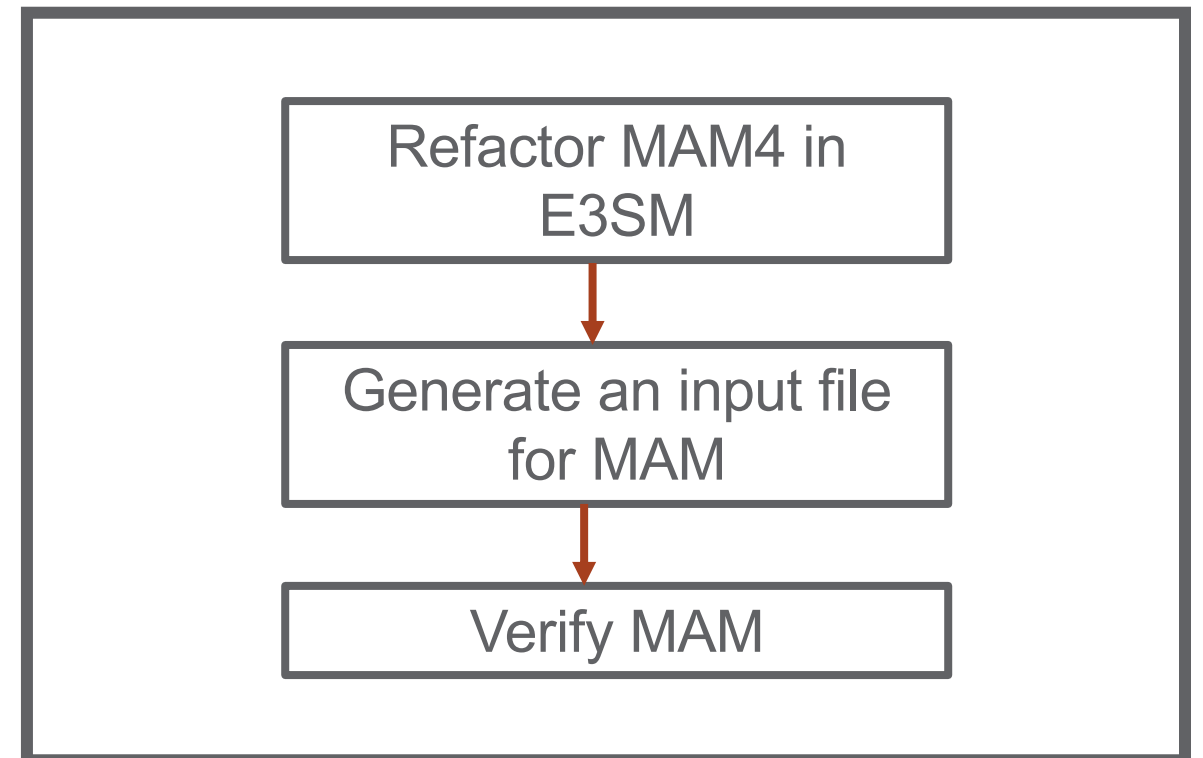
Approach

- Refactor MAM4 processes within E3SM using ultra coarse resolution (ne4)
- For verification, write a grid point data to a file and drive MAM code using this data as input

New capabilities and scientific significance

- This workflow tests the refactored process with a huge number of input and boundary conditions to increase code coverage
- All the latest bug fixes are included with the process
- Verification task is streamlined

Verification Workflow:



Next Steps:

- Automate the workflow and add plotting capabilities using python scripts

Creating cross-validation workflows for aerosol parameterizations

Qiyang Yan, James Overfelt, Jeffrey Johnson, Hui Wan

Objective

- To compare new and existing implementations of MAM parameterizations *qualitatively* and *quantitatively*

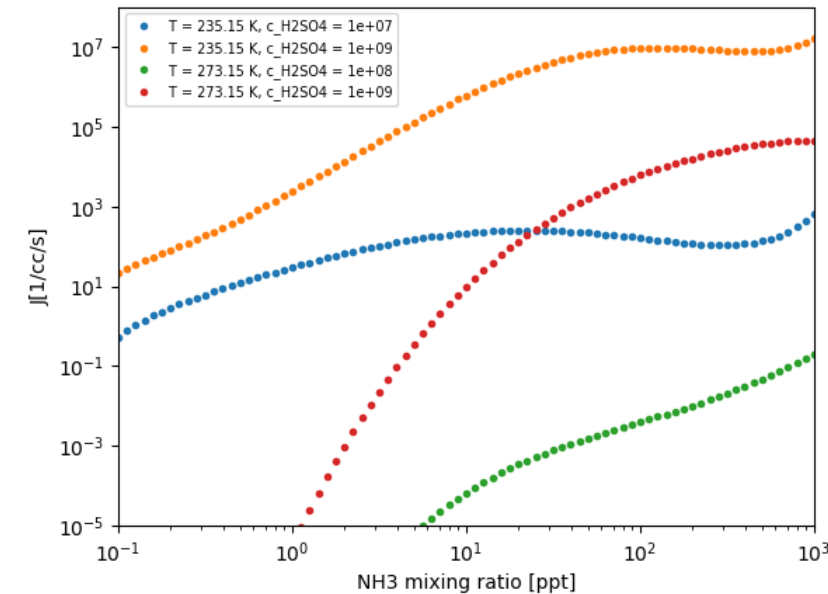
Approach

- Develop a tool that generates **ensembles** for testing parameterizations and produces structured output for “apples-to-apples” comparisons
- Build workflows to test individual and integrated components of parameterizations within MAM

New capabilities and scientific significance

- Developed and documented [Skywalker](#), a simple library for constructing ensembles and running them on parameterizations written in C++ and Fortran
- Created a cross-validation workflow that uses Skywalker to validate parameterizations developed for MAM

Nucleation Rate



Skywalker writes Python data for easy plotting and numerical comparisons

```
Norms for difference of output.uptkaer[0]:
  Absolute: L1: 0.00033819 L2: 7.52132e-05 Linf: 2.9124e-05
  Relative: L1: 0.038085 L2: 0.0560729 Linf: 0.127181
Norms for difference of output.uptkaer[1]:
  Absolute: L1: 7.82253e-05 L2: 1.7126e-05 Linf: 6.7271e-06
  Relative: L1: 0.0192867 L2: 0.0279906 Linf: 0.0678261
```

Next Steps:

- Publicize and support Skywalker as a community tool
- Continue using and developing validation workflows to compare and understand parameterizations

MAM simplification for computational performance improvement

Jianfeng Li, Kai Zhang, Qiyang Yan, and Balwinder Singh

Objective

- Improve the computational performance of MAM4 by simplifying some aerosol processes

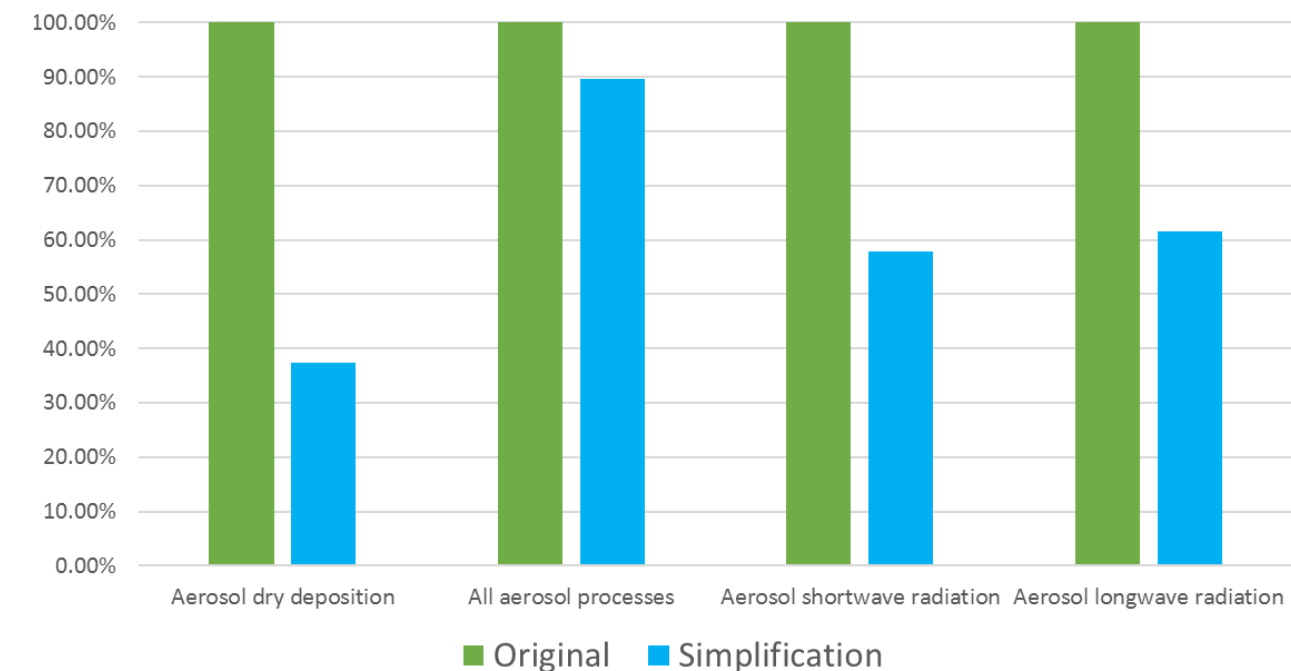
Approach

- Remove the sedimentation calculation for small particles (Aitken, primary carbon, and accumulation modes) above the surface model layer
- Remove the calculation of aerosol optical properties for Aitken and primary carbon modes

Results

- Time for aerosol dry deposition calculation module reduced by 63%
- Time for aerosol optical property calculation reduced by ~40%
- Generally, < 2% change in global mean aerosol burden due to the MAM simplification
- < 2% change in total aerosol AOD and has negligible impacts on aerosol radiative forcing (shortwave and longwave)

Computational Cost



Next Steps:

- Merge the modification to the EAGLES maint-1.0 branch and then EAGLES master (E3SMv2)
- Further E3SM simulations to evaluate the computational performance enhancement by MAM simplification and examine its impact on the aerosol budget and radiation balance

Developing an Earth System Model Aerosol-Cloud Diagnostics (ESMAC Diags) Package to Evaluate Aerosols, Clouds and Aerosol-Cloud Interactions in E3SM

Shuaiqi Tang, Jerome D. Fast, Kai Zhang, Joseph C. Hardin, Adam C. Varble, John E. Shilling, Fan Mei, Maria A. Zawadowicz and Po-Lun Ma

Objective

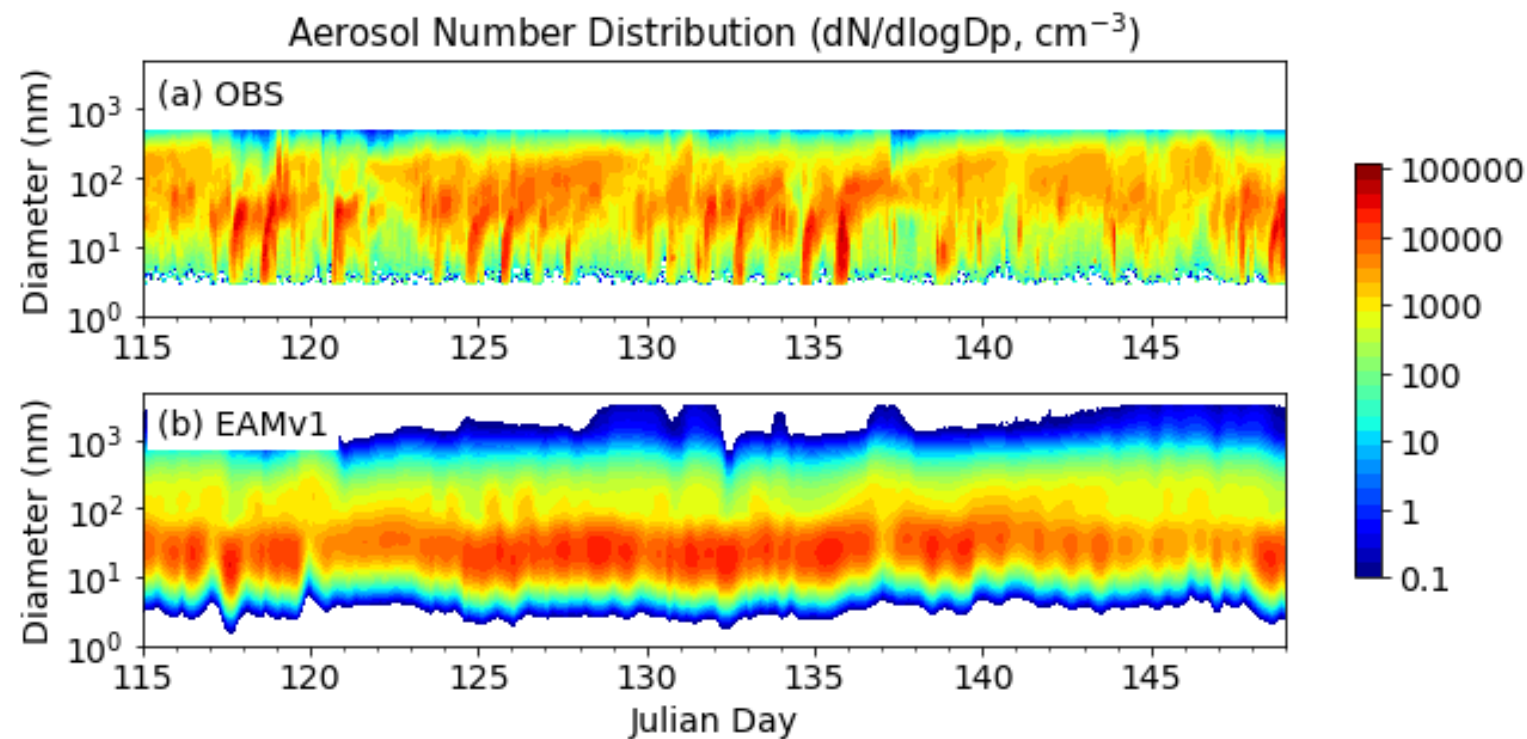
- To evaluate model performances, provide insights into model deficiencies to guide future model development.

Approach

- Develop a Python-based diagnostics package to facilitate the routine evaluation of aerosols, clouds and aerosol-cloud interactions in E3SM.

New capabilities and scientific significance

- The diagnostics cover 6 field campaigns in 4 geographical regions: Eastern North Atlantic (ENA), Central U.S. (CUS), Northeastern Pacific (NEP) and Southern Ocean (SO).
- ESMAC Diags v1 is released focusing on aerosol evaluation with aircraft, ship, and surface measurements, mostly in-situ.



Next Steps:

- ESMAC Diags v2 is being developed to include long-term ARM and satellite measurements, with more diagnostics and metrics for clouds and aerosol-cloud interactions.

Statistical Evaluation of ACI Processes in E3SM

Adam Varble, Po-Lun Ma, Matt Christensen, Johannes Mülmenstädt, Shuaiqi Tang, Jerome Fast

Objective

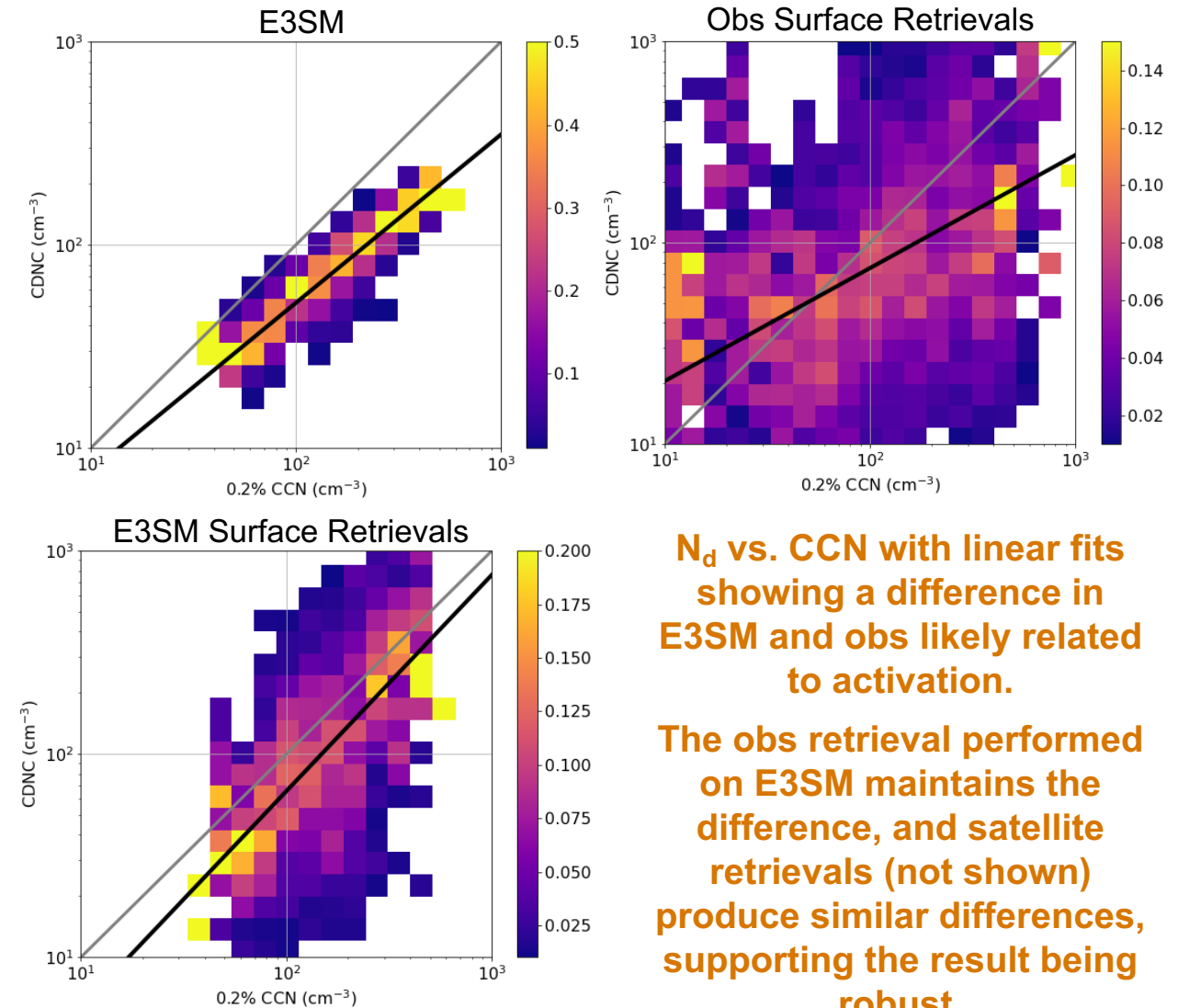
- Compare ACI relationships modulating cloud radiative effects in obs and E3SM to guide E3SM development

Approach

- Coupled surface, satellite, and aircraft retrievals over 4 distinctive regions starting with ENA

New capabilities and scientific significance

- Cloud retrievals (both in obs and E3SM) vary greatly by method, highlighting the need for our multi-perspective approach for robust comparisons
- E3SM cloud albedo susceptibility is too negative due to overly strong LWP adjustment
- $dA/d\ln N_d$ (too weak) and $d\ln N_d/d\ln \text{CCN}$ (too strong) offset to yield a reasonable Twomey effect
- Albedo difference partly due to higher N_d (activation), weaker inversions (SST and/or subsidence?), and smaller R_{eff} for a given N_d (assumed DSD)



N_d vs. CCN with linear fits showing a difference in E3SM and obs likely related to activation.

The obs retrieval performed on E3SM maintains the difference, and satellite retrievals (not shown) produce similar differences, supporting the result being robust.

Next Steps:

- Expand and implement into the open-source ESMAC-Diags package.



There are many more great work to show, but I know I am running out of time for the webinar today...

- Yu Yao: Giant CCN
- Laura Fierce: PartMC-MAM comparison
- Matt Christensen: Lagrangian analysis
- Yunpeng Shan and Jiwen Fan: 3-moment P3
- Mike Schmidt: Chemical solver
- Guangxing Lin: Cloud-borne aerosols
- Bin Zhao: SOA
- Johannes Muelmenstaedt: Cloud-top entrainment
- Xiquan Dong: ENA data analysis and model evaluation
- Roj Marchand: Southern ocean data analysis and model evaluation
- Colleen Kaul and Kyle Pressel: LES data generation
- Charlotte Beall: Evaluation using simulators
- Hui Wan: Detailed documentation of MAM, testing and verification



Summary

- We are committed to deliver better (scientifically robust) and faster (computationally efficient/affordable) aerosol/ACI parameterizations fully connected within EAMxx.
- We have made significant progress on developing improved treatments for aerosols and ACI as well as new diagnostics/evaluation toolkit.
- We have made significant progress on refactoring and converting the MAM aerosol microphysics code to work with EAMxx.
- Next steps
 - Develop improved treatments for other aerosol/ACI processes
 - Develop interface routines to fully connect aerosols within EAMxx
 - Robust scientific evaluation to increase confidence on fidelity
 - Integrate the improved treatments into EAMxx