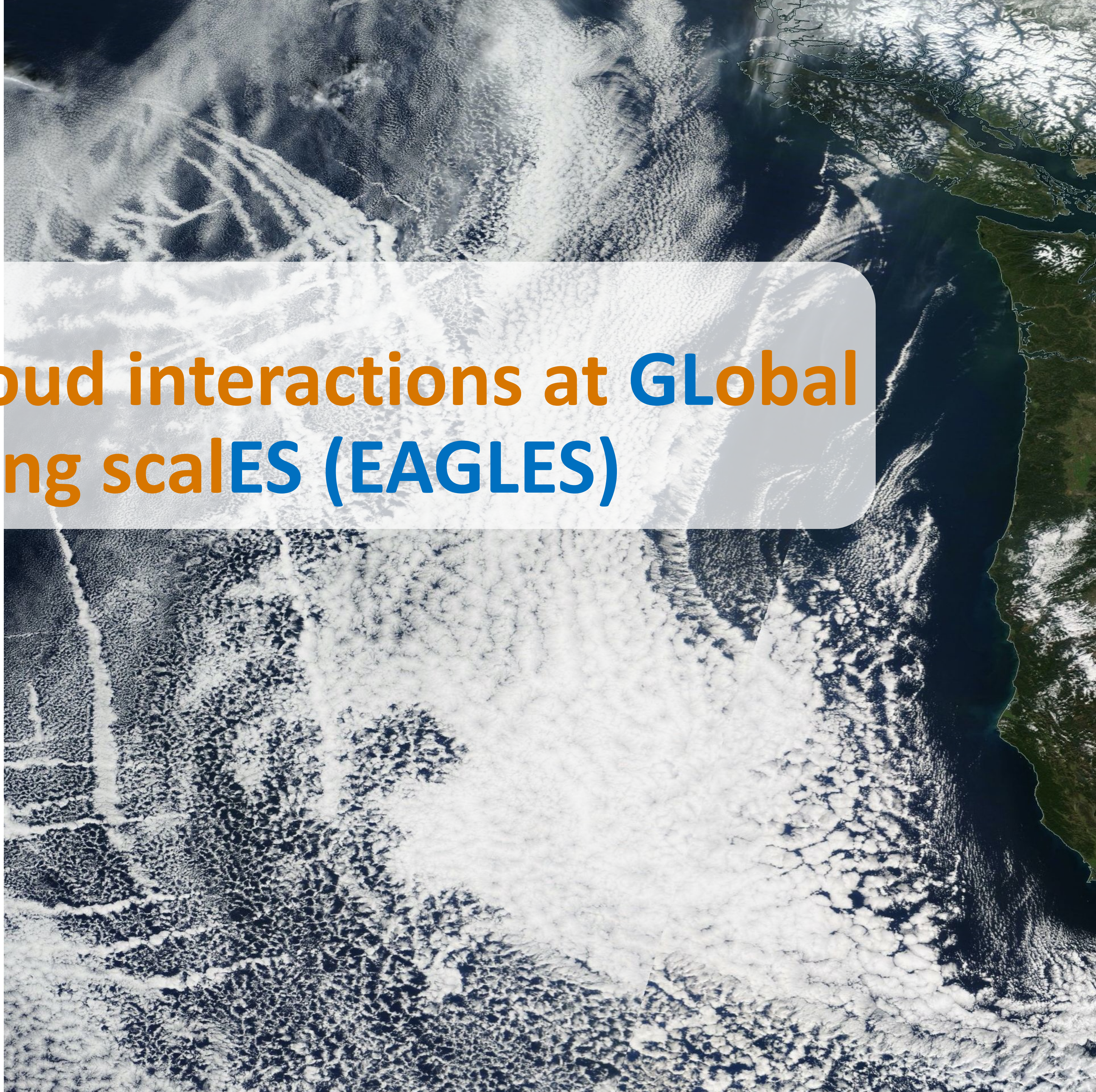
Enabling Aerosol-cloud interactions at GLobal convection-permitting scalES (EAGLES)

Po-Lun Ma

The EAGLES Project Team

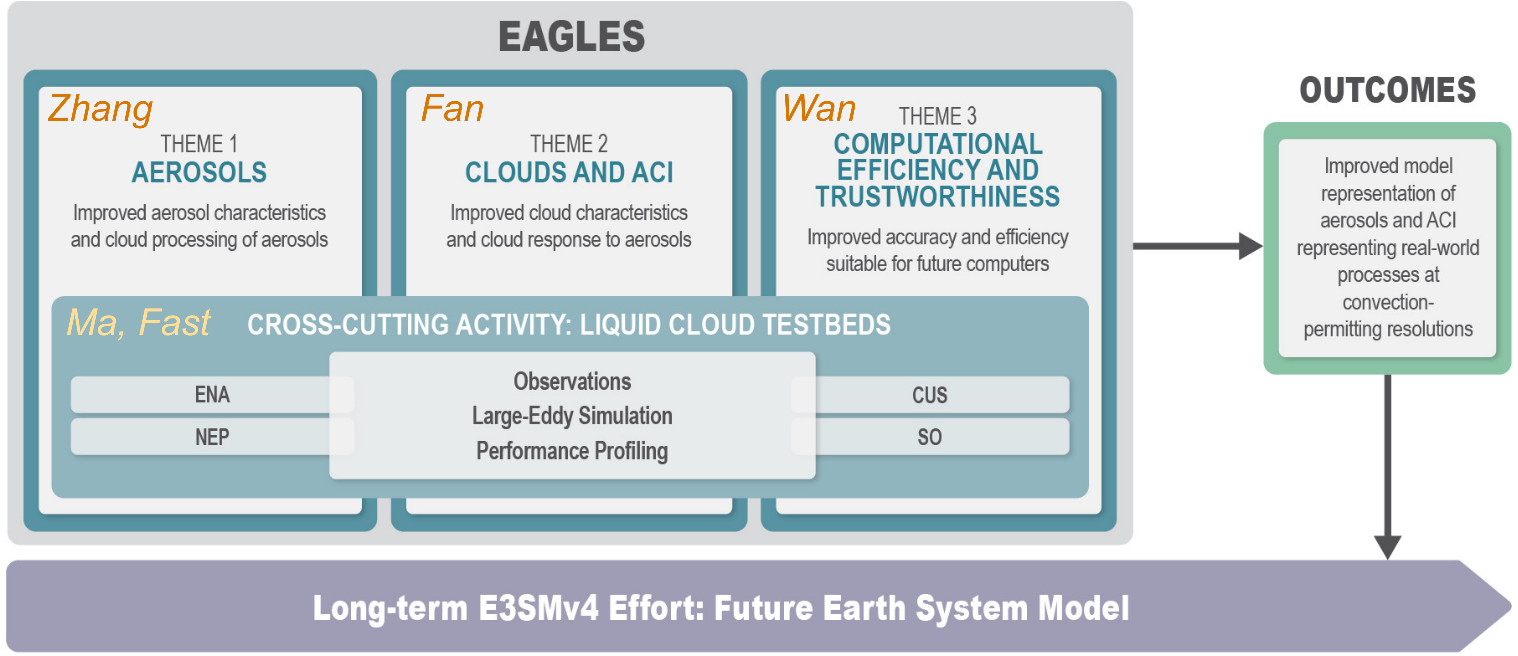


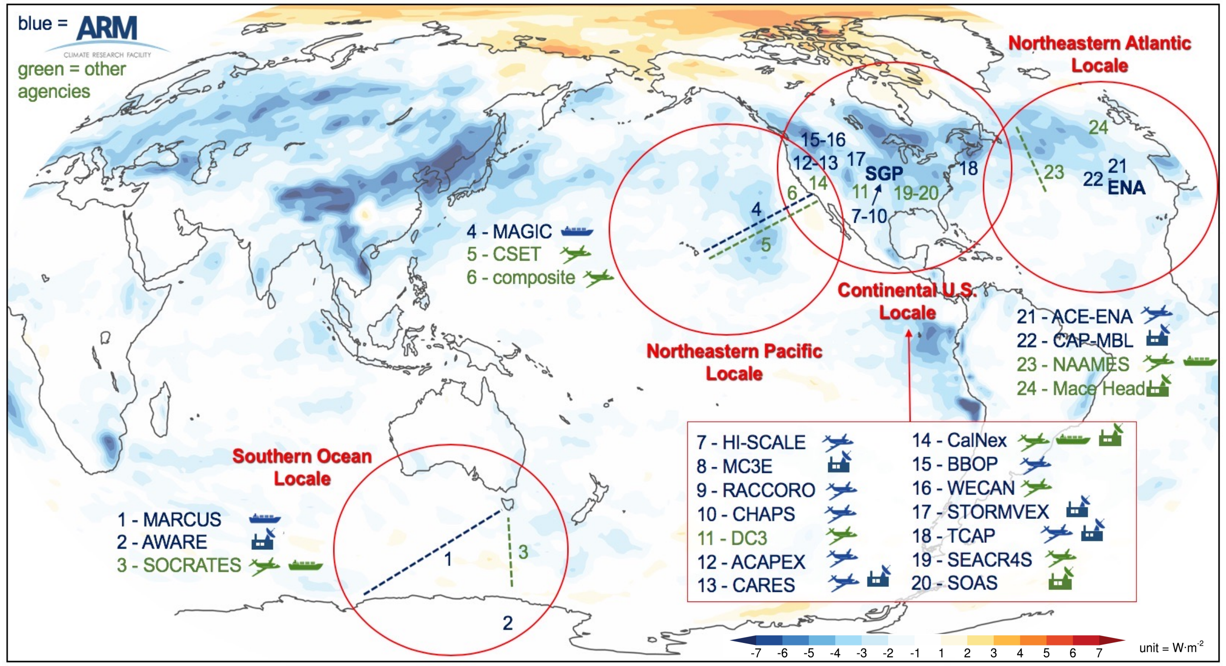
June 21, 2021

EAGLES

3 model development themes (Aerosol, Clouds, Computation)
1 cross-cutting activity (Testbeds)
Develop 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**





The EAGLES Team

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University of California, Irvine: Mike Pritchard

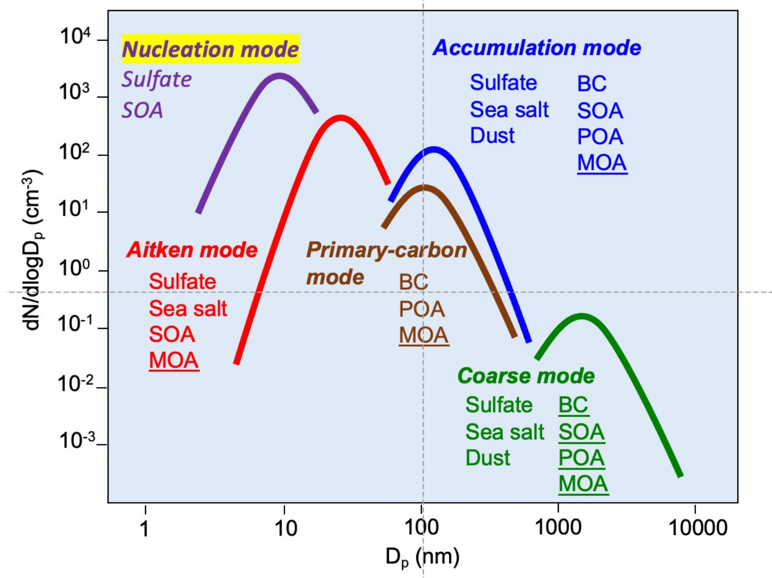
Friends/Unfunded Collaborators: Jim Randerson (UCI), Nicole Remer (UIUC), and others

Progress overview

- **Addressing the structural deficiency in modeling aerosols and ACI in E3SM**
  - **Develop and refine 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**
- **Integrating observationally based process-oriented constraints for ACI in parameterization development**
  - Develop an **automated aerosol and ACI diagnostics package**, **process-oriented metrics**, and **decomposition analysis framework** for model-data comparison and parameterization refinement
- **Performing a large LES ensemble covering a wide range of aerosol, cloud, and meteorological regimes**
  - Deploy a newly developed computationally performant LES model "**PINACLES**" to provide aerosol, cloud, precipitation, and meteorological data across regimes **for ML emulation, parameterization development, and model evaluation**
- **Developing AI-assisted parameterization**
  - New physically regularized **ML-based parameterizations** for aerosol and ACI processes produce **stable E3SM simulations.**
  - Use new AI/ML techniques to **address model structural deficiency**
- **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
  - Refactor and transplant aerosol code to **C++/kokkos**

Representing ultra-fine aerosols

Kai Zhang, Jian Sun, Jerome Fast, Bin Zhao, Shuaiqi Tang, Po-Lun Ma, et al



Objective

- Improve the background aerosols associated with new particle formation

Approach

- Add a new nucleation mode and treat the particle growth
- Use ARM measurements to evaluate and constrain the new treatment

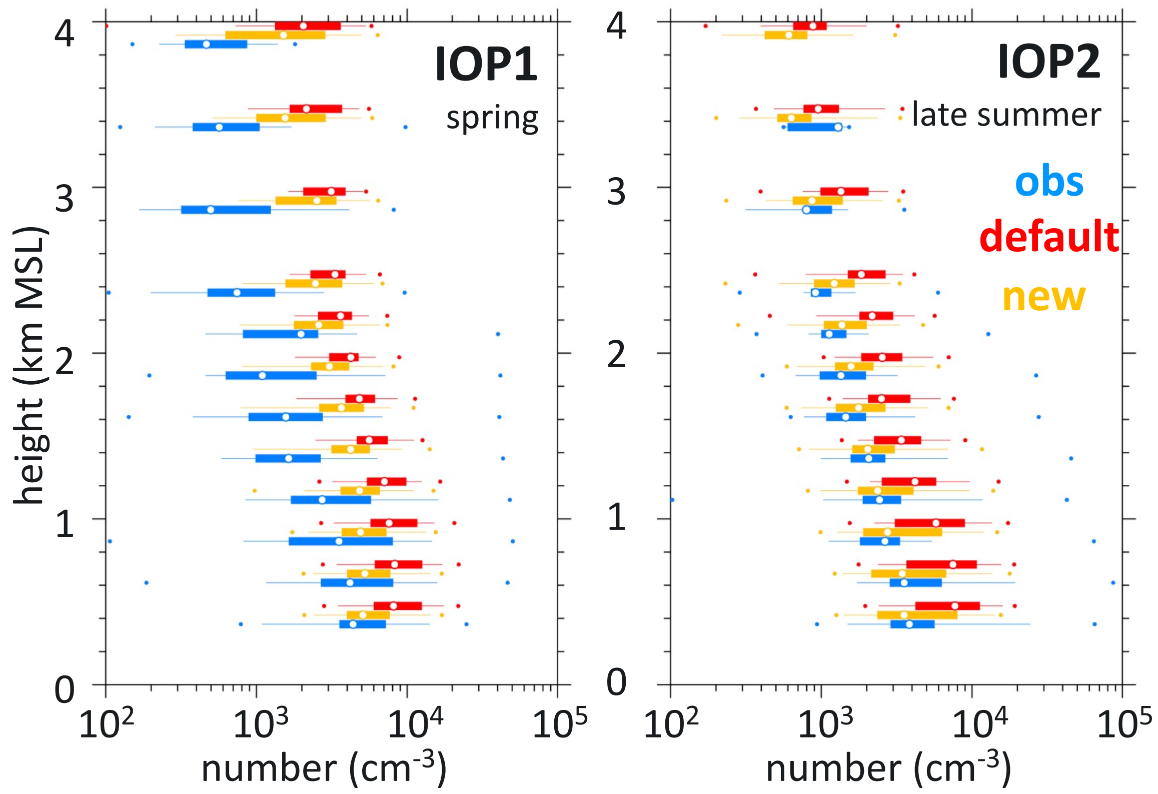
New capabilities and scientific significance

- Explicitly treat the growth, coagulation, and transport of newly-formed particles
- Merged aerosol size distribution from different instruments

Next Steps:

- Evaluate model simulations in different regions
- Sensitivity test and refine the parameterization

Number Concentration Percentiles (diameter > 10 nm)



New treatment (with the nucleation mode aerosols) produces better aerosol number simulations (in better agreement with observations)

Representing the organic-mediated new-particle formation (NPF) in E3SM

Bin Zhao, Manish Shrivastava, Kai Zhang, Po-Lun Ma, Balwinder Singh, Jerome Fast

Objective

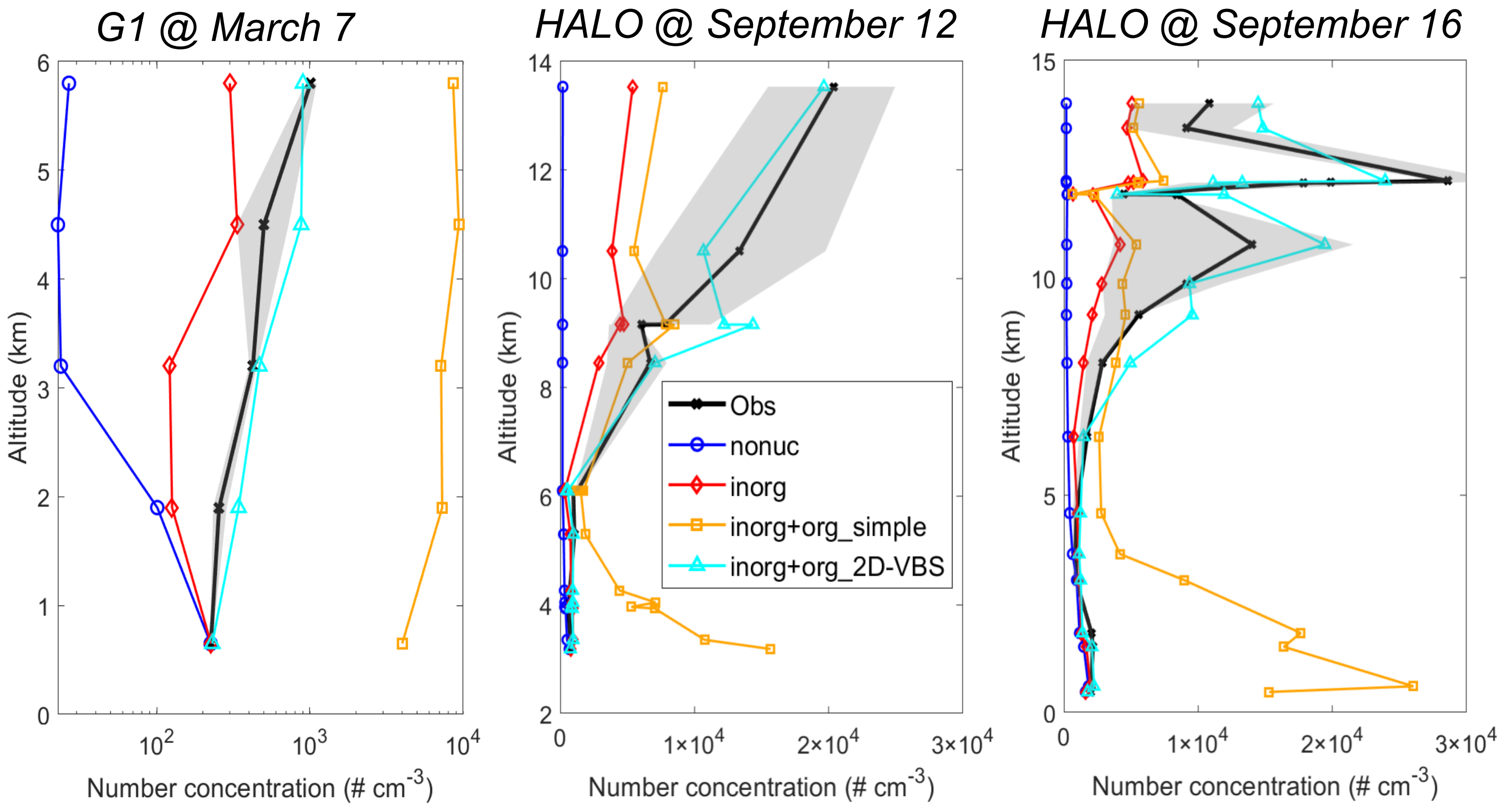
- To represent the organic-mediated NPF, an important NPF pathway

Approach

- Incorporate an organic-mediated NPF parameterizations and a novel radical two-dimensional volatility basis set (2D-VBS) in E3SM to simulate the formation chemistry and thermodynamics of extremely low volatility organics that drive NPF.

New capabilities and scientific significance

- Developed the parameterizations of 3 organic-mediated NPF pathways
- Determined the chemical reactions that form the nucleating organics, based on the radical 2D-VBS with experimentally-constrained parameters
- The work is expected to improve global aerosol number budget and help better quantify aerosol radiative forcing
- The organic–mediated NPF has been implemented in E3SM EAGLES code base.



Zhao et al., PNAS, 2020

Incorporation of organic-mediated NPF improves simulation

Next Steps:

- Evaluate against observations in different testbeds

Representing wildfire aerosols

Xiaohong Liu, Zheng Lu, Ziming Ke, Allen Hu, Jiwen Fan, Kai Zhang, Po-Lun Ma, et al

Objective

- Improve the representation of the injection height of wildfire aerosols

Approach

- Calculate fire plume rise and aerosol injection height based on fire properties and ambient meteorological conditions

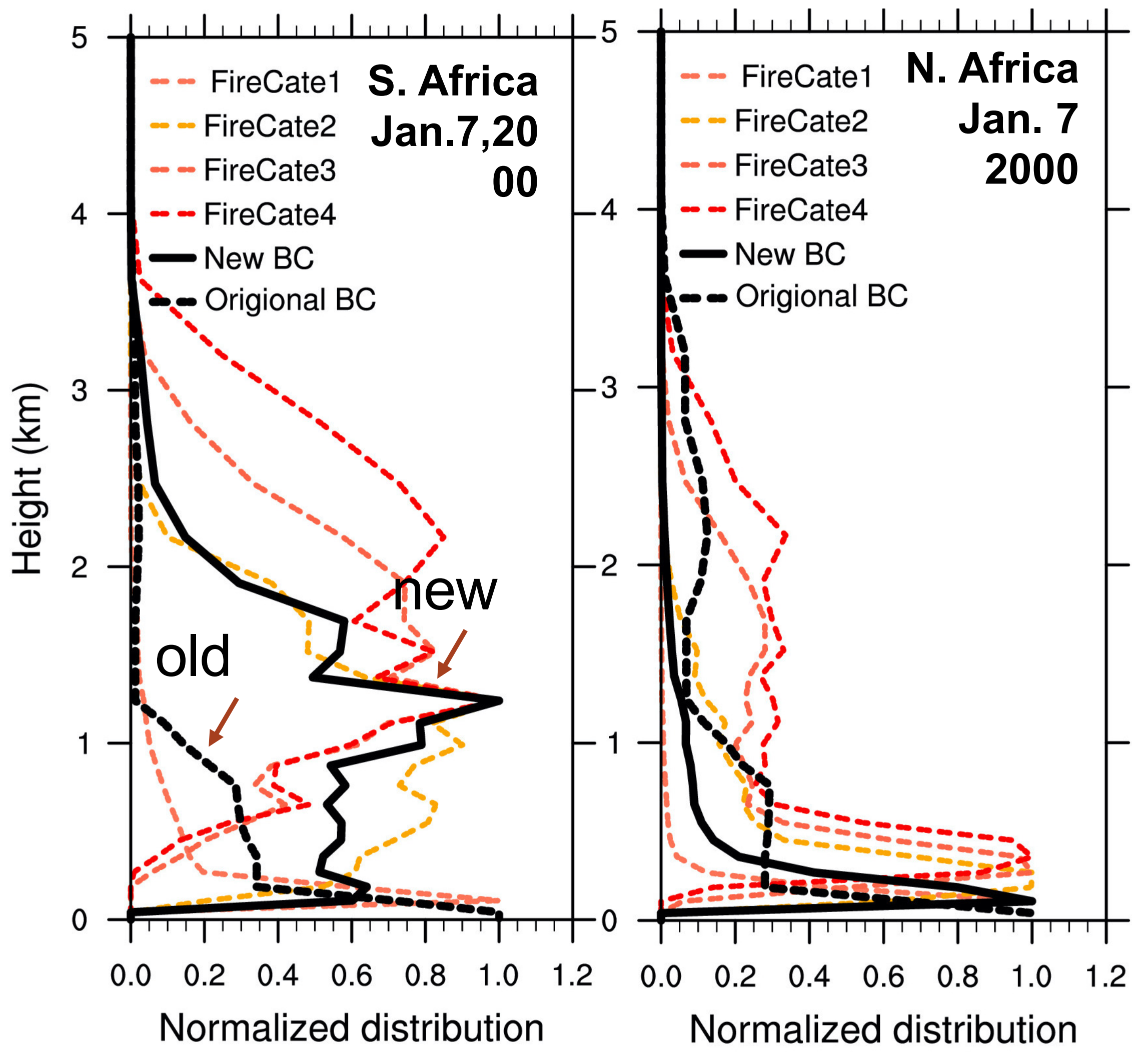
New capabilities and scientific significance

- Vertical distributions of wildfire aerosols are predicted rather than prescribed.
- The distribution of wildfire aerosols as well as their impacts on radiation and clouds are now better represented in E3SM.

Next Steps:

- Evaluation against observations
- Incorporate fire diurnal cycle and generate new fire emission maps.

Calculated and prescribed BC profiles



Aerosols are elevated to higher altitude using the new (prognostic) treatment of wildfire aerosol injection height

Fully prognostic treatment of cloud-borne aerosols

Guangxing Lin, Kai Zhang, Po-Lun Ma, Balwinder Singh, Jian Sun, Hailong Wang, et al

Motivation

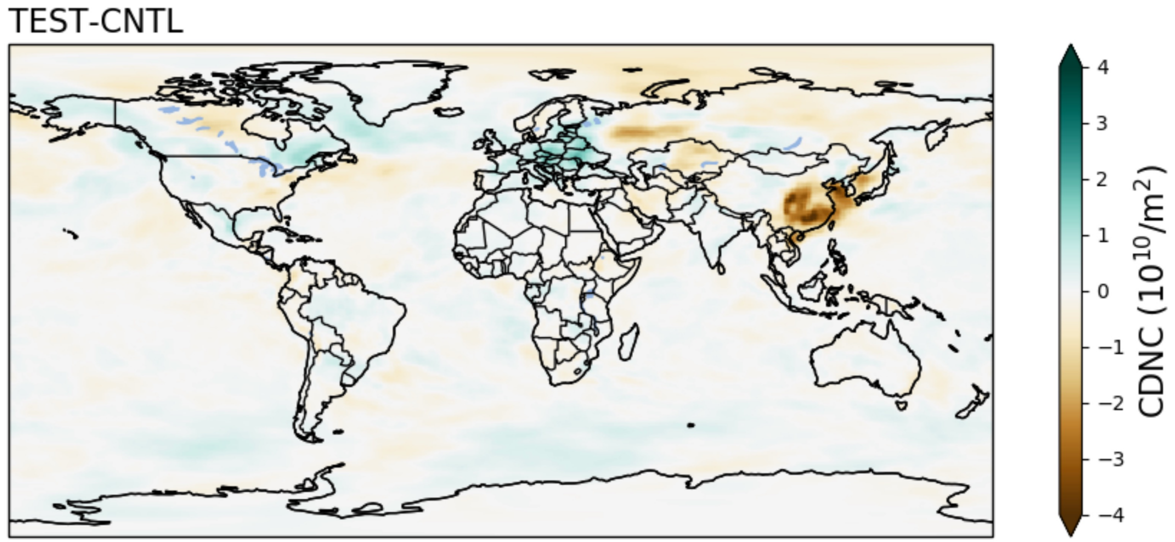
- The treatment of neglecting the advection of cloud-borne aerosols is designed for coarse-resolution models. At convection-permitting scales, this treatment is expected to produce large errors.

Approach

- Implement the advection of cloud-borne aerosols in E3SM
- Assess its impacts on aerosols, clouds, and aerosol radiative effects

Next Steps:

- Assess the resolution sensitivity of the new treatment
- Evaluate the model against observations
- Assess the impacts on aerosol radiative effects



Significant reduction of cloud droplet number in East Asia after accounting for advection of cloud-borne aerosols in E3SMv1 running at ne30 resolution

Improving aerosol activation using physically regularized deep neural network

Sam Silva, Po-Lun Ma, Balwinder Singh, Mike Pritchard, et al

Objective

- Improve aerosol activation in E3SM using novel machine learning techniques (e.g., deep neural network)

Approach

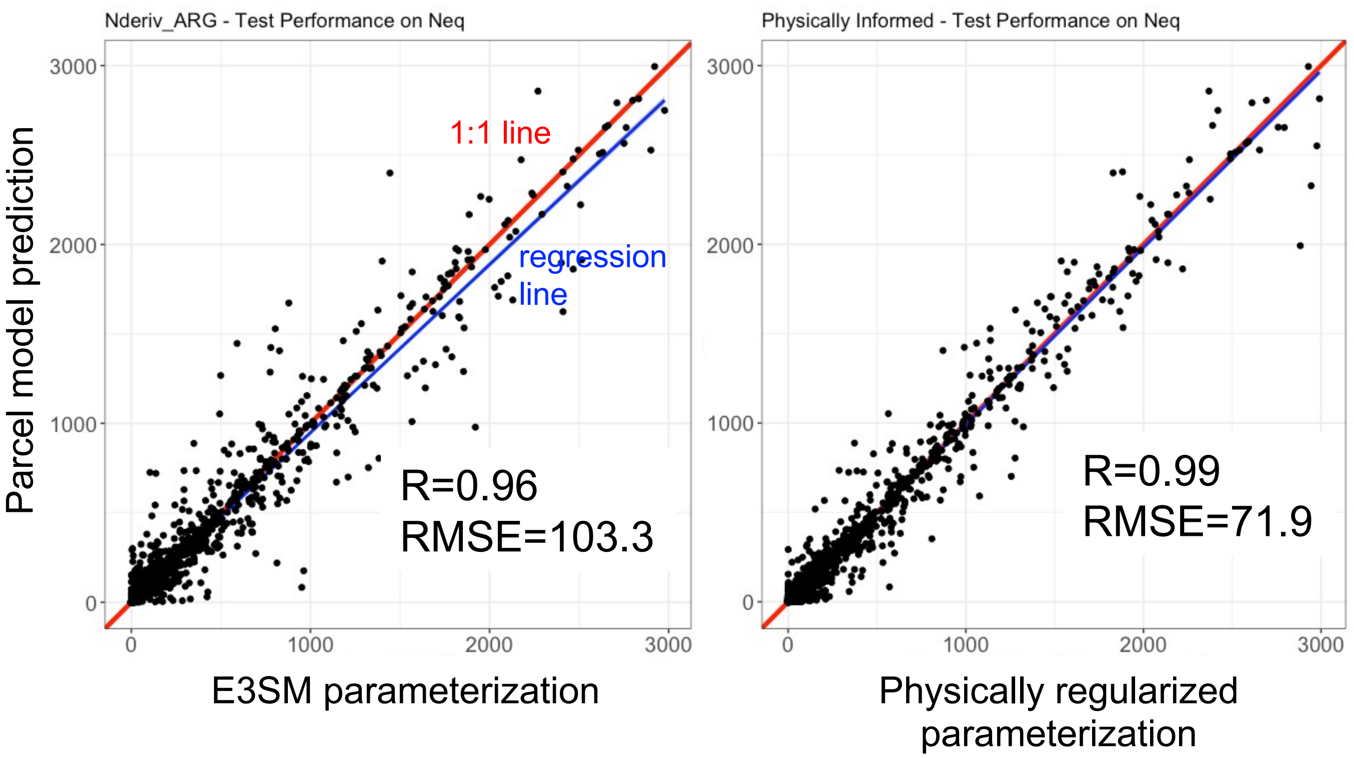
- Use various machine learning techniques to emulate activation from cloud parcel model
- Implement the emulator in E3SM using the Fortran-Keras Bridge (FKB) library

New capabilities and scientific significance

- Workflow for physically regularized emulator building
- Workflow for fast implementation of emulator in E3SM
- Stable E3SM simulations with the new activation emulator

Ongoing effort

- Extend from single mode to multiple mode treatment
- Importance sampling based on Earth's climate



New DNN-based activation corrects the default E3SM's bias in over-predicting activation in high-activation regime, potentially reduce the ERFaci.

Silva et al. (2021), *Geosci. Model Dev.*, doi:10.5194/gmd-14-3067-2021.

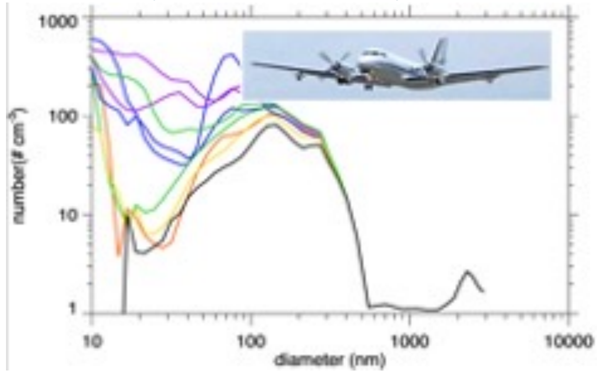
Develop globally suitable, faster, and better warm rain parameterization for ESMs

Kyle Pressel, Colleen Kaul, Jacob Shpund, Jiwen Fan, Mikhail Ovchinnikov, Jerome Fast, Jamin Rader, Sam Silva, Adam Varble, Po-Lun Ma, et al

Background: Warm rain has **significant impact** on climate; parameterization based on a **single cloud regime**

Approach: **ML emulation** trained on large eddy simulation **(LES) and observations from various regimes**

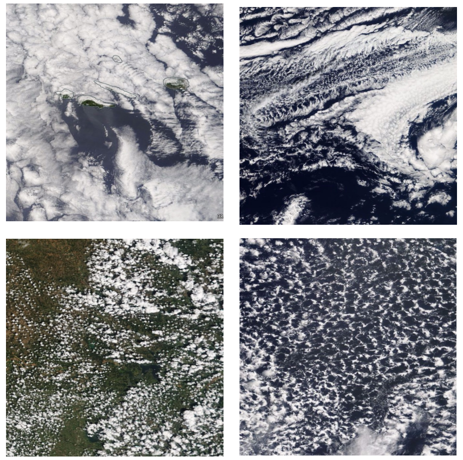
ARM



Aircraft measurements of aerosols, clouds, precipitation, and meteorology

PINACLES

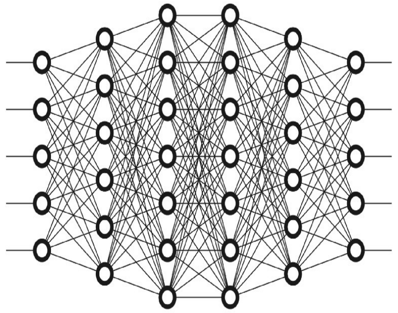
World's largest LES ensemble provides information on aerosols, clouds, precipitation, and meteorology



Training Dataset

Various regimes: coupled vs uncoupled boundary layer, different seasons, range of aerosol conditions, etc.

How do we train on different datasets (from models and observations)?



Machine learning emulation

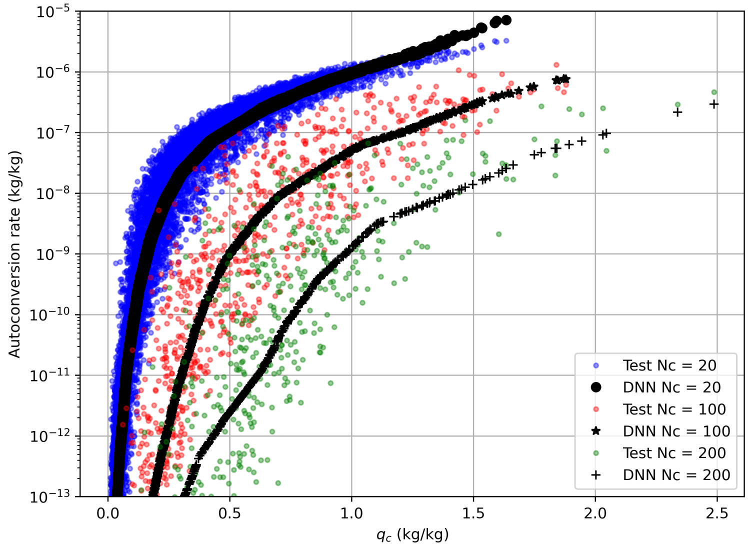
E3SM Energy Exascale Earth System Model

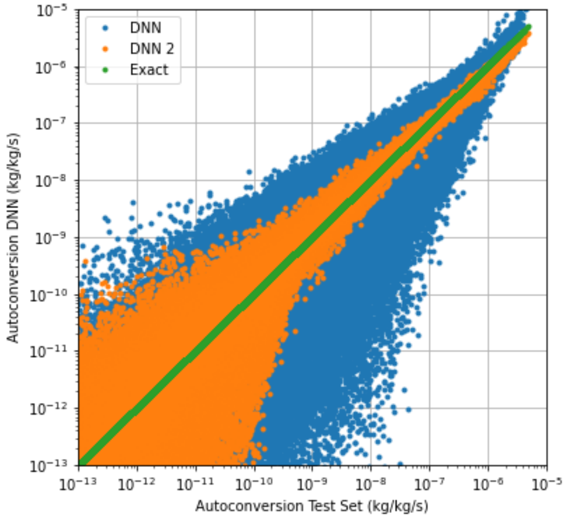
Accurate and computationally efficient treatments

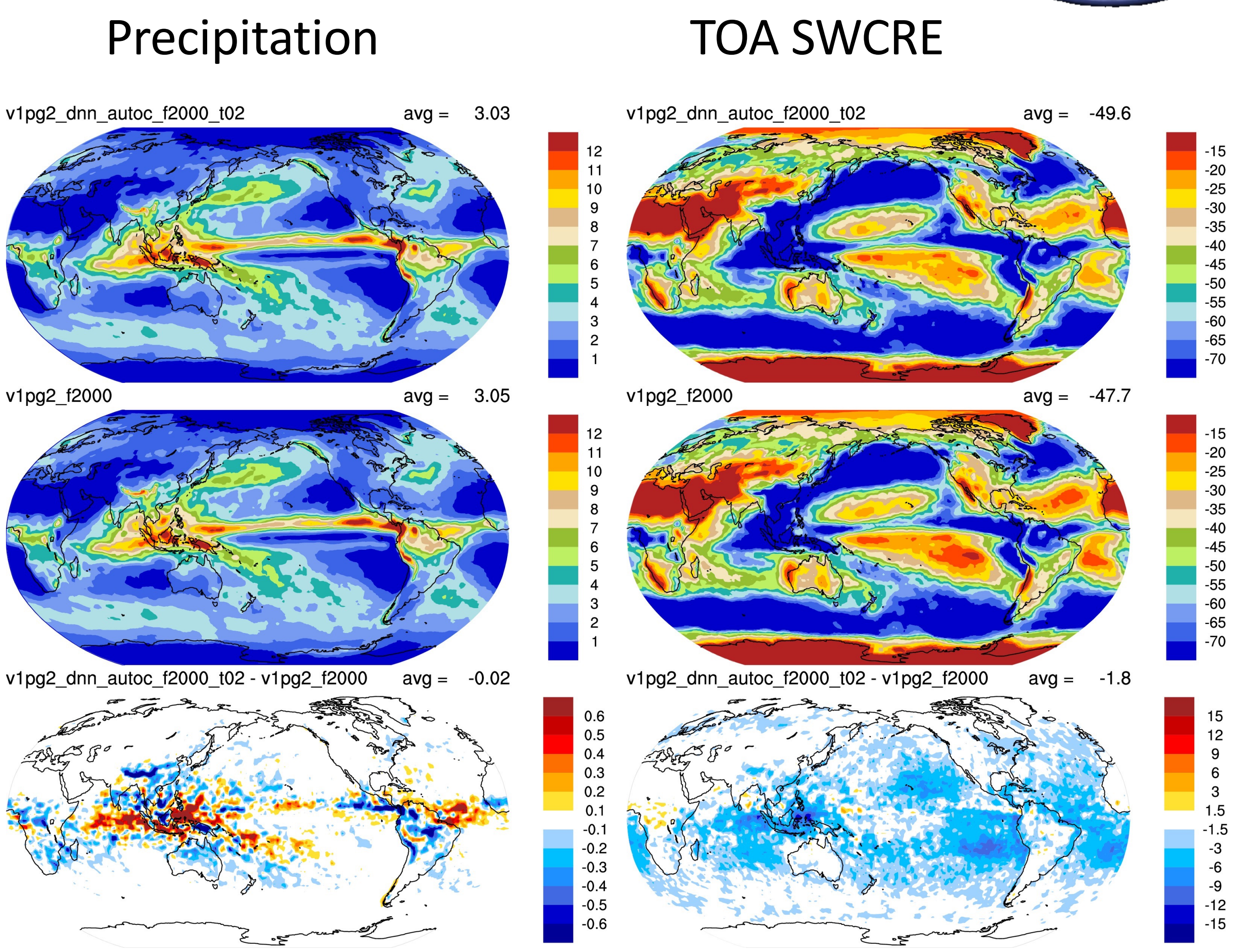
Information lost due to structural deficiency. Ongoing research to determine the necessary level of complexity.

Initial results show some success in emulating autoconversion

- The training data generated by the simulations described in the previous slide are used to train a deep neural network, with **three dense hidden layers**.
- The training dataset is composed of more than **5 million samples**.
- Initial training showed that a DNN mapping of $q_c, N_c, q_r, N_r \rightarrow \left(\frac{\partial q_c}{\partial t}\right)_{auto}, \left(\frac{\partial N_c}{\partial t}\right)_{auto}$ proved effective. This will be extended to prediction of $\left(\frac{\partial N_r}{\partial t}\right)_{auto}$.





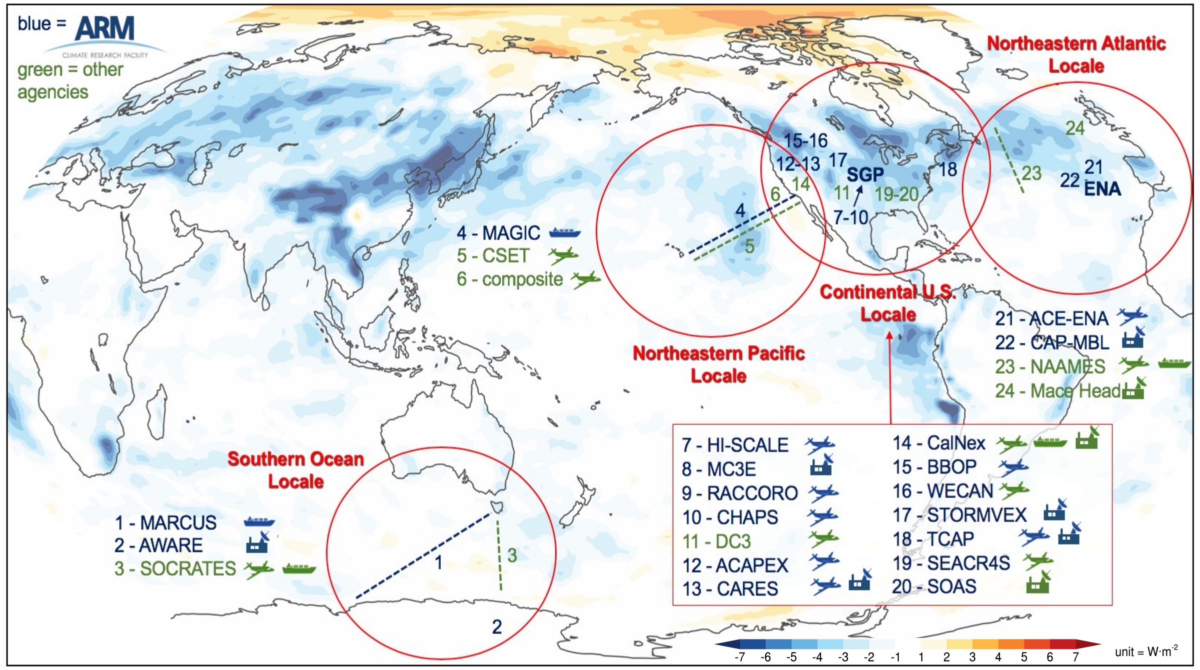


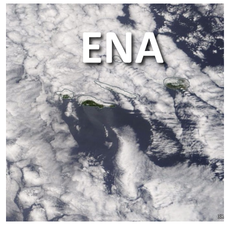
Reasonable climate simulation without adding computational cost.

Integrating observations and process-oriented diagnostics in parameterization development

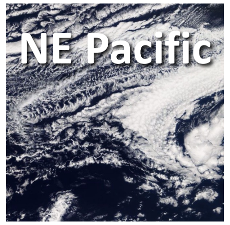
Adam Varble, Shuaiqi Tang, Matt Christensen, Johannes Muelmenstaedt, Xiquan Dong, Roj Marchand, Jerome Fast, Po-Lun Ma, et al

- Motivated by the need to better integrate **observational constraints** and **process understanding** into model development, we have begun development of a new Python-based liquid cloud ACI diagnostics package for robust evaluation of both state and processes.
  - Surface-based and aircraft measurements are coupled with satellite retrievals
  - Analyzed variables are extensive to account for co-variabilities
  - Various retrievals and outputs are intercompared to address potential retrieval biases.
  - Incorporate controls for coupling of clouds to the surface.
  - Minimize dataset/model resolution and sampling differences.
  - Applicable to future, differing resolution model versions.
- While new aerosol and cloud parameterizations are being developed and implemented in EAGLES, this framework allows us to **routinely test and track** how each process treatment impacts ACI relative to observations, providing guidance for adjustment and refinement.





diverse subtropical marine BL clouds susceptible to aerosol



transitions in Sc to trade-wind Cu regimes

continental convective clouds with high aerosol concentration

marine BL clouds with low aerosol concentrations

Aerosol Diagnostics

Covering 6 field campaigns over 4 testbed regions

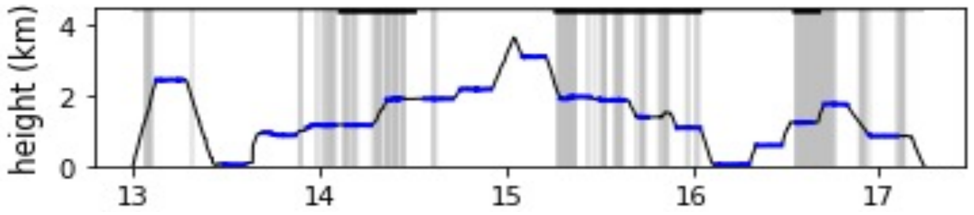
Shuaiqi Tang, Jerome Fast, et al

Mean statistics

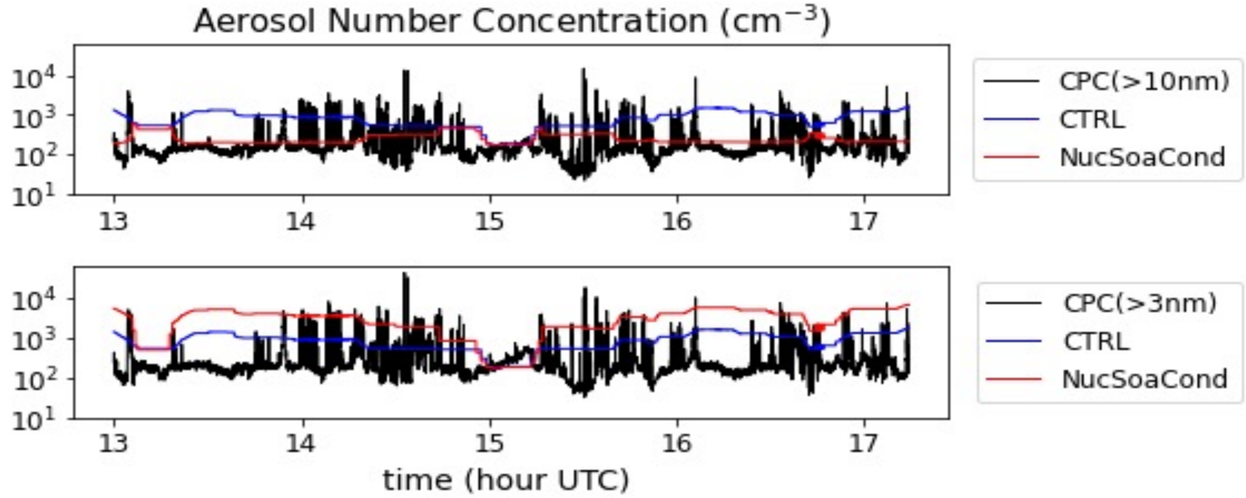
statistics of Aerosol Number Concentration comparing with CPC(>10nm). sample size 977

---	CTRL	NucSoaCond	OBS
mean	4896.33	3589.28	3333.24
bias	1563.09	256.04	
RMSE	3148.87	2647.14	
corrcoef	0.1405	0.1829	
P_corr	0.00	0.00	

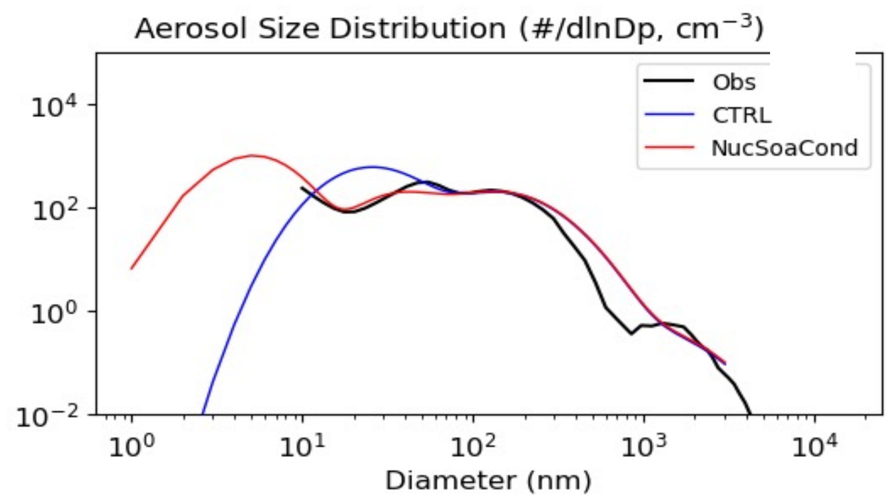
Time series



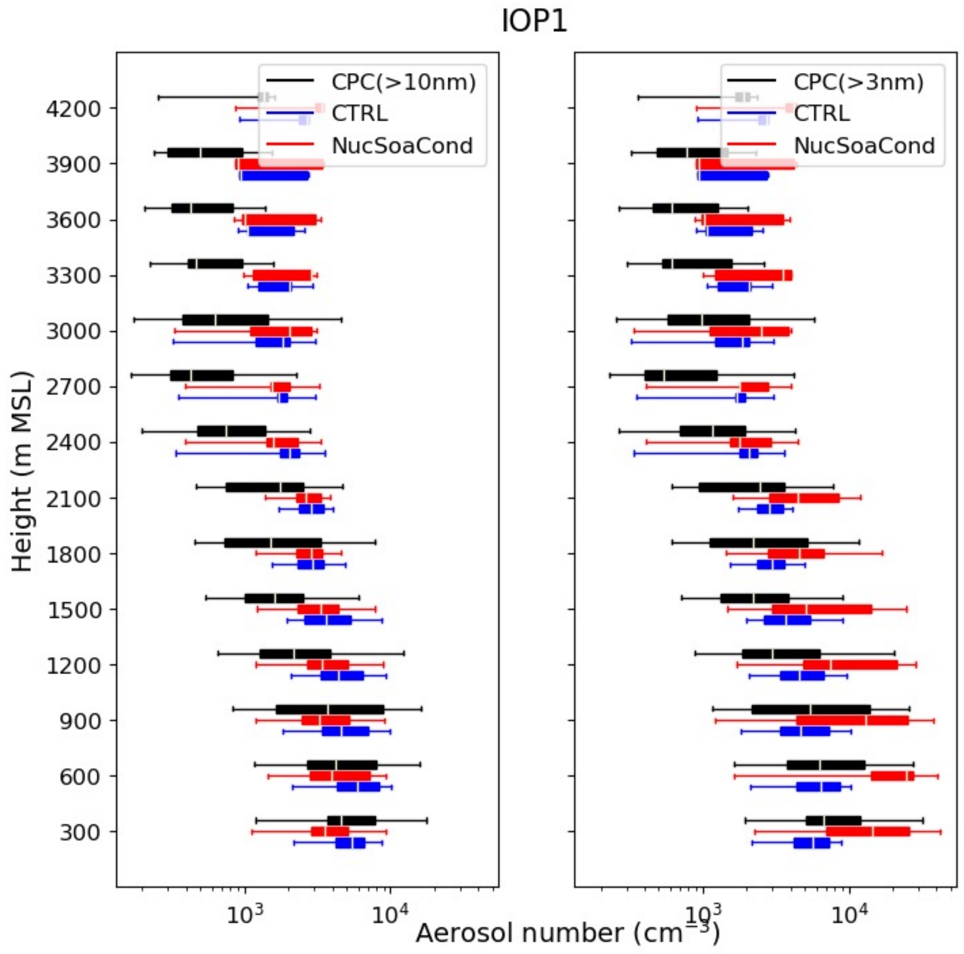
Thick black: CVI mode
Gray: cloud flag
Thin black: flight track
Blue: flight legs



Mean size distribution



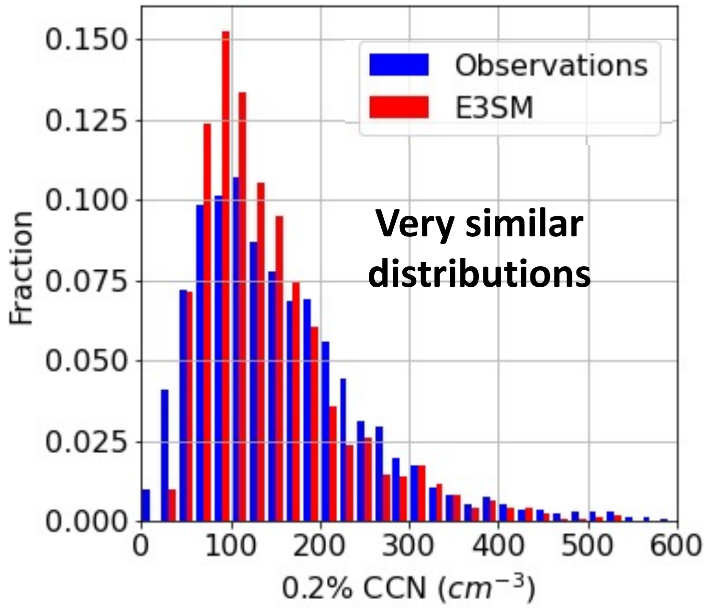
Percentiles with height



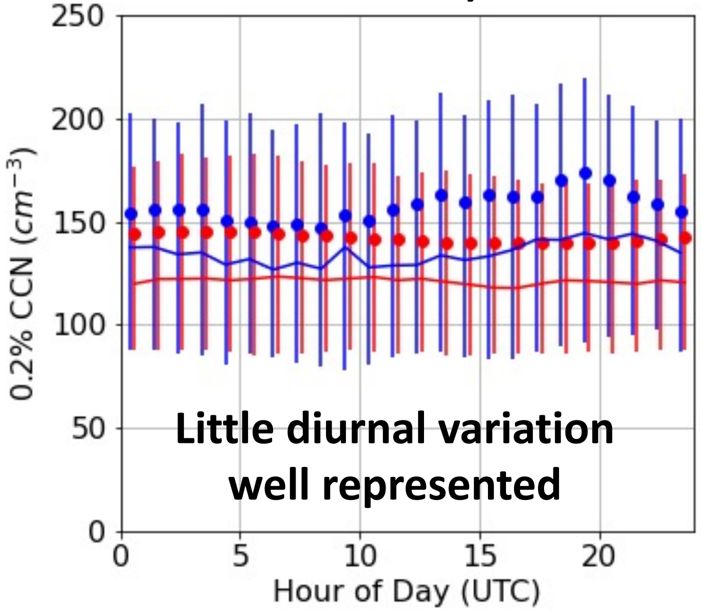
ACI Diagnostics

Adam Varble et al.

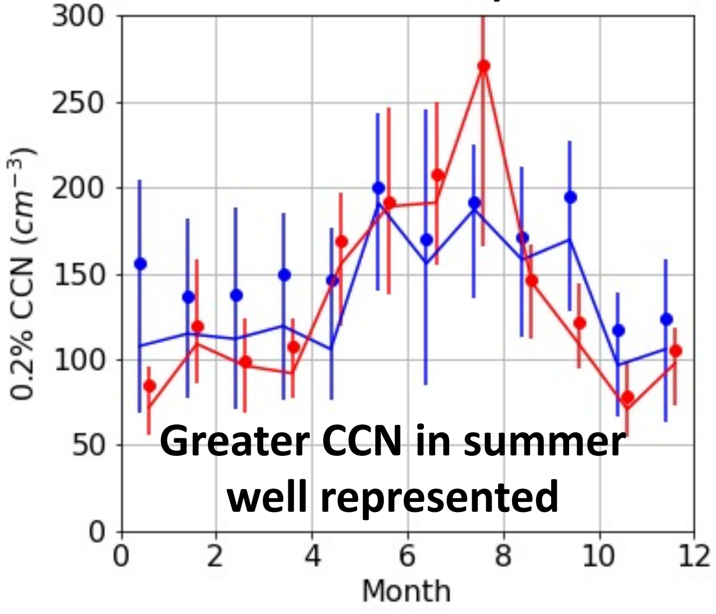
PDF

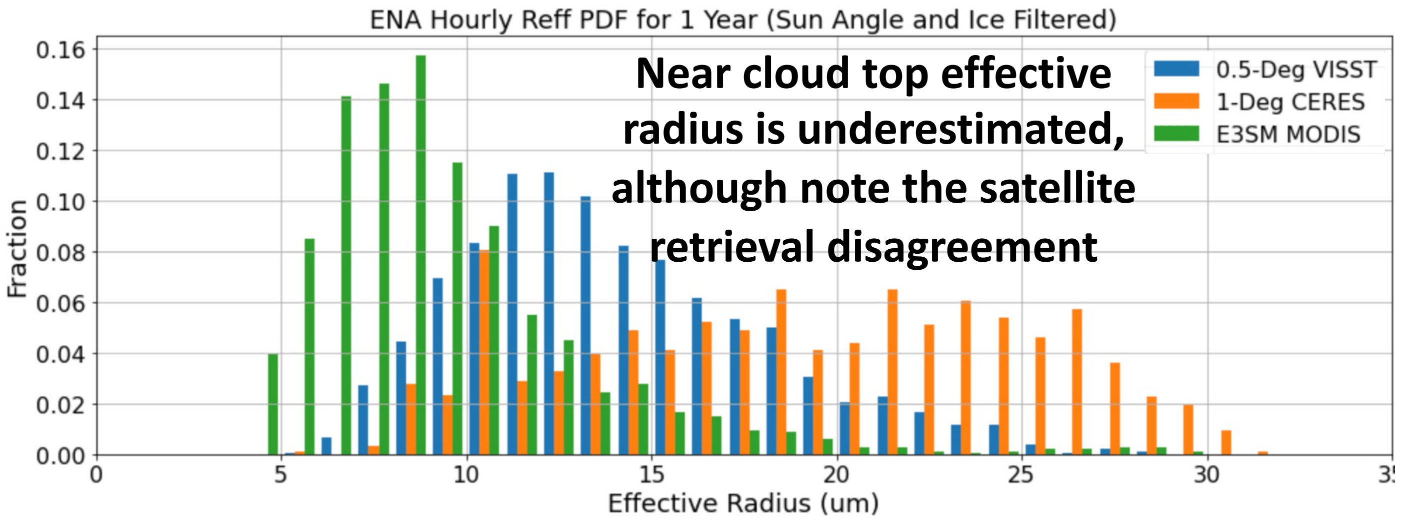


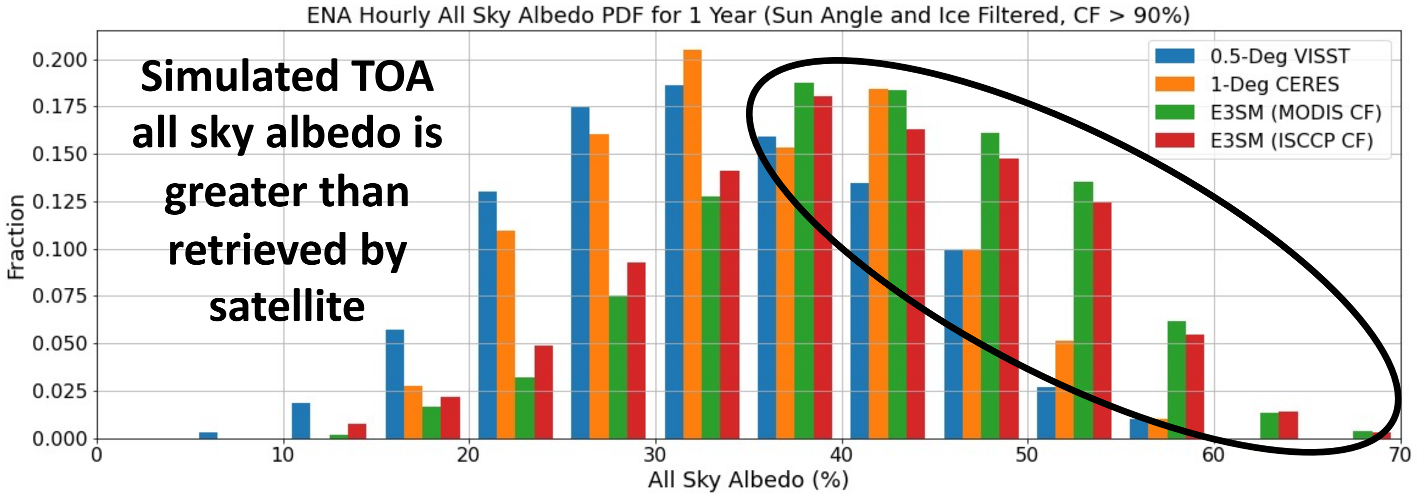
Diurnal Cycle



Seasonal Cycle







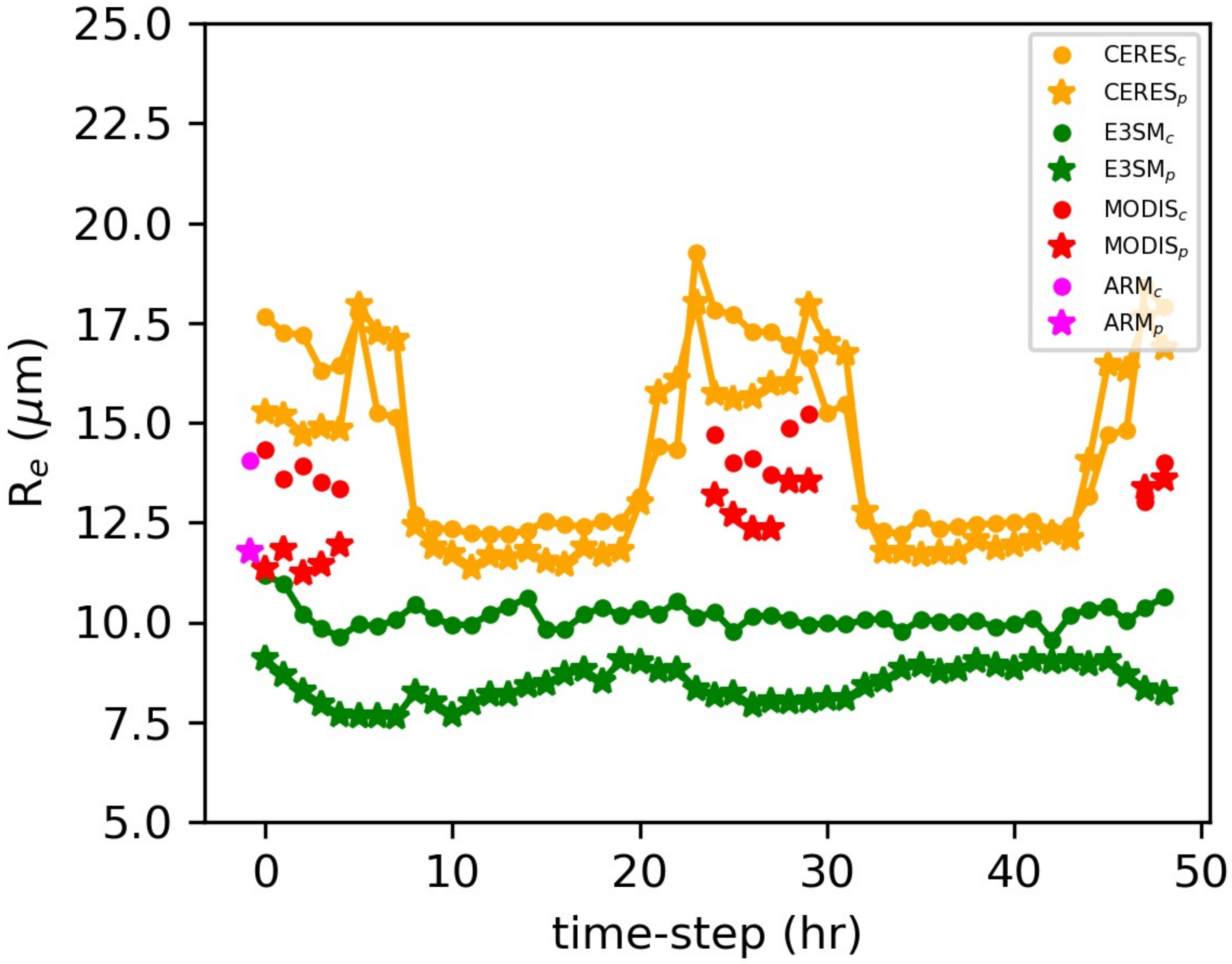
Lagrangian analysis of droplet effective radius (R_e)

Matt Christensen et al

Polluted: CCN > 113 cm³
Clean: CCN < 113 cm³

} **E3SM** value at t=0

3.7-µm Effective Droplet Radius



- ARM and MODIS cloud droplet effective radius are in excellent agreement!
  - CERES SYN is biased high
  - E3SM is biased low

- Droplet effective radius is smaller in polluted conditions in all datasets.
  - ➢ Larger concentration of CCN results in smaller and more numerous cloud droplets (Twomey effect).
  - ➢ 18% decrease in polluted clouds

- ΔR_e decreases over the trajectory on average.
  - ➢ Dilution and removal by precipitation

Summary

- We have made significant progress in the development of **aerosols and ACI process representation**, **evaluation toolkit**, and **analysis framework**.

- Ongoing effort is to improve understanding and refine model fidelity through better **model-data integration** and perform robust assessment of aerosols and ACI at **convection-permitting resolution** (i.e., dx = 3km).

- We look forward to learn from you and collaborate with you on improving the understanding and predictability of aerosols and ACI!