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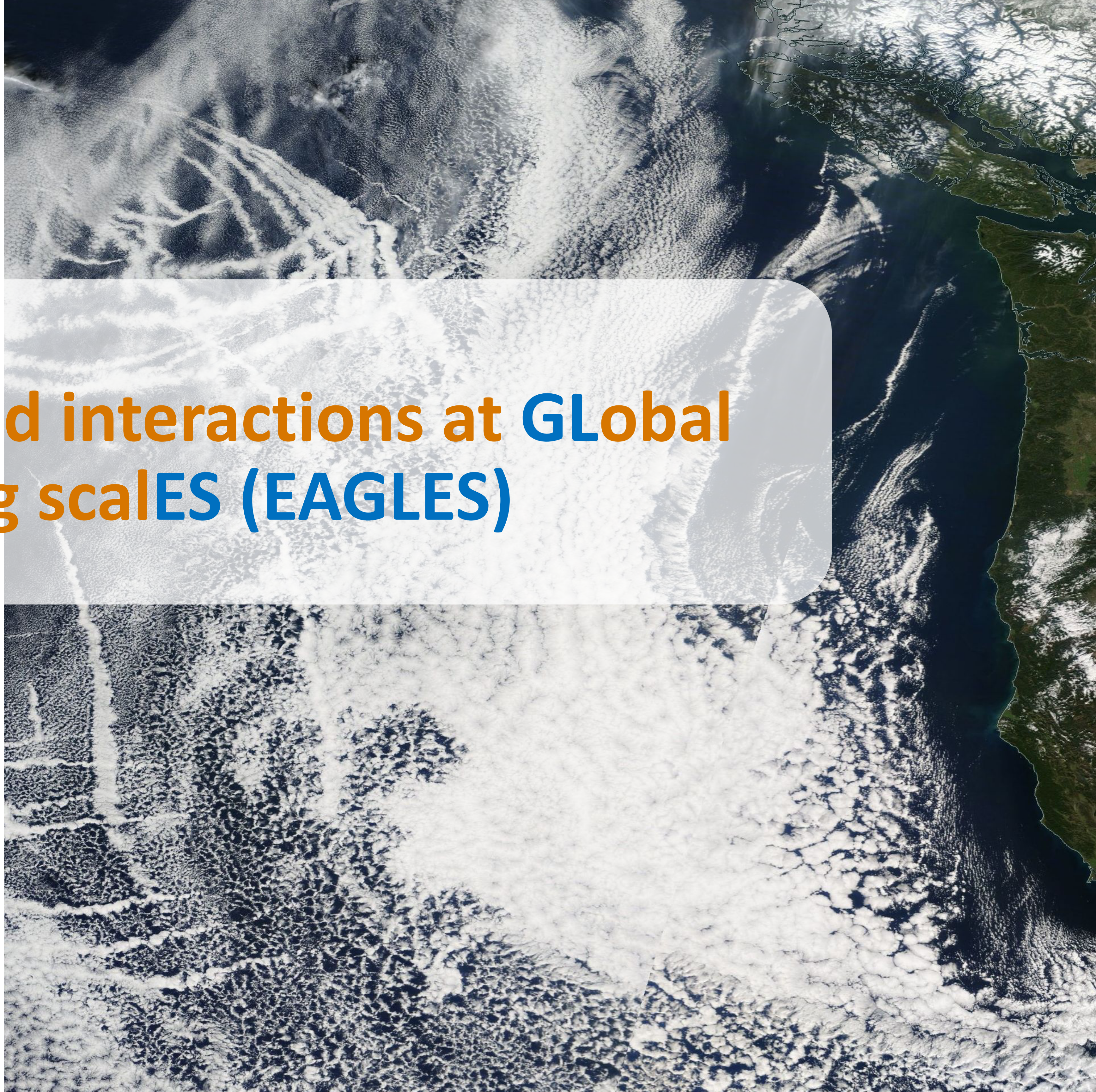
Enabling Aerosol-cloud interactions at GLobal convection-permitting scalES (EAGLES)



Po-Lun Ma

Atmospheric Sciences and Global Change
Pacific Northwest National Laboratory

October 27, 2020

U.S. DEPARTMENT OF ENERGY BATTELLE

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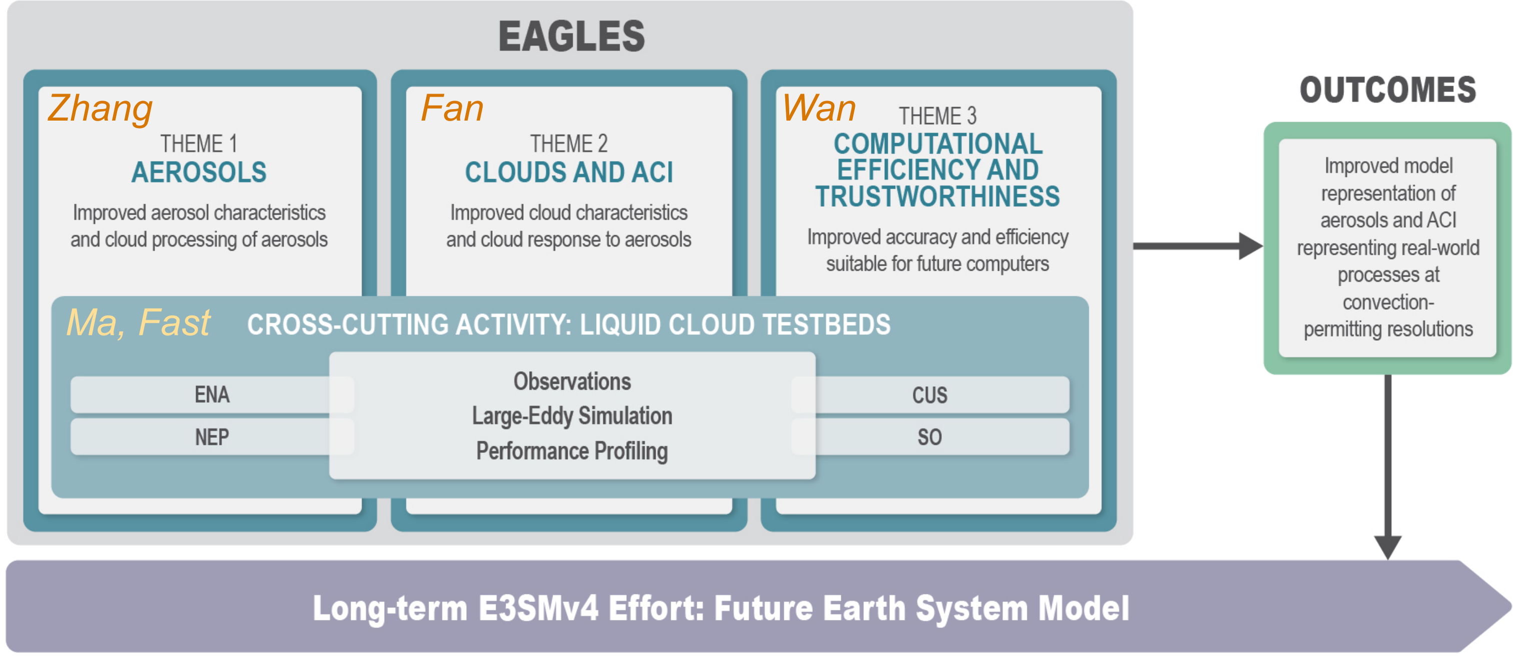
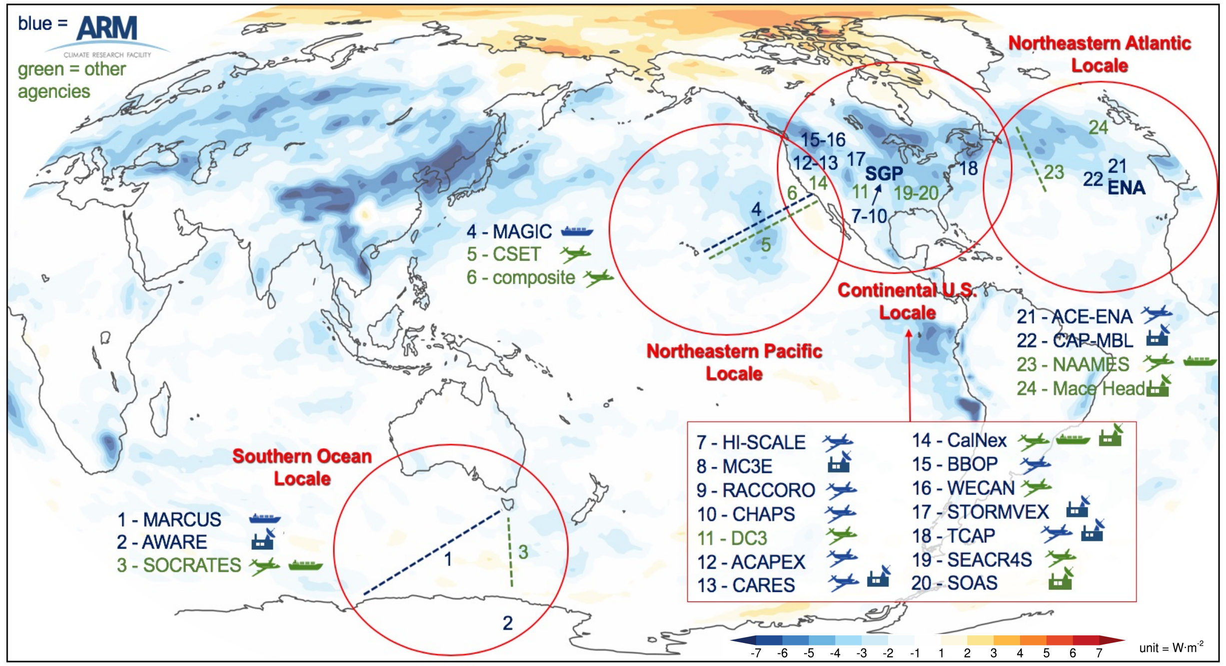
EAGLES

3 model development themes (Aerosol, Clouds, Computation)
1 cross-cutting activity (Testbeds)
Deliver improved representation to run on DOE's GPU-based computers

Goal: To increase confidence in, and understanding of, the role of aerosols and aerosol-cloud interactions in the evolution of the Earth system using new modeling techniques that are scientifically robust and computationally efficient for global convection-permitting simulations envisioned for E3SMv4





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TEXAS A&M UNIVERSITY

THE UNIVERSITY OF ARIZONA

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UNIVERSITY of WASHINGTON

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What a great team!

PNNL: Po-Lun Ma, Jiwen Fan, Hui Wan, Jerome Fast, Kai Zhang, Adam Varble, Balwinder Singh, Bill Gustafson, Bin Zhao, Chris Jones, Colleen Kaul, Guangxing Lin, Hailong Wang, Jacob Shpund, Joe Hardin, Jian Sun, Johannes Muelmenstaedt, Kyle Pressel, Manish Shrivastava, Mikhail Ovchinnikov, Phil Rasch, Sam Silva, Shixuan Zhang, Shuaiqi Tang, Susannah Burrows

SNL: Andy Salinger, Jeff Johnson, Pete Bosler, Mike Schmidt

Texas A&M University: Xiaohong Liu, Zheng Lu, Ziming Ke

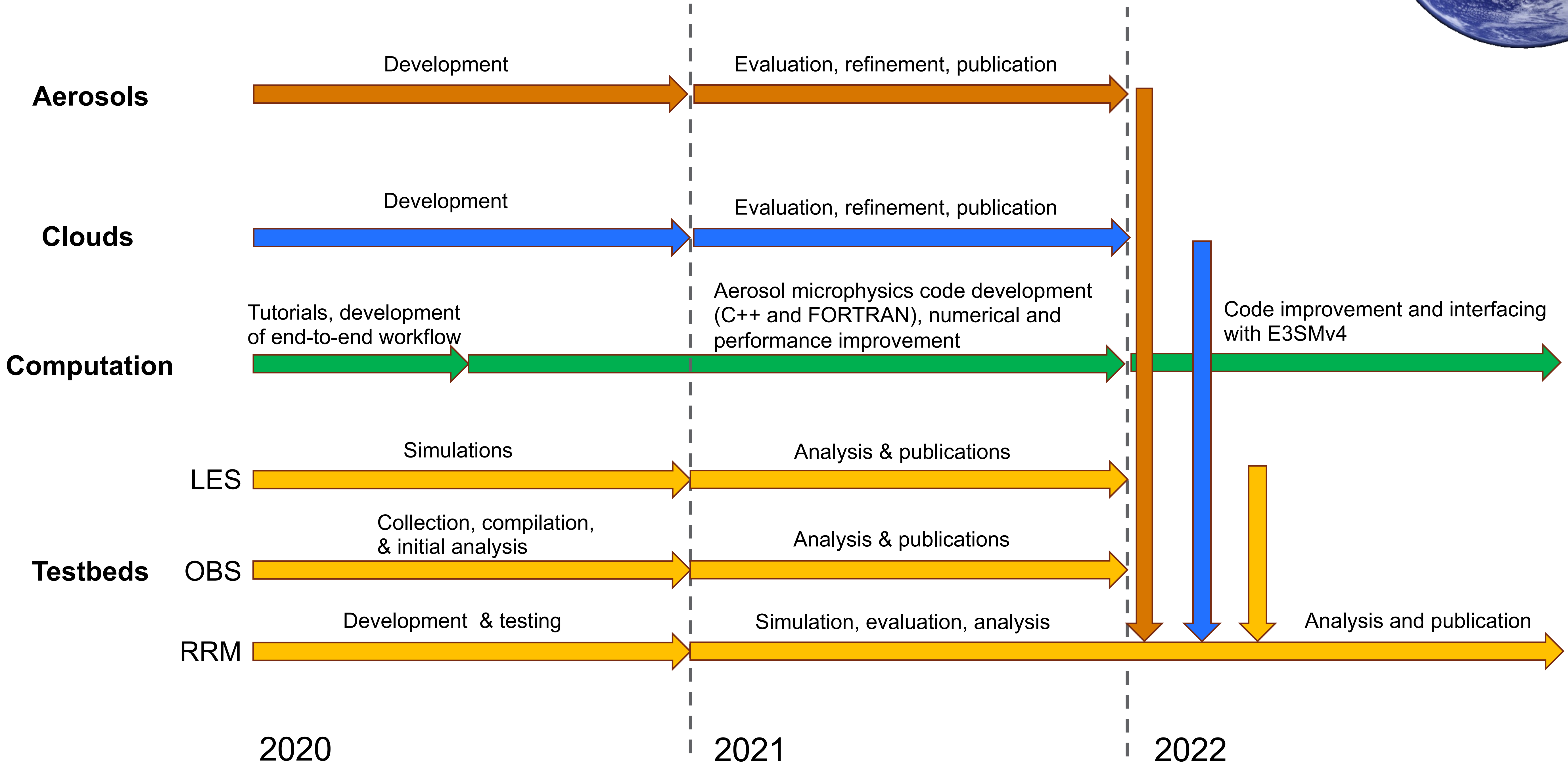
University of Arizona: Xiquan Dong, Baike Xi, Jordann Brendecke, Xiaojian Zheng, Peng Wu

University of Wisconsin-Milwaukee: Vince Larson, Brian Griffin, Niklas Selke

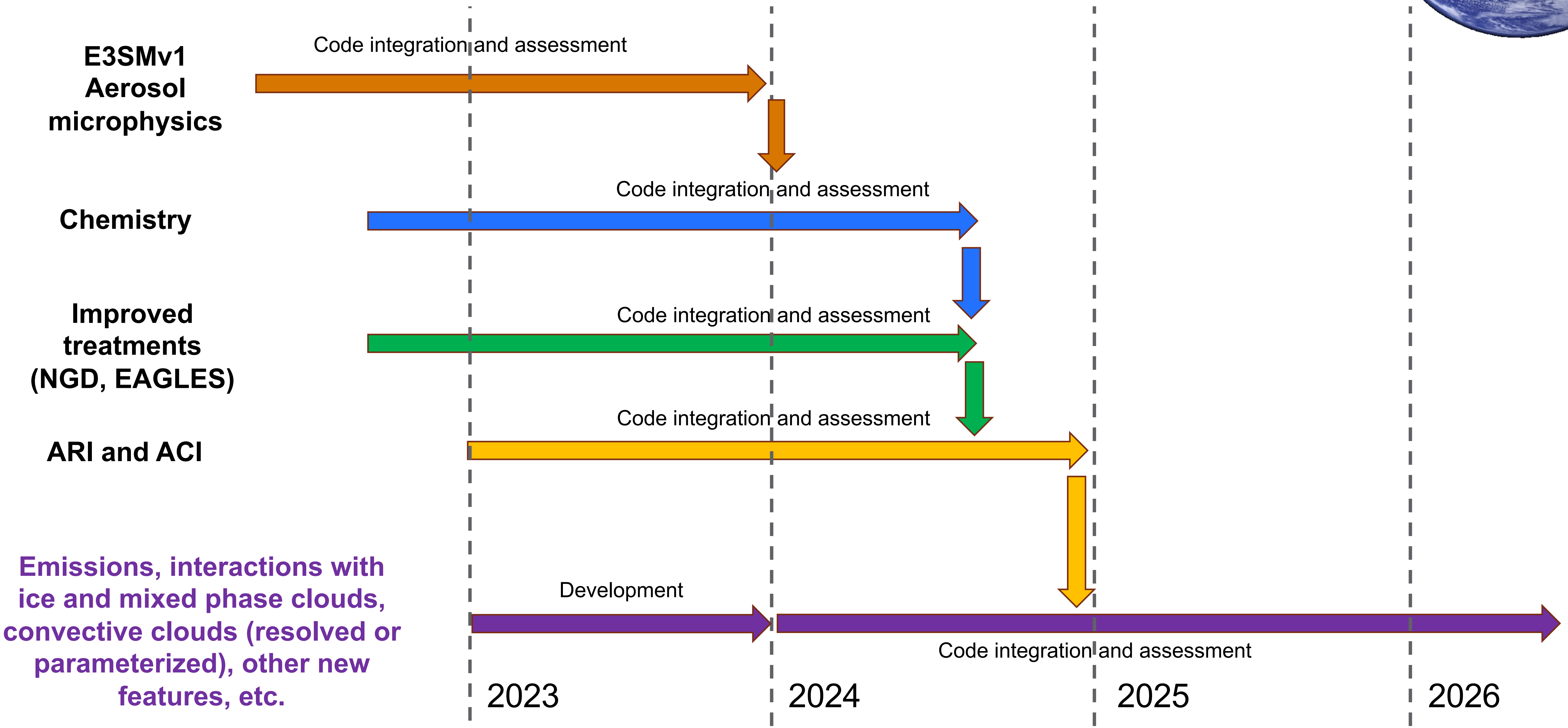
University of Washington: Roj Marchand, Chris Bretherton

University of California, Irvine: Mike Pritchard, S. Karthik Mukkavilli

Timeline of activities



Integration with E3SMv4



Discussion in D4S1 BR4 (Aerosols breakout session)

Accomplishments in FY21

- **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** using RRM
- **Streamlining the "machine learning (ML)-to-E3SM" workflow**
  - New physically regularized **ML-based parameterizations** for aerosol activation, precipitation, turbulence and clouds, etc., **implemented in E3SM**
- **Performing a large LES ensemble covering a wide range of aerosol, cloud, and meteorological regimes**
  - Use a newly developed computationally efficient LES model "PINACLES" to provide aerosol, cloud, precipitation, and meteorological data across regimes **for machine learning emulation, parameterization development, and model evaluation**
- **Integrating observationally based process-oriented constraints for ACI in parameterization development**
  - Develop an **automated aerosol and ACI diagnostics package** and **process-oriented metrics** based on ARM, satellites, and other observations to guide the model development
- **Modernizing software for DOE's GPU-based computers**
  - Redesign the code package to **improve efficiency, accuracy, and trustworthiness** using modern modeling techniques, better numerics, and testing and verification tools
  - Prepare the code for porting 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

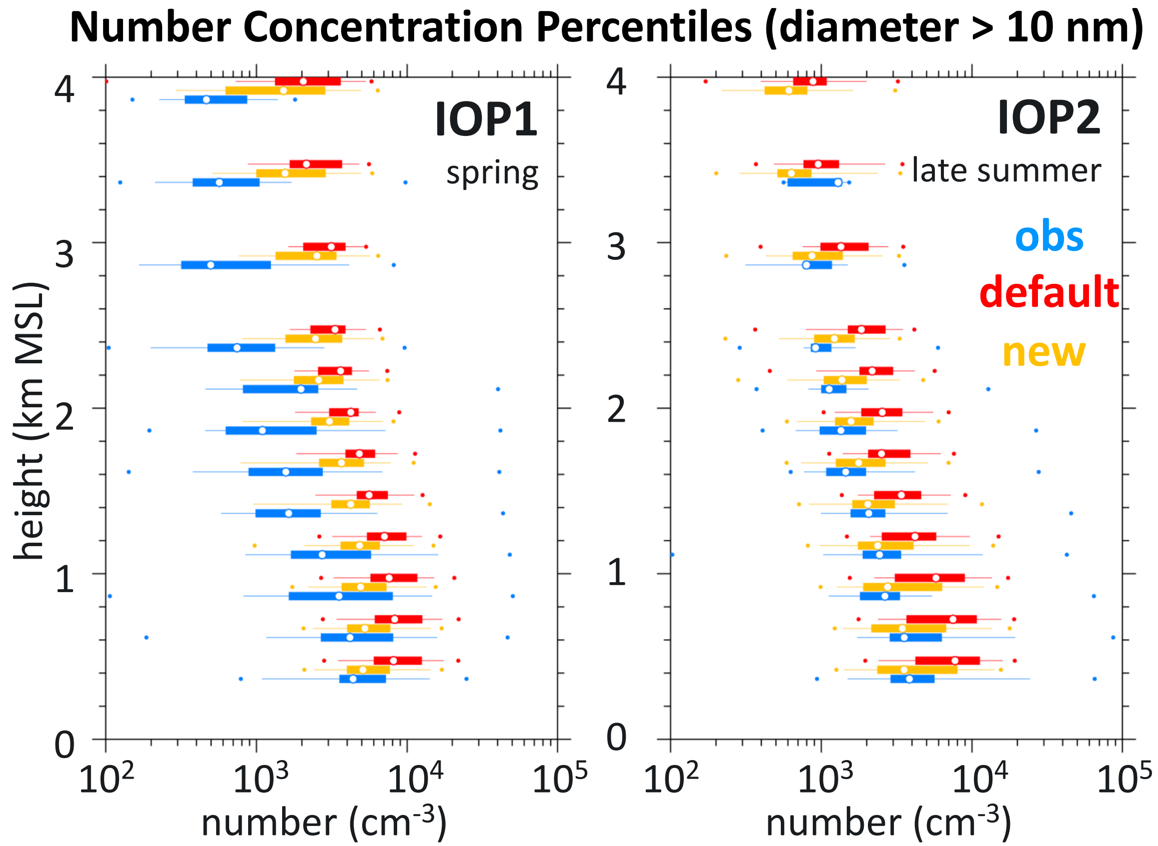
- Add a new nucleation mode and treat the particle growth
- Use ARM measurements to evaluate and constrain the new treatment

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 areas
- Assess the effects of organics in various processes



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

See more details in Kai Zhang's poster and Shuaiqi Tang's poster

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

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

Objective

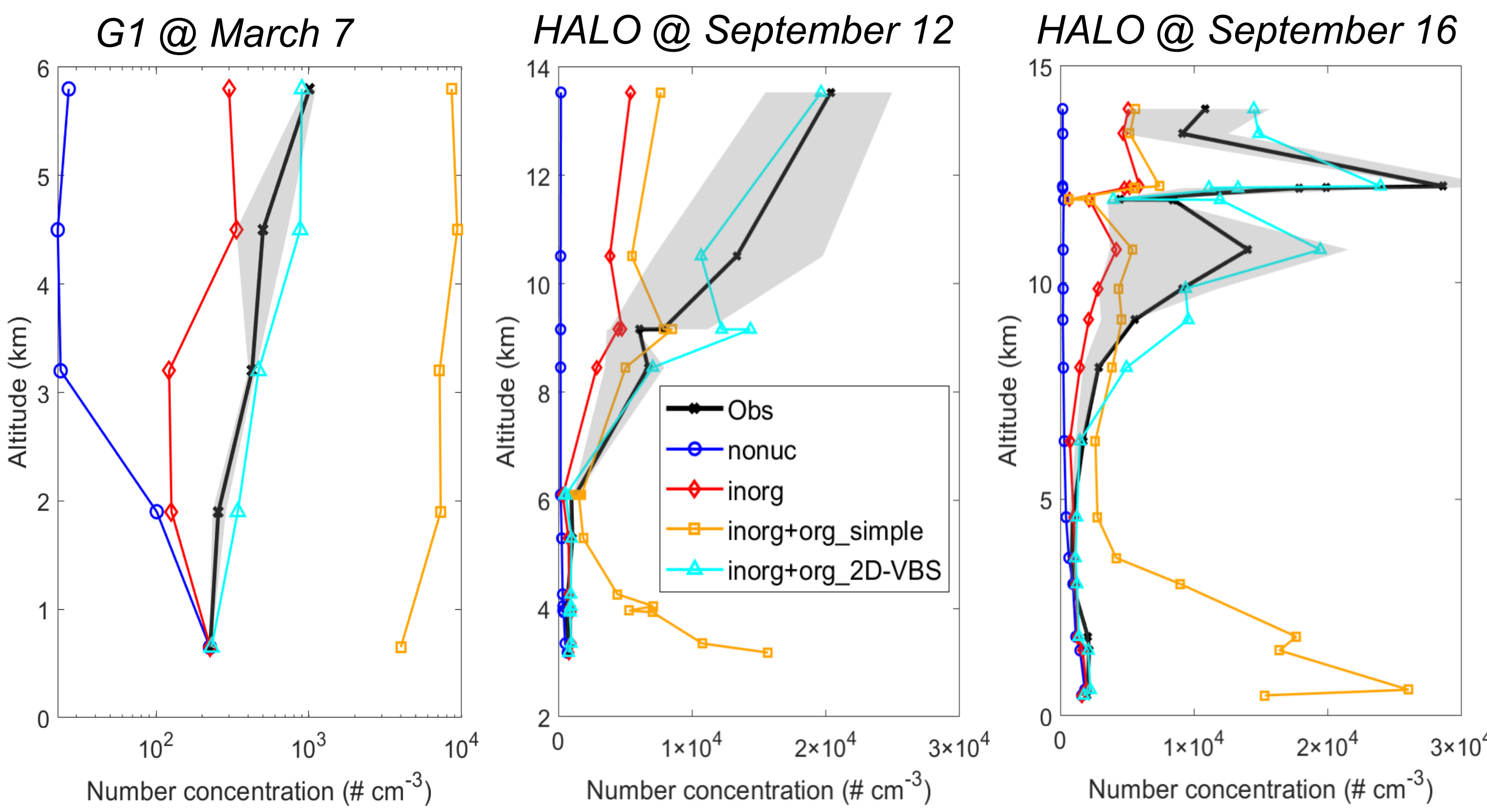
- To represent the organic-mediated NPF, an important and even dominant NPF pathway

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 the predictive understanding of global aerosol number budget and help better quantify aerosol radiative forcing



Zhao et al., PNAS, 2020

Incorporation of organic-mediated NPF improves simulation

Next Steps:

- Incorporate the organic-mediated NPF in E3SM
- 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

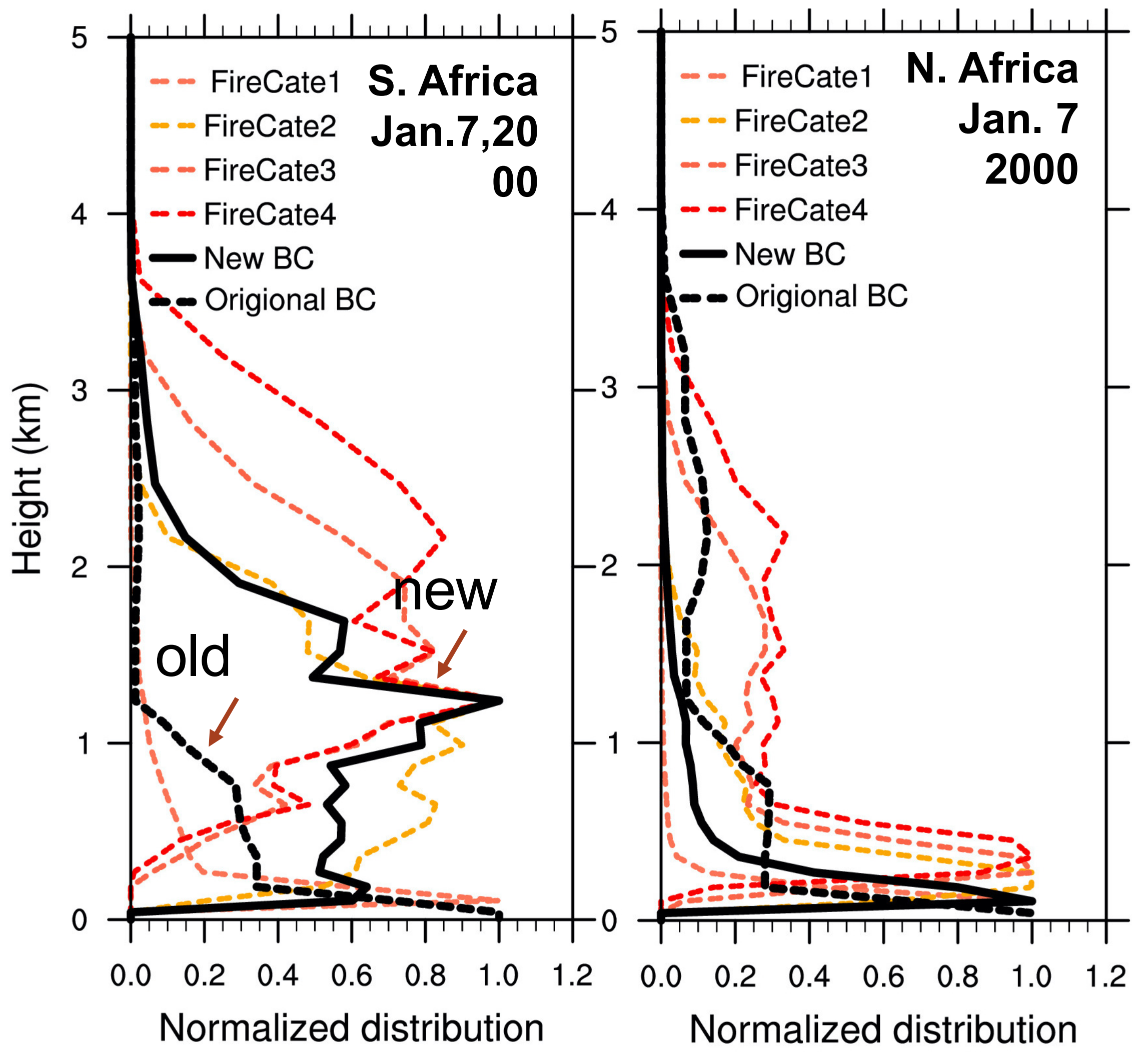
New capabilities and scientific significance

- 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:

- Evaluate the plume-rise model with 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

See more details in Xiaohong Liu's poster

Fully prognostic treatment of cloud-borne aerosols

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

Motivation

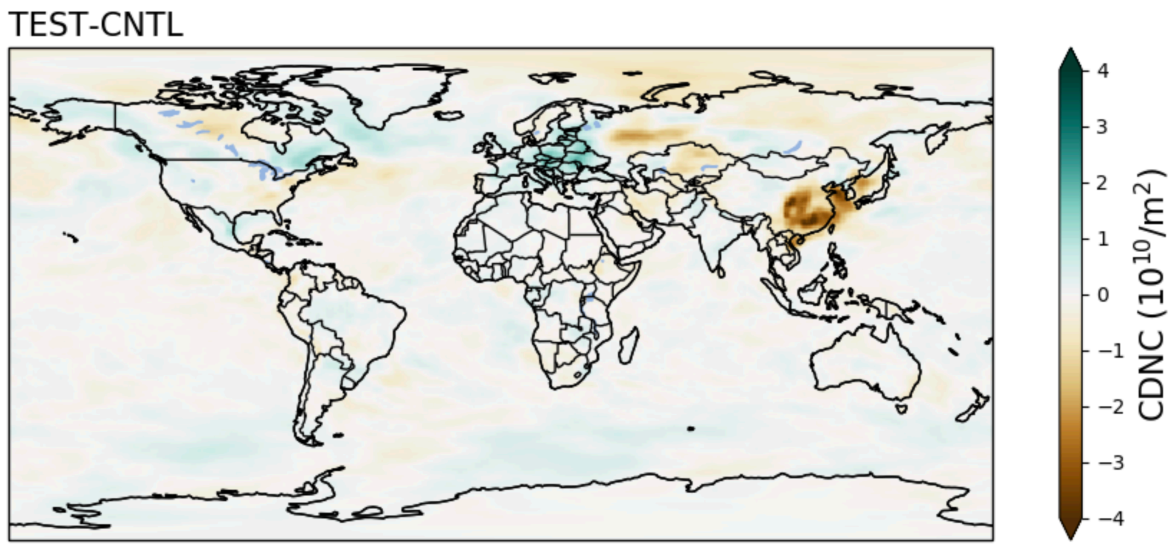
- The treatment of neglecting the advection of cloud-borne aerosols is designed for coarse-resolution models. At convection-permitting scales, this treatment is expected to produce large errors.

Approach

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

Next Steps:

- Run RRM to 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

See more details in Guangxing Lin's poster

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

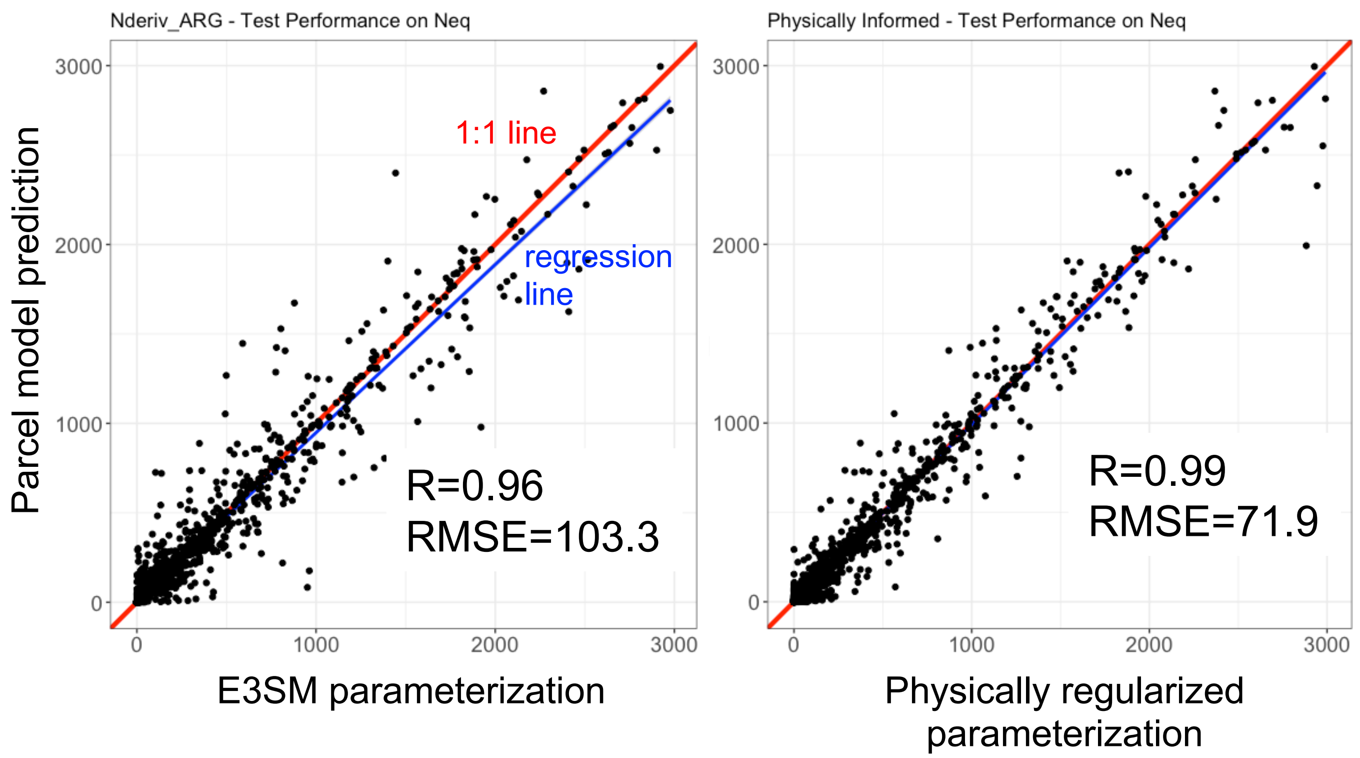
- Use various machine learning techniques to emulate activation from cloud parcel model
- Implement the emulator in E3SM using the Fortran-Keras Bridge (FKB) library

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

Next Steps:

- Extend from the single mode to multi mode treatment of aerosols when building the emulator
- 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.

More details in Sam Silva's oral presentation and Balwinder Singh's poster

Improving the turbulence effects on activation

Brian Griffin and Vince Larson

Objective

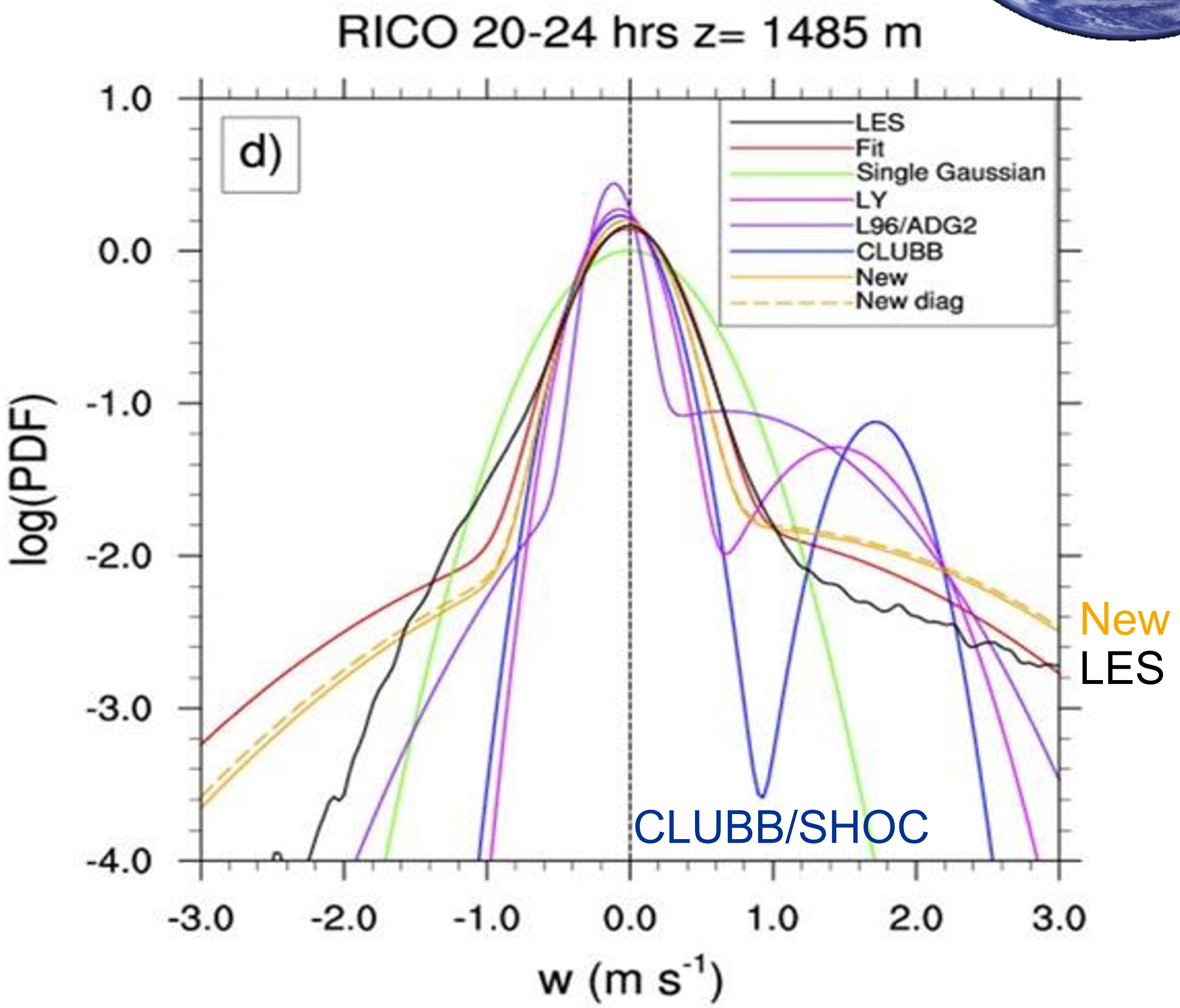
- To improve the parameterization of subgrid-scale updrafts that drive aerosol activation

Approach

- Improve the subgrid-scale double Gaussian PDF shape of velocity that is used by CLUBB and SHOC
- Sample the velocity PDF and feed them into aerosol activation

New capabilities and scientific significance

- A new multivariate, double-Gaussian PDF shape is being developed that represents strong updrafts more realistically
- Non-interactive convergence tests using an increasing number of samples has been carried out.



New updrafts PDF agrees better with LES

See more details in Brian Griffin and Vince Larson's poster

A high-performance aerosol library

Jeff Johnson, Pete Bosler, Balwinder Singh, Hui Wan

Objective

- Develop a modern software package for aerosols

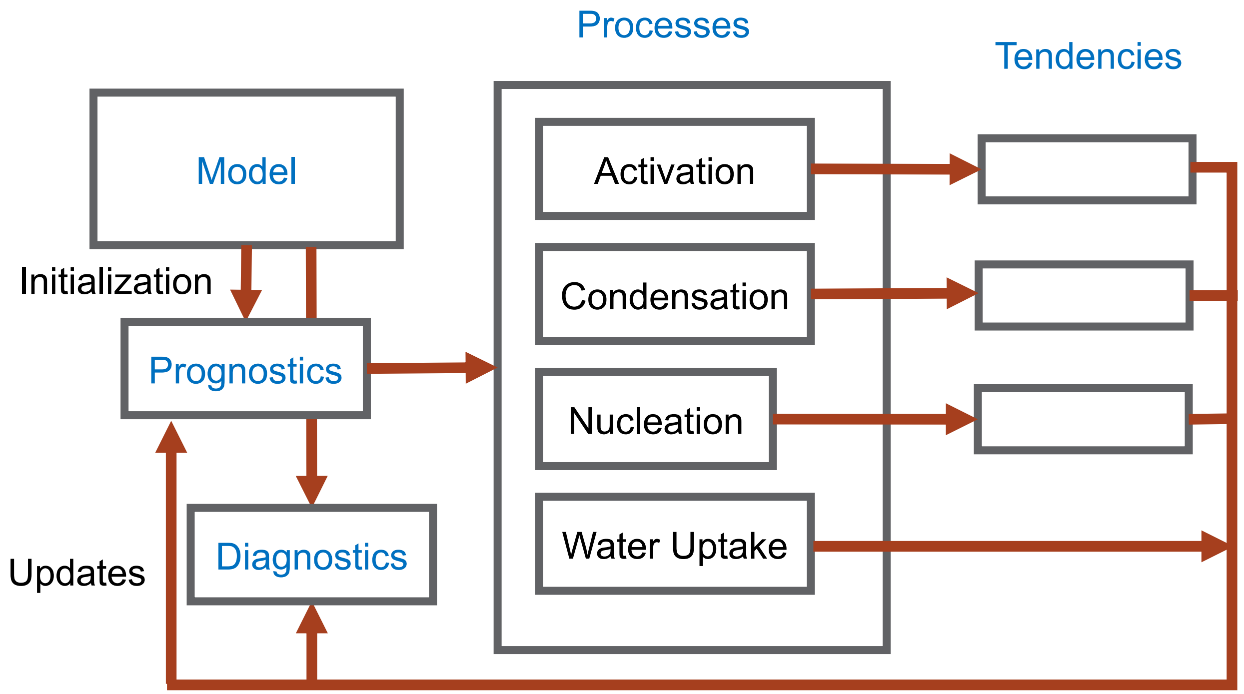
Approach

- Develop a set of building blocks (library) and a driver to verify their correctness and performance

Software design

- Model – Stores parameters that define the physical characteristics of an aerosol system and the surrounding atmosphere
- Prognostics – Stores prognostic variables that define the system's instantaneous physical state (similar to physics_state)
- Diagnostics – Stores diagnostic variables needed by various parameterizations (similar to physics_buffer)
- Tendencies – Stores time derivatives for prognostic variables at a given time (similar to physics_ptend). Accumulated into Prognostics during time integration
- Process – Implements a parameterization that computes tendencies or updates diagnostics for a state at a given time

Host Atmosphere Model



The host model assembles building blocks, allowing parameterization transplant!

See more details in Jeff Johnson's poster

Integrating observationally based process-oriented constraints for ACI in model development

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

Goal

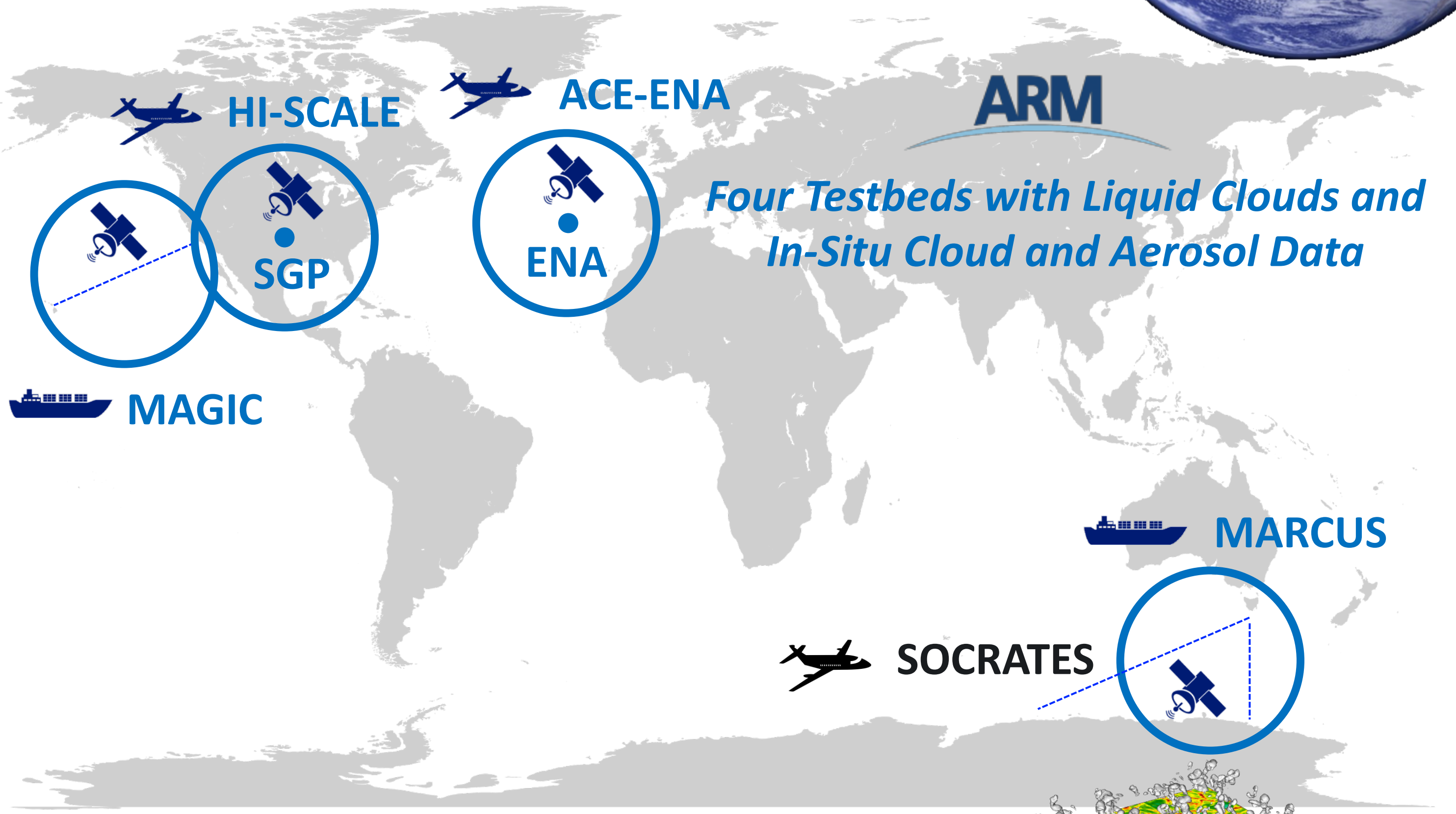
- Develop emergent constraints for ACI
- Routinely use emergent constraints to keep track of their evolution through model development

Approach

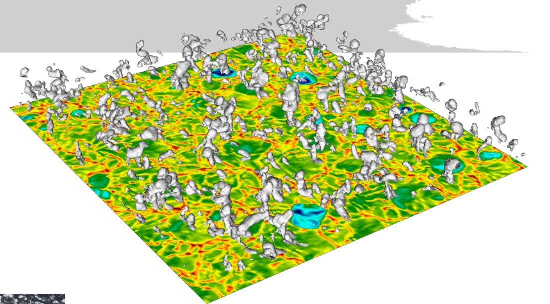
- Develop an open source Python package to evaluate ACI in Earth system models across scales.
- Combine ARM site, aircraft, ship, and satellite data to analyze meteorology, radiation, liquid clouds, and aerosol statistics and relationships
- Use machine learning techniques to develop ACI metrics

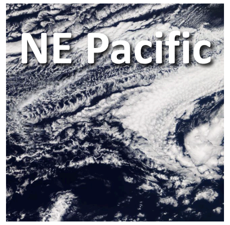
Next Steps

- Assess predictability of each metrics
- Routine evaluation provides insights into model development



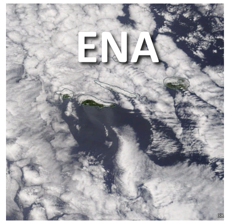
LES cases at all four testbeds that provide extensive information needed for parameterization development and evaluation





transitions in Sc to trade-wind Cu regimes

continental convective clouds with high aerosol concentration



diverse subtropical marine BL clouds susceptible to aerosol

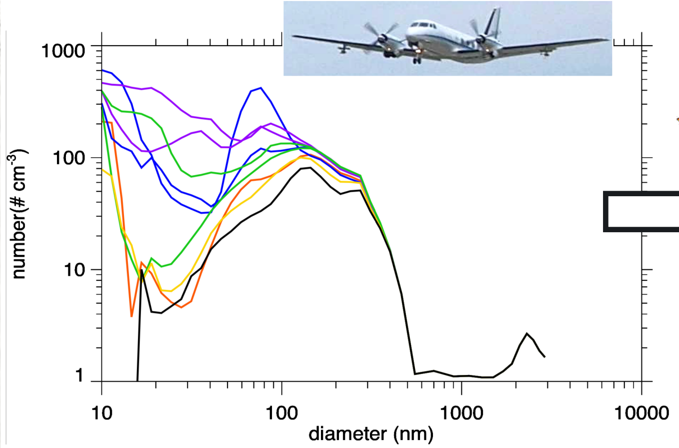
marine BL clouds with low aerosol concentrations

More details in Adam Varble’s oral presentation in D4S1 BR4 (Aerosols breakout session)

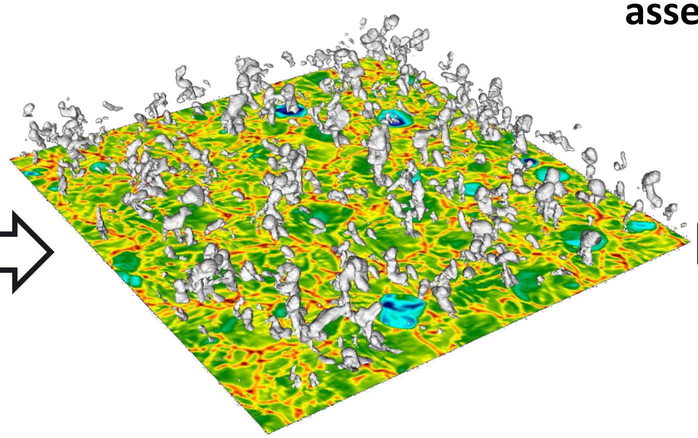
Use large eddy simulations to provide guidance for Earth system model development

Kyle Pressel, Colleen Kaul, Jacob Shpund, Jiwen Fan, Mikhail Ovchinnikov, Po-Lun Ma, et al

Objective: Develop robust data sets using large eddy simulation (LES) for machine learning emulation, parameterization development, and model evaluation

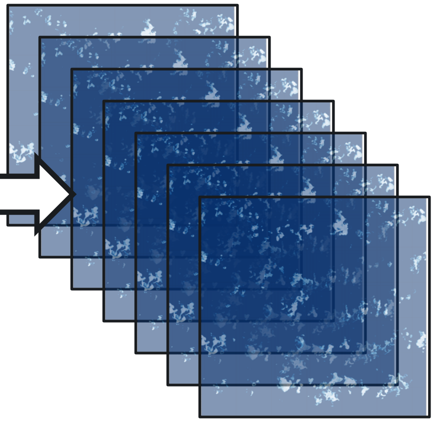


Observed Aerosol Size Distribution



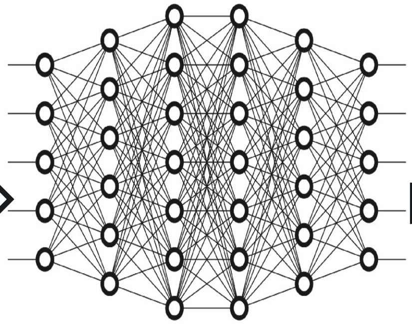
Simulated SGP Boundary Layer Clouds and ACI

assess fidelity using ARM data



Training Dataset:

multiple cases: coupled vs uncoupled boundary layer, different seasons, range of aerosol conditions, etc.



Machine Learning Emulation

Computationally Efficient Treatments

E3SM
Energy Exascale Earth System Model

Approach

- Develop a new computationally efficient LES model, **P**redicting **IN**teractions of **A**erosol and **C**louds in **L**arge **E**ddy **S**imulation (**PINACLES**), at least 10x faster than WRF-LES, coupled with spectral bin microphysics (**SBM**)

Next steps

- Complete the **large LES ensemble** to provide robust data sets for a wide range of aerosol, cloud, and meteorological regimes
- Evaluation against ARM data (in addition to other LES cases)
- Use **deep neural network** to emulate cloud, precipitation, and and turbulence characteristics
- Use LES to evaluate E3SM

More details in Kyle Pressel's poster and Colleen Kaul's poster

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