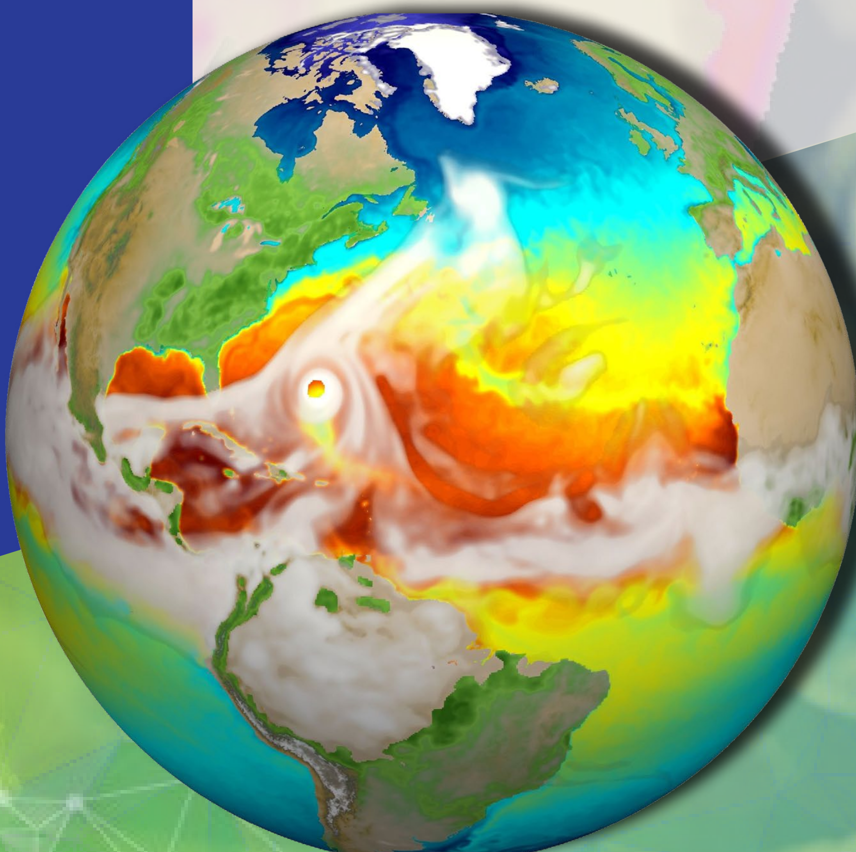
E3SM
Energy Exascale
Earth System Model

Earth System Model Development – Energy Exascale Earth System Model

2020 PRINCIPAL INVESTIGATOR MEETING REPORT



U.S. DEPARTMENT OF ENERGY | Office of Science

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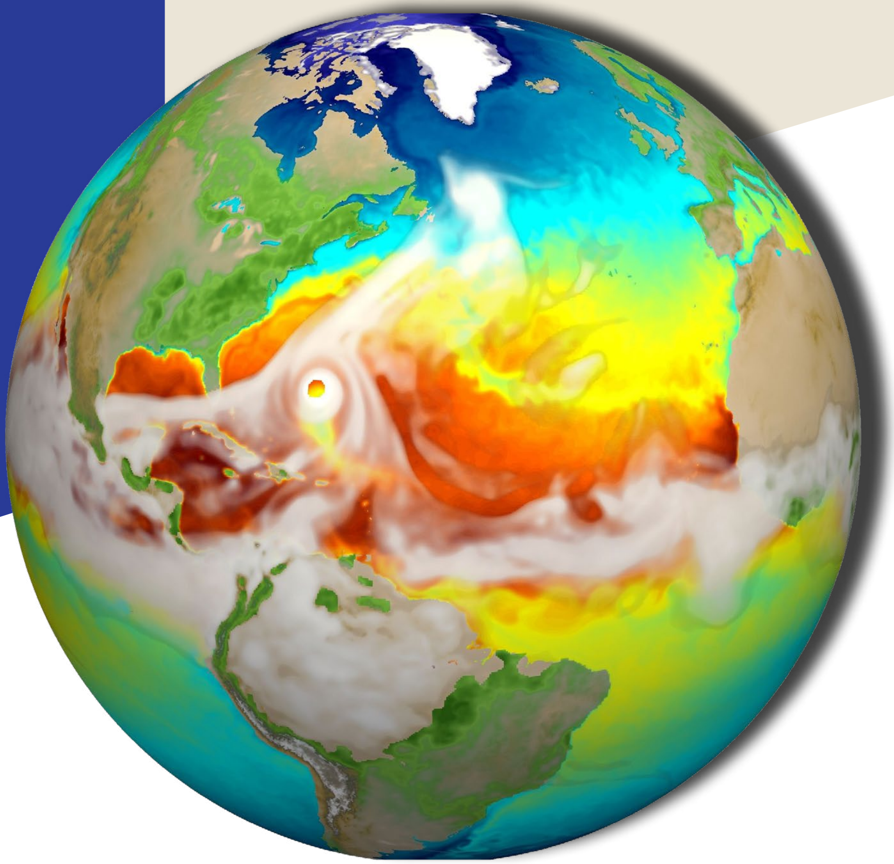

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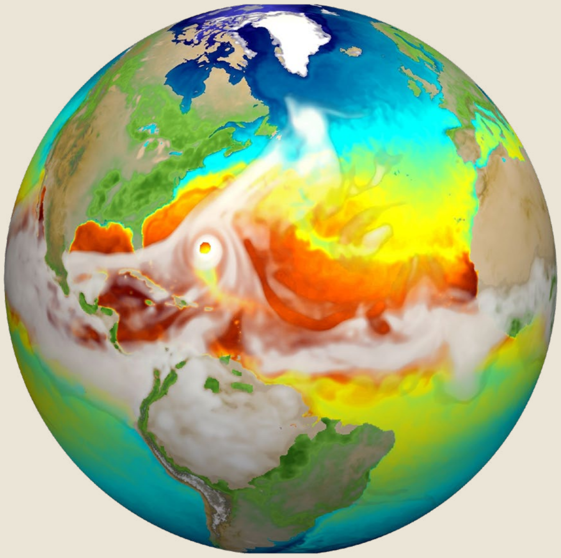
EARTH SYSTEM MODEL DEVELOPMENT – ENERGY EXASCALE EARTH SYSTEM MODEL

2020 PRINCIPAL INVESTIGATOR MEETING REPORT



Convened by

U.S. Department of Energy
Office of Science
Biological and Environmental Research Program

October 26 – 29, 2020

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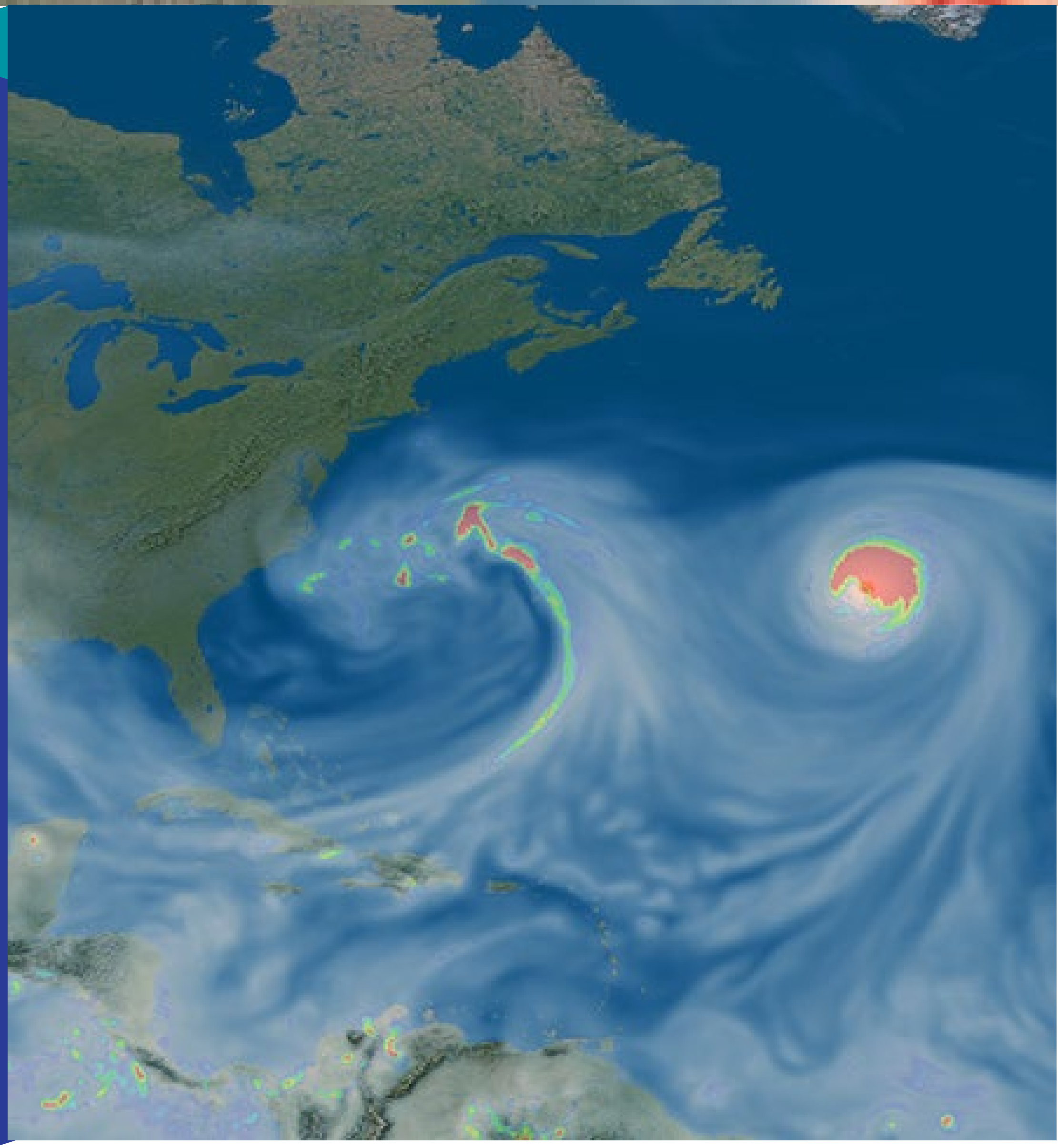

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The meeting organizers and Steering Committee would like to thank all the scientists who energetically participated in the meeting discussions and generously contributed their time and ideas to this important activity for the U.S. Department of Energy's Office of Biological and Environmental Research. We would like to specifically thank the speakers who gave keynote and invited talks (Nils Wedi, Oliver Fuhrer, Walter Hannah, Mike Pritchard, Laure Zanna, Nicole Riemer, and Baylor Fox-Kemper), and those who served as session co-chairs (Ben Bond-Lamberty, Peter Bosler, Susannah Burrows, Peter Caldwell, Kate Calvin, Anand Gnanadesikan, Chris Golaz, Matthew Hoffman, Jennifer Holm, Rob Jacob, Phil Jones, Vince Larson, Wuyin Lin, Zhengyu Liu, Po-Lun Ma, Mark Petersen, Robert Pincus, Steve Price, Mike Pritchard, Jim Randerson, Andrew Roberts, Andy Salinger, Sarat Sreepathi, Qi Tang, Peter Thornton, Luke Van Roekel, Hui Wan, and Shaocheng Xie). We are thankful to the Oak Ridge Institute for Science and Education (ORISE); Holly Davis, E3SM Communication Specialist and E3SM Managing Editor; and Tanya Reshel, E3SM Communication Team, LLNL, for organizing the logistics and supporting workshop participants during the meeting. The report was prepared by the E3SM Communications Team at Lawrence Livermore National Laboratory with assistance from LLNL's TID Department, for which we are thankful.

EXECUTIVE SUMMARY

As part of the U.S. Department of Energy (DOE) Office of Biological and Environmental Research (BER), the Earth System Model Development (ESMD) program area supports significant research in Earth system model development, including major efforts in the Energy Exascale Earth System Model (E3SM) project. Convened virtually on October 26–29, the 2020 ESMD-E3SM Principal Investigator (PI) Meeting provided a forum to survey ESMD sponsored research, recent progress made by the ESMD science team and the broader Earth system modeling community within and outside of DOE, foster interactions across ESMD projects, and discuss research gaps and opportunities for future advancements.

Besides E3SM, ESMD is also supporting three major coordinated efforts led by DOE labs (Enabling Aerosol-cloud interactions at GLobal convection-permitting scalES (EAGLES), Interdisciplinary Research for Arctic Coastal Environments (InteRFACE) and Integrated Coastal Modeling (ICoM)), eight projects under Scientific Discovery through Advanced Computing (SciDAC)—a partnership between BER and the Advanced Scientific Computing Research (ASCR) program—and thirteen university projects, as well as two early-career award projects. The virtual format of the meeting promoted broader participation, with more than 300 attendees and about 200 oral and poster presentations.

DOE program managers kicked off the first day of the meeting with overviews of DOE's Earth and Environmental Systems Science Division (EESSD), the three program areas of the Earth and Environmental System Modeling (EESM) program—ESMD, Regional and Global Model Analysis (RGMA), and MultiSector Dynamics (MSD)—and the Data Management (DM) activity. The first and second days of the meeting featured the E3SM project, a major DOE investment in Earth system modeling with over 120 project team members across eight DOE national laboratories and several universities. The E3SM executive committee and leadership team presented overviews of the project, its science and computational goals, and the current status and future directions of the core groups and next generation development (NGD) subprojects. These presentations provided the backdrop for facilitating interactions between the E3SM project and other projects across the ESMD portfolio, many of which are contributing to developing or improving components of the E3SM model. The second and third days featured overviews and updates from the DOE lab-led projects, SciDAC projects, university projects, and early-career award projects on modeling wide-ranging processes in the Earth system. The meeting also featured two keynote talks and two invited presentations highlighting important advances in global cloud-resolving modeling in the international and broader DOE Earth system modeling community, using different approaches. Besides oral presentations, scientists across ESMD presented posters showcasing more specific aspects and the scientific and technical progress of the projects.

Taking advantage of the broad participation of the ESMD science team, the meeting provided ample time for breakout discussions. While some breakout sessions focused on components of Earth system models (atmosphere, ocean, land), others focused on coupled processes of the Earth system (water cycle, biogeochemistry, cryosphere), and crosscutting topics (computational science, machine learning/artificial intelligence). The challenges, opportunities, and needs discussed in the breakout sessions provide useful information for guiding future directions in ESMD research. By summarizing the oral presentations and breakout discussions and including the presentation slides, posters, and abstracts, this report is intended to be a valuable resource for the meeting participants and the broader Earth system modeling community.

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INTRODUCTION

The present report is based on a meeting convened virtually on October 26–29, 2020, in response to a need for communication and coordination of activities among the U.S. Department of Energy's (DOE) Office of Biological and Environmental Research (BER) Earth System Model Development (ESMD) program area and Energy Exascale Earth System Model (E3SM, https://e3sm.org) project. The purpose of the meeting was to present an overview and foster interactions between the E3SM project and its "Ecosystem" projects that ESMD supports, i.e., the ESMD projects that work on an aspect of E3SM or work with E3SM data or perform E3SM simulations.

More than 300 U.S. and international scientists attended the meeting and researchers presented a record number of studies—about 200. The meeting started with an introduction to the structure of BER's Earth and Environmental Systems Sciences Division (EESSD) and an overview of the ESMD program area, followed by an update and status report from the E3SM project. The E3SM Executive Committee presented a high-level overview of the project and each of the E3SM groups gave a status report on their progress. Next, the Ecosystem projects presented their work and goals. Throughout the meeting, there were several invited talks and two longer, keynote talks. There was also time for several breakout sessions focused on challenges, opportunities, and needs in different model components (like atmosphere, ocean, land, and computation), as well as breakouts focused around the E3SM groups and their goals and challenges.

The virtual meeting was held through Zoom sessions, with discussions encouraged over dedicated Slack channels. The discussion of posters during the designated poster sessions occurred on Slack channels organized by topic, culminating in participants voting for the Best Poster Award. Additionally, four people received the E3SM Outstanding Achievement Award. Continuing the tradition of home-grown entertainment, the E3SM band, the Deep Dives, performed three songs which had been previously recorded.

OVERVIEW OF BER EESSD PROGRAMS

Xujing Davis, program manager of the Earth System Model Development (ESMD) program area, briefly welcomed meeting participants on behalf of the PI-meeting steering committee. She concisely described (Presentation-1 – Davis) the role of ESMD at DOE as one of the three program areas (with Regional & Global Model Analysis [RGMA]) and MultiSector Dynamics [MSD]) in the Earth and Environmental System Modeling (EESM) program. EESM is part of the Earth and Environmental Systems Sciences Division (EESSD), led by Gary Geernaert under the Office of Science's Biological and Environmental Research (BER) Office, managed by Sharlene Weatherwax (see Figure 1).

EESSD: Earth and Environmental Systems Science Division, Gary Geernaert

Gary Geernaert, director of EESSD, kicked off the meeting with his **welcoming remarks**. He pointed out that the national labs are tackling some of the most difficult modeling and prediction challenges facing DOE and the nation. He also noted that the progress and priorities associated with lab discussions and workshops over the next couple of years will likely influence the content of the division's strategic plan. Because **machine learning (ML)** is highly likely to be a component in the next plan, Geernaert also expressed that ML is not a cure for everything but its promise is worth exploring. He is willing to initiate that process. He thanked everyone for all the hard work they have contributed during the past year. He ended on a very positive note, stating that he expects that team members will keep up their momentum and imaginations as a way to drive the future and keep efforts focused. He is excited about the direction in which the program is heading.

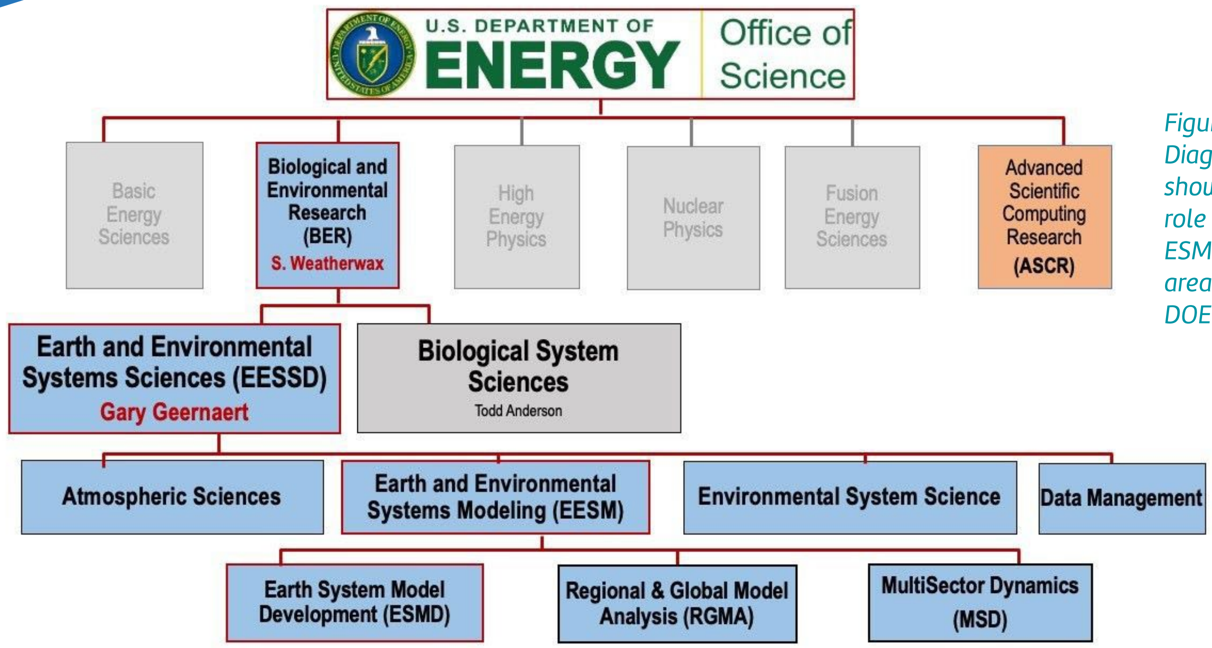


Figure 1. Diagram showing the role of the ESMD program area within the DOE structure.

ESMD: Earth System Model Development, Xujing Davis

Xujing Davis followed Geernaert's remarks by presenting an **Overview of the Earth System Model Development (ESMD) Program Area** (Presentation-1 - Davis) including its goal, strategies, portfolio, and future vision. The goal of EESM (ESMD, RGMA, and MSD) is to develop and demonstrate advanced modeling and simulation capabilities, to enhance the predictability of the Earth system over multiple temporal and spatial scales. Within this scope, the goal of ESMD focuses on the development of the Energy Exascale Earth System Model (E3SM) and its subcomponents to address the grand challenge of actionable predictions of the changing Earth system, emphasizing the most critical scientific questions facing the nation and DOE. To fulfill this goal, ESMD supports research activities via three types of funding instruments: (1) Scientific Focus Areas (SFAs) led by DOE labs; (2) university awards via Funding Opportunity Announcements (FOAs) and (3) Scientific Discovery through Advanced Computing (SciDAC) projects, which is a partnership between BER and the Advanced Scientific Computing Research (ASCR) program.

ESMD's FY20 budget is $44 M. The current portfolio mainly includes:

- **Four SFAs** (**E3SM**, Enabling Aerosol-cloud interactions at GLobal convection-permitting scalES (**EAGLES**), Interdisciplinary Research for Arctic Coastal Environment (**InteRFACE**) and Integrated Coastal Modeling (**ICoM**)),
- **Eight SciDAC projects** and
- **Thirteen university awards**.

See the ESMD Program Area Projects and Presentation Links appendix for more details, including additional ESMD-related nonstandard projects like the Early Career Awards, the Land Climate Process Teams (CPTs), and the Community Emissions Data System (CEDS).

As Figure 2 shows, the E3SM SFAs account for 62% of the ESMD budget and are the central drivers for E3SM development, with focused scientific questions and well-defined short and long term goals and strategies. The E3SM project consists of scientists from eight DOE labs and multiple universities. Advances from other ESMD projects contribute to E3SM developments in various ways on different time frames. Other SFAs (i.e., non-E3SM SFAs) aim to either tackle challenges in E3SM development (e.g., EAGLES is working on the parameterization of aerosols and aerosol-cloud interactions) or address DOE emerging priorities (e.g., InteRFACE and ICoM are addressing coastal processes). DOE entrains fresh knowledge and talent from the academic community through university awards. The SciDAC projects focus on developing innovative computational methods, tools, and algorithms for Earth System Models via collaborations among researchers in Earth science and computational science.

Davis introduced the ESMD projects in detail, including the major achievements of the four SFAs during the past year. She noted the date of the overview presentations of all the projects in the meeting agenda and congratulated the two ESMD PIs/E3SM scientists, Mathew Hoffman from LANL and Benjamin Sulman from ORNL, who received the prestigious DOE Early Career Awards.

Finally, Davis described the role of ESMD at DOE and in the US and global environment. She noted some of the collaborative research activities between ESMD and other DOE programs, as well as other agencies and international entities. She envisioned that ESMD will continue to support E3SM development by:

1. strengthening E3SM's core effort, not only within ESMD itself, but also in conjunction with RGMA and MSD in EESM;
2. enhancing E3SM's integration with other DOE programs within EESSD and ASCR; and
3. further coordinating and collaborating with US and global institutions and organizations.

By doing this, ESMD will continue to contribute to national and global endeavors in advancing Earth system modeling capability and Earth system predictability while addressing DOE's mission.

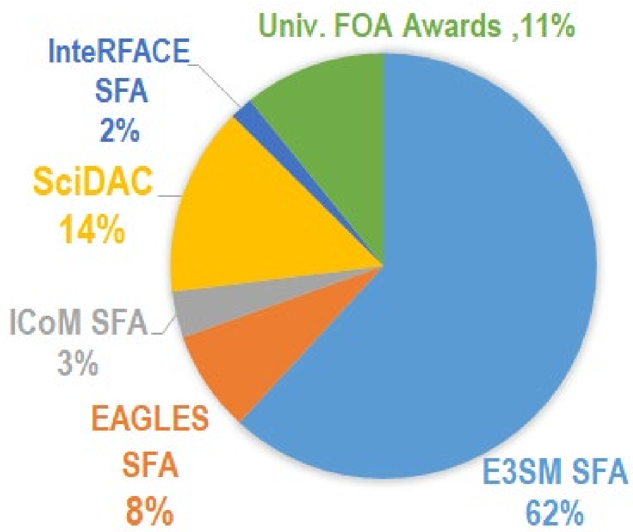


Figure 2. Breakdown of ESMD Fiscal Year 2020 (FY20) Budget.

RGMA: Regional & Global Model Analysis, Renu Joseph

There are three program areas within the Earth and Environmental System Modeling (EESM) program: Earth System Model Development (ESMD), Regional & Global Model Analysis (RGMA), and MultiSector Dynamics (MSD). Together, these program areas aim to develop and demonstrate advanced modeling and simulation capabilities to enhance the predictability of the Earth system over multiple temporal and spatial scales (Fig. 3). In this session, program managers from RGMA, MSD as well as the crosscutting Data Management (DM) activity presented an overview of the research activities in their program areas and some linkages with ESMD activities.

An **Overview of RGMA** was presented by **Renu Joseph** (Presentation - Joseph), the program manager of projects in the RGMA portfolio. The goal of the RGMA program area is to enhance predictive and process-level understanding of variability and change in the Earth system by advancing capabilities to design, evaluate, diagnose, and analyze global and regional Earth-system models informed by observations. To address science-relevant questions, RGMA projects use a multimodel approach centered on E3SM and a hierarchy of models of varying levels of complexity.

Over the past 10 years, the RGMA budget has been relatively flat. RGMA projects are highly productive, with a publication rate of about 120 peer-reviewed papers per year.

The RGMA portfolio consists of (1) Scientific Focus Areas (SFAs), which are large projects led by a DOE National Laboratory or joint collaborations between a DOE National Laboratory and academia; (2) cooperative agreements; and (3) university-led projects funded through Funding Opportunity Announcements (FOAs) and jointly-funded interagency projects. The science themes addressed by these projects include (a) water cycle, (b) extreme events, (c) variability and change, (d) high-latitude feedbacks, (e) cloud processes, and (f) analysis of biogeochemical feedbacks.

The following projects represent the core activities of the RGMA portfolio:

1. **Water Cycle and Climate Extremes Modeling (WACCEM):** designed to advance robust predictive understanding of water-cycle processes and hydrological extremes and their multidecadal changes
2. **Calibrated and Systematic Characterization, Attribution, and Detection of Extremes (CASCADE):** designed to advance understanding of natural and anthropogenic influences on multiscale climate extremes in observations and models
3. **Reducing Uncertainty in Biogeochemical Interactions through Synthesis and Computation (RUBISCO):** designed to identify and quantify interactions between biogeochemical cycles and the Earth system and quantify and reduce uncertainties in Earth system models (ESMs) associated with these interactions
4. **High-Latitude Application and Testing (HiLAT-RASM):** designed to reduce uncertainty in modeling and enhance predictive understanding of high-latitude and environmental change and its global consequences
5. **Program for Climate Model Diagnosis & Intercomparison (PCMDI):** designed to measure model performance, reduce uncertainties in their predictions,

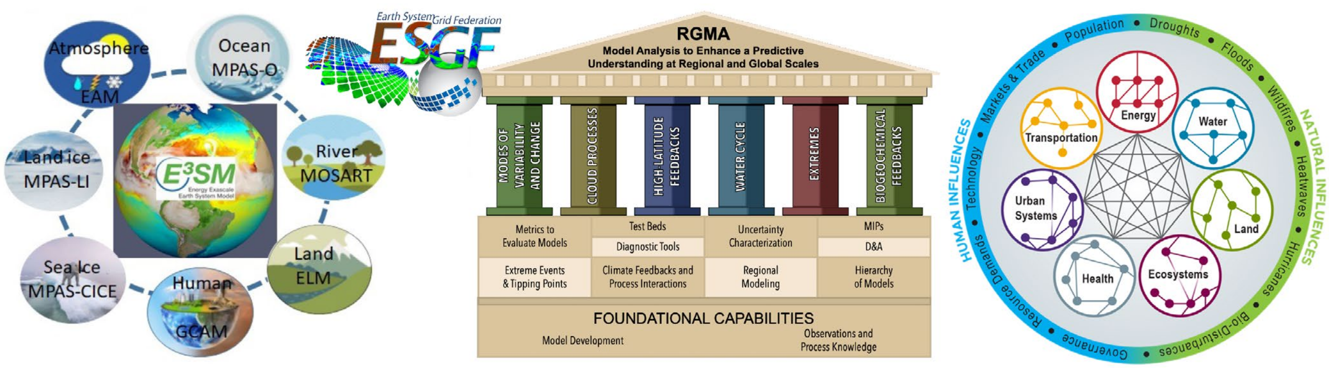


Figure 3. The three program areas within the EESM: ESMD (left), RGMA (center) and MSD (right). The Earth System Grid Federation (ESGF) is a Scientific Focus Area (SFA), supported by the DM activity, which is closely related to EESM. The goal of EESM is to develop and demonstrate advanced modeling and simulation capabilities in order to enhance the predictability of the Earth system over multiple temporal and spatial scales.

and determine the pathways for their improvement using model ensembles of today and tomorrow

6. **Cooperative Agreement To Analyze variability, change and predictability in the Earth SysTem (CATALYST):** designed to perform foundational research toward advancing a robust understanding of modes of variability and change using models, observations, and process studies
7. **Interdisciplinary Research For Arctic Coastal Environments (InteRFACE):** designed to understand how the coupled, multiscale feedbacks among land processes, sea ice, ocean dynamics, coastal change biogeochemistry, atmospheric processes, and human systems will control the trajectory and rate change across the Arctic coastal interface
8. **Integrated Coastal Modeling (ICoM):** designed to understand the impact of large-scale drivers of extreme hydrological events, surface-atmosphere interactions on coastal processes, and their long-term changes
9. **A Framework for Improving Analysis and Modeling of Earth System and Intersectoral Dynamics at Regional Scales (HyperFACETS):** designed to understand how well ESMs, integrated human–Earth system models, and available datasets perform for relevant quantities and what drivers and processes are the most important in ensuring model performance

These core activities benefit from university projects developed in collaboration with DOE labs to enhance lab activities.

The relationship between the RGMA projects and ESMD activities can be described as a two-way street: (1) the advanced capability of E3SM and its simulations from ESMD can be used by RGMA projects to address their science goals and (2) new RGMA knowledge can benefit E3SM development.

A survey of researchers working on RGMA projects revealed that E3SM is being used to address science questions related to (a) modes of climate variability (e.g., air-sea interaction and MJO, ENSO and connections to other modes of variability, AMOC and high-latitude variability), (b) the Arctic and Antarctic (e.g., heat transport, connections to lower latitudes, polar amplification, sea-ice loss, delivery of warm water to Antarctic and Greenland ice shelves, storm regions, permafrost, benthic habitats, and wave attenuation in coastal regions), (c) tropical cyclones (e.g., African easterly waves, factors controlling landfalling and genesis) (d) extreme precipitation and weather events (e.g., processes controlling extreme precipitation, impacts of model biases and resolution on simulation of weather extremes, and future changes), clouds and radiation (e.g., ITCZ and cloud-radiative interactions, the role of dynamics-radiation coupling on weather extremes and climate sensitivity), and (e) biogeochemistry (e.g., ocean carbon uptake, carbon-cycle feedback, the CO_2 fertilization effect, and the impacts of plant biogeochemical responses on water-cycle processes).

RGMA projects conduct model intercomparison studies and contribute to CMIP6 experiments by evaluating how E3SM simulations compare with other simulations from coordinated model experiments (e.g., DECK and HighResMIP) as well as other model simulations (e.g., WRF-Arctic, ATS-MOSART, UK Met Office Unified Model, RASM, and UWIN-CM).

The HiLAT-RASM project has been developing a version of E3SM with a high-resolution grid over the Arctic. This configuration shows promising results with respect to key metrics.

The Catalyst project, in collaboration with a university project focused on multiyear predictability and prediction in ocean eddy-resolving coupled models, will conduct initialized predictions with E3SM.

To develop a fundamental understanding and synthesis of the mechanisms that energize Pacific decadal variability in ESMs, RGMA researchers are contributing an E3SMv1 large ensemble. The ensemble is generated using a unique initialization strategy.

The RUBISCO project is applying different versions of E3SM to address questions related to deforestation/afforestation, AMIP-style ENSO simulations, and LS3MIP offline land simulations with multiple atmospheric reanalysis and factorial forcing.

RGMA researchers have been developing integrated tools and science for event analysis, packaged as the Coordinated Model Evaluation Capabilities (CMEC). CMEC allows any ESM output saved in the Climate Model Output Rewriter (CMOR) format to be compared with observations or other models using any or all community evaluation toolkits, such as TECA (Toolkit for Extreme Climate Analysis), PMP (PCMDI Metrics Package), and ILAMB/IOMB (International Land Model Benchmarking/International Ocean Model Benchmarking).

To facilitate easy access to CMIP6 model output and observations, RGMA researchers organized a collection of selected variables on NERSC's high performance computers (HPC) and made it available to DOE-supported projects.

MSD: MultiSector Dynamics, Bob Vallario

The MultiSector Dynamics (MSD) program area was presented by **Bob Vallario** (Presentation - Vallario), the program manager of projects in MSD in Earth and Environmental System Modeling (EESM). The goal of the MSD program area is to explore the complex interactions and potential coevolutionary pathways within the integrated human–Earth system, including natural, engineered, and socioeconomic systems and sectors. To achieve this goal, the program identified three strategic objectives: (1) Identify forces and patterns that reveal the combination of factors, varying by geographies, that contribute most significantly to patterns of development in transregional, regional, and subregional landscape evolutions, including interactions and interdependencies among natural and built environments and human processes and systems; (2) Identify the characteristics of interacting natural and built environments and human processes that lead to stabilities and instabilities across systems, sectors, and scales, and deliver new insight into the role of strong interdependencies, feedbacks, and compounding influences and stressors; (3) Explore how development patterns, stabilities, instabilities, and system resilience may evolve within multisector, multiscale landscapes as a result of future forces, stressors, and disturbances, and reveal what pathways, characteristics, and risk profiles may emerge from gradual and abrupt transitions.

MSD research priorities include domain emphases on (a) coastal dynamics, (b) integrated water cycle, (c) connected infrastructure, (d) urban/landscape morphology, and (e) resource development. Priorities within MSD include development and use of

- Functional, collaborative community-of-practice and working group structure;
- Hierarchical frameworks and use-inspired tools (emulators and sensitivity research);
- Distributed science mechanisms (i.e., open-source models, software couplers, interoperability, modular methods, community data and computation);
- Complexity-theory science (e.g., networks, collective behavior, evolution and adaptation, pattern formation, systems theory, and machine learning);
- Scenario methods and development with implications for uncertainty framing/analysis, complex storylines, and modeling experiments;
- Model resolution fit-for-purpose details across spatial and temporal scales (e.g., energy, water, land, economics, population, land use, and technology); and
- Significant coupled-systems behaviors, such as those found among energy, water, land, and socioeconomic systems with nonlinear responses, e.g., induced extremes.

MSD projects consist of two Scientific Focus Areas (SFAs), two projects led by individual DOE national laboratories, and three university cooperative agreements:

1. **Integrated Multisector, Multiscale Modeling** SFA (IM3): focused on understanding the evolution, vulnerability, and resilience of interacting human and natural systems and landscapes due to long-term influences and short-term shocks, from local to regional scales
2. **Global Change Intersectoral Modeling System** SFA (GCIMS): focused on the long-term evolution of the coupled human–Earth system at regional to global spatial scales and seasonal to multidecadal timescales, including the interplay between influences, responses, and feedbacks and linkages within E3SM
3. **Integrated Coastal Modeling** (ICoM): designed to deliver a robust predictive understanding of coastal evolution that accounts for the complex, multiscale interactions among physical, biological, and human systems, including interactions involving coastal development, critical infrastructure, natural systems, adaptations, and resulting risk and resilience
4. **Interdisciplinary Research for Arctic Coastal Environments** (InteRFACE): focused on enhancing the understanding of interactions between natural and societal changes in the Arctic such as the coevolution of transportation, resources development, and human systems (Fig. 4)
5. **Program on Coupled Human–Earth Systems** (PCHES): ffocused on building a next-generation integrated suite of science-driven modeling and analytic capabilities and a more expanded and connected community of practice, for analysis of compound stressors related to

integrated energy–water–land systems dynamics and interdependent structures

6. **Integrated Global System Modeling** (IGSM): designed to develop a multi-system modeling framework to explore compounding stressors and tipping points at regional scales, with a particular focus on land-use and land-cover change, water resources, and potential energy-systems and transportation-sector transitions

7. **A Framework for Improving Analysis and Modeling of Earth System and Intersectoral Dynamics at Regional Scales** (HyperFACETS): designed to advance scientific understanding of processes at the atmosphere–water–energy–land interface to fundamentally improve the ability to perform credible climate modeling of particular regions and processes relevant to those regions and to strengthen stakeholder input in model development evaluation

MSD and ESMD are linked by the direct participation of personnel in activities supported by the two program areas (e.g., the chief scientist for MSD's GCIMS SFA is a task leader for E3SM, the E3SM chief scientist is one of the HyperFACETS' co-PIs, and the ESMD program manager is invited as a speaker/panelist at MSD meetings) as well as common science goals such as

- Fine-scale work in IM3 (perennial bioenergy crops for the Community Terrestrial Model), now being adopted for the land component, ELM, in E3SM;
- The Global Change Analysis Model (GCAM), developed by GCIM provides emissions and land-use data to E3SM and E3SM provides productivity information to GCAM; and
- Plans to link GCAM's water components in E3SM.

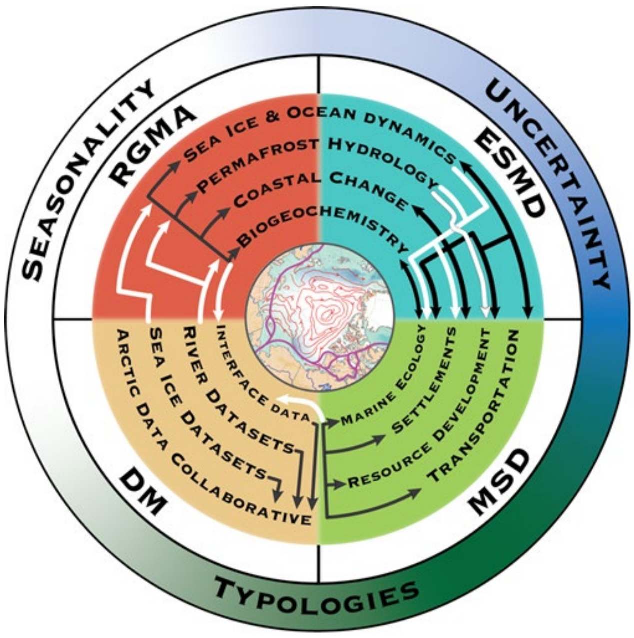


Figure 4. Schematic diagram showing how the ESMD, RGMA, MSD program areas and DM activity work together to support the InteRFACE SFA.

DM: Data Management, Jay Hnilo

The **Data Management (DM) program area** was presented by **Jay Hnilo** (Presentation - Hnilo), the program manager of projects in the Data Management portfolio. The massive volumes of data resulting from modeling and observational activities within DOE's Environmental System Science projects and the demand for data security require coordinated efforts for archiving and dissemination. DM activity supports the Earth System Grid Federation (ESGF) and the Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) projects.

ESGF is an international collaboration that manages the first-ever decentralized database for handling climate science data, with multiple petabytes of data at dozen of federated sites worldwide. It supports the Coupled Model Intercomparison Project (CMIP), whose protocols enable periodic assessments carried out by the Intergovernmental Panel on Climate Change (IPCC). ESGF uses a system of geographically distributed peer nodes (> 70) which are independently administrated, yet united by common protocols and interfaces. ESGF has more than 2,500 science users per year. The number of publications using data stored by ESGF is about 750 annually.

The data archives managed by ESGF include

- The IPCC CMIP3 and CMIP5 archive used in the IPCC AR4 and AR5 reports and the CMIP6 data archive used in the upcoming IPCC AR6 report;
- Multimodel datasets managed and distributed by the BER-funded PCMDI project;
- The DOE E3SM project, which currently distributes 330 TB of model output publicly to researchers; and
- The input4MIPs and obs4MIP data sets managed and distributed by PCMDI.

Between September 2019 and September 2020, users downloaded 135,637,177 files, with a total size of 9.5 PB. The users were distributed across the world, with China responsible for the majority of the activity in Asia. E3SM data access through ESGF shows increased activity over last year, from a peak rate of 745 GB/week in April 2019 to 33 TB in October 2020.

The ESGF CMIP6 search portal uses a faceted search, or users can perform a text search by entering their search term in the text box.

ESS-DIVE is a data service that allows scientists access to long-term, spatially dense, high-quality observational data sets coupled with simulations to understand and predict ecosystem behavior over timescales spanning decades to centuries. The data service was launched on April 1, 2018. ESS-DIVE uses web and programmatic storage of data packages deployed with semiautomated curation. The standardized metadata enables the data to be searchable via a broad range of cross-agency search engines. The data service is built on Metacat and Metacat UI developed by NCEAS/DataONE and is designed using Findable, Accessible, Interoperable, and Reusable (FAIR) principles. On ESS-DIVE, 373 data sets are available with 76 published in the second quarter of fiscal year 2020 (Q2 FY20), and over 28,000 downloads of data were downloaded as of March 2020 (the end of Q2 FY20).

ESS-DIVE data sets are highly diverse, consisting of multidisciplinary data (e.g., vegetation, geomorphology, hydrology, geochemistry, spectroscopy, mineralogy, fluxes, and drone/AUV), multiscale data (e.g., molecular [nm - um], lab/sample [cm - 1 m], field [10 m - 1 km], watershed [1 - 10 km], and regional [10 - 100's km]), multitemporal data (e.g., rapid [sec - hours], frequent [hours - days], infrequent [weeks - months], and rare [years]), and heterogeneous formats (e.g., model output, in-situ measurements, and satellite estimates).

INVITED TALKS

The meeting's steering committee invited several scientists to give talks at the meeting. The two longest of these invited talks were denoted as keynote talks. Other invited talks were shorter and occurred in the plenary sessions and various breakout sessions. The two invited talks in the plenary sessions and the keynote talks are described below. Invited presentations in the breakout sessions are described in their most-relevant report sections (see the list below).

Nils Wedi: A baseline for global weather and climate simulations at 1 km resolution

The first keynote speaker, **Nils Wedi**, is the Head of Earth System Modelling at the European Centre for Medium-Range Weather Forecasts (ECMWF). Wedi presented "A baseline for global weather and climate simulations at 1 km resolution", the ECMWF's effort in pushing the frontier of simulating planet Earth with unprecedented resolution by testing its GPU-based model at 1-kilometer resolution for four simulated months on DOE's Summit supercomputer. He summarized parallel efforts to improve performance and portability while handling this increasing complexity for the different existing and emerging applications of ECMWF's Integrated Forecasting System (IFS), also known as the "European model." He described recent efforts towards increasing realism with storm-scale resolving simulations. In particular, Wedi presented the effects of explicitly simulating deep convection on the atmospheric circulation and its variability, as assessed by comparing the 1.4 km simulation to equivalent well-tested and calibrated global simulations at 9 km grid spacing, with and without parametrized deep convection (Fig. 5). Wedi's talk initiated great audience interest and Q&A discussions on the session's Slack channel afterwards. This is not surprising, since E3SM is heading in the same direction, i.e., pushing the higher-resolution frontier in exascale computing environment.

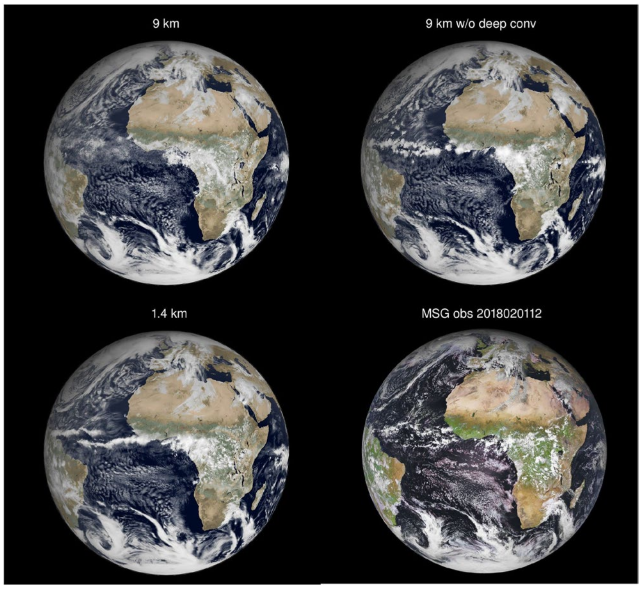


Figure 5. Simulated visible satellite images of the 9 km simulation with (top left) parametrized deep convection and (top right) without parameterized deep convection (meaning the deep convection was explicitly simulated) and (bottom left) of the 1.4 km simulation with explicitly simulated deep convection. The verifying visible Meteosat Second Generation (MSG) satellite image is also shown (bottom right), at the same verifying time. Simulations are based on three-hourly accumulated shortwave radiation fluxes, leading to a lack of sharpness (in the images only) as compared to the instantaneous satellite image (Wedi, 2020).

Oliver Furher: Learning how to forget: how high-level abstractions can help bridge the gap between productivity and performance

Keynote speaker **Oliver Fuhrer** from the Federal Institute of Meteorology and Climatology MeteoSwiss, and Vulcan Inc. presented "Learning how to forget: how high-level abstractions can help bridge the gap between productivity and performance." Fuhrer pointed out that although the weather and climate community has set ambitious goals to reach global km-scale modeling capability on future exascale high-performance computing (HPC) systems, current state-of-the-art models are executed using much coarser grid spacing and only a few of the productive weather and climate models are capable of fully exploiting modern HPC architectures with hybrid node designs. Alongside rapidly evolving HPC hardware, new associated programming models are being introduced and no de-facto standard has been adopted. Fuhrer's presentation focused on higher-level abstraction using domain-specific languages (DSLs) (Fig. 6). Based on efforts made so far on the European COSMO (Consortium for Small-scale Modeling) model and NCEP's FV3GFS (Global Forecast System with Finite Volume Dynamical

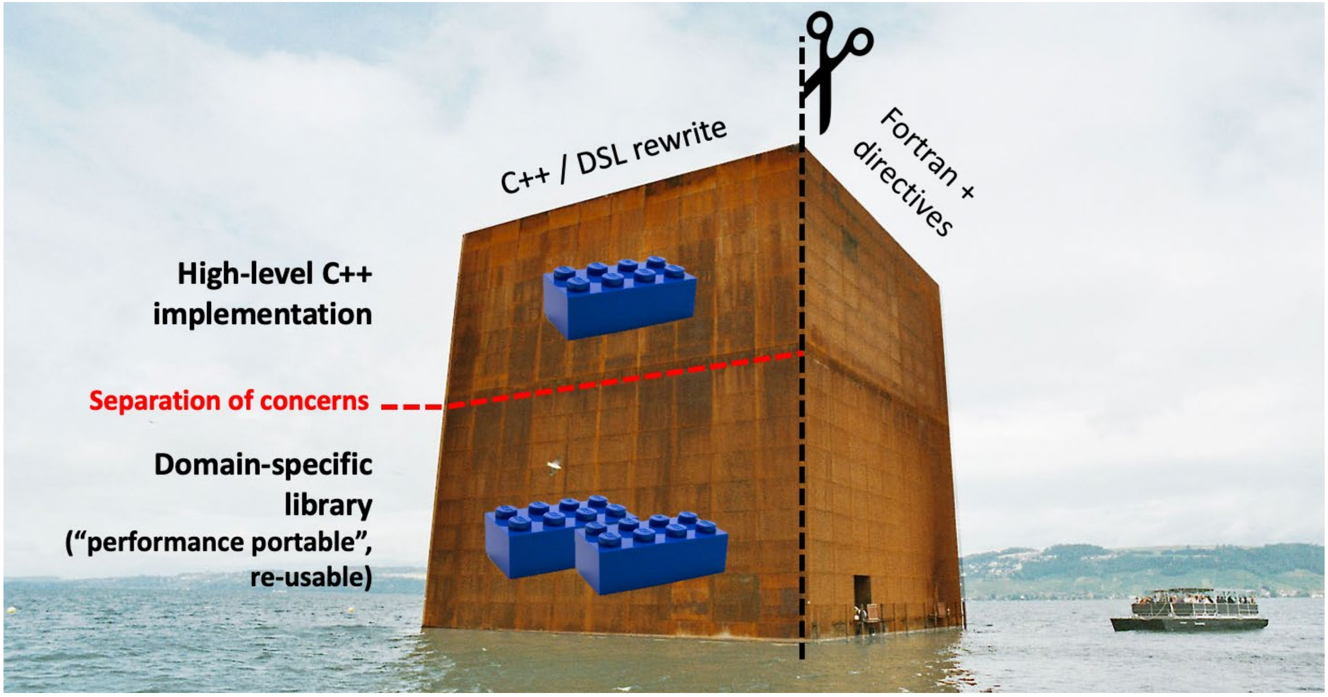


Figure 6. Porting the COSMO model to an acceleration-based higher architecture by replacing physical parametrization and data assimilation with code using Fortran with directives, and a dynamical core with C++ and a DSL that abstracts the hardware architecture (Fuhrer, 2018).

Core, version 3) model, Fuhrer pointed out that (1) DSLs have the potential for achieving a good balance between performance, portability, and productivity (at the price of generality); (2) optimizing for data movement on different hardware targets can require a higher level of abstraction in geophysical codes; and (3) there are no turnkey solutions, but existing tools and libraries can be exploited.

Walter Hannah: A Multiscale Modeling Framework for E3SM

Invited speaker **Walter Hannah** from Lawrence Livermore National Laboratory (LLNL) presented results and future plans for A Multiscale Modeling Framework for E3SM (E3SM-MMF), developed as part of DOE's Exascale Computing Project (ECP). The MMF approach embeds a cloud-resolving model (CRM) in each grid column of an atmospheric general-circulation model to provide an explicit representation of clouds and cloud radiative effects. This ECP effort is aimed at making E3SM-MMF viable for climate simulations through hardware and algorithmic acceleration. Hannah discussed progress and future plans to address E3SM-MMF performance portability challenges

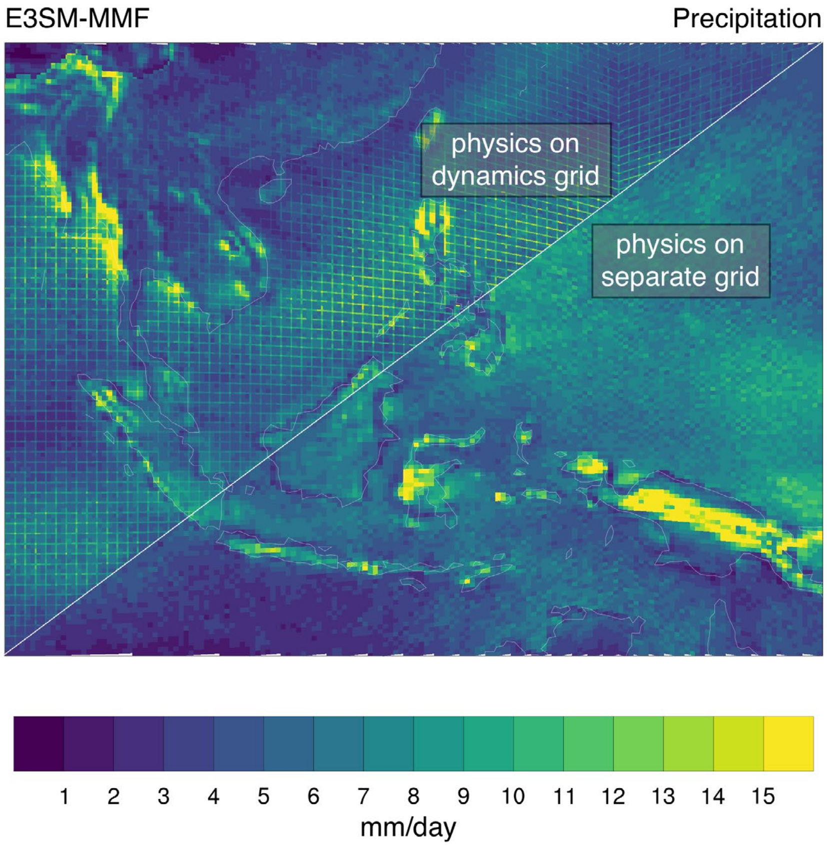
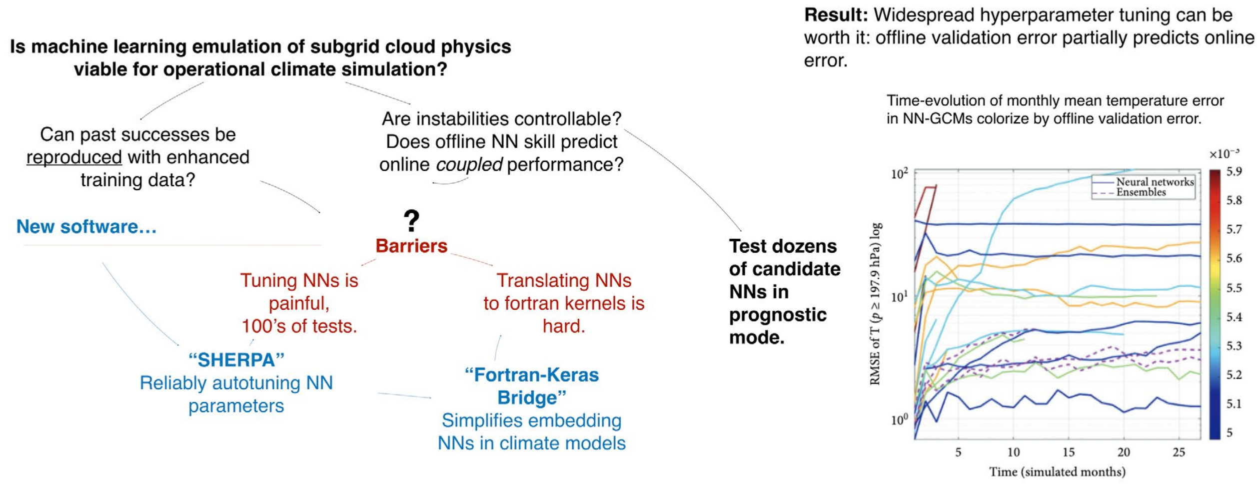


Figure 7. Comparison of five-year precipitation climatology for E3SM-MMF using the 120np4 (top left) and ne120pg2 (bottom right) physics grids. The grid imprinting bias caused by E3SM's spectral element dynamical core (top left) has been removed by using the physgrid implementation (bottom right).



Ott, Pritchard et al., *Scientific Programming*, 2020.

Figure 8. Challenges and recent progress in using neural networks (NNs) to emulate convection with real geography.

for exascale machines. The presentation also highlighted numerical challenges, in particular a grid imprinting bias caused by E3SM's spectral element dynamical core, which motivated development of the new "physgrid" in E3SMv2 (Fig. 7). Hannah concluded that E3SM-MMF will be viable for climate experiments in E3SMv4: the MMF is well suited for utilizing GPUs; performance will be portable across current and upcoming DOE machines; the throughput is on par with traditionally parameterized models; and explicit convection can overcome long-standing parameterization issues.

Mike Pritchard: Towards robust neural network parameterizations of convection: advances in stability, credibility, and software

Invited speaker **Mike Pritchard** from the University of California, Irvine presented "Towards robust neural network parameterizations of convection: advances in stability, credibility, and software." The MMF framework discussed in the previous invited presentation, also known as superparameterization, is computationally expensive. Pritchard and his group have been investigating the viability of using deep learning to emulate the behavior of CRMs to produce highly accurate yet inexpensive parameterizations of atmospheric convection. Going beyond earlier successes in using neural networks (NNs) to emulate convection on aquaplanets, Pritchard presented recent progress in physically constraining NN-based parameterizations, improving numerical stability of prognostic simulations using such parameterizations, and emulating convective activities in an atmosphere with real geography. He demonstrated that using new software such as Sherpa and the Fortran-Keras bridge allows for reliable autotuning of NN parameters and simplifies embedding NNs in climate models, which facilitates ensemble testing of NN-coupled climate models (Fig. 8). These can contribute to further progress in obtaining physically-constrained NN parameterizations in prognostic simulations with real geography.

Additional invited talks presented in the breakout sessions include the following:

- "Update on Eddy Energy Climate Progress Team (CPT)" by Laure Zanna in the Ocean Breakout Session, Luke Van Roekel, Zhengyu Liu
- "Enhancing aerosol predictions on the global scale with particle-resolved modeling and machine learning" by Nicole Riemer in the Aerosols Breakout Session, Po-Lun Ma, Qi Tang
- "Scale aware parameterizations" by Baylor Fox-Kemper in the Ocean + Coastal Modeling Breakout Session, Luke Van Roekel, Andrew Roberts.

To learn more, see these breakout session summaries which include relevant related information.

E3SM OVERVIEW

The Energy Exascale Earth System Model is an ongoing, state-of-the-science Earth system modeling, simulation, and prediction project that optimizes the use of DOE laboratory resources to meet the science needs of the nation and the mission needs of DOE (Leung, 2020).

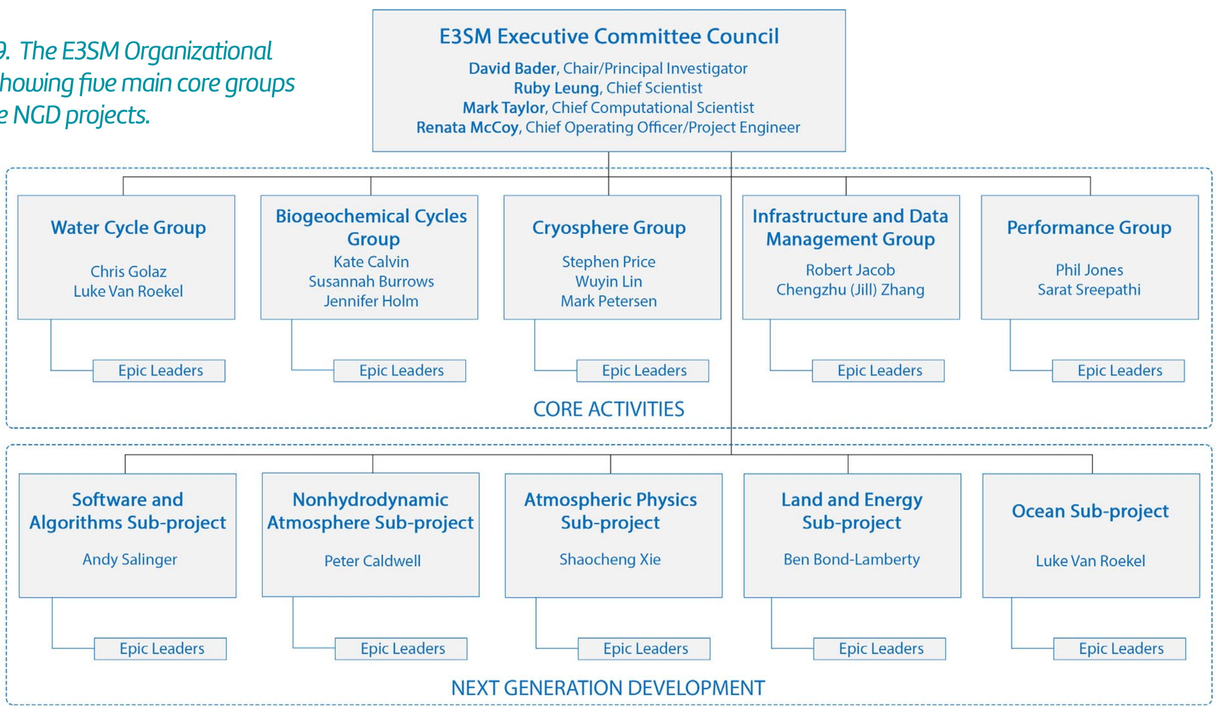
It contains aspects of both higher-risk research and more straightforward, but still complex, model development. Accordingly, the project devotes efforts in two main types of subprojects (Fig. 9):

- **Core activities** encompassing completion of the v2 model and execution of the v2 simulation campaign
- **Next-generation development (NGD) activities** develop new science and computational capabilities for E3SM versions v3 and v4 with a path for integration into E3SM within five years.

The core activities include three science groups centered around the simulation campaigns: the water-cycle, biogeochemical-cycles, and cryosphere groups, as well as two software-engineering-related groups: the performance group and the infrastructure and data-management group.

NGD activities consist of five main sub-projects, namely, the software and algorithms, nonhydrostatic atmosphere (also known as SCREAM—a simple cloud-resolving E3SM atmospheric model), atmospheric physics, land and energy, and the ocean NGDs. Additionally, the Berkeley ice-sheet initiative for climate extremes (BISICLES) NGD is a smaller effort on dynamical land-ice model development.

Figure 9. The E3SM Organizational chart, showing five main core groups and five NGD projects.



E3SM Overview and Status from Executive Committee

The session was dedicated to an overview of the Energy Exascale Earth System Model (E3SM) Project by the executive committee, consisting of Dave Bader, Ruby Leung, Mark Taylor and Renata McCoy.

E3SM Status, Dave Bader

In the first talk, **Dave Bader**, lead PI and chair of the governing council, introduced (Presentation-1 - Bader) the project's long-term goal of developing Earth system models that address the grand challenge of actionable predictions of Earth system variability and change, with an emphasis on the most critical scientific questions facing the nation and DOE. Conceptually, the E3SM project

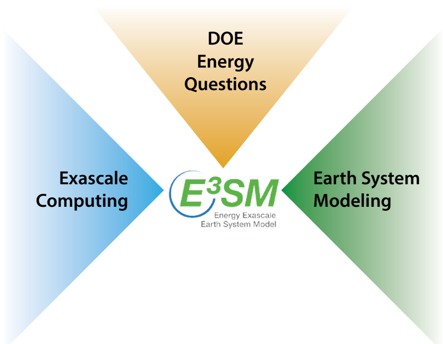


Figure 10. Conceptual diagram depicting the rationale for the E3SM modeling system: "A DOE Model for the DOE Mission on DOE Computers."

describes its vision as a DOE project for the development and deployment of Earth system models for the DOE mission on current and future generations of DOE computational systems in the Office of Science Leadership Facilities (Fig. 10). Bader additionally explained the E3SM paradigm in which multiple versions of the E3SM model are developed in parallel with new versions released approximately every three years. Since many developments require much longer than three years to fully implement and test, this philosophy prevents delays in model releases while waiting for a new feature to be added. Further, it allows some riskier approaches to be tried and tested that may ultimately prove unfeasible. The final part of Bader's presentation was a tentative plan to allow four years for the integration of the version 4 (v4) model, essentially in parallel with the integration of v3, which will take a year. The v4 model is specifically designed for Leadership Facility exascale computer architectures and will be drastically different in coding structure and programming model from versions 1–3.

Science, Ruby Leung

Ruby Leung, E3SM chief scientist, explained (Presentation-1 - Leung) how the overall project goals for DOE mission science result in science questions that drive priorities in model development and capstone simulation campaigns in the water cycle (WC), biogeochemistry (BGC) and cryosphere (CRYO) (Fig. 11).

Leung then detailed the evolution of the increased demands upon the modeling system with each successive campaign. V1 simulations were designed and analyzed to get a full understanding of the modeling system's strengths and weaknesses in simulating key aspects of the WC, BGC, and CRYO campaigns. V2 science-campaign simulations were designed around use-inspired science, primarily enabled by regionally-refined meshes (RRMs) across all model components. V3 model development is focused on further bias reduction and more advanced use-inspired science, with the inclusion of the Global Change Analysis Model (GCAM), a multisector dynamics code that represents many human activities and their impacts on the environment. V4 is a transformational model

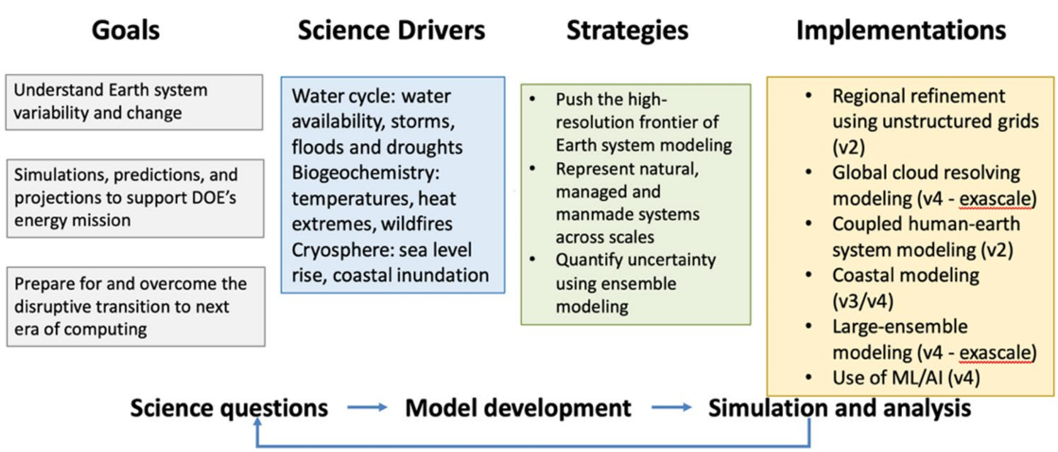


Figure 11. Pathway from science goals to model development and application.

with simulation capabilities across multiple scales, from convection-permitting to global. Making use of the hybrid CPU-GPU architectures, v4 will enable very large ensemble simulations of 100 or more members for probabilistic estimation of future climate states, including the ability to model the increased frequency of major storm events.

Computational Science, Mark Taylor

Mark Taylor, E3SM chief computational scientist explained (Presentation - Taylor) that DOE is taking the lead among US science and technology agencies to deploy useable exascale systems for science and engineering applications. Examples of these new systems are OLCF's Frontier and NERSC's Perlmutter, to be deployed in 2021, followed by ALCF's Aurora in 2022. Broadly, aspects of E3SM computational improvements are achieved through close collaboration among three Office of Science programs, with E3SM supported by BER, SciDAC supported by BER and ASCR, and the Exascale Computing Project (ECP) funded by ASCR. The key architectural feature to achieve exascale performance will be a reliance on graphical processing units (GPUs) coupled tightly on a node with more traditional central processing units (CPUs), known as a heterogeneous architecture. GPUs exhibit a three-times (3x) speedup per watt over CPUs, but only in high-workload regimes. Unfortunately, typical climate model simulations operate in mostly low-workload regimes, even after they are refactored for efficient performance on heterogeneous architectures. E3SM v4 will be designed to work on both heterogeneous machines and more traditional HPC homogeneous CPU clusters. The project will make use of exascale hybrid architectures for 100+ member large-ensemble experiments at traditional resolutions and single very-high-resolution convective-scale simulations, both of which achieve the high-workload threshold.

E3SM Communication and Support for E3SM Ecosystem Projects, Renata McCoy

Renata McCoy, E3SM's chief operating officer and project engineer, presented (Presentation-2 - McCoy) the final talk of the session, describing E3SM communication work and support for E3SM Ecosystem Projects. She started by describing different levels of support for the project, Ecosystem and external users. E3SM has a special relation to the Ecosystem Projects, which are ESMD-funded projects that work with E3SM data or on some aspect of E3SM development. Projects that develop code to be eventually included in E3SM need to be aware of the strict rules that the E3SM project enforces before such code can be considered for possible inclusion in the E3SM code base. She further explained how the E3SM project fully realizes and embraces the importance of making the model source code, data, and application software tools publicly available. Several of her slides included web links to documentation and software available for model development, execution, and analysis of results. McCoy's presentation also included policies and practices for communicating with and informing the scientific community and public about the project's research and all of its stages, including future plans. In addition to a publicly accessible project website containing extensive documentation and information (e3sm.org), the project publishes an electronic newsletter, "Floating Points," to which people may subscribe by emailing listserv@lists.llnl.gov with "subscribe E3SM-news" in the body of the email.

E3SM Future Versions v3/v4

Dave Bader started the session with an overview of the council's draft strategy for v3 and v4 of E3SM. The project will commence parallel, but coordinated, development of the v3 and v4 model versions, with a v3 release date scheduled for June 2023 and a v4 release date of June 2026. The motivation for this approach is to assure that the v4 (exascale) version of E3SM is complete and thoroughly tested on the yet-to-be-delivered hybrid CPU-GPU systems at Office of Science Leadership Computing Facilities. The differences in machine architecture and the programming model required for exascale machines requires new or completely refactored code for major portions of the model, particularly the E3SM Atmosphere Model (EAM). Concurrently, the next generation of E3SM, v3, will be developed to incorporate new features and improved process representations over v2. While the computational architecture and data structures will be similar to v2, v3 will have substantially more capability to simulate a wider range of the phenomena required for the v3 science campaign.

The roadmap for both versions is shown conceptually in Figure 12. Starting with v2 on the left, v4 replaces EAMv2 with the new nonhydrostatic v4 prototype, nicknamed SCREAM for "Simple Convection-Resolving E3SM Atmospheric Model," written from the ground up in C++/Kokkos and developed by the Nonhydrostatic Atmosphere Next-Generation Development (NGD) subproject. The C++/Kokkos programming model enables the code to run on both traditional CPU architectures and exascale

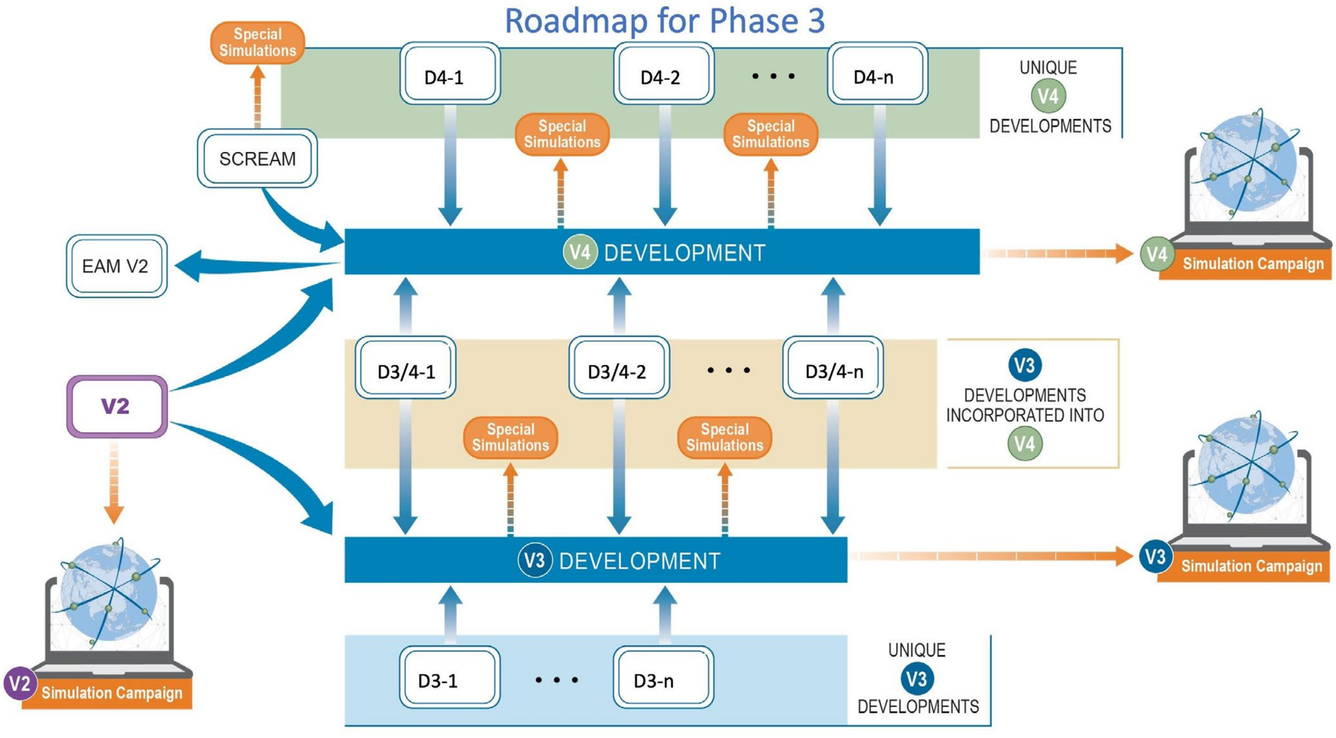


Figure 12. Conceptual diagram of the E3SMv3 and E3SMv4 Road Maps. "D3-1", "D3-2", to "D3-n" are labels for distinct new development features in v3, such as convection, radiation, cloud physics, and river chemistry. Similarly, "D4-1" to "D4-n" are distinct features developed for v4. "D3/4-1" to "D3/4-n" are features from v3 that will be incorporated into v4.

heterogeneous architectures, such as the Frontier machine scheduled for deployment at the Oak Ridge Leadership Computing Facility (OLCF) in 2021. Programming in C++/Kokkos unlocks more levels of parallelism to efficiently exploit the CPU-GPU architectures. The increase in efficiency comes at the cost of code complexity, as shown in Figure 13. Although capable of running very high horizontal-resolution atmosphere simulations in the convection-resolving and convection-permitting regimes (at 3 km grid cell size), EAMv4 will also be capable of running at resolutions more typically found in climate-model simulations, i.e. 10 km and larger. While release of the full model is scheduled for 2026, the project envisions special simulations with early developmental versions of EAMv4 and E3SMv4 starting as soon as 2021.

The development of v3 will result in a single codebase for all v3 science campaigns. The starting point for v3 is v2 + NGD Land and NGD Atmosphere features and improvements. Other developments, e.g., some Ocean NGD improvements or outside contributions, are possible. From a performance standpoint, v3 will run efficiently on traditional homogeneous distributed-memory machines. Because its data structures and programming model are the same as v2, external developments from the Ecosystem and Collaborator projects will be incorporated more easily into v3. It is hoped that some new features will be sufficiently flexible to go into both v3 and v4. The talk concluded with Bader emphasizing that many questions remain, such as whether organizational changes may be needed. Decisions will need to be made about the programming model for other components that will not be refactored in C++/Kokkos.

The second talk in the session was given by **Ruby Leung**, who described the science strategy implementation through the end of the project's Phase 3 in 2025. The science questions include aspects to address model biases, understand model behaviors, and advance use-inspired science. She explained how the science goals are translated into E3SM science drivers and strategies leading to the simulation campaigns for versions v2, v3 and v4 (Fig. 11). The v3 model will implement improvements from the Land/Energy and Atmospheric Physics NGD subprojects to expand the breadth of actionable-science simulations relevant to the DOE mission. The v4 Nonhydrostatic Atmosphere Model (SCREAM), Software/Algorithms, and possible new NGD-subproject research activities will be incorporated into the v4 development stream.

The integration of the Land/Energy and Atmospheric Physics NGD developments will produce a single v3 code base for all three simulation campaigns. The applications will span across a range of resolutions, including regionally-refined meshes (RRMs) for the atmosphere and ocean components to balance computational costs and model accuracy. EAMv3 will have more scale-aware physics and improved aerosol representations, while the ocean component will contain improved representations of mesoscale eddies, waves, and vertical mixing. The Land/Energy NGD will contribute important new parameterizations for land-atmosphere interactions and a unified land-river-ocean grid for coastal modeling.

Leung presented a series of slides on the next level of detail for the three E3SM science drivers and how they will be addressed with v3 and v4 of the model. The v3 Water Cycle Campaign will have an extended focus on climate sensitivity, especially now that a WCRP-sponsored review (Sherwood et al., 2020) revealed that E3SM and several other models have equilibrium sensitivity outside the scientific best estimates of their range. For the v4 Water Cycle Campaign, the focus will be on better quantification of uncertainty with very large ensembles (N>100) and exploring climate processes and feedbacks at the high-resolution frontier. V4 will be capable of short simulations of 3 km in the atmosphere, coupled to an ocean with mesoscale eddy resolution (3 km to 30 km depending on latitude).

For the BGC Campaign, v3 and v4 capabilities will include gas-phase atmospheric chemistry, nitrate aerosols, and stratospheric sulfate aerosols in the atmosphere. The ocean component will simulate seafloor BGC, while the land component will incorporate dynamic vegetation, crops, naturally occurring methane, an improved fire model and representations of managed disturbances. Nutrient flow from the land to the ocean and better representation of lakes will be simulated by the river model. Particularly noteworthy is better coupling to GCAM to incorporate two-way interactions with energy, water, and food systems. GCAM, supported by the BER MultiSector Dynamics Program, is a global model that represents the behavior of, and interactions among, the energy system, the economy, and the Earth system.

The v3 and v4 Cryosphere simulation campaigns will focus on coastal processes, ice sheets, and sea-level rise. These will be enabled by the integration of capabilities from SciDAC, E3SM, the CICE Consortium, and coastal (InterFACE and ICoM) projects. Fully-dynamic ice-sheet representations of the Greenland and Antarctic ice sheets, tides, and icebergs will be among the features of the next-generation models.

The session concluded with a discussion led by the Executive Committee of the preliminary plans presented during the session and summarized above. The comments received will be used to revise and improve the strategy in the Phase 3 proposal.

Figure 13. Comparison of model code written in FORTRAN (top) and C++/Kokkos (bottom).

Original F90

```fortran
kloop_sedi_c2: do k = k_qxtop,k_qxbot,-kdir

   qc_notsmall_c2: if (qc_incld(k)>qsmall) then
      !-- compute Vq, Vn
      call get_cloud_dsd2(qc_incld(k),nc_incld(k),mu_c(k),rho(k),nu,dnu,   &
           lamc(k),tmp1,tmp2,lcldm(k))

      nc(k) = nc_incld(k)*lcldm(k)
      dum = 1._rtype / bfb_pow(lamc(k), bcn)
      V_qc(k) = acn(k)*bfb_gamma(4._rtype+bcn+mu_c(k))*dum/(bfb_gamma(mu_c(k)+4._rtype))
      V_nc(k) = acn(k)*bfb_gamma(1._rtype+bcn+mu_c(k))*dum/(bfb_gamma(mu_c(k)+1._rtype))

   endif qc_notsmall_c2
   Co_max = max(Co_max, V_qc(k)*dt_left*inv_dzq(k))

enddo kloop_sedi_c2
```

Ported to C++/Kokkos

```cpp
Kokkos::parallel_reduce(
  Kokkos::TeamThreadRange(team, kmax-kmin+1), [&] (int pk_, Scalar& lmax) {
    const int pk = kmin + pk_;
    const auto range_pack = scream::pack::range<IntSmallPack>(pk*Spack::n);
    const auto range_mask = range_pack >= kmin_scalar && range_pack <= kmax_scalar;
    const auto qc_gt_small = range_mask && qc_incld(pk) > qsmall;
    if (qc_gt_small.any()) {
      // compute Vq, Vn
      Spack nu, cdist, cdist1, dum;
      get_cloud_dsd2<false>(qc_gt_small, qc_incld(pk), nc_incld(pk), mu_c(pk), rho(pk), nu, dnu, lamc(pk), cdist,
      nc(pk).set(qc_gt_small, nc_incld(pk)*lcldm(pk));
      dum = 1 / (pack::pow(lamc(pk), bcn));
      V_qc(pk).set(qc_gt_small, acn(pk)*pack::tgamma(4 + bcn + mu_c(pk)) * dum / (pack::tgamma(mu_c(pk)+4)));
      if (log_predictNc) {
        V_nc(pk).set(qc_gt_small, acn(pk)*pack::tgamma(1 + bcn + mu_c(pk)) * dum / (pack::tgamma(mu_c(pk)+1)));
      }

      const auto Co_max_local = max(qc_gt_small, -1,
                                    V_qc(pk) * dt_left * inv_dzq(pk));
      if (Co_max_local > lmax)
        lmax = Co_max_local;
    }
}, Kokkos::Max<Scalar>(Co_max));
team.team_barrier();
```

Overview of E3SM Core Groups Progress and Future Directions

This session featured presentations by the group leads of the five E3SM Core Groups (Water Cycle, BGC, Cryosphere, Performance, and Infrastructure), focusing on the progress made during E3SM's Phase 2 (2018–2020) and future development direction. For summary papers on the Water Cycle standard/low-resolution, Water Cycle high-resolution, and BGC v1 models, see Golaz et al. (2019), Caldwell et al. (2019), and Burrows et al. (2020), respectively.

Note: The authors underscored below presented the work.

E3SM Water Cycle Group

Chris Golaz and **Luke Van Roekel** presented the **E3SM Water Cycle Group Overview** (Presentation-1 - Golaz) on the progress towards the E3SM v2 and the considerable effort dedicated to improving the model's computational performance and physical fidelity. As a highlight, they noted that the low-resolution configuration (100 km atmosphere, 30–60 km ocean) of E3SMv2 is nearly twice as fast as E3SMv1. The fidelity of the simulated climate in E3SMv2 is generally comparable to E3SMv1, with some notable improvements. In particular, regional sea surface temperature (SST) biases and Atlantic meridional overturning circulation (AMOC) biases are reduced in E3SMv2 with the introduction of new ocean-mesh (Fig. 14) and sea-ice features. In the atmosphere, cloud and precipitation biases are reduced through careful calibration of the existing cloud parameterizations and improved representation of the deep convection trigger. New land and river features in E3SMv2 provide capabilities such as inundation and irrigation/water management to address v2 Water Cycle science questions.

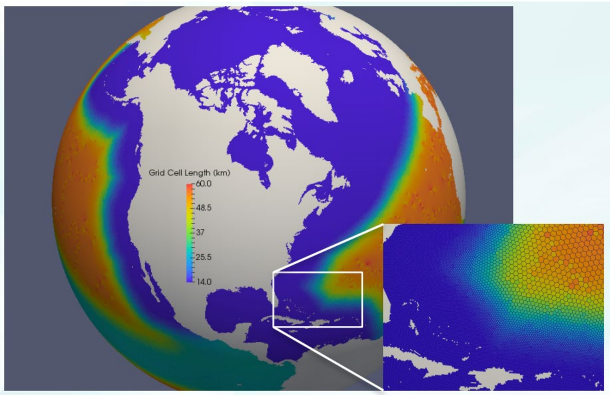


Figure 14. A key feature of E3SM v2 is a regionally refined capability, shown here with ocean mesh cell resolutions ranging from 60 km (orange) to 14 km (cobalt blue) along the North American coast and in the North Atlantic and Arctic oceans, compared to the base standard low-resolution mesh in E3SM v1.

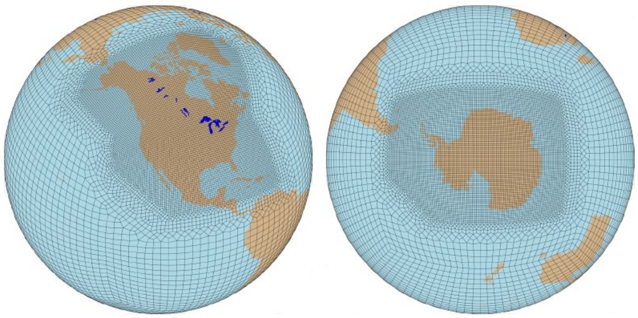


Figure 15. New RRMs in the E3SM Atmosphere Model (EAM) developed as part of E3SMv2. Water Cycle RRM on left, Cryosphere RRM on right.

They also highlighted the new regionally-refined meshes (RRMs) developed as part of E3SMv2. Relative to the low-resolution, the atmosphere resolution over North America has increased to 25 km. Figure 15 shows the atmosphere model RRM developed for the v2 simulations of the Water Cycle and Cryosphere campaigns. In the ocean, the resolution for v2 simulations will be increased to 14 km near the North American coast and in the North Atlantic and Arctic oceans. Single-component simulations with such RRM capability demonstrate similarity to global high-resolution simulations at a fraction of the computational cost. Lastly, the central Water Cycle science questions and simulation campaign were presented.

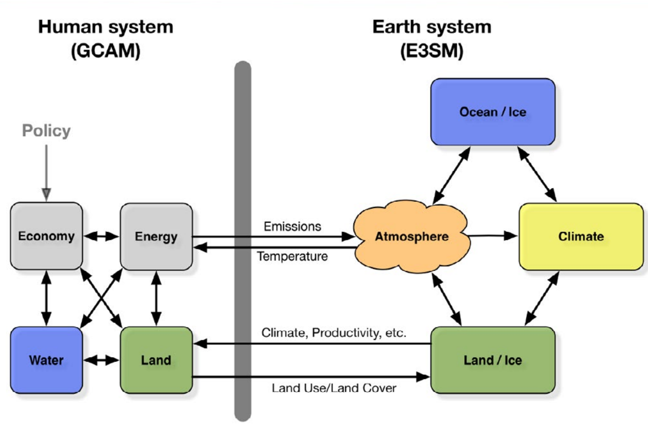


Figure 16. Enhancements in the coupling of the human system (GCAM) with the Earth system (E3SM), showing GCAM supplying land use/land cover changes, CO_2 emissions and non-CO_2 emissions and concentrations, and E3SM providing changes in land productivity to GCAM.

E3SM BGC Group

Kate Calvin and **Susannah Burrows** discussed the **E3SM BGC Group Overview** (Presentation - Calvin), providing an update on progress and plans. They began by introducing the overarching science question addressed by the BGC Group: "How do the biogeochemical cycles interact with other Earth system components to influence energy-sector decisions?" They reported on the status of v1 simulations, including a discussion of the progress towards publishing the data on ESGF (the Earth System Grid Federation) and documenting the results in a series of peer-reviewed publications. They reported on the status of the E3SM BGC-related v2 model development and simulation plan.

Specifically, they presented updates on energy-relevant developments, highlighting a new capability to couple the GCAM with E3SM (Fig. 16), as well as several developments in the land/river model for core simulations (soil erosion, stream temperature, vegetation scheme, and variable soil thickness) and the use of a new vegetation dynamics model (Functionally Assembled Terrestrial Ecosystem Simulator, or FATES) and a crop model for offline sensitivity simulations. E3SMv2 also features new development of biogeochemistry in the ocean and sea-ice models, including incorporation of the MARine Biogeochemistry Library (MARBL) and other ocean/ice capabilities. Additionally, fixes have been added to the atmosphere model to conserve carbon.

The v2 simulation plan will include active biogeochemistry in the atmosphere, land, ocean, and sea ice using low-resolution and the regionally-refined model configurations, branching from the Water Cycle v2 model tag. Simulation modes will include one-way coupling (CMIP-like) and two-way coupling of human–Earth system interactions (Fig. 17) featuring high bioenergy production under scenarios of high and low fossil-fuel CO_2 emissions and different cropland and forest cover.

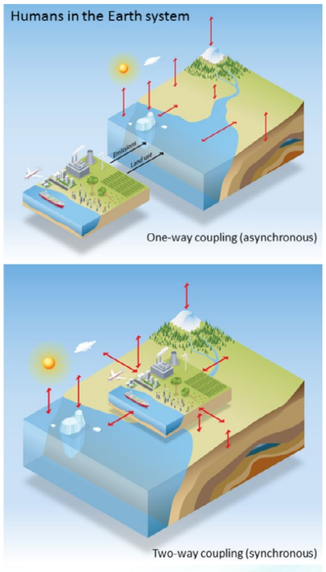


Figure 17. The E3SM v2 BGC campaign will include traditional (CMIP-like) one-way (asynchronous) coupling as well as two-way (synchronous) coupling between the human and Earth systems.

E3SM Cryosphere Group

Steve Price, **Wuyin Lin** and **Mark Petersen** presented the **E3SM Cryosphere Group Overview**, (Presentation-1 - Price) in which they summarized the group's E3SMv1 simulation campaign efforts during the past year, in the areas of model simulation, model analysis, model development, and publications, aimed at addressing the v1 science question, "What are the impacts of ocean-ice shelf interactions on melting of the Antarctic Ice Sheet (Fig. 18), the global climate, and sea level rise?" They highlighted specific successes and discussed ongoing difficulties and areas of concern (e.g., model biases). They also summarized planned efforts under the v2 simulation campaign and proposed potential science foci for consideration under the Cryosphere campaign in Phase 3 of E3SM. In particular the work on E3SMv1 low-resolution configuration revealed that more effort than anticipated was needed to get a reasonable Southern Ocean climate and stable ice-shelf melt rates under pre-industrial forcing. The group has identified and addressed important model biases and noted the importance of producing physically realistic sub- ice-shelf circulation that influences ice-shelf melt rates and instabilities. The group will complete simulations featuring the capability of ice-ocean interactions using historical quadrupling of atmospheric CO_2 ($4xCO_2$), and Shared Socioeconomic Pathways (SSP) forcing.

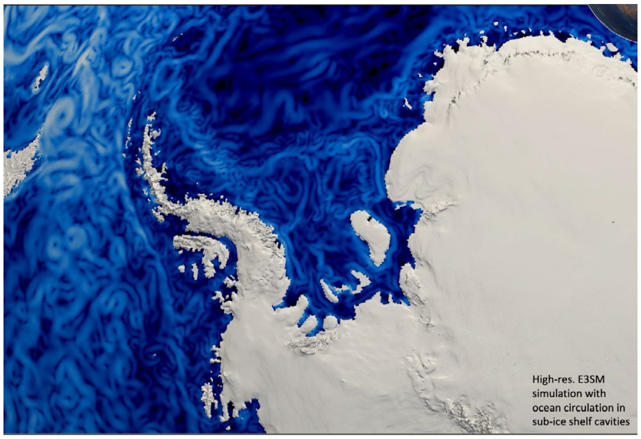


Figure 18. Ocean circulation beneath ice shelves showing ocean and ice interaction around Antarctica in a high-resolution E3SM simulation.

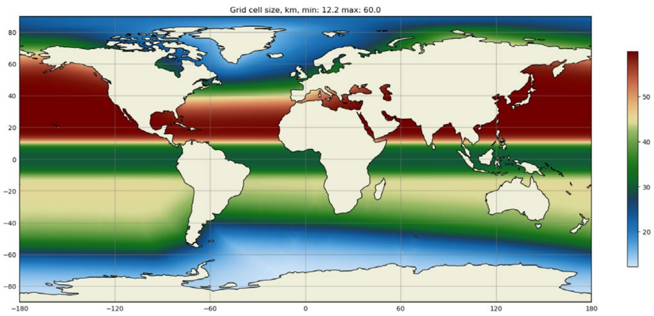


Figure 19. One of E3SMv2's Cryosphere Southern Ocean RRMs showing a band of high-resolution grid cells around Antarctica (see Poster-1 – Asay-Davis).

The initial results with the v2 configuration, using both high and variable resolution (Fig. 19), show that

- a better Southern Ocean climate and stable/realistic melt rates using SORRM (Southern Ocean RRM) exist in v2; initial simulations look good (out to ~60 years),
- important coupled-model biases (atmosphere, ocean, and sea ice), identified from analysis of a high-resolution simulation, are likely to appear in v2 as well as v1, and
- final v2 tunings are needed before scientists can proceed further.

E3SM Performance Group

Phil Jones and **Sarat Sreepathi** presented the **E3SM Performance Group Overview** (Presentation-1 – Jones) summarizing the Performance Team's progress since the last meeting and describing plans for future work. They emphasized the improvements in throughput (Fig. 20) for simulations running on currently-used machines, ongoing work on standard benchmarking and profiling, and performance tools. They also discussed the preparation for new architectures by gaining access to early prototype versions of DOE's next-generation machines. Performance metrics and throughput on standard high-resolution benchmark cases were presented, showing good scaling. Substantial improvement was achieved in input/output (I/O) performance and incremental improvement was made on in-node performance. They highlighted a new infrastructure, PACE (Performance Analytics for Computational Experiments), to provide an executive summary of experiment performance. Finally, kernel extraction and characterization work was presented for detailed GPU characterization.

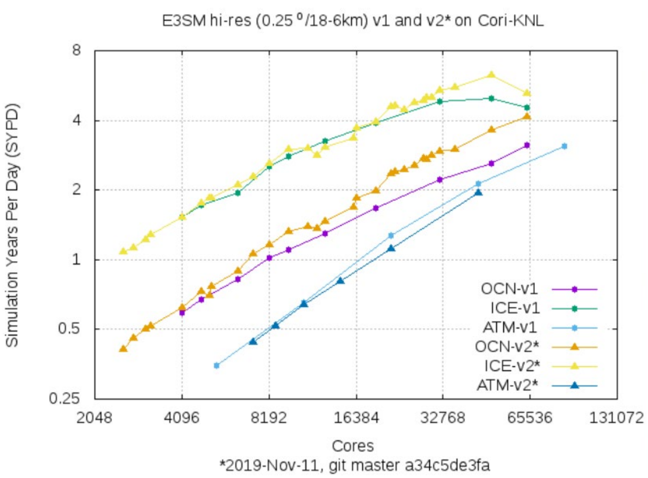


Figure 20. Throughput of E3SM simulations with standard high-resolution benchmark cases showing improvements in ocean, ice, and atmosphere components.

E3SM Infrastructure and Data Management Group

Robert Jacob and **Chengzhu (Jill) Zhang** presented the **E3SM Infrastructure Group Overview** (Presentation – Jacob) detailing the Infrastructure Group's progress during Phase 2. They explained the group's responsibility to maintain and support all E3SM software, manage datasets, and define, document, and manage the processes and procedures used in software development. They briefly described the model-development process and testing strategy, pointing out recent and upcoming changes like new Travis-CI testing. Currently supported machines and expected, upcoming machines' specifications and capabilities were presented. They noted that the Infrastructure Group has published most of the v1 simulation data to ESGF and established procedures and programs to streamline future publication. New features in diagnostic (Fig. 21) and analysis tools will enhance and speed up the analysis of E3SMv2 simulations.

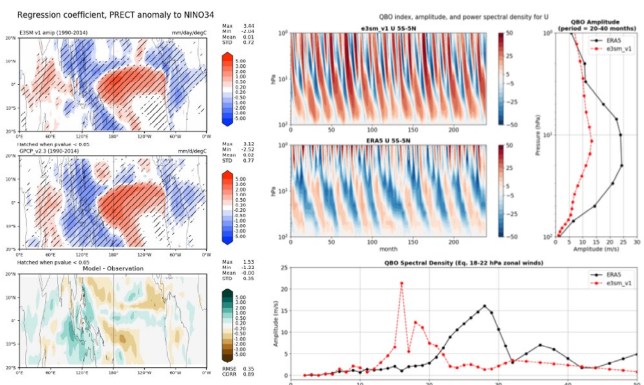


Figure 21. The E3SM Diagnostics Package, e3sm-diags, added El Niño–Southern Oscillation (ENSO) diagnostics and quasi-biennial oscillation (QBO) evaluations.

Overview of E3SM Next-Generation Development Groups

This session included updates from five Next Generation Development (NGD) projects within E3SM.

NGD Nonhydrostatic Atmosphere

First, **Peter Caldwell** provided an update (Presentation – Caldwell) on the **Nonhydrostatic Atmosphere NGD**. This subproject, which involves about twenty people, is developing the Simple Cloud-Resolving E3SM Atmosphere Model (SCREAM), a new atmospheric model written in C++/Kokkos. SCREAM is an optional atmosphere model now and is planned to be the default E3SM atmosphere model for the v4 release. This programming model will enable the future E3SM atmosphere to run on both CPUs and GPUs, thus future-proofing the model. SCREAM includes parameterized turbulence but resolves convection directly; aerosols are prescribed for now, with the intention that the EAGLES project will develop a candidate aerosol package to be considered for future E3SM versions.

Two years after the project kickoff, SCREAM is still well on track to deliver on its goals. SCREAMv0 exists as a Fortran 90 implementation using the existing EAM infrastructure, and DYAMOND1 simulations show that its skill is similar to other current convection-resolving global climate models (Fig. 22). SCREAMv0 is expected to provide a platform for tackling science goals. In parallel, efforts are ongoing to port SCREAM codes into the C++/Kokkos framework to meet the computational goals of the subproject. For more information on additional SCREAM runs, see Caldwell et al. (2021).

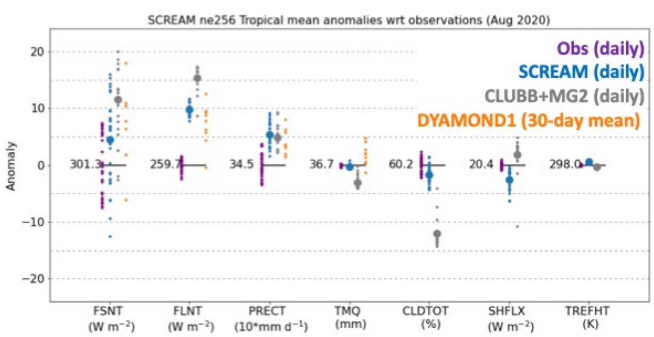


Figure 22. Tropical mean bias for DYAMOND1 period (Aug 1–Sept 10, 2016) from SCREAMv0 at 12 km (ne256) compared to runs from other modeling centers.

NGD Atmospheric Physics

Next, **Shaocheng Xie** provided an update (Presentation - Xie) on the **Atmospheric Physics NGD**, which is focused on the v3 model release. This NGD development concentrates on conventional-resolution simulations which require parameterization of deep and shallow convection and naturally lend themselves towards more complex physics. Additionally, this subproject aims to enhance scientific goals focused on coupling across the Earth system.

One major effort in the Atmospheric Physics NGD is focused on improving the model's cloud physics, in particular, its deep convection schemes via parallel efforts. The first effort focuses on enhancing the current Zhang-McFarlane scheme. Two additional efforts focus on evaluating the potential use of a unified turbulence/convection parameterization in E3SM. These include an improved version of the CLUBB parameterization and the multi-plume EDMF scheme.

Additionally, the team is working with SCREAM to test the potential for some of the SCREAM parameterizations to be used in the v3 model. These include the SHOC turbulence parameterization and the P3 cloud microphysics scheme (see Fig. 23). Initial evaluation shows that the P3 microphysics reduces biases in both the geographic distribution of mean precipitation and in the precipitation probability density function (PDF).

To enhance the coupling across the Earth system, the team is adding improvements to aerosols and interactive chemistry. The UCI chemistry scheme has already been implemented and efforts are underway to implement improvements to the aerosol scheme.

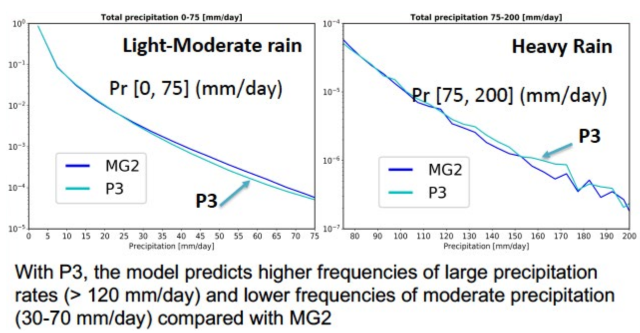


Figure 23. Frequency of precipitation comparison between the new P3 cloud microphysics and the old MG2 implementation.

NGD Software and Algorithms

Andy Salinger provided an update (Presentation – Salinger) on progress and plans for the **Software and Algorithms NGD**. This NGD focuses on five tasks: (1) improve model throughput on exascale machines, (2) improve developer productivity, (3) create a culture of verification, (4) leverage DOE computational-science investments, and (5) entrain talented computational scientists into E3SM.

In terms of improving model throughput, E3SM developers have been working on a semi-implicit barotropic solver for the ocean. These improvements have led to a 2.55-times (2.55x) speedup for the barotropic mode and a 1.74-times (1.74x) speedup of MPAS-Ocean at scale (see Fig. 24).

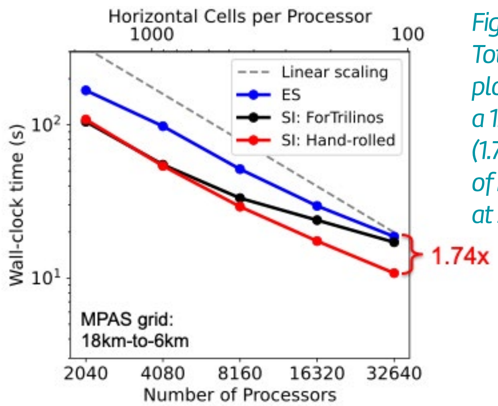


Figure 24. Total runtime plot showing a 1.74-times (1.74x) speedup of MPAS-Ocean at scale.

For the atmosphere, the implementation of semi-Lagrangian tracer transport has sped up the model by 2–3 times and a new atmospheric chemistry solver has reduced the cost of the UCI chemistry model by 33%. Scientists have also developed exponential time-differencing Runge-Kutta methods for the nonhydrostatic models, which enable large and accurate time steps. A new strategy for "coupled" partitioning decreases the time needed to compute parallel mesh intersections. Next, this NGD has developed a machine-learning-based testing framework for climate reproducibility. This framework can detect whether changes in parameters lead to climate-changing results. It has been tested in MPAS-Ocean and efforts are underway to use it within EAM. Finally, researchers have started a new optimization/uncertainty-quantification-based calibration effort.

NGD Land and Energy

Ben Bond-Lamberty provided an update (Presentation – Bond-Lamberty) on progress and plans for the **Land and Energy NGD**. This NGD includes four broad areas: coupling between the human (GCAM) and Earth system (E3SM) models; hydrology and plant hydraulics; natural and anthropogenic disturbance; and vegetation dynamics, canopy processes, and photosynthesis. These developments are designed to be incorporated in future versions of E3SM used by all three science campaigns. For the human–Earth system coupling area, the v2 efforts focused on land and carbon are wrapping up now. These efforts were designed to facilitate easy extension for v3 NGD plans, which focus on water and crops. However, some rethinking of the tools used in the interface may be required. Efforts are ongoing in this area to add bioenergy crops to the E3SM land model (ELM); these crops have been added but additional work is needed to better match simulation results to observations. Several developments have been made in MOSART, the river routing model used by E3SM, including the addition of stream temperature and soil erosion. Efforts in this NGD are also aiming to simplify and improve the fire model. This research includes

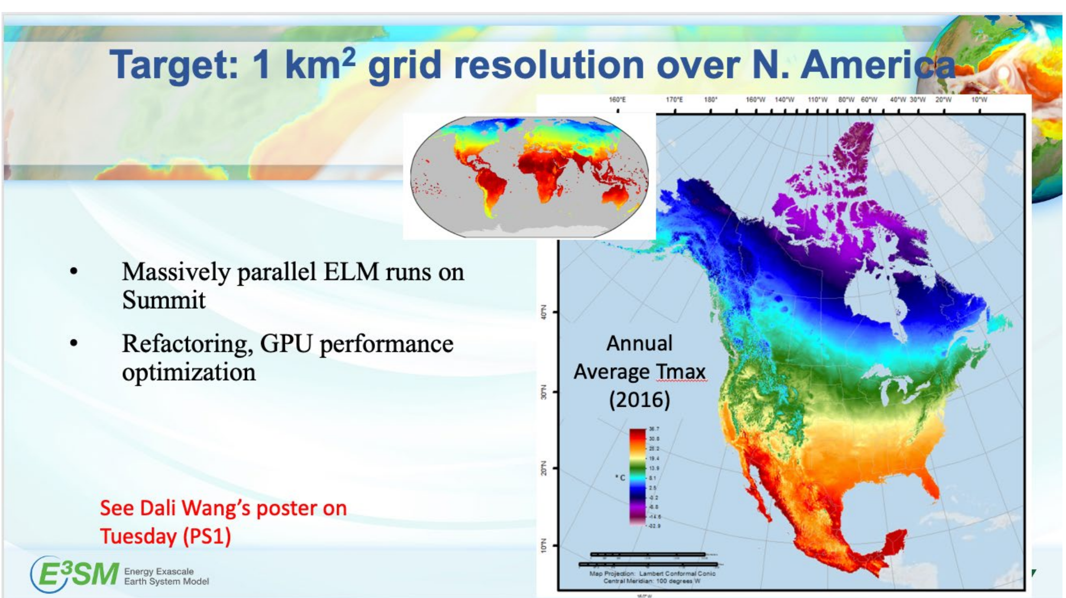


Figure 25. Slide from Ben Bond-Lamberty's talk showing the high resolution (1 km) 2016 annual average Tmax result from an E3SM Land Model (ELM) run.

improvements to the representation of emissions from fire and a machine-learning approach to modeling fire. For plant hydraulics, scientists have developed a tree-level hydrodynamic model. For managed disturbance, researchers have been adding harvesting into FATES, the dynamic vegetation model used by E3SM. Finally, progress has been made on running a very-high-resolution (1 km) version of ELM on Summit (see Fig. 25).

NGD Ocean

In the last presentation of the session, **Luke Van Roekel** provided an update (Presentation - Van Roekel) on the newly-established **Ocean NGD**. The goals of this effort are to (1) create an Earth system model that can accurately simulate waves from coastal to global oceans for decadal simulations, (2) utilize variability to improve coastal predictability of E3SM, and (3) examine the impact of uncertainty in these predictions.

To achieve these goals, the project needs to develop an exascale-ready version of WaveWatch3 (WW3) (see Fig. 26) and an exascale-ready version of MPAS-Ocean for ultra-large ensembles. Additionally, efforts will be required to optimize the unstructured-mesh capability, to understand where high resolution is necessary, and to develop improved and scale-aware physics parameterizations.

The proposed developments will support possible v4 science questions for each of the major science campaigns. Water Cycle goals will be supported by targeting exascale and improving support for large ensembles and RRMs. Cryosphere goals will be supported through improvements to sea level rise predictability. Biogeochemistry goals will be supported through improved exchanges between the atmosphere and ocean/sea ice.

Improvements to the model infrastructure are also planned, including efforts to de-obfuscate MPAS, make improvements to the data layout and model structure, and achieve performance improvements through reductions in communication and passive tracer supercycling. Additionally, the project will explore new programming models, such as Kokkos, FLeCSI, and/or OpenMP.

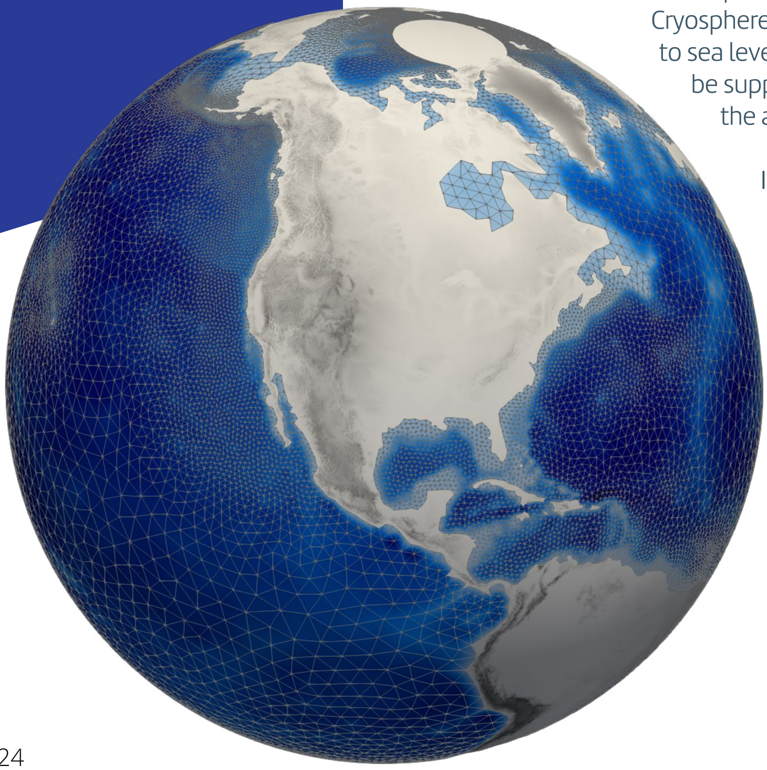


Figure 26. Global unstructured WaveWatchIII mesh (Brus et al., 2020).

E3SM Tools

The final session of the meeting featured presentations from E3SM Infrastructure and Performance Groups focusing on E3SM tools to support E3SM model development and evaluation activities. This session started with an overview (Presentation - Zhang) of the E3SM workflow and major tools (Fig. 27). The presentations that followed covered tools to facilitate running the model (CIME control system), simulation data post-processing and analysis (NCO, E3SM_diags, MPAS_analysis, and E3SM_unified), data management (zstash, and e3sm_to_cmip), and computational performance archiving and analysis (PACE). To help new E3SM and ecosystem projects users, a brief introduction, how-to instructions, and where to get help/documentation were presented for each tool.

Presentations

The CIME Case Control System by Rob Jacob: CIME (Common Infrastructure for Modeling the Earth) provides a Case Control System (CCS) for configuring, compiling and executing Earth system models. CCS is the workflow control code for creating an experiment in a CIME-enabled model like E3SM (and CESM). CCS is written in Python with XML files for configuration. It allows configuring, building and running an experiment with a handful of commands. The normal CCS development workflow creates an out-of-the-box case and then customizes it for the user's science. With a specific source code version (git hash) and the compset (component set) and grid, one can exactly reproduce an out-of-the-box case. The run_e3sm script is a way to put all the commands to create and modify base cases in one csh file and can be used to exactly reproduce the simulations being conducted.

NCO by Charlie Zender: NCO (netCDF Operators) are command-line operators to manipulate and analyze netCDF and HDF files. Many performance-enhancing functionalities were added to the NCO package for optimizing its use to E3SM component model output (EAM, ELM, MPAS-SI, MPAS-O). The most common use of NCO are generating climatologies, performing regridding, and time-series extraction.

e3sm_diags by Jill Zhang: e3sm_diags (E3SM diagnostics package) is a Python-based diagnostics package for comprehensive E3SM diagnostics. It mostly focuses on atmospheric analyses (including those key sets available from NCAR's AMWG package) with ongoing effort to support more land and river variables. The e3sm_diags package is configurable, extendable, and saves provenance. Streamflow, QBO and diurnal cycle analyses have been recently added.

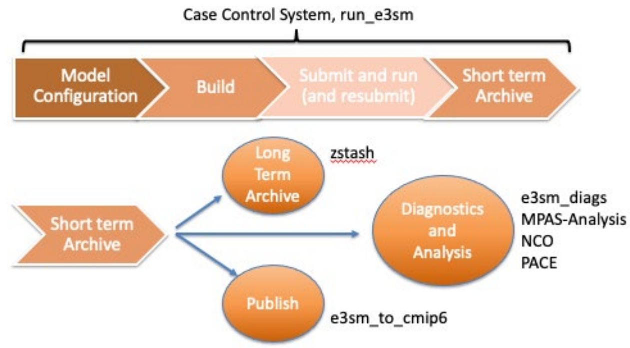


Figure 27. E3SM workflow and primary tools.

MPAS_analysis by Xylar Asay-Davis: MPAS_analysis covers analysis for simulations produced with MPAS components: MPAS-SI and MPAS-O. It is also a Python package with up-to-date analysis datasets. New evaluation capabilities include eddy kinetic energy, time series of volume transport, and ocean basin means of temperature and salinity.

zstash by Ryan Forsyth: zstash is an HPSS long-term archiving solution for E3SM. Zstash is written entirely in Python using standard libraries. Standard tar files are generated locally before transfer to HPSS. Checksums (md5) are computed on-the-fly during archiving and verified on extraction. Metadata are stored in a sqlite3 index database, enabling faster retrieval for target files. Zstash has parallel extraction and verification for increased performance. All E3SMv1 production simulations have been archived on NERSC's HPSS using zstash.

e3sm_to_cmip by Sterling Baldwin: e3sm_to_cmip (Presentation - Baldwin) is an extensible and portable Python package for the conversion of E3SM data to the MIP (Model Intercomparison Project) format. e3sm_to_cmip is able to take atmosphere, land, sea-ice, and ocean variables as input and convert them into CMIP compliant datasets. The package has been used to produce more than 1,800 datasets published to CMIP6.

All of the diagnostics/post-processing tools discussed here are available through a single Conda package, **e3sm_unified**. The e3sm_unified environment has been installed on all the E3SM-supported machines and simple instructions for activating it are provided. Tutorials and documentation are publicly available to new external users including information on how to install e3sm_unified on their own machines.

PACE by Sarat Sreepathi: PACE (Performance Analytics for Computational Experiments) provides an executive summary of E3SM performance, facilitating the following functions: interactive analyses and deep-dives into experiments and application subregions; tracking performance benchmarks and simulation campaigns of interest; performance research on load balancing and process layouts; and identification of bottlenecks to inform targeted optimization efforts. It has tracked more than 37,332 experiments and 1 million+ model-input files. Users use https://pace.ornl.gov to search for existing experiments using case, compset, grid, or user, etc.

Resources

E3SM Tools

- Main pages for all the E3SM tools: https://e3sm.org/resources/tools/

CIME

- GitHub repo: https://github.com/ESMCI/cime
- Documentation: http://esmci.github.io/cime/index.html

NCO

- GitHub repo: http://github.com/nco/nco
- Documentation: http://nco.sourceforge.net/nco.html

e3sm_diags

- GitHub repo: https://github.com/E3SM-Project/E3SM_diags
- Documentation: https://e3sm-project.github.io/e3sm_diags/_build/html/master/index.html

MPAS_analysis

- GitHub repo: https://github.com/MPAS-Dev/MPAS-Analysis
- Documentation: https://mpas-dev.github.io/MPAS-Analysis/stable/
- MPAS-analysis tutorial: https://mpas-dev.github.io/MPAS-Analysis/latest/tutorials/getting_started.html

zstash

- GitHub repo: https://github.com/E3SM-Project/zstash
- Documentation: https://e3sm-project.github.io/zstash/_build/html/master/index.html
- Tutorial: https://e3sm-project.github.io/zstash/_build/html/master/tutorial.html

e3sm_to_cmip

- GitHub repo: https://github.com/E3SM-Project/e3sm_to_cmip
- Documentation: https://github.com/E3SM-Project/e3sm_to_cmip/blob/master/README.md
- Getting started with CWL: https://e3sm-project.github.io/e3sm_to_cmip/html/cwl.html

e3sm_unified

- GitHub repo: https://github.com/E3SM-Project/e3sm-unified
- Documentation: https://e3sm.org/resources/tools/other-tools/e3sm-unified-environment/

PACE

- PACE portal: https://pace.ornl.gov/
- Videos
  —Web portal features video
  —Data upload video

E3SM ECOSYSTEM PROJECTS UPDATE

Closely associated with E3SM are the ESMD-supported research efforts called the "**E3SM Ecosystem**" projects. E3SM Ecosystem projects are closely-related, currently-funded BER Earth System Model Development (ESMD) projects that work on some aspect of E3SM development or work with E3SM data or its simulations. They receive money through the three main funding opportunities: Science Focus Areas (SFAs), University and Early Career Projects, and SciDAC Projects.

Science Focus Area (SFA)

E3SM Ecosystem projects are projects outside the main E3SM development project that are complementary to or coordinated with E3SM work. This session featured four Ecosystem projects funded partially through the Earth and Environmental System Modeling (EESM) program. Ecosystem projects funded through the Scientific Discovery through Advanced Computing (SciDAC) and Exascale Computing Project (ECP) programs were presented in dedicated sessions. The four projects in this session each crosscut various aspects of E3SM and are expected to feed back into E3SM in versions 3 or 4 (~5 year timeframe).

EAGLES: Enabling Aerosol-cloud interactions at GLobal convection-permitting scalES

The first project presented was the Enabling Aerosol-cloud interactions at GLobal convection-permitting scalES (EAGLES) project, which was covered by two presentations. In the first talk (Presentation-1 - Ma), **Po-Lun Ma** gave an overview of the project. EAGLES is focused on improving the representation of aerosols and aerosol-cloud interactions for global convection-permitting simulations targeted by E3SMv4. The scientific goal is to improve the understanding of, and confidence in, the role of aerosols and aerosol-cloud interactions in the evolution of the Earth system. The project sets up four geographic regions—Northeast Pacific, Central United States, Northeast Atlantic, and Southern Ocean—for model evaluation and assessment at a lower computational cost. Early achievements include prototyping improved treatments of ultra-fine particles, secondary organic aerosols, cloud-borne aerosols, giant particles, wildfire aerosols, dust, deep neural network (DNN) emulation of aerosol activation, refactored aerosol microphysics code, autoconversion emulation based on a newly developed computationally efficient Large Eddy Simulations (LES), and improved turbulence for aerosol activation. A preliminary diagnostics package using satellite and Atmospheric Radiation Measurement (ARM) data has been developed to facilitate routine model evaluation during model development. Code integration, evaluation, and analysis are ongoing. Figure 28 illustrates the overall approach consisting of three model-development themes and a cross-cutting activity.

The second talk of the session, given by **Sam Silva**, (Presentation - Silva) focused on the development of physically regularized machine-learning emulators of aerosol activation within the EAGLES project. There is clear observational evidence for aerosol activation, notably from ship tracks, but explicitly simulating the chemical and physical processes relevant to aerosol

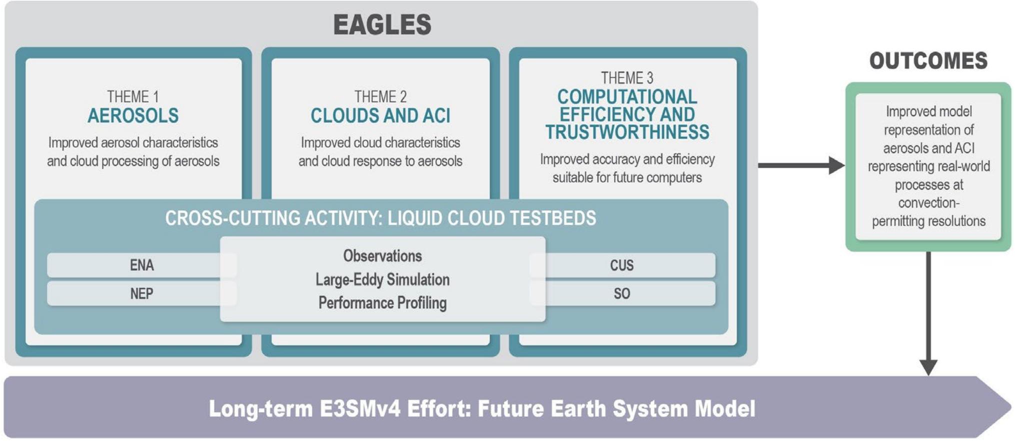


Figure 28. Enabling Aerosol-cloud interactions at GLobal convection-permitting scalES (EAGLES) project's approach, which includes three model-development themes and a cross-cutting activity.

activation is too computationally expensive for global Earth system models. The existing parameterization for aerosol activation in E3SM, ARG2000, is twenty years old, and while skillful and fast, it has well-understood limitations. This project has been investigating replacing the ARG2000 parameterization with a machine-learning emulator trained on a full, detailed reference cloud-parcel model of aerosol activation (parcel activation model). The emulator matches the reference simulations reasonably well, with better accuracy than the ARG2000 scheme, and most errors are within a factor of two. A second deep neural network was developed to include a simple regularization term that explicitly adds physics knowledge and avoids overfitting. The regularized machine-learning approach is much more accurate and fixes important local biases and potentially addresses some errors in extrapolation beyond the training data. This machine-learning approach runs smoothly in E3SM without causing the model to crash; however, it leads to many more cloud droplets, as compared to the existing aerosol activation parameterization (ARG2000). While the elevated cloud-droplet number concentration is expected given the properties of the deep neural networks and the ARG2000 scheme, further testing and development is ongoing.

ICoM: Integrated Coastal Modeling

The third talk, by **Elizabeth Hunke**, (Presentation - Hunke) described the Integrated Coastal Modeling (ICoM) project. ICoM focuses on modeling coastal evolution, including the tools and datasets needed to account for the multiscale interactions among physical, biological, and human systems (see Fig. 29). The project has a geographic focus on the Mid-Atlantic region, especially the Delaware/Susquehanna basin, and takes advantage of the regional mesh refinement

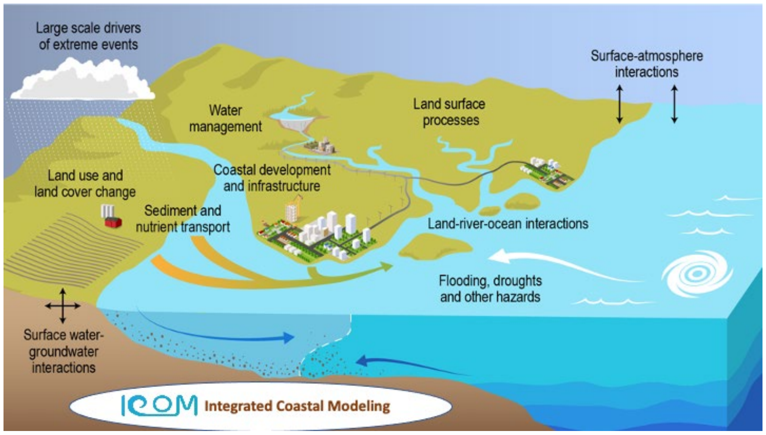


Figure 29. Integrated Coastal Modeling (ICoM) addresses the multi-scale interactions among physical, biological, and human systems.

in E3SM. The project is supported through the Regional & Global Model Analysis (RGMA), MultiSector Dynamics (MSD), Earth System Model Development (ESMD) and Subsurface Biogeochemical Research (SBR) program areas within BER. A goal of the project is cross-cutting hazard modeling and understanding the impacts of coastal development. A key development for this work is enabling two-way coupling between the model components for land (ELM), rivers (MOSART), and ocean (MPAS-O). For example, two-way coupling between land and river models leads to an increase in the maximum daily runoff in most regions. MOSART-Urban has been successfully validated offline for several urban watersheds with different levels of urbanization. To enable this more complete coupling between components, the project has developed a unified unstructured mesh, based on the MPAS Voronoi mesh format, that aligns with component boundaries so that no interpolation between components is required. These new, unified, unstructured meshes enable multiscale physics to be captured through variable resolution grids and for tight coupling between the ocean, land, and river models. The new mesh requires additional work to make sure that watersheds and rivers are properly routed across the landscape; the "stream-burning" capability within the HexWatershed model can produce robust flow direction even at coarse spatial resolution for hydrologic simulations. Water and sediment discharges are being tested on the new mesh. A unifying application area is in estuarine dynamics, which requires a range of new ocean-model development activities. These include tides with self attraction and loading, improved bottom drag, and topographic wave drag, which are being implemented in MPAS-O for a number of scientific reasons, e.g., sensitivity to climate change, impact on coastal flooding hazard assessments, impact on mixing, interactions with sea ice and floating ice shelves, etc. The implementation of the General Ocean Turbulence Model (GOTM) and a hybrid sediment transport model delivers to MPSA-O the capacity of simulating key estuarine processes. A novel, local time-stepping scheme enables efficient simulations on multi-resolution meshes. A number of numerical experiments will be conducted as part of this ESMD model development activity. A new collaborative project will explore ICoM's models' ability to produce conditions conducive to hypoxia in the Chesapeake and Delaware estuaries.

InteRFACE: Interdisciplinary Research for Arctic Coastal Environment

The fourth talk, given by **Andrew Roberts**, (Presentation - Roberts) summarized the Interdisciplinary Research for Arctic Coastal Environment (InteRFACE) project focused on improving fundamental understanding of changes in arctic coastal systems. The Arctic Ocean presents unique modeling challenges, with 10% of the Earth's runoff draining into 1% of its ocean volume. Internal variability is large in this region, which requires many model ensemble members to provide meaningful results. To address these challenges, an Arctic-focused configuration of E3SM has been developed using the regional refinement capability of MPAS and coordinating with the Water Cycle Campaign of E3SM. One year into the project, core model developments in InteRFACE are focused on ocean mixing, benthic biogeochemistry, landfast ice, wave-ice interaction, and permafrost hydrology in E3SM. These developments aim to add new capabilities to E3SM focused on improved polar ocean stratification and carbon fluxes, and coastal interactions affected by sea ice. One notable improvement includes a new ocean mixing scheme, where the K-Profile Parametrization (KPP) was replaced by the Assumed Distribution Higher-Order Closure (ADC) method (Poster - Garanaik), which is far less dependent on vertical resolution, so changing the vertical resolution in the ocean does not

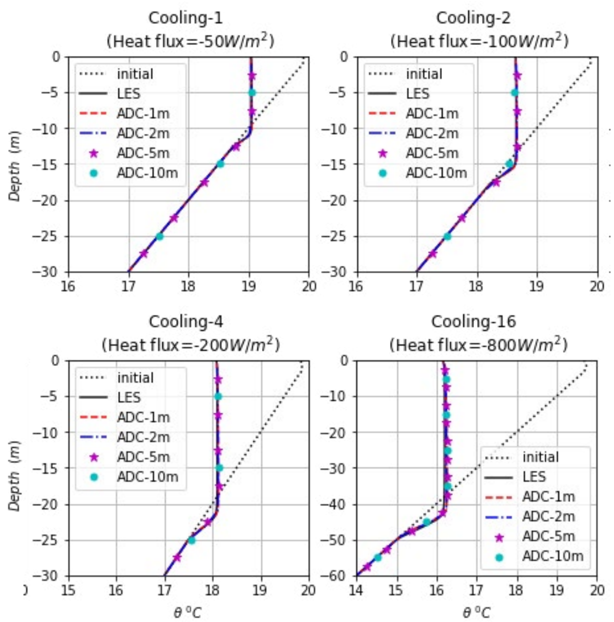


Figure 30. Evolution of mean temperature profiles for the ocean-surface-boundary layer obtained from the one-dimensional Assumed Distribution Higher-Order Closure (ADC) with different vertical resolutions (1m, 2m, 5m, and 10m) and forcings (heat fluxes of -50 to -800 W/m2), verified against the Large Eddy Simulations (LES) (solid black line) and the initial stratification (dotted black line). All forcing scenarios show that the ADC method agrees well with the LES method. ADC replaced the K-Profile Parametrization (KPP) ocean-mixing scheme since ADC is far less dependent on vertical resolution, making ocean mixing robust to changes in resolution. Image courtesy of Garanaik, Robey, Smith, Van Roekel and Li.

affect the resulting ocean mixing. Figure 30 shows a very close match between the LES (black line) and the E3SM simulations with the new ADC closure method (colored lines). In another InteRFACE development effort, the Advanced Terrestrial Simulator (ATS) is being coupled with MOSART as a proof of concept to understand the impact of permafrost on the land-ocean freshwater flux. These developments are being informed by parallel groups within InteRFACE working on the RGMA and MSD programs to ensure applicability of model developments in answering science and economic questions for the rapidly evolving Arctic region.

COMPASS-GLM: Coastal Observations, Mechanisms, and Predictions Across Systems and Scales, Great Lakes Modeling

The final talk in the session, given by **Ian Kraucunas**, (Presentation - Kraucunas) provided an overview of the Coastal Observations, Mechanisms, and Predictions Across Systems and Scales - Great Lakes Modeling (COMPASS-GLM) project. This project is focused on performing modeling at both regional and watershed scales, with a long-term goal of informing Earth system model development. The regional-scale work focuses on atmosphere-land-lake interactions, while the watershed-scale modeling focuses on nutrient removal and transport. COMPASS also includes a measurement-focused project that includes field work and site-scale modeling in both the Great Lakes and Mid-Atlantic regions (Fig 31). COMPASS will leverage and inform a number of other BER projects including ICoM, ExaSheds, IDEAS-Watershed, and E3SM. A future goal of the project is a regionally-refined configuration of E3SM that includes the Great Lakes resolved at 1 km resolution with enhanced representation of biogeochemical processes at the terrestrial-aquatic interface.

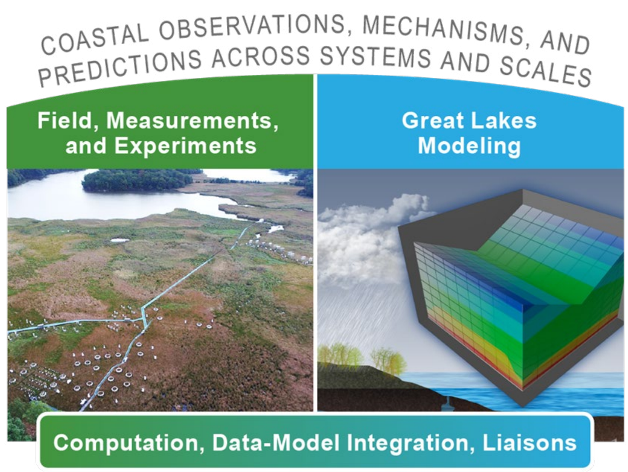


Figure 31. Overview of the COMPASS project.

University and Early Career Projects

This session was dedicated to University Projects within the ESMD program area. There are seven newly funded projects and eight other currently active projects. Each of the principal investigators (PIs) of the seven new projects gave a short presentation on the planned research for the coming years. The PIs of the active projects presented their current research results. The topics covered a wide range, from atmospheric physics parameterization, to data assimilation, to ocean model development and biogeochemistry.

Sea-level change is an important parameter for climate change and coastal management. **Matt Hoffman** described planned work to include regional modeling of sea level into E3SM (Presentation - Hoffman). The presence of an ice sheet attracts water towards the coast and pushes down the land. As ice sheets melt, the result is that sea levels change with a global pattern, falling locally and rising the most on the other side of the planet from the ice sheet. Including such feedback is important for correctly simulating sea-level rise in vulnerable areas, but requires simulating many processes not currently included in E3SM. This project will take steps towards including such processes.

Benjamin Sulman presented plans on simulating estuarine wetland vegetation and biogeochemistry in the E3SM Land Model (ELM) (Presentation - Sulman). Estuaries are characterized by interactions between freshwater from rivers and saltwater from the ocean and are important for carbon and nitrogen sequestrations. However, estuaries and estuarine wetlands are not currently represented in E3SM. This model-development project will introduce salt marsh and mangrove vegetation types and simulate chemical and biological interactions in wetland sediments. It will enable quantitative estimates of nitrogen removal, carbon sequestration, and greenhouse gas emissions from estuarine wetlands at estuary to continental scales.

Francois Primeau described a newly funded project aimed at initializing carbon-cycle processes within E3SM (Presentation - Primeau). Because the carbon content of oceans and soils can take many centuries to adjust to changes in climate, Earth System Models (ESMs) often show a drift in the carbon balance between the ocean, atmosphere, and land. The drift is significant in comparison to the anthropogenic uptake of carbon by land and ocean. This project uses simulations of idealized tracers to develop an approximate transport matrix that can then be inverted for the steady state of the system, eliminating the possibility that changes in the carbon cycle under climate change reflect changes in drift.

Atmospheric radiation parameterization is an important part of any ESM. In his talk (Presentation - Pincus), **Robert Pincus** described plans to update the radiation parameterization in E3SM and implement key improvements to ensure it is efficient and accurate. The enhancement of accuracy includes treating the first-order effects of a spherical atmosphere, including refraction and extended path lengths, in calculations of the direct solar beam and accounting for correlations between gases and clouds in the spectral dependence of scattering and absorption.

Parameter tuning in climate modeling is ad hoc, informed largely by global satellite products; it is a top-down approach. By contrast, process-level constraints can provide new insights for improving parameterization schemes; it is a bottom-up approach. In his talk (Presentation - Van Lier-Walqui), **Marcus Van Lier-Walqui** presented an approach combining process-level constraints with global climatology using Bayesian statistics and machine learning to improve the warm rain process representation in E3SM. The project aims to develop a system for evaluating both structural and parametric microphysical choices, thus paving the way for an integrated top-down and bottom-up climate model improvement.

Record levels of burning in 2018 and 2020 in the California ecosystems pose immense challenges for mitigating and adapting to climate change. **Jim Randerson** presented his project focused on investigating the interactions between land use, fires, and dust as drivers of global climate change (Presentation - Randerson). The goal is to improve the representation of fire and dust in E3SM, create new fire and dust emissions time series, and examine the impacts of fire-dust-land interactions on future climate feedbacks.

Johannes Westerink described a project aimed at embedding high-resolution models of coastal embayments within E3SM (Presentation - Westerink). Tidal variations in such embayments are critical for many uses of the coastal zone, including flood protection, energy production and navigation, but properly simulating such features (and the extent to which they dissipate tidal energy) requires much finer resolution than even the high-resolution versions of the current model. The goal of the project is to extend the capabilities of MPAS-Ocean to include coastal flooding using recently developed subgrid techniques.

The eight currently active University Projects were presented next with research covering a wide range of topics from atmospheric model physics to ocean biogeochemistry. **Guang Zhang** presented results from his project on enhancing convection parameterization in E3SM (Presentation - Zhang). A stochastic convection parameterization scheme was incorporated into the Zhang-McFarlane scheme to account for stochasticity of convection in E3SM at both low (1-degree) and high (0.25-degree) resolution . The inclusion of stochastic convection parameterization decreased the occurrence of light rain and increased the occurrence of heavy rain, largely correcting the “too much light rain and too little heavy rain” problem in the model. There was not much difference in the mean state of rainfall distribution.

Joao Teixeira described a new unified boundary layer and convection parameterization using the multi-plume Eddy-Diffusivity/Mass-Flux (EDMF) approach in the E3SM model. The goal of the project is to reduce key biases related to the atmospheric boundary layer and boundary layer clouds in E3SM. The EDMF scheme makes use of the surface-layer probability density function (PDF) of thermodynamics and Monte Carlo sampling of the PDF to produce multiple plumes. The plumes are determined by surface properties. The results show that using the Simplified Higher-Order Closure (SHOC) scheme with EDMF improved the representation of the planetary boundary layer (PBL) and shallow convection in several aspects.

The effect of mesoscale organization is not represented in E3SM. **Jack Chen** presented results from the project focused on evaluating the effects of organized mesoscale heating on the Madden-Julian Oscillation (MJO) and precipitation in E3SMv1 (Presentation - Chen). A parameterization representing the dynamical and physical effects of the circulation associated with organized convection, referred to as multiscale coherent structure parameterization (MCSP), has been implemented in E3SMv1. The free parameters in the MCSP were tuned based on the findings from high resolution (1 km) WRF simulations. The MCSP enhances the Kelvin wave spectrum and improves the simulation of the MJO in E3SMv1.

Xiangyu Huang described the effects of a more realistic treatment of surface spectral emissivity, ice-cloud optics, and ice-cloud longwave (LW) scattering implemented in RRTMG_LW and RRTMGP_LW of E3SMv2 (Presentation - Huang). This treatment resulted in more heating of the atmosphere column and increased LW cloud radiative forcing. In the global-energy budget, large effects of this improved treatment were seen in both the top of atmosphere (TOA) and surface longwave fluxes; it reduced biases from the CERES-EBAF observations by about 1 Wm-2 for both the outgoing longwave radiation (OLR) and surface net longwave flux.

Shu Wu described the progress on implementing an online data-assimilation system within E3SM (Presentation - Wu). A particular challenge in developing such systems is estimating the covariance matrix whereby the impact of an observation is propagated within the model. The approach taken here was to run a relatively small number of simulations to estimate the time-varying part of this covariance matrix, while using the results of a large ensemble to precompute the stationary part of this matrix to much higher accuracy.

Sagar Rathod reported on a project examining the impact of aerosol iron on climate, via its reflection of solar radiation, and biogeochemical cycling, by providing a key nutrient for oceanic photosynthesis and carbon fixation (Presentation - Rathod). While the anthropogenic impacts on both effects are small on a global scale, this work shows that, locally, increased iron deposition from anthropogenic sources can increase productivity by up to 15% and produce changes in the shortwave forcing on the order of 0.5 W/m2 over East Asia.

Xiaoming Xu presented results quantifying the impact of agriculture, in particular systems including livestock, on the carbon cycle (Presentation - Xu). A significant amount of the carbon fixed in plants is used as feedstock for animals. This work described a synthesis looking at the impact of the entire cycle of harvesting, feedstock, and manure on nitrogen and carbon-cycle dynamics. It was estimated that about 2.5 Pg of carbon are involved in the production of feedstock and that the net release of carbon from agricultural facilities is comparable to that associated with land-use and land-cover change.

Anand Gnanadesikan reported on work done to isolate the impact of lateral mixing in the ocean on Earth system modeling within E3SM (Presentation - Gnanadesikan). The lateral mixing due to mesoscale eddies was omitted from E3SMv1 owing to numerical instabilities, which have been diagnosed and fixed. This presentation highlighted the role of convective-region lateral mixing as having disproportionate impacts on biogeochemical cycling in the oceanic interior, which affects the character of deep-ocean convection.

SciDAC Projects

The Principal Investigators of the SciDAC projects provided overviews of their projects.

Phil Jones presented the "**Coupling Approaches for Next Generation Architectures (CANGA)**" project (Presentation-2 - Jones), which investigates new algorithmic and computational approaches for coupling processes and components in Earth System Models like E3SM. Asynchronous Many-Task (AMT) models have advantages for managing complexity, load balancing, and fault tolerance in coupled Earth System Models. In addition, they permit a coupling of subcomponents at the process level rather than coupling large components. Preliminary results from the exploration of these systems were presented. Some algorithmic improvements in the remapping of fields were described. Also presented were improvements in how a coupled system is advanced in time in a stable and accurate manner.

Peter A. Bosler presented the project, "**Compact, Performance-Portable Semi-Lagrangian Methods for E3SM**" (Presentation - Bosler). The project develops semi-Lagrangian (SL) algorithms and associated software for passive tracer transport in E3SM, aiming at (a) high performance on the advanced architectures of current and anticipated DOE Leadership Computing Facility (LCF) computing platforms, and (b) achieving the fundamental required traits of a climate model's transport scheme: conservation, accuracy, tracer consistency, shape preservation, and computational efficiency. Integrating SL transport into E3SM frequently requires algorithmic improvements in other parts of the code (time stepping, in particular) and exposes opportunities for investigating non-hydrostatic effects and radiative-convective equilibrium at high resolution. The presentation discussed the impacts and applications of this work on the E3SM Atmosphere Model version 2 (EAMv1). Also presented was ongoing work with MPAS-Ocean targeted at the version 3 biogeochemistry science campaign.

Hui Wan presented the project, "**Assessing and Improving the Numerical Solution of Atmospheric Physics in E3SM**" (Presentation - Wan), which addresses numerical issues in parameterizations. The first efforts in the project used a hierarchy of models with different levels of complexity to demonstrate that time-step convergence is a relevant concept, despite the fact that parameterizations are often considered empirical and/or pragmatic. Revisions of numerical algorithms that address convergence issues can lead to a more consistent representation of the physics and significant impacts on the simulated long-term climate. Recent efforts have focused on the current and planned versions of EAM. Significant progresses included the quantification and

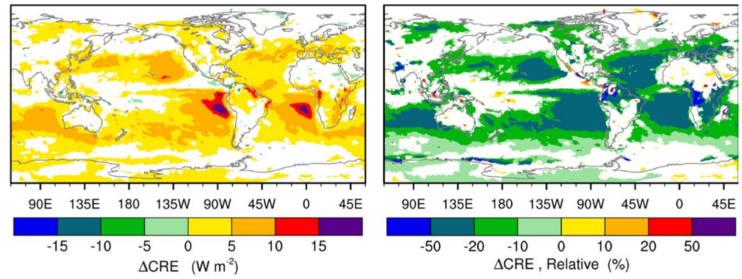


Figure 32. EAMv1 simulates substantially less subtropical clouds and weaker cloud radiative effects when model time steps are shortened. Important progress has been made to identify and address the root causes of this sensitivity. The left and right panels show the absolute and relative changes, respectively, in the 10-year mean total cloud radiative effect when time steps in EAMv1's 1-degree present-day simulation are shortened to 1/6 of the default values.

attribution of time-step sensitivities in present-day climate simulations (Fig. 32) and improvements in the numerical coupling of various atmospheric processes.

Lili Ju presented "**Parallel Exponential Time Differencing Methods for Ocean Dynamics**" (Presentation - Ju). Exponential time differencing has been numerically proven to be an effective and efficient approach for time integration of the ocean dynamics. It allows use of large time-step sizes much beyond the CFL (Courant–Friedrichs–Lewy) time-step restriction, while still maintaining good numerical stability. Its main cost lies in the calculation of the products of matrix exponentials and vectors. The presentation reported on recent progress in developing and implementing scalable parallel exponential time-differencing algorithms within the MPAS framework. The benefits of the new algorithms were demonstrated with simulations of the rotating shallow-water equations and the primitive equations.

Takanobu Yamaguchi presented "**Enhanced Low Cloud Representation in E3SM with Framework for Improvement by Vertical Enhancement (FIVE) and Future Plan**" (Presentation - Yamaguchi). FIVE is a novel method that embeds an auxiliary column with a fine vertical grid in the grid column of the host atmospheric model and computes selected one-dimensional processes thereon. The first set of efforts in this project demonstrated that high vertical resolution similar to that used in large eddy simulations can significantly improve E3SMv1's simulation of low clouds that have important climatic impacts. It was also shown that FIVE can yield similar improvements while limiting computational cost (Fig. 33). The second phase of the project focuses on incorporating an Adaptive Vertical Grid (AVG) into E3SMv1-FIVE, tackling remaining "stubborn" low-cloud types, and developing FIVE towards the global cloud-resolving E3SMv4. Important recent progress includes the development of a 2D Hadley circulation model with E3SMv4 physics as a testbed to assess FIVE's performance. A new FIVE implementation strategy was proposed and the implementation of FIVE into the 2D Hadley circulation model is ongoing.

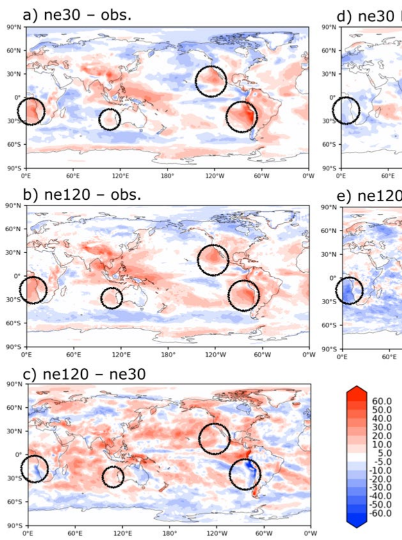


Figure 33. Differences in shortwave cloud radiative effect show that (i) improving horizontal resolution from ne30 (100 km mesh) to ne120 (25 km mesh) produces some coastal stratocumulus (panels a, b, and c), (ii) FIVE with ne30 does not produce the coastal stratocumulus (panels a and d), and (iii) ne120-FIVE significantly improves coastal stratocumulus as well as other subtropical low clouds (panels b and e). A combination of the Regionally Refined Model and FIVE would be a cost-effective method to mitigate the coastal stratocumulus problem.

Stephen Price presented the project "**Probabilistic Sea Level Projections from Ice Sheet and Earth System Models (ProSPect)**" (Presentation-2 - Price), which aims to address limitations to DOE's ice sheet models (ISMs) and Earth System Model (E3SM) that currently limit their application towards probabilistic sea-level projections. Project focus areas include the improvement of (1) missing or inadequate ISM physics, (2) partial or missing coupling between ISMs and ESMs, (3) ISM initialization methods targeting coupled ISM and ESM simulations, (4) ISM uncertainty quantification towards probabilistic sea-level projections, and (5) the computational performance of ISMs on next-generation HPC architectures. In this presentation, progress in several project areas was presented, including (1) the simulation of fracture and calving through the use of damage mechanics, (2) the addition and validation of new subglacial hydrology models and their impact on simulation realism and uncertainty quantification approaches, (3) the coupling and impact of ice-sheet and solid-earth models, (4) new E3SM capabilities for simulating ice-sheet surface mass balance in E3SM, and (5) DOE ice-sheet-model contributions to improved projections of future sea-level rise (Fig.34).

Adrian Turner presented "**Discrete Element Model for Sea Ice (DEMSI)**" (Presentation - Turner), a project that aims to develop a new sea-ice component for E3SM using a discrete-element method where parcels of sea ice are represented as finite-sized Lagrangian particles. It is expected this methodology will improve model performance on next-

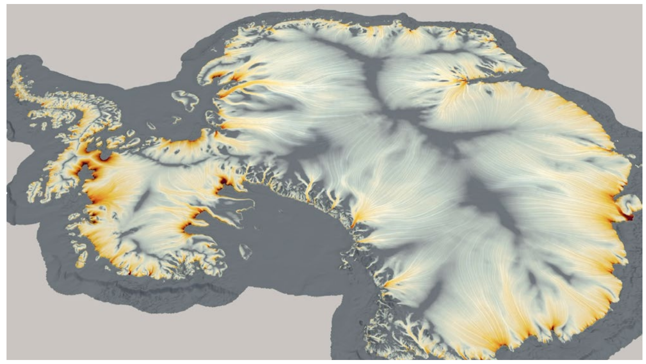


Figure 34. DOE MALI ice-sheet model's simulation of Antarctic ice-sheet collapse caused by the instantaneous and sustained removal of all fringing ice shelves starting from the present day. This is one of a number of contributions from the international CMIP6/ISMIP6 effort towards projecting/bounding future sea level rise from ice sheets. The image shows streamlines of ice flow with color indicating relative ice speed (the speed increases from gray to white, orange, and red). Fastest speeds are seen in ice streams and outlet glaciers and along the retreating ice-sheet margin.

generation DOE heterogeneous computing architectures and improve model dynamical fidelity by explicitly representing complex contact physics. Simulations were presented to demonstrate DEMSI's ability to represent ridging and sea-ice convergence, to ameliorate the effect of this ridging on particle distribution by remapping techniques, and to simulate sea ice on the basin scale. The model's performance on heterogeneous architectures was also demonstrated.

Gautam Bisht presented "**Development of Terrestrial Dynamical Core (TDycore) for the E3SM to Simulate Water Cycle**" (Presentation - Bisht), a project that aims to advance the state-of-the-art modeling of terrestrial hydrological and thermal processes by enabling the inclusion of lateral subsurface transport of water and energy in the E3SM Land Model (ELM). The TDycore is expected to be rigorously verified, spatially adaptive, scalable, and validated for a wide range of cases. The open-source TDycore library has been developed using the Portable Extensible Toolkit for Scientific Computing (PETSc) to numerically solve the discretized equations. The terrain-following ELM meshes are nonorthogonal with approximately 10^6 differences in horizontal and vertical length scales, which render first-order spatial discretization methods inaccurate. The TDycore supports three second-order spatial discretization methods and four temporal discretization schemes. A code-agnostic verification and validation framework to benchmark the TDycore has been developed. The TDycore has been coupled to ELM and idealized simulation with the coupled model has been performed. In collaboration with the Exascale Computing Project (ECP), TDycore has successfully used PETSc's support for heterogeneous computing architectures on DOE's Summit supercomputer.

BREAKOUT SESSIONS FOCUSED ON CHALLENGES, OPPORTUNITES, AND NEEDS

The purpose of the breakout sessions was to brainstorm some ideas that can benefit the E3SM development in each component (e.g., atmosphere, ocean, land, and computation) and its interaction with other components.

Atmosphere Breakout, Peter Caldwell, Vince Larson

Many challenges for the E3SM Atmosphere Model (EAM) were identified in this session. In particular, **Chris Golaz** provided a summary of the main biases in E3SM (Presentation-2 - Golaz). For precipitation, they are double ITCZ, dry Amazon, dry central US, and excessive amount over the Maritime Continent and regions of high topography. The main top-of-atmosphere radiative biases are

1. too little stratocumulus,
2. overly bright clouds over the Southern Ocean, and
3. overly-strong aerosol indirect effect and climate sensitivity, leading to underpredicted surface temperatures between 1960 and 2000.

Fixing these model biases should be a number-one priority for the E3SM development.

Interestingly, Golaz used comparison against the best and worst CMIP6 models to show that most of E3SM's main biases are shared by other models. This implies that E3SM's problems are not due to a particular choice of parameter setting or code implementation, but instead arise from the foundational assumptions made in contemporary Earth system modeling. Jiwen Fan pointed out that coarse resolution is a common feature of CMIP models and could easily be responsible for many of these shared biases. If true, the SCREAM model may provide a path to surmounting these problems.

Ross Dixon also gave a talk (Presentation - Dixon) showing that both E3SMv1 and its cousin CAM6 report unrealistically large supersaturations after MG2 microphysics calculations. This result was met with surprise by MG2 designers, who noted that their scheme ends with a calculation to remove excess cell-average supersaturation. Dixon found that reducing the model timestep was effective at reducing excessive supersaturations. Understanding and fixing this

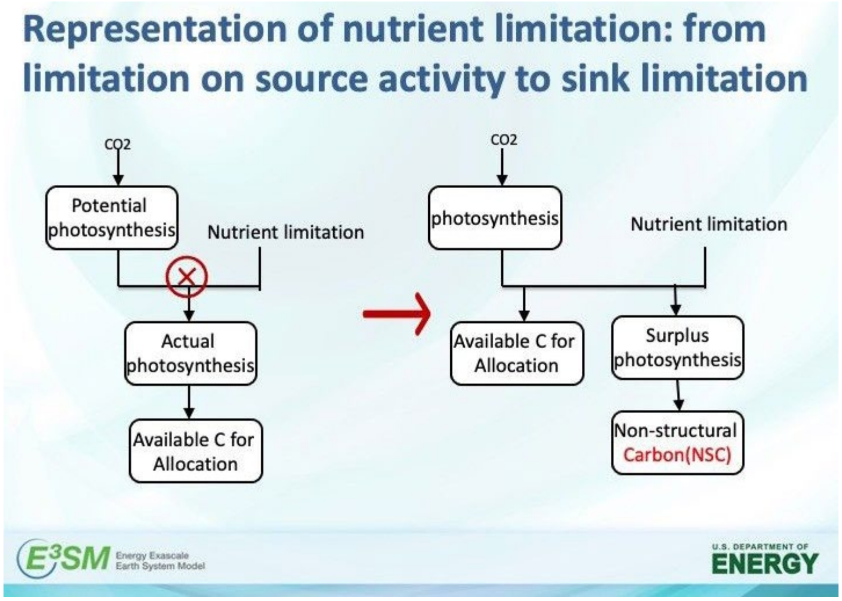


Figure 35. Schematic of the representation of nutrient limitation in CLM4.5/ELMv0 (left) and ELMv1 (right). In CLM4.5/ELMv0, photosynthesis is instantaneously down-regulated due to nutrient limitation. In ELMv1, nutrient limitation does not directly affect photosynthesis, but rather constrains plant growth; the extra photosynthesized carbon enters a nonstructural carbon pool.

supersaturation problem is low-hanging fruit for improving model realism.

Another challenge for EAM is the ability of parameterizations to provide accurate results across a wide range of resolutions. Peter Caldwell argued that getting schemes to behave accurately over all scales is much harder than developing different schemes for spatial regimes where that process is/isn't resolved. In this context, scale awareness would mean that researchers should be aware of the scale at which their parameterizations are appropriate. He claimed that effort would be better spent providing good parameterizations within regimes than forcing schemes to work outside the regime they naturally fit in. E3SM's Regionally-Refined Model (RRM) capability provides a case that may force E3SM to develop scale-aware schemes. Chris Golaz pointed out that spatial-resolution sensitivity is often really due to the need to use shorter timesteps at finer resolutions and at least for the 25–100 km scale difference used in E3SMv2 RRM efforts, simply ensuring a common physics timestep at all resolutions was sufficient to damp down resolution sensitivities. In the future, E3SM will likely want RRM grids which span from 3 km in some locations to 100 km in others. This span is clearly too large to handle with a single set of tuning parameters; Peter Caldwell suggested that in this scenario the model should be tuned to work well at 3 km and nudging used in the 100 km areas to prevent inappropriate tuning/physics at that scale from degrading the simulation.

Oksana Guba suggested that model robustness is another grand challenge for E3SM. For E3SM to be used for decision support, we need to be sure its predictions aren't artifacts of poorly designed numerical schemes or coding errors. This requires increased focus on unit tests and in particular, tests of mathematical convergence. Such testing would also hopefully protect the model against instabilities/crashes, which are hard to track down. E3SM has steadily been moving towards more thorough testing, but much more work is needed.

Finally, **Charlie Zender** pointed out that using a spherical earth rather than a flat-plane assumption for radiation would fix known regional biases of 1 W/m2 amplitude (reported by Michael Prather), potentially fixing some of the E3SM longstanding biases noted earlier.

Land Breakout, Ben Bond-Lamberty, Jim Randerson

Xiaojuan Yang – talk on global benchmarking of ELM v1
The E3SM Land Model v1 (ELMv1) has a prognostic Phosphorus (P) cycle and prognostic Carbon-Nitrogen-Phosphorus (CNP) interactions. Interestingly, the implementation of P generally improves performance, although there are a few degradations (e.g. burned area); it also improves simulated spatial distribution of biomass. At a global scale, incorporating P improves simulated historical land carbon accumulation. How about compared to other CMIP6 models? **Xiaojuan Yang** noted (Presentation – Yang) that there are no clear winners; some models do better on a set of variables, some on other variables.

She also posed an interesting question: how can scientists be sure their models are doing the right thing for the right reason? Researchers need to think beyond benchmarking with ILAMB. For example, results from the Free-Air Carbon dioxide Enrichment (FACE) experiments can be compared against global model runs simulating 200 ppm above current ambient CO_2 concentrations. Yang argued that scientists can also contrast nutrient limitation in the Community Land Model (CLM) v4 and 4.5 with ELM v1, an approach supported by, e.g., Prescott et al. (2020); she has found that models have similar gross primary production (GPP) responses to elevated CO_2, but very different leaf area index (LAI) responses (Fig. 35).

Finally, Yang noted that scientists need to think beyond carbon. For example, modelers should leverage resources such as GOLUM-CNP, a series of internally consistent, observationally based global datasets first published by Wang et al. (2018). ELMv1 shows general agreement with GOLUM's high tropical N and P uptake, but also some significant differences; there's a similar story with nitrogen use efficiency, which exhibits general model/data product agreement in spatial patterns, but not magnitudes. Finally, Yang reminded the audience that other literature values might be useful too. Researchers shouldn't confine themselves just to global datasets; synthesis efforts that are not "wall-to-wall" in spatial extent can still provide useful constraints to models.

Open Discussion
What are the grand challenges in land modeling?
The breakout then turned to an open discussion of the grand challenges in land modeling. One theme is clearly how the intersection of disturbance and soil biogeochemistry affects the carbon cycle and how this complicates modeling. For example, Earth System Models typically don't track disturbances at a granular-enough level, meaning that long-acting disturbance effects are lost over time (although ELM's novel "spawn new soil columns" capability improves this significantly). Data on 14C turnover time could be a great constraint for models as well.

A second area revolves around subgrid heterogeneity—the ability to run hyper-resolution, disaggregating pools and fluxes in response to high-resolution climate forcing. Several participants raised an interesting caveat: how much can be gained if the atmosphere model uses a coarser grid? One problem is that scientists don't know the critical resolution; uncertainty is related to the initial state and transient boundary conditions (e.g. land use/land cover change). One attendee noted that in atmospheric science there is a power spectrum, and one can see breaks which mean a different parametrization/implementation is needed. Is there something like that for the land model? It's unclear. Further points raised on this issue included the following:

- Interesting hotspot processes may happen on scales of less than 1 m, and modelers risk losing all the signal if averaging. Highly nonlinear responses to soil moisture varying over small scales is one example.
- The hydrological unit is also important: e.g. snow cover is variable in both space and time, and how it interacts with and/or drives biogeochemical hotspots is unclear.
- A lot of work has been done on climate downscaling, but there is a limit at some point in terms of numerical fidelity and precision limitations.
- Again borrowing concepts from atmospheric sciences, researchers look at mean values, not mean + perturbation, higher-order moments.
- Going from coarse resolution to fine spatial resolution means that three-dimensional effects become increasingly important; for example, the lateral process driven by hydrology (surface runoff carries debris, etc.).

Another theme revolved around being able to run models for thousands of years—in particular, being able to easily run model ensembles over long time periods. Considerations raised include:

- Such ensembles are critical for longer-term questions that are important to humans as a species, but at first glance the computational requirements seem prohibitive; how can researchers deal with this?
- Can scientists come up with Reduced Order Models (ROMs) or Machine Learning (ML) surrogates? The surrogate model work under the E3SM Land UQ (Uncertainty Quantification) effort is very relevant here.
- What about combining topographical representation with vegetation for joint distribution? One developer noted that this is partly the purpose of the new nested sub-grid hierarchy in ELM. The GFDL model has a similar scheme, but overall this is unusual in the Earth System Modeling community. Finally, participants noted that such a representation helps make use of datasets at different resolutions (e.g. elevation) vs. soil type.

Ocean Breakout, Luke Van Roekel, Zhengyu Liu

The purpose of this session was to discuss grand challenges in ocean modeling. Most of the discussion was focused on how to better understand and model unresolved processes in the ocean (Fig. 36).

The processes shown in Figure 36 are essential to the climate system. Mesoscale eddies can be resolved in shorter simulations, but it is not feasible to resolve them in large ensembles of projections, which are essential to DOE mission needs. In this session, participants discussed how to physically understand these processes, what tools are needed, and how to foster collaborations to accelerate understanding.

The session began with an overview of the work being done by the **Eddy Energy Climate Process Team (CPT)**. Invited speaker **Laure Zanna** discussed the various approaches being taken by the CPT to parameterize mesoscale eddies in ocean models. Most of their work is proceeding within the context of eddy-energetics schemes. These schemes will be constrained via high-resolution simulations and observations. Zanna also presented some intriguing new directions for mesoscale eddy parameterization, using non-Newtonian methods (similar to the LANS-alpha model) and physics-informed machine learning.

The discussion identified several important focus areas for ocean models: (1) mesoscale and submesoscale eddies and symmetric instabilities, (2) where non-Boussinesq and non-hydrostatic capabilities are truly needed in the ocean model, (3) scale-aware physics, and (4) data assimilation that can be used for optimizing model parameters as a first step in machine learning, in addition to the estimate of the ocean state. While the Eddy Energy CPT is poised to make great strides in mesoscale eddy parameterization, submesoscale eddies and symmetric instability parameterization remains a largely unexplored frontier.

Models like E3SM are uniquely poised to lead simulations of the global to coastal ocean, but progress must be made in creating or adapting parameterizations to be scale-aware, where eddies are fully resolved in some regions and fully parameterized in others. It is also desirable to have flexibility in where non-hydrostatic pressure is computed, as this is a large computational expense. This requires not only knowing where non-hydrostatic pressure is important, but also requires advances in numerical algorithms to solve the Poisson equation for pressure regionally. Application of

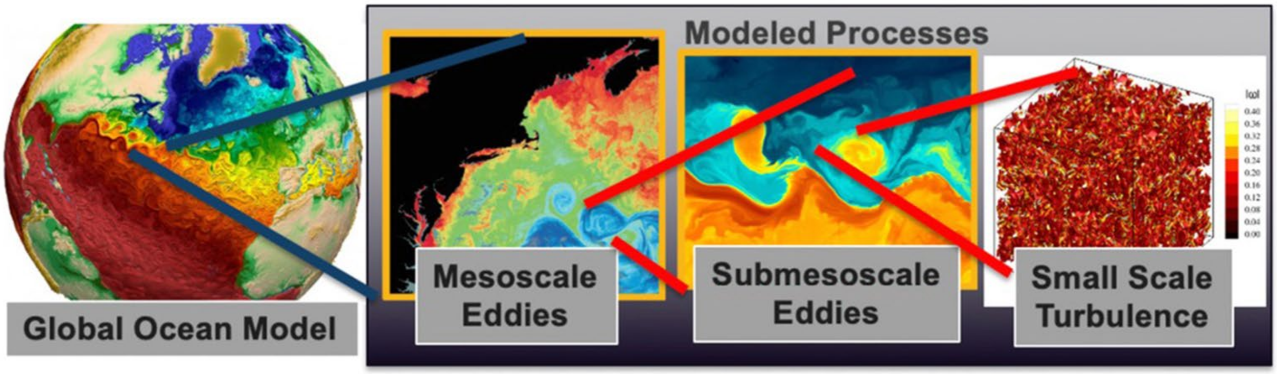


Figure 36. Schematic of scales of oceanic motion. The left panel is from an MPAS-Ocean simulation with high resolution (18 km near the equator and 6 km near the poles). Moving from left to right progressively zooms in to illustrate smaller scales of motion. The left three images show a bird's-eye view, while the rightmost image is a 3D view. Mesoscale eddies (6–100 km in diameter) are most prominent in the upper 2000 meters of the ocean where horizontal buoyancy gradients are strong and are easily seen in the MPAS-Ocean simulation as Gulf Stream rings. Submesoscale eddies (100 m–10 km) are most prominent in the upper ocean and often form on the edge of mesoscale eddies. Small-scale turbulence (<100 m) is often confined to the upper ocean but can exist throughout the global ocean.

machine learning and artificial intelligence, including data assimilation for parameter optimization, could help constrain where non-hydrostatic pressure is important. Recent advances in mesoscale eddy parameterization also suggest physics-informed machine learning could provide a path toward scale-aware parameterizations.

To make progress in these essential areas it is critical that E3SM be able to receive input and developments from community researchers. For this to happen, it is imperative to develop an infrastructure that allows outside researchers to run and modify E3SM without significant time and effort from E3SM staff. This will require clear documentation on running the model and associated workflows. For E3SM to receive developments back from the community, the E3SM team must clearly publicize coding, testing, and design standards.

Progress in key areas also requires a model with flexible configurations. Simple, lightweight test cases are needed to allow for the rapid testing of new ideas. To make an idealized configuration that also applies to the coupled system, work is needed to determine the minimum set of processes and feedbacks needed to understand the model. The need for a hierarchy of models and configurations extends beyond the dynamical model to the biogeochemical cycles (BGC) configuration as well. Here a reduced set of BGC variables will allow for rapid testing and will open avenues to the interaction of BGC and ocean physics.

Participants in this breakout session recommend the following:

1. Redoubling the effort on understanding the processes within the model is needed. This will help determine which advances are needed in which regions. These advances will likely require scale-aware parameterizations that vary in complexity from region to region.
2. It was agreed that physics-informed machine learning is likely to play a large role in determining what advances are needed and potentially contribute to new parameterizations as well. Given a model configuration, data assimilation also provides a method for optimizing model parameters.
3. The advances required to address key challenges require community engagement. An investment is needed to make community involvement easier. This will likely be a nontrivial, upfront cost, but will lead to lower cost over the longer term.

Computational Science Breakout, Phil Jones, Peter Bosler

Computational Science Grand Challenges

In this breakout session, the goal was to identify a set of big-picture issues, opportunities, and challenges related to computational science in Earth system modeling and E3SM. The focus was directed at the approximate five-year time horizon or longer, E3SM versions 4 and beyond.

The session co-chairs devised some guiding questions to frame the discussion and provide scope for the session. These questions were grouped into four areas representing the broad range of work needed to perform and support computational science, including exascale-hardware challenges, algorithmic improvements, supporting infrastructure and workflow, and documentation.

Presentation
Before opening the discussion, **Andrew Bradley** gave a talk (Presentation - Bradley) that exemplified work combining algorithmic improvement, optimized implementation, and rigorous testing to increase the throughput of the atmosphere model by a factor of two. Bradley presented his work on new semi-Lagrangian transport schemes with high computational efficiency, defined as the highest accuracy for given computational resources. The semi-Lagrangian algorithm permits longer time steps with a fixed communication volume independent of time step. The scheme can be further optimized with a Communication Efficient Density Reconstructor (CEDR) and an upwind communication pattern, both of which greatly reduce communication. From a solution standpoint, the scheme also has low dissipation, better conservation, and converges at the expected second order, with much-higher order implementations planned. Future work will implement this algorithm in the ocean model.

Discussion Questions
Prior to the start of the breakout session, a number of questions were posed to help guide the discussion. These questions, grouped into four general topic areas are repeated here for context.

A. Grand Challenges & Barriers for Exascale Computing and Beyond
1. What are the grand challenges and barriers, with respect to computing, that are specific to Earth system modeling?
   a. What kind of strategies and efforts might break these barriers?
   b. What recent opportunities and advances in algorithms, performance optimization, programming models, and software engineering could E3SM leverage and integrate?
2. How do we keep E3SM at the forefront of scientific development and computing?
   a. What level of programming knowledge/ability can we realistically expect from the broader E3SM community?
   b. How can we facilitate the requisite learning and training required to achieve these new skill levels?
   c. What level of abstraction properly balances portability and performance while also encouraging performant programming practice from developers?

B. Algorithms
Some of our best successes have come from algorithm development, not hardware.
1. What parts of E3SM present the best opportunities for algorithmic improvements?
2. Are any of our current algorithmic choices limiting performance or progress?
3. What algorithmic approaches to coupling, both between components (e.g., atmosphere–ocean) and within components (e.g. physics–dynamics), would improve accuracy, stability, and software workflow?

C. Workflow, Testing, & Infrastructure
1. What improvements are needed in DevOps (e.g., git workflow, build system, test coverage, test frequency, test design, handling test failures)?
2. What are the pain points in our current workflow?
   a. GitHub
   b. Build systems
   c. Model configuration, incl format (xml, yaml, nml), compatibility of options
3. How can we improve our testing, from unit tests through system verification of complex nonlinear dynamics?
   a. Given that bit-for-bit reproducibility may not be guaranteed on future architectures, how do we move beyond BFB testing? What characterizes "statistically equivalent" model climates?
   b. Can we make verification a standard practice, uniformly across E3SM?
4. Is there parallelism in our workflow that we are not taking advantage of? How do we use the extreme parallelism in new architectures to include more of the scientific workflow?

D. Documentation
1. How can we improve E3SM-specific, computationally-focused on-boarding of new personnel?
   a. Many Confluence how-to guides exist, but how many are outdated?
   b. Suppose a new postdoc has experience with MPI-based software before. Could this person, using only the existing documentation, build and run an existing E3SM test case and do some cursory data analysis (e.g., plotting) in a reasonable amount of time?
2. What are the big holes in our current documentation? How do we incentivize documentation from developers?

Discussion Summary
The time for discussion was very short (only ~40 minutes) and it would be impossible in that time to capture the views of the 30 or more participants or prioritize the most pressing needs or grand challenges across the broad scope of computational science. However, the topics that were discussed are summarized here. These should not be considered

consensus opinions, just a summary of topics that were discussed.

Exascale Challenges

One of the biggest challenges for exascale computing, noted in numerous presentations during the week and mentioned during this session, is the need to provide more work per node to effectively utilize the additional parallelism within accelerators and future devices. Earth system models typically have thin workloads, particularly at the strong scaling limit. Algorithmic innovation will be needed to solve this problem and simply porting existing models will be insufficient.

Related to the architectural challenges is the lack of a robust, standard programming model, or even a machine model or abstraction. A number of programming models and Domain-Specific Languages (DSLs) were presented during the week by participants and keynote speakers. There is a strong need to provide portable programming models to shield developers from the rapid change and different approaches in hardware. However because the machines continue to undergo substantial evolution, it is likely that programming models and abstractions will also evolve and developers may not be able to expect a convergence in programming models. It was also noted that current programming models are having difficulty achieving buy-in by scientific developers, causing multiple versions of codes and divergence in development.

Another challenge will be the continuing imbalance in storage and input/output (I/O) speeds compared to computational power. While SCORPIO has significantly improved I/O performance, additional algorithm and workflow innovation will likely be needed to overcome these bottlenecks. New machines are also introducing innovation in file systems, moving away from spinning disk arrays, and this will also require developers to adapt. Some ideas for I/O included,

- Asynchronous I/O (also known as non-sequential I/O)—offloading I/O tasks to operate concurrently
- Generalizing specifications to allow flexibility, e.g., to describe which fields are written, how frequently, at what resolution, etc.
- Down-sampling high-resolution data
- Compression of data
- Less frequent output, with supplemental reruns of targeted intervals to provide high-frequency data.

It was also noted that identifying all the desired fields has already been problematic and has required expensive re-computation for current high-resolution production simulations.

Algorithmic Challenges

Algorithms provide the best means for improving model throughput and performance. A number of algorithm suggestions arose during the discussion.

Remapping is a general capability that is useful for a number of algorithms across the model, and optimal, accurate, and robust algorithms for remapping would have high impact. This includes not only remap used in transport or coupling, but also in upscaling or downscaling for land meshes, runoff, particle-based methods (e.g., DEMSI), and in spin-up applications.

There were discussions related to meshing also during this session. The current sea-ice model is constrained to the full ocean mesh in the present model and an early win could relax this constraint to use sea-ice meshes that only cover the polar regions. Other suggestions included a range of land meshes and the use of the regionally-refined mesh (RRM) with land. Coupling to the runoff component can be an issue. For the coastal components, projects are using a unified land/ocean mesh.

Time-step constraints continue to be a bottleneck at high resolution and continued work in this area could significantly improve throughput. Verification at the coupling level with different time steps has also been a source of error. Related to that, the spin-up and initialization of models is also problematic, with some model components (especially deep ocean and biogeochemical fields) requiring centuries of spin-up for a proper initial state. Ongoing research in advanced spin-up techniques are needed. Anderson acceleration was suggested as one example.

Development Workflow and Testing

There was some discussion of the current configure/build/run workflow. It was recognized that the system is sophisticated but can sometimes be painful for developers, and fragile. However, some of that fragility is often associated with changes in the software stack or machine downtime that are not under the project's control and are instead caused by the management of particular machines or centers. This can create problems when machines involved in testing are down, because this can interrupt testing for lengthy periods. There were complaints with Cori's downtime due to management of that machine. It was also noted that there were ambitions early on to cover a fairly large set of supported compiler and machine options, but that this is increasingly difficult with available resources. All of these unavoidable problems are amplified for advanced architectures for which the project has early access.

A number of participations were eager to try the singularity container and this may simplify some of the software-stack-related problems that are often encountered.
For the development workflow, it was noted that the rate of one pull request per day represented a lot of churn, though some fraction of this churn is related to configurations and not necessarily source code. While current testing is fine and remains important, additional coverage and a wider variety of tests, including true property tests like mass conservation and additional unit tests across E3SM, are needed.

Intercomparison with competing models, for both physical and computational performance, may be useful to understand how well the E3SM model is doing. The project already has its own standard benchmarks, but might need to add community-related benchmarks. This also needs to include scientific benchmarks like skill scores. It's difficult to get this data from other centers/groups, so intercomparison will take some effort.

Staffing, Training, and Documentation

The project continues to have difficulty hiring and retaining staff with advanced computing expertise. Historically, developers who have both application and computational experience have been much more likely to become long-term team members and contributors than computer scientists with no expertise in the climate application space, but these hybrid individuals are hard to find. The project needs to identify better means to either recruit or train from within. To be successful, E3SM will also need to train a broader team, including most active developers, on some important aspects of computational performance and programming models. At the same time, the E3SM team will need to develop programming-model abstractions that help guide application developers in the proper direction. Discussion participants noted that they had difficulty even understanding aspects like the host/device model and related memory spaces, and thus had trouble identifying issues when trying to use accelerators. As the project moves toward more of a C++ code base and related programming models or DSLs, additional training will be needed to understand aspects of C++ and programming-model interfaces. Some participants noted that earlier access to code in development and using unit tests as examples helps in understanding the code and what developers are trying to do. Testing can also give rapid feedback on new development.

Like many Earth system models, there are aspects of the model in which there is only a single expert, or developers are using code in which they have no internal expertise (e.g., third-party or community-developed code). This can be risky, but it is not feasible to have complete redundancy. How should this risk be managed?

Documentation is also important for spinning up new staff and new users. It seems that most users can be up and running in roughly a day (once computer accounts have been obtained) with current documentation, but developers who need access to testing and other aspects can find the documentation less up to date.

Machine Learning/Artificial Intelligence Breakout, Ruby Leung, Mike Pritchard

The goals of this session were to: (1) survey the current and planned use of machine learning/artificial intelligence (ML/AI) across projects supported by ESMD and (2) discuss the challenges and prospects of using ML/AI approaches in improving E3SM and its use in addressing the E3SM science drivers. A brief survey was conducted before the meeting to collect information from the E3SM leadership team and the PIs of 20 university projects and ecosystem projects (e.g., SciDAC). The survey included the following questions:

1. Which project(s) are you working on?
2. Have you used (or planning to use) ML/AI in your projects?
3. If yes:
    a. What science or modeling questions are you addressing or planning to address?
    b. How is ML/AI being used or planned to be used to address your questions?
    c. In your application of ML/AI, what strengths and weaknesses have you identified?
4. If no, can you tell us why?
5. Which areas of E3SM do you think can benefit from ML/AI in the current (CPU) and future (GPU and CPU) computing phases?
6. What steps/strategies are needed to make good use of ML/AI in E3SM development?

During the breakout session, the survey results were briefly summarized in a presentation by Ruby Leung. To kick off discussion of the challenges and prospects of using ML/AI for improving E3SM and its applications, Guang Zhang, Robert Pincus and Michael Pritchard were invited to give brief remarks from their ML/AI experiences and perspectives. After the remarks, Michael Pritchard and Ruby Leung led an open discussion with 40–50 participants in the session. The breakout session is summarized below.

1. Summary of survey presented by Ruby Leung (Presentation - Leung - Pritchard):
    a. Responses from six members of the E3SM leadership team and the PIs of eight university and ecosystem

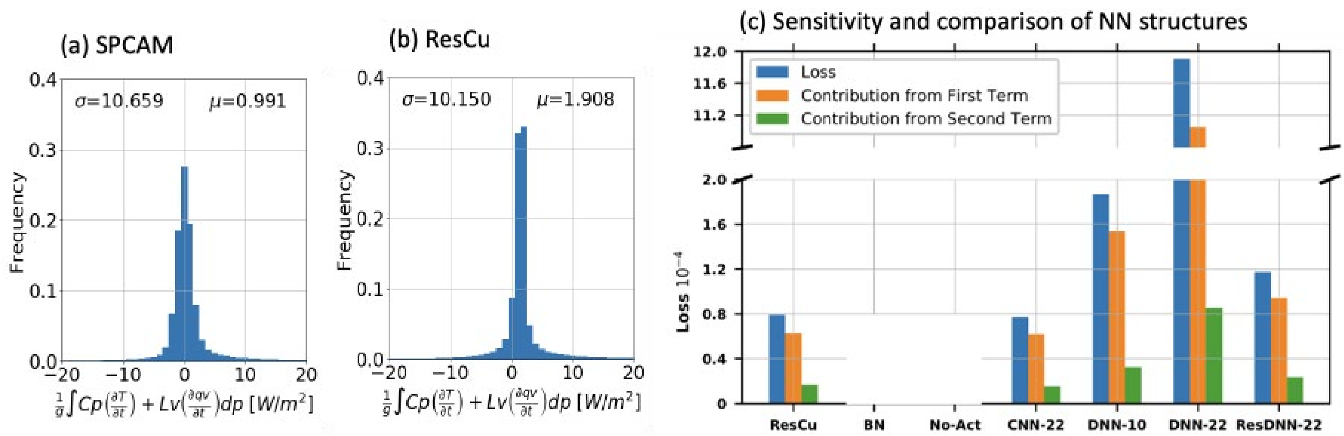


Figure 37. Training a residual convolutional neural network (ResNet)—called ResNet for convection (ResCu) in this study—using simulations from the superparameterized Community Atmosphere Model (SPCAM) to represent moist physics. The probability density function (PDF) of column-integrated moist static energy change (x-axis) for (a) SPCAM and (b) ResCu, showing good agreement between the two. (c) The total loss (blue bar) and contributions from mean squared error (orange bar) and penalty for violations of column-integrated moist static-energy conservation (green bar) for different neural-network architectures. (Source: Han et al., 2020)

projects were received.

b. About 80% of the responses indicated that ML/AI is being used or planned to be used.

c. About 40% of the uses relate to developing/emulating parameterizations; ~20% relate to model sensitivity and uncertainty quantification (UQ) analysis; and the remaining uses relate to analysis/evaluation of model outputs, process understanding, and generation of input and model evaluation data.

d. On development/emulation of parameterizations, processes being parameterized or scheduled to be parameterized include aerosols, aerosol-cloud interactions, radiation, ocean sediment, ocean mesoscale eddies, and wildfires.

e. Areas where E3SM can benefit from ML/AI:

   i. Parameterizations: subgrid physics, reduced complexity parameterizations, bias-correction rather than complete solutions, scale-aware parameterizations, and leveraging satellite data.

   ii. Sensitivity, UQ, model tuning: parameter estimation, observation constrained model tuning, autotuning, and online learning.

   iii. Analysis/evaluation: in-situ verification and online selective data output.

2. Remarks by Guang Zhang, Robert Pincus, and Michael Pritchard:

a. Guang Zhang showed an example of using a neural network to emulate superparameterization, suggesting that ML can be very accurate (Figs. 37a & 37b). He noted some challenges in ML/AI approaches for parameterization development, including how to make ML/AI obey the laws of physics, how to produce stable integration, the need to improve interpretability, and determining how complex ML-based emulators should be. For this last challenge, Guang showed a comparison of the accuracy of emulating the superameterization using different neural network (NN) approaches, showing some sensitivity of the accuracy to the NN structures (Fig. 37c). He noted opportunities to further advance the use of ML/AI, including the availability of big data (observations, simulations) and advances in algorithms and hardware.

b. Robert Pincus remarked on the importance of asking whether it is appropriate to use ML to address certain questions. As an example, using ML to solve the radiative-transfer equation is a bad idea because there are physical laws behind radiative transfer, but ML can be judiciously used to speed up the empirical bits and correct for errors in the formulation. He noted that physical understanding is key to the generalizability of parameterizations, and to support prudent uses of ML/AI, robust infrastructure to efficiently evaluate ML models within Fortran/C++ is needed.

c. Michael Pritchard showed an example of NN-assisted analysis of the finest scale of complexity in large-domain superparameterized cloud-resolving model (CRM) simulations using "self-supervised" learning (Presentation-2 - Pritchard). In this example, a Variational Autoencoder (VAE) uncovered "latent spaces" in the simulations that are interesting to analyze (Figure 38). More specifically, a VAE can

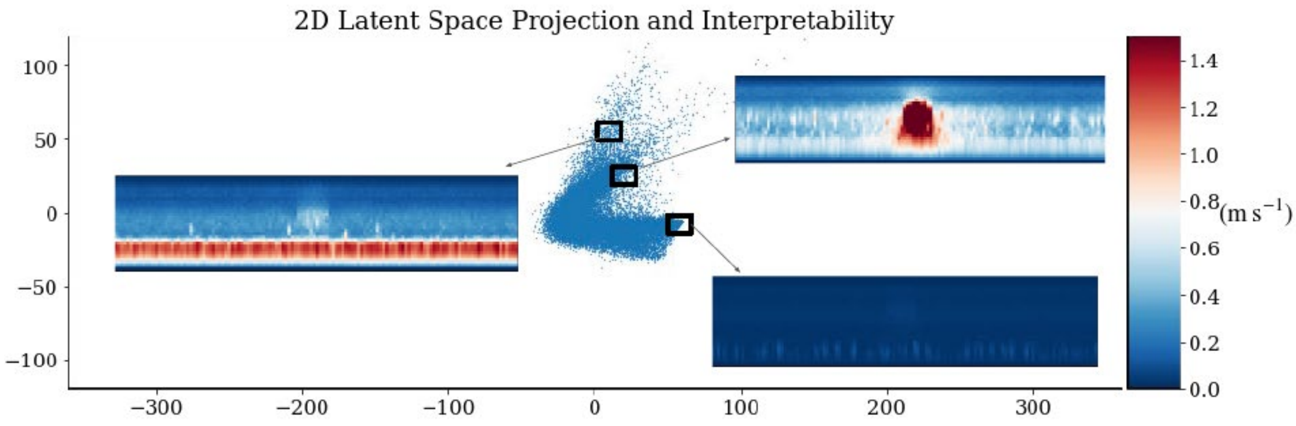


Figure 38. Visualization of the latent space originally in dimension 1024, but reduced to dimension 2 by principal component analysis. The standard deviations of different types of convection the VAE learns to cluster are embedded near corresponding clusters. This suggests the VAE learns an interpretable clustering of the data, with means and variances both contributing to the results. (Source: Mooers et al., 2020)

reconstruct details of convective organization allowing a data-driven classification, as well as objective anomaly detection, with the latter identifying two mesoscale convective systems coexisting in a single CRM array as an extreme event, showing the usefulness of a VAE in defining what is extreme and rare in large datasets, with attention to spatial patterns. Pritchard also remarked on the linked ML infrastructure challenges going beyond the limits of a single GPU to handle big data and hefty NN architectures.

3. The following topics were covered during the open discussion:
   a. Complexity of ML-based emulators: On how complex ML-based emulators need to be, it was noted that extensive hyperparameter tuning should be performed for a fair comparison of different NN architectures while probing their limits. Extensive tuning is needed because there is a spread in the NN fit akin to the spread from an ensemble representing a range of fit potentials, but this is underreported. However, iterating towards a skillful NN may be more computationally expensive than the parameterization it was intended to emulate. There is a need to balance computational efficiency with accuracy and advancing hardware-accelerated NN backends is needed to address computational efficiency.
   b. Judicious use of ML emulation: On whether emulating radiative transfer or other processes with underlying equations and physics makes sense, it was noted that ML emulation is not abandoning the equations, but rather emulating their coupled effects on scales that are otherwise unapproachable. The latter plays to an advantage of NNs in being able to summarize overwhelming complexity and internal correlation.
   c. Physics constraints: On the need to constrain ML approaches by physics, a question was raised as to whether ML can be used to infer the physics.
   d. Observations for ML parameterization development: Given that many examples of using ML/AI for parameterization development are based on emulation of superparameterized or global cloud resolving simulations, a question was raised as to whether ML can make use of observations for parameterization development. It was noted that the use of observations in parameterization development is particularly pertinent for processes, such as in biology, for which there are no known physical laws or equations. To make use of observations for parameterization development, there is a general need to develop datasets with multiple variables and high spatiotemporal resolution. It was also noted that observations have been used in the context of Bayesian inference or surrogate-accelerated Bayesian inference, but it is not clear if such constraints are enough.
   e. Interpretability: On interpretability of ML/AI approaches, it was noted that tools are available but some may be more useful for classification problems, rather than the regression problems that are more relevant for ML parameterization development. Layerwise relevance propagation was one example.
   f. ML/AI methods for parameterization development:
      i. A question was raised as to whether traditional statistical inference (e.g., Bayesian parameter estimation) may be included as ML.

  ii. There are other classes of generative models or partial-differential-equation (PDE)-based neural systems like the sparse identification of nonlinear dynamics (SINDY) or relevance vector machine (RVM)—a new analytic parameterization that can be used to interrogate rather than be used as a black-box model. Generative adversarial networks (GANs) are unsupervised, while their conditional counterparts, conditional GANs (cGANs), are mostly supervised. GANs have a use in data augmentation.
  iii. Stochastic emulators: crude percentile classifiers paired with percentile-specific NNs are fascinating approaches.
  iv. There are Bayesian networks where the outputs of a NN can be a probabilistic distribution, but they don't scale particularly well. Nonetheless this is an underexplored and promising form of ML that likely deserves increased attention.
  v. There is a big road block in using a Bayesian approach to improve ML models, because for Bayesian inference, structural uncertainty is typically not explored. It was noted that a NN is a cost-effective approach that can be used to emulate the set of many interacting processes.
  vi. On what discriminates ML from traditional statistics, it was noted that there is important overlap, but two ML/AI elements are not reflected in its semantics: (1) scalable efficient training algorithms and (2) a more generic structure of the code that does the prediction, and thus an associated appealing flexibility of ML/AI.

g. Generalizability: A question was raised regarding how much confidence one can have using models with ML parameterizations for projecting the future when conditions outside the training samples may be encountered. It was noted that the same question may also apply to physically based parameterizations that have been tuned to reproduce the historical past. Finding strategies to rephrase extrapolation questions (through targeted renormalization of inputs and outputs) as interpolations may hold promise and is beginning to be explored.

h. Decision support: A question was raised regarding the use of NN for informing real-time decisions, where there is a lot of interest stemming from other fields such as astrophysics or particle physics event detection. In that context the speedup of NN algorithms compared to heuristic algorithms has practical advantages for decision making. In the climate context, a speedup is also desirable, but for the purpose of doing more explicit climate simulations. This analogy was fun to articulate.

i. Human–Earth system interactions: On the use of ML to represent human–Earth system interactions, it was noted that there is interest in collaborative efforts in this community to tackle infrastructure challenges in ML-E3SM integration.

4. Summary of key points
  a. The discussion in the breakout session highlighted a few areas of shared interest in the community, including,
    i. ML approaches constrained by physics;
    ii. Using ML to tease out some physics between the inferred relationships;
    iii. Collaborative efforts to tackle infrastructure challenges in ML-E3SM integration; and
    iv. Evolving principled practices towards robustness, interpretability, and the stable integration of NN parameterizations.
  b. The discussion also highlighted a few shared frustrations:
    i. What is good enough? At some point, the ML emulator gets so fancy that it costs more than what it was emulating; and
    ii. How confident can scientists be on the generalizability of ML emulators trained using observations or highly detailed simulations of present-day conditions?

BREAKOUT SESSIONS FOCUSED ON CURRENT AND FUTURE DIRECTIONS

The goal of these breakout sessions was to share research and ideas, while also brainstorming solutions to challenges on subjects related to the E3SM groups or development areas.

Water Cycle Breakout, Chris Golaz, Luke Van Roekel

The Water Cycle breakout consisted of two parts. In the first, four updates were provided to show a small subset of the work accomplished under the v1 analysis campaign and v2 model development. In the second part, there was a broad discussion on future directions for Water Cycle v3 and v4.

Presentations

Two presentations were given on analysis of the v1 simulation campaign. **Xue Zheng** detailed a study of the future projection scenario ensemble (SSP585) (Presentation – Zheng). Comparisons to CMIP6 models show that E3SM is often an outlier, for example, sea ice disappears in Northern Hemisphere winter before 2100. Consistent with this sea-ice loss, E3SM warms very quickly in the projection. Figure 39 shows the zonally averaged temperature from the historical simulation and the SSP585.

The temperature change (middle panel) shows a Northern Hemisphere cooling through much of the historical period, followed by very rapid warming in the SSP585. In the CMIP6 mean, this cooling and rapid warming are not as evident. This result is consistent with a strong aerosol-cloud effect, as well as a large equilibrium climate sensitivity (and transient climate response) in E3SMv1. **Salil Mahajan** detailed work examining the influence of model resolution on ENSO teleconnections to precipitation extremes (Presentation – Mahajan). This work found that the high-resolution model (25 km atmosphere, 18 to 6 km ocean) was better able to simulate ENSO teleconnections to precipitation extremes over the Southeast US, as shown in Figure 40.

LeAnn Conlon discussed the work she is leading in developing a metric to assess how well E3SM simulates the connection of SST variability to precipitation over the North American HUC-2 (Hydrologic Unit Code 2) regional watersheds (Presentation – Conlon). Good progress has been made; the metric is being applied to high resolution v1 output and observations. In the near future, the metric will be finalized and integrated into E3SM-Diags so it is available to assess all new E3SM simulations.

Andrew Bradley detailed the extensive work done for the E3SM atmosphere model (Presentation – Bradley). The switch to the physics grid (pg2) has resulted in large performance gains. He also discussed semi-Lagrangian transport which improves performance without degrading accuracy. With these improvements implemented, EAMv2 is roughly twice as fast as v1.

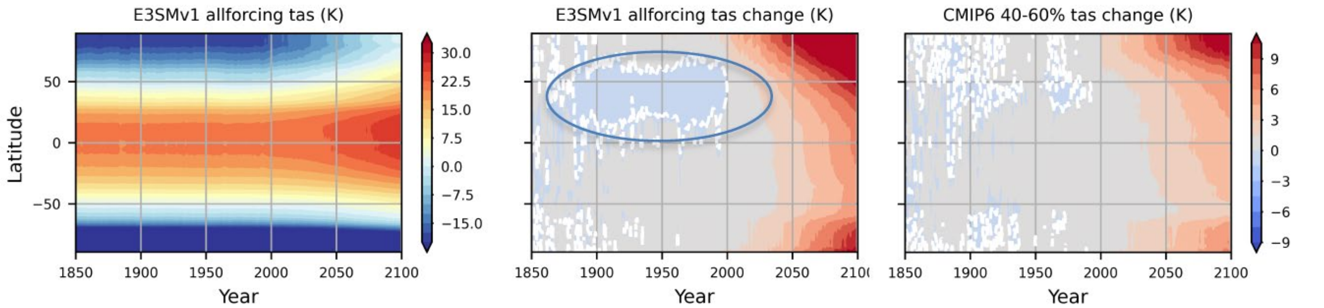


Figure 39. Left: time evolution of zonal mean surface-air temperature between 1850 and 2100 in E3SMv1 (historical + SSP585). Middle: temperature anomalies relative to 1850 conditions. Right: same but for CMIP6 model within 40 to 60% percentiles of temperature range.

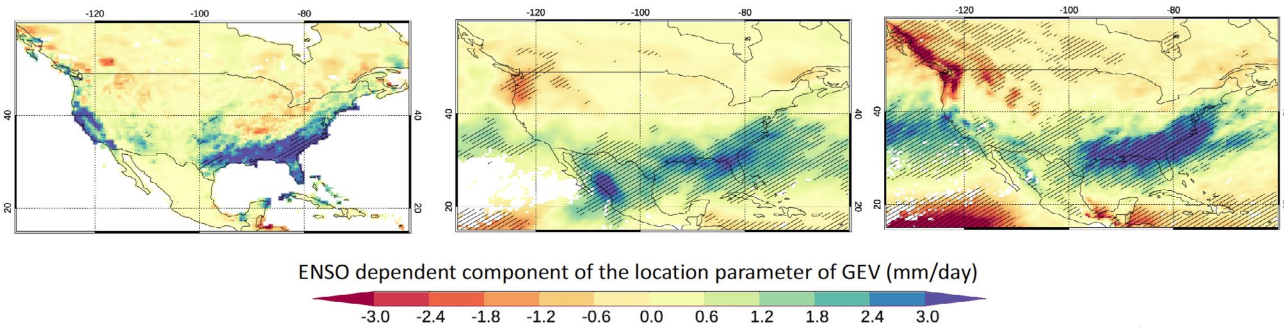


Figure 40. ENSO teleconnections to winter precipitation extremes. ENSO-dependent (ENSO Longitudinal Index, ELI) component of the location parameter of the generalized extreme value (GEV) model for winter season (November–February) daily maximum precipitation rate (mm/day) for CPC gauge-based analysis data (1979–2018, left panel), low-resolution historical simulation ensemble (1979–2014, middle panel) and high-resolution model 1950 control simulation (98 years, right panel). Hatching represents statistical significance at the 5% level.

Discussion

The discussion was centered around possible future directions for the Water Cycle Group going into v3 and v4. The discussion was motivated by three questions:

- What DOE relevant Water Cycle science questions is E3SM uniquely suited for?
- What other relevant science could E3SM claim?
- What developments are needed to achieve this science?

From the discussion, a few key themes emerged: how to best address DOE relevant questions, how best to leverage E3SM's unique regionally refined mesh capability, and how to utilize upcoming Exascale resources.

DOE Mission-Relevant Questions and the Water Cycle Group

Climate change in the Earth System will directly impact the nation's energy infrastructure, energy use, and production at different spatiotemporal scales. For example, water availability and storm surges can negatively impact energy production capacity.

To address questions like these, DOE needs a model skilled at simulating the Earth's hydrological cycle. The hydrological cycle is itself tightly coupled to the energy cycle of the Earth, requiring skill in predicting all aspects of the climate, including clouds and radiation. For the energy infrastructure, water availability over land, runoff, and storm predictions need to be as accurate as possible now and in the future.

One potential role for the Water Cycle Group is understanding the role of land-atmosphere interactions on water availability and security. High-elevation headwater source regions play a particularly important role, as they influence all the downstream regions and eventually the oceans. New topographic and disturbance-related sub-grid units on land, as well as emerging capability for high-resolution land simulations, will enable a more realistic representation of headwater regions under a changing climate. There will be a need to balance atmosphere resolution versus topographic features to optimize realism in storm-track accuracy (from increased resolution) and topographic runoff effects (from improved land features).

Leveraging Regionally Refined Mesh (RRM) Capabilities

Several participants pointed out that the E3SM model is unique in its capability of using regionally refined meshes (RRM) in all its components. This is a strength that should be pursued since it aligns well with DOE Mission needs.

Given the v2 focus of resolution over North America, part of the discussion centered on how best to leverage RRM over North America. It was suggested that E3SM should consider a **large ensemble with a RRM resolution of 1/8 or 1/4 degree over North America**. Over the Western US, where topography plays a considerable role, a resolution of 14 km (~1/8 of a degree at the equator) or higher is desirable to realistically capture the evolution of the snowpack, coupling it to river flow, and provide a good assessment of climate variability.

Current plans for the Water Cycle v2 simulation campaign include RRM simulations (1 deg - ¼ deg over North America), but with a relatively small ensemble. Beyond v2, E3SM is aggressively moving to efficiently run on exascale computers, which will enable both higher RRM resolution and a larger ensemble size.

At present, the design of RRM requires a significant amount of expert judgment and subjectivity. Moving beyond v2, it is critical to address where resolution is actually needed. Some potential research avenues to address this question include

- Green's function: try all regions and combine them to explore impact, similar to regional SST perturbation cloud feedback work, e.g., Zhou et al. (2017); and
- Use of machine learning and artificial intelligence to learn from high-resolution simulations.

To make significant progress in understanding Water Cycle questions, the broader scientific community must be engaged. Internal and external users should have the flexibility to design new RRM grids for specific science questions. This will require streamlining and better documenting the process of generating new grids and all associated input files. Significant progress has been made in that direction, but additional improvements are needed. The group should also strive to reduce the need for manual retuning of the components' dynamical cores and physics parameterization as the resolution changes.

Using Exascale Resources: Ultra-Large Ensembles
Presently, E3SMv4 is targeting 100, possibly 1000, ensemble members with RRM on upcoming exascale architectures. Analyzing the output from 100 to 1000 members will be very difficult, as current approaches will not scale to such a large ensemble. This will represent a major infrastructure challenge that DOE is well positioned to tackle.

Ensemble members will be differentiated based on

- RRM grids (ocean and atmosphere),
- Initial conditions (IC), and
- Physics perturbations (PPE) with credible configurations, not simply brute force PPE (which typically have unrealistic climates). The goal would be to have 10+ distinct configurations developed with the help of machine-learning techniques.

The large ensemble would allow the E3SM project to explore uncertainties in present-day and future simulations.

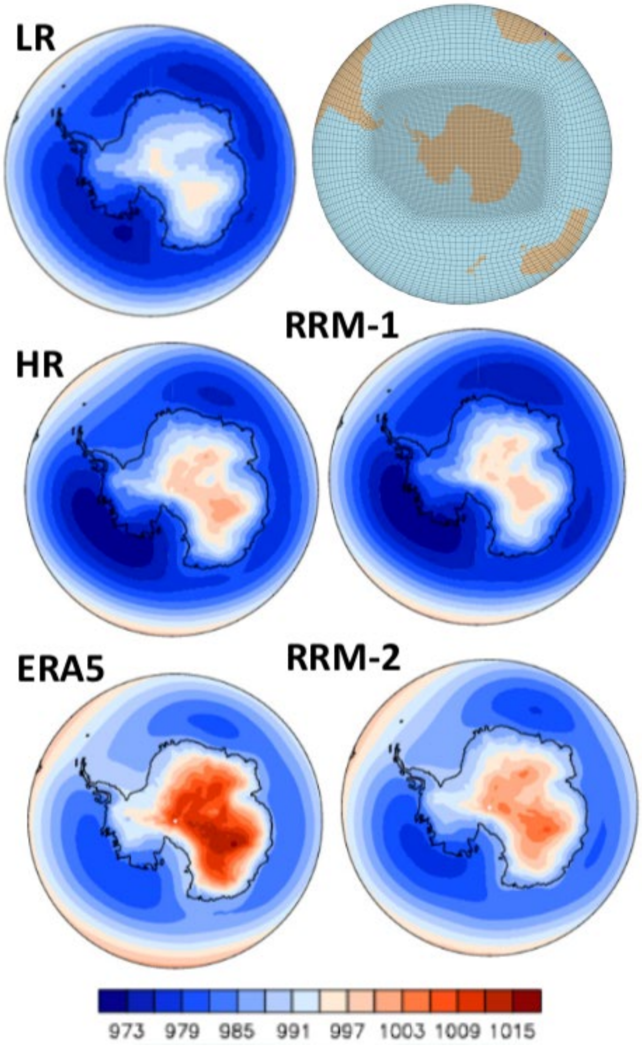


Figure 41. 2010–2012 mean annual sea-level pressure from EAMv2 alpha using low-resolution (LR), high-resolution (HR), and a regionally refined mesh (RRM; upper right) configurations. LR, HR and RRM-1 use identical tuning, while RRM-2 uses an improved tuning. RRM-2 demonstrates a significant improvement, relative to reanalysis, over both LR and uniform HR simulations.

Cryosphere Breakout, Steve Price, Mark Petersen, Wuyin Lin

Overview
This breakout session focused on a number of distinct but related topics of importance to broader Cryosphere Simulation Campaign efforts, including (1) a review (three detailed presentations) of E3SM's current status with respect to simulating important aspects of polar climate, (2) a discussion of current polar-climate biases in E3SM and what efforts need to be undertaken during the reminder of Phase 2 (and over the long term) to address them, and (3) a review of current Cryosphere Campaign short- and long-term metrics, both in terms of progress towards them and whether they need refinement.

Current Polar Climate in E3SM and Biases
The discussion of E3SM's polar climate and its biases was structured around three presentations. These included an assessment of atmospheric simulations over the Antarctic using regional refinement, an overview of polar climate in E3SM versions 1 and 2, and a first look at E3SM's skill at simulating the drivers of surface melt on the Greenland ice sheet.

Wuyin Lin provided an initial assessment of E3SMv2 in simulating the atmospheric climate over the southern polar region (Presentation Zhang_Lin). The broad goals of this assessment were: (1) to provide an initial benchmark for tracking Southern Ocean and Antarctica climate metrics in E3SMv2 and beyond (see additional discussion below), and (2) to assess the effectiveness and improvements resulting from regional refinement in the atmosphere over Antarctica. E3SMv2-alpha versions produce a similar southern polar climate to E3SMv1, with improvements over v1 seen in some candidate v2

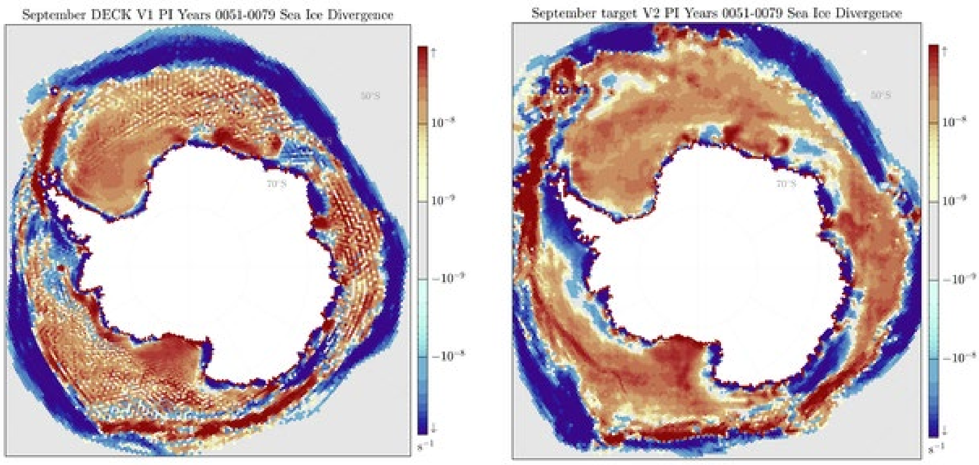


Figure 42. Illustration of improvements in sea-ice and ocean coupling from E3SMv1 (left) to v2 (right), shown here for the Southern Ocean. In v1, the sea-ice divergence field demonstrates noise at the grid scale, which affects sea-ice melt rates and dynamics. In E3SMv2 (right), this noise is no longer present.

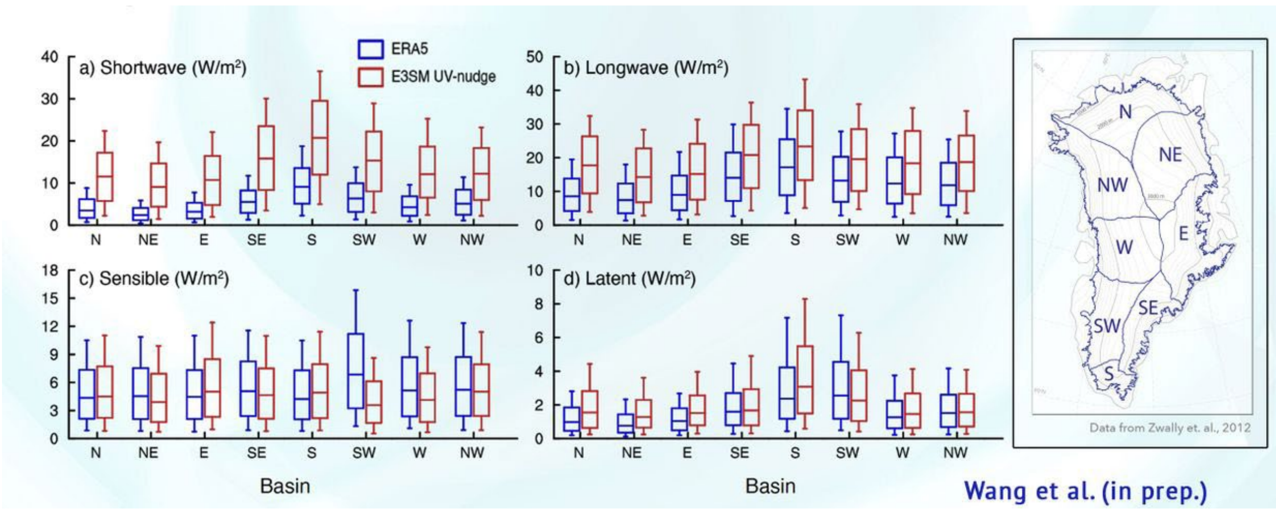


Figure 43. Comparison of various factors controlling Greenland ice-sheet surface melting in E3SM (red) vs. in ERA5 reanalysis (blue).

configurations. The comparison of simulations using different resolutions (including regional refinement over Antarctica) and tunings indicate that simulation results in v2 will be sensitive to both resolution and model parameter changes. Clear improvements were identified in several southern polar-climate metrics in global, high-resolution simulations. These improvements are generally reproduced under simulations using regional atmospheric refinement over Antarctica. Additional tuning on top of current Water Cycle efforts is expected to result in further regional improvements that should benefit v2 Cryosphere simulations (see Figure 41). Important biases that will require attention include too strong Southern Ocean winds (which worsen at high resolution) and an expression of the Southern Annular Mode (SAM) in regionally-refined atmosphere configurations. In high-resolution simulations, SAM is worse than the low-resolution counterpart.

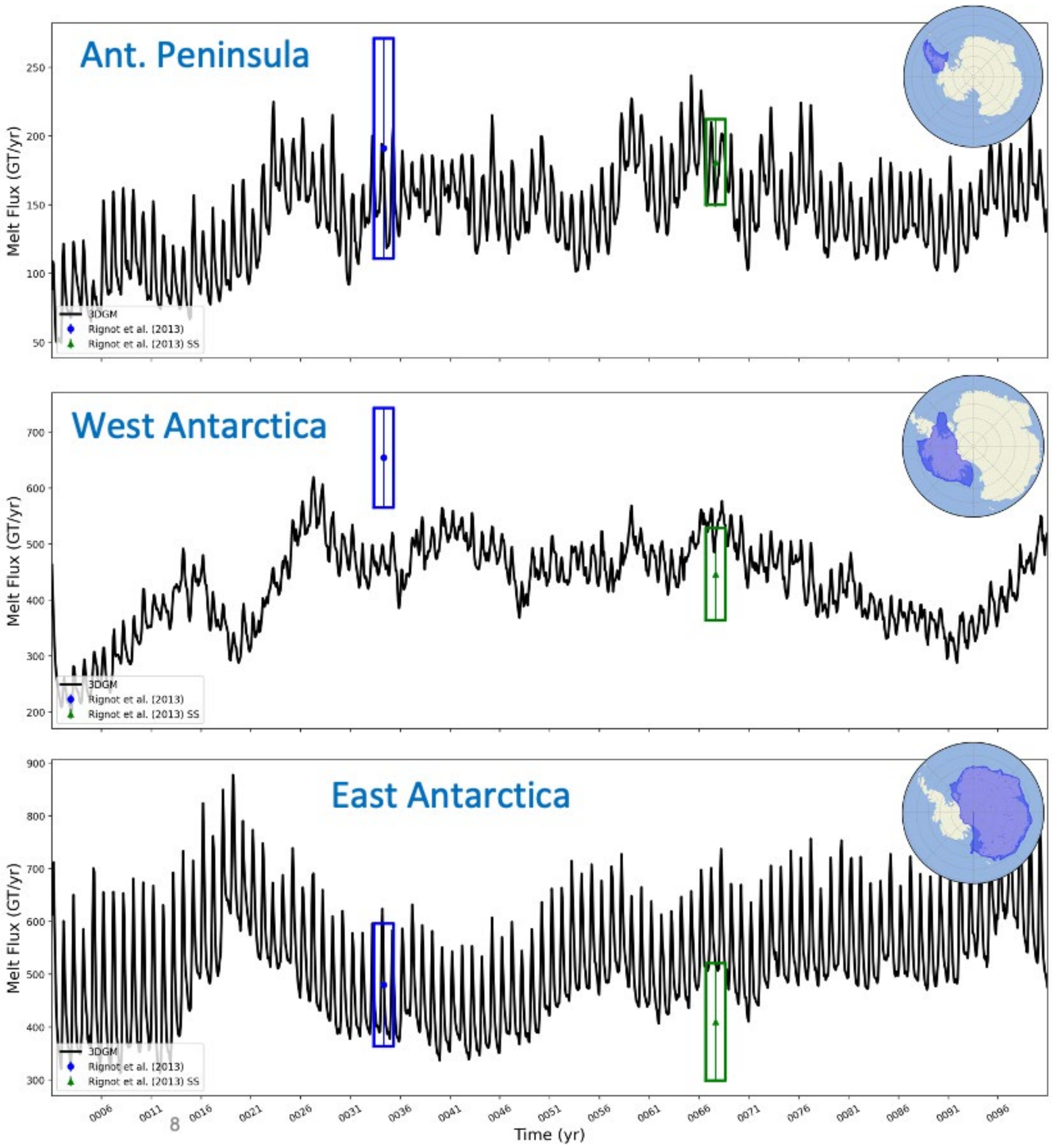
Andrew Roberts provided a summary of polar-climate biases in E3SMv1 and alpha versions of v2, assessed primarily via sea-ice model metrics (Presentation - Roberts). Upgrades in v2 relative to v1 include (1) an improved and consistent treatment of the snow-surface radiation balance over both land and sea ice, (2) improvements in the morphology of snow on sea ice, and (3) consistent ocean and sea-ice freezing temperatures, with the third improvement appearing to have the largest impact. A number of other bug fixes have also been implemented and tested in v2 (see Figure 42). While these fixes do not appear to have a large impact on simulations, they have removed some uncertainties about their importance, which is a critical step for narrowing down what else might be behind persistent biases. In general, v2-alpha versions have more sea ice in the Antarctic and less in the Arctic, relative to v1, possibly due to a surface-radiation bias in the high-latitude north. These biases will be targeted primarily by improving the coupling between the sea ice and ocean. Also of note are significant advances in assessing E3SM-modeled sea-ice extent and thickness, including model sampling via an ICESat and ICESat2 satellite emulator and the conversion of these samples into skill scores with respect to observations.

Wenshan Wang reported that the primary driver of surface melt on the Greenland ice sheet at seasonal and diurnal timescales is shortwave radiation, which is strongly controlled by the solar zenith angle and the albedo (Presentation - Wang). On sub-seasonal timescales, sensible heat and shortwave radiation dominate, both of which are enhanced during katabatic wind events. Relative to ERA5 reanalysis (Fig. 43), E3SM shows similar spatial patterns of surface melt driven by both sensible heat and shortwave radiation. Surface energy and other meteorological fields also vary with wind direction in E3SM similar to ERA5. Biases in E3SMv1 include overestimates of sub-seasonal variability in shortwave heating caused by overestimates in ice-sheet surface albedo and atmospheric humidity. The former bias will be at least partially addressed via ongoing snowpack model improvements occurring in partnership with the SciDAC ProSPect project.

Review of Cryosphere Campaign Short- and Long-Term Metrics

Progress was noted for both of the campaign's short-term actionable metrics. In terms of improving the ability to simulate and assess "ice sheet freshwater flux to the ocean," E3SM can now calculate realistic sub- ice-shelf melt fluxes and the variability at a range of spatial and temporal scales. Comparing those fluxes to observations—at the individual ice shelf, regional, and whole ice-sheet scale —is something already regularly done when conducting standard simulation analysis (see Figure 44). Comparing the variability in those fluxes to recently available observations will be a focus of future work. Also of note are improvements to the snowpack model in E3SM (as part of the SciDAC ProSPect project) that will allow the realistic simulation of surface-mass balance over the Greenland and Antarctic ice sheets. This capability is

Figure 44. Variability in Antarctic sub-ice-shelf melt flux to the ocean over the course of a century-long E3SM simulation under steady preindustrial forcing. Blue and green boxes represent the ranges from observational estimates of Rignot et al. (2013).



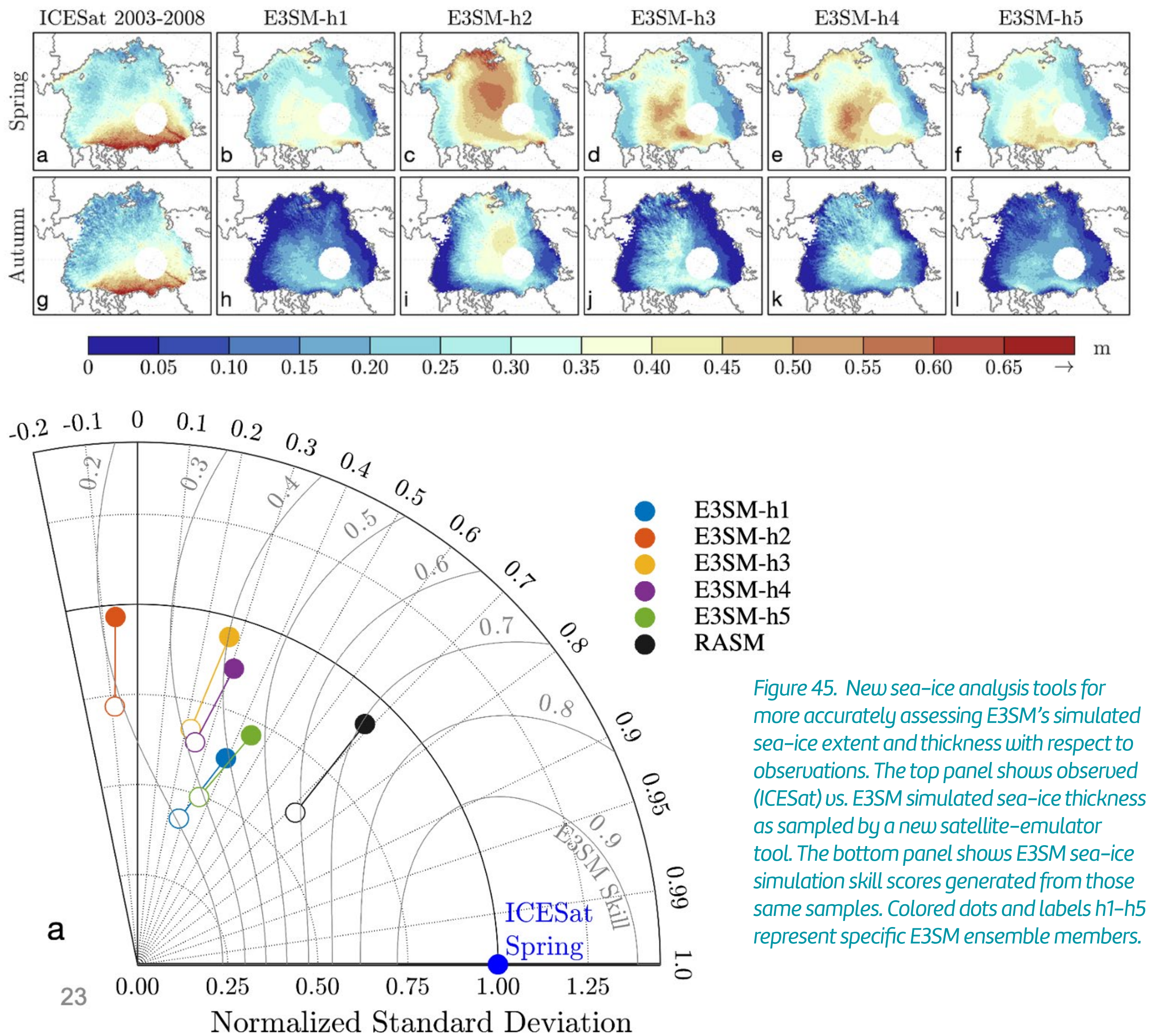


Figure 45. New sea-ice analysis tools for more accurately assessing E3SM's simulated sea-ice extent and thickness with respect to observations. The top panel shows observed (ICESat) vs. E3SM simulated sea-ice thickness as sampled by a new satellite-emulator tool. The bottom panel shows E3SM sea-ice simulation skill scores generated from those same samples. Colored dots and labels h1–h5 represent specific E3SM ensemble members.

currently being implemented and tested within E3SM. In terms of assessing and improving E3SM's skill at simulating "Antarctic atmospheric forcing," E3SM scientists have characterized the most important aspects of the Southern Ocean and Antarctica atmospheric climate in E3SMv1, including winds, precipitation, and various aspects of the Southern Annular Mode. Similar characterization of the v2 model, including regionally refined configurations, is currently underway, as discussed above.

With respect to longer-term project metrics, one long-term goal for the Cryosphere Campaign is to be able to quantify the contribution of land ice to global and regional sea level. This involves being able to simulate, within E3SM, the relevant climate forcing (surface and submarine mass balance, as discussed above) and also ice-sheet evolution in response to that forcing. Progress in this area has primarily occurred under the SciDAC ProSPect project, using DOE's standalone ice-sheet models in collaboration with international, multi-model inter-comparison efforts under the CMIP6 ISMIP6 effort. A number of high-profile publications from these efforts are expected to be part of the next IPCC assessment report (AR6). Also relevant are E3SM efforts under the Cryosphere Campaign that have identified "tipping points" for large Antarctic ice shelves that have the potential to lead to order-of-magnitude increases in submarine melting and, as a result, significant increases in the Antarctic ice sheets' dynamic mass loss to the ocean. A second longer-term project goal is for E3SM to be able to simulate historical decadal trends in sea-ice cover (towards confidence in future projections). This includes being able to assess the variability in sea-ice cover at seasonal to decadal timescales and decadal trends in sea-ice cover since the late 1970s. To this end, it was noted that E3SM now can much more accurately compare modeled and simulated sea-ice extent and thickness, using a new satellite emulator, and incorporate that information into formal skill-score metrics for assessing model improvements over time (see Figure 45).

Infrastructure and NGD Software and Algorithms Breakout, Rob Jacob, Andy Salinger

The breakout session on topics associated with the E3SM Core **Infrastructure Group** and the E3SM **NGD Software and Algorithms** subproject was facilitated by the leads of those two groups, Rob Jacob and Andy Salinger. The time was split evenly between presentations and discussions.

Presentations

The three presentations scheduled for this session addressed very different algorithmic and software topics.

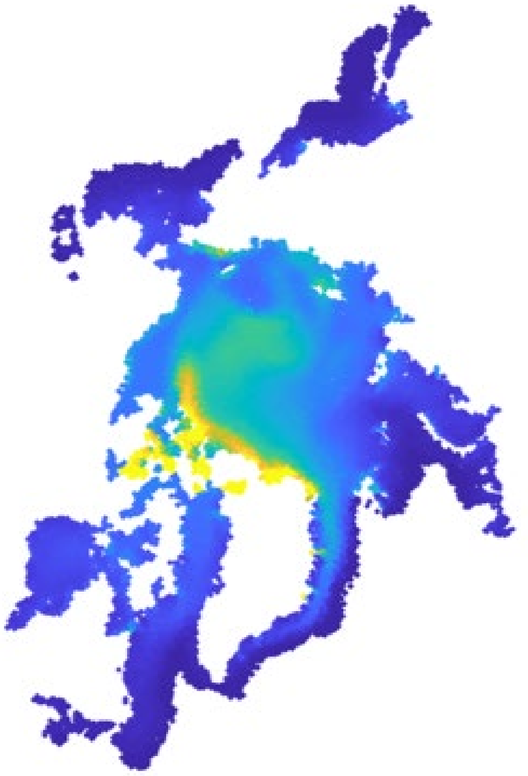


Figure 46. Sea-ice thickness from an Arctic basin-scale simulation with DEMSI.

The first talk (Presentation - Peterson) was by **Kara Peterson**, the ASCR-lead of the Discrete Element Sea Ice Model (DEMSI) SciDAC project, which is developing a novel particle-based sea-ice model. This approach is promising in its potential to better address sea-ice physics and map better to exascale architectures for the very high-resolution regime, as compared to the current PDE-based model. Peterson presented progress on algorithm development, including a moving least-squares approach to coupling the particle solution to the ocean grid and verification of a particle-to-particle remapping scheme (Fig. 46). She also presented her team's approach to performance portability, using the Kokkos programming model, including some initial GPU results.

A second talk by **Menno Veerman** (Presentation - Veerman) was entitled "Using neural networks to predict atmospheric optical properties for radiative transfer computations." This talk explored the use of machine learning as a surrogate for part of the expensive radiative-transport model (Fig. 47). Using established code to generate the training data, Veerman trained several neural-net configurations of various complexity and expense as emulators for the full implementation, for both shortwave and longwave cases. The results were promising, showing a potential for speedup. The current results show a tradeoff in accuracy versus speed, where the simplest emulators provided a large speedup, but with some modest errors in the emulation, and the most complex emulators produced very good accuracy but limited speedup. Promising areas for future refinement were presented.

Sterling Baldwin of the Infrastructure group gave the third talk, (Presentation - Baldwin) on "Converting E3SM model output to the CMIP6 data standard." Baldwin discussed his e3sm_to_cmip Python script, which converts atmosphere, land, sea-ice, and ocean variables into CMIP-compliant data sets, with strict tests of compliance with CMOR metadata. The tool has already been used to publish 1800 E3SM data sets to CMIP6.

Discussion

The remaining time in the breakout was an open discussion, facilitated by Jacob and Salinger, the breakout leads.

A discussion was prompted by the question, "What is missing from the current E3SM Infrastructure?" The group discussed the use of project disk space on Compy, and the choices of setting quotas versus automated purging of old files. The current practice tends to keep the disk at 90% full, but it was noted that some filesystems don't do well at that level. It was recommended that team members use Globus Online for moving files to NERSC, but there was a request for a more complete "turnkey" solution which presumably would

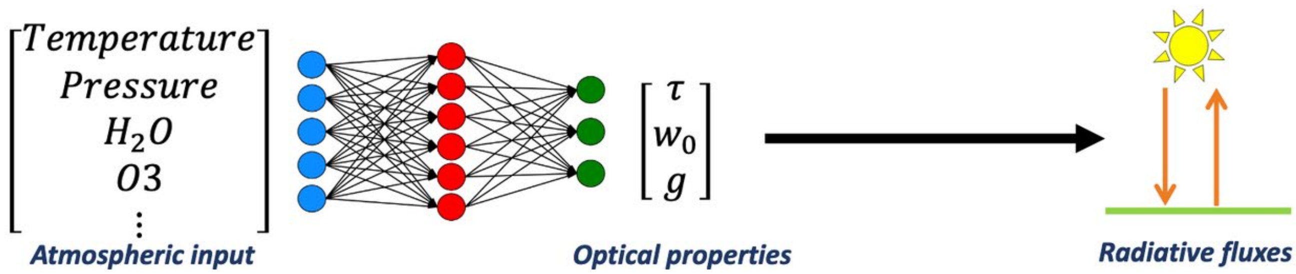


Figure 47. Schematic showing location of proposed neural network in the calculation of radiative fluxes from atmospheric input.

move files to NERSC, put them on tape, and delete them from Compy. Another option proposed was to keep expanding the file system, since adding more disk space is inexpensive.

There was also a discussion about the ownership of the software design of the E3SM Land Model (ELM). There is a lack of documentation for developers, who are currently pointed to the old CESM Land Model (CLM) documentation. Even a simple user's guide would be an improvement over the current situation. Since there are probably only three people on the E3SM team who understand the code, it would be good to make it easier for others to come up to speed. Complicating the process of learning the code is the fact that there is a lot of duplicated code and high-level if statements.

This brought up a larger point: it is not clear within E3SM's management structure who would have the authority to decide to clean up ELM. The structure of the project focuses on campaigns, so who makes high-level decisions about individual components? NGDs?

Participants discussed whether a code coverage tool would be useful to see how broadly the test suite touches the source code, and the consensus was that it would be nice but not critical or urgent. It is clear that not all features BER scientists are interested in are tested, but the key features used in production simulations are. Overall, there were no glaring issues identified that the team needs to address, a striking improvement over just a few years ago when the new E3SM infrastructure team and new software stack were struggling to catch up with user needs.

Another discussion topic was on provenance—the capturing of enough data about a science run that it can be reproduced—spanning the source code, input data sets, and namelist configurations. Participants discussed the potential of extending the Performance Analytics for Computational Experiments (PACE) capability, which was developed to harvest performance data, to capture all necessary provenance information. One issue is that a campaign might consist of several simulations, and it would be helpful to view them as one. CIME and by extension PACE consider an individual experiment (a job that ran on a supercomputer) as a separate entity. A set of related experiments could be grouped by case names to aggregate data for simulation campaigns; however, agreement on conventions is needed. Recently, the case_group attribute has been added to create_newcase (CIME) to pave the way towards a more robust solution. There was a brief discussion of the need to revisit provenance capture in the future, as this capability has presently evolved as a byproduct of PACE's primary goal of capturing performance data.

Finally, it was noted that there should be continued efforts to make the native model output CF compliant.

Aerosols Breakout, Po-Lun Ma, Qi Tang

Oral Presentations

Kai Zhang and several EAGLES project team members (Guangxing Lin, Shuaiqi Tang, Bin Zhao, Zheng Lu, Xiaohong Liu, Jeff Johnson) gave an introduction (Presentation - Zhang) on the development of new features for E3SMv4, including the model design and evaluation of nucleation-mode aerosols, organic-mediated new-particle formation, the prognostic treatment of cloud-borne aerosols, anthropogenic dust, wildfire aerosols, and the software design of the aerosol code. Initial code implementation is complete. New aerosol treatments show improvement in several aspects: (1) including nucleation-mode aerosols improves the simulation of background aerosol-number concentration, (2) the organic-mediated new-particle formation treatment improves the vertical profile of aerosol-number concentration over the central U.S., (3) the prognostic treatment of cloud-borne aerosols produces significant reduction of cloud-droplet-number concentration, (4) representing the injection height of wildfire aerosols improves the vertical distribution of aerosols, and (5) incorporating the anthropogenic dust associated with land-use land-cover changes enhances global dust emissions.

Nicole Riemer, an invited speaker, introduced machine-learning emulation of the aerosol mixing state, which has significant impact on aerosol optics and aerosol hygroscopicity and, hence, the concentration of cloud-condensation nuclei (Presentation - Riemer).

The team used PartMC, a particle-resolved aerosol model to provide explicit simulation of aerosol composition for a machine-learning algorithm to learn the aerosol mixing state. The emulator then predicted the mixing state using ambient conditions obtained from CESM (Fig. 48). Comparing the mixing state between CESM/MAM4 and the machine-learning emulator is part of the ongoing investigation. Aerosol mixing state is likely to be sensitive to time stepping, wet scavenging, model resolution, and aging timescale. The metrics for evaluating the aerosol mixing state should be developed and clearly defined.

Li Xu presented effects on wildfire aerosols using an online fire-emission model in E3SM (Presentation - Xu). Initial results show reasonable aerosol distribution in fire regions. Figure 49 shows that the wildfire aerosols change the near-surface climate in many ways, including radiative flux, temperature, and humidity.

The fire model can be emulated by machine-learning techniques (done by Qing Zhu at LBNL), which is very useful for understanding past and present climate but may need more considerations before using it for climate projections. One simplification in the current design is that plume chemistry is not considered, though it can be investigated in the future.

Adam Varble introduced a new diagnostics package being developed for the evaluation of simulated aerosols, clouds, and aerosol-cloud interactions (Presentation - Varble). He demonstrated how a process-oriented evaluation of E3SM was possible using combined observations from ARM and satellite retrievals.

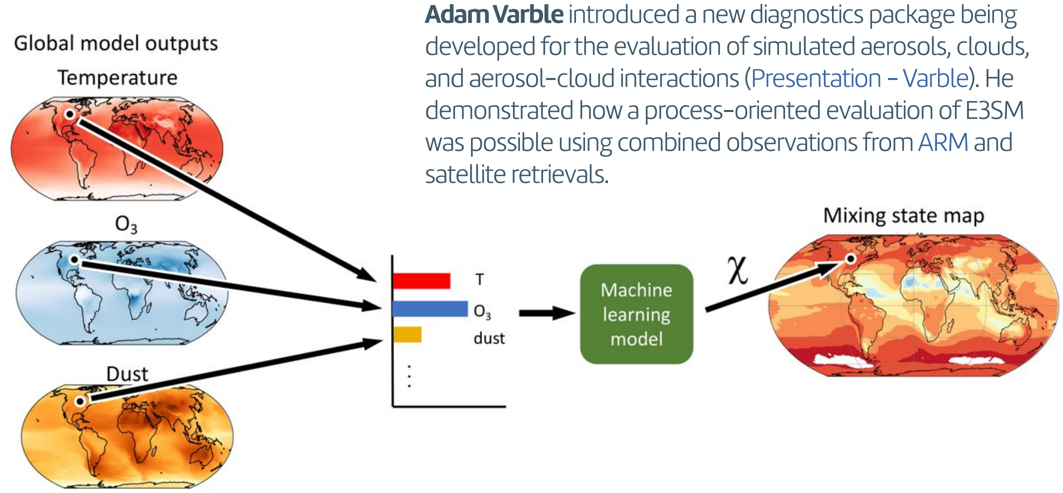


Figure 48. Workflow for building a machine-learning emulator using PartMC and CESM data.

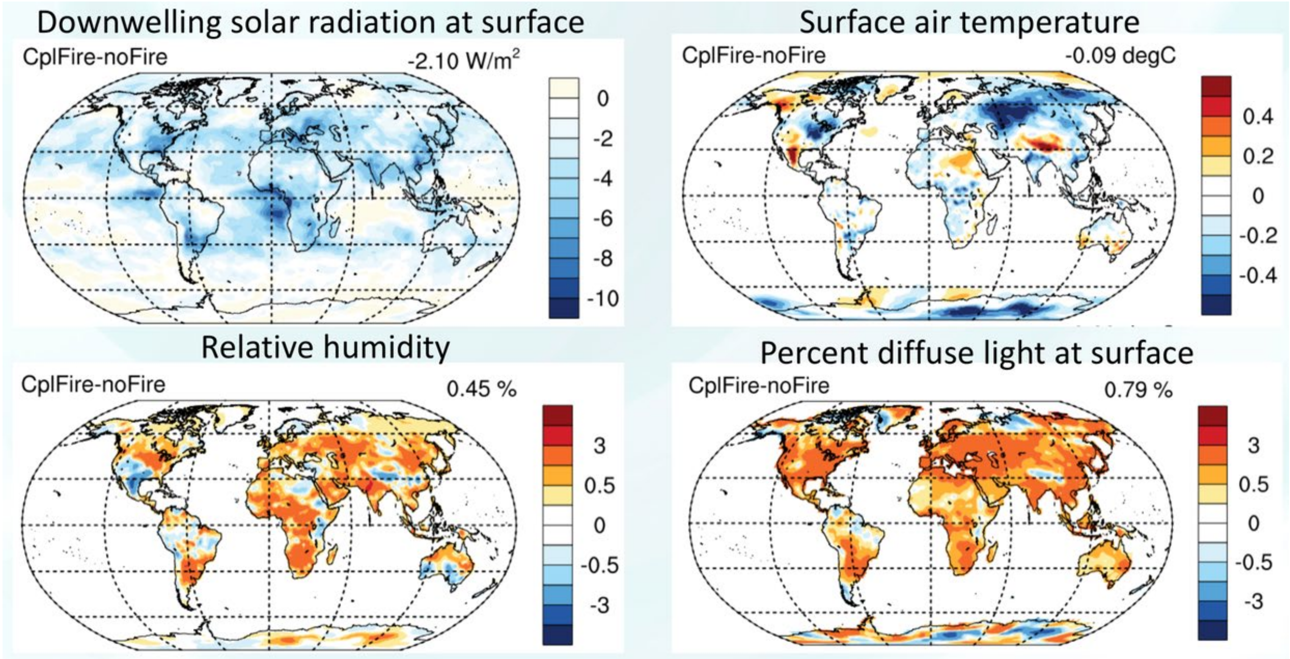


Figure 49. Wildfire-aerosol-induced difference in downwelling solar radiation at surface, surface-air temperature, relative humidity, and precent diffuse light at surface.

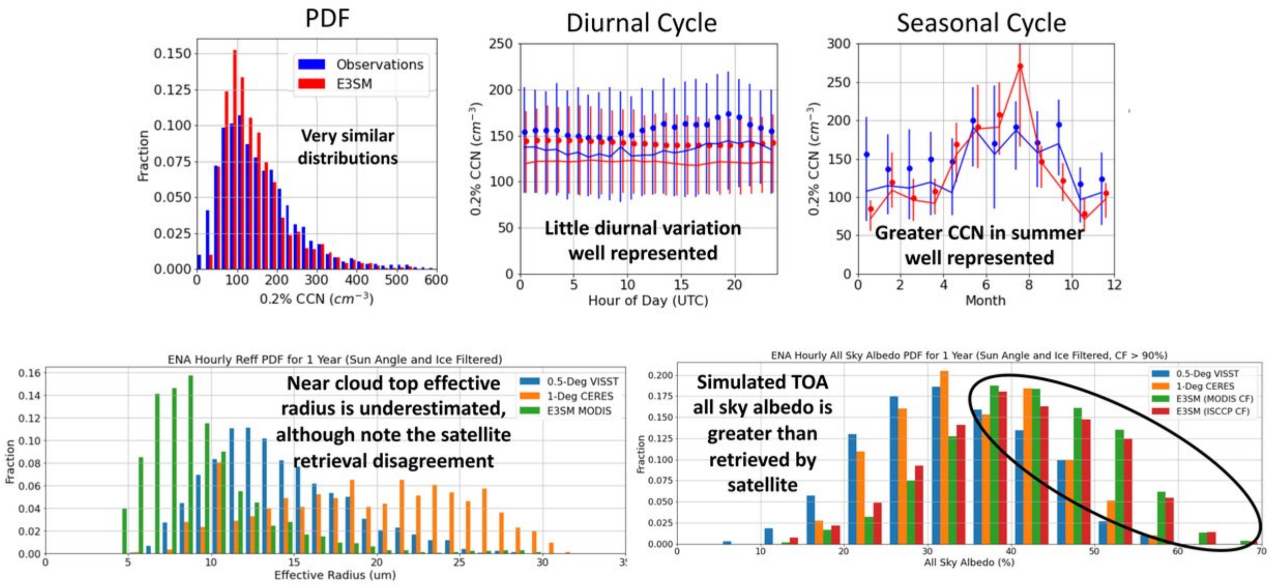


Figure 50. Sample diagnostics comparing E3SM and observations, including the occurrence frequency of cloud-condensation nuclei (CCN), the diurnal cycle, the seasonal cycle, the occurrence frequency of cloud droplet effective radius, and the occurrence frequency of albedo.

Preliminary results (Fig. 50) for the ARM Eastern North Atlantic site show that E3SM produces good simulations of cloud-condensation nuclei, liquid-water path, and rain rates. However, E3SM underestimates the detectable cloud fraction, effective radius, and lower tropospheric stability, and overestimates cloud optical depth, albedo, and rain frequency. These diagnostics provide insight into model representations of aerosol-cloud processes and aid parameterization adjustment and refinement.

Discussion

The group had a productive discussion of gaps, connections, and opportunities for aerosol modeling in E3SMv4 running global-convection-permitting (e.g., dx = 3 km) simulations on DOE's GPU machines. The group concluded that a good software design is critical. The new aerosol code needs to be flexible and easy to test new features and have a clean interface with the host model. The EAGLES project team has designed the code infrastructure that meets the need, but inputs from the community are always welcome.

Hailong Wang introduced the ongoing aerosol efforts in NGD-Atmospheric Physics (including new treatments of prognostic stratospheric sulfate, nitrate aerosol, dust, and secondary organic aerosol), and led the discussion on integrating these efforts into the EAGLES branch for E3SMv4. Most of the integration is already done or easy to do. One challenging task is the integration of the nitrate aerosol treatment, which will require further investigation and a large number of code changes for coupling with chemistry and Modal Aerosol Module (MAM).

The group discussed connections between two efforts on improving wildfire aerosols. Li Xu and the UC-Irvine team focus on improving wildfire aerosol-emission rates, while EAGLES focuses on improving the vertical distribution of wildfire aerosol emissions. Both teams see an opportunity to collaborate by integrating the two efforts so that a complete treatment for wildfire aerosol emissions can be implemented in E3SM.

At high resolution, 3D radiation (e.g., the reflection of radiation from clouds in neighboring cells) might be important. Currently E3SM still uses two-stream approximation and neglects 3D radiative effects, but there are 3D radiation efforts occurring at ECMWF, the Canadian Climate Center, and in the LES community. If E3SM plans to do 3D radiation in the future, aerosol optics will need to be redone to provide more information regarding the phase function (not just the extinction, single-scattering albedo, and asymmetry factor needed for two-stream approximation).

The last item discussed was the chemistry-mechanism code. One familiar package is KPP (which is used by Joshua Fu's new chemistry solver). Nicole Riemer and collaborators are developing a new package "Chemistry Across Multiple Phases (CAMP)", which is runtime configurable, and a GMD paper is in preparation. Riemer is working with software engineers at Barcelona Supercomputer Center to make CAMP run on GPU machines. Jeff Johnson and Mike Schmidt from the EAGLES project are assessing CAMP and a few other options.

NGD Nonhydrostatic Atmosphere and Performance / Exascale Readiness Breakout, Peter Caldwell, Sarat Sreepathi

Presentations

The first talk of this breakout session, given by **Youngsung Kim** (Presentation - Kim), provided a deep dive on GPU performance with a case study using SAM++. Next, **Luca Bertagna** described the performance portability progress for SCREAM (Simple Cloud-Resolving E3SM Atmosphere Model), E3SM's ultra-high resolution non-hydrostatic atmosphere model (Presentation - Bertagna). **Gunther Huebler** gave the final talk suggesting a potential pathway for performing long-term climate simulations on OLCF's Summit supercomputer (Presentation - Huebler).

Discussion

Several tasks were identified which are low-hanging fruit for performance improvement. One of those is switching the MPAS Sea Ice to not run in tropical regions where there is never sea ice. Currently, ice columns on each core are drawn randomly from around the world for load balancing and the ice code exits quickly from columns with no ice; so it is unclear how this would help, except in the strong scaling limit where each core has few ice columns to load balance over. Another suggested easy way to improve performance is to reduce unneeded resolution. This may look like a lower model top or coarser vertical-grid spacing, or it may look like a coarser horizontal mesh. On one hand, modelers should definitely be cognizant of the resolution needed to answer a particular science question and use the coarsest acceptable resolution that achieves that objective. On the other, (1) defining that minimum required resolution is hard to do without running at higher resolution, (2) E3SM was built on the goal of high resolution, and (3) higher resolution is necessary to supply the parallelism required for modern computers. Another easy performance win is to cull the project's output files (both restarts and default history tapes) because although PIO2 improves write speed, writing is still expensive (in terms of compute time, memory, and post-processing time).

Several more time-intensive but potentially high-payoff changes were proposed. In his presentation, Gunther Huebler talked about using microphysics subcolumns to provide extra work on GPUs while reducing model biases. The possibility of extending these subcolumns to include radiation was floated, but Walter Hannah said his experience with the multiscale modeling framework (MMF) showed that radiation subcolumns had little impact on model solution. E3SM has been moving away from subcolumns, so changing course would require Executive Council buy in. More sophisticated timestepping was also brought up as a potential win. Mark Taylor pointed out that the dycore timestepping is already very efficient, so the only avenue for future improvement would be adaptive timestepping. Since atmospheric physics is very sensitive to timestep, adaptive timestepping would be hard. Better timestepping within subcycled atmospheric physics (e.g. rain sedimentation) is a potential win, but affects only small portions of model time. Doing radiation in parallel with other atmospheric processes (or as its own component in parallel with all other components) is likely to provide large improvement for a moderate amount of work. Finally, the ability to use single (or half!) precision was brought up as a definite area for model speedup. Figuring out what variables/calculations could be done in lower precision and which need double precision is the key task here.

Several important infrastructure campaigns were also discussed. One is improving/expanding unit testing, including mathematical convergence. This is necessary for building the confidence needed to use E3SM for decision support and should reduce the number of model crashes. Another task is developing hardware-utilization metrics and tools to help optimize GPU performance. Finally, the ability to run large ensembles efficiently as a single executable for INCITE (Innovative and Novel Computational Impact on Theory and Experiment)-class simulations will be important in Phase 3 of the project. The team has the ability to do this now (via the model's "multi-instance" capability) but this capability needs to be hardened/improved and the tools to postprocess ensemble data quickly need to be developed.

Another topic discussed was the need to strengthen the team's INCITE proposals and include more ambitious requests. In the past, the team has struggled to utilize INCITE's GPU machines for compelling science. Furthermore, there is a need to think about science campaigns that are more aligned with hardware. This should improve (and is improving) as SCREAM and MMF mature. Another example would be G-cases that are more aligned with correct resolutions. Finally, there was some discussion about the need to quantify the project's numerical-precision requirements to take advantage of emerging mixed-precision architectures.

BGC + NGD Land Breakout, Kate Calvin, Ben Bond-Lamberty

Implementation and Evaluation of 3D Radiative Transfer Parameterizations to Represent Topographic Effects in the E3SM Land Model

In this talk (Presentation - Hao), **Dalei Hao** started by noting that the world is mountainous, leading to large topographic effects on radiation-transfer models. All CMIP6 Earth System Models (ESMs) use a plane-parallel (PP) radiation-transfer

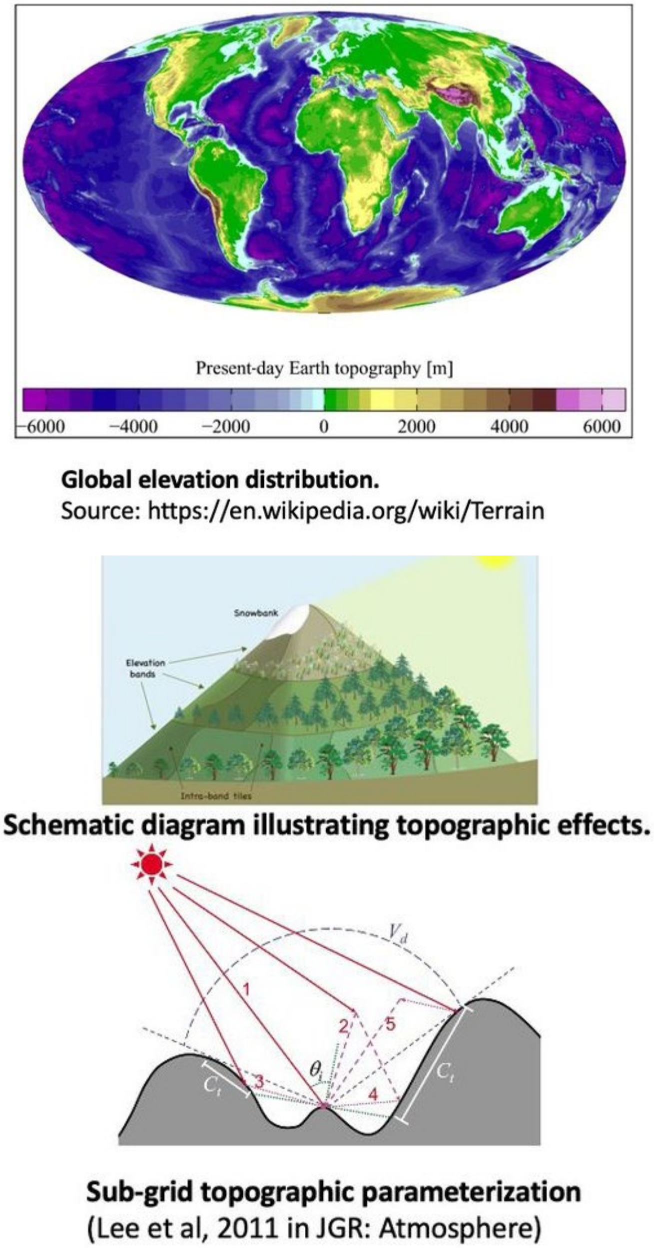


Figure 51. Summary information from the "Implementation and Evaluation of 3D Radiative Transfer Parameterizations to Represent Topographic Effects in ELM" presentation.

scheme for atmosphere–land exchange and do not account for the effects of surface topography. Hao's study implemented a 3D sub-grid radiation transfer parameterization, taking advantage of the E3SM Land Model's (ELM's) new topography-based sub-grid structure (Fig.51). One goal of the study was to consider the influence of arbitrary topography without degrading performance, using a sub-grid parameterization based on Lee et al. (2011). To test the influence of topographic effects, two simulations were conducted—one with, and one without, these effects for the Tibetan Plateau. The results were evaluated with remote-sensing data, using Random Forest models to evaluate parameter importance. The key findings include,

- The topography-induced albedo difference between the PP and 3D methods at 0.125 degree resolution was ±20% in some instances, the winter topography-induced surface temperatures varied by ±1 K, the topography-induced net solar-radiation difference could be larger than 20 W/m^2, the latent-heat-flux difference was smaller than ±10 W/m^2, the sensible-heat-flux difference could reach up to ±10 W/m^2, and the topography-induced snow-cover difference was smaller than ±10%.
- The results of the MODIS evaluation showed that ELM-PP overestimated direct albedo in most regions, whereas the 3D parameterizations (ELM-3D) showed a smaller bias than ELM-PP. For diffuse albedo, ELM-3D had a similar or slightly larger bias than ELM-PP. For snow cover and surface temperature, ELM-3D was closer to MODIS estimates in winter. For latent-heat flux, both showed large biases compared to the MODIS data.
- As spatial resolution increases, the topographic effects on albedo become more and more obvious, especially in winter.

In summary, topography had nonnegligible effects on surface-energy balance and snowmelt; the topographic effects have seasonal variations and are related to spatial scale; and considering topography in ELM improves consistency with MODIS data. Future work includes

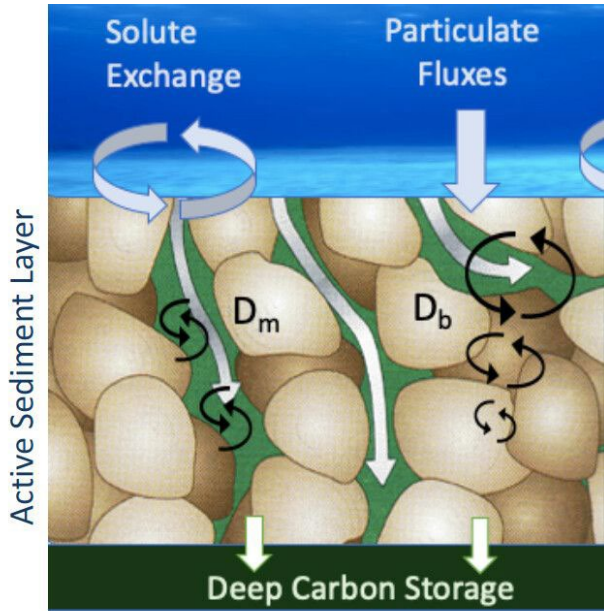


Figure 52. Illustration of the mixing and transport processes included in the ocean-benthos diagenetic model created as part of the InteRFACE project. Dm within the active sediment layer represents molecular diffusion of solutes and Db represents biodiffusion of solids and solutes.

accounting for sub-grid topographic heterogeneity in ELM, developing parameterizations for black carbon (BC) and dust mixing in snow and the associated light-absorption and scattering processes, implementing multilayer canopy energy transfer accounting for tracers (e.g., dust and BC) in the canopy air space, accounting for the topographic effects on longwave radiation, and performing a land-atmosphere coupled run.

Modeling Arctic Seafloor Biogeochemistry in E3SM for InteRFACE

In the next talk (Presentation - Jeffery), **Nicole Jeffery** commented that coastal carbon pools are big, with a great deal of primary production and important coastal impacts. In particular, the Arctic food web has large socioeconomic impacts, motivating the work she presented on modeling seafloor biogeochemistry as part of the InteRFACE project. The mixing and transport aspects of the ocean benthos diagenetic model (Fig. 52) have two parts: (1) a benthic submodule which consists of a ~30 cm active layer, 35 solid and solute biogeochemical tracers, sinking particulate fluxes (including both sedimentation and chemical precipitation), and diffusive exchanges of solutes with ocean-bottom waters and (2) interior mixing within sediments, which includes molecular diffusion of solutes (D_m) and biodiffusion of solids and solutes (D_b). The reactive processes of the ocean-benthos diagenetic model includes organic-matter decomposition, which fuels the reactive transformations in the sediments and is microbiologically mediated, but microbial biomass is not explicit in the kinetics. Rather, kinetics follow the preferred oxidants O_2, NO_3, MnO_2, $Fe(OH)_3$, and SO_4, and when oxidants are depleted, particulate organic matter (POM) decomposes through methanogenesis (CH_4). Particulate inorganic carbon dissociation of calcite, aragonite, and 15% mg-calcite is included, as are 19 secondary reactions.

A test case is in progress. Though not in the Arctic, the Arkona Basin in the Baltic Sea is data rich, which is useful for testing the 1D prototype model, built in MATLAB and based on Reed et al. (2011)'s benthos model, Krumins et al. (2013)'s carbonate-chemistry model, and the MPAS-Sea Ice BGC model. Jeffery and her team are also working on a benthic submodule in MPAS-Ocean and have ported the MATLAB code to Fortran. They are currently working on verifying the port against the 1D prototype version. The current version is active for all MPAS-Ocean grid cells, but they prefer it to be active only in the coastal/shelf -zone cells. The current model has many limitations, which will be addressed in the production version, assisted by ongoing ICoM work that will address sediment flux issues.

Climate Responses to Emissions Reductions Caused by COVID-19 Lockdowns and Restrictions

Next, **Hailong Wang** presented collaborative work looking at

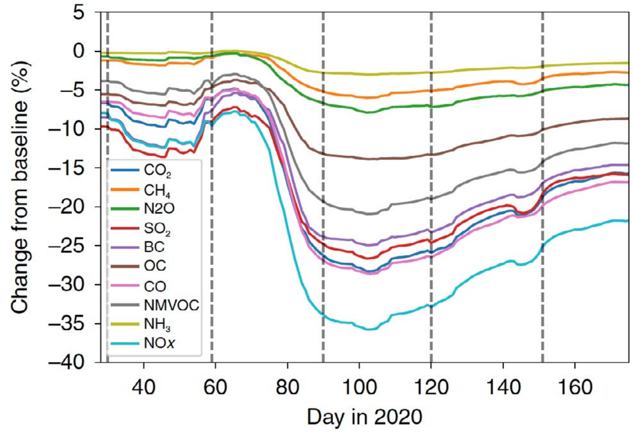


Figure 53. Percentage of globally averaged emission changes for the considered species as a function of the day in the year 2020, where Day 1 is January 1, 2020. The changes are for fossil fuel CO_2 emissions and total anthropogenic emissions from the other sectors. The vertical grey dashed lines mark the first day of the months February to June to aid orientation. From Forster et al. (2020).

COVID-19's impact on weather and climate (Presentation - Wang). The COVID-19 lockdown and restrictions led to sudden large reductions in greenhouse gas (GHG) and pollutant emissions (Fig. 53). Forster et al. (2020) found a short-term cooling associated with less GHGs and short-term warming associated with fewer aerosols, based on a simple energy-balance model. Though there is a need to look at climate responses involving both fast and slow processes, at the moment it is practical to look only at near-term impacts and fast processes. Wang described one effort, the CovidMIP (COVID Model Intercomparison Project), which is using a number of climate models to examine the following questions:

- What is the impact of these emissions reductions on climate?
- What do different recovery scenarios look like?

E3SM's participation includes looking at the near-term impact of COVID-lockdown emissions reductions by creating a simulation branched from the SSP2-4.5 scenario (Shared Socioeconomic Pathway 2 with 4.5 W/m2 forcing in 2100 - a medium forcing category) and run for five years, with 10 ensembles. Currently there is no plan to look at longer-term impacts of recovery scenarios such as a branch from SSP2-4.5 at January 1, 2020 run for 30 years instead of five (with 10 ensemble members). Similar to Forster et al. (2020), the estimated radiative forcing (ERF) and temperature change increase initially until approximately 2023, then both decrease, with corresponding changes in aerosol optical depth (AOD), cloud-droplet number, and moisture. The key results of the simulations include the following:

- The global mean surface temperature increases slightly,

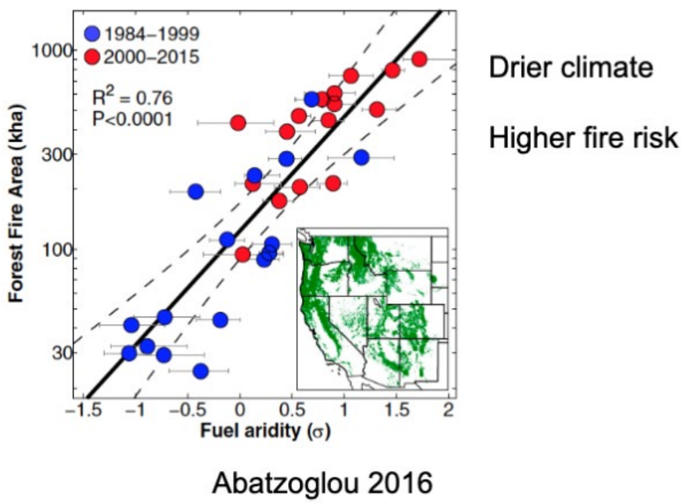


Figure 54. Relationship between forest fire area and fuel aridity for two time periods: 1984 to 1999 and 2000 to 2015, from Abatzoglou and Williams (2016). A drier climate, signaled by increasing fuel aridity, correlates to increased fire risk.

peaking in 2022, though regional warming or cooling effects are more significant with the Arctic experiencing amplified warming initially before reversing in 2023-2024.

- For the first couple of years, precipitation changes significantly in the tropics and the Intertropical Convergence Zone (ITCZ) shifts northward. These trends reverse in 2023. There are significant (large) regional changes in the mid-latitudes. A comparison of E3SM's simulations to the Community Earth System Model's (CESM's) simulations shows that the changes in the ITCZ are not exactly in phase and the ITCZ signals in 2020 is less clear in CESM.
- Surface warming is consistent with net radiative forcing.

In summary, scientists have completed all the planned simulations, which show interesting results. The international team will contribute the simulations to the CMIP6 community for a potential inclusion in the IPCC's AR6 report. The team plans to analyze simulations from all 13 modeling centers and focus on high-latitude changes, since this is where the greatest changes occur.

E3SM Wildfire Fire Surrogate Model Based on Machine Learning

Qing Zhu presented the next talk (Presentation - Zhu), which examines the accuracy of the current E3SM fire model with respect to burn area and whether machine learning (ML) can help improve accuracy. A drier climate leading to higher fires motivates this study, which follows other work such as that by Abatzoglou and Williams (2016) (Fig. 54). The current fire model is adequate, but specific regions show large biases; for example, the pan tropics are overestimated and the northern temperate areas are underestimated.

Scientists took inputs (ignition factors, etc.) and coupled them with process representations (e.g., fire duration), leading to outputs such as burn area. Researchers tuned 10 E3SM wildfire model parameters, which was very time consuming, and unfortunately did not work very well, so they tested modeling nonlinear relationships using a deep neural network (DNN) for 14 widely used Global Fire Emissions Database (GFED) wildfire regions. This ML approach reproduced the original E3SM wildfire behavior with high accuracy (Pearson correlation p=0.91; Coefficient of determination R2=0.79), though researchers noted that Africa has very high fire activity, which can dominate the results, so they recommend using region-specific models. Next, scientists fine-tuned the DNN with GFED observations from 2001 to 2010 and saw very good latitudinal performance. It also had high accuracy and was much less (99% less) computationally demanding. It prognostically simulated the 2011 to 2015 global burn area and was fast, accurate, and flexible. This hybrid approach (pre-train DNN with E3SM model outputs, fine-tune DNN with GFED data) combines the process-based model that has strong physical constraints and the data-driven model that has high prediction accuracy and provides E3SM with a reliable wildfire module.

Since the DNN is a black box, which is hard to interpret and puts focus on back-tracing, and may not be physically reasonable, scientists are currently working on a physically-constrained neural network (NN) to make sure the model can generate reasonable results based on cause-and-effect relationships.

Open Discussion

During the open discussion, the group asked the question "What are the missing couplings or uncertainties the team should focus on?" Responses included that numerical coupling itself is often ignored and the coupling method chosen changes results. Scientists were forced to use wrong parameters to make the model right. At some point, researchers will no longer be able to add processes to improve the model.

A somewhat tongue-in-cheek suggestion was made: "What about throwing out all our process models for DNNs?" The responses included:

- Is a hybrid approach important to explore? If so, there are some real challenges.
- Anthropogenic activities are areas where humans can exert control over CO_2 emissions by changing their behavior. The model needs to represent anthropogenic activities in a way that captures the control humans exert.
- Scientists need to incorporate knowledge into ML approaches so models can't incorporate arbitrary information (the model must stay physically guided).
- But climate change is moving us into novel states, and ML

is likely to be less accurate in predicting the future.

- Combine them both! Keep our cool process-based physics, but why can't we add in ML for say allocation, nutrient uptake? (A number of attendees seconded this.)
- E3SM's plant hydraulics could probably really benefit from ML, especially in cases when numerical solver crashes occur due to nonconvergence when simulating conductance and transpiration in very dry soils.
- Data quality is also an issue and can hugely distort training.

The scale issue is very important—e.g., site-scale parameters being used for global-scale simulations. For example, scientists can ignore lateral fluxes in a coarse resolution model, but these fluxes should not be ignored at high resolution. The models should have scale awareness.

Finally, lateral fluxes (water, land, river, etc.) pose a hard problem and are a big challenge. Solving this requires close coordination among many groups and disciplines.

Ocean + Coastal Modeling Breakout, Luke Van Roekel, Andrew Roberts

This session featured three talks highlighting future opportunities for E3SM development for global to coastal ocean simulations: (1) tides and their impact on the Earth system by **Brian Arbic** and **Johannes Westernik** (Presentation - Arbic_Westerink), (2) sources of sub-grid mixing and scale-aware parameterizations by **Baylor Fox-Kemper**, and (3) near- and long-term possibilities for new MPAS-Ocean discretizations by **Sarah Calandrini** and **Darren Engwirda** (Presentation - Engwirda).

Tides

Tides are being implemented in E3SM as part of the Integrated Coastal Modeling (ICoM) project. The first stage of development has resulted in a geopotential function and runtime harmonic analysis in MPAS-Ocean for each of the largest semidiurnal (M2, S2, N2, K2) and diurnal (K1, O1, Q1 and P1) tidal constituents. An example of the M2 tidal amplitude and phase is shown in Figure 55. Bottom drag, topographic wave drag, and self attraction and loading are now under development within MPAS-Ocean, each of which is necessary for tidal accuracy. Beyond these basic physical elements, critical questions remain to be answered as to the required ocean model resolution and mesh transitions within a fully coupled Earth system to adequately represent tides in the climate system. Coastal/shelf tides have a substantial back-effect on open-ocean tides, and therefore shelf tides are important not only for their own sake, but also because they feed back onto the open ocean. As a consequence, mesh design and variable time stepping are important in the efficient representation of tides within a moderate-resolution global model. Owing to basin resonance, simple use of regional refinement may be far less accurate than bathymetrically-defined mesh resolution on the unstructured MPAS-Ocean grid. The Atlantic basin is particularly sensitive to resolution and geometry, and it has been demonstrated that Antarctic ice-shelf cavities significantly affect sea level on the North American Atlantic coast. This opens the way for investigating the impact of bathymetry and cavity geometry on global tides within baroclinic tidal versions of MPAS-Ocean in E3SM, and their impact on global climate variability. Collaborations are currently being established with experts in mixing and sea-ice model simulations with the E3SM ecosystem.

Ocean Mixing

The discussion was motivated by an examination of the distribution of ocean model resolution from every IPCC assessment report, as shown by the blue dots in Figure 56. The black dashed line is a fit to the median resolution, the red line is a fit the finest resolution and the blue line assumes Moore's law continues to hold. The vertical axis shows three critical regimes: the mesoscales, the submesoscales, and

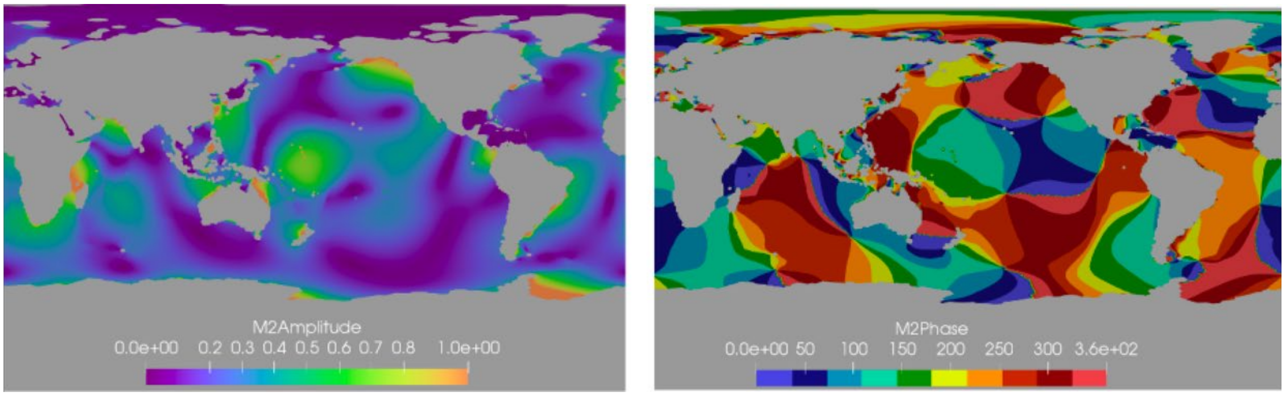


Figure 55. Example of the M2 amplitude (m) and phase (degrees) in MPAS-Ocean after the first stage of ICoM development. (Courtesy of Steven Brus)

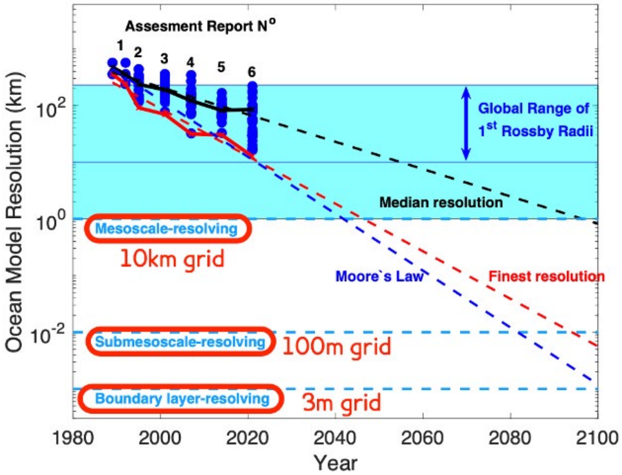


Figure 56. Ocean model resolution from every IPCC assessment report. (Courtesy of Baylor Fox-Kemper)

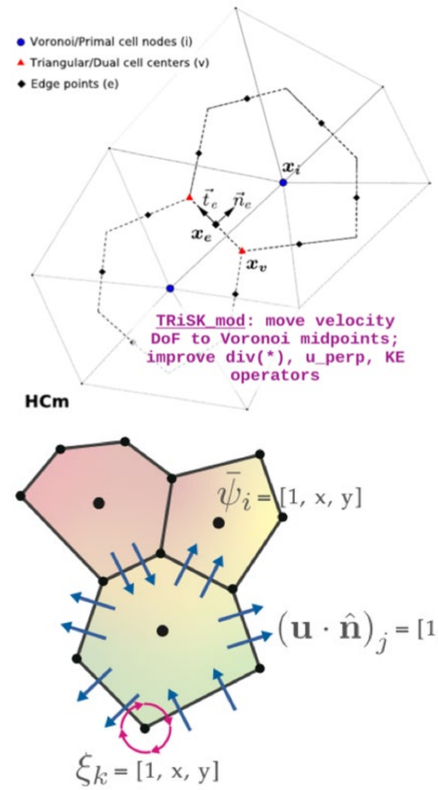


Figure 57. Two new possibilities for MPAS-Ocean discretizations. (Courtesy of Darren Engwirda and Sara Calandrini)

boundary-layer turbulence. All these regimes are critical to represent in ocean models.

This figure shows clearly that scientists cannot simply assume that they will be able to directly resolve these processes in Earth System Model projections. Following the finest resolution, mesoscales will not be directly resolved regularly until 2040, submesoscales until 2090, and boundary layer turbulence beyond 2100. Parameterizations will be a mainstay of ocean models for the foreseeable future.

Mesoscale eddies are dominant in the forward cascade of enstrophy. Models that only partially resolve the mesoscales may not accurately represent this cascade. Often, models use a simple constant coefficient biharmonic-momentum diffusivity to account for this missing sink. However, this can lead to excessive dissipation. The quasi-geostrophic (QG) Leith scheme, which is flow aware, yields an appropriate cascade and dramatically improves the energetic balance in the ocean. However, for non eddy-resolving resolutions, the QG Leith scheme can lead to an inaccurate enstrophy cascade. This represents a special challenge for E3SM, with an unstructured mesh, where mesoscales may be fully resolved in select regions.

Submesoscale eddies are dominant drivers of mixed-layer restratification. These processes are at the very bottom of the hydrostatic regime. The Fox-Kemper et al. (2011) parameterization for submesoscale eddies has some scale-aware components, e.g., the scaling of the horizontal buoyancy gradient, but the parameterization is incomplete. As an example, observations have shown surface convergence in the presence of submesoscale eddies, which current parameterizations are unable to capture. At a slightly smaller scale, symmetric instabilities, which form along fronts, are strong drivers of turbulent vertical-momentum fluxes. Models that do not account for these instabilities exhibit excess momentum fluxes. Current parameterizations of symmetric instability require resolved fronts; extending this to global ocean models remains an open question.

As E3SM moves toward a global to coastal ocean capability, work is needed to make these parameterizations scale and flow aware. Further, some of these processes interact, e.g., submesoscales and symmetric instability both derive their instability from horizontal buoyancy gradients in the upper ocean. It is unclear how interaction of these processes alters parameterizations.

MPAS-Ocean Discretizations and Meshing
Two possibilities for new MPAS-Ocean discretizations were presented, as shown in Figure 57.

The plot on the left tweaks the location of the normal velocity along the edge. Currently MPAS places the velocity at the midpoint of the edge. This was done to ensure geostrophic balance, as the appropriate reconstruction of the tangential velocity relies on the normal velocity's being at the midpoint of the edge. The proposed change would move the normal velocity to the Voronoi midpoint. This can improve the order of accuracy of the model, but may degrade conservation of critical properties in the model.

The longer-term discretization, on the right, proposes to borrow some ideas from Discontinuous Galerkin models. In this framework, the number of velocity degrees of freedom is effectively doubled in the dynamical core. Two points would be placed along each edge. This would allow for a higher-order reconstruction along the edge, which would increase the order of accuracy of quantities like vorticity/enstrophy. This would again increase the order of accuracy of the model. Questions remain in this discretization. With double the velocity degrees of freedom, the model becomes more computationally intensive. However, the higher order of accuracy could allow for a reduction in the number of grid cells required. It is also again unclear how many and how much of the mimetic nature of MPAS can be retained.

NGD Atmosphere Breakout, Shaocheng Xie, Susannah Burrows

The NGD-Atmosphere breakout session consisted of three oral presentations about new atmospheric-physics developments and an open-discussion session with the emphasis on upcoming major activities organized by the Atmospheric Physics NGD subproject and coordination with Biogeochemistry (BGC) project.

Presentations

The session started with a major update on the recent developments of atmospheric chemistry and aerosols by **Qi Tang** and **Hailong Wang** (Presentation – Tang). Significant progress has been made in these areas. The advanced University of California–Irvine (UCI) fast chemistry with 32 species has been implemented in E3SMv1 (Fig. 58), which will provide some chemical mechanisms required for aerosols and BGC coupling.

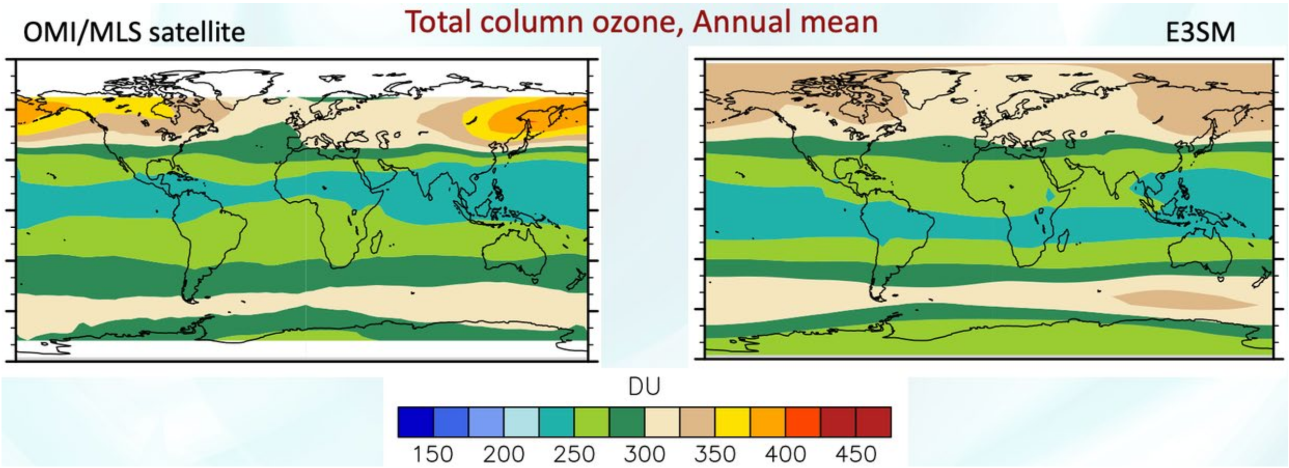


Figure 58. Annual mean geographic patterns of the total column ozone (DU) from the fast chemUCI (full chemistry) test (right) are encouraging compared with satellite observations (left).

The advanced gas-aerosol module MOSAIC has also been implemented in E3SMv1 and coupled with MOZART chemistry and a modified four-mode Modal Aerosol Module (MAM4) for nitrate and other aerosols. The treatment of Secondary Organic Aerosols (SOA) has been improved and stratospheric sulfate aerosols are now represented by a new aerosol module MAM7S (i.e., MAM4 plus three modes for stratospheric sulfate). New dust-emission and dry-deposition schemes are being tested. These individual new developments will be integrated into the same code base and coupled to the new UCI chemistry (Fig. 59).

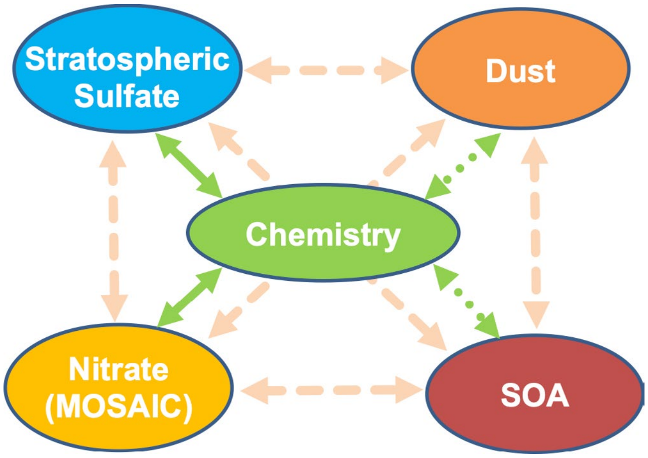


Figure 59. New aerosol developments and their connections to full chemistry for E3SMv3.

Chris Terai showed (Presentation – Terai) the coupling of a Simplified-High-Order-Closure (SHOC) turbulence and shallow-convection scheme with the Zhang-McFarlane (ZM) deep-convection scheme which has been tested for simplifying the current turbulence and shallow convective processes represented by the Cloud Layers Unified by Binormals (CLUBB) with the goal of developing a single code base for future E3SM versions. Initial tests using SHOC show improvements in stratocumulus clouds along the coastline in the Eastern Pacific, but a worsening in the simulation of precipitation over the Tropical Western Pacific (Fig. 60).

Initial results on the impact of land-surface heterogeneity on turbulence and boundary layer clouds were presented by **Po-Lun Ma** (Presentation-2 - Ma). This research is currently supported by the Coupling of Land and Atmospheric Subgrid Parameterizations (CLASP) project. This study has shown that representing subgrid-scale variability of the land-surface can lead to enhanced vertical mixing and a deeper planetary boundary layer (PBL) (Fig. 61), which in turn affects clouds and precipitation.

Discussion

These presentations were followed by organized discussions of several topic areas. One important discussion topic was the major Atmospheric Physics NGD subproject activity on evaluating four candidate convection schemes for E3SMv3, which will start early next year. The code base used for the comparison will be E3SMv3 with the new P3 cloud microphysics. The tests include both 1-degree and 0.25-degree AMIP simulations to evaluate the performance of the convective schemes across different scales. Some suggestions from the discussion include (1) +4K experiments for clouds and cloud feedback in a changing climate, (2) metrics for the assessment, (3) ensemble runs for addressing uncertainties in a single climate simulation, and (4) fairness of the comparison, since the model is tuned around a single set of parameterizations. The feedback obtained from the discussion is being incorporated into the convection assessment plan.

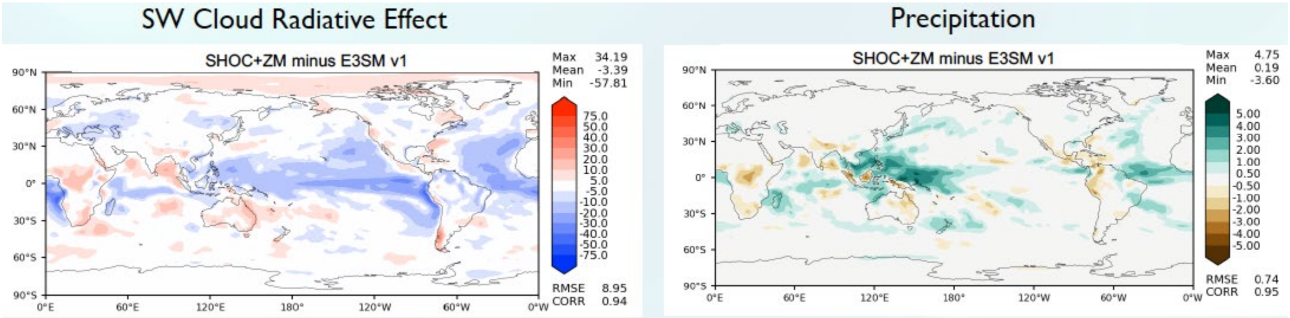


Figure 60. Annual mean difference map of shortwave cloud radiative effect (left) and precipitation rate (right) show more reflection from marine stratocumulus, but also more rainfall over the Tropical Western Pacific in the simulation that couples SHOC with ZM when compared to E3SMv1.

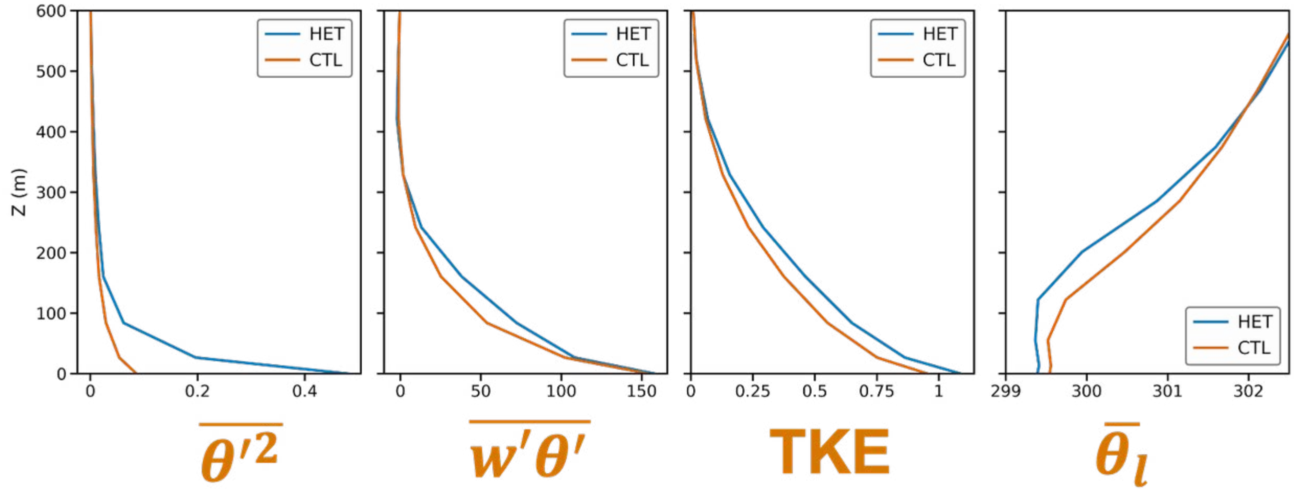


Figure 61. HET denotes the simulation with land-surface heterogeneity applied; CTL is the control simulation. The impact of surface temperature variance extends to about 200 m height. The corresponding buoyancy generates positive temperature flux, resulting in an increased turbulent kinetic energy (TKE) and enhanced vertical mixing.

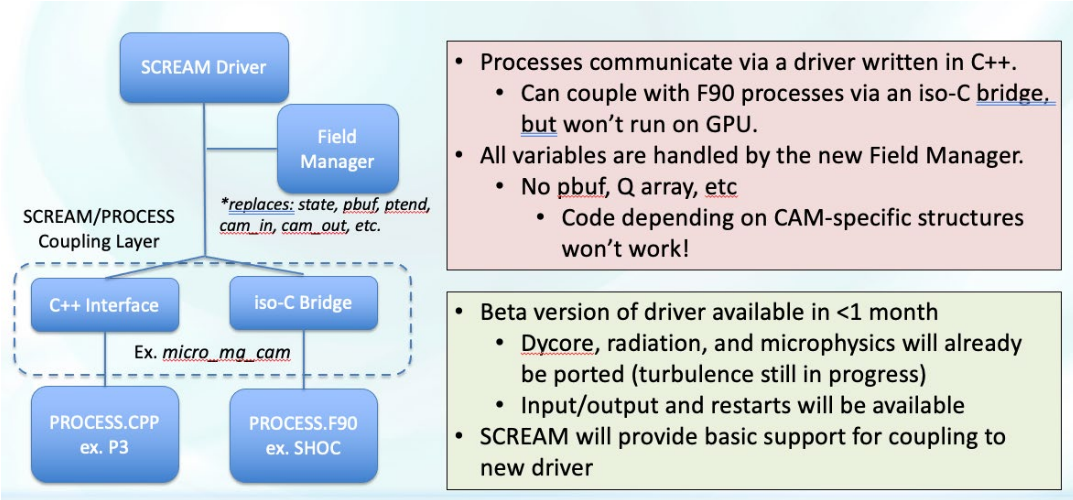


Figure 62. SCREAM – Process Coupling Infrastructure.

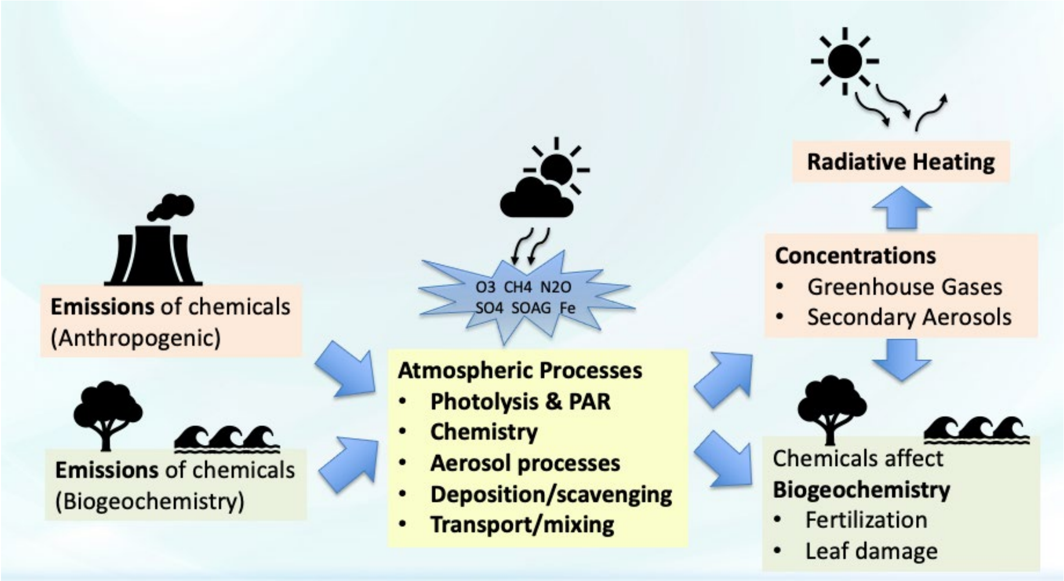


Figure 63. Photolysis affects radiative heating and biosphere.

Another discussion topic was the coupling of new NGD atmosphere developments with the new atmospheric driver that is being developed by the Simply Cloud-Resolving E3SM Atmosphere Model (SCREAM) team for managing both Fortran and C++ atmospheric modules for v3. **Aaron Donahue** provided a quick update on the new atmospheric-driver development, which can run Fortran code on CPUs (see Fig. 62). More follow-up discussion is planned for future NGD atmosphere teleconference meetings.

Coordination with BGC was another major topic scheduled for the open discussion. **Susannah Burrows**, deputy Group Leader for the E3SM BGC group and Co-Chair of the breakout session, presented gaps and opportunities for BGC and the Atmospheric Physics NGD (Presentation - Burrows_Calvin).

The science questions BGC emphasizes are how changes in carbon, methane, and other nutrients impact, and interact with, climate and the coupled Earth system. The BGC team is interested in collaborating with Atmospheric Physics NGD researchers on relevant capabilities being developed, which includes the improved representations of SOA, dust, and chemistry. Figure 63 demonstrates how photolysis affects radiative heating and the biosphere.

Collaboration with ESMD and the university projects funded by DOE climate programs was also briefly discussed. The university principal investigators (PIs) were encouraged to participate in some of the NGD-directed activities when they are interested.

E3SM AWARDS

Figure 64. Photos left to right, top to bottom: awardees Andrew Bradley, SNL, Pat Worley, ORNL, Aaron Donahue, LLNL, Darin Comeau, LANL. Presenting Awards: Sharlene Weatherwax, DOE, and Xujing Davis, DOE.

Sharlene Weatherwax, the Associate Director of Science for BER, recognized this year's "unsung heroes" on the E3SM Team. At the meeting, she announced and presented E3SM Outstanding Achievement Awards to Andrew Bradley, Patrick Worley, Aaron Donahue and Darin Comeau (Fig. 64) for the following contributions:

Andrew Bradley
For algorithmic work, performance improvements, and bug fixes spanning the atmosphere and ocean components and coupling infrastructure, including a 2x improvement in computational efficiency on all architectures.

Patrick Worley
For his meticulous attention to detail and diligence in performing root-cause analysis of seemingly intractable problems and applying his encyclopedic knowledge of E3SM codebase to develop performant solutions.

Aaron Donahue
For essential development of the EAMv4 (SCREAM) integration and infrastructure code, including the creation of the model's input/output capability and management of process coupling, while also serving as a code integrator and tester.

Darin Comeau
For playing a critical role in the v1 cryosphere simulation campaign and in the development and testing of new v2 model configurations—and for being one of the most flexible, diverse, and reliable members of the E3SM team.

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APPENDIX A: EARTH SYSTEM MODEL DEVELOPMENT (ESMD) FUNDED PROJECTS

**See the PDF version of the document (https://l.ead.me/bc6Ix1) to follow the links provided in the Links column.

Table 1. E3SM SFA Leadership Team

Leader, Lab	Group	Links**
Dave Bader, LLNL	Executive Committee – Council Chair	Abstract-1 – Bader Presentation-1 – Bader
Ruby Leung, PNNL	Executive Committee – Chief Scientist	Abstract-1 – Leung Presentation-1 – Leung
Mark Taylor, SNL	Executive Committee – Chief Computational Scientist	Abstract – Taylor Presentation – Taylor
Renata McCoy, LLNL	Executive Committee – Project Engineer / Chief Operating Officer	Abstract – McCoy Presentation-2 – McCoy
Jean-Christophe (Chris) Golaz, LLNL Luke Van Roekel, LANL	Core Group: Water Cycle	Abstract – Golaz Presentation-1 – Golaz
Katherine Calvin, PNNL Susannah Burrows, PNNL	Core Group: Biogeochemical Cycles	Abstract – Calvin Presentation – Calvin
Steve Price, LANL Wuyin Lin, BNL Mark Petersen, LANL	Core Group: Cryosphere	Abstract-1 – Price Presentation-1 – Price
Philip Jones, LANL Sarat Sreepathi, ORNL	Core Group: Performance	Abstract-1 – Jones Presentation-1 – Jones
Robert Jacob, ANL Chengzhu (Jill) Zhang, LLNL	Core Group: Infrastructure and data management	Abstract – Jacob Presentation – Jacob
Peter Caldwell, LLNL	NGD Group: Nonhydrostatic Atmosphere	Abstract – Caldwell Presentation – Caldwell
Shaocheng Xie, LLNL	NGD Group: Atmospheric Physics	Presentation – Xie
Benjamin Bond-Lamberty, PNNL	NGD Group: Land and Energy	Abstract – Bond-Lamberty Presentation – Bond-Lamberty
Andrew Salinger, SNL	NGD Group: Software and Algorithms	Abstract – Salinger Presentation – Salinger
Luke Van Roekel, LANL	NGD Group: Ocean	Abstract – Van Roekel Presentation – Van Roekel

Table 2. Non-E3SM SFAs

PI, Institution	Title	Links**
Ian Kraucunas, PNNL Elizabeth Hunke, LANL - (ESMD lead)	Integrated Coastal Modeling (ICoM)	Abstract - Hunke Presentation - Hunke BER website
Joel Rowland, LANL Andrew Roberts, LANL)- (ESMD component)	Interdisciplinary Research for Arctic Coastal Environment (InteRFACE)	Abstract - Roberts Presentation - Roberts BER website
Po-Lun Ma, PNNL	Enabling Aerosol-cloud interactions at GLobal convection-permitting ScalES (EAGLES)	Abstract-1 - Ma Presentation-1 - Ma BER website

Table 3. University Projects (designates projects awarded in FY20)*

PI, Institution	Title	Links**
Atul Jain, UIUC	Investigating the impacts of changes in land cover and land management on climate using ACME	Abstract - Xu Presentation - Xu
Joao Teixeira, UCLA	The Multi-Plume Eddy-Diffusivity/ Mass-Flux (EDMF) Unified Parameterization: Stratocumulus and the Transition to Cumulus Boundary Layers	Abstract - Teixeira
Xianglei Huang, U. of Michigan	Incorporate more realistic surface-atmosphere radiative coupling in E3SM	Abstract - Huang Presentation - Huang
Zheng-Yu Liu, OSU	Developing Coupled Data Assimilation Strategy for Understanding Model Bias and Extreme Climate Events in E3SM	Abstract - Wu Presentation - Wu
Anand Gnanadesikan, JHU	Parameterizing the Impact of Mesoscale Eddies on Earth System Process in the Energy Exascale Earth System Model	Abstract - Gnanadesikan Presentation - Gnanadesikan
Jadwiga Richter, UCAR	Improving Momentum Transport Processes in E3SM	Abstract - Chen Presentation - Chen
Guang Zhang, UCSD	Enhancing Convection Parameterization for Next Generation E3SM	Abstract - Zhang Presentation - Zhang
Tami Bond, CSU	Collaborative Proposal: Fire, dust, air and water: Improving aerosol biogeochemistry interactions in ACME	Abstract - Rathod Presentation - Rathod
*Marcus van Lier-Walqui, Columbia U & NASA Hugh Morrison, UCAR	Improving the Parameterization of Cloud and Rain Microphysics in E3SM using a Novel Observationally-Constrained Bayesian Approach	Abstract - Van Lier-Walqui Presentation - Van Lier-Walqui
*Joannes Westerink, UND	Efficiently Resolving the Terrestrial-Aquatic Interface in E3SM with Sub-Grid Methods to Improve Coastal Simulations	Abstract - Westerink Presentation - Westerink
*Robert Pincus, Columbia U.	Improving the Capabilities and Computational Efficiency of the RTE+RRTMGP Radiation Code	Abstract - Pincus Presentation - Pincus
*Francois Primeau, UC Irvine	Improving the initial state of biogeochemical components in Earth System Models	Abstract - Primeau Presentation - Primeau
*James Randerson, UC Irvine	Interactions between land use, fires and dust as drivers of global climate change	Abstract - Randerson Presentation - Randerson

Table 4. SciDAC Projects

PI, Institution	Title	Links**
Adrian Turner (LANL)	A New Discrete Element Sea-Ice Model for Earth System Modeling: Phase 2	Abstract - Turner Presentation - Turner
Hui Wan (PNNL)	Assessing and Improving the Numerical Solution of Atmospheric Physics in E3SM Phase 2	Abstract - Wan Presentation - Wan
Philip Jones (LANL)	Coupling Approaches for Next Generation Architectures (CANGA)	Abstract-2 - Jones Presentation-2 - Jones
Peter Bosler (SNL)	Non-Hydrostatic Dynamics with Multi-Moment Characteristic Discontinuous Galerkin Methods (NH-MMCDG) Phase 2	Abstract - Bosler Presentation - Bosler
Stephen Price (LANL)	Probabilistic Sea-Level Projections from Ice Sheet and Earth System Models	Abstract-2 - Price Presentation-2 - Price
Gautam Bisht (PNNL)	Development of terrestrial dynamical cores for the ACME to simulate water cycle	Abstract - Bisht Presentation - Bisht
Takanobu Yamaguchi (NOAA)	Adaptive Vertical Grid Enhancement for E3SM ("Phase 2")	Abstract - Yamaguchi Presentation - Yamaguchi
Lili Ju (USC) Max Gunzburger (FSU)	Efficient and Scalable Time-Stepping Algorithms and Reduced-Order Modeling for Ocean System Simulation	Abstract - Ju Presentation - Ju

Table 5. Early Career Projects (designates projects awarded in FY20)*

PI, Institution	Title	Links**
*Matthew Hoffman (LANL)	Creating a Sea-Level-Enabled E3SM: A Critical Capability for Predicting Coastal Impacts	Abstract - Hoffman Presentation - Hoffman
*Benjamin Sulman (ORNL)	Simulating Estuarine Wetland Function: Nitrogen Removal, Carbon Sequestration, and Greenhouse Gas Fluxes at the River-Land-Ocean Interface	Abstract - Sulman Presentation - Sulman

Table 6. Land Climate Process Teams (CPTs) and CEDS

PI, Institution	Title	Links**
Po-Lun Ma (PNNL)	Parameterizing the effects of sub-grid land heterogeneity on the atmospheric boundary layer and convection: Implications for surface climate, variability and extremes	Abstract-2 - Ma Presentation-2 - Ma
Gautam Bisht (PNNL)	3-D Land Energy and Moisture Exchanges: Harnessing High Resolution Terrestrial Information to Refine Atmosphere-to-Land interactions in Earth System Models	Abstract - Bisht Presentation - Hao
Steven Smith (PNNL)	Emissions Data for Earth System Models: CEDS Updates and Emissions Sensitivity Evaluation	Project Description Project Site

APPENDIX B: TALKS PRESENTED AT THE ESMD–E3SM PI MEETING

D1S1 denotes Day 1, Session 1. D1S2 denotes, Day 1 Session 2, etc. For details on when the talks were presented, see the Meeting Agenda.

D1S1 – Session Chairs: Xujing Davis, Renata McCoy

Welcome

Gary Geernaert, Director of BER Earth and Environmental Systems Science Division (EESSD)

Xujing Davis, Program Manager of the Earth System Model Development (ESMD)

A Brief Overview of the ESMD in Supporting the E3SM Development, Presentation-1 - Davis

Renata McCoy, E3SM Chief Operating Officer

Meeting Sessions, Logistics, and Etiquette, Presentation-1 - McCoy

Keynote

A Baseline for Global Weather and Climate Simulations at 1 km Resolution, Nils Wedi, ECMWF, Abstract - Wedi, Presentation - Wedi

E3SM Awards Announcement, Sharlene Weatherwax, Associate Director of Science for Biological and Environmental Research

D1S2 – Session Chairs: Dave Bader, Cristiana Stan

E3SM Overview

E3SM Status – Dave Bader, Abstract - Bader, Presentation-1 - Bader

Science - Ruby Leung, Abstract - Leung, Presentation-1 - Leung

Computational Science - Mark Taylor, Abstract - Taylor, Presentation - Taylor

E3SM Communication and Support for E3SM Ecosystem Projects - Renata McCoy, Abstract - McCoy, Presentation-2 - McCoy

E3SM v3/v4

Dave Bader, Ruby Leung, Mark Taylor, Presentation-2 – Bader, Presentation-2 – Leung

D1S3 – Session Chairs: Ruby Leung, Renata McCoy

E3SM Core Groups Progress during E3SM Phase 2 and Future Direction

E3SM Water Cycle Group - Chris Golaz, Luke Van Roekel, Abstract - Golaz, Presentation-1 - Golaz

E3SM BGC Group - Kate Calvin, Susannah Burrows, Abstract - Calvin, Presentation - Calvin

E3SM Cryosphere Group - Steve Price, Wuyin Lin, Mark Petersen, Abstract-1 - Price, Presentation-1 - Price

E3SM Performance Group - Phil Jones, Sarat Sreepathi, Abstract-1 -Jones, Presentation - Jones

E3SM Infrastructure and Data Management Group- Robert Jacob, Chengzhu (Jill) Zhang, Abstract - Jacob, Presentation - Jacob

D1S4 – Session Chairs: Kate Calvin, Susannah Burrows

E3SM Next Generation Development Group (NGDs) Update

NGD Nonhydrostatic Atmosphere – Peter Caldwell, Abstract – Caldwell, Presentation – Caldwell

NGD Atmospheric Physics – Shaocheng Xie, Presentation – Xie

NGD Software and Algorithms – Andy Salinger, Abstract – Salinger, Presentation – Salinger

NGD Land and Energy – Ben Bond-Lamberty, Abstract – Bond-Lamberty, Presentation – Bond-Lamberty

NGD Ocean – Luke Van Roekel, Abstract – Van Roekel, Presentation – Van Roekel

Day 1 Wrap-up – Xujing Davis

D2S1 – Introduction to Day 2 – Xujing Davis, Christiana Stan

DOE Regional & Global Model Analysis Program Area (RGMA) Overview and Its Linkages to ESMD – Renu Joseph, Presentation – Joseph

DOE MultiSector Dynamics Program Area (MSD) Overview and Its Linkages to ESMD – Bob Vallario, Presentation – Vallario

DOE Data Management Program Area Overview and Its Linkages to ESMD – Jay Hnilo, Presentation – Hnilo

D2S2 – Session Chairs: Shaocheng Xie, Matthew Hoffman

Ecosystem Projects Update

Enabling Aerosol-Cloud Interactions at GLobal Convection-Permitting ScalES (EAGLES) – Po-Lun Ma, Abstract-1 – Ma, Presentation-1 – Ma

Physically Regularized Machine Learning Emulators of Aerosol Activation, EAGLES – Sam Silva, Abstract – Silva, Presentation – Silva

Integrated Coastal Modeling (ICoM) – Elizabeth Hunke, Abstract – Hunke, Presentation – Hunke

Interdisciplinary Research for Arctic Coastal Environment (InterFACE) – Andrew Roberts, Abstract – Roberts, Presentation – Roberts

Coastal Observations, Mechanisms, and Predictions Across Systems and Scales – Great Lakes Modeling (COMPASS-GLM) – Ian Kraucunas, Presentation – Kraucunas

D2S3 – Session Chairs: Guang Zhang and Anand Gnanadesikan

Overview of FY20 Awards (via FOAs)

1. Creating a Sea-Level-Enabled E3SM: A Critical Capability for Predicting Coastal Impacts – Matthew Hoffman, Abstract – Hoffman, Presentation – Hoffman
2. Simulating Estuarine Wetland Vegetation and Biogeochemistry in ELM – Benjamin Sulman, Abstract – Sulman, Presentation – Sulman

3. Modern Radiation for DOE Modeling Efforts - Robert Pincus, Abstract - Pincus, Presentation - Pincus
4. Improving the Initial State of Biogeochemical Components in Earth System Models - Francois Primeau, Abstract - Primeau, Presentation - Primeau
5. Combining Process-Level Constraints with Global Climatology using Bayesian Statistics and Machine Learning to Improve the Warm Rain Process Representation in E3SM - Marcus Van Lier-Walqui, Abstract - Van Lier-Walqui, Presentation - Van Lier-Walqui
6. Research Challenges Related to New Extremes in California Wildfires - James Randerson, Abstract - Randerson, Presentation - Randerson
7. Sub-Grid Scale Methods Nearshore and across the Coastal Floodplain to Overcome Resolution Limitations in MPAS-O - Joannes Westerink, Abstract - Westerink, Presentation - Westerink

Update from other active University Awards

University Projects

1. Evaluation of the Effects of Stochastic Convection Scheme in E3SMv1 - Guang Zhang, Abstract - Zhang, Presentation - Zhang
2. A New Unified Boundary Layer and Convection Parameterization in the E3SM Model: The Multi-Plume Eddy-Diffusivity/Mass-Flux (EDMF) Approach - Joao Teixeira, Abstract - Teixeira
3. Effects of Organized Mesoscale Heating on the MJO and Precipitation in E3SMv1 - Jack Chen, Abstract - Chen, Presentation - Chen
4. Assessing an Improved Treatment of the Surface-Atmosphere Longwave Radiative Coupling in the E3SM v2 - Xianglei Huang, Abstract - Huang, Presentation - Huang
5. System Design and Evaluation of a Real Time Online Hybrid Data Assimilation System Based on E3SM - Shu Wu, Abstract - Wu, Presentation - Wu
6. Atmospheric Radiative and Oceanic Biological Productivity Responses to Anthropogenic Combustion-Iron Emission in the 1850-2000 Period - Sagar Rathod, Abstract - Rathod, Presentation - Rathod
7. Global Carbon Fluxes Induced by Management Practices on Agricultural Land - Xiaoming Xu, Abstract - Xu, Presentation - Xu
8. Mesoscale Eddy Parameterization Affects the Linearity of Responses to Increased CO_2 - Anand Gnanadesikan, Abstract - Gnanadesikan, Presentation - Gnanadesikan

Day 2 Wrap-Up before posters – Xujing Davis

Introduction to Day 3 – Xujing Davis

D3S1 – Session Chairs: Mark Taylor, Hui Wan

Keynote

How High-Level Abstractions Can Help Bridge the Gap between Productivity and Performance, Oliver Fuhrer (Federal Institute of Meteorology and Climatology MeteoSwiss), Abstract - Fuhrer, Presentation - Fuhrer

Overview of the Scientific Discovery through Advanced Computing (SciDAC) Projects

Announcement of 2021 SciDAC PI Meeting, Randall Laviolette, the ASCR Program Manager of SciDAC

SciDAC projects

1. Coupling Approaches for Next Generation Architectures (CANGA) - Philip Jones, Abstract-2 -Jones, Presentation -2 - Jones

2. Compact, Performance-Portable Semi-Lagrangian Methods for E3SM - Peter Bosler, Abstract - Bosler, Presentation - Bosler
3. Assessing and Improving the Numerical Solution of Atmospheric Physics in E3SM - Hui Wan, Abstract - Wan, Presentation - Wan
4. Parallel Exponential Time Differencing Methods for Ocean Dynamics - Lili Ju, Abstract - Ju, Presentation - Ju
5. Enhanced Low Cloud Representation in E3SM with Framework for Improvement by Vertical Enhancement and Future Plan - Takanobu Yamaguchi, Abstract - Yamaguchi, Presentation - Yamaguchi
6. Probabilistic Sea Level Projections from Ice Sheet and Earth System Models (ProSPect) - Stephen Price, Abstract-2 - Price, Presentation-2 - Price
7. Discrete Element Model for Sea Ice (DEMSI) - Adrian Turner, Abstract - Turner, Presentation - Turner
8. Development of Terrestrial Dynamical Core for the E3SM to Simulate Water Cycle - Gautam Bisht, Abstract - Bisht, Presentation - Bisht

Invited Talks

1. Results and Future Plans for the Multiscale Modelling Framework in E3SM, Walter Hannah, Presentation - Hannah
2. Towards Robust Operational Neural Network Parameterizations of Convection in Climate Models — Advances in Stability, Credibility and Software, Mike Pritchard, Presentation-1 - Pritchard

Day 3 Wrap-up before posters and short break - Xujing Davis, Renata McCoy

Session Chairs:

- **D3S2-BR#1 - Peter Caldwell, Vince Larson**
- **D3S2-BR#2 - Ben Bond-Lamberty, Jim Randerson**
- **D3S2-BR#3 - Luke Van Roekel, Zhengyu Liu**
- **D3S2-BR#4 - Phil Jones, Peter Bosler**
- **D3S2-BR#5 - Ruby Leung, Mike Pritchard**

Parallel Sessions: 1st Breakout #D3S2

1. Atmosphere (BR#1 - Breakout Room #1)
   a. Extreme Supersaturation in CESM2 and E3SMv1 Simulations: Sensitivity to Time-Stepping and Impact on Model Climate - Ross Dixon (U of A), Abstract - Dixon, Presentation - Dixon
   b. Atmospheric Biases in E3SMv2 - Chris Golaz (LLNL), Presentation-2 - Golaz
2. Land (BR#2)
   a. Global Benchmarking of ELM v1: ILAMB and Beyond - Xiaojuan Yang, Abstract - Yang, Presentation - Yang
3. Ocean (BR#3) 2020-10-28 ESMD/E3SM PI Meeting -- Ocean Breakout Session
   a. Update on Eddy Energy Climate Progress Team (CPT) - Laure Zanna (invited)
4. Computational Science (BR#4) 2020-10-28 ESMD/E3SM Computational Science Breakout Session
   a. High-Order, Property-Preserving, Semi-Lagrangian Tracer Transport in E3SM - Andrew Bradley (SNL), Abstract - Bradley, Presentation - Bradley
5. ML/AI (BR#5)
   a. Results From a Survey on ML/AI Use Across the ESMD Projects - Ruby Leung and Mike Pritchard, Presentation - Leung - Pritchard

b. Three Five-Minute Remarks (Robert Pincus, Guang Zhang, Mike Pritchard) P: ML-questions.pdf, Presentation-2 - Pritchard

c. Discussion

Introduction to Day 4 – Xujing Davis, Renata McCoy
Session Chairs:

- **D4S1-BR#1 - Chris Golaz, Luke Van Roekel**
- **D4S1-BR#2 - Steve Price, Mark Petersen, Wuyin Lin**
- **D4S1-BR#3 - Rob Jacob, Andy Salinger**
- **D4S1-BR#4 - Po-Lun Ma, Qi Tang**

Parallel Sessions: 2nd Breakout #D4S1

1. Water Cycle (BR#1 - Breakout Room #1)
   a. Presentations
      i. Model Resolution Sensitivity of Simulated ENSO Teleconnections to Winter Precipitation Extremes Over the US in E3SM - Salil Mahajan, Abstract - Mahajan, Presentation - Mahajan
      ii. Creation of an SST Metric for E3SM - LeAnn Conlon, Abstract - Conlon, Presentation - Conlon
      iii. High-Order, Property-Preserving Physics-Dynamics-Grid Remap in E3SM - Andrew Bradley, Abstract - Bradley, Presentation - Bradley
      iv. E3SMv1 DECK Future Projections Under the High-Emission SSP5-8.5 Scenario - Xue Zheng, Abstract - Zheng, Presentation - Zheng
   b. Group Discussion: v3 / v4 directions.
2. Cryosphere (BR#2) 10-29-2020: E3SM All-Hands meeting Cryosphere Breakout
   a. Presentations:
      i. Assessment of Atmospheric Simulations Over the Antarctica with E3SM Regional Refinement Model - Wuyin Lin, Abstract - Lin, Presentation Zhang_Lin
      ii. The Polar Climate of E3SM Versions 1 and 2 - Andrew Roberts, Abstract - Roberts, Presentation - Roberts
      iii. E3SM's Skill at Simulating the Drivers of Surface Melt on the Greenland Ice Sheet - Wenshan Wang, Abstract - Wang, Presentation - Wang
   b. Group Discussion:
      i. Discussion of known and anticipated biases in v2 and plans for mitigating them
      ii. v3 and v4 Cryosphere science questions and model configuration
      iii. Review and discussion of Cryosphere campaign actionable metrics
3. Infrastructure and NGD Software and Algorithms (BR#3)
   a. A Performance Portable Discrete Element Sea Ice Model - Kara Peterson, Abstract - Peterson, Presentation - Peterson
   b. Using Neural Networks to Predict Atmospheric Optical Properties for Radiative Transfer Computations - Menno Veerman, Abstract - Veerman, Presentation - Veerman

c. Converting E3SM Model Output to the CMIP6 Data Standard – Sterling Baldwin, Abstract – Baldwin, Presentation – Baldwin
d. Discussion
   i. What do you think is missing/broken in current infrastructure?
   ii. How do we expand PACE to cover all provenance needs?

4. Aerosols (BR#4)
   a. Aerosol Model Development for the Future-Generation E3SM at Convection-Permitting Scales – Kai Zhang, Abstract – Zhang, Presentation – Zhang
   b. Enhancing Aerosol Predictions on the Global Scale with Particle-Resolved Modeling and Machine Learning – Nicole Riemer (invited), Presentation – Riemer
   c. Wildfire Aerosol Climate Effect Using Online Fire Emission Coupling in E3SM – Li Xu, Abstract – Xu, Presentation – Xu
   d. Integrating Observations and Process-Oriented Diagnostics to Constrain Aerosol-Cloud Interactions in Earth System Model Development – Adam Varble, Abstract – Varble, Presentation – Varble

Session Chairs:

D4S2-BR#1 – Peter Caldwell, Sarat Sreepathi

D4S2-BR#2 – Kate Calvin, Ben Bond-Lamberty

D4S2-BR#3 – Luke Van Roekel, Andrew Roberts

D4S2-BR#4 – Shaocheng Xie, Susannah Burrows

Parallel Sessions: 3rd Breakout #D4S2

1. NGD Nonhydrostatic Atmosphere and Performance / Exascale Readiness (BR#1 – Breakout Room #1) 2020-10-29 ESMD/E3SM NGD Nonhydrostatic Atmosphere + Performance/Exascale Readiness Breakout Session
   a. GPU Performance Deep Dive: Case Study Using SAM++- Youngsung Kim, Abstract – Kim, Presentation – Kim
   b. Performance-Portability Progress for an Ultra-High Resolution Non-Hydrostatic Atmosphere Model in E3SM – Luca Bertagna, Abstract – Bertagna, Presentation – Bertagna
   c. A Potential Pathway for Performing Long-Term Climate Simulations on Summit – Gunther Huebler, Abstract – Huebler, Presentation – Huebler
2. BGC and NGD Land (BR#2)
   a. Implementation and Evaluation of 3D Radiative Transfer Parameterizations to Represent Topographic Effects in the E3SM Land Model – Dalei Hao, Abstract – Bisht, Presentation – Hao
   b. Modeling Arctic Seafloor Biogeochemistry in E3SM for InteRFACE – Nicole Jeffrey, Abstract – Jeffery, Presentation – Jeffery
   c. Climate Responses to Emissions Reductions Caused by COVID-19 Lockdown and Restrictions – Hailong Wang, Abstract -Wang, Presentation – Wang
   d. E3SM Wildfire Fire Surrogate Model Based on Machine Learning – Qing Zhu, Abstract – Zhu, Presentation – Zh u
3. Ocean and Coastal Modeling (BR#3)
   a. Tides in the Earth System – Brian Arbic, Joannes Westerink (Joint talk), Presentation – Arbic_Westerink

b. Scale-Aware Parameterizations – Baylor Fox-Kemper (Invited)
c. Can We Improve the Numerical Formulation Used in MPAS-Ocean? – Darren Engwirda, Abstract – Engwirda, Presentation – Engwirda
d. Discussion on Future Plans for E3SM:
   i. Important Outcomes by 2025
      - Regional-scale SLR projections, include ice-sheet-sourced SLR
      - Robust variability, change, and overturning matching observations
   ii. Ocean Physics
      - Scale-aware physics
      - Non-Boussinesq approximation
      - Mixing with explicit tides and waves
   iii. Ocean Coupling
      - Scale-aware coupling of land hydrology and land-Ice ocean coupling
      - Scale-aware atmospheric coupling and waves
      - Embedded sea ice
   iv. Oceanographic and Coastal Community Integration with E3SM:
      - Collaboration contacts within E3SM and past experiences with collaborations
      - Defining expectations for community developments (design document, code and testing standards)
      - Defining E3SM expectations (final testing and integration)

4. NGD Atmosphere (BR#4)
   a. Updates on the Interactive Chemistry and Aerosols for E3SM – Qi Tang/Hailong Wang, Abstract – Tang, Presentation – Tang
   b. Understanding the Land-Atmosphere Interactions at Grid and Sub-grid Scales in E3SM – Po-Lun Ma, Abstract-2 – Ma, Presentation-2 – Ma
   c. Evaluating the Climate of Coupling SHOC with ZM – Chris Terai, Abstract – Terai, Presentation – Terai
   d. Open discussion
      i. V3/v4 directions
         1. Coordination between NGD-atm and BGC, Presentation – Burrows_Calvin
         2. Options for convection
         3. New atmospheric driver/GPUs
      ii. Interaction with broader ESMD efforts

D4S3 – Session Chairs: Shaocheng Xie, Jennifer Holm, Robert Pincus
E3SM Tools
Infrastructure and Performance Tools Talks, Abstract – Zhang, Presentation – Zhang
Presentations:

1. Overview and Case Control System – Rob Jacob
2. NCO – Charlie Zender
3. E3SM_diags – Chengzhu (Jill) Zhang, Abstract – Zhang
4. MPAS_analysis – Xylar Asay-Davis
5. e3sm_to_cmip – Sterling Baldwin, Presentation – Baldwin
6. zstash – Ryan Forsyth
7. Performance Archiving and Analysis (PACE) – Sarat Sreepathi

Poster Awards Announcement (Xujing Davis)
D4S4 – Session Chairs: Ruby Leung, Peter Thornton
Report from Day 3 breakouts
Reports from breakouts x 8
Meeting Wrap-Up – Gary Geernaert, Xujing, Renata, Cristiana, Dave, Ruby, Mark and Guang, Presentation-2 – Davis

APPENDIX C: POSTERS PRESENTED AT THE ESMD–E3SM PI MEETING

**See the PDF version of the document (https://Lead.me/bc6Ix1) to follow the links provided in the Links column.

	Presenter	Poster Title	Links**
1	Asay-Davis, Xylar	Designing Regionally Refined Ocean and Sea-ice Meshes for the E3SM v2 Cryosphere Science Campaign	Abstract-1 - Asay-Davis Poster-1 - Asay-Davis
2	Asay-Davis, Xylar	E3SM Ocean and Sea-Ice Diagnostics with MPAS-Analysis	Abstract-2 - Asay-Davis Poster-2 - Asay-Davis
3	Balaguru, Karthik	Analysis of Eastern Subtropical North Pacific SST Bias in the E3SM	Abstract - Balaguru Poster - Balaguru
4	Beydoun, Hassan	Quantifying the Response of Anvil Cloud Fraction to Sea Surface Warming in SCREAM-RCE	Abstract - Beydoun Poster - Beydoun
5	Bishnu, Siddhartha	A Suite of Verification Exercises for the Barotropic Solver of Ocean Models	Abstract - Bishnu Poster - Bishnu
6	Bisht, Gautam	Development of a Soil-Plant-Atmosphere Continuum Model With Support for Heterogenous Computing Architectures	Abstract - Bisht Poster - Bisht
7	Bogenschutz, Peter	Efficient Configurations: Single Column and Standalone Cloud-Resolving Models	Abstract - Bogenschutz Poster - Bogenschutz
8	Brunke, Michael	Attribution of E3SMv1's Snowpack Biases and Errors in Trends to Temperature and Precipitation over the Contiguous U.S.	Abstract - Brunke Poster - Brunke
9	Calandrini, Sara	A Modified TRiSK Scheme to Address Instabilities Found in MPAS-Ocean	Abstract - Calandrini Posters - Calandrini
10	Cameron-Smith, Philip	A Photolysis Scheme That Understands Clouds: Fast-J	Abstract - Cameron-Smith Poster - Cameron-Smith
11	Cao, Zhendong	Implementation of Turbulence and Sediment Transport Models in MPAS-Ocean	Abstract - Cao Poster - Cao
12	Capodaglio, Giacomo	Local Time-Stepping Schemes for Global to Coastal Simulations in MPAS-Ocean	Abstract - Capodaglio Poster - Capodaglio
13	Comeau, Darin	Preliminary Results Using Regionally Refined Ocean and Sea-Ice Meshes for the E3SM v2 Cryosphere Science Campaign	Abstract-1 - Comeau Poster-1 - Comeau

	Presenter	Poster Title	Links**
14	Comeau, Darin	Summary of the Cryosphere v1 Simulation Campaign Overview Manuscript	Abstract-2 - Comeau Poster-2 - Comeau
15	Drewniak, Beth	ELM-Crop in Coupled Model Framework	Abstract - Drewniak Poster - Drewniak
16	Eldred, Christopher	Progress Towards a New CRM for E3SM-MMF	Abstract - Eldred Poster - Eldred
17	Engwirda, Darren	'Unified' Ocean-Land-River Modelling Using Compatible Unstructured Meshes	Abstract - Engwirda Poster - Engwirda
18	Fan, Jiwen	Impact of a New Cloud Microphysics Scheme on Simulations of Mesoscale Convective Systems in E3SM Regionally Refined Model (RRM)	Abstract - Fan Poster - Fan
19	Fang, Yilin	Towards Mechanistic Unraveling of Plant Physiological Response to Increasing Vapor Pressure Deficit	Abstract - Fang Poster - Fang
20	Fang, Yuanhao	Improving the Representation of Lateral Flow in E3SM Land Model	Abstract - Fang Poster - Fang
21	Feng, Yan	Influence of High-Latitude Dust on Aerosol Concentrations and Deposition in the Arctic	Abstract - Feng Poster - Feng
22	Forsyth, Ryan	Zstash v0.4.2: HPSS Long-Term Archiving Tool	Abstract - Forsyth Poster - Forsyth
23	Chien, Rong-You	Verification of High-Efficiency Chemistry Numerical Solver in the Global Model Using E3SM	Abstract - Fu_Joshua Poster - Chien Video - Chien
24	Garanaik, Amrapalli	A New Eddy Diffusivity Parameterization for Ocean Models Using Assumed Distribution Higher-Order Closure (ADHOC)	Abstract - Garanaik Poster - Garanaik
25	Guba, Oksana	A Framework to Evaluate IMEX Schemes for Atmospheric Models	Abstract - Guba Poster - Guba
26	Hager, Alexander	Stable Channelized Subglacial Drainage Beneath Thwaites Glacier, West Antarctica	Abstract - Hager Poster - Hager
27	Hamilton, Douglas	Modeling the Ferrous Wheel (the Iron Cycle) and Anthropocene Changes in Ocean BGC	Abstract - Hamilton Poster - Hamilton
28	Harrop, Bryce	Evaluating the Water Cycle Over CONUS Using Multiple Metrics for the Energy Exascale Earth System Model (E3SM) Across Resolution	Abstract - Harrop Poster - Harrop
29	Hillebrand, Trevor	Retreat of Humboldt Glacier, North Greenland	Abstract - Hillebrand Poster - Hillebrand

	Presenter	Poster Title	Links**
30	Hoffman, Matthew	Sensitivity of Coupled Solid Earth - Ice Sheet Modeling of Thwaites Glacier to Earth Rheology and Coupling Timescale	Abstract - Hoffman Poster - Hoffman
31	Holder, Christopher	Using Neural Network Ensembles to Differentiate Biology and Physics in Earth system Models	Poster - Holder
32	Holm, Jennifer	ELM-FATES Progress Updates: Impacts of Modeling Global Vegetation Demography and Dynamic Plant Competition	Abstract - Holm Poster - Holm
33	Hunke, Elizabeth	CICE Consortium Progress and Plans	Abstract - Hunke Poster - Hunke PowerPoint w/ narration - Hunke
34	Jeffery, Nicole	A Key Role for DON Remineralization in Arctic Sea Ice	Abstract - Jeffery Poster - Jeffery
35	Johnson, Jeffrey	A High-Performance Modal Aerosol Dynamics Library Based on MAM	Abstract - Johnson Poster - Johnson
36	Kang, Hyun-Gyu	A Barotropic Mode Solver for MPAS-Ocean Using ForTrilinos	Abstract - Kang Poster - Kang
37	Kaul, Colleen	Liquid Cloud Testbed Simulations Using a Novel Large Eddy Simulation Capability	Abstract - Kaul Poster - Kaul
38	Ke, Ziming	Improving the E3SM Representation of the Stratospheric Aerosol Forcing Induced by Volcanic Eruptions	Abstract - Ke Poster - Ke
39	Larson, Vincent	Development of a New Subgrid PDF Shape for E3SM: Current Status	Abstract-1 - Larson Poster-1 - Larson
40	Larson, Vincent	Parameterization of Deep Convection in E3SM with Higher-Order Closure	Abstract-2 - Larson Poster-2 - Larson
41	Lee, Hsiang-He	A Novel Modeling Framework to Improve Stratocumulus by Increased Horizontal and Vertical Resolution	Abstract - Lee-HH Poster - Lee-HH
42	Li, Hongyi	MOSART-Urban: a Semi-Distributed Regional Urban Flood Modeling Framework	Abstract-1 - Li Poster-1 - Li
43	Li, Hongyi	MOSART-Lake: Development and Global Validation	Abstract-2 - Li Poster-2 - Li
44	Liao, Chang	A Hexagonal Mesh-Based Routing Method for Land Surface and Hydrologic Models	Abstract - Liao Poster - Liao
45	Lin, Guangxing	Improving the Prognostic Treatment of Cloud-borne Aerosols in E3SM	Abstract - Lin-G Poster - Lin-G

	Presenter	Poster Title	Links**
46	Lin, Wuyin	Evaluation of E3SMv1 Simulated Surface Winds Over the Southern Ocean and the Antarctica	Abstract – Lin-W Poster – Lin-W
47	Lee, Doo Young	Evaluation of Wintertime Pacific North America Teleconnection in E3SM	Abstract – Lee-DY Poster – Lee-DY
48	Liu, Weiran	Performance of Hydrostatic and Nonhydrostatic Dynamical Cores in a Forecast Diagnostic Package	Abstract – Liu-W Poster – Liu-W
49	Liu, Xiaohong	Improving Simulations of Biomass Burning Smoke and Anthropogenic Dust in E3SM	Abstract – Liu-X Poster – Liu-X
50	Mahajan, Salil	Machine Learning Approaches to Ensure Statistical Reproducibility of MPAS-O	Abstract – Mahajan Poster – Mahajan
51	Maltrud, Mathew	Development of Regionally Refined Ocean/Sea Ice Meshes for E3SMv2	Abstract – Maltrud Poster – Maltrud
52	Martin, Daniel	E3SM BISICLES Next Generation Development (NGD)	Abstract-1 – Martin Poster-1 – Martin
53	Martin, Daniel	Space-Time Adaptivity for Climate Models	Abstract-2 – Martin Poster-2 – Martin
54	Nadiga, Balu	Quantification of Non-Hydrostatic Effects and the Role of Vertical Resolution in HOMME	Abstract – Nadiga Poster – Nadiga
55	Petersen, Mark	MPAS-Ocean Testing and Verification	Abstract – Petersen Poster – Petersen
56	Pressel, Kyle	A Novel Python Based Large Eddy Simulation Capability Designed to Generate Training Data for Machine Learning of Microphysical Process Rates	Abstract – Pressel Poster – Pressel
57	Price, Stephen	Towards a Coupled Greenland Ice Sheet in E3SM	Abstract – Price Poster – Price
58	Qian, Yun	Using PPE Simulations and Parametric Sensitivity Analysis to Better Understand Cloud Physics and Parameterization in EAM Over Different Regions and Cloud Regimes	Abstract – Qian Poster – Qian
59	Reeves Eyre, Jack	Sensitivity of E3SM Energy and Water Cycles to Ocean Surface Flux Algorithm DesignValidation	Abstract – ReevesEyre Poster – ReevesEyre
60	Ren, Tong	Impact of Cloud Longwave Scattering on Radiative Fluxes Associated with the Madden-Julian Oscillation in the Indian Ocean and Maritime Continent	Abstract – Ren Poster – Ren
61	Ricciuto, Daniel	Quantifying Drivers of Uncertainty in Land Model Predictions at Global Scales Using Machine Learning	Abstract – Ricciuto Poster – Ricciuto

	Presenter	Poster Title	Links**
62	Riley, William	Impacts of Nitrogen and Phosphorus Co-Limitation on Global Carbon Cycling	Abstract - Riley Poster - Riley
63	Sargsyan, Khachik	Physics-informed Machine Learning for Uncertainty Quantification in E3SM Land Model	Abstract - Sargsyan Poster - Sargsyan
64	Schneider, Adam	Improving Snow Compaction and Firn Densification on E3SM's Ice Sheets	Abstract - Schneider Poster - Schneider
65	Shi, Xiaoying	Quantifying the Long-Term Changes of Land Water Availability and Their Driving Factors	Abstract - Shi Poster - Shi
66	Shpund, Jacob	Evaluation of the Predicted Particles Properties (P3) Microphysical Scheme in E3SM	Abstract - Shpund Poster - Shpund
67	Singh, Balwinder	Implementation and Testing of a Deep Neural Network Emulator for Aerosol Activation in E3SM	Abstract - Singh Poster - Singh
68	Sinha, Eva	Modeling Bioenergy Crops in ELM	Abstract - Sinha Poster - Sinha
69	Song, Xiaoliang	Implementing and Improving Convective Microphysics Parameterization in E3SMv1	Abstract - Song Poster - Song
70	Steyer, Andrew	Exponential Integrators for the HOMME-NH Nonhydrostatic Dycore	Abstract - Steyer Poster - Steyer
71	Sun, Xiaoming	Hydrostatic and Non-Hydrostatic Convective Self-Aggregation in E3SM	Abstract - Sun Poster - Sun
72	Tan, Zeli	Estimates of Global Erosional Sediment, Carbon, Nitrogen and Phosphorus Fluxes	Abstract - Tan Poster - Tan
73	Tang, Jinyun	Different Numerical Coupling Strategies Lead to Diverging Carbon-Nutrient Interactions	Abstract - Tang-J Poster - Tang-J
74	Tang, Qi	Evaluation of the Interactive Stratospheric Ozone (O3v2 Module) for the E3SM Version 2	Abstract-1 - Tang-Q Poster-1 - Tang-Q
75	Tang, Qi	Regionally Refined Model Updates for the E3SMv2 Atmosphere Model	Abstract-2 - Tang-Q Poster-2 - Tang-Q
76	Tang, Shuaiqi	Evaluating Ultrafine Aerosol Nucleation Mode in E3SM with In-Situ Aircraft Measurements at SGP and ENA	Abstract - Tang-S Poster - Tang-S
77	Terai, Christopher	Capabilities and Remaining Challenges for SCREAM Evaluation	Abstract - Terai Poster - Terai

	Presenter	Poster Title	Links**
78	Tesfa, Teklu	Impacts of New Atmospheric Forcing Downscaling Methods and Topography-Based Subgrid Structure on E3SM Simulations	Abstract - Tesfa Poster - Tesfa
79	Thornton, Peter	Climate-Carbon-Nutrient Feedbacks Under a Future Climate Change Scenario in the E3SM v1.1 Model with Coupled Biogeochemistry	Abstract - Thornton Poster - Thornton
80	Wang, Dali	Massively Parallel Ultra-Scale E3SM Land Model Development on Summit	Abstract - Wang Poster - Wang
81	Wolff, Zachary	Effects of Spectrally Varying Cryospheric Surface Emissivity on Atmospheric Longwave Radiation	Abstract - Wolff Poster - Wolff
82	Wu, Mingxuan	New Development and Evaluation of E3SM-MOSAIC: Spatial Distributions and Radiative Effects of Nitrate Aerosol	Abstract - Wu Poster - Wu
83	Xu, Donghui	Land River Two-Way Coupling Development in E3SM	Abstract - Xu Poster - Xu
84	Yoshida, Ryuji	A 2-D Framework for Accelerating the Development of Physics Schemes in High Resolution Global Modeling	Abstract - Yoshida Poster - Yoshida
85	Zhang, Chengzhu (Jill)	Introduction to E3SM Diagnostics Package (e3sm_diags v2)	Abstract - Zhang-C Poster - Zhang-C
86	Zhang, Kai	Effective Aerosol Forcing in E3SMv1 and E3SMv2 Candidates	Abstract-1 - Zhang-K Poster-1 - Zhang-K
87	Zhang, Kai	Improving the Representation of Ultra-fine Aerosols in the E3SM Atmosphere Model	Abstract-2 - Zhang-K Poster-2 - Zhang-K
88	Zhang, Tong	Ice Sheet Model Mesh-Resolution Dependence of Damage Advection and Calving	Abstract - Zhang-T Poster - Zhang-T
89	Zhou, Tian	New Features in E3SM V2 to Address Human Impacts on Extreme Hydrologic Events	Abstract-1 - Zhou Poster-1 - Zhou
90	Zhou, Tian	Simulating River Processes in a Coupled Earth System	Abstract-2 - Zhou Poster-2 - Zhou

APPENDIX D: GROUP PICTURE

More than 300 people registered for the meeting and approximately 200 attended each day. Participants were not required to turn on their cameras and some chose not to participate in the picture-taking sessions or missed them, so the group photo collage includes a subset of all attendees.


Luke Van Roekel
Marcus van Lier-Wal...
Michael Prather
Francois Primeau
Hailong Wang
Ziming Ke
Anand Gnanadesika...
Peter's iPad
Julian Grindeanu
Jennifer Holm
James Randerson
rjeffery
Kate Calvin
Mindo Choi
Xiaoming Xu
Mark Petersen
Hsiang-He Lee
Wuyin Lin
Elizabeth Hunke
Holly Davis
Joannes Westerink
Shu Wu
Wenshan Wang
Alice
Detelina Ivanova
Charlie Zender
Dalei Hao
Philip Cameron-Smit...
Vijay Mahadevan
Xylar Asay-Davis
Milena Veneziani
Mike Pritchard
Ask to Unmute
Carolyn Begeman
Kristin Barton
Shuaiqi Tang
Jerome Fast
Bill Gustafson
Liu, Xiaohong
Michael A Brunke
dwirasae
Zhengyu Liu
takamitsu3
Po-Lun Ma
Lu, Zheng
Adam Varble
Baylor Fox-Kemper
Brian K Arbic
dengwirda
Laure Zanna
SM PI MEETING

ABBREVIATIONS AND ACRONYMS

ADC .... Assumed Distribution Higher-Order Closure
ALCF .... Argonne Leadership Computing Facility
AMOC .... Atlantic meridional overturning circulation
AMWG .... Atmospheric Model Working Group
AMT .... Asynchronous Many-Task
AOD .... Aerosol Optical Depth
AR6 .... IPCC's Sixth Assessment Report (AR6)
ARM .... Atmospheric Radiation Measurement
ASCR .... Advanced Scientific Computing Research
ATS .... Advanced Terrestrial Simulator
AVG .... Adaptive Vertical Grid
BER .... Biological and Environmental Research, a DOE program
BFB .... Bit-For-Bit
BGC .... "BioGeochemical Cycles" if referring to the E3SM BGC Group and model; "Biogeochemistry" if using BGC in a more general scientific context.
CAM6 .... Community Atmosphere Model Version 6
CAMP .... Chemistry Across Multiple Phases
CANGA .... Coupling Approaches for Next Generation Architectures
CASCADE .... Calibrated And Systematic Characterization, Attribution, and Detection of Extremes
CATALYST .... Cooperative Agreement To Analyze variabiLity, change and predictabilitY in the earth SysTem
CCN .... Cloud Condensation Nuclei
CCS .... Case Control System
CEDR .... Communication Efficient Density Reconstructor
CEDS .... Community Emissions Data System
CERES-EBAF .... CERES Energy Balanced and Filled (EBAF) climate data
CESM .... Community Earth System Model
CFL .... Courant-Friedrichs-Lewy convergence condition in mathematics
cGANs .... Conditional Generative Adversarial Networks
CIME .... Common Infrastructure for Modeling the Earth
CLASP .... Coupling of Land Atmospheric Subgrid Parameterizations
CLM .... Community Land Model
CLUBB .... Cloud Layers Unified By Binormals
CMEC .... Coordinated Model Evaluation Capabilities
CMIP6 .... Coupled Model Intercomparison Project Phase 6
CMOR .... Climate Model Output Rewriter
CNP .... Carbon-Nitrogen-Phosphorus
COMPASS .... Coastal Observations, Mechanisms, and Predictions Across Systems and Scales
COSMO .... COnsortium for Small-scale MOdeling
COVID-19 .... COronaVIrus Disease 2019
CovidMIP .... COVID Model Intercomparison Project

CPTs.................................. **C**limate **P**rocess **T**eams
CPU.................................. **C**entral **P**rocessing **U**nit
CRM.................................. **C**loud **R**esolving **M**odel
CTL.................................. **C**on**t**ro**l** Simulation
DECK................................. **D**iagnostic, **E**valuation and **C**haracterization of **K**lima (DECK) experiments used in CMIP6
DEMSI............................... **D**iscrete **E**lement **M**odel for **S**ea **I**ce
DevOps.............................. Set of practices that combines software development (**Dev**) and IT operations (**Ops**)
DM.................................... **D**ata **M**anagement, a DOE activity within EESSD
DNN.................................. **D**eep **N**eural **N**etwork
DOE.................................. **D**epartment **o**f **E**nergy
DSLs................................. **D**omain-**S**pecific **L**anguage**s**
DYAMOND........................ **DY**namics of the **A**tmospheric general circulation **M**odeled **O**n **N**on-hydrostatic **D**omains
E3SM................................ **E**nergy **E**xascale **E**arth **S**ystem **M**odel
EAGLES............................. **E**nabling **A**erosol-cloud interactions at **GL**obal convection-permitting scal**ES**
EAM.................................. **E**3SM **A**tmosphere **M**odel
ECMWF............................. **E**uropean **C**entre for **M**edium-Range **W**eather **F**orecasts
ECP.................................. **E**xascale **C**omputing **P**roject
EDMF................................ **E**ddy-**D**iffusivity/**M**ass **F**lux
EESM................................. **E**arth and **E**nvironmental **S**ystem **M**odeling, a DOE program within EESSD
EESSD............................... **E**arth and **E**nvironmental **S**ystems **S**ciences **D**ivision of DOE
ELM.................................. **E**3SM **L**and **M**odel
ENSO................................ **E**l **N**iño-**S**outhern **O**scillation
ERA5................................. ERA5 reanalysis dataset
ESGF................................. **E**arth **S**ystem **G**rid **F**ederation
ESM.................................. **E**arth **S**ystem **M**odel
ESMD............................... **E**arth **S**ystem **M**odel **D**evelopment, a DOE program area within EESM
ESS-DIVE.......................... **E**nvironmental **S**ystems **S**cience **D**ata **I**nfrastructure for a **V**irtual **E**cosystem
FACE................................. **F**ree-**A**ir **C**arbon dioxide **E**nrichment
FAIR.................................. **F**indable, **A**ccessible, **I**nteroperable and **R**eusable
FATES............................... **F**unctionally **A**ssembled **T**errestrial **E**cosystem **S**imulator
FIVE.................................. **F**ramework for **I**mprovement by **V**ertical **E**nhancement
FLeCSI.............................. **FLe**xible **C**omputational **S**cience **I**nfrastructure
FOA.................................. **F**unding **O**pportunity **A**nnouncement
GANs................................ **G**enerative **A**dversarial **N**etwork**s**
GCAM............................... **G**lobal **C**hange **A**nalysis **M**odel
GCIMS.............................. **G**lobal **C**hange **I**ntersectoral **M**odeling **S**ystem
GEV.................................. **G**eneralized **E**xtreme **V**alue
GFDL................................ **G**eophysical **F**luid **D**ynamics **L**aboratory
GFED................................ **G**lobal **F**ire **E**missions **D**atabase
GHG.................................. **G**reen**h**ouse **G**as
GOTM............................... **G**eneral **O**cean **T**urbulence **M**odel
GPP.................................. **G**ross **P**rimary **P**roduction
GPU.................................. **G**raphics **P**rocessing **U**nit
HDF.................................. **H**ierarchical **D**ata **F**ormat
HiLAT-RASM.................... The **Hi**gh **L**atitude **A**pplication and **T**esting of Earth System Models (HiLAT) team is collaborating with the **R**egional **A**rctic **S**ystem **M**odel (RASM) project

HighResMIP .... **High Res**olution **M**odel **I**ntercomparison **P**roject
HPC .... **H**igh-**P**erformance **C**omputing
HPSS .... **H**igh **P**erformance **S**torage **S**ystems
HR .... **H**igh **R**esolution
HUC-2 .... **H**ydrologic **U**nit **C**ode **2**
HyperFACETS .... A Framework for Improving Analysis and Modeling of Earth System and Intersectoral Dynamics at Regional Scales
IC .... **I**nitial **C**onditions
ICESat2 .... **I**ce, **C**loud, and Land **E**levation **Sat**ellite-**2**
ICoM .... **I**ntegrated **Co**astal **M**odeling
IFS .... **I**ntegrated **F**orecasting **S**ystem, an ECMWF global numerical weather prediction model
IGSM .... **I**ntegrated **G**lobal **S**ystem **M**odeling
ILAMB/IOMB .... **I**nternational **La**nd **M**odel **B**enchmarking/**I**nternational **O**cean **M**odel **B**enchmarking
IM3 .... **I**ntegrated **M**ultisector, **M**ultiscale **M**odeling
INCITE .... **I**nnovative and **N**ovel **C**omputational **I**mpact on **T**heory and **E**xperiment
input4MIPs .... **Input**s for **M**odel **I**ntercomparison **P**roject**s**, specifically the boundary condition and forcing datasets for CMIP6
InteRFACE .... **Inter**disciplinary **R**esearch **f**or **A**rctic **C**oastal **E**nvironments
I/O .... **I**nput/**O**utput
IPCC .... **I**ntergovernmental **P**anel on **C**limate **C**hange
ISMs .... **I**ce **S**heet **M**odel**s**
ITCZ .... **I**nter**t**ropical **C**onvergence **Z**one
Kokkos .... A programming model in C++ for writing performance portable applications targeting all major HPC platforms.
KPP .... **K**-**P**rofile **P**arametrization
LAI .... **L**eaf **A**rea **I**ndex
LANL .... **L**os **A**lamos **N**ational **L**aboratory
LBNL .... **L**awrence **B**erkeley **N**ational **L**aboratory
LCF .... **L**eadership **C**omputing **F**acility
LES .... **L**arge **E**ddy **S**imulations
LLNL .... **L**awrence **L**ivermore **N**ational **L**aboratory
LR .... **L**ow **R**esolution
LW .... **L**ong**w**ave radiation
MALI .... **M**PAS-**A**lbany **L**and **I**ce model
MAM4 .... four-mode **M**odal **A**erosol **M**odule
MARBL .... **MAR**ine **B**iogeochemistry **L**ibrary
MATLAB .... A proprietary programming language and numeric computing environment
MCSP .... **M**ultiscale **C**oherent **S**tructure **P**arameterization
MG2 .... **M**orrison and **G**ettelman version **2** microphysics
MJO .... **M**adden-**J**ulian **O**scillation
MIP .... **M**odel **I**ntercomparison **P**roject
ML .... **M**achine **L**earning
MMF .... **M**ultiscale **M**odeling **F**ramework
MODIS .... **Mod**erate Resolution **I**maging **S**pectroradiometer (satellite imaging sensors)
MOSART .... **MO**del for **S**cale **A**daptive **R**iver **T**ransport
MOZART .... **M**odel for **OZ**one **A**nd **R**elated chemical **T**racers
MPAS-O .... **M**odel for **P**rediction **A**cross **S**cales-**O**cean

MPAS-SI........................ **M**odel for **P**rediction **A**cross **S**cales–**S**ea **I**ce
MPI .... **M**essage **P**assing **I**nterface
MSD................................ **M**ulti**S**ector **D**ynamics, a DOE program area within EESM
NCAR.............................. **N**ational **C**enter for **A**tmospheric **R**esearch
NCO .... **N**etCDF **O**perators tool
NERSC............................ **N**ational **E**nergy **R**esearch **S**cientific **C**omputing **C**enter
netCDF........................... **Net**work **C**ommon **D**ata **F**orm
NGD................................ **N**ext **G**eneration **D**evelopment (of the E3SM model)
NNs .... **N**eural **N**etwork**s**
obs4MIP.......................... **Obs**ervations for **M**odel **I**ntercomparisons **P**roject
OLCF.............................. **O**ak **R**idge **L**eadership **C**omputing **F**acility
OLR................................. **O**utgoing **L**ongwave **R**adiation
OpenMP .... **Open** **M**ulti–**P**rocessing (OpenMP) application processing interface (API)
ORNL.............................. **O**ak **R**idge **N**ational **L**aboratory
P3.................................... **P**redicted **P**article **P**roperties microphysics parameterization scheme
PACE............................... **P**erformance **A**nalytics for **C**omputational **E**xperiments
PBL .... **P**lanetary **B**oundary **L**ayer
PCHES............................ **P**rogram on **C**oupled **H**uman **E**arth **S**ystems
PCMDI............................ **P**rogram for **C**limate **M**odel **D**iagnosis & **I**ntercomparison
PDE................................. **P**artial **D**ifferential **E**quation
PDF .... **P**robability **D**ensity **F**unction
PETSc............................. **P**ortable **E**xtensible **T**oolkit for **Sc**ientific Computing
PI...................................... **P**rincipal **I**nvestigator
PIO2................................ **P**arallel **I**nput/**O**utput (I/O) library, version **2**
PMP................................ **P**CMDI **M**etrics **P**ackage
PNNL.............................. **P**acific **N**orthwest **N**ational **L**aboratory
PP..................................... **P**lane **P**arallel
PPE .... **P**hysics **Pe**rturbations
ProSPect .... **Pro**babilistic **S**ea Level **P**roj**ect**ions from Ice Sheet and Earth System Models
QBO .... **Q**uasi–**b**iennial **O**scillation
QG.................................... **Q**uasi–**g**eostrophic
ResNet........................... **Res**idual Convolutional Neural **Net**work
RGMA............................. **R**egional & **G**lobal **M**odel **A**nalysis, a DOE program area within EESM
ROM .... **R**educed **O**rder **M**odels
RRM................................ **R**egionally **R**efined **M**esh
RUBISCO........................ **R**educing **U**ncertainty in **B**iogeochemical **I**nteractions through **S**ynthesis and **Co**mputation
RVM................................ **R**elevance **V**ector **M**achine
SAM................................ **S**outhern **A**nnular **M**ode
SBR................................. **S**ubsurface **B**iogeochemical **R**esearch
SciDAC .... **Sci**entific **D**iscovery through **A**dvanced **C**omputing
SCORPIO......................... **S**oftware for **C**aching **O**utput and **R**eads for **P**arallel **I/O**
SCREAM .... **S**imple **C**loud–**R**esolving **E**3SM **A**tmosphere **M**odel
SFA .... **S**cientific **F**ocus **A**reas
SHOC.............................. **S**implified **H**igher–**O**rder **C**losure
SINDY............................. **S**parse **I**dentification of **N**onlinear **Dy**namics
SL .... **S**emi–**L**agrangian
SOA................................. **S**econdary **O**rganic **A**erosols
SORRM .... **S**outhern **O**cean **R**egionally **R**efined **M**esh

SPCAM .... **S**uper**p**arameterized **C**ommunity **A**tmosphere **M**odel
SSP .... **S**hared **S**ocioeconomic **P**athways forcing
SST.................................. **S**ea **S**urface **T**emperature
SW .... **S**hort**w**ave radiation
TECA................................ **T**oolkit for **E**xtreme **C**limate **A**nalysis
TDycore .... **T**errestrial **Dy**namical **Core**
TKE .... **T**urbulent **K**inetic **E**nergy
TOA................................. **T**op **o**f **A**tmosphere
UQ................................... **U**ncertainty **Q**uantification
UWIN–CM .... **U**nified **W**ave **IN**terface–**C**oupled **M**odel
VAE .... **V**ariational **A**uto**e**ncoder
WACCEM .... **Wa**ter **C**ycle and **C**limate **E**xtremes **M**odeling
WRF .... **W**eather **R**esearch and **F**orecasting model
WW3................................ **W**ave**W**atch**III**
ZM .... **Z**hang–**M**cFarlane convection parameterization scheme

For More Information

Earth and Environmental Systems Science Division (EESSD)

https://science.osti.gov/ber/Research/eessd

Gary Geernaert (Director of EESSD)

Earth System Model Development (ESMD)

https://climatemodeling.science.energy.gov/program/earth-system-model-development

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Energy Exascale Earth System Model (E3SM)

https://e3sm.org

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E3SM Code

https://github.com/E3SM-Project/E3SM

E3SM Data

https://e3sm.org/data/