E3SM Energy Exascale Earth System Model

E3SM: The Energy Exascale Earth System Model

Phase 2, 2018-2022

The Energy Exascale Earth System Model (E3SM, e3sm.org) is a coupled Earth system model (ESM) designed for use across a wide range of resolutions. Supported by the U.S. Department of Energy (DOE), it is tailored for energy-relevant research and runs efficiently on DOE high-performance computers.

E3SM Version 1 (E3SMv1) was released to the broader scientific community in April 2018, and E3SMv2 was tagged in September 2021. E3SM is an open-development project and is engaging a growing community of scientists.

E3SM PROJECT MISSION, GOAL, AND SCIENCE

E3SM's Mission is to reliably project decade-to-century-scale climate changes that could critically impact the U.S. energy sector. Current focus areas include changes in:

- Water availability for energy production;
- Extreme temperatures as influenced by biogeochemistry (via CO_2), with impacts on the power grid;
- Energy resource potentials for hydropower, wind, solar, and bioenergy; and
- Sea-level rise from melting ice sheets that threatens coastal energy infrastructure.

To provide actionable science, E3SM features:

- Multi-resolution capabilities and improved process representations to enhance model fidelity and representation;
- Representations of human-Earth interactions to support scenario-based modeling; and
- Ensemble modeling to quantify simulation and projection uncertainties.

E3SM Science is organized around three science drivers with simulation campaigns focused on water cycle, biogeochemistry, and cryosphere research. Each campaign employs unique model configurations optimized to address the associated research challenges by varying their choice of biogeochemical species, use of variable-resolution meshes, and targeted sensitivity experiments.

As a fully-coupled ESM, E3SM integrates models of the atmosphere (EAM), land (ELM), river (MOSART), ocean (MPAS-O), sea ice (MPAS-SI), and land ice (MALI). The development of E3SMv1, along with aspects of model evaluation and applications, has been documented in 50 peer-reviewed papers in an American Geophysical Union (AGU) Special Collection.

E3SM PHASE 2 ACTIVITIES

During Phase 2 (2018-2022), major parallel efforts have been devoted to:

- Evaluating and analyzing simulations from the E3SMv1 simulation campaigns;
- Developing E3SMv2 to address v2 science questions; and
- Developing new capabilities for integration in E3SM v3 and v4.

Evaluation and Analysis of E3SMv1 Simulations

Water Cycle

As part of the water cycle simulation campaign, E3SMv1 has been used to produce CMIP6 DECK simulations and subsets of the ScenarioMIP and DAMIP simulations at "low resolution" (also called "standard resolution," 100 km for atmosphere and land and 30-60 km for ocean and sea-ice) and HighResMIP simulations at "high resolution" (25 km for atmosphere and land and 6-18 km for ocean and sea ice). The simulations have been evaluated using a wide range of water-cycle metrics, with a focus on water availability in

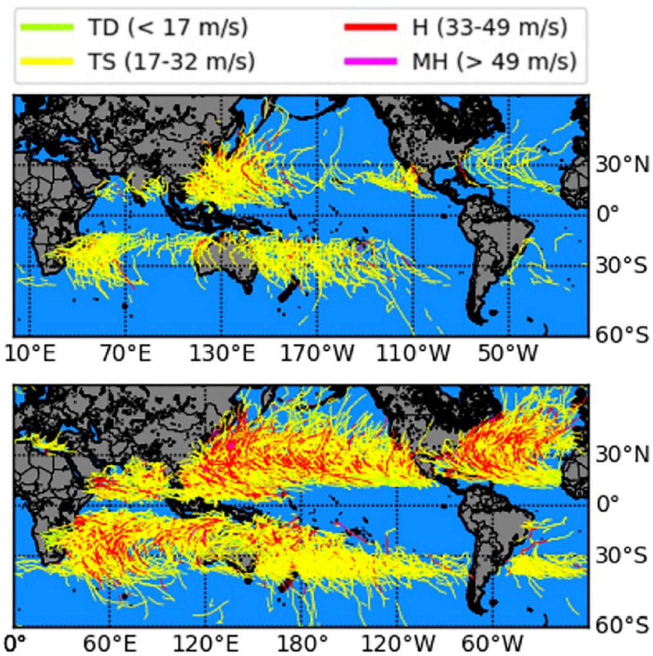

Figure 1: Global distribution of tropical cyclone tracks simulated by E3SMv1 at low (top) and high (bottom) resolution color-coded based on the along-track intensity for tropical depression (TD), tropical storm (TS), hurricane (H), and major hurricane (MH). (Caldwell et al., 2019). At high resolution, E3SMv1 simulates more hurricanes and major hurricanes, which compares better to observations.

river basins across the contiguous U.S. The all-forcing and single-forcing experiments and low- and high-resolution simulations have been analyzed to address the v1 water cycle science questions of the drivers of past and future water cycle changes and the impact of model resolution on simulating water-cycle processes (Figure 1), respectively.

Biogeochemistry

Including representations of biogeochemistry, E3SMv1.1 has been used to produce CMIP6 DECK simulations and a subset of the C4MIP simulations at "standard resolution" (Figure 2). Featuring two approaches to model nutrients in the land component, analysis has been performed to address the v1 biogeochemistry science question of the contribution of structural uncertainty in modeling nutrient limitations to uncertainty in carbon-climate feedbacks. Simulations that include only the radiative effect and only the plant physiological effect of CO_2 have been compared to understand their relative contributions to Earth system changes.

Cryosphere

With a new and unique capability to model ocean-ice shelf interactions, E3SMv1.2 is being further developed to address the largest remaining uncertainty in projections of future sea-level rise, the contribution from Antarctic ice sheet mass loss. E3SMv1.2 simulations at "standard resolution" demonstrate stable, realistic Antarctic sub-ice shelf melt fluxes over century-length timescales that are within the range inferred from observations. Simulations with and without explicit representation of ocean-ice shelf interactions have been used to address the v1 cryosphere science question, i.e., the impacts of ocean-ice shelf interactions on Antarctic ice sheet melt rates and Southern Ocean water-mass properties.

The E3SMv1 and E3SMv1.1 DECK simulations have been used in the Intergovernmental Panel on Climate Change (IPCC) AR6 WGI report. Standard model outputs from the simulations discussed above are available on the Earth System Grid Federation (ESGF).

Development of E3SMv2

Building on E3SMv1, version 2 of E3SM has been developed with a focus on improving modeling skill and computational performance. The former has been achieved through improvements in and better tuning of physics parameterizations for processes such as clouds and convection. Additionally, E3SMv2 features a new nonhydrostatic atmospheric dynamical core for high-resolution modeling.

Improvements in computational performance have been achieved by using a faster tracer transport scheme and using different grids for atmospheric physics and dynamics

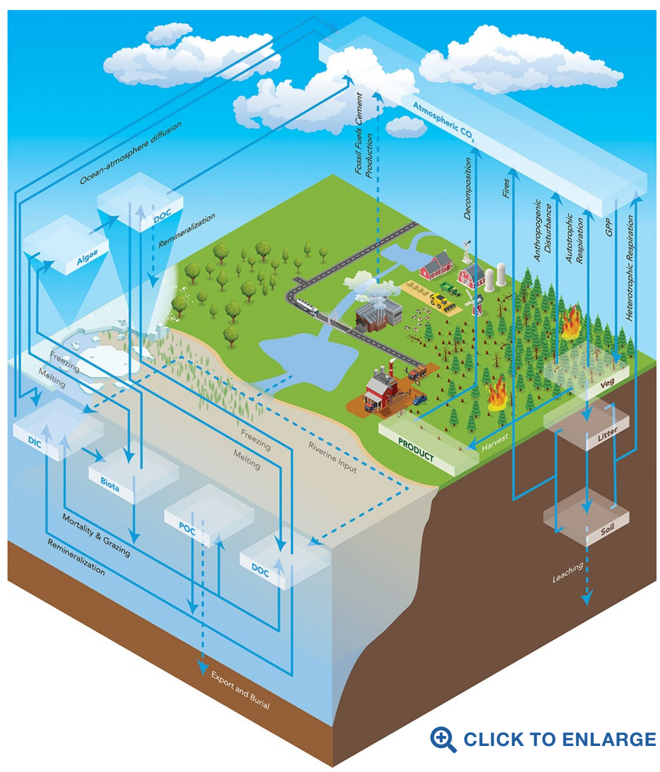

Figure 2: Global carbon cycle in the E3SMv1.1-BGC model, with major carbon pools (boxes) and fluxes (arrows). Dashed lines indicate fluxes that are either prescribed inputs to model carbon pools or losses which are not tracked further in the model. (Burrows et al., 2020).

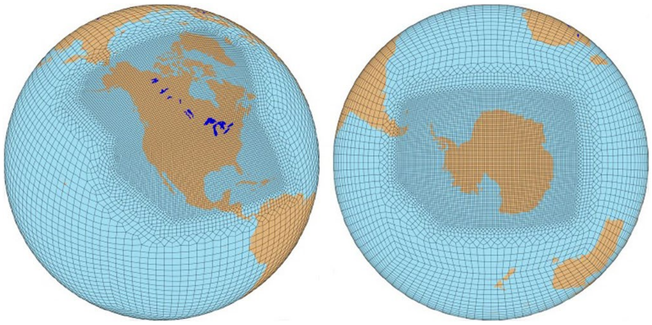

Figure 3: Regionally-refined meshes (RRMs) with high resolution over North America (left) and Antarctica (right) and their surrounding oceans. The number of grids in these RRMs is ~1/6 the number of grids in a global high-resolution mesh, making RRMs more computationally affordable for high-resolution modeling in regions of interest.

calculations. Notable improvements of E3SMv2 include reducing the global precipitation bias by ~20%, with larger reductions in regions such as the Amazon, and doubling the computational throughput compared to E3SMv1.

Two regionally-refined meshes (RRMs) with high resolution over North America and Antarctica have been tested to support the v2 water cycle and cryosphere simulation campaigns, respectively (Figure 3). These configurations offer significant computational savings compared to global high-resolution simulations, while improving the simulations within the RRM, such as improved Gulf Stream strength in the North America RRM (Figure 4) and more realistic sub-ice-shelf melt rates in the Antarctica RRM (Figure 5).

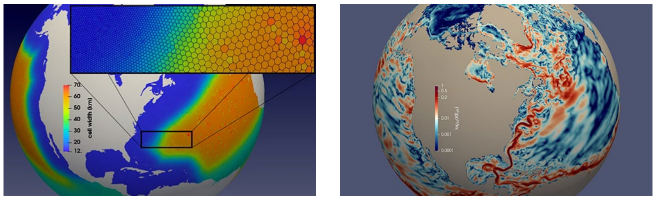

Figure 4: With resolution increasing from 60 km (orange) in the open ocean to 14 km (cobalt) near the coast (left), the strength and separation of Gulf Stream that meanders along the east coast of North America and the Loop Current in the Gulf of Mexico are well simulated in the North America RRM (right).

Biogeochemistry in E3SMv2 features several new developments, such as the capability to simulate CO_2 concentration in a prognostic mode, representing water use and management, coupling of E3SM with the Global Change Analysis Model (GCAM) to represent human-Earth interactions, and incorporating the Marine Biogeochemistry Library (MARBL), a modular framework for representing biogeochemistry, into MPAS-O.

Infrastructure (Figure 6) surrounding E3SMv2 has many improvements over v1, including: a shorter and simplified run_e3sm script for one-command model use, more features in the CIME Case Control System for tracking and controlling simulations, new diagnostics in E3SM's

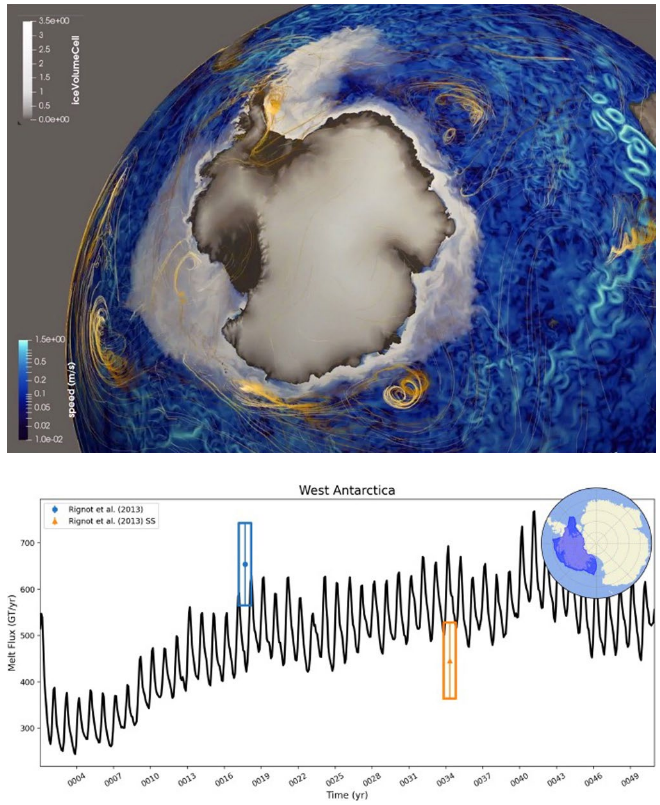

Figure 5: Top: Atmospheric winds (warm-colored streamlines), ocean eddies (cool background colors), and sea ice concentration (grey/white) over Antarctica and the Southern Ocean in a simulation using the Antarctica RRM. Bottom: At high resolution, sub-ice shelf melt rates in West Antarctica are realistically simulated (blue and orange bars indicate the range supported by observations), showing variability at multiple timescales.

main analysis packages (MPAS-Analysis and E3SM Diagnostics), new and improved tools for managing output (zstash and E3SM_cmip), a website for exploring performance data from simulations (PACE), a workflow tool zppy that exploits the E3SM analysis environment (E3SM Unified), and speedup and automation of all common post-processing and analysis tasks for E3SM simulations.

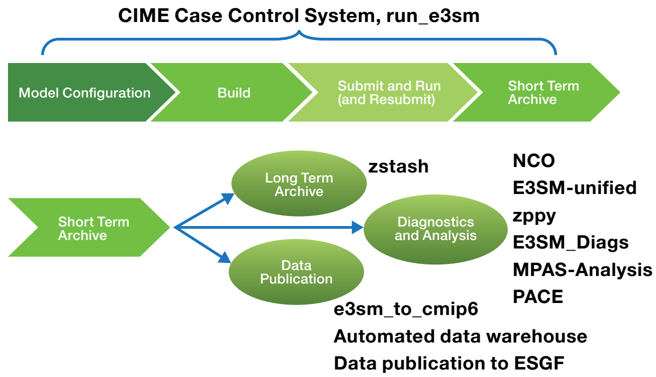

Figure 6: E3SMv2 includes better infrastructure support for every phase of model development.

For comparison with E3SMv1, version 2 is being used to perform CMIP6 DECK simulations, which will also be used in combination with simulations designed for the v2 simulation campaign to address the v2 science questions:

- *Water Cycle:* What are the relative impacts of global climate forcing versus regional effects of human activities on flood and drought risk in North America?
- *Biogeochemistry:* What are the implications of different energy futures for the biogeochemical cycle through changes in land use and land cover, water availability, and extreme events?
- *Cryosphere:* How will the atmosphere, ocean, and sea ice systems mediate sources of sea-level rise from the Antarctic ice sheet over the next 30 years?

Next-Generation Development for E3SMv3/v4

The E3SM project aims for future model generations with major innovations in both model processes and computational performance and a much higher resolution (e.g., 3-km resolution for the global atmosphere and even higher resolution regionally using RRMs).

Long-term scientific goals include the ability to more accurately capture the statistics of extreme weather events, coastal features such as biogeochemical changes and inundation due to storm surge and sea-level changes, the projection of land-use and land-cover changes based on socio-economic pathways, dynamic ice sheets as coupled Earth system model components, and decadal trends in sea ice.

In support of these goals, new approaches and capabilities to model aerosols and chemistry, radiation, convection, boundary-layer turbulence, and cloud microphysics are under development. These efforts have already yielded improvements in simulating the probability distribution of rain rates, tropical waves, ozone, and other aspects of atmospheric simulations.

The nonhydrostatic atmospheric dynamical core in E3SMv2 enables ultra-high-resolution modeling to better simulate clouds and convection. Combined with physics parameterizations tested for ultra-high resolution, the **Simple Cloud-Resolving EAM (SCREAM)** has been used to perform global simulations at 3-km grid spacing (Figure 7), for participation in the **DYAMOND** Initiative on the intercomparison of global storm-resolving models.

The SCREAM model is being rewritten from Fortran to the C++ language. Using the Kokkos C++ library, the C++ code can run efficiently on both CPU and GPU machines. The C++ version of the nonhydrostatic atmospheric dynamical core used in SCREAM **achieves excellent throughput** at 3 km grid spacing on the Summit GPU architectures. The C++ implementation outperforms the original Fortran implementation on conventional CPU architectures, achieving performance portability.

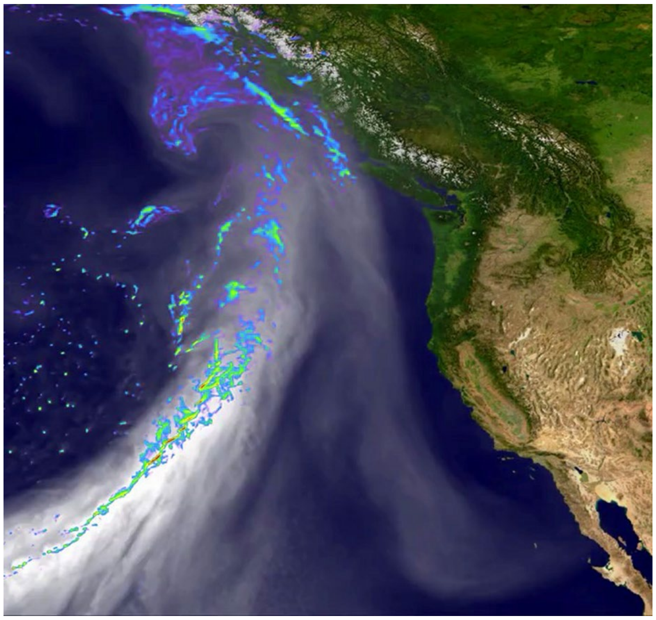

Figure 7: An atmospheric river in a SCREAM global simulation at 3 km grid spacing. Gray shading is column water vapor, and colors are precipitation. Atmospheric rivers are responsible for most of the flooding events in the U.S. West Coast.

The SCREAM model provides the foundation for future versions of E3SM for multi-resolution applications ranging from the “standard resolution” to coupling of a cloud-resolving atmosphere and an eddy-resolving ocean.

The land and biogeochemistry treatments are being improved to represent lateral subsurface water flows, more realistic vegetation, and terrestrial-aquatic processes. Human energy and agricultural management practices, as well as unmanaged fire disturbances, are being incorporated in ELM-MOSART. Massively parallel ELM runs at 1-km grid spacing over North America have been demonstrated on GPU machines.

Ocean and cryosphere advances being developed include the addition of a wave model (Figure 8) and other coastal processes, two-way coupling of dynamic, variable, and adaptive mesh ice-sheet models, and the coupling of critical new ice-sheet model physics to climate processes. New approaches to model mesoscale and sub-mesoscale eddies are being investigated. Passive tracer supercycling has improved computational efficiency for modeling ocean biogeochemistry.

Software and algorithm development have focused on improving the computational performance of the semi-Lagrangian transport scheme and the ocean barotropic and baroclinic solvers. Surrogate construction for automating the tuning of E3SM is being explored to support model calibration and uncertainty quantification.

E3SM PROJECT ECOSYSTEM AND CODE

The E3SM core project involves coordination among more than 100 scientists from eight DOE national laboratories and a number of universities. E3SM is also being developed and used broadly across university and laboratory investigators supported by various non-E3SM DOE programs. Model computational work is also performed by projects that receive Advanced Scientific Computing Research (ASCR) support, including the SciDAC BER-ASCR partnership projects and ASCR's Exascale Computing Initiative.

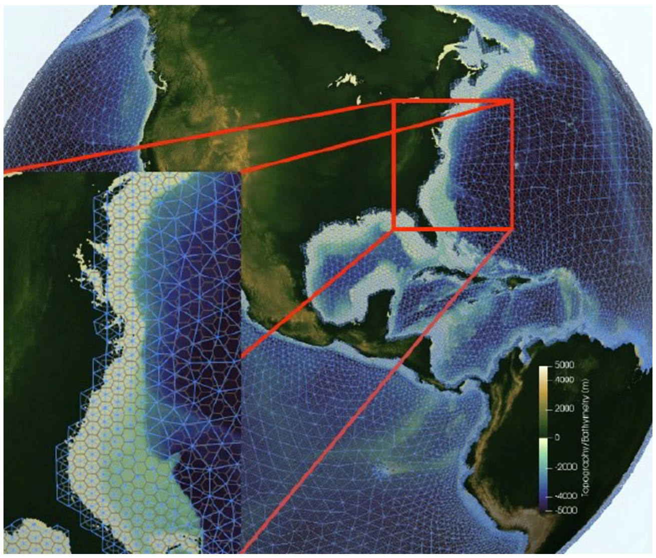

Figure 8: A new, unstructured wave modeling mesh capability for Wavewatch III, developed by E3SM. A new algorithm has also been developed to ensure perfect overlap of the ocean and wave meshes near the coast (inset) to ensure accurate transmission of fluxes between components.

PROJECT SUPPORT

The E3SM project is sponsored by the Earth System Model Development program area of the Earth and Environmental Systems Modeling Program within the Earth and Environmental Systems Sciences Division under DOE's Office of Science Biological and Environmental Research (BER). The project maintains important collaborations with other BER and ASCR activities.

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E3SM information, code, simulation configurations, model output, and tools to work with the output are available at:
https://e3sm.org

Model code may be accessed on the GitHub repository at:
https://github.com/E3SM-Project/E3SM

Model output data are accessible through the DOE Earth System Grid Federation at:
https://esgf-node.llnl.gov/projects/e3sm

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