E3SM-v2-v3-plans_Nov2017

Plans for E3SM-v2.0 and v3 developments

The features listed in this document are under active E3SM development or planning.

Coupled E3SM simulations with v2

The focus of v2 will be on infrastructure and computational performance improvements, bug-fixes, etc. The major scientific activity will be around a set of simulations with regional refinement over North America, extending up into the boreal and permafrost regions.

Atmosphere v2-v3 Plans

Developments Already Started:

1. An Elevation Class decomposition will be used for each column of the atmosphere and land model to diagnose the vertical displacement of air parcels flowing through the grid cell. Energy and moisture conservation produces an orographic tendency for model state variables, influenced by differing vertical displacements for each elevation class. Physical parameterization produce tendencies for a subcolumn characterizing each elevation class. The different elevation classes also affect snow-cover and water flow at the surface.
2. Improve the treatment of secondary organic aerosols, brown carbon, and nitrate aerosols (aerosol components that are crudely treated or missing in the current model).
3. Introduction of a simple reactive photochemistry, appropriate for improved aerosol representations and a first treatment of Methane chemistry.
4. Continuing improvements to the internal consistency between convection, clouds, and aerosols
5. Changes in numerical methods in the model to
   - better treat the pressure gradient term in the vicinity of orography
   - reduce time discretization errors in physics parameterizations

Under consideration:

1. Other convection and turbulence parameterizations will be considered
2. Revisions to the surface flux calculations may occur to improve consistency with the turbulence treatment, and to account for processes that are currently neglected (e.g. surface gustiness, and sub-grid inhomogeneities in surface properties)
3. The SciDAC developed non-hydrostatic dycore may be integrated into E3SM to allow the model to be used in v3 at higher horizontal resolution, especially for regionally refined configurations. It retains most aspects of the current hydrostatic dycore: spectral elements

and finite differences, terrain following hybrid pressure coordinate with new prognostic equations for potential temperature, geopotential height and vertical velocity.
4. Alternate vertical coordinates are being considered to reduce computational artifacts associated with the current hybrid pressure, eta coordinate system.
5. We hope to improve the integration of atmospheric processes with other model components, particularly
    - exchange of biogeochemical components between the ocean and cryosphere
6. Improve existing diagnostics, and develop new ones.
7. The DOE BER ECP project is developing a configuration of E3SM that uses a multiscale modeling framework (MMF) with GPU acceleration of the SAM CRM as a superparameterization. This configuration may be available in 2020 and may be considered by E3SM for v3.

Land v2-v3 Plans

We have developments planned in several areas for v2 and v3:

1. We will develop the ability to use high-resolution watershed delineation with topographically defined sub-watershed units.
2. For hydrology and thermal processes, several developments are planned, including
    a. introducing or improving representation of inundation, water management, and runoff generation;
    b. stream temperature, riverine sediment and nutrient transport;
    c. coupling soil, root, and plant hydrology
    d. variably saturated flow models (VSFM and PFLOTRAN)
    e. a framework to account for lateral subsurface exchanges and processes (e.g., water and tracer transport)
    f. topographic effects on surface radiation
    g. Variable soil depth coupled with soil hydrology and root
3. For biogeochemistry and vegetation process modeling, we are planning to develop or enhance
    a. coupled C, N, and P dynamics and improvements to plant-microbe nutrient competition
    b. wetland hydrology and biogeochemistry, including CH4 improvements
    c. explicit microbial processes for C and nutrient cycling
    d. vegetation carbon and nutrient storage, transport, allocation, and root, leaf, and other plant traits
    e. multi-phase, multi-substrate, and multi-consumer vertically-resolved reactive transport (BeTR and PFLOTRAN)
    f. nitrification, denitrification, fixation, and leaching representations
    g. Dynamic vegetation using FATES
4. We are planning several developments in the crop model, including
    a. improved plant date trigger and growing season length
    b. additional crop types
    c. improved fertilizer application
5. For Land Use and Land Cover developments, we will
    a. develop improved historical LU/LCC drivers and mechanisms
    b. include future LU/LCC driven by a human component
6. For uncertainty quantification and benchmarking, we will continue to develop and apply the V1 UQ and benchmarking (ILAMB) frameworks.

Ocean Model v2-v3 Plans

1. Isopycnal-like vertical coordinates (adiabatic interior) that tracks the bottom of the ocean mixed layer (diabatic surface).
2. Turbulent eddy kinetic energy mesoscale closure (from SciDAC multi scale)
3. High order transport (from SciDAC LEAP)
4. Thin walls approach for bottom bathymetry
5. Extend into coastal ocean dynamics (tides, non-hydrostatic, wetting/drying)

* Here and below, indicates development that will take place within or in conjunction with SciDAC 4 projects (2017-2022)

Sea Ice Model v2-v3 Plans

1. Snow-on-sea-ice model
2. Icebergs in MPAS-CICE
3. Coupling of icebergs to land ice model (via calving)

4. Unified ridging and form drag (work with Andrew Roberts/RASM)
5. MPAS-CICE Sea-ice buoy simulator (Use the LIGHT framework infrastructure to build a sea-ice buoy simulator in MPAS-CICE)
6. A new Discrete Element Method sea ice model *
7. Radiation in CICE (optionally) handled by (extended) SNICAR

Land Ice Model v2-v3 Plans

1. Improved calving schemes *
2. Improved ice sheet spin-up / initialization techniques *
3. Update heat balance code to use enthalpy formulation
4. Subglacial hydrology model(s) for Greenland and Antarctica *
5. Basal processes models, improved basal "sliding" models, and necessary optimization capabilities to initialize these *

Ocean-ice Biogeochemistry v2-v3 Plans

1. Couple marine biogenic aerosol emissions to CAM, with influence on sea spray plus surfactant effects on sea-air gas transfer
2. Sediment BGC module necessary for the iron cycle, acidification/carbon cycling and benthic denitrification
3. Extend ecosystem complexity to allow adaptation to future climate, including explicit bacteria groups, variable stoichiometry for different autotrophs, and multiple zooplankton groups
4. Extend ecodynamics/chemistry schemes to unify soil, river, coastal and open ocean environments
5. Iron and colloidal chemistry interacting with macromolecular organics in both ocean and sea ice
6. Sea ice model: inorganic carbon chemistry for a fully coupled carbon cycle simulation, includes full gas exchange with the atmosphere

Ice / Ocean Coupling V2-V3 Plans

1. Change coupling to correctly account for salt transfer between ocean and sea-ice without using a salinity reference
2. Finish development / testing of wetting-drying for land ice / ocean coupling *
3. Dynamic land, ocean, sea-ice masks to allow for evolving calving front *
4. New / updated iceberg treatment (consistent with evolving calving front in land ice and sea ice models)
5. Gravitationally consistent SLR model and sea-level coupled to ice sheet evolution (i.e., ice sheet "sees" spatially and time varying sea-level and responds dynamically) *

Performance v2-v3 Plans

1. GPU acceleration (likely OpenACC) enabled in major components
2. Threading of MPAS-CICE
3. Threading and vectorization optimized for Intel Phi (many-core) architectures
4. Atmospheric superparameterization (SAM) implemented on GPUs
5. New transport schemes optimal for large tracer counts
6. Evaluation, prototyping and potential implementation of new programming models and infrastructure (e.g. Kokkos data structures and parallel abstractions, Legion task-parallel model) for exascale

Workflow v2-v3 Plans

1. Data Management
    a. ESGF: provenance capture for publication; publish climatologies and diagnostic outputs.
    b. netCDF4 compression/chunking to reduce data size/accelerate access time
2. Diagnostics, Analysis and Metrics
    a. Additional diagnostics and enhanced provenance capture reproducibility.
    b. Improved and additional graphics display options.
    c. Geometrically exact regridding to/from rectangular grids
3. Provenance Capture
    a. Deploy provenance database to capture all workflow componenent execution details.
4. Processflow
    a. CIME integration and verification.
    b. Automated data archive
    c. Automated creation and publication of diagnostic and evaluation output
    d. Automated publication to ESGF
5. Dashboard/UI
    a. Integration of all workflow components, including diagnostics, viewer, provenance, processflow integration, ESGF publication and model simulation.

Software Engineering and Coupler v2-v3 Plans

1. System for adding and running unit tests for all components. Code coverage measurements.
2. New, faster, more standard build system, including support for mixed Fortran and C++.
3. New, faster more flexible coupler with online interpolation and dynamic load balancing.
4. Greater support for runtime configuration of cases.
5. Climate reproducibility testing, statistical techniques for distinguishing between roundoff level and true climate altering changes.
6. Improved code design across all of E3SM – modularity, data structures, code reuse, code standards.
7. Expand verification practice and evidence: correctness, convergence order verification.
8. Support for in-situ analysis.
9. Faster and more scalable data models
10. Continuous improvement:
    a. Expand test coverage so no bug or loss of functionality slips through twice
    b. Expand functionality of case and test scripts to meet user's needs
    c. Take opportunities to improve the code development and integration process and documentation
    d. Improve rigor and speed of processes of dealing with failed tests and changed test baselines