Present and Future Computing Requirements for IMPACTS and CLIMES
(Investigation of Magnitudes and Probabilities of Abrupt Climate Transitions)
(Center at LBNL for Integrative Modeling of the Earth System)

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NERSC BER Requirements for 2017
September 11-12, 2012
Rockville, MD
1. Project Description

**IMPACTS PI:** William Collins

**IMPACTS leads:** William Riley (boreal), Philip Cameron-Smith (clathrates), William Lipscomb/Steve Price (land ice), and Ruby Leung (droughts)

- Scientific objectives of IMPACTS
  - **Project the risk of abrupt climate change over the 21st Century**
    - Disintegration of marine ice sheets
    - Melting permafrost leading to releases of CO2 and CH4
    - Destabilization of methane deposits in Arctic-circle oceans
    - Large-scale megadroughts in North America
  
- Enhance global models of these rapid climate transitions
1. Project Description (cont.)

**CLIMES PI:** William Collins

**CLIMES leads:** David Romps (fast physics), William Collins (extreme/local change), William Riley and Jeffrey Chambers (terrestrial Earth systems)

• **Scientific objectives of CLIMES**

  • **Advance simulations of climate forcing, response, and feedback:**
    - *Ultra high-resolution global climate simulation*
    - *Frameworks for robust regional climate modeling*
    - *Quantification of critical uncertainties in the carbon cycle*
    - *Representation of clouds, aerosols, and the cryosphere in climate models*

  • **Advance projections of climate mitigation measures:**
    - *Improved representations of human-Earth system interactions*
    - *Integrated assessment model development, intercomparison, and diagnostics*
Contributions to CESM Science and Capabilities

**Radiation:**
- LBNL led the integration of the ASR-funded RRTMG radiation parameterizations into the DOE-NSF CESM.
- RRTMG is included in the public release of CESM.

**iESM:**
- LBNL led the integration of the BER-funded GCAM IA model into the DOE-NSF CESM.
- LBNL has shared this capability with iESM ST.

**Abrupt Climate Change:**
- LBNL led the integration of the 1D TOUGH+ model for ocean hydrates into the DOE-NSF CESM.
- LBNL heads the development of terrestrial CH4 cycle with treatments of permafrost, thermokarst, peat, etc.
1. Project Description (cont.)

- **Our present focus in IMPACTs is to perform:**
  - 1\textsuperscript{st} coupled projections of Earth’s methane cycle
  - 1\textsuperscript{st} sea-level rise projections including Antarctica
  - Simulations of the future of western forests
Dynamics of Antarctica and Sea-Level Rise

**IMPACTS: Investigation of the Magnitudes and Probabilities of Abrupt Climate TransitionS**
Implementation of Land-Ice/Ocean Interface in POP

**Objectives:**
- Projections of sea-level rise due to Antarctic and Greenland ice sheets
- Examine abrupt climate feedbacks related to land-ice/ocean interactions

**Implementation:**
- Adding *dynamic* land-ice/ocean interface to POP
  - partial cells
  - immersed boundaries
- Developed efficient algorithms for representing turbulent ocean boundary layers under ice shelves

**Experiments:**
- Underway: expts. with fixed, idealized geometries for model comparison
- Next: expts. with fixed, realistic geometries for data comparison

*IMPACTS: Investigation of the Magnitudes and Probabilities of Abrupt Climate TransitionS*
Atmospheric Impact of Methane Clathrate Emissions

**Objective:**
- Study the impact of methane clathrate emissions on the atmosphere.

**Implementation:**
- Implemented Fast Methane Chemistry in CESM1_0_beta14, using CAM4 physics and RRTMG radiation.

**Simulation Experiments:**
- **Control Case:** CESM, full ocean, fast methane chemistry, 2 degree resolution.
- **Arctic Methane Emission Case:** Simulating Arctic Methane Emission (22% increase),
  - Impacts CH₄, T, rainfall, air-quality.
- **Uniform Methane Emission Case:** 22% increase in emissions spread uniformly,
  - Impacts depend on emission location.

**Methane Increase from Arctic Clathrates**
- (a) 100 year zonal mean
- (b) 20 year zonal mean
- (c) 20 year Uniform Emission Case

**Change in Surface Air Temperature**
- 100-year difference between Arctic methane emission & control cases

*IMPACTS: Investigation of the Magnitudes and Probabilities of Abrupt Climate TransitionS*
Inclusion of a Terrestrial CH$_4$ Model into CESM1 (CLM4Me)

Objectives:
• Identify uncertainties
• Predict 21$^{\text{st}}$ century CH$_4$ emissions
• Quantify potential for abrupt feedbacks.

Implementation:
• Vertically resolved biochemical model
• 2 reactions and 3 transport processes
• Implementation designed to integrate with future land model improvements.

Experiments:
• Compared present CH$_4$ emissions to 15 sites and 3 atmospheric inversions.
• Identified critical uncertain parameters
• Showed declines in high-latitude inundation may limit 21$^{\text{st}}$ century increases in emissions
• Developing subgrid peatland ecosystem model

Comparison of CH$_4$ emissions from CLM4Me and several atmospheric inversions.

RCP 4.5 emissions from vegetated ecosystems without old soil carbon source.

**IMPACTS: Investigation of the Magnitudes and Probabilities of Abrupt Climate TransitionS**
Belowground Carbon Processes

**Objectives:**
- Represent processes responsible for growth and loss of permafrost C, which is a large (>1000 Pg) and vulnerable fraction of the terrestrial C pool.

**Implementation:**
- Developed vertically-resolved belowground biogeochemistry, mixing.
- Improved SOM dynamics, growth of Permafrost C pools.
- Improved N cycle at high latitudes leads to better productivity.

**Experiments and Next Steps:**
- Equilibrium experiments, sensitivity to parameters and model structure.
- Next Steps: Future scenarios; Coupling between soil and wetland biogeochemistry; coupled soil BGC and soil physics.

*IMPACTS: Investigation of the Magnitudes and Probabilities of Abrupt Climate TransitionS*
The Role of Surface Water – Groundwater Interactions on Long Term Droughts

Objectives:
- Study the role of surface water – groundwater interactions on long term droughts

Implementation:
- Implemented the VIC runoff and groundwater parameterizations to CLM4
- CLM4 has been coupled to WRF using the CCSM flux coupler

Experiments and Results:
- CLM4VIC-ground has been applied to flux tower sites for comparison with CLM4 and CLM4VIC and showed improvements in simulating seasonal soil moisture
- WRF-CLM has been configured for the US using a new global 0.05° CLM input data
- WRF-CLM simulates realistic precipitation and surface temperature in North America
- WRF-CLM will be used to perform numerical experiments to study the role of surface water – groundwater interactions on long term droughts

Comparison of CLM4, CLM4VIC, and CLM4VIC-ground at Tonzi, CA

IMPACTS: Investigation of the Magnitudes and Probabilities of Abrupt Climate TransitionS
Impacts of Great Basin Dust on North American Summer Monsoon Precipitation

Objectives:
- Study the impacts of dust on North American summer monsoon precipitation

Implementation:
- WRF-Chem is used to conduct numerical experiments using the modal MADE/SORGAM scheme coupled with the GOCART dust emission scheme

Experiments and Results:
- Simulations were performed for April – September of 1995 – 2009 at 36km resolution with and w/o dust
- The simulated dust concentration and AOD compare well with observations
- Dust from the Great Basin induces surface cooling of 1 W/m² and atmospheric heating of 0.4 W/m²
- Dust heating of 0.3 K/day in the lower atmosphere strengthens the low-level meridional winds, leading to a 10-40% increase in NAM precipitation

IMPACTS: Investigation of the Magnitudes and Probabilities of Abrupt Climate TransitionS
1. Project Description (cont.)

• Our present focus in CLIMES is to create:
  – New and more robust simulations of climate extremes
  – Enhanced models of regional moisture and precipitation
  – Better representations of carbon-cycle processes
  – First coupled energy-climate models with 2-way interactions
Reactive transport modeling-CLM4BeTR

Objectives:
• Uniform implementation of vertically-resolved underground biogeochemistry
• Multiphase description of C-Nutrient dynamics, gaseous, aqueous, sorbet

Implementation:
• Operator splitting approach
• Two-layer bi-directional modeling of atmosphere-surface exchange for different tracers, e.g. NH₃, N₂O, CH₄
• Evaluation against analytical results (successful) and measurement data

Experiments and :
• Tested single-point simulation of N₂O, CO₂ transport with vertically resolved C and N biogeochemistry
• Test the functionality of isotope fractionation and merge with CLM4Me
iESM Schematic

Integrated Earth System Model

Details of Land Use/Land Cover Change Downscaling

- Prognostic Land Use Classes from GCAM
  - Forests: managed & unmanaged
  - Food and Fiber: 9 types
  - Bioenergy: 2 types (grass & poplar)
  - Pasture: Non-Arable

- Land Use Transitions (GLM Optimization Scheme)
  - Primary vegetation
  - Secondary forests
  - Crops (food, fiber, fuel)
  - Pasture

- CLM Plant Functional Type Transition Matrix

Sea Ice
Ocean
Atmosphere
iESM Coupling:
Emulation of Sneaker-net Coupling

Status:
• We emulate sneaker-net using 15-year timesteps.
1. Project Description (cont.)

- By 2017 we expect to:
  - Develop probabilistic risks of abrupt climate change
  - Conduct local and regional projections of extreme rainfall
  - Simulate the CO₂/CH₄/N₂O feedbacks in a warmer climate
  - Develop more integrated scenarios for climate mitigation
1. Project Description (cont.)

- **Performance enhancement to support developments**
  - SLR: >10X for high-resolution land-ice / ocean models
  - Extremes: 10 to 30X for superparameterized models
  - Chemistry: 10X for reactive chemistry and transport
  - Scenarios: 10 to 100X for scenario development
2. Computational Strategies

• We climate simulation computationally using models that solve the Euler equations, constituent equations, and 1\textsuperscript{st} of thermodynamics for ocean, atmosphere, and ice.

• The primary code we use is the DOE-NSF joint Community Earth System Model (CESM):
  \url{http://www.cesm.ucar.edu/}

• Distinctive features of simulations:
  \begin{itemize}
  \item \textit{Duration}: Centuries to millennia
  \item \textit{Time steps}: Minutes (atmosphere) to hours (ocean)
  \item \textit{Experiments}: Response to time-evolving boundary conditions
  \item \textit{Metrics}: Non-deterministic statistics of the solutions
  \end{itemize}
2. Computational Strategies (cont.)

• **CESM is comprised of 4 (now 5) components and a coupler:**
  - Atmosphere: (200 x 288 x 30 = 1.7e6)
  - Ocean: (180 x 360 x 40 x 0.7 = 1.8e6)
  - Sea & land ice (= ocean/land grids)
  - Land (200 x 288 x 10 x 0.3 = 1.7e5)

• **The dynamical frameworks are / are evolving to:**
  - Atmosphere: Spectral element dycore on cubed sphere (SNL)
  - Ocean: Unstructured mesh/Voronoï tessellation (LANL)

• **Implementation of parallelism:**
  - Choice of MPI, OpenMP, MPI/OpenMP hybrid throughout.
  - Components run in arbitrary mix of serial and parallel processor layouts.
  - Parallel NetCDF for I/O.
2. Computational Strategies (cont.)

• **Our biggest computational challenges are:**
  - Ensemble sizes required for uncertainty quantification (1000s)
  - 100x increase in throughput required for cloud/eddy-resolving models
  - Barrier to long-time integrations from flat trends in clock rates

• **Current implementations exhibit scaling to \(O(10^5)\) processors:**
  - CESM scales to 30K Cray / 60K Blue Gene cores (*Dennis et al, 2012*)
  - Spectral element dycore scales to 256K processors (*Taylor et al, 2011*)

• **Major changes anticipated / contemplated by 2017:**
  - GPU implementation of CESM components (underway for OLCF Titan)
  - New atmospheric/ocean dycores: focus on refinement, scalability
  - Implementation of stochastic parameterizations in atmosphere/ocean
  - AMR techniques for land ice
3. Current HPC Usage (see slide notes)

- **Machines currently running CESM:**
  - Major Facilities: NERSC, NCCS / OLCF, ALCF, NCSA, NCAR
  - Architectures: Cray XE/XT, IBM Power Series, IBM Blue Gene, Linux cluster

- **Hours used in 2012:**
  - IMPACTS/CLIMES: XX / YY M Core-hours
  - Other users: O(XXX) Core-hours at NCCS, ~40M for IPCC, ~140M @ NCAR

- **Typical parallel concurrency and run time, number of runs per year:**
  - Timing data: [http://www.cesm.ucar.edu/models/cesm1.0/timing/](http://www.cesm.ucar.edu/models/cesm1.0/timing/)
  - Hopper cores: 2064 (for 1-degree resolution)
  - Hopper core-hours: 2063 core-hours per year of simulation
  - Hopper throughput: 24.01 simulation years per wall clock day
  - Number of years/year: 4000 to 10000 simulation years / calendar year
3. Current HPC Usage (see slide notes)

- **Data read/written per run and data resources used**
  - In IPCC AR5 production runs, 56.2 GB/sim. month and 675 GB/sim. Year
  - Storage system: HPSS, 3.46M SRUs = 725 TB

- **Memory used per (node | core | globally)**
  - 135 GB (1850 carbon/nitrogen compset, (Intel Benchmark, for HPC Advisory Council)

- **Necessary software, services or infrastructure**
  - UNIX like operating system (LINUX, AIX, OSX)
  - csh, sh, perl, and xml scripting languages
  - subversion client version 1.6.11 or greater
  - Fortran 90 and C compilers. pgi, intel, and xlf are recommended options.
  - MPI (although CESM does not absolutely require it for running on one processor only)
  - netcdf 3.6.2 or greater
  - Earth System Modeling Framework (ESMF) (optional) 5.2.0p1
  - pnetcdf (optional) 1.1.1 or newer
4. HPC Requirements for 2017
(Key point is to directly link NERSC requirements to science goals)

- **Compute hours needed (in units of Hopper hours)**
  - 2012 ERCAP request = 11.9M (CLIMES) + 26.3M (IMPACTS) = 38.2M
  - Estimate for 2017 = (8/2) * 38.2M = 150M

- **Changes to parallel concurrency, run time, number of runs per year**
  - Parallelism : 2K -> 20K processors per integration
  - In principle, 100K processors per integration feasible

- **Changes to data read/written**
  - Data per sim. Year = $8^{(2/3)} \times 56\text{Gb/sim. year} = 200\text{ GB/sim. Year}$
  - Total volume = $4 \times 725\text{TB/calendar year} = 3\text{ PB / calendar year}$

- **Changes to memory needed per ( core | node | globally )**
  - Memory required = $4 \times 135\text{ GB} = 540\text{ GB for entire simulation}$
5. Strategies for New Architectures

• Our strategy for many-core architectures is collaboration with FASTMATH and SUPER Institutes via SciDAC climate apps:
  – Transport and advection (led by ORNL)
  – Land ice (LANL)
  – Multiscale physics and integration w/new dycores (LBNL)

• To date we have prepared for many core by implementing capabilities for arbitrary hybrid MPI / OpenMP parallelism and end-to-end MPMD architecture.

• The CESM project is committed to porting to MIC machines, including the TACC Stampede machine based on Knights Corner.
5. Summary

• What new science results might be afforded by improvements in NERSC computing hardware, software and services?
  • Better understanding of land-ice dynamics of Antarctica and implications for SLR
  • Exploratory studies of multiscale climate dynamics from cloud/eddy to global scales
  • Model/data fusion for studies of the carbon cycle and carbon-climate feedbacks
  • Linking robust national energy strategies to needed advances in climate science

• Recommendations on NERSC architecture, system configuration and the associated service requirements needed for your science
  • “Leading without bleeding” procurement strategy of NERSC works well for our apps, since we can leverage substantial DOE and NSF investments in performance portability.
5. Summary

• NERSC generally refreshes systems to provide on average a 2X performance increase every year. What significant scientific progress could you achieve over the next 5 years with access to 32X your current NERSC allocation?
  • Advances towards global eddy-resolving projections of sea-level rise
  • Initial exploration non-hydrostatic cloud-system-resolving climate models
  • Development of regional-to-global carbon/water/climate analyses of the Earth system
  • Integrated climate/energy scenarios for the Sixth IPCC report and national assessments

• What "expanded HPC resources" are important for your project?
  • Integration of provenance tracking throughout software / project / data cycles.
  • “Rendering engines” (hardware and/or MPP software) for exabyte data sets
  • Multi-terabyte/second networks to key partners including LCFs, NCAR, etc.