PROGRESS REPORT 2008

A Scalable and Extensible Earth System Model for Climate Change Science otherwise known as the SciDAC2 CCSM Consortium Project

Department of Energy Office of Biological and Environmental Research Scientific Discovery through Advanced Computing Scientific Application of the Climate Change Prediction Program (Dr. Anjuli Bamzai, program manager)



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1 Introduction[†]

This project employs multi-disciplinary teams to accelerate development of the Community Climate System Model (CCSM), based at the National Center for Atmospheric Research (NCAR). A consortium of eight Department of Energy (DOE) National Laboratories collaborate with NCAR and the NASA Global Modeling and Assimilation Office (GMAO). The laboratories are Argonne (ANL), Brookhaven (BNL) Los Alamos (LANL), Lawrence Berkeley (LBNL), Lawrence Livermore (LLNL), Oak Ridge (ORNL), Pacific Northwest (PNNL) and Sandia (SNL). The work plan focuses on scalablity for petascale computation and extensibility to a more comprehensive earth system model. Our stated goal is to support the DOE mission in climate change research by helping ...

To determine the range of possible climate changes over the 21st century and beyond through simulations using a more accurate climate system model that includes the full range of human and natural climate feedbacks with increased realism and spatial resolution.

Over the five years of the project, we endeavor to support this goal through four integrated areas:

- 1. Extend the capabilities of the Community Climate System Model (CCSM) to include representations of biological, ecological, chemical, and aerosol processes that will allow scientists and policy-makers to simulate climate and climate change using a comprehensive Earth system model,
- 2. Provide the necessary software and modeling expertise to rapidly integrate new methods and model improvements,
- 3. Pursue the development and evaluation of innovative methods in the coupled context of the CCSM, and
- 4. Improve the performance, portability and scalability of the CCSM on available and future computing architectures for use in national and international assessments of climate change.

Key objectives are to develop, integrate and evaluate the CCSM (through comparison with observed data), enhance the performance of the CCSM, making it the leading comprehensive earth system model on scalable computer architectures. Our management plan defines roles and responsibilities to assure that our work remains coordinated, focused, and compatible with the objectives of the CCSM Scientific Steering Committee, while supporting the DOE Climate Change Prediction Program (CCPP).

As part of the DOE Scientific Discovery through Advanced Computing (SciDAC) program, the "CCSM Consortium" (or the SEESM) works collectively with applicable parts of the whole SciDAC infrastructure development efforts, namely the Centers for Enabling Technologies (CETs) the Scientific Application Projects (SAPs), and SciDAC Institutes. This project acts as a focal point for collaborations with related efforts

[†] A complete list of acronyms is given in Appendix A.

sponsored by other agencies, such as the NASA Earth System Modeling Framework (ESMF), NASA Carbon Assimilation projects within the GMAO at Goddard Space Flight Center, and NOAA atmospheric model development projects at the Geophysical Fluid Dynamics Laboratory (GFDL). The project also has a collaborative relationship with the DOE Climate Change Research Division programs. As part of the Climate Change Prediction Program we work with researchers from the DOE Atmospheric Science Program (ASP), the Atmospheric Radiation Measurement (ARM) and the DOE Terrestrial Carbon Program (TCP).

2 Objectives

The approach of the SciDAC2 CCSM Consortium project is to work in collaboration with NCAR to develop and maintain the CCSM as a state-of-the-art climate model optimized for performance, portability, and climate change science application on a range of parallel computer architectures. The project seeks to facilitate the CCSM's use to gain the best possible scientific understanding of climate variability and global change on decadal to century time scales. This project works to implement scalable algorithms and conform to modern software engineering practices and modular, open development of each component of the CCSM and of the coupled system as an Earth System Model. Efficient parallel execution for high-throughput climate simulations at multiple resolutions will be achieved through flexible model configurations and optimized utilities and algorithm libraries. The completeness of the model will also be extended through the development of new physical parameterizations, with particular focus on the global carbon cycle and terrestrial land and ocean ecological processes and atmospheric chemistry and aerosol coupling with climate. Ocean and cryosphere model developments are integrated with the CCSM and evaluated in the coupled context through close collaboration with the LANL Center for Ocean and Ice Modeling (COSIM). With collaborative links to the DOE Climate Change Research Divisions programs in Aerosol Science (ASP) and Terrestrial Carbon (TCP) we seek to advance the capability of the CCSM in conjunction with the latest developments in process modeling and with the benefit of DOE's extensive measurement campaigns in the Atmospheric Radiation Measurement (ARM) program.

3 Summary of Accomplishments

This past year (2008) has been marked by intensive, ongoing model development work in preparation for the CCSM4 model science freeze in October 2008 and in preparation for a model release for use in the IPCC AR5 work of 2009 and 2010. Of course, ongoing scientific research from this project may be included in CCSM5. Two of the major additions, indirect aerosols and a land ice sheet model, represent important milestones for this project and for higher fidelity in modeling the earth's climate.

3.1 Coupled Model Developments

Under SEESM, coupled model development efforts have targeted the creation of a new coupling architecture that permits extensive code reuse among CCSM components and eliminates the need for existing separate stand-alone drivers. The resulting design now permits CCSM to run on new low memory, massively parallel peta-scale hardware, smaller Linux clusters and even single laptop computers. As a result, a single coupling architecture is now used in an end-to-end model development cycle, from running single processor single-column calculations to developing new model parameterizations to running high-resolution eddy-resolving simulations on thousands of cores. The resulting model system is now easier to debug and port and has greater flexibility in achieving optimal efficiency and performance for specific resolutions, component configurations and target architectures.

SEESM efforts have also targeted the continual porting, performance evaluation and performance optimization of the model system as it has evolved towards the creation of CCSM4. Finally, SEESM contributions have been critical to the creation and resulting simulations of a high resolution eddy-resolving CCSM.

3.1.1 Evaluating the Interim Model CCSM3.5

A decadal climate projection between 1980 and 2030 using a nominal 0.5deg resolution in the atmosphere and land components has been performed using the Community Climate System Model, version 3.5. The mean climate is compared to a companion simulation using a nominal 2deg resolution in the atmosphere and land components. The increased atmosphere resolution has several benefits, and produces a significantly better mean climate. The maximum sea surface temperature biases in the major upwelling regions, including the West Coast of the USA, are reduced by about 60%. There are improved precipitation patterns over North America, mostly due to the better resolved orography, and this leads to better river flows in several North American rivers. There are also improvements in the summer Asian monsoon and eastern tropical Pacific precipitation. The atmospheric circulation in the Arctic also improves, which leads to a better regional sea ice thickness distribution in the Arctic Ocean.

The figure in the highlight shows the difference between the sea surface temperature (SST) in the two runs and a climatology (Levitus et al. 1998)¹ and PHC data in the Arctic (Steele et al. 2001)². It shows the SST bias for the 2deg run, which is very typical of errors found in previous CCSM runs. The largest positive SST errors of more than 6deg C are in the three major upwelling regions off the west coasts of North and South America and off Southern Africa. The bottom panel from the 0.5deg run shows that the SST errors in the upwelling regions are very significantly reduced. They are reduced by

 ¹Levitus, S., T. Boyer, M. Conkwright, D. Johnson, T. O'Brien, J. Antonov, C. Stephens, and R. Gelfeld, 1998: Introduction, Vol 1, World Ocean Database 1998, NOAA Atlas NESDIS 18, 346pp.
 ²Steele, M., R. Morley, and W. Ermold, 2001: PHC: A global ocean hydrography with a high-quality Arctic Ocean. J. Climate, 12, 2079--2087.

about 60% off North and South America, and the area of biases larger than 2deg C is very significantly reduced in all three upwelling regions. The globally-averaged SST bias in the 0.5deg run is now very small when compared to the observations.

The 0.5deg atmospheric resolution resolves orography much better, and this helps to produce stronger surface winds in the upwelling regions that are better aligned along the coasts. This immediately increases the coastal upwelling, which reduces the SST. The colder SST and surface atmospheric temperature allows more stratus clouds to form,

which shield the sunlight reaching the ocean, which further reduces the SST. Thus, the positive feedbacks between the ocean and atmosphere that led to the large positive SST errors are strongly alleviated in the 0.5deg run. The CCSM project has spent much effort in trying to reduce these upwelling region SST biases in previous model versions by changing atmosphere and ocean parameterizations. This has never worked satisfactorily, and the only known way to reduce these biases is to use much finer resolution in the atmosphere.

The highlight figure also shows there are large SST errors in the North Atlantic, where the path of the Gulf Stream is too far south, and in the region of the Kuroshio separation, which is too far north off Japan. In the 0.5deg run, shown in Fig 1b, the error in the North Atlantic remains, but the Kuroshio separation is improved and the SST bias reduced significantly, again probably due to improved atmospheric winds. The SST improvements in the 0.5deg run are reflected in reduced temperature biases over the upper ocean down to about 400 m. Below that depth, the biases are comparable in the two runs.



Highlight: Two different atmospheric model resolutions are being supported in CCSM4, a 2 degree and a 0.5 degree. The graphic shows the difference between the SST in a) 2deg run, and b) 0.5deg run and observations Improvements are seen especially in coastal upwelling regions.

Reference: Gent, P, S. Yeager, R. Neale, S. Levis, D. Bailey, Improvements in a Half Degree Atmosphere/Land Version of the CCSM, in preparation.

3.1.2 A New Coupler for CCSM4: Coupler 7

The coupler developed under the previous SciDAC, CCSM3/cpl6, was a significant improvement over earlier couplers but still lacked some desired features³. The multiple-program configuration of CCSM3 and its routing through the cpl6 main driver limited the options for load balancing the model, and the coupler's main driver and the software layers of cpl6 were seen by end-users as too complex to modify. Under SEESM, we have contributed extensively to the development of an entirely new coupler architecture called cpl7 that addresses these limitations. This project built on work performed towards the end of the last SciDAC, namely the clean separation of initialization and runtime methods within each component of CCSM and construction of a prototype sequential execution system using "dead" models.

The new coupling architecture extensively utilizes MCT datatypes⁴ and functionality and consists of three main categories of software. The first is a driver that calls the initialization and run methods of the component models and all coupler functions. The second is the collection of modules for coupler-specific functions such as regridding, atmosphere/ocean flux calculations, merging and diagnostics. The final category is a translation layer that converts data between MCT and internal model datatypes. The translation layer sits between the initialize and run calls in the driver and the model's implementation of those routines. The separation of driver datatypes and code from model datatypes and code and the isolation of the driver code at the top of the software stack of the entire model also makes it easier to try different coupling software packages or frameworks by re-implementing the driver, interface and coupler layers using those of the new package.

Another significant feature of cpl7 is the capability to utilize processor/model configurations that were not provided by the CCSM3/cpl6 architecture. The new CCSM4/cpl7 system is a single executable system that provides new flexibility in running model components sequentially, concurrently, or in a mixed sequential/concurrent mode. The cpl7 driver runs on all the processors of a model simulation and controls the time sequencing, processor concurrency, and exchange of boundary data between components. In the cpl7 architecture all model components can run on subsets of the driver processors and the component processor layouts can be determined at run time from simple user editable files. This design permits the model system to have significant flexibility in setting up an appropriate component layout in order to achieve optimal performance and efficiency for a specific model simulation. In particular, component layouts are now



³Craig, A.P., R. Jacob, B. Kauffman, T. Bettge, J. Larson, E. Ong, C.Ding, Y. He, "CPL6: The New Extensible, High Performance Parallel Coupler for the Community Climate System Model", IJHPCA Vol. 19, No. 3, pp. 309-327, 2005

⁴Larson, J. R. Jacob, E. Ong, "The Model Coupling Toolkit: A New Fortran90 Toolkit for Building Multiphysics Parallel Coupled Models,", IJHPCA, Vol 19, No. 3, pp. 277-291, 2005

supported where all components run concurrently on non-overlapping processor sets, where all components run sequentially on the same processor set or where components run in a hybrid sequential/concurrent layout. Furthermore, the new design guarantees that the results of a given simulation are bit-for-bit regardless of the component processor layouts chosen.

The design of the cpl7 architecture also provided several other improvements to the cpl6 system. The elimination of several datatypes that existed in the cpl7 design, such as the "contract" and "bundle" has produced a more easily modifiable architecture. In addition, exposing fundamental MCT datatypes such as AttributeVector and Router at high levels in the code allows for the data and control flow within the driver to be more easily followed and limited the amount of new code that needed to be developed, thus enhancing maintainability

Important new functionality has also recently been incorporated into cpl7. First, the cpl7 architecture now supports the ability to run the atmosphere and land on different grids and is being used to carry out the first set of non-aqua planet simulations where CAM-HOMME is on a cubed sphere grid, CLM is on a regular latitude/longitude grid and the ocean and ice are on identical displaced pole grids. Secondly, the new land ice component has been added to the coupling infrastructure thereby permitting the GLIMMER land-ice model to couple into the system.

The new coupler has been validated and will be used in upcoming production runs of CCSM4 and included in the public release of CCSM4.

3.1.3 Software Engineering for CCSM4

An important aspect of the software engineering activity is the porting, maintenance, and periodic performance evaluation of the evolving code base. In this capacity, SEESM works closely with the CCSM software engineers at NCAR (CSEG), members of the CCSM Software Engineering Working Group (SEWG), and the CCSM component model developers. We also work closely with the Scalability SAP described in section 3.4.1.

This activity is tied closely to the target platforms, currently the IBM BG/P and the Cray XT4 and XT5 available at the major DOE computing centers at Oak Ridge National Laboratory, Lawrence Berkeley National Laboratory and Argonne National Laboratory. Major activities within the past 2.5 years include the following:

1 Characterization of the computer system performance, including evaluation of the numerical and performance impacts of the many compiler and MPI environment variable options, and development of algorithmic workarounds when existing approaches are not efficient on a given platform. Examples of the latter are the development of an SMP-aware version of the *allreduce* collective and latency-hid-ing implementations of the halo update for use in the POP ocean model.

- 2 Building on the flow-control algorithms developed within the scalability SAP to implement collective algorithms that do not fail when large numbers of processes are sending to one or to a small number.
- Platform-specific debugging. For example, significant resources were expended 3 identifying an MPI library bug that occurred approximately once every 3 wallclock hours in CCSM runs. (This issue has since been resolved by the vendor.)
- Benchmarking configuration options, to 4 understand the performance impact of fications that are being proposed for inclusion in the model (see side-bar highlight).
- 5 Continuing development and maintenance of the timing library used to document model performance. (This library is built on top of the GPTL timing library, created and maintained by Jim Rosinski, now at ORNL)
- 6 Continuing development and maintenance of the Model Coupling Toolkit used in the new coupler, cpl7. There have been three major releases of MCT under

These data were from April, 2008, and so do not SEESM, 2.3, 2.4, and 2.5. The improve-necessarily represent performance of the most recent versions of CAM. ments included performance enhance-

ments that both lowered the memory cost and increased the communication efficiency of critical functions and new functionality to support cpl7, including the ability to use unordered *GlobalSegmentMaps* and new options for using MCT-World and Accumulator. The mpi-serial replacement library incorporates more of the MPI library and is a key technology for supporting serial and "laptop" configurations of CCSM.

3.1.4 High Resolution Configurations of CCSM

We have made a variety of important contributions to enable the effective operation of CCSM at high resolution. A number of these have been under the Scalability SAP and are discussed in section 3.4.1. Here we discuss one of the most important requirements for

Highlight: Performance results for CAM show the increasing cost of including more vertical levels (C1-C6), the new processes and other code modi- a new radiation package (C0r), a number of new formulations of physical processes (C2-C5), and full tropospheric chemistry (C6). Data shown were collected on a Cray XT4 with quad-core nodes, but similar data were also collected on the IBM BG/P.



very high resolution – parallel I/O. We additionally report on a SciDAC-enabled ultrahigh-resolution CCSM simulation that is currently in progress.

3.1.3.1 Parallel I/O

The typical I/O paradigm throughout CCSM has been for the master task of each component to handle all interactions with disk. Increases in resolution, model complexity and processing speed coupled with the trend of decreasing memory per processor (e.g., BG/L) make this paradigm non-viable – not only because of the time required to accomplish the I/O, but also because of the memory required to hold the data. We have developed a parallel I/O capability (PIO) and started deploying it through the most critical parts of CCSM. This has been a community-wide effort with extensive contributions from both within and outside of SciDAC. Starting with the original design by John Dennis, SciDAC has had primary responsibility for the development of the PIO software and accompanying test suite, with deployment in the atmosphere and ocean components having significant non-SciDAC contribution (from both Jim Edwards and John Dennis). The PIO software has already enabled calculations that otherwise could not have gone forward (aqua planet CAM calculations with HOMME dycore on BG/L, modal aerosol CAM calculations at high resolution on ORNL Jaguar) and is critical to the future of CCSM, particularly on the emerging multi-core architectures. Further information is provided in section 3.4.1 (Scalability SAP).

3.1.3.2 Ultra-high-resolution coupled climate simulation⁵

An ultra-high-resolution coupled climate simulation using CCSM4/cpl7 is being carried out on the LLNL Atlas (Opteron/Infiniband) machine. This is the first simulation of its kind carried out in the US and was undertaken as a collaborative effort involving contributions from DOE/SciDAC, LLNL and NCAR. The atmosphere is at 0.25-deg resolution and the ocean uses a 0.1-deg tripole grid. Particular benefits of such a calculation include realistic simulation of strong, narrow mean currents and of mesoscale eddies, which affect not only ocean heat transport but also atmospheric circulation (e.g., storm tracks), and more accurate depiction of air-sea feedbacks resulting from explicit resolution of a greater range of scales. The calculation has run for 11 years using 4048 processors. We find more realistic energy levels and position of ocean currents and are also able to simulate the cold wake in the ocean sea surface temperature following a typhoon. The accompanying figure shows the computed variability of the sea surface height (bottom), which shows excellent agreement with satellite observations (top). This calculation would not have been possible without model improvements brought about through SciDAC contribution and the collaboration of research staff in the SciDAC CCSM Consortium.

⁵This non-SciDAC funded work. Computer time on Lawrence Livermore National Laboratory's Atlas machine was provided under LLNL's Multiprogrammatic and Institutional Computing Initiative.



The computed variability of the sea surface height (bottom), shows excellent agreement with satellite observations (top)

3.2 Atmospheric Chemistry and Aerosols

3.2.1 Fast Chemistry for Climate Change Modeling

In response to the needs of the CCSM community for the next IPCC simulations and other long climate simulations, we have developed, implemented, and validated fast chemical mechanisms that retain the most important chemical interactions and responses for climate simulations. In particular, we have just developed a super-fast mechanism that solves a reduced set of chemical ODE equations for troposphere only, while for the stratosphere, we have connected our super-fast chemistry to a linearized ozone capability

(Linoz), which was developed by M. Prather (UC Irvine) and implemented in CAM by Jean-Francois Lamarque. This capability provides the minimum needed to study the variability in methane lifetime, along with interactive ozone and sulfate aerosols with a cost of only 40% increase in CAM computational cost (including computational performance improvements by Mirin and Worley, q.v. section 3.4.1), compared to 450% for a full chemistry capability..

chemical mechanisms against a full atmospheric chemistry mechanism, and sensitivity to emission perturbations are sufficiently similar. We have integrated the super-fast mechanism into the trunk of CAM as a standard option, which will make this capability an option for the IPCC AR5 simulations, and make it available to the general science community.

To further improve the performance of the super-fast chemistry, we have tested various tropopause definitions to determine the best scheme that handles tropopause folds and the ozone hole. The best definition appears to be the Stobie algorithm.

To further validated and understand our interactive chemistry sensitivity, we have run simulations with and without interactive chemistry totaling several centuries (with a

Highlight: Our "super-fast" atmospheric chemistry We have validated both our fast and super-fast capability in CAM provides consistency and feedbacks for: ozone, and sulfate aerosol mass at a fraction of the computational cost of full chemical simulations. The computational cost has been reduced from 450% to 40% verified that both the mean concentrations and on the same number of processors. Other mechanisms include full stratospheric chemistry, methane, and nitrous oxide. The plot shows the validation of our fast ozone chemistry in the stratosphere.



Reference: P.Cameron-Smith, P.Connell, A.Mirin, C.Chuang, J.-F.Lamarque, P.Hess, F.Vitt, "A Fast Chemical Mechanism and Performance Improvements Coupled Chemistry-Climate Simulations", for in preparation.

slab ocean to avoid spurious temperature contrasts), including comparison of our CAM results with shorter simulations of the whole atmosphere by the WACCM model. Analysis is ongoing, but we see significant differences in both the mean and variability of temperature. In particular, the interannual variability in the polar stratosphere is more than doubled for some seasons, which has implications for detection of climate change signatures in the stratosphere and possibly Antarctic surface temperatures.

3.2.2 Aerosol Representation

Aerosols in CAM3 are represented in terms of an external mixture of different aerosol types (sulfate, soil dust, sea salt, hydrophobic and hydrophilic organic carbon and black carbon), each with a specified size distribution. Observations tell us that most aerosol particles are composed of internal mixtures of multiple components, as primary and nucleated particles age through coagulation and condensation of secondary material.

3.2.2.1 The Modal Method

To replace the externally-mixed treatment in CAM with an internally-mixed treatment, we have implemented a modal aerosol model (MAM), which represents the aerosol in terms of internal mixtures of primary and secondary material for each of three log-normal modes, with the total number and the mass of each component predicted for each mode⁶ (Easter et al., 2004). This treatment required the introduction of new processes, such as particle nucleation and coagulation, and representations of existing processes in terms of internal mixtures, such as aerosol optical properties. Although this aerosol representation assumes all fresh primary particles are instantaneously mixed internally with secondary material and also uses a single coarse mode to represent coarse soil dust and sea salt, it yields similar CCN concentrations and aerosol optical depths compared with simulations using a more for two coarse modes each for soil dust and sea salt and adds a separate mode for primary carbonaceous aerosol. This suggests that the three-mode MAM, which is 50% slower than

Highlight: Point-by-point comparison of anthropogenic increase in Cloud Condensation Nuclei (CCN) concentrations at a supersaturation of 0.1%, as simulated by the 3-mode and 7-mode representations of the aerosol in CAM.



Reference: Gettelman, A., H. Morrison, and S. J. Ghan, 2008: A new two-moment bulk stratiform cloud complete seven-mode representation that allows microphysics scheme in the NCAR Community Atmosphere Model (CAM3), Part II: Single-column and global results. J. Climate, 21, 3660-3679.

the older bulk representation and 50% faster than the seven-mode MAM, can be used for century climate simulations that require representations of aerosol direct and indirect effects. The anthropogenic aerosol direct and indirect effects on the energy balance are somewhat sensitive to details such as the size distribution of anthropogenic primary particles and the parameterization of particle nucleation, but we have been able to achieve global mean estimates as small as -1.0 W/m2 for indirect and -0.5 W/m2 for direct effects. This opens the door for adoption of the MAM as the aerosol representation for CAM4, although the final decision has not yet been made. We have been actively involved with the rest of the CCSM development team in the evaluation and tuning of CAM and CCSM in preparation for the final decision on the configuration of CCSM4. Further work is needed to support the capability of reading MAM aerosol concentrations from history rather than calculating all aerosol processes, so that ensembles of CCSM simulations can be performed more rapidly.

⁶Easter, R. C., S. J. Ghan, Y. Zhang, R. D. Saylor, E. G. Chapman, N. S. Laulainen, H. Abdul-Razzak, L. R. Leung, X Bian and R. A. Zaveri, 2004: MIRAGE: Model description and evaluation of aerosols and trace gases, J. Geophys. Res., 109, D20210, doi: 10.1029/2004JD004571.

3.2.2.2 The Quadrature Method of Moments SAP

The method of moments tracks lower-order moments for any number of aerosol particle populations during the course of a simulation. Normally the equations governing moment evolution are not closed and, furthermore, it is not obvious how to evaluate aerosol physical and optical properties from moments. Both of these problems are solved using the quadrature method of moments (QMOM). In essence, from the tracked set of moments we obtain an equivalent number of representative quadrature points and it is these that provide both closure (dynamics) and a highly accurate and efficient "shorthand" representation of the aerosol for determination of physical and optical properties.

Progress under this SAP has been made in the following areas:

- QMOM aerosol module design and validation [McGraw et al., 2008]
- Correction of moment sequences for errors during advective transport [McGraw, 2007]
- Determining statistical complexity of real atmospheric aerosols and the level of detail needed for their representation in models [Zhang et al., 2008]
- Module development and testing in the GISS climate model [Bauer et al., 2008]

Future plans focus on testing and development of QMOM for CCSM5. Design and validation of the aerosol module is nearly complete and the third year of the BNL SAP will focus mainly on module construction and testing. Module integration and testing will be carried out first using the GISS climate model, in collaboration with Dr. Susanne Bauer of NASA GISS, prior to it its delivery for use with the CCSM. This schedule



Validating the QMOM against benchmark particle-resolved (PR) simulation for general mixing of soot-sulfate populations. Dots: 1000-particle samples from 100,000-particle PR simulation. Circles: quadrature abscissas from QMOM. Linear dot arrays and green circles: external mixture of fixed-composition soot-rich and sulfate-rich populations. Scattered points and blue circles: bivariate generally mixed population. Panel a: short time behavior. Panel b: longer time behavior and approach to internal mixing at large size. Cloud activation (CCN spectra) and optical properties computed from the quadrature abscissas and weights (only abscissas are indicated here) agree well with results from the PR simulation.

follows the original BNL SAP proposal plans and takes full advantage of the already in place BNL-GISS collaboration and QMOM aerosol model framework MATRIX, which will also be used for the new module construction [Bauer et al., 2008].

3.2.3 Aerosol Direct and Indirect Effects

The primary purpose of adding aerosols to the CCSM is so that direct (through scattering and absorption of solar and terrestrial radiation) and indirect (through impacts on cloud microphysics) effects of aerosols on the energy balance can be treated. In addition, simulation of the aerosol life cycle provides the opportunity to treat the effects of aerosol deposition on snow albedo and the biogeochemistry of the land and ocean.

To treat aerosol direct effects for the modal aerosol model we have introduced the parameterization of Ghan and Zaveri (2007), which calculates the optical properties of an aerosol composed of multiple log-normal modes, each composed of an internal mixture of multiple components including aerosol water, with the aerosol water diagnosed from the relative humidity, dry mode radius, and mass concentration and hygroscopicity of all components.

To treat aerosol indirect effects we have extended the prognostic droplet number treatment of Gettelman et al. (2008) to couple with the MAM, following the treatment developed and tested in earlier versions of CAM [Ghan et al., 1997⁷; Easter et al., 2004⁸; Ghan and Easter, 2006⁹]. Droplet nucleation is expressed in terms of the MAM internally-mixed variable-size aerosol representation [Abdul-Razzak and Ghan, 2000¹⁰]. Droplet formation and aerosol activation are treated consistently at cloud base in terms of a transfer of interstitial aerosol to the cloud-borne phase, with vertical mixing of droplets and cloud-borne aerosol above cloud base [Ghan and Easter, 2006]. Droplet number is related to cloud optical depth as described by Gettelman et al. (2008).

3.2.4 Historic Emissions and Scenario Development

Other atmospheric chemistry tasks include the simulation of pre-industrial to 2100 using AC&C emissions. J.-F. Lamarque has developed simulations using the CAM with MOZART chemistry to help define proposed scenarios for AR5 for a chemical climate

⁸ibid

⁷Ghan, S. J., L. R. Leung, R. C. Easter, and H. Abdul-Razzak, 1997: Prediction of droplet number in a general circulation model. *J. Geophys. Res.*, *102*, 21,777-21,794.

⁹Ghan, S. J., and R. C. Easter, 2006: Impact of cloud-borne aerosol representation on aerosol direct and indirect effects. *Atmos. Chem. & Phys.*, *6*, 4163–4174.

¹⁰Abdul-Razzak, H., and S. J. Ghan, 2000: A parameterization of aerosol activation. Part 2: Multiple aerosol types. *J. Geophys. Res.*, 105, 6837-6844.

model. He has also created and begun to evaluate a stratosphere-troposphere chemistry version of CAM3 (see Lamarque, 2008) and perform transient simulations from 1960-2100.

3.3 Coupled Climate and Biogeochemistry

3.3.1 Carbon and Land Modeling

Project activities in terrestrial biogeochemistry have included software development; collaboration on the development of experimental protocols, evaluation metrics, and output metadata standards; performing simulations at DOE's Leadership Computing Facilities using the Climate End Station (CES); post-processing of model output for distribution via the Earth System Grid (ESG); collaboration on the development of analysis and diagnostic tools; and publication of experimental designs, interim analyses, and scientific model evaluation of CLM biogeochemistry model results. Most of these efforts have focused on the Carbon-Land Model Intercomparison Project (C-LAMP), a major component of the activities of the CCSM BGCWG, and relied on significant community involvement.

Software development activities included vectorization of new CLM model code for use on the Cray X1E at ORNL, implementation of science modifications to CLM to support the first set of C-LAMP simulations, and CASA' modifications designed to support a second set of C-LAMP simulations using pre-release versions of CLM4, which will be included in a MODIS remote sensing products. future CCSM4 release. C-LAMP (see



Month of Maximum Leaf Area Index (LAI), a comparison of models with

http://www.climatemodeling.org/c-lamp) consists of a carefully crafted experimental protocol designed to elucidate the performance of models over the 20th century, a set of model evaluation metrics for comparison against best-available satellite- and groundbased measurements, a prototype diagnostics package based on those metrics, and a database of publicly available model results that can be used by the scientific community for their own studies. This project completed the first set of C-LAMP simulations using the CLM-CASA' and CLM-CN, totaling over 16,000 years and ~50TB of saved output,

published a subset of these data on the ESG, and performed a detailed analysis of Experiment 1 results. The C-LAMP diagnostics are now a standard part of CLM model evaluation as part of the Land Model Working Group's diagnostic package.

Other activities include a developing collaboration with Jian Huang's group at UTK (a SciDAC visualization project), contributions to the NACP syntheses, and international presentation of benchmarking activities at international C⁴MIP meetings, iEMSs conference, and Marie Curie/iLEAPS workshops. This work is serving as a prototype for a wider international model benchmarking and intercomparision activity associated with IPCC AR5 and CMIP5.

3.3.2 Advanced Marine Biogeochemistry Modeling

A majority of the SciDAC effort in marine geochemistry simulation has been directed toward the construction of a sulfur-earth system model, as reviewed in [Elliott, 2009]. But several subprojects are deserving of mention as well. In preparation for the insertion of DMS and general sulfur cycle packages, an independent trace gas module was attached to POP. It is driven by ecodynamics quantities computed in the POP/CCSM carbon cycle and imported in order to determine source sink terms locally [Elliott et al. 2008]. A variety of trace greenhouse gases have been simulated via the new set of subroutines, including carbon monoxide, carbonyl sulfide, methyl halides, methane, and several low molecular weight nonmethane hydrocarbons [Elliott et al. 2008; Chu et al. 2008]. The global marine methane geocycling developed is now being applied to provide the backdrop for continental shelf clathrate hydrate destabilization runs. With sea ice disappearing rapidly in the Arctic Ocean, it has become apparent that POP will require close biogeochemical coupling to the CICE marine cryospheric dynamics code. Accordingly, ice algal and general skeletal layer biogeochemistry routines have been developed within CICE [Roberts et al. 2008; Deal et al. 2009]. A common theme cutting across all the above research is that accurate simulation of marine trace gas processing will soon demand simulation of the microbial ecology of the bulk ocean. Bacteria control not only the major transformations of the carbon and nitrogen cycles in the sea, but also the formation and decomposition of a wide variety of direct and indirect greenhouse gases. Examples include carbon monoxide, methane and dimethyl sulfide. In fact the key uncertainties in methane clathrate hydrate destabilization will involve bacterial consumption rates. These issues and the modeling which will be required are discussed in the overview paper [Elliott, 2008b], and links to DOE genomics studies through marine metagenomics of the bacteria are dealt with in the report Graber et al. (2008), on which SciDAC team members served as co-chairs and co-authors.

3.3.3 Sulfur Cycle Coupling

Building on the capabilities from several parts of this SciDAC project (atmospheric chemistry & aerosols, oceans and ocean biogeochemistry, model coupler, and the 'performance SAP' project) we have worked on interactive trace gas-climate connections

within CCSM to create a first generation Earth system model (ESM) for the sulfur cycle. Our goal is to quantify the CLAW hypothesis feedback loop in the coupled oceanatmosphere model (ie production of ocean DMS is oxidized in the atmosphere and affects clouds and thereby ocean biogeochemistry and climate).

Several different indirect greenhouse gases and aerosol/albedo forcing agents have been simulated in ocean component surface waters. First, a modular subroutine set was developed which could ingest marine ecodynamic and carbon cycling information from standard CCSM biogeochemistry in order to drive the processing of arbitrary climate-reactive compounds. The coding was tested initially on indirect forcers such as carbon monoxide, carbonyl sulfide, nonmethane hydrocarbons and volatile halogenated organics [Chu et al. 2008; Elliott 2008a; Elliott et al. 2008], followed by our focus on the geocycling of marine dimethyl sulfide. A surface ocean





sulfur cycle model was developed and tested which is fully compatible with the standard CCSM carbon ecology [Elliott et al. 2007; Elliott 2009]. The sulfur model was applied initially in a study of DMS sea-air transfer coefficients, inspired by the direct tropical flux measurements of Huebert and company. It was determined that eliminating the contribution of an interfacial bubble bypass improved the global distribution of flux to the atmosphere [Elliott 2009].

Our POP sulfur geocycling was entered in the first international intercomparison of global marine DMS models. A publication describing the results is in preparation by the organizers, at Laval University in Quebec. The concentrations generated by POP were found to be superior to those of other large scale simulations, as judged against the major climatology (Kettle) and statistically based approaches.

However, because the Kettle data was used to help develop these DMS models, we have independently validated this capability by comparing the resultant distribution of sulfate aerosol calculated by our atmospheric chemistry models with atmospheric sulfate observations, and compared the results with the same analysis using other DMS emission estimates (from models and observations). In this way we have demonstrated that our DMS model does as well as the best climatology, and is better than the other models we tested (in prep by LLNL for submission to GRL). It also appears that there may be a systematic over estimate of DMS concentrations in the Kettle climatology for the southern ocean.

We have spun-up our ocean sulfur mechanism in CCSM, with the atmosphere driven by 355 and 970 ppm carbon dioxide, representing contemporary and future scenarios (A1Fi). Dramatic changes in mixed layer DMS concentration are apparent in a warmer world. Gyre concentrations fall by order tens of percent, and habitats for high latitude organisms shift toward the poles. Furthermore, by comparison with earlier studies conducted in (or driven by) climate change calculations, it is clear that as ecological structure of the sulfur cycle approaches a realistic level of detail, global DMS reductions and regional variability are both enhanced. The SciDAC biogeochemistry group is currently developing a series of surface ocean metabolic schemes which mimic the diversity of such models across the international community. These too will be inserted into present/future CCSM simulations and are expected to demonstrate that loss, habitat shifts and variability are all related to model sophistication.

Among the newest sulfur reactions incorporated into POP are several uniquely suited to simulation of the dynamic DMS situation, including specialized geocycling by tropical and polar phytoplankton, dissolved organic matter chemistry as it relates to bacterial demand versus DMS processing yield, and climate interactive ultraviolet stress. The SciDAC group hopes to capitalize on these developments by encouraging and participating in ensemble analysis of global DMS models. The latest and most realistic reaction channels will also be run inside CCSM with flow from the ocean coupled to atmospheric sulfate aerosol chemistry.

With the components now tested and validated, chemistry capabilities. we are working to run the full sulfur-ESM to study the biogeochemistry-aerosol-cloud interactions that will estimate the strength of the CLAW hypothesis, building on some uncoupled sensitivity tests we have already carried out in the CAM model. **Reference:** P.Cameron-S

Looking to the next generation of our sulfur ESM, we have concurrently been working on



Highlight: Estimates of dimetyl sulfide (DMS) emissions from the oceans varies widely. This plot shows the emission rate from the various models and climatologies that we intercompared using atmospheric sulfate aerosol observations and our atmospheric chemistry capabilities. The best matches with observations were for the brown and green curves, which are from our ocean sulfur model and the Kettle climatology, respectively, using a new air-sea transfer parameterization we implemented. Note: the solid green area shows the ocean surface area at each latitude.

Reference: P.Cameron-Smith, S.Elliot, "Intercomparison of DMS models and climatology using atmospheric sulfate observations", in preparation.

the design of ice algal and ice domain biogeochemistry models in coupled POP/CICE [Deal et al. 2009]. These will not only increase the fidelity of high latitude sulfur cycle simulations, but also of carbon and nutrient processing. Gap algal layers within sea ice may well be related to destabilization and coverage loss through absorption of energy in the interior.

3.4 Scalable Performance of the CCSM

3.4.1 Scalability SAP

The Science Application Partnership (SAP) project "Performance Engineering for the Next Generation Community Climate System Model" addresses fundamental structural impediments to performance and performance scalability of the CCSM, for both current and future model configurations. Thus far the SAP has focused primarily on three areas: porting the CCSM to the IBM BG/L; improving performance scalability of the atmosphere component, and developing and implementing a parallel I/O facility within the CCSM. While other aspects of CCSM performance are also important, and are being evaluated and addressed within the Science Application project, these particular tasks were deemed by project management to be the most critical and most appropriate for the SAP personnel. Highlights so far include the first port of the CCSM to the BG/L and a more than doubling of the performance of the atmosphere component.

3.4.1.1 Next Generation Architectures

When the project began, the target platforms for the Science Application project were IBM Power4 and Power5 SMP clusters, the Cray X1E, and the dual-core Cray XT3. It was recognized, however, that the IBM BG/L, emphasizing an order of magnitude increase in parallelism but relatively slow processor cores and limited memory per core, was likely to be researchers undertook the first port of CCSM (version 3 with the CPL6 coupler) to the BG/L and succeeded in executing a case with a 48x96x26 atmosphere grid and a 320x384x40 ocean grid on 1024 processors. In collaboration with CCSM software engineers, the porting effort then moved to development versions of the CCSM. Several instances of (very) large memory requirements were identified and eliminated, as were a number of bugs that manifested themselves only at scale. Success on this front led to the IBM BG/P being designated an official target for CCSM4.

Highlight: A performance comparison is made between (a) the latest version of CAM with many of the SAPinspired modifications removed and run at the maximum "pre-SAP" MPI parallelism, (b) the latest version of the code optimized with respect to the new options but utilizing the same MPI and OpenMP parallelism as for version 'a', and (c) the maximum performance observed out to the maximum available parallelism. Results are from a Cray XT5 with 8-way SMP nodes, presented for more representative of future architectures. SAP both MPI-only and hybrid MPI/OpenMP experiments. The problem configuration is FV on a 384x576x26 grid, providing a maximum parallelism for version 'a' of 1024 MPI processes (and up to 8192 threads when also using OpenMP). For version 'c', throughput continues to increase up to 9984 MPI processes without OpenMP, and up to 3328 MPI processes when using 8 threads per process. We see that the performance more than doubles as a result of these modifications.



3.4.1.2 Atmosphere Component

The atmosphere component of the CCSM is the Community Atmosphere Model (CAM). It is characterized by two computational phases: the dynamics, which advances the evolution equations for the atmospheric flow, and the physics, which approximates subgrid phenomena. Multiple options are supported for the dynamics. For the fourth IPCC assessment, a spectral Eulerian (EUL) algorithm on a 128x256x26 latitude/longitude/vertical grid was used. For the upcoming fifth assessment, a finite volume (FV) algorithm will be used with 96x144x26 and 384x576x26 latitude/longitude/ vertical grids. The new configurations will also include new physical processes, including chemistry packages that increase the number of advected tracers from 3 to somewhere between 20 and 120.

The FV dynamics supports a two-dimensional domain decomposition: latitude/vertical in one phase of the code and latitude/longitude in another. Prior to the SAP contributions, the decomposition was limited to no fewer than 3 latitude, 3 longitude, and 3 vertical levels per MPI process. In contrast, the physics can use as many MPI tasks as there are horizontal grid points. However, the code required that a uniform number of MPI processes be used throughout. OpenMP was applied to the same loops parallelized with MPI, so was limited in its ability to address the scalability restrictions.

Through the SAP, a process can now be assigned as few as one vertical level. Equally important, the parallelism restrictions in one phase (latitude/vertical, latitude/longitude, physics) no longer constrain the others. For the smaller FV target resolution we can now use 832 MPI processes in the latitude/vertical dynamics decomposition and 13,824 MPI processes in the physics. Another important innovation is the ability to parallelize the tracer advection (by decomposing over the tracer index) within the dynamics when more processes are allocated to the physics than to the latitude/vertical phase.

With the ability to exploit so much additional parallelism, a number of algorithms with poor scalability (memory or complexity) became evident, and required replacement. Finally, at scale and when running on systems with significantly different performance characteristics, the choices of MPI communication algorithm and implementation become very important. Both new algorithms and new algorithm implementation options (flow control, blocking vs. non-blocking, collective vs. point-to-point, etc.) have been implemented that have further improved performance. As shown in the sidebar, the performance more than doubles as a result of these modifications for problems of interest.

3.4.1.3 Scalable Parallel I/O

PIO is a high-level parallel I/O library developed for use in CCSM but general enough to be suitable for use in other applications. The SAP personnel have contributed to virtually all aspects of the PIO effort, but have been responsible primarily for the core PIO software.

The PIO interface was designed to closely follow those of NetCDF and pNetCDF, and its back end can invoke either MPI-IO or pNetCDF to accomplish parallel disk I/O. To achieve optimal performance, pNetCDF requires that the image of an MPI process' data on disk be rectangular in shape. We have chosen to implement the PIO interface for one-dimensional arrays of user data and wherever necessary employ a data rearrangement step accomplished via the introduction of a new PIO "box-rearranger". The box-rearranger also provides an explicit aggregation capability, allowing data to be rearranged to an arbitrary subset of the processes prior to the underlying parallel library operation. Use of PIO increases the read and write bandwidths to disk and permits a significant reduction in the required memory per MPI process compared to the original methods. This is critical for architectures that have small memory to core ratio (e.g., BG/L or BG/P). CCSM development efforts are already encountering memory limitations due to architecture and/or resolution requirements and cannot go forward without the PIO library. For example, the very high resolution experiments described in section 3.4.2 would not have been possible without PIO.

PIO has been tested on a wide variety of platforms and we have found relative performance to be highly platform-dependent. A recently completed comprehensive test suite should aid in diagnosing the best strategy for a given machine, which is one of the foci of future work.

3.4.1.4 Other SAP Activities

The SAP has been able to improve performance and performance scalability of CAM significantly. Additional optimization opportunities will likely become apparent once CCSM4 has been frozen and released in the next few months. However, the current atmosphere dynamics algorithms all utilize a latitude/longitude horizontal grid and suffer from intrinsic scalability limitations that can only be worked around. Further significant performance gains are expected to require moving to new dynamical algorithms, such as the spectral element dynamics described in section 3.4.2 and the new FV-cubed sphere dynamical algorithm from Lin (GFDL) and Putman(NASA), both of which use a cubed sphere horizontal grid. SAP personnel have collaborated in an initial performance evaluation of the cubed sphere FV dynamics on the Cray XT4, and have contributed to the integration of the spectral element dynamics into CAM, enabling dynamics based on a non-latitude/longitude grid to utilize the numerous physics load balancing algorithms. The SAP participates in ongoing development activities with the developers of both alternative dynamics algorithms. As these advanced dynamical algorithms mature, SAP personnel expect to be at the forefront of identifying and addressing their performance issues within the CCSM, especially at scale.

3.4.2 Evaluation and Integration of CAM with Unstructured Grids

The main objective of the SciDAC2 Consoritum project is to develop a first generation Earth system model based on the Community Climate System Model (CCSM). The envisioned Earth system model will require petascale computing facilities, so we are

devoting significant resources to ensure the CCSM is ready to fully utilize DOE's petascale computers. The largest bottleneck to petascale performance in the CCSM is the scalability of the atmospheric dynamical core, and thus a component of this project is focused on integration and evaluation of petascale-ready dynamical cores in the CCSM. The traditional dynamical cores in the CCSM use latitude/longitude grids which limits their scalability due to the clustering of grid points near the poles. Petascale performance at the planned resolutions will require scalability to O(100,000) processors and this is driving us to consider dynamical cores and algorithms based on more spatially uniform grids such as the cubed-sphere and other geodesic grids. We have completed the integration of the highly scalable HOMME atmospheric dynamical core into CAM, the atmospheric component of the CCSM. This work was initiated in FY 07 and required addressing many technical and software engineering issues. *This is the first non-latitude/longitude dynamical core to be integrated into CAM* and thus served as the first test of much of the new software engineering being done in CAM to allow for arbitrary grids.

3.4.2.1 CAM/HOMME Aqua Planet Simulations

Dynamical cores such as HOMME have previously undergone extensive evaluation using idealized atmospheric flows with known reference solutions. To evaluate HOMME in CAM, with the full suite of physical subgrid parametrizations, we can no longer rely on reference solutions and instead used the recently developed Williamson equivalent resolution methodology for the standardized Aqua planet test case ^{11, 12}. This required a suite of runs at different resolutions using the full CAM model, but without the land, ocean and ice components in the CCSM. Initial aqua planet results revealed three areas where the numerical methods in HOMME needed improvements in order to perform well when coupled with the many subgrid physics parametrizations used in CAM:

- 1 The numerics in HOMME did not conserve mass or energy, which we addressed by developing a new *compatible* formulation of spectral elements (Taylor et al., 2007), making HOMME the first dynamical core in the CCSM to conserve both mass and energy without the use of ad-hoc fixers.
- 2 The original limiter based dissipation mechanisms in HOMME resulted in noticeable grid imprinting in the solution, which we eliminated by replacing the limiters with an isotropic hyper-viscosity operator. This makes the HOMME dynamics quite similar to the CAM-Eulerian dynamical core.
- 3 We replaced the original oscillatory tracer advection scheme with a conservative, non-oscillatory and sign-preserving advection operator in the horizontal directions (Taylor et al. 2009), coupled with a Lagrange+remap approach to handle the

¹¹Williamson, D. L., *Convergence of aqua-planet simulations with increasing resolution in the Community Atmospheric Model, Version 3*, Tellus **60**, 2008.

¹²Williamson, D. L., *Equivalent Finite Volume and Spectral Transform Horizontal Resolutions Established for Aqua-planet Simulations*, Tellus **60**, 2008.

vertical coordinate. The vertical remap uses a cubic reconstruction with monotonicity constraints algorithm from the UK Met. Office.

With these improvements we were able to show that the CAM with the HOMME dynamical core produces a climate with the more traditional finite volume and Eulerian dynamical cores (Taylor et al. 2008).

Highlight: The CAM atmospheric component has been the primary obstacle to scaling on massively parallel HPC machines. The cubed sphere grid on which the remarkably similar to that produced by CAM spectral element discretization lives provides a solution for the scaling problem of the poles as well as improved accuracy for the dynamical simulation. This dynamical core is showing excellent strong (and weak) scaling on a variety of systems and performing well on Aqua planet idealized tests.



Reference: M. A. Taylor, J. Edwards, A. St.Cyr, Petascale Atmospheric Models for the Community Climate System Model: New Developments and Evaluation of Scalable Dynamical Cores, J. Phys. Conf. Ser. 125 (2008). Highlights of this work were featured in the Scientific Discovery section on the SciDAC website, a BER Weekly research report and an ASCR News Note.

We also used the aqua planet configuration to establish the excellent scalability of CAM-HOMME. At a 0.25 degree resolution (average grid spacing at the equator) CAM-HOMME runs well on up to 86,000 processors of LLNL's BG/L (see Highlight). The results strongly suggest at higher resolutions we will easily scale well past the O(100,000) processors necessary to achieve petascale performance on DOE's newer platforms. This scalability allowed us to perform several multi-year ultra high-resolution simulations (using 56,000 BG/L processors for 1 week). *The combination of high resolution and conservation properties of CAM/HOMME allowed the CCSM, for the first time, to capture the observed Nastrom-Gage transition in the kinetic energy spectrum.*



Kinetic energy as a function of wave number k from two highresolution aqua planet simulations (0.25 and 0.125 degree average grid spacing at the equator). The black lines illustrate slopes of k^3 and $k^{5/3}$. The highest resolution simulation has a clear well resolved transition from the k^3 to the $k^{5/3}$ regime.

3.4.2.2 AMIP Simulations

Our current goal is to evaluate the CCSM model using the HOMME dynamical core with AMIP simulations. We are using the new tri-grid feature of the CCSM flux coupler which allows the CCSM to utilize different grids for the atmosphere, land, and ocean/ice modes. We have completed preliminary simulations with the CCSM, coupling CAM-HOMME, CLM and the CCSM data ocean and ice models (see Figure). A complete set of simulations and detailed analysis of the results will be one of our key goals for FY09.



A snapshot of precipitable water (kg/m^2) from a CCSM simulation using the HOMME cubedsphere dynamical core with a 2 degree average grid spacing at the equator.

3.4.2.3 NCAR ASP 2008 Summer Colloquium on Numerical Techniques for Global Atmospheric Models.

SciDAC team member Mark Taylor was one of four organizers of this two week colloquium surveying the latest developments in petascale-ready numerical methods for Atmospheric General Circulation Models. The agenda included a successful student-run dynamical core inter-comparison project, attended by close to forty graduate students. Eleven modeling groups, including those from international modeling centers, collaborated in the development of a suite of standardized test cases focused on the key capabilities needed for these models. Working with the modeling groups, the students performed all the simulations on NCAR's IBM Bluevista supercomputer and conducted analysis and visualization of the results.

3.5 Ice Sheet Model Integration

William Lipscomb, in consultation with NCAR scientists, has made significant progress toward integrating a dynamic ice sheet model in CCSM:

- 1. The GLIMMER ice sheet model was incorporated in CCSM3.5, a developmental version, and is now being migrated to CCSM4. The ice sheet surface mass balance is computed in the land model (CLM) and passed to the ice sheet component through the coupler, and the new ice sheet geometry is returned to the land model.
- 2. A new surface-mass-balance scheme for ice sheets was implemented in CLM. Atmospheric fields are downscaled to each of ~10 elevation classes, and a separate mass balance is computed in each elevation class. This approach is more physically realistic and energetically consistent than GLIMMER's positivedegree-day scheme, and is computationally much cheaper than calculating the surface mass balance on the finer ice-sheet grid.
- 3. A suite of planned climate change experiments with has been developed for IPCC AR5. Initial experiments with a dynamic Greenland ice sheet are under way. Funding was obtained for a postdoc, Miren Vizcaino, to collaborate with SciDAC researchers in running and analyzing these experiments.

In addition, Lipscomb and LANL postdoc Stephen Price have been developing "higherorder" ice sheet flow models that are valid for fast-moving ice streams and outlet glaciers as well as for slow-moving interior ice:

- 1. The higher-order GLAM model developed by Price and Tony Payne has been debugged and tested for idealized geometries and is now giving realistic ice velocities in standalone simulations of the Greenland ice sheet.
- 2. An incremental remapping transport scheme originally developed for LANL sea ice and ocean models has been added to GLAM, allowing longer time steps on finer grids.
- 3. GLAM has been rewritten so that it can be implemented in GLIMMER in spring 2009.
- 4. John Dukowicz, working with Lipscomb and Price, has developed a novel variational approach to deriving consistent approximations for ice sheet dynamics (Dukowicz et al., 2009). This approach provides a foundation for more robust and efficient discretization and solution schemes, which will be developed and tested during the next year.

In order to promote collaborations with the broader ice sheet modeling community, a workshop entitled "Building a next-generation community ice sheet model" (Lipscomb et al., 2009) was held at LANL in August 2008. This workshop led to the creation of a developers' web site (http://oceans11.lanl.gov/trac/CISM) and the formation of six ongoing focus groups working on various aspects of model development and application (software design, data sets, hydrology, calving, ice-ocean interactions, and sea-level assessment). The goal of these efforts is to develop a Community Ice Sheet Model (CISM) to aid in predicting sea-level rise. CISM will be based on GLIMMER and will ultimately replace GLIMMER as the ice-sheet component of CCSM.

3.6 Ocean Model Development and Evaluation

Much of the work in ocean model development has been a continuing effort to merge various developments on the main LANL POP repository with the parameterization and other improvements on the NCAR CCSM POP repository. LANL improvements for high resolution ocean simulation have been incorporated into an official hrpop branch in CCSM in the process of creating a supported high resolution configuration. In addition, a new version of the POP parallel infrastructure was developed and implemented in both the LANL and CCSM versions of POP. The new infrastructure included new scalable algorithms for allocating and distributing domains among processing elements and for performing halo updates on tripolar ocean grids. In addition, improved halo update routines for multi-dimensional arrays were implemented. Finally, the new infrastructure fixed some bugs in the existing halo updates for cases where land point elimination resulted in information loss on the corners of domains. As part of this process, unit tests for the infrastructure were updated and more robust testing in both low and high resolution configurations have been performed. Because the sea ice model (CICE) shares this infrastructure, the new CICE 4.0 release also contains these infrastructure improvements.

Merging of model physics and other modifications continues and some preparations for the eventual transition to the next generation HYbrid Coordinate POP (HYPOP) model are under way. In addition, we are beginning to explore changes that may be necessary for both hybrid computing architectures (e.g. Roadrunner) and for future variableresolution grids.

Ocean model evaluation has taken three tracks. As mentioned in previous sections, ocean spinups with the full ocean ecosystem and trace gas modules are being performed. Comparisons of these simulation results to observed DMS data is described above. A second set of simulations has been focused on developing an appropriate initial state for the ultra-high resolution coupled climate system also described above, in collaboration with J. McClean (LLNL/Scripps) and F. Bryan (NCAR). These simulations have built on our previous experience in eddy-resolving ocean simulation, but utilize a new 0.1-degree tripole grid. These simulation results have been compared to both previous eddy-resolving simulations on displaced-pole grids as well as observational data. Finally, in collaboration with F. Bryan, S. Peacock (NCAR) and J. McClean (LLNL/Scripps) , we have performed a long (over 100 years) eddy-resolving simulation with a set of passive tracers, including CFCs, transit time distribution functions (TTDs) and Lagrangian floats. These tracers will provide additional metrics for comparison with observations as well as provide information on ventilation times and flow pathways in the ocean.



Relative vorticity at 15m depth in a global eddy-resolving simulation.

4 Future Plans

While the challenge of scaling to several thousands of cores has been met, the project will continue to pursue the more ambitious goal of tens of thousands of execution threads. With millions of processors available on machines very soon, we must more aggressively include implicit methods with parallel solver technologies in our modeling framework. The factors of two performance improvement become harder and harder to find without allowing the algorithms to fundamentally change. As we move past sockets with 4- 16 cores, another programming paradigm must be found. This project has not begun any experimentation for this regime so the current hybrid programming model will likely persist through the duration of the project.

The Earth System Model and CCSM4 will prove enormously useful in the upcoming IPCC AR5 so we expect to be somewhat refocused on supporting and collecting results for that effort. Multi-century studies in a production setting rely on optimized codes that run efficiently on thousands of processors with fast parallel I/O. Analyzing the results of the control simulations and further studies is the final stage of our Integration and Evaluation task.

Work on the next version of the model and refinements for Earth system simulations will occupy our focus once the production CCSM4 is well established. Our more advanced topics involving the carbon and sulfur cycle, aerosols and new dynamical cores will provide the focus of the last two years of the project. According to our tracking of project tasks we are slightly more than 50% complete (TRAC) on most topics.

We hope to continue our close relationship with the efforts defined in the two SAPs, with appropriate re-scoping past their three year period.

5 Publications

- S. R. Alam, R. F. Barrett, M. R. Fahey, J. A. Kuehn, J. M. Larkin, R. Sankaran, and P. H. Worley, "Cray XT4: An Early Evaluation for Petascale Scientific Simulation," in Proceedings of the ACM/IEEE International Conference for High Performance Computing, Networking, Storage and Analysis (SC07), Reno, NV, November 10-16, 2007 (accepted).
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6 Coordination of the Project^{*}

Coordination of the SciDAC2 project must take place at several levels.

- 1. It is necessary to coordinate contributions from several DOE labs in each of many topic areas (see Table 1 below).
- 2. SciDAC activities must follow DOE OBER's Climate Change Prediction Program (CCPP) objectives.
- 3. Activities in DOE labs must be coordinated with related activities at NCAR and NASA and NOAA, to avoid duplication of effort and to insure that DOE contributions are both timely and relevant to the overall CCSM goals.
- 4. SciDAC activities ultimately must be compatible with the overall vision for CCSM determined by the collection of CCSM Working Groups (WGs) and the CCSM Scientific Steering Committee (SSC).
- 5. As part of the DOE SciDAC program, this SciDAC Consortium project is expected to interact with and benefit from research and development activities in the rest of the SciDAC program, namely, the other SciDAC Computer Science and Mathematics projects of the Centers for Enabling Technology (CETs) and SciDAC Institutes.
- 6. Finally, we are expected to be responsive to the US Climate Change Science Plan and to participate and support Assessment activities such as the U.N. Intergovernmental Panel on Climate Change (IPCC).

Clearly, for DOE laboratory scientists to be effectively involved in so many aspects of CCSM, it is imperative that they participate actively in relevant activities. Most important is involvement in the Working Groups as members or, if possible, as co-chairs. This is where alternative approaches are evaluated and compared prior to making recommendations to the SSC. Attendance at the annual summer CCSM Workshops provides a unique opportunity to see the "big picture" of CCSM's progress. Obviously, if the opportunity arises, it can be very helpful to serve as a member of the CAB or SSC.

6.1 Coordination among DOE Labs

This SciDAC Consortium project involves different subsets of eight DOE laboratories contributing to different aspects of CCSM development and evaluation (see Table 1). The nomenclature used to describe different managerial responsibilities is explained here.

Coordination will take place by means of weekly teleconference calls, periodic project working meetings. Problems will be dealt with via email, telephone and mini-teleconference calls. Semi-annual meetings will be held. One will take place in conjunction with the annual CCSM Workshop on the Monday immediately preceding late June meeting. The second will be held in conjunction with the periodic CCPP program review and Science team meeting. A project web page is maintained at <u>http://www.scidac.org/CCSM</u>.

^{*} Full names, affiliations, and primary interests and roles of individuals referred to in this document are listed in Appendix B.

6.1.1 Principal Investigators

The PIs, John Drake (ORNL) and Phil Jones (LANL), will coordinate all aspects of the project among the participating DOE laboratories and corresponding activities at NCAR and NASA and NOAA. The PIs are responsible for (a) monitoring progress of SciDAC tasks, (b) negotiating the roles of the DOE labs relative to one another and NCAR, and (c) insuring through discussions with CCSM management that SciDAC contributions are compatible with CCSM objectives. The PIs will provide semi-annual reports on the progress of the project to the DOE program sponsors. These will include highlights of the project and status of scheduled tasks and milestones. Drake and Jones will also be liaisons to NCAR and CCSM management for the coordination of the project.

6.1.2 Laboratory Site Contacts

Each participating DOE lab has a designated Site Contact for the project, whose purview cuts across all topics being pursed at that laboratory. It is the responsibility of the Site Contacts to communicate issues to the PIs, help manage ongoing activities at their labs and to monitor progress within the lab, and oversee budgets. Site Contacts and their NCAR and NASA and NOAA counterparts are listed (italicized) in the second row of Table 1.

Highlight: SCIDAC supported modeling study of atmospheric CO2 to be used to support NASA satelitte mission (Contact: David Erickson). The monthly anthropogenic CO₂ flux estimates are used to model atmospheric CO₂ concentrations using meteorological fields from the NASA GEOS-4 data assimilation system. The study found that the use of monthly resolved fluxes makes a significant difference in the seasonal cycle of atmospheric CO₂ in and near those regions where anthropogenic CO₂ is released to the atmosphere.

> (w/ff98_seasonal - w/ff98_fixed at LEF, MLO, and SPO



e: D. J. Erickson III, R. T. Mills, J. Gregg, T. J. Blasing, F. M. Hoffman, R.J. Andres, M. Devries, Z. Zhu and S. R. Kawa. (**2008**). An estimate of monthly global emissions of anthropogenic CO₂: The impact on the seasonal cycle of atmospheric CO₂, *J. Geophys. Res.*, 113, G01023, doi:10.1029/2007JG000435.

Торіс	NCAR	NASA	NOAA	ANL	BNL	LANL	LBNL	LLNL	ORNL	PNNL	SNL
Site Contacts	Gent	Rood	Lin	Jacob	McGraw	Jones	Wehner	Cameron -Smith	Drake	Ghan	Taylor
Biogeochemistry	Mahowald					Elliott			Hoffman		
Aerosols and Atm Chem	Lamarque/Co nnely				McGraw	Elliott		Cameron -Smith	Erickson	Ghan	
Integration	Vertenstein	Sawyer		Jacob		Lipscomb		Mirin	Worley		Taylor
Evaluation	Gent			Jacob		Maltrud	Wehner	Cameron -Smith	Erickson	Ghan	
Scalability	Craig		Kerr	Loy				Mirin	Worley		Taylor
Performance	Craig			Loy					White		

Table 1. Laboratory Site Contacts are responsible for overseeing all activities at their respective institutions and high-level coordination among institutions. Major topic areas are listed in the first column, (in bold) Team Coordinators.

6.1.3 Topic Leaders

In each topic area, the PIs have appointed one of the Topic Leaders to coordinate and provide input to the periodic progress reports. The role is to monitor progress and coordinate work among the DOE labs, NCAR, NASA and NOAA.

6.2 Coordination with CCSM

The management structure of the CCSM project at NCAR has three parts: the Scientific Steering Committee (SSC), the CCSM Advisory Board (CAB), and a collection of Working Groups, each devoted to a component model, scientific research area, or other aspect of CCSM. Detailed information about the CCSM management structure and scientific plans is available on-line at http://www.cgd.ucar.edu/csm.

6.2.1 Working Groups

The topic areas listed in Table 1 fall within the scope of the CCSM Working Groups (WG). Each working group consists of scientists who come together to work on topics in which they share common interest. Membership in any WG is open to all persons having an interest in the topic. The WGs allow scientists to participate in cooperative research, compare different approaches, and minimize unnecessary duplication. The WGs present their research and recommendations, preferably based on consensus, to the SSC, which has the authority to accept or reject any recommendation. The SSC may also call for further research before any decision is made. Thus, it is imperative that SciDAC personnel be involved closely in the activities of relevant WGs.

6.2.2 Scientific Steering Committee

The CCSM Scientific Steering Committee (SSC), is chaired by Dr. Peter Gent, who is also an investigator on the SciDAC team. Steve Ghan, Bill Collins and Mariana Vertenstein are also members of the SSC and Co-Investigators on this project. The SSC provides scientific leadership for the CCSM project, including oversight of activities of working groups, coordination of model experiments, decision making on model definition and development, and encouragement of external participation in the project. The SSC determines what working groups should be organized and oversees the activities of these working groups. The co-chairs for each working group are appointed by the SSC. The major scientific responsibility of the SSC is to decide which components and/or parameterizations should be included in future versions of CCSM. Proposals for new components and/or parameterizations should come from the appropriate working groups, together with appropriate reasons for the recommended changes and documentation of the results. It is worth noting that most SciDAC scientists have no access to the SSC as a unit, so the only mechanism that presently exists for communication between SciDAC and the SSC is conversations with individual members of the SSC. That seems sufficient for now.

6.2.3 CCSM Advisory Board

In addition to the SSC, CCSM has an Advisory Board (CAB) that meets twice annually to review the progress and status of the CCSM program. The CAB then writes a report (letter) to the President of UCAR, the Director of NCAR, and the Leader of the Climate and Global Dynamics Division. In January, 2002, John Drake became a member of CAB, taking over from Bob Malone, who served a three-year term starting in 1998.

6.3 Coordination with CCPP

In its present form, the DOE Climate Change Highlight: SCIDAC supported modeling study of marine Prediciton Program (CCPP) comprises numerous university grants plus three major projects: the climate change project at NCAR (Warren Washington, PI); the Program for Climate Model Diagnosis and Intercomparison (PCMDI) at LLNL (David Bader, Director); and the Climate, Ocean and Sea Ice Modeling (COSIM) project at LANL (Phil Jones, PI). PCMDI is playing an important role in evaluation and validation of CCSM. Thus strong ties already exist between CCPP, CCSM, and the SciDAC CCSM Consortium. Progress Reports to the CCPP program director, Dr. Anjuli Bamzai, will be provided semiannually by the PI's, utilizing information from the Topic Coordinators. In

aerosols in CAM4: Mike Long, PhD student DOE/Global Change Education Program (GCEP) at University of Virgina. The objectives is to 1) Test and benchmark a comprehensive multiphase chemical mechanism across a relevant scope of chemical regimes and range in aerosol size bins to determine the dominant chemical reaction modes, 2) Using these modes in conjunction with the full mechanism, evaluate the efficiency-versus-accuracy and stability-versus-stiffness characteristics of the array of implicit ODE solvers in the Kinetic PreProcessor, and 3) Implement MECCA as a module into the CCSM and investigate the numerical and performance implications of detailed multiphase chemistry coupled to the suite of dynamical cores in CAM4.

Reference: Long, M., W. C. Keene and D. J. Erickson III, 'An inter-comparison of marine aerosol production parameterizations in CAM 3.5', CCSM Workshop, Breckenridge, CO, June 16-19, 2008.

addition, we anticipate a review in the second or third year of the program. The PI's will keep the present management plan updated and provide periodic highlights to Dr. Bamzai.

Within the DOE Climate Change Research Division that sponsors the CCPP, there are three other programs with which we have collaborative links. The Terrestrial Carbon Program sponsors measurements and process model development for terrestrial carbon cycle. Mac Post (ORNL) is a collaborator and advisor to this project regarding biogeochemical developments. In addition, the Aerosol Science Program sponsors work in Robert McGraw (BNL)'s group who is a Co-Investigator for this project. The Atmospheric Radiation Measurement program (ARM) is also important for providing data and validition of the Single Column Radiation Model that is a unit in the atmospheric physics model of the CCSM.

6.4 Coordination with SciDAC Program Elements

The full SciDAC program within DOE spans a wide range of applications, of which climate modeling is the largest. Cross-cutting activities in numerical methods, adaptive grids, mathematical libraries, data management, and computational performance optimization are supported by Centers for Enabling Technology (CETs) as well as SciDAC Institutes which are lead by University collaborations. Collaborations between the SciDAC CCSM Consortium and several of the SciDAC CETs and Institutes have been established. Table 4 lists those most pertinent to the SciDAC CCSM Consortium project, along with the lead investigators at each institution; the Principal Investigator of each CET or Institute is in bold. Tasks in collaboration with other SciDAC projects are tracked along with other project tasks. Note that the Geodesic Climate Model project led by David Randall (CSU) is another SciDAC Climate project funded by OBER. The Earth System Grid is a CET.

ISIC/NC	NCAR	ANL	LANL	LBNL	LLNL	ORNL	Other
Earth Sys Grid	Middleton	Foster			Williams	Bernholdt	
PERI				Lucas		Worley	
SDM CET		Ross		Shoshani		Samatova	
ITAPS CET					Diachin		
TOPS CET					Woodward		Keyes (Columbia)
APDEC CET				Colella	Brown		

Table 4. SciDAC projects pertinent to CCSM Consortium. PI names in **bold**.

6.4.1 Scientific Application Partnerships

Two SAP's have been funded by the DOE ASCR Office in conjunction with this project. These are of three year duration and focused on a particular mathematical or computer science task within the proposal. Bob McGraw (BNL) leads the SAP on Aerosol Dynamics and Pat Worley (ORNL) leads the SAP on Scalability. These are tightly integrated with our project and will be considered members of the Consortium, though they will have reporting requirements in addition those requested by OBER program director Anjuli Bamzai. The DOE OASCR program manager for the SAPs is Lali Chatterjee. The PI's will be accountable and assist in responses to both program managers.

6.4.2 Computational Climate End Station and the INCITE Program

The computational resources for the project are provided through the DOE Office of Science INCITE program. This project is one of several teaming to form a Computational Climate End Station that coordinates development and simulation schedules between the NLCF at ORNL, NERSC and the LCF at ANL. Dr. Warren

Washington is the PI and Chief Scientist of the Computational Climate End Station allocation and John Drake is the Chief Computational Scientist. Each year of the project we have applied for computational resources through the competitive proposal process of the INCITE program. The current allocation for 2009 is 35M node hours on the Cray XT5 at ORNL. This includes the required development time as well as preliminary production runs for the IPCC AR5 using CCSM4. Lawrence Buja and Trey White provide oversight and management support and coordination.

Appendices

A. Acronyms

ANL	Argonne National Laboratory
CCSM	Community Climate System Model (NCAR and other institutions)
CET	Center for Enabling Technology (SciDAC program element)
CICE	Sea ice model (LANL)
DAO	Data Assimilation Office (NASA)
DOE	Department of Energy
ESMF	Earth System Modeling Framework (NCAR and other institutions)
HPCC	High Performance Computing and Communications (multi-agency
	program)
ISIC	Integrated Software Infrastructure Center (SciDAC)
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LLNL	Lawrence Livermore National Laboratory
MCT	Model Coupling Toolkit (ANL)
NASA	National Aeronautics and Space Administration
NCAR	National Center for Atmospheric Research
NSF	National Science Foundation
ORNL	Oak Ridge National Laboratory
PCMDI	Program for Climate Model Diagnosis and Intercomparison (LLNL)
POP	Parallel Ocean Program (LANL)
PNNL	Pacific Northwest National Laboratory
SAP	Scientific Application Partnership
SciDAC	Scientific Discovery through Advanced Computing (DOE program)
SCRIP	Spherical Coordinate Remapping and Interpolation Package (LANL)
SSC	CCSM Scientific Steering Committee

B. Names, affiliations, and primary interests

The following table contains the full names, affiliations, primary interests and roles (in the context of this management plan) of individuals referred to in this document. Names in italics identify people *not* funded under the SciDAC CCSM Consortium project.

Last name	First name	Laboratory	Primary Interest	Primary role
Atherton	Cyndi	LLNI	Chemistry, aerosols	Co-I: Constortium, ASP
Bader	David	LLNL	Global modeling	CCPP Chief Scientist
Bernholdt	David	ORNL	SW Engineering	CCA and ESG
Bonan	Gordon	NCAR	Land-surface model	Co-Ch: Land WG
Cameron-Smit	hPhilip	LLNL	Chemistry, aerosols	Co-I: Consortium
Chung	Cathy	LLNL	Aerosols	Co-I: Consortium, ARM
Collela	Phil	LBNL	Applied math	PI: APDEC CET
Collins	Bill	NCAR	Aerosols, Evaluation	Co-I: Consortium

Last name	First name	Laboratory	Primary Interest	Primary role
Conley	Andrew	NCAR	Chemistry, Aerosols	Co-I: Consortium (New)
Craig	Tony	NCAR	SW Engineering	Co-I: Consortium
Doney	Scott	NCAR	Biogeochemistry	Co-Ch: Biogeo WG
Drake	John	ORNL	Atmospheric dynamics	PI: Consortium
Diachin	Lori	LLNL	Meshing software	PI: SciDAC ITAPS CET
Elliott	Scott	LANL	Ocean biogeochemistry	Co-I: Consortium
Erickson	David	ORNL	Chemistry, Evaluation	Co-I: Consortium
Evans	Kate	ORNL	Dynamics, Methods	Co-I: Consoritum(New)
Fung	Inez	Berkeley	Biogeochmistry	Collaborator, advisor
Gent	Peter	NCAR	Ocean model	CCSM Chief Scientist
Ghan	Steve	PNNL	Atmospheric model	Co-I: Consortium
Hoffman	Forrest	ORNL	Land-surface model	DOE lead: Land
Hunke	Elizabeth	LANL	Sea-ice model	Co-Ch: Polar Cli WG
Jacob	Rob	ANL	Coupler, SWE	Co-I: Consortium
Keyes	David	Old Dominion	Applied math	PI: TOPS ISIC
	Jean-			Co-I: Consortium (on leave)
Lamarque	Francios	NCAR	Chemistry	
Larson	Jay	ANL	Coupler, SWE	Collaborator
Lin	<i>S. J.</i>	GFDL	Atmospheric dynamics	Collaborator
Lipscomb	William	LANL	Ice sheet	Co-I: Consortium
Loy	Ray	ANL	Scalability on BG/L	Co-I: Consortium
Lucas	Bob	LBNL	Performance	PI: SciDAC PERI
Malone	Robert	LANL	Hydrologic cycle	Co-PI: Consortium
Maltrud	Mat	LANL	Ocean analysis	Co-I: Consortium
McGraw	Bob	BNL	Aerosol dynamics	PI: SAP
Middleton	Don	NCAR	Earth system grid	Co-I: Earth Sys Grid
Mirin	Art	LLNL	Atmospheric model	Co-I: Consortium
Post	Mac	ORNL	Carbon land processes	TCP, advisor
Putman	Bill	NASA/DAO	Dynamics FV	Collaborator
Randall	David	CSU	Coupled model	PI: Geodesic Grid CM
Rood	Ricky	UMich-NASA	Global modeling	advisor
Sawyer	Will	NASA/GMAO	SW Engineering	Co-I: Consortium
Shoshani	Ari	LBNL	Data grid	PI: SciDAC SDM CET
Taylor	Mark	SNL	Scalability	Co-I: Consortium
Washington	Warren	NCAR	Coupled model	Co-I: Consortium, CCWG
Wehner	Michael	LBNL	Performance, evaluation	Co-I: Consortium
Williams	Dean	LLNL	Diagnostic tools	Co-PI: ESG
White	Trey	ORNL	Performance	Co-I: Consortium
Woodward	Carol	LLNL	Solvers	Co-I: TOPS CET
Worley	Pat	ORNL	Scalability, integration	Co-I: PERF ISIC