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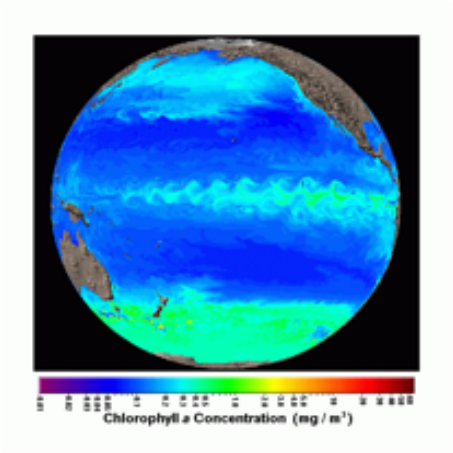
SciDAC CCSM Consortium Final Summary Report (2001-2006)



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Acronyms

SciDAC	Scientific Discovery through Advanced Computing
ANL	Argonne National Laboratory
GFDL	Geophysical Fluid Dynamics Laboratory
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LLNL	Lawrence Livermore National Laboratory
NCAR	National Center for Atmospheric Research
ORNL	Oak Ridge National Laboratory
PNNL	Pacific Northwest National Laboratory
CAM	Community Atmospheric Model
CCSM	Community Climate System Model
CLM	Community Land Model
CICE	Sea Ice Model
CSIM	Community Sea Ice Model
POP	Parallel Ocean Program
CPL6	Coupler Program Six

Executive Summary

The "Collaborative Design and Development of the CCSM for Terascale Computers" was a five-year Scientific Discovery through Advanced Computing (SciDAC) project that started in 2001. The project goal was to advance the state of the art in climate modeling by adding to the functionality of the model as well as designing the model to take advantage of the modern scalable high performance computing systems. The project was undertaken as a collaboration between six U.S. Department of Energy (DOE) laboratories: Los Alamos National Laboratory (LANL), Argonne National Laboratory (ANL), Lawrence Livermore National Laboratory (LLNL), Oak Ridge National Laboratory (ORNL), Pacific Northwest National Laboratory (PNL), and Lawrence Berkeley National Laboratory (LBNL). The National Center for Atmospheric Research (NCAR) is the National Science Foundation (NSF) collaborator and Goddard Space Flight Center - Data Assimilation Office is a National Aeronautics and Space Administration (NASA) collaborator.

In this, our final progress report, we examine progress from the perspective of the five years duration of the SciDAC project. We attempt to evaluate progress toward our original objectives and evaluate the benefit of the "SciDAC Consortium" to the CCSM, the focal point of this entire project. We also examine various aspects of the management of such a large cooperative program, including the degree of cooperation among the six U.S. Department of Energy national laboratories, one National Aeronautics and Space Administration Office, and NCAR.

This project directly supported the DOE Strategic Science Goal Five of maintaining World-Class Scientific Research Capacity in Climate Change Research. It did this by delivering improved climate models for policy makers to determine safe levels of greenhouse gases for the Earth System. The specific impact of this project was in

- Providing the tools required to perform climate change predictions and analysis of variability through feedbacks with the physical climate system, the carbon cycle and biogeochemical cycles that improve the fidelity and accuracy of high end coupled climate simulations,

- Providing the software frameworks and advanced software practices that enhance the ability of DOE researchers to test hypotheses, develop new process models and understand the environmental interactions with climate change.

- Maintaining state of the art, production ready, community simulation capabilities (specifically, the CCSM) on DOE supercomputers.

The SciDAC CCSM project webpage may be found at *http://www.scidac.org* and the full CCSM project pages may be found at *http://www.ccsm.ucar.edu*.

There were two main goals of the SciDAC CCSM Consortium Project. One goal was to improve computational performance and portability of the CCSM model. At the start of the SciDAC program, the physical component models (atmosphere, ocean, sea-ice and land) in CCSM were able to take advantage of the many processors in a parallel supercomputer. The coupler, responsible for managing the interaction and communication between components, was restricted to a single node. Over the past five years, we successfully developed a new coupler for CCSM which can use multiple processors of the parallel supercomputers typically used for climate model integrations. To create a parallel coupler, we created two new software libraries. The Model Coupling Toolkit (MCT) handles the complex routing of data between each component model and the coupler and also provides a generic sparse matrix capability used for the interpolation of data between components. The Mulit-Program Handshaking (MPH) library provides the infrastructure for dividing the processor space and creating high-level communication objects for the coupler and each component model in the CCSM. Both of these libraries formed the basis for the new coupler program, cpl6 which SciDAC also helped develop. We have recently modified cpl6 further to allow more flexibility in defining the different chemical species passed through the coupler for biogeochemical models.

The re-appearance of vector computers like the Earth Simulator and Cray X1 required a coordinated effort of software developers and vendors to produce a vectorized version of the CCSM3. Considerable effort was devoted to gaining good vector utilization while maintaining or improving the performance on cache based computing platforms. The land surface and sea ice models were largely rewritten for improved performance while still maintaining an extensible design. A load balancing scheme for atmospheric column physics calculations was added as an option, which along with user control of the vector length, allows for 10-30% performance gains on the vector architectures. On non-vector systems,the improvements from load balancing are even greater than on vector systems. A similar scheme was independently adopted in the ocean model and has recently been introduced into the ice model.

A second main goal of this project was the addition of new algorithms and new physical parameterizations necessary for future climate simula-

tions. SciDAC researchers aided in testing and improving a new finite-volume method for atmospheric dynamics. The project also evaluated two approaches to assessment of climate change impacts at the regional scales. One approach was to run a very high resolution (as fine as 0.5x0.625 degrees) simulation of the atmosphere using the latest version of CAM (version 3) with both the Eulerian and finite-volume dynamical cores. Another approach used a subgrid orography scheme developed under this project to treat land and atmospheric processes at finer scale within a global model and has been used to downscale the simulated climate to 5 km resolution for more than a century of climate change. For the ocean model, partial bottom cells and new horizontal grids have been introduced and work continues on a new ocean model with hybrid vertical coordinates that should greatly improve the simulation of deep ocean properties.

An important focus of recent work was the addition of atmospheric chemistry, together with land and ocean biogeochemistry to enable simulations of the full carbon and sulfur cycles and their feedbacks on the physical climate system. Tropospheric chemistry capability was extended in the atmosphere model through development and implementation of a "fast" chemical mechanism that is 3-4 times faster than our existing "full" chemical mechanism, inclusion of interactive sulfur cycles within both the "fast" and "full" ozone mechanisms, and significant improvements to the representation of nitrate, sea- salt, and secondary organic aerosols. This tropospheric chemistry code is now incorporated into the main CCSM archive, and has been connected to the land and ocean biogeochemistry components. In the ocean model, an ecosystem model was implemented and extended to include trace gases like dimethyl sulfide that are important in the formation of sulfate aerosols. The land model includes either the CASA' (Fung) or the CN (Thornton) extensions to provide an interactive carbon cycle that links to the atmosphere through the new coupler. These improvements are being used to examine the effect of nitrogen deposition on land biogeochemistry and the sensitivity of the atmosphere to aerosol emissions. A representation of aerosol indirect effects is also being added to the interactive chemistry version of CAM3.

To demonstrate the feasibility of fully coupled modeling at this level, a prototype Earth System Model was assembled with the consequent extensions required in the software engeineering design. This work met our primary FY05 milestone for DOE and will be used for CCSM experiments with interactive carbon and sulfur fluxes.

Abstract

The purpose of this multi-disciplinary project was to accelerate the development of the Community Climate System Model (CCSM), a computer model of the Earth's climate that combines component models for the atmosphere, ocean, land and sea ice. There were two goals to this project. The first goal was to improve software design and engineering of the CCSM and its component models and improve performance portability across the wide variety of computer architectures required for climate assessment simulations. This goal was accomplished with the release of the CCSM3.0 and its use across a variety of vector and scalar high performance computational platforms for the simulation of climate change scenarios for the Intergovernmental Panel on Climate Change (IPCC) Fourth Assessment Report. The second goal was to accelerate the introduction of new numerical algorithms and new physical processes within CCSM models. The recent introduction of atmospheric chemistry and ocean ecosystems, along with new formulations and algorithms for ocean and ice dynamics, extends the ability of the model to simulate complex climate interactions and feedbacks. Improving the representations of biogeochemical processes and the carbon cycle supports the DOE's Climate Change Prediction Program. Active participation in the CCSM working groups, collaboration with key NASA and NSF research centers and cooperation with the Earth System Modeling Framework were coordinated with the CCSM Scientific Steering Committee in this multi-lab, multi-agency collaborative effort.

Chapter 1

INTRODUCTION

The "Collaborative Design and Development of the CCSM for Terascale Computers" was a five-year Scientific Discovery through Advanced Computing (SciDAC) project that started in 2001. The project goal was to advance the state of the art in climate modeling by adding to the functionality of the model as well as designing the model to take advantage of the modern scalable high performance computing systems. The project was undertaken as a collaboration between six U.S. Department of Energy (DOE) laboratories: Los Alamos National Laboratory (LANL), Argonne National Laboratory (ANL), Lawrence Livermore National Laboratory (LLNL), Oak Ridge National Laboratory (ORNL), Pacific Northwest National Laboratory (PNL), and Lawrence Berkeley National Laboratory (LBNL). The National Center for Atmospheric Research (NCAR) is a National Science Foundation (NSF) collaborator and Goddard Space Flight Center Global Modeling and Assimilation Office is a National Aeronautics and Space Administration (NASA) collaborator.

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1.1 Overview of Progress

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The re-appearance of vector computers like the Earth Simulator and Cray X1 required a coordinated effort of software developers and vendors to produce a vectorized version of the CCSM3. Considerable effort was devoted to gaining good vector utilization while maintaining or improving the performance on cache based computing platforms (Sections 2.2.1, 2.2.2,2.2.3, 2.2.4). The land surface (Sec. 2.2.2) and sea ice (Sec. 2.2.4) models were largely rewritten for improved performance while still maintaining an extensible design. A load balancing scheme for atmospheric column physics calculations was added as an option, which along with user control of the vector length, allows for 10-30% performance gains on the vector architectures (Sec. 2.2.1). A similar scheme was independently adopted in the ocean model and has recently been introduced into the ice model (Sec. 2.2.4).

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To demonstrate the feasibility of fully coupled modeling at this level, a prototype Earth System Model was assembled with the consequent extensions required in the software engineering design. This work met our primary FY05 milestone for DOE (Sec. 2.4.5) and will be used for CCSM experiments with interactive carbon and sulfur fluxes.

1.2 Background

The effort to develop and support a community model for climate studies began about twenty years ago. The first Community Climate Model (CCM), CCM0A, was actually only an atmospheric model and was described by Washington in 1982 [54]. This model was followed by CCM0B [56] and a sequence of models that displayed steady improvement in the fidelity of the simulated climate: CCM1 in 1987, CCM2 in 1992, and CCM3 in 1995. The introduction of CCM2 marked a new philosophy with respect to implementation. The CCM2 code was entirely restructured to satisfy three major objectives: greater ease of use, including portability across a range of computational platforms; conformance to a plug-compatible physics interface standard; and the incorporation of single-job multitasking capabilities.

The Community Climate System Model (CCSM) project started in January 1994 and led to the release of CCSM version 1.0 (CCSM1) in 1996, which coupled atmosphere, ocean, land surface, and ice model components. Various aspects of the model are described in a special issue of the Journal of Climate (Climate Systems Model, 1998). Concurrent with this activity, a group led by Warren Washington at NCAR developed the Parallel Climate Model (PCM) to enable century-long climate simulations on scalable parallel computers [55]. The PCM was a coupled model with many of the same components as CCSM1. It played an important role in the DOE sponsored simulations, and considerable effort was invested to achieve good parallel performance. Both models were among the first coupled models to perform century long simulations without the need for "flux correction" to compen-

sate for climate drift. This was viewed in the scientific community as a major step in modeling the Earth system.

This SciDAC project is partly responsible for the merging of the CCSM series with the PCM series as part of the CCSM2 release in May 2002. As in PCM, many of the model components were based on DOE model developments. In particular, the POP ocean model, developed at LANL, became the ocean circulation model of the coupled system, and the LANL CICE sea ice model formed the core of the Community Sea Ice Model (CSIM) of CCSM. The LSM (land surface model) was replaced with the Community Land Model (CLM2) and the NASA finite-volume (FV) dynamical core was added to the atmospheric model as part of the SciDAC CCSM collaboration. Several ongoing developments within this SciDAC project made fundamental contributions to subsequent releases of the model, including the development of a new coupling technology, the glue that holds the component models together.

The CCSM3 was released in June 2004 with major contributions from this project. It is being heavily used for the U.S. contribution to the IPCC Fourth Assessment Report due out in 2007, contributing over 10,000 years of climate simulation and over 100TB of output. This effort will have long standing implications in climate science and policy and may be the largest set of simulation experiments in the open scientific arena. The CCSM3 is now, arguably, the premier coupled climate model in the world and should provide a strong scientific basis for policy makers in discussions of climate change, climate variability and predictability.

As more research scientists invest their efforts using and extending community models, the capabilities available to other researchers increase. This compounding of the investment in a community model is already yielding significant discoveries and advances. We will show in this report how our project contributed both to the infrastructure necessary for such a community resource and to the scientific capabilities required for future simulations of the Earth's climate system.

Chapter 2

TECHNICAL PROGRESS

The project started with an emphasis on software engineering and performance as we focused on adapting to new computer architectures, meeting short term performance objectives for the IPCC simulations and on developing the necessary software engineering infrastructure for later model improvements. After a mid-term review and the release of the CCSM for IPCC, focus shifted towards model improvements and the incorporation of chemistry and biogeochemistry.

2.1 Software Engineering

The project started with an emphasis on software engineering practice in order to lay the groundwork for incorporating our changes into the CCSM code base and to improve our own internal software engineering practices. To sustain accelerated development, two objectives must be achieved and maintained in the CCSM. These are model extensibility and performance portability. The objective of model extensibility is to facilitate the development of component models by reducing the time and effort required to replace a module of specified functionality with another module containing an alternative treatment with the same or increased functionality. This requires a clear statement of the requirements that the model and all of the modules comprising it must satisfy. To achieve "plug and play" interchangeability of modules requires a clear statement of the global structure of the model and standardized definitions of the module interfaces.

Personnel from the project were major contributors to the new CCSM Software Engineering Working Group (SEWG). We participated in the creation of design and requirement documents for each of the existing compo-

nent models. We have also continued a formal software engineering approach with other revisions and extensions to accommodate the expanding requirements for a chemical climate model. The practice of developing design documents for the software architecture and for new additions to the model allowed a broader development team including DOE software engineers to contribute directly to the NCAR CCSM code developement efforts. New testing and verification mechanisms allowed external developers to check-in code in the CCSM repository. Establishing and participating in Change Review Boards (CRBs) greatly facilitated coordination among developers and assured high software quality. These initiatives, in collaboration with the NCAR CCSM Software Engineering Group and Bill Collins as Chief Scientist for the CCSM, contributed to the release of the model in June 2004.

In addition to the DOE laboratory staff participating in the development of the CCSM, this SciDAC project funded several efforts and four software engineers in the NCAR Software Engineering Group.

A full time testing engineer, Wei Yu, was funded by SciDAC (1 FTE) from May 2004 to February 2005. He was responsible for all CCSM system testing and was instrumental in carrying out the testing needed for the successful release of CCSM3.0 in June 2004. In addition, he provided extensive testing as part of the preparation for the IPCC simulations carried out over the last year. Having a full-time test engineer was also greatly beneficial to the porting of CCSM to new platforms. His work was critical to the development of new CCSM run scripts and automated testing scripts that accompanied the release and that were used in the IPCC simulations. Due to his efforts, model bugs were detected earlier and much more extensive testing was performed on the released code than in previous releases.

A second software engineer, Jeff Lee (1 FTE), started in January 2005 and was funded by SciDAC as the Biogeochemistry Working Group Software Engineering Liaison. His main task was to make the modifications to the code required to conduct the C4MIP simulations (Coupled Carbon Cycle Model Intercomparison Project). The terrestrial and ocean carbon cycle codes were developed within the component models and needed to be linked in a specific fashion in order that the CCSM could participate in this important intercomparison project. He has had to rapidly become familiar with both the CCSM3 model components and the associated CCSM3 build and run scripts. As part of the requirements for the C4MIP experiments, he implemented a CO_2-cycle module into CAM3 that transported CO_2 traces and that read and time interpolated CO_2 flux data. He also modified the CAM radiation code to permit use of spatially varying CO_2 and modified

CAM, CLM and the flux coupler to permit the exchange of CO_2 between CAM and CLM. He was instrumental in helping to prepare the input data required by the experiments by creating the necessary CO_2 and Sea Surface Temperature (SST) input datasets. Finally, he carried out numerous debugging tests of the CCSM system for the specific CCSM configuration required for the experiments.

A third software engineer, Nancy Norton (.925 FTE), was funded by SciDAC since February 2005 to serve as the CCSM Ocean Model Working Group Software Engineering Liaison. She performed ocean-model development, served as the gate keeper for the CCSM ocean model code and maintained an internal ocean-model web page that provided extensive documentation of ocean model changes. In the final years of the project, she worked on the incorporation of the Hybrid Coordinate Ocean Model (HYCOM) and POP2 into CCSM3, requiring modifications to various CCSM3 scripts as well as integrating CCSM3 communication routines into HYCOM.

A fourth software engineer, Mariana Vertenstein (.1 FTE), is the head of the CCSM software engineer group and was funded by SciDAC since October 2004 to coordinate Biogeochemistry Working Group software activities as well as collaboration with the SciDAC group on carbon modeling. She helped develop the new interfaces that will be used to exchange biogeochemical tracers between atmosphere, land and ocean components and coordinated the coding changes and accompanying testing required for the C4MIP experiments. She worked on developing the extensibility of the current CCSM system to facilitate the performance of new biogeochemical experiments using CCSM3.

2.2 Performance

A second objective for our accelerated development was performance portability, defined as the ability to maintain good performance across a wide variety of computer architectures without needing to support multiple versions of the underlying source code. Performance portability is important so that productivity and active use of the model can be maintained despite the rapid technological changes in computing. These technological changes apply to hardware architectures as well as software practices and programming paradigms. The explosion of capabilities from the massively parallel computer architectures has posed great challenges for software engineers and computational scientists. This proposal followed a software engineering approach that is yielding a single version of the CCSM that runs on the myriad

computer platforms with parameters that are set to optimize for particular hardware features. Since the hardware features and memory hierarchies are becoming increasingly specialized, this is particularly challenging.

The biggest test of our approach came in 2005 with the re-emergence of vector supercomputers in major scientific research facilities. The Japanese Earth Simulator at the Frontier Center and the ORNL Cray X1 offered substantial compute resources to climate modelers and the CCSM3 IPCC simulations required that vector performance be provided within the model. The decision of the DOE Office of Advanced Scientific Computing to pursue the development of petascale computing capabilities also underscores the need for a solid software engineering and parallel algorithm base to develop and extend new climate models. This project has laid the groundwork.

2.2.1 Atmosphere Model Performance

Spectral Dynamical Core and Physical Parameterization Performance Optimizations and Benchmarking

We worked closely with NCAR software engineers on a number of functionality and optimization activities for both the spectral dynamical core and the model physics. An early task was the integration of conflicting NEC, Cray, and non-vector system optimizations, reducing the amount of system-specific code. We also made changes that now allow both OpenMP and SSP-mode to be used with both the finite-volume and spectral dynamical cores on the Cray X1. As further changes to CAM proceeded over the life of this project, periodic reexamination of CAM performance on the Cray X1 was required with occasional (re)introduction of vectorization as needed.

In addition to vector modifications, a number of general optimizations were incorporated into CAM, including reducing the number of array allocations and deallocations in performance sensitive code. We also added MPI-1 collective operators and MPI-2 and Co-Array Fortran one-sided message runtime options for implementing the matrix transposes used in the spectral transform and in the physics load balancing. Finally, the domain decomposition algorithm in the dynamical core was generalized to improve load balance when using a reduced grid. We made a careful study of the sources of load imbalance in the current physical parameterizations and the impact of the current physics load balancing strategies on overall performance.

To evaluate these performance improvements, we benchmarked versions of CAM on the Cray X1 and XD1, Power 4 cluster with HPS, and SGI Altix,

using both the standard T42 and T85 spectral dynamical core benchmarks and a benchmark problem similar to how CAM was run for the IPCC simulations. Some of these results are reported in a paper in the special issue on software engineering in climate and weather models in the International Journal of High Performance Computing Applications [186].

Finite-Volume Dynamical Core Optimization and Utilization

The introduction of a new finite-volume dynamical core required substantial performance analysis and subsequent optimizations to ensure the new dynamical core could be evaluated and used for future climate simulations. A journal article covering the various improvements and optimizations to the finite- volume dynamical core is included in a special issue on climate modeling of the International Journal of High Performance Computing Applications [180]. An inter-agency (DOE, NASA, GFDL, NCAR) finite-volume dynamical core working group, whose main aim was to coordinate software implementations of the finite-volume dynamical core enabled the merging of the ESMF- and NCAR-based versions, resulting in a more robust implementation of the dycore and a wider distribution of the modifications below.

One improvement we implemented was a multi-two-dimensional domain decomposition methodology, whereby the dynamical advance within a flux volume is decomposed in latitude- vertical, and the remapping in longitude-latitude. The latitude-vertical decomposition avoids nonlocal subdomain references, which would otherwise occur at the high latitudes if decomposing in longitude. The longitude-latitude decomposition perfectly suits the remapping, which treats each vertical column separately. The decompositions are connected by transposes using the Pilgrim and Mod_comm libraries. This work required development of irregular communication routines for Mod_comm to handle more general communication patterns, particularly those that arise with the transposes. These routines support use of intermediate buffers to enable contiguous data transfers, as well as direct use of MPI derived data types. We also added the ability to include ghost zones in the transposes and generalized the Mod_comm to support MPI-2 one-sided communications and (for the Cray X1) Shmem communications. In the end, neither MPI-2 nor shmem were superior to traditional two-sided MPI on the Cray X1. The fact that the Cray X1 implementation of MPI is not thread safe negated a potential advantage of MPI-2.

Another improvement was a faster method for computing the geopotential, which previously had required 8 transposes per dynamics time step. A

new method was introduced that reduces communication four-fold, but at the expense of not preserving bit-for-bit agreement across vertical decompositions.

Similar to the spectral core, changes for vectorization were added for improved performance on the Cray X1 and the Earth Simulator. This involved moving latitude loops to the lowest level, reordering loops, and performing logical tests in advance in conjunction with indirect indexing to separate the conditional operations from the vectorizing arithmetic. We could not adequately vectorize the polar filters due to limited concurrency at fine domain decomposition.

To evaluate performance improvements and scalability of the model, we carried out a section-by-section performance analysis over a range of resolutions. For 0.5x0.625x26L we compared 32-processor and 2944-processor scenarios on IBM Seaborg. Overall there was a 25-fold speedup in going to the finer domain decomposition. The biggest bottleneck was the land model; it did not have a large enough computational load to effectively utilize that many processors. We found that the transposes accounted for only 3% of the overall computer time at 2944 processors. Even the geopotential calculation, with its semi-global communication and frequent execution, increased its fractional time within the dycore from 21% to only 26%. This suggests that load imbalance more than communication overhead is the main factor limiting scalability of the multi-two-dimensional-decomposition approach.

We extended the performance and scalability comparison of FV-CAM on other leading architectures, including the Cray X1, Earth Simulator, IBM Power5, Cray XT3 and Itanium 2 cluster. The analysis included throughput measurement and monitoring of communication trends. We found that, on a processor by processor basis, the Cray X1 was the fastest, with the Earth Simulator roughly 25% slower. We also analyzed the benefits and drawbacks of OpenMP. On the Cray X1 at coarse domain decomposition we observed a tangible benefit; however for fine domain decomposition the vector lengths were sufficiently reduced so as to worsen rather than improve performance. We found OpenMP to allow effective use of a larger processor count on the IBM and SGI Origin platforms but to be only marginally faster on Linux platforms.

As a step toward measuring the increased cost of atmospheric chemistry, we monitored the increase in computer time when advecting hundreds to thousands of tracers. We found the additional cost per tracer to be minimally 1 to 2 per cent, so that advecting an additional 50 to 100 fields would double the CAM run time. This is without consideration of optimizations that might be relevant at very large tracer count.

Performance History

Documenting performance improvements in an evolving code can be difficult. Changes that add, for example, new processes to the physics can increase the amount of work required in a simulation. Such complexity-changing modifications invalidate performance optimization comparisons between versions of the code before and after the modification. Periodically the problem specification or dynamical core of most interest also changes. It is often not possible to run the new problem specification using older versions of the code, requiring the redefinition of baseline performance using the current production version of the code. A version control system is essential for this type of study as it documents the code evolution. Subversion [57] is used with CAM currently, having replaced CVS in December 2005. One positive side effect of introducing performance optimizations as compile-time and run-time options is that new versions of the code can be run in the "old way", so that the performance impact of the introduction of a performance tuning option can still be quantified.

The left graph in Figure 2.1 describes the performance improvement between June 2001 and November of 2002 on a IBM Power 4 cluster. During this time period the Power 4 cluster had an IBM SP Switch2 interconnect between nodes. The benchmark problem T42 L26 uses a 64x128x26 (latitude by longitude by vertical) computational grid and the Eulerian dycore, which were the production settings at the time of the experiments. The "original settings" curve is the performance when setting the optimization options to emulate the way that CAM version 1.0 was run in June 2001. Note that the performance improvements include increasing the number of processors tLhat could be used effectively from 64 to more than 256.

The right graph in Figure 2.1 describes the performance improvement attributable to the performance optimization options introduced between June 2001 and May 2004 on the IBM Power 4 cluster, now using the IBM HPS interconnect, on an IBM p575 cluster, and on a Cray X1. Results are for the new production problem size of T85 L26, which uses the EUL dycore and a computational grid of size 128x256x26.

So far we have described the impact of performance optimizations in the physics and in the EUL dycore. Over the same period of time the NASA finite-volume dycore was integrated with CAM, a two-dimensional (2D) domain decomposition option was implemented, and a number of finite-volume communication optimization options were added. finite-volume was not available in CAM prior to this work and many of the optimizations were introduced simultaneously. In consequence, no baseline exists against which

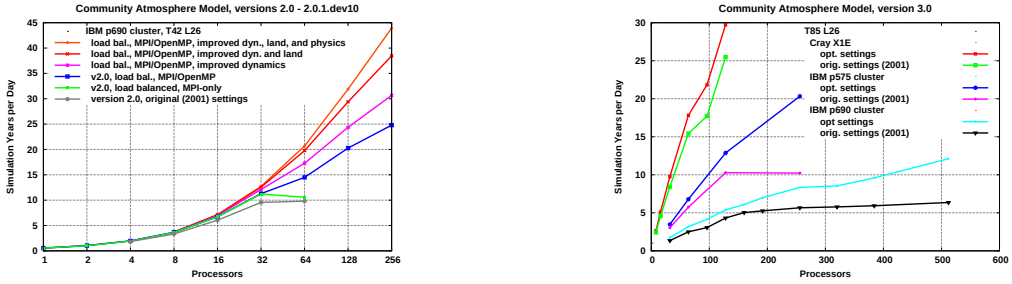

Figure 2.1: CAM Eulerian performance history.

to evaluate these optimizations. Figure 2.2 contains plots examining CAM performance sensitivities to two of the finite-volume-specific tuning options.

The left graph in Figure 2.2 compares CAM performance when using MPI-2 one-sided and MPI-1 two-sided communication requests with varying levels of thread parallelism. The experimental platform is the SGI Origin3800. The benchmark problem (1x1.25 L26) uses a 181x288x26 computational grid. MPI-2 one-sided communications and thread level parallelism are not performance enhancers on all target platforms, and it is important for performance portability that the communication protocol be an option.

The right graph in Figure 2.2 illustrates the performance impact of the 2D domain decomposition on performance on three platforms: the Cray X1, the Cray XT3, and the IBM Power 4 cluster. The benchmark problem (0.5x0.625 L26) uses a 361x576x26 computational grid. Performance is graphed for the original one-dimensional (1D) decomposition, a 2D decomposition where four processes are applied to the new dimension, and a 2D decomposition in which seven processes are applied to the new dimension.

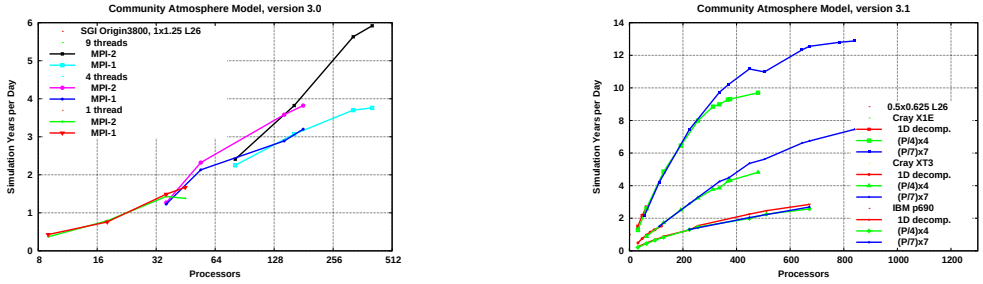

Figure 2.2: CAM finite-volume performance optimizations.

The 1D decomposition is limited to 120 MPI processes for this benchmark. The 2D domain decomposition increases MPI scalability significantly, but with diminishing performance returns for high processor counts. For the IBM Power 4 cluster, the 1D domain decomposition with OpenMP parallelism is more efficient at increasing scalability than is the 2D decomposition with OpenMP parallelism up to the indicated number of processors.

The most recent performance engineering efforts involved (re)vectorizing CAM while not degrading performance on the nonvector systems. The target vector systems are the Cray X1 and the Earth Simulator. These two systems have somewhat different performance sensitivities, and maintaining performance portability between them has required careful testing. Figure 2.2.1 illustrates the performance history for three benchmark problems and processor counts on the X1 from May 2005 to May 2006. The versions named on the X-axis were developed on the X1, and often include changes that eliminate performance degradations that crept in since the previous X1-oriented modification. For each named version, we also measured per-

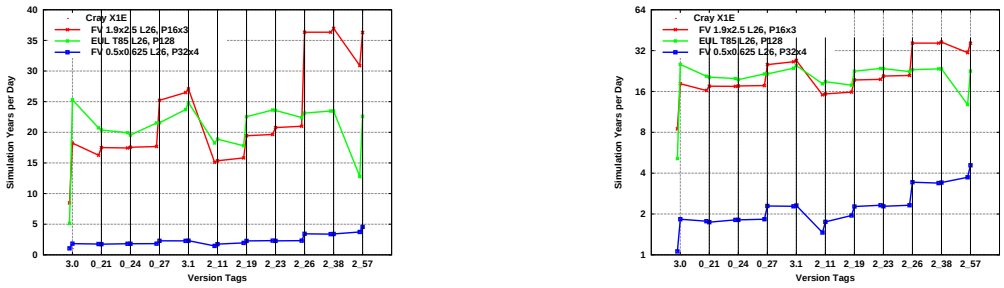

Figure 2.3: CAM vector performance history: March 2005 to March 2006.

formance for the immediately preceding version. The name of each version is of the form "3.X_Y". The "3." is dropped from the name in the graph where it improves readability. The two graphs contain the same data, but the one on the right uses a logarithmic Y-axis. From this it should be clear that maintaining vectorization is a significant performance advantage and requires ongoing monitoring as new code is introduced. The new benchmark problem, 1.9x2.5 L26, has a 96x144x26 computational grid and is the initial production resolution for the finite-volume dycore within CCSM.

2.2.2 Land Model Performance

The CLM incorporates a hierarchical subgrid data structure composed of grid cells, land units, columns, and plant functional types (PFTs). Each grid cell contains one or more land units, each land unit contains one or more columns, and each column contains one or more PFTs. The land unit is intended to capture the broadest spatial patterns of physically distinct

surface types including bare ground, vegetation, lakes, and glaciers. The column subdivides the potential variability in the soil and snow state variables within a single land unit while the PFT further subdivides columns based on their biophysical and biogeochemical differences due to broad categories of vegetation.

The objectives of the land surface efforts are to establish and improve software design and documentation, develop and implement selected frameworks and interfaces for utilities and communications, optimize the performance of the model on target platforms and new computer architectures, improve subgrid scale parameterizations, and provide support to NCAR and the CCSM Land Model Working Group. Identified as high priority tasks early in the project were: the development of a Requirements Document, the design and implementation of a flexible cache-friendly decomposition, and the improvement of the subgrid scale orography for precipitation and runoff. In addition, the design, development, and implementation of a new coupling interface between the land model and the atmosphere model were suggested as high priority tasks. This coupling interface is used when CAM is run in standalone mode since it requires the land model in order to run. In the first half of the project, effort was focused on these tasks.

Identified as an objective in the second half of the project was the vectorization of the land model for use on the Earth Simulator and the Cray X1 architectures. A single source code is required that gives reasonable performance on both scalar and vector machines. Because the data structures and code were developed for scalar platforms, vectorization of the model required implementation of new data structures and modifications to all parts of the existing model code. Significant effort has been applied to this task.

Grid cells in CLM, the highest level in the subgrid scale hierarchy, correspond to physics columns in the atmosphere. A new data structure called "clumps" was created to group land grid cells into cache-friendly portions and to provide a load-balanced decomposition of the land surface. Clumps contain a varying number of grid cells because the work associated with each is proportional to the number of PFTs contained therein. Because a grid cell can not span multiple clumps, a perfect load balance may not be achieved, depending on the distribution of PFTs among grid cells.

Two new data structures, *clump2chunk* and *chunk2clump*, are initialized after both the atmosphere and the land models have performed their decompositions (Figure 2.4). These data structures may be re-initialized at any time if the physics or land decompositions change, thereby supporting future dynamic load balancing algorithms. Multiple MPI gathers and scatters were replaced by a single *MPI_alltoallv()* before and after each call to

the land model driver routine.

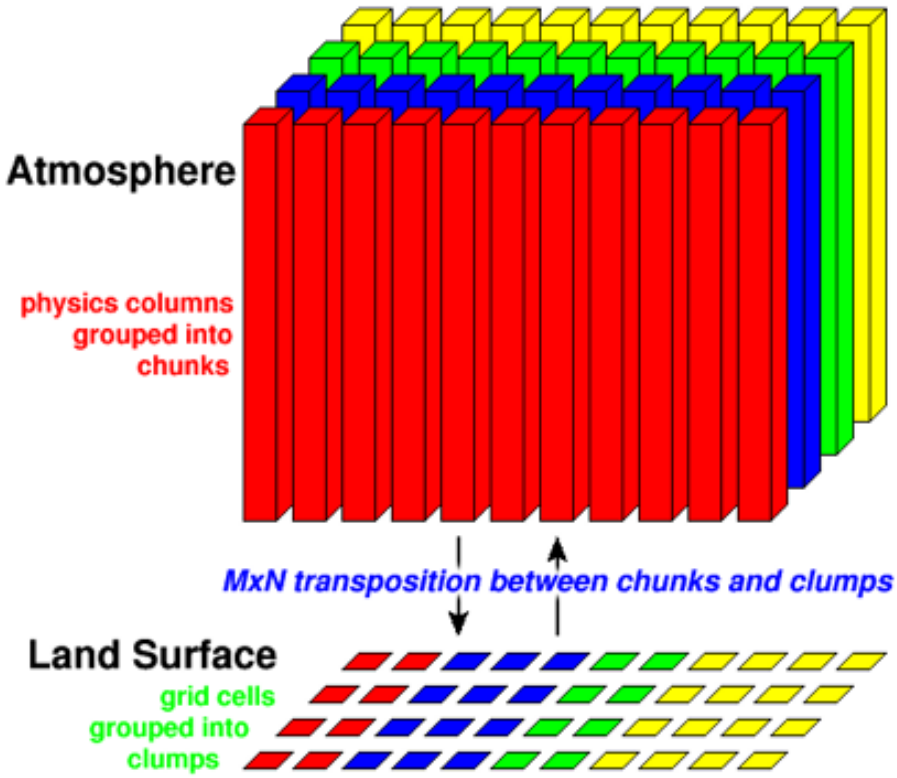

Figure 2.4: Mapping of physics columns grouped into chunks to land surface grid cells grouped into clumps.

Performance tests for the new interface were run on the IBM Power 4 at ORNL using a modified CAM2.0.1 with CLM2.0 at T42 resolution and 26 levels with the Eulerian dynamical core for 720 time steps. Mean total communications time was reduced by a factor of 7 to 9, depending on configuration. Since communication time is attributed to the land model, the improved interface reduces total land model run time. The total land model runtime consumed by communications was significantly reduced (see Figure 2.5). Even greater performance improvements would be realized at higher resolutions. On 256 processors of the IBM Power 4 at ORNL with a CAM chunk size of 16 ($pcols$=16), the new CAM/CLM interface increases the number of simulation years per day from 31 to 38. The new interface was made available to the public in the CAM2.0.2 release.

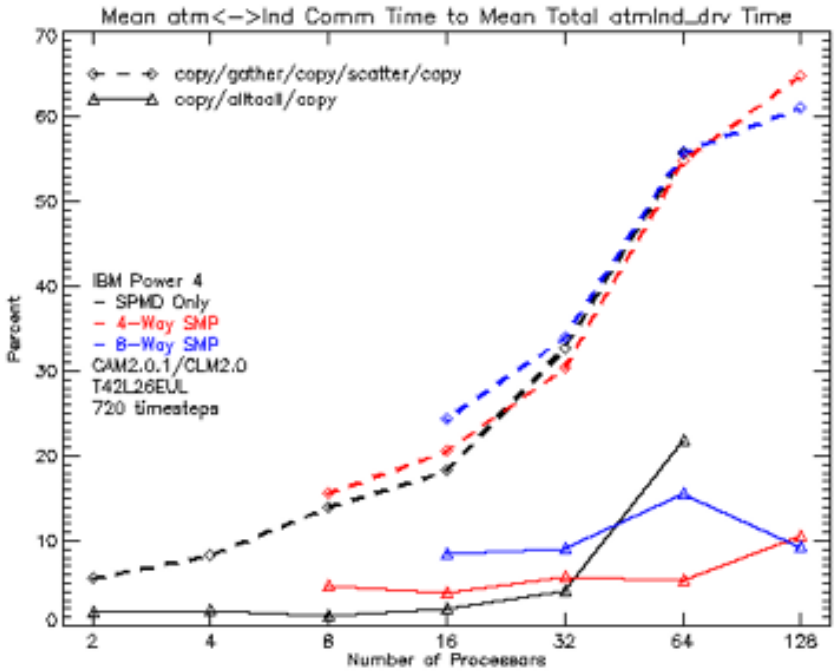

Figure 2.5: Mean atmosphere/land communications time to mean total land model run time.

2.2.3 Ocean Model Performance

At the start of our SciDAC work, the Parallel Ocean Program was at version 1.4.3 and was being adopted by CCSM version 2. This version of POP already performed quite well on vector architectures and was portable across a variety of both vector- and scalar-based computing systems. However, performance on scalar architectures suffered due to memory bandwidth limitations exacerbated by the choices of data structures and coding style. Instead, a new design based on a more flexible data decomposition scheme was developed and the new code was released in 2004 as POP version 2.0.

In POP 2.0, a sub-blocked data decomposition scheme was adopted in which the logically-rectangular domain is broken up into two-dimensional Cartesian blocks. The size of these blocks can be chosen to maximize vector lengths on vector machines or can be small to provide cache blocking on scalar processors. The blocks are then distributed across processing nodes based on the amount of work per block in an attempt to balance the computational load. Blocks containing all land points are dropped from the domain altogether, eliminating unnecessary work that was being performed in previous POP versions. Multiple blocks can be assigned to each node and OpenMP parallelism is available for operating on multiple blocks within a node; message passing continues to be used between nodes. This combination of land point elimination, load balancing and cache-blocking resulted in up to a 30% improvement in performance for high-resolution ocean simulations; performance at coarser resolution did not improve as much due to lower numbers of land blocks and block sizes that were already small in production configurations [172]. In order to estimate optimal block sizes, a performance model of POP 2.0 was developed [174], though this has not seen effective use beyond the initial validation.

The release of POP 2.0 did not occur in time to make the code freeze for CCSM3, so a modified 1.4.3 version was used for all of the IPCC assessment runs and for much of the performance tuning. During the last year of the project, a large effort has been expended to re-sychronize the LANL and NCAR versions and migrate changes from the CCSM 1.4.3 version into the 2.0 version of the model. To prevent further divergence, a public Subversion repository has been established at LANL so that the NCAR Oceanography section can make some modifications directly and can track LANL changes more quickly. Such a mechanism has been needed for some time, but was difficult due to earlier LANL computer security regulations.

Performance of various versions of the POP model were analyzed by project scientists as a part of this project and supported by collaboration

with the SciDAC performance evaluation center (PERC, with Pat Worley as part of both projects). POP 1.4.3 was ported and benchmarked on the Cray XD1 and Cray XT3. POP performance measurements were repeated on the Cray X1, tracking performance changes in the X1 sysytem software, and on the Power 4 cluster, evaluating the performance impact of the HPS ("Federation") interconnect. The good small message performance of the XD1 makes POP performance on the XD1 similar to POP performance on the SGI Altix up to 64 processors. The current poor small message performance on the XT3 seriously limits POP performance on the XT3, but this is expected to improve significantly over the next 6 months. On the X1, performance of the collective communication routines have continued to improve, and use of Co-Array Fortran to improve performance is less important than it was a year ago. The Power 4 results are improved over those collected on the earlier version of the system using the IBM SP Switch2 interconnect. However the HPS interconnect primarily increases performance for large messages, so the POP performance improvement was not significant. Figure 2.6 summarizes the performance for the "x1" benchmark across a range of systems.

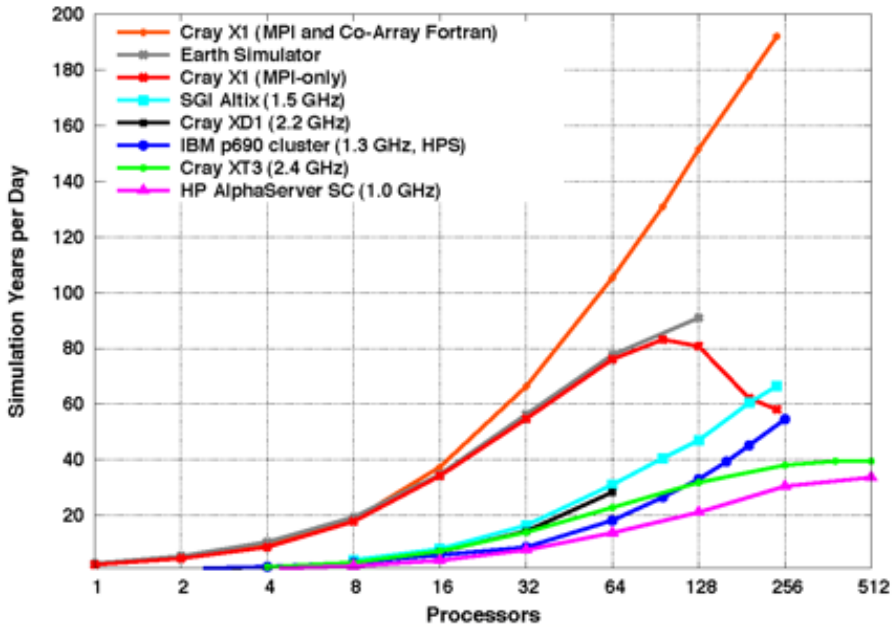

Figure 2.6: Comparison of POP performance and scalability on multiple platforms.

Analysis of POP 2.0 by project scientists at ANL involved instrumenting POP with MPE calls for visualization using the Argonne-developed Jumpshot tool. The performance of this instrumented version of POP was studied using ANL's Jazz linux cluster. Figure 2.7 shows an example Jumpshot display, showing the performance impact of small messages within POP. POP 1.4.3 and POP 2.0 were also ported to the ANL Bluegene/L (BGL) System and benchmarks were run to compare POP performance on BGL to other high-end systems (Figure 2.9). For the "x1" benchmark, with sufficient number of processors the BGL performance just exceeds that of the HP AlphaServer, both in simulation throughput (measured in model years per wall-clock day) and in the barotropic phase considered separately. Performance differs from the Cray X1 by a factor of approximately 16, an expected result given the lightweight processor design of BGL. Furthermore, tests were run using co-processor ("CO") mode of the BGL, where only one processor of each node participates in the computation and the other handles communication. Performance may be improved using virtual ("VN") mode, in which both processors are used for the application at the cost of splitting the node's memory. VN mode was not available at the time of testing but will be after system software upgrades. As the BGL runtime environment matures, tools such as Jumpshot will be brought to bear to study parallel performance.

In addition to the analysis above, additional peformance studies were carried out by NCAR scientists, Japanese scientists (as part of an Earth Simulator collaboration) and computer hardware vendors (as part of procurement benchmarking). All of these efforts have lead to code improvements that are being incorporated as part of a POP version 2.1 release in progress.

2.2.4 Sea Ice Model Performance

Early in the project, it was recognized that the LANL CICE model adopted for CCSM3 would not perform well on vector architectures due to the structure of the ice thermodynamics. In the version at that time, the thermodynamics driver called individual subroutines for each process and for each individual horizontal point (i.e. the subroutine calls sat within the loop over all horizontal points). For performance on the Cray X1 and the Japanese Earth Simulator, a significant effort was made to restructure the thermodynamics and push the horizontal loops within subroutines. Additional performance bottlenecks were identified in the use of the ice mask, resulting in the use of merged vectors of ice points rather than checking the mask

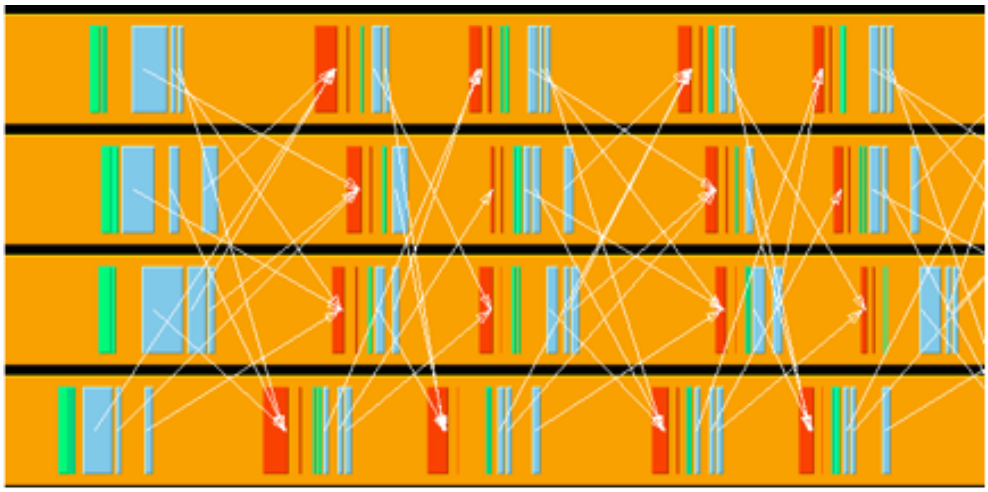

Figure 2.7: Jumpshot analysis of the instrumented POP 2.0 code running a test case on 4 processors. The image shows MPI communications at the end of the barotropic driver. Horizontal bars correspond to individual processors, the horizontal axis representing time. The gold background represents time spent in the barotropic solver. Colored vertical bars represent time spent in various MPI calls: *MPI_Isend()* (light blue), *MPI_Irecv()* (turquoise), and *MPI_Waitall()* (red). Directed arrows connect MPI send and receive operations on source and target processors, respectively.

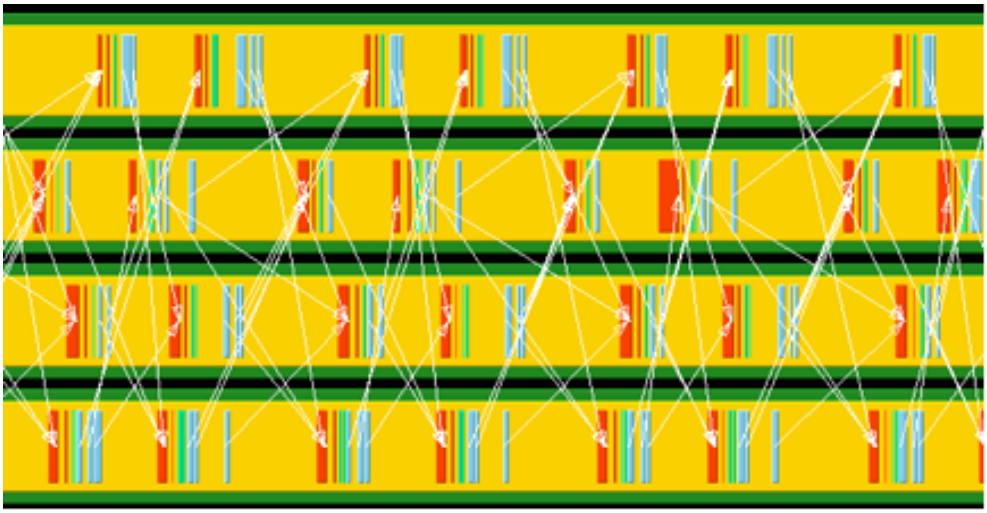

Figure 2.8: Jumpshot visualization of the POP baroclinic solver. The yellow background is the boundary condition calculation within the baroclinic solver (green). Color coding of time spent in *MPI_Isend()*, *MPI_Irecv()*, and *MPI_Waitall()* is the same as that used in Figure 2.7.

value at individual points. These changes not only enabled vectorization but improved performance of the CICE code on other platforms and were included in a CICE 3.1 release.

Later, it was decided to import the POP 2.0 infrastructure into the CICE model. The primary driver for this effort was the need to support tripole grids and remain compatible with the ocean. It will also give the CICE model the ability to eliminate regions of the globe where no ice is likely to form (e.g. the tropics). Further, it will promote code reuse between the two component models and enable easier ocean-ice standalone simulations. The new code is currently being tested in preparation for a 4.0 release of CICE.

2.2.5 Coupler and Utility Performance

As mentioned earlier, when this project started, a critical bottleneck to CCSM was related to how the physical component models were coupled together. The existing coupler was a serial code and communications between components and the coupler required all-to-one gathering of distributed arrays. In addition, CCSM software engineers were finding many cases where the CCSM model of concurrent multiple executables was not portable. To

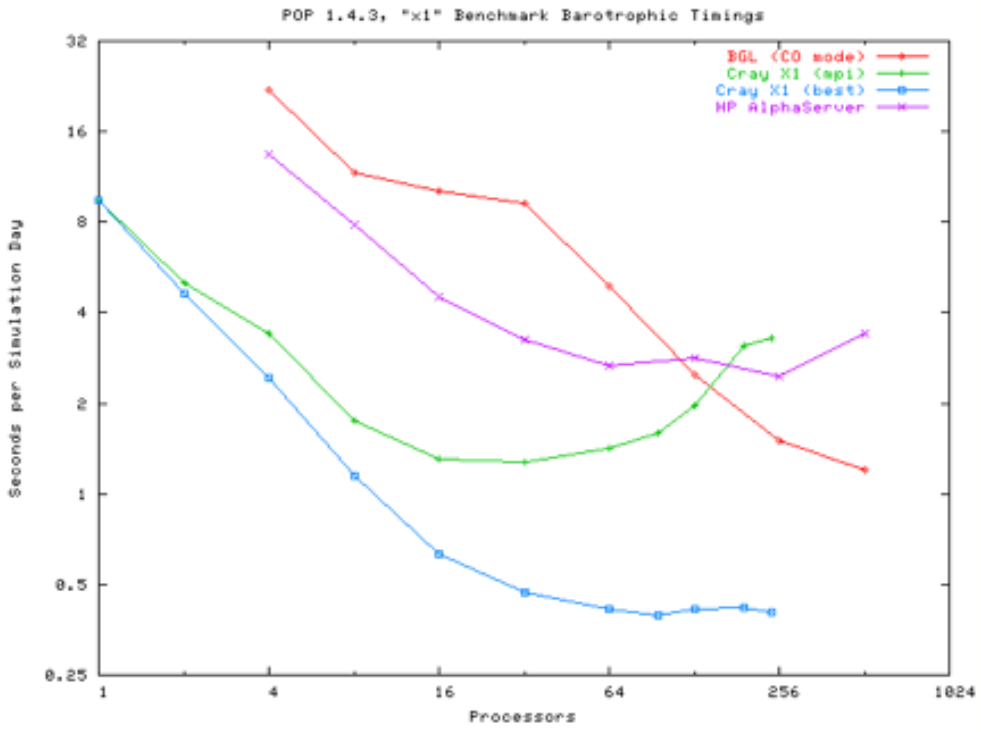

Figure 2.9: Comparison of timings for the barotropic phase of the POP x1 benchmark on the Argonne BlueGene/L, ORNL Cray X1 and Pittsburgh Supercomputer Center HP AlphaServer platforms. Performance of the barotropic phase is determined by the small message performance for large numbers of processors and limits the performance scalability of POP.

address these issues, this project developed new software libraries like MCT and MPH and collaborated on the development of a new coupler, named CPL6. The release of CCSM 3.0 in June of 2004 marked the debut release for CPL6, and also corresponded to the release of MCT 2.0.1. Several papers on these efforts appeared in a special issue of the International Journal of High-Performance Computing Applications and are likely the first time the coupling infrastructure of a climate model has been reported in detail in a refereed journal [175], [171].

Model Coupling Toolkit

The Model Coupling Toolkit (MCT) is a software library for constructing parallel coupled models from individual parallel models. MCT was created to address the challenges of creating a parallel coupler for the Community Climate System Model (CCSM). Each of the submodels that make up CCSM is a separate parallel application with its own domain decomposition, running on its own set of processors. This application contains multiple instances of the $M \times N$ problem, the problem of transferring data between two parallel programs running on disjoint sets of processors. CCSM also requires efficient data transfer to facilitate its interpolation algorithms. MCT was created as a generalized solution to handle these and other common functions in parallel coupled models. MCT s implementation of the data transfer infrastructure needed for a parallel coupled model is documented in [171]. The performance of MCT scales satisfactorily as processors are added to the system. However, the types of decompositions used in the submodels can affect performance. MCT's infrastructure provides a flexible and high-performing set of tools for enabling interoperability between parallel applications.

Development of MCT resulted in numerous incremental releases (listed at *http://www.mcs.anl.gov/mct/changes.html*) and four major releases. The important features added to MCT in these releases were: support for vector platforms, support for both 32- and 64-bit reals in the MCT API, a port to the SGI Altix platform, and a new, autoconf-based build system. Support for vector platforms such as the Cray X1, NEC SX series (including specific build system support for the Earth Simulator), and Fujitsu VPP was added to MCT by building upon and enhancing modifications to MCT's sparse matrix-vector multiplication facilities by our Earth Simulator collaborators from Fujitsu, CRIEPI, and NEC. The expansion of the MCT API to comprise variable real-number precision was accomplished by explicitly typing all real variables in MCT using Fortran's kind() facility, and now allows

MCT to be used to couple models that may be using differing real-number representations.

The four major releases of MCT were: version 2.0.0 (April 23, 2004), which was the first major release to feature the new MCT build system, and was originally the targeted release for CCSM 3.0; version 2.0.1 (May 24, 2004), which included some minor bug fixes and was the version distributed with CCSM 3.0; version 2.0.2 (July 11, 2004), which incorporated more bug fixes; and version 2.1.0 (February 14, 2005), which included Cray X1 compiler directives to improve vector performance on this platform and slight alteration of some AttrVect query methods to allow CPL6 to handle exceptions. This version also marked the debut of Babel-based multilingual bindings for MCT, which are available as a separate download and are described in detail below.

Expansion of MCT's programming model beyond Fortran was accomplished in prototype form by leveraging work from the Common Component Architecture's (CCA) SciDAC-funded Center for Component Technology for Terascale Simulation Software. We wrote a restricted description of the MCT API in the scientific interface definition language (SIDL). This version of the MCT API is restricted in the sense that SIDL does not support the use of optional arguments, whereas Fortran does, and MCT uses this feature. The MCT SIDL API is processed using the Babel language interoperability tool (another CCA product) to automate the creation of interlanguage glue code, resulting in both C++ and Python bindings for MCT. We have created a working purely C++ example that uses MCT to perform parallel coupling. Collaborators at the University of Chicago have created a corresponding working Python example, and are working on a Python version of MCT.

Also recently completed but not yet released is a serial MPI-compatibility library to support MCT on platforms that do not have MPI installed. This will be used for benchmark comparisons, eliminating the unnecessary overhead of MPI. It will also be useful for code development of MCT-based models on workstations and laptops. Typical "stub" libraries do not support complex MPI behaviors such as immediate-mode sends and receives (e.g. *MPI_Isend()*, *MPI_Irecv()*). This library supports them as well as providing complete MPI- handle support for Fortran MPI-based packages such as MCT.

For the coupler and coupled system, we have worked to:

- develop a single-executable CCSM with concurrent component scheduling;

- develop a sequentially scheduled "event-loop" version of CCSM;
- complete changes required to implement a biogeochemical cycle in CCSM; and
- improve the ice-coupler communication speed in CCSM through masked data transfer.

For MCT, the project:

- finished testing and released a version of MCT that operates in the absence of MPI;
- implemented on-line generation of interpolation matrix elements using either a sequential version of SCRIP or a parallel implementation; and
- incorporated OpenMP directives in the code to improve scaling and full use of available resources when MCT is used in a hybrid parallel environment.

We have prepared two important documents to support users of CPL6 and CCSM developers who intend to extend or modify the coupled model: "CPL6 API Reference Manual," which documents CPL6's interfaces, and "CPL6 User's Guide, Source Code Reference and Scientific Description," which offers valuable information to CPL6 develpors. An MCT Users' Guide is available, and we have added a CCSM Web support site:
http://www.mcs.anl.gov/mct/CCSM_MCT.html

Multi-Program Handshaking

A critical task for effectively running multi-executable applications on distributed memory architectures is a handshaking process that enables each component model to get the necessary information about other component model executables. A general-purpose multi-program handshaking (MPH) library was developed to handle the handshaking process so that different executables communicate as if they are parts of the same single executable. This makes use of the advanced multi-program multi-data (MPMD) mode of many HPC platforms. MPH enables different executables to recognize each other and sets up a registry of executable names and communication channels among different components.

We identified five effective execution modes and developed MPH to support these modes.

1. Single-Component, Single-Executable application

2. Multi-Component, Single-Executable application

3. Single-Component, Multi-Executable application

4. Multi-Component, Multi-Executable application

5. Multi-Instance, Multi-Executable application

MPH provides the key infrastructure for integrating separate executables together. It provides functionalities for component name registration, resource allocation and communication channels initialization between independent components. MPH also supports component joining, inter-component communication, inquiry on multi-component environment, and redirection of input and output. MPH provides a flexible, versatile mechanism for these tasks, which are foundations for larger software tools and frameworks.

MPH provides a convenient framework to do the ensemble simulations. A multi-instance executable is a special type of executable. It differs from regular single-component and multi-component executables in that this particular executable is replicated multiple times (multiple instances) on different processor subsets. This enables running ensembles simultaneously as a single job, with ensemble averaging done on the fly. Not only is this an effective way of using existing computing resources, it also reduces the potential human error by reducing the number of jobs that need to be monitored. This could eliminate large data output and storage for post- processing averaging, and enables on-the-fly nonlinear ensemble statistics that are otherwise impossible to compute as a post-processing step.

All MPH functionalities are currently working on IBM SP, SGI Origin, HP AlphaServer SC, and Linux clusters. MPH is adopted in the Coupler Component (CPL6) in CCSM 3.0 public released version (June 2004) and subsequent development versions. It is also used by many models for coupling model components, including Model Coupling Toolkit (MCT), NCAR MM5/WRF models, and Colorado State University (CSU) Geodesic Grid Model. MPH also facilitates multi-instance ensemble simulations (with each instance as a model component within an executable), used by applications in European Centre for Medium- Range Weather Forecasts (ECMWF), the Edinburgh Parallel Computing Centre (EPCC), NCAR, and many others including a Monte Carlo code running on 1024 processors.

Concurrent Single-executable CCSM Development

The current CCSM is a multi-executable system running under the MPMD mechanism.We have developd a concurrent single-executable version of CCSM that coexists with the multi-executable option.

Design issues that have been resolved are:

- Co-existence of multi-executable and single-executable modes. This is accomplished by redesigning the top level CCSM structure. Only a minor redesign of top level source code is necessary to switch between MPMD and SPMD modes. For the single-executable, a master program is also added.

- Flexible switching among different model options: real model, data model, and dead (mock) model.

- Allowing different number of OpenMP threads set on different components. For the single-executable, this is set from each component dynamically at runtime (instead of using environmental variables for multi-executables).

- Allowing MPI tasks per node set differently on different components. This is systematically resolved by using task geometry and MPMD command files.

We also developed a module-based approach to solve name conflict issues associated with single-executable CCSM. The module-based approach uses a wrapper module and "use module only" renaming variables on the fly. The key idea is localization of global symbols. The wrapper module is used to hide stand-alone subroutines of a component model so they become local entities of the wrapper module, and no global names are generated for these subroutines. There is minimal renaming when different component modules are used in a same file. This solution is less tedious than adding a prefix to all subroutine names.

As of 2006, the Single-executable CCSM worked on NERSC IBM SP3 (Seaborg), and NCAR IBMs SP4 (Bluesky), NCAR IBM SP5 (Bluevista), and ORNL Cray-X1 (Phoenix). Both modified single-executable and modified multi-executable CCSM generate bit-for-bit results when compared with the original multi-executable CCSM for all model configurations. Preliminary performance data shows run time within 10% difference from original multi-executable CCSM runs.

Detailed information about the MPH library and single-executable CCSM is available from: *http://hpcrd.lbl.gov/SCG/acpi/MPH/* and *http://hpcrd.lbl.gov/SCG/acpi/SE*.

Parallel I/O

In the first half of the project we integrated our parallel I/O library (ZioLib) into CAM. In our most recent work, we integrated/incorporated the parallel netCDF library developed at ANL and Northwestern University under the Scientific Data Management project of SciDAC for use in distributed memory computers. This provides a full parallel I/O capability that will be maintained. We found it is more efficient and convenient to incorporate parallel netCDF directly into CAM instead of going through the extra layer of ZioLib.

CAM3.0 uses sequential I/O by gathering all 3D fields into a master task and writing them from that task. Using parallel netCDF, no such collective gathering is necessary. Therefore, not only is the I/O speed improved, but the large memory requirement on a single node for such gathering is also lifted. Overall, the new implementation speeds up I/O by a factor of 4 with T85L26 resolution. Some timing results are given in the table below:

Processors	Writers	16	32	64	128
T42-resolution					
Serial netCDF (s)		52	54	55	55
Parallel netCDF (s)	M4	34	66	40	46
	M2	30	64	44	68
T85-resolution					
Serial netCDF (s)		272	276	283	281
Parallel netCDF (s)	M4	106	90	74	79
	M2	80	83	80	88

Table 2.1: In the table, times are in seconds. We list the total number of processors, the number of processors in a MPI-task (M4 refers to 4 processor per MPI-task). The most relevant timing is on 64 processor with M4, which is the most common configuration for production runs. For this configuration, the history file output reduces from 283 seconds to 74 seconds. We expect more significant speedup for higher resolutions.

The first implementation was for the Semi-Lagrangian dynamical core version of CAM3.0 for all history related input and output, and confirmed

bit-for-bit agreement of the generated history output files with those generated with the existing CAM. These modifications have now been extended to the other dynamical cores as well. The changes made in the source are extensive because all parallel netCDF subroutines are different from their sequential counter parts and several new ones are also introduced. Most of the netCDF I/O interface has been changed to parallel netCDF I/O interface. Besides making CAM compatible and consistent with parallel netCDF, the major scheme/algorithmic change is in the subroutine *dump-field* which writes out the history file.

2.3 Physical Model Developments

After the release of the CCSM3 model, the emphasis of the project changed somewhat with more focus on extension of the model to new scientific capabilities. These improvements are described below for each model component. The most significant model improvements were for atmospheric chemistry and land and ocean biogeochemistry. Because these changes are more extensive, they are described in a later section while this section focuses on physical model improvements.

2.3.1 Atmosphere Model Development

Downscaling and Subgrid Orography Scheme

For many applications of climate models, such as estimating the impacts of global climate change, the grid size of global climate models is too coarse to provide information that is directly useful. For example, in regions with complex terrain much of the spatial structure of precipitation occurs on scales less than 50 km, and for snow water (which is heavily relied on as a natural reservoir of water but is sensitive to climate change) variability on scales down to 5 km are important. Such scales are far finer than is practical for the ensembles of multi-century simulations that are currently and for the next five years expected to be used to project future climate change. Thus, the climate impacts community has had to and will continue to rely on a variety of methods for downscaling global climate simulations to scales between 5 and 50 km.

During this project we applied the Leung and Ghan (1995, 1998) subgrid orography scheme to the NCAR CAM and used it to downscale global climate change for a full century. The scheme, which applies all of the atmospheric and land surface physics to each of a moderate set of elevation classes

within each grid cell and then in postprocessing distributes the climate for the elevation classes according to the high-resolution distribution of surface elevation, was first developed by Leung and Ghan using a regional climate model (Leung and Ghan, 1999a,b). We applied the scheme to a branch from a prototype of CAM3 [369], and then maintained the branch throughout the project as the developmental trunk of CAM was updated. Since the subgrid scheme lies between the column physics and the dynamics, separate applications of the scheme are required for each dycore; we applied the scheme to the Euler and Finite-Volume dycores in CAM. Figure 2.10 compares the global distribution of the simulated and observed annual precipitation at 20 km resolution.

Recognizing the potential large load imbalance introduced by the heterogeneous distribution of the number of elevation classes in each grid cell, we introduced a static load balancing scheme that distributes the number of elevation classes (and hence columns for atmospheric and land surface physics calculations) uniformly across all processors both within and between computational nodes ([162]).

To demonstrate the potential value of the subgrid scheme, we drove this version of CAM using ocean surface conditions and CO_2 concentrations from a CCSM simulation of the IPCC A1B scenario [96]. The ocean surface conditions (surface temperature and sea ice cover) were adjusted to correct for the bias in the CCSM simulation for the period 1980-2000 [78]. The 2x2.5 resolution simulation was initialized at the year 1977 and run through year 2100. It was evaluated for the period 1980-2000 by comparing with high-resolution (2.5 minute) gridded analyses of station measurements of precipitation, surface temperature, and (for the Western U.S.) snow water equivalent (Ghan et al., [77]) for ten selected regions with complex terrain. Our analysis of the climate change (Ghan et al., [78]) focused on the same climate variables for the same ten regions and for the periods 2040-2050 and 2090-2100. Figure 2.11 shows the change in precipitation between the periods 1980-2000 and 2080-2100. We found snow water reductions (compared with the period 1980-2000) exceeding 50% in many regions, but also found the snow loss in some regions is artificially limited by an upper bound on snow water that is applied in the CLM to compensate for the absence of any treatment of snow loss by downslope slides.

One major weakness of the subgrid scheme is the neglect of the rain shadow effect; precipitation within a grid cell is assumed to be the same on the windward and lee sides of mountain ranges. To address this weakness we developed a rain shadow scheme that distinguishes between elevation classes on the windward and lee sides of mountain ranges, with precipitation from

the classes on the windward side depleting cloud water from classes on the lee side, and with the precipitation distributed across the grid cell according to the wind direction.

Although we coded the rain shadow scheme in CAM, we did not test it because the SciDAC leadership decided to terminate this downscaling work at the end of the project. We instead focused our effort on updating the scheme in CAM so that it could be merged onto the developmental trunk of CAM before the end of the project. However, discussions with the land model working group (which of the CCSM working groups would benefit most from the downscaling scheme) and with the CCSM Science Steering Committee led to the conclusion that the subgrid scheme should not be merged with the developmental trunk because of the lack of software engineering support available to support it as the CLM adopts a grid that is independent of the CAM grid.

During the last six months of the project we focused on a second straightforward application of the subgrid scheme. We performed a ten-year CAM simulation with the subgrid scheme at 1x1.25 resolution, and saved CAM history that was then used to provide boundary conditions for a 15 km resolution simulation of the Western U.S. by the regional climate version of the NCAR Weather Reseach and Forecasting (WRF) model. The CAM history was mapped to the same 15 km resolution as the WRF simulation for direct comparison with gridded observations at the same resolution. A second WRF simulation was also performed using National Center for Environmental Prediction analysis for boundary conditions. At least one and perhaps three papers will be written based on these simulations.

Simulations:

- 2x2.5 CAM/CLM with subgrid scheme years 1980-2000.
- 2x2.5 CAM/CLM with subgrid scheme years 1977-2100 of IPCC A1B scenario.
- 1x1.25 CAM/CLM with subgrid scheme years 1994-2003.
- 15 km WRF Western U.S. 1994-1999 NCEP boundary conditions.
- 15 km WRF Western U.S. 1994-1999 CAM boundary conditions .

High-Resolution Climate Simulations with the CAM2 and CAM3 Atmosphere Models

Another approach to getting improved solutions for use in regional climate prediction is to increase the resolution of the global model. We performed

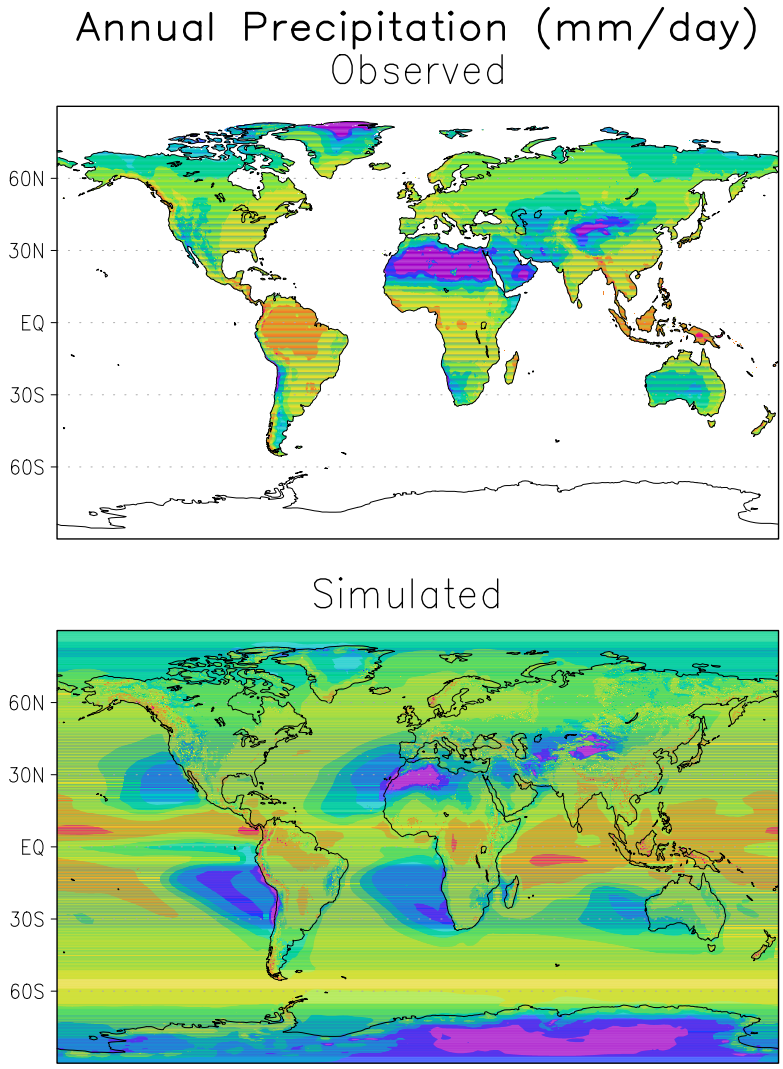

Figure 2.10: Downscaled global annual precipitation observed and simulated

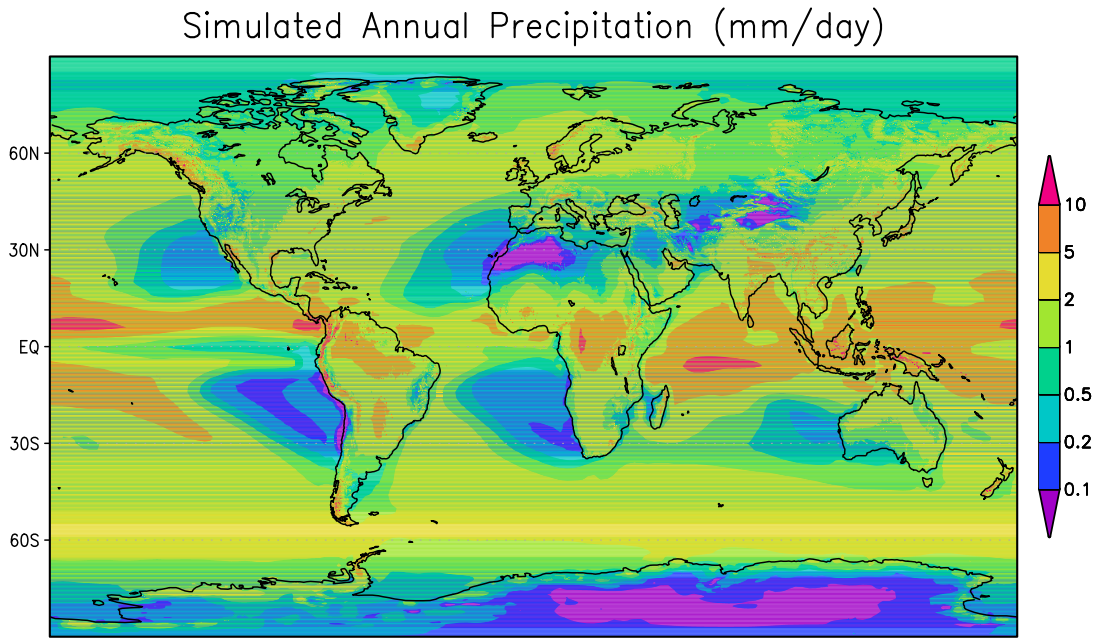

Figure 2.11: Change in downscaled simulated global annual precipitation between the periods 1980-2000 and 2080-2100.

and analyzed simulations of the global climate using the CAM2 and CAM3 global atmospheric climate models at spatial resolutions ranging from 2.0 x 2.5 to 0.4 x 0.5 degrees. In both models, configurations based on the Finite Volume dynamical core were evaluated with both the multi-year time-averaged climate and (in CAM2) simulated climatic responses to the 1997-1998 El Nino. Analysis of 20 meteorological quantities shows that the multi-year time-average climate in the CAM2 model has much less sensitivity to spatial resolution than is found in identical analyses of results of two related models, CCM3 and FVGCM. In simulations of the 1997-1998 El Nino, the CAM2 model reproduces largescale patterns of anomalies of temperature, precipitation, surface pressure, and zonal wind speed. However, regional-scale anomalies are often not accurately reproduced, and anomalies are not clearly more accurate at high resolution (0.5 x 0.625 deg.) than at coarse resolution (2.0 x 2.5 deg.). The response to El Nino of vertical distribution of clouds in the tropical Pacific is qualitatively correct but much smaller than the observed response. Analysis of CAM3 results shows similar sensitivity to resolution as in CAM2. The resolution-sensitivity of the finite-volume configuration of CAM3 used here is remarkably similar to that seen in configurations using the Eulerian spectral dynamics, and very different from that seen in a configuration using an embedded cloud-system resolving model instead of cloud parameterizations. This suggests that the resolution sensitivity is determined more by "physics" than by dynamics.

Models and Simulations

We performed simulations of the global climate with two versions of the CAM. With CAM2 we performed and analyzed simulations at spatial resolutions of 2.0 x 2.5 deg., 1.0 x 1.25 deg, 0.5 x 0.625 deg, and 0.4 x 0.5 degrees. With CAM3, we performed AMIP simulations at spatial resolutions of 2.0 x 2.5 deg., 1.0 x 1.25 deg, and 0.5 x 0.625 degrees.

The default configurations of CAM2 and CAM3 use Eulerian spectral dynamics at T42 truncation, corresponding to a horizontal grid size of 2.8 x 2.8 deg. In the simulations discussed here, the models were configured using the Finite-Volume dynamical core. This dynamical formulation was developed at the NASA Goddard Space Flight Center. With CAM2, we performed simulations at the following four spatial resolutions: B32 (2.0 deg. x 2.5 deg.), C32 (1.0 deg. x 1.25 deg.), D32 (0.5 deg. x 0.625 deg.), and 0.4 deg. x 0.5 deg. CAM2 simulations used 32 levels in the vertical. In all of our simulations, the model was forced with prescribed sea surface temperatures (SSTs) and sea-ice extents. Two simulations used observed monthly-mean SSTs corresponding to the years 1980 through 1990. The other two used climatologically-averaged monthly-mean SSTs, which were

obtained by time-averaging observed SSTs for the years 1980 through 1990. Salient features of our CAM2 simulations are shown in Table 2.2.

Resolution	Prescribed SSTs	Number of Years Analyzed
B32	Climatology from AMIP [2]	10 years
C32	AMIP [2]	10 years (1980 through 1990)
D32	AMIP [2]	5 years (1980 through 1990)
0.4 degree x 0.5 degree	Climatology from AMIP [2]	5 years

Table 2.2: Properties of CAM2 simulations

With CAM3, we performed simulations at three spatial resolutions: B (2.0 deg. x 2.5 deg.), C (1.0 deg. x 1.25 deg.), and D (0.5 deg. x 0.625 deg.):

- "b26," using the standard CAM3 finite-volume model with grid spacing of 2.0 x 2.5 deg (latitude/longitude);
- "c26," using the standard CAM3 finite-volume model with grid spacing of 1.0 x 1.25 deg (latitude/longitude); and
- "d26," using the standard CAM3 finite-volume model with grid spacing of 0.5 x 0.625 deg (latitude/longitude).

All model configurations used 26 levels in the vertical in the GCM. All were driven by prescribed, observed, yearly-varying SSTs for the period 1979-1999. Parameter values in the b26, c26, and d26 model configurations independently tuned. The b26 configuration was tuned thoroughly by researchers at NCAR. We performed less comprehensive retunings of the c26 and d26 configurations. In these processes, several cloud-related parameters were adjusted with the goal of optimizing simulated energy fluxes.

Evaluation of the CAM2 multi-year time-averaged climate

We compared 22 simulated climate quantities to corresponding observations (or reanalysis), using Taylor diagrams. Prior to comparison, a monthly-mean climatology was calculated for each variable from the model output and from the observations or reanalysis, by averaging monthly-mean results over all available years. Also each simulated variable was regridded to the grid of the corresponding observation (which varies from observation to observation).

A Taylor diagram was plotted for results of all CAM2 simulation (Fig 2.3.1). In order to show how the agreement between the simulated variable and the observation depends on model resolution, the dots corresponding to the different simulations of a same variable were connected by arrows

(the arrows go from one resolution to the next finer resolution, for example from 2 x 2.5 to 1 x 1.25). The *zg500, ta850* and *tas* variables show a very good agreement with observations across the different resolutions. Other variables such as *prw, rsut, rsutcs*, or *hus850* also show a relatively good agreement with the observations. On the other hand, the *clt, ta200, tauv, va200, va850, hfls* and *pr* variables agree relatively poorly with observations. It has to be noted though, that the apparent ability of the model to simulate a specific variable may for some variables depend strongly on the reference observation chosen. Different observational data sets sometimes differ significantly from one another, and a variable that has a good agreement with a set of observations may have a poor agreement with another. This can be the case for variables such as *hfls, tauu* or *tauv*.

For most variables, the agreement of the model with the observations either does not improve or improves very little from the B32 simulation (2 degrees x 2.5 degrees) to the finest-resolution (0.4 degree x 0.5 degree) simulation.

The same exercise was performed for two global climate models that are closely related to CAM2. The CCM3 model is the immediate predecessor to CAM2; we analyzed results of this model obtained using Eulerian spectral dynamics at T42 and T170 truncations (resolutions of 2.8 deg and 0.7 deg, respectively). As configured for our simulations, CAM2 differs from CCM3 in both dymanics and aspects of the model physics. The CCM3 results are shown in Fig. 2.3.1. These results show greater sensitivity to spatial resolution than results of CAM2 do. We also analyzed results of the NASA/NCAR Finite-Volume General Circulation Model (FVGCM; *http://gmao.gsfc.nasa.gov/sci_research/NASanCAR/*). We ran this model at the B32 and D32 resolutions (2.0 x 2.5 deg, and 0.5 x 0.625 deg, respectively.) This model uses the same physics as CCM3, and the same finite-volume dynamical core as we used in CAM2. The FVGCM results are shown in Fig. 2.3.1. In the FVGCM results, most variables agree better with the observation in the higher resolution simulation (most arrows point toward the point of reference). Thus, the FVGCM results show more sensitivity to spatial resolution than both the CAM2 results and the CCM3 results.

Simulated response to 1997-1998 El Nino in CAM2

We assessed how well the CAM2 model simulates the effects of El Nino on climate at model resolutions of 2 degrees x 2.5 degrees and 0.4 degree x 0.5 degrees. We did not predict the occurrence of El Nino, but rather its climatic consequences (precipitation anomalies, etc). At both B32 and D32 resolutions, we performed ensembles of 5 simulations forced with prescribed

observed sea surface temperatures (SSTs) from 1997-1998, when the most recent, largest, and best-observed El Nino occurred. For comparison, we also performed ensembles of simulations forced by muti-year average (climatological) monthly-mean SSTs.

At the global scale the model is able to simulate the main spatial patterns of the DJFM El Nino precipitation anomaly (not shown). However, the details of these patterns are often misrepresented.

At the 2 degrees x 2.5 degrees resolution (Fig. 2.3.1), the CAM2 model simulates the general pattern of El Nino induced precipitation anomalies in the U.S.; however these anomalies are generally too weak (Figure 2.3.1). At 0.4 degree x 0.5 degrees (Fig. 2.3.1), the agreement between the model and the observations seems to get worse. In particular, the precipitation increase over the Pacific Ocean and over the west coast of the U.S. is almost totally absent. This seems to be due to an overestimation by the model of the climatological precipitation over these regions.

As for precipitation, the CAM2 correctly simulates the gross spatial patterns of DJFM El Nino-induced anomalies of skin temperature, sea level pressure, and the eastward wind speeds at 20,000 Pa and 85,000 Pa. However, the regional details of these anomalies are often poorly represented. None of these simulated anomalies showed any obvious improvement when the CAM2 resolution was increased from 2.0 degrees x 2.5 degrees to 0.4 degree x 0.5 degrees. For some variables, such as precipitation, the model results are worse at the higher resolution. This is generally consistent with the model's weak sensitivity to resolution in simulating the time-averaged present climate.

The El Nino phenomenon has a strong signature on clouds. In particular, it changes the vertical distribution of clouds over certain regions, especially the tropical Pacific Ocean. We evaluated the ability of the model to simulate El-Nino induced changes in vertical distribution of clouds, using the approach of Cess et al. [3]

First we plotted vertical profiles of the cumulative cloud frequency, the frequency of clouds found above a given altitude, for both the climatological DJFM season and for the 1997-1998 DJFM (El Nino) season (Figs 2.3.1).

Over the tropical Pacific, the observed cumulative cloud frequency goes from low values at 15 km to values close to 100% (sky totally cloudy), when integrated vertically over the whole column near the surface, in all cases. For the Western Pacific region (Fig 2.3.1), the vertical profile of the observed cumulative cloud frequency strongly shifts to the left from the 1985-1991 DJFMA climatology to the 1997-1998 DJFMA seasonal mean. This indicates that the amount of high clouds decreased during the 1998 El Nino

event over the Western Pacific, while the amount of low clouds increased. On the contrary, over the Eastern Pacific region (Fig. 2.3.1), the cumulative cloud frequency remains low above the altitude of 3 km (it reaches the value of 40% at about 3 km) in the climatological DJFMA season, while it is strongly shifted to the right (the value of 40% is now reached at 13 km) in the 1997-1998 DJFMA season. Similarly, this indicates that the amount of high clouds dramatically increased over the Eastern Pacific during the 1997-1998 El Nino event, while the amount of low clouds decreased.

For CAM2, over the Western Pacific (Fig. 2.3.1), the vertical profile of the simulated climatological cumulative cloud frequency is in relatively good agreement with observations, as it shows a domination of high clouds at both resolutions. However, in the 1997-1998 DJFM season, the vertical profiles of simulated cumulative cloud frequency do not show as large a decrease in high clouds or an increase in low clouds as is seen in the observations. Over the Eastern Pacific (Fig. 2.3.1), the difference between the vertical profiles of cumulative cloud frequency in the climatological and the El Nino simulations is greater, but there are still large misrepresentations. We also noticed that the CAM2 model tends to underestimate the total cloud cover, as the cumulative cloud frequency does not reach values close to 100 % near the surface.

In summary, although the CAM2 model is able to simulate the large-scale spatial patterns of the climate response to El Nino, the details of this response are often misrepresented. For example, over the Western U.S., the positive precipitation anomaly is underestimated at the 2 degrees x 2.5 degrees resolution and is almost nonexistent at 0.4 degree x 0.5 degree. Simulated El Nino-induced changes in the vertical distribution of clouds in the tropical Pacific are qualitatively correct but smaller than observed changes.

Global- and annual-mean precipitation amounts are nearly identical in all CAM3 simulations. This is not especially surprising, given that all use the same, prescribed SSTs, which will tend to produce the same evaporation rates. Similarly, zonal- and annual-mean precipitation is quite similar in these simulations (Figure 2.3.1); differences among them in this quantity are smaller than differences between any simulation and the Xie-Arkin observations [31]. Simulated mid-latitude maxima in precipitation associated with storm tracks are higher than observed and are located too far poleward; however, this is the case in both conventional and MMF-based simulations.

In the tropical Pacific region, the parameterized model configurations have difficulty representing the shape of the ITCZ in both DJF and JJA; this well-known double ITCZ problem is insensitive to increasing spatial

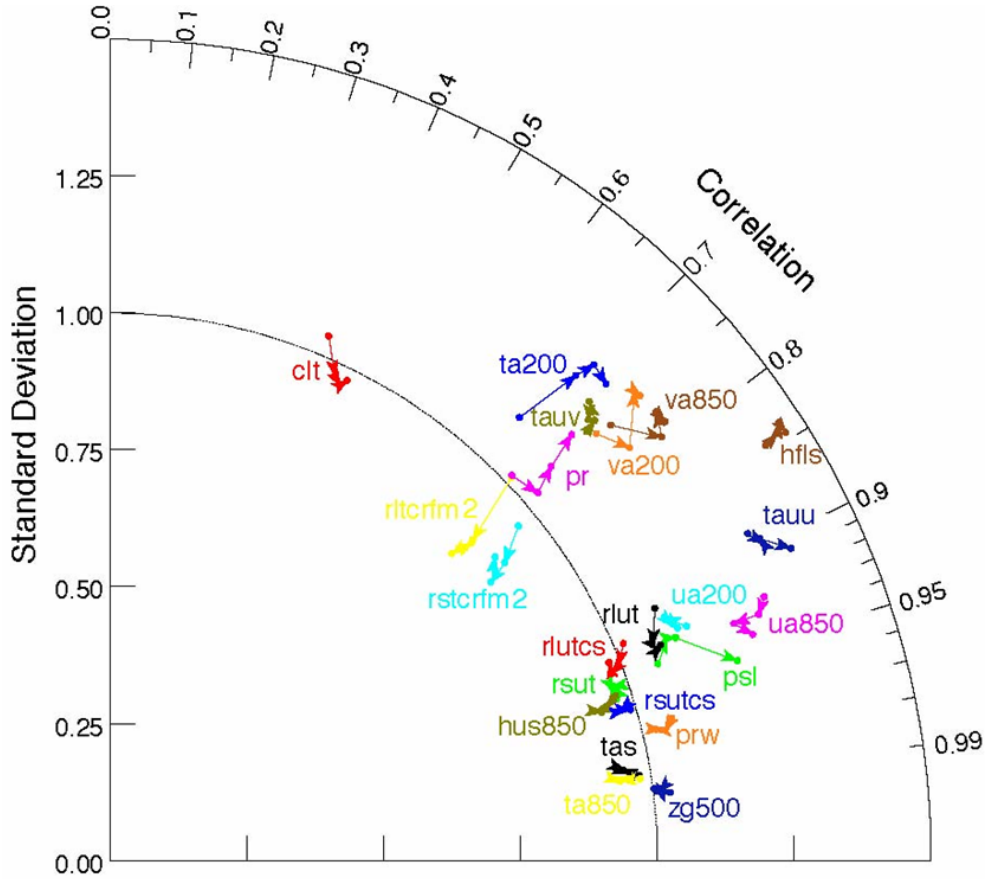

Figure 2.12: Taylor diagram representing the CAM2 simulations at all four resolutions. The arrows go successively from B32 to C32, from C32 to D32, and from D32 to 0.4 x 0.5; they show for each variable how the agreement of the simulations with the observations or reanalysis evolves across the resolutions.

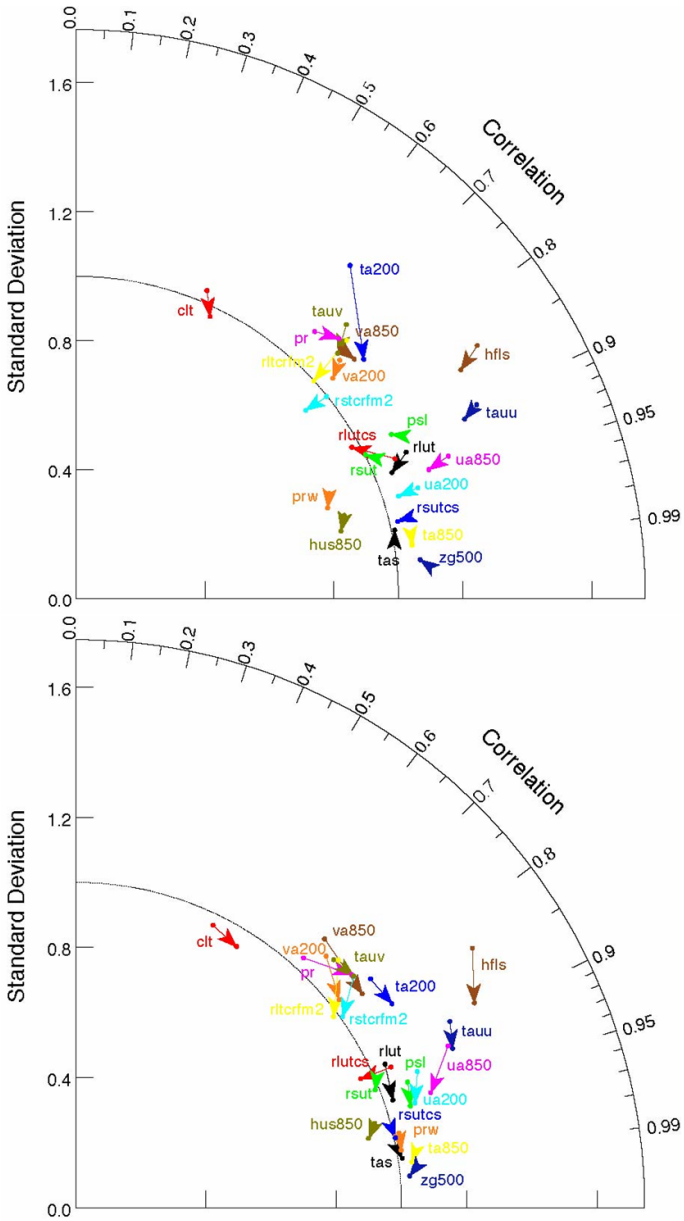

Figure 2.13: Taylor diagrams for the CCM3 model ((a) CCM3 at T170 vs. CCM3 at T42, the arrows go from T42 to T170) and for the FVGCM model at 0.4 degree x 0.5 degree vs. FVGCM at 2 degrees x 2.5 degrees ((b) the arrows go from 2 x 2.5 to 0.4 x 0.5).

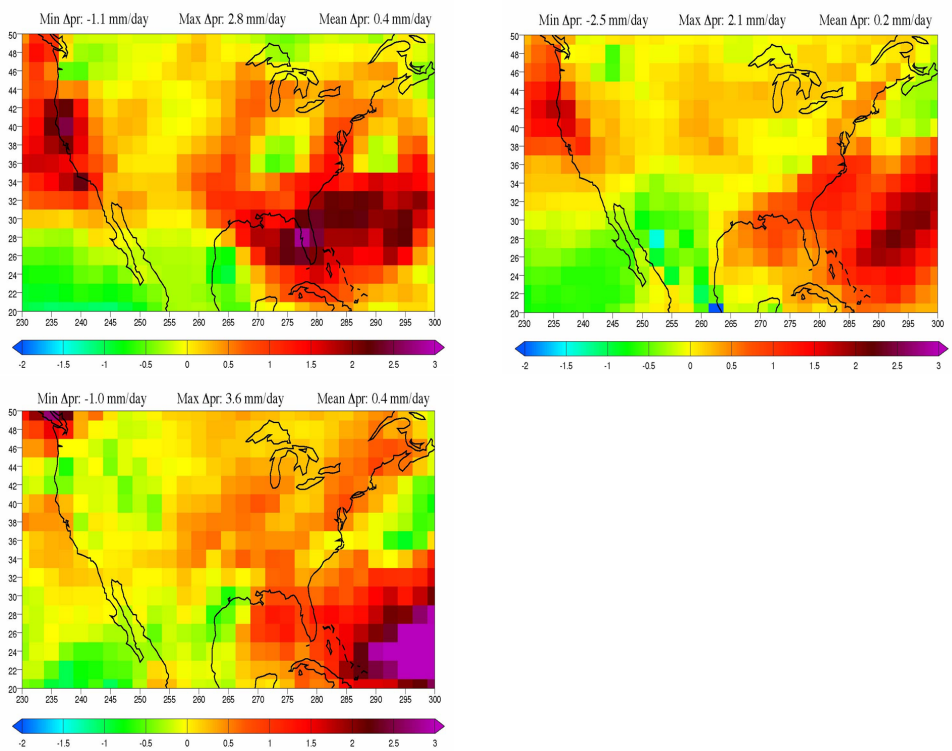

Figure 2.14: Precipitation anomaly for the 1997-1998 DJFM, over the continental U.S. (a) CMAP observation, (b) 2 degrees x 2.5 degrees, (c) 0.4 degree x 0.5 degree regridded to 2 degrees x 2.5 degrees.

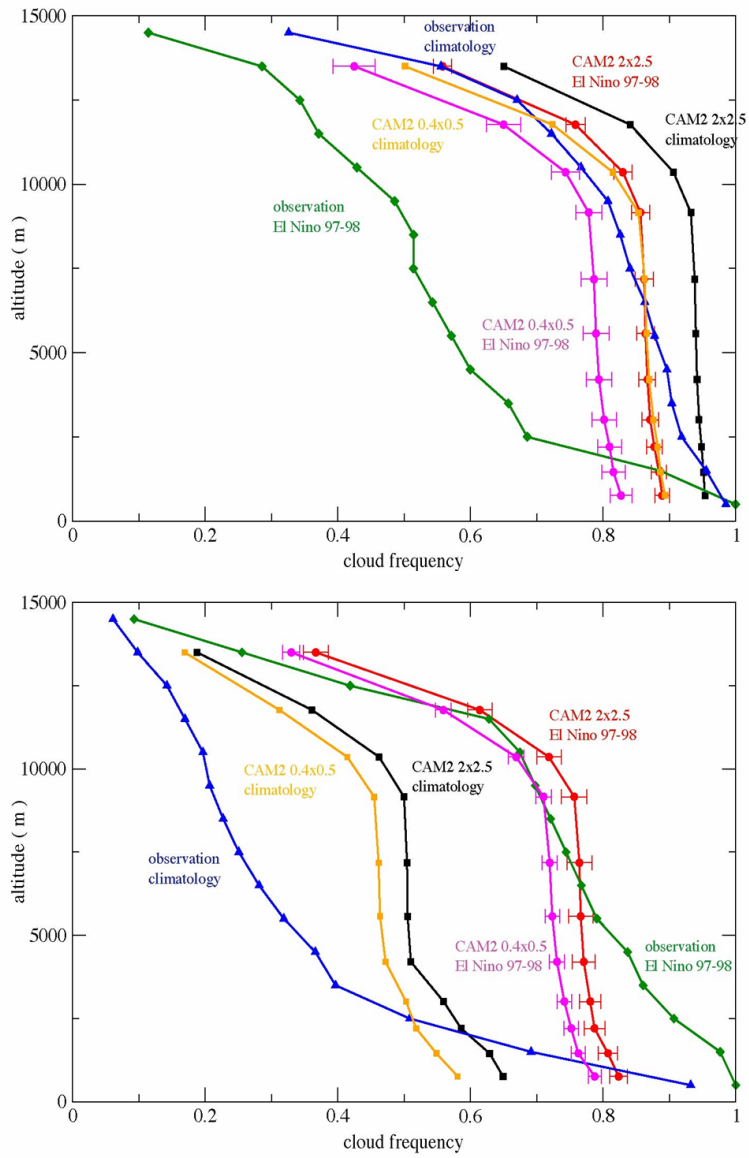

Figure 2.15: Vertical profiles of the cumulative cloud frequency over the tropical Pacific. The observational data were provided by Cess et al., (a) Western tropical Pacific, (b) Eastern tropical Pacific.

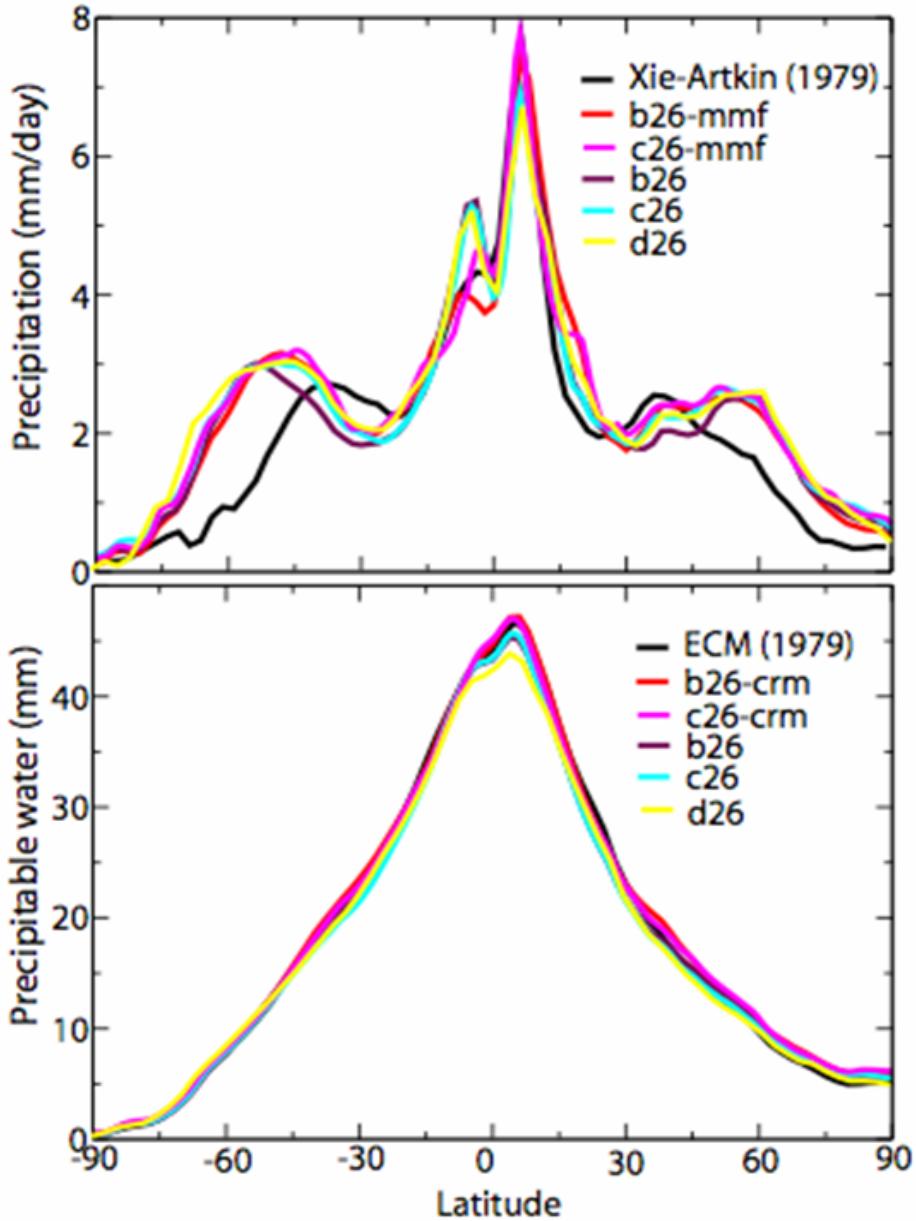

Figure 2.16: Top: Simulated zonal- and annual-mean precipitation for 1979, compared to the Xie-Arkin observational data set. Bottom: Simulated zonal- and annual-mean precipitable water for 1979, compared to ECMWF reanalysis.

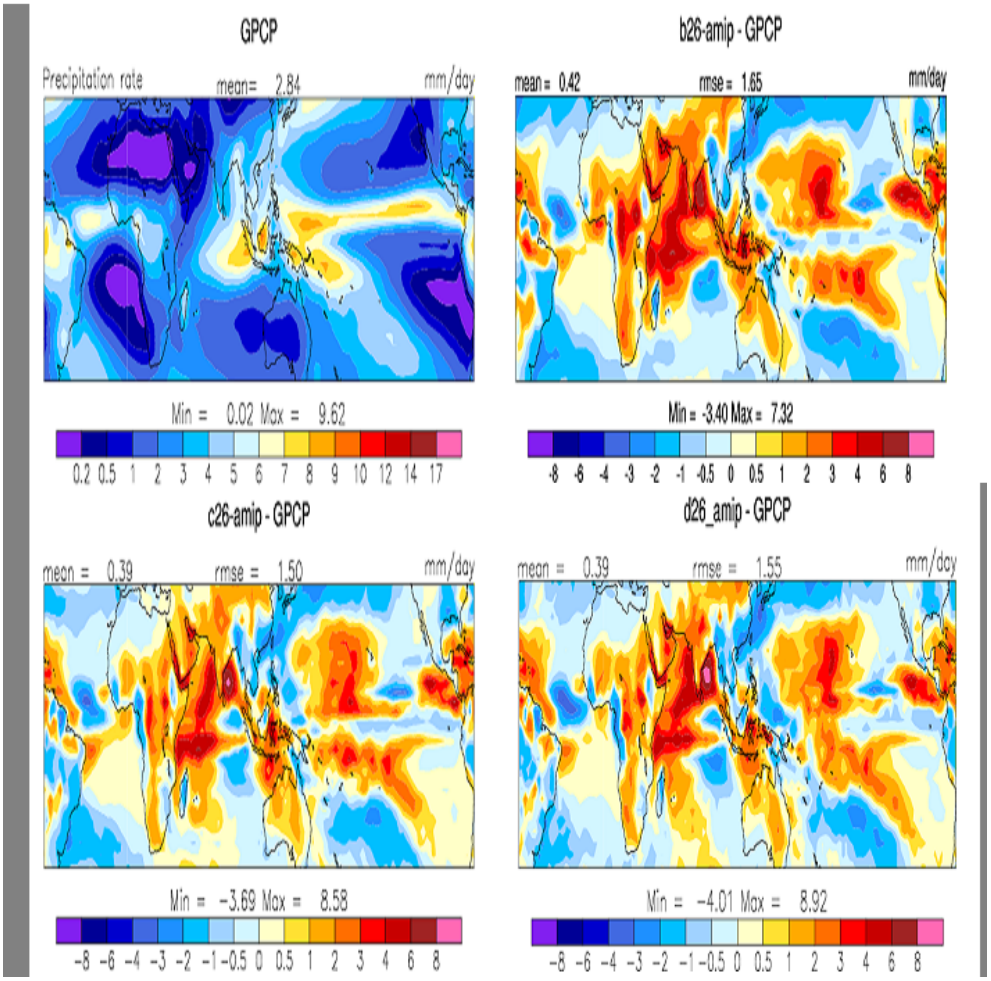

Figure 2.17: Annual-mean precipitation for 1979, in FPCP observations (top left), in simulations with CAM3 (top right and bottom row).

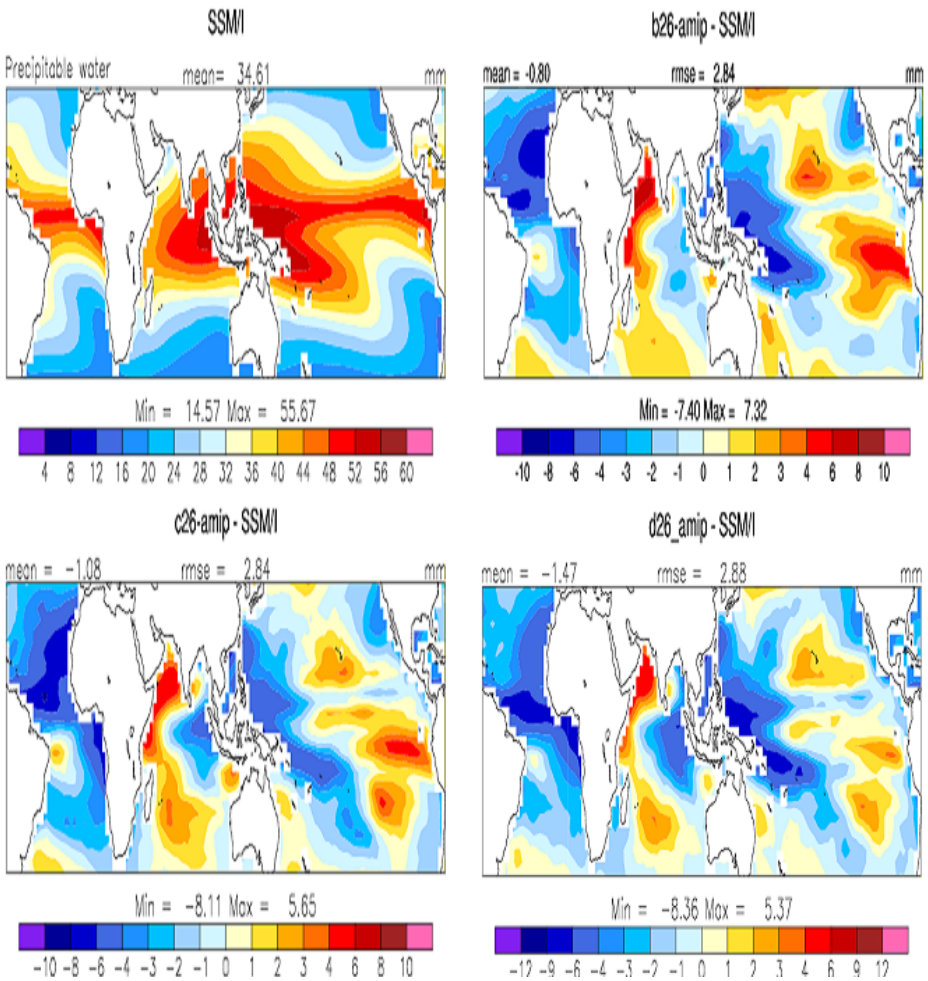

Figure 2.18: Annual-mean precipitable water for 1979, in SSM/I observations (top left), in simulations with parameterized version of CAM3 (top right and bottom row).

resolution in our simulations, and is also present in the very high resolution coupled model described by Sumi [27]. Similarly, Hack et al., [11] show that the double ITCZ problem is largely insensitive to horizontal resolution in the Eulerian spectral configuration of CAM3, when run with prescribed SSTs and also when coupled to ocean and sea ice models. (As is typical, the problem itself is worse in the coupled models.) This indicates improved representation of some convective processes.

Relative impact of parameterized physics vs. dynamics on sensitivity to horizontal spatial resolution

The cause of the weaker sensitivity to horizontal resolution is not immediately obvious. Our CAM2 and CAM3 results can be compared with previous studies with CCM3 [7]. Parameterized physics as well as dynamics are different between the two models. The relatively strong resolution-sensitivity in the FVGCM model (which uses CCM3 physics with finite-volume dynamics) suggests that resolution-sensitivity is determined primarily by dynamics, rather than parameterized physics. We can test this hypothesis by comparing our findings to those of Hack et al., [11], who examined the sensitivity to resolution in a configuration of CAM3 using the Eulerian spectral dynamics (i.e., this configuration uses the same parameterized physics as we did, but different dynamics). Our c26 and b26 CAM3 simulations are comparable to the T85 and T42 simulations of Hack [11]. We examined the resolution dependence of the vertical temperature structure, net long-wave and short-wave top of model fluxes (Figures 2.3.1 and 2.3.1, precipitation (Figure 2.3.1), and surface wind stresses (Figure 2.3.1), and compared to results of [11]. In general, differences between our c26 and b26 simulations are very similar to differences between the T85 and T42 simulations of Hack et al. This is perhaps expected of quantities that are strongly influenced by parameterized physics. It is more remarkable, however, that surface wind stresses also exhibit very similar sensitivities to resolution in the finite-volume vs. Eulerian spectral model configurations.

The hypothesis that parameterized physics primarily determines resolution sensitivity is confirmed by comparing *c26mmf* – *b26mmf* to *c26* – *b26* differences with the T85 – T42 differences seen by Hack [11]. The resolution sensitivity seems to be more similar in the simulations that use the same physics (i.e. in *c26* – *b26* and T85 – T42) than in simulations that use the same dynamics (i.e. *c26mmf* – *b26mmf* and *c26* – *b26*). This is true even of surface wind stresses (Figure 2.3.1).

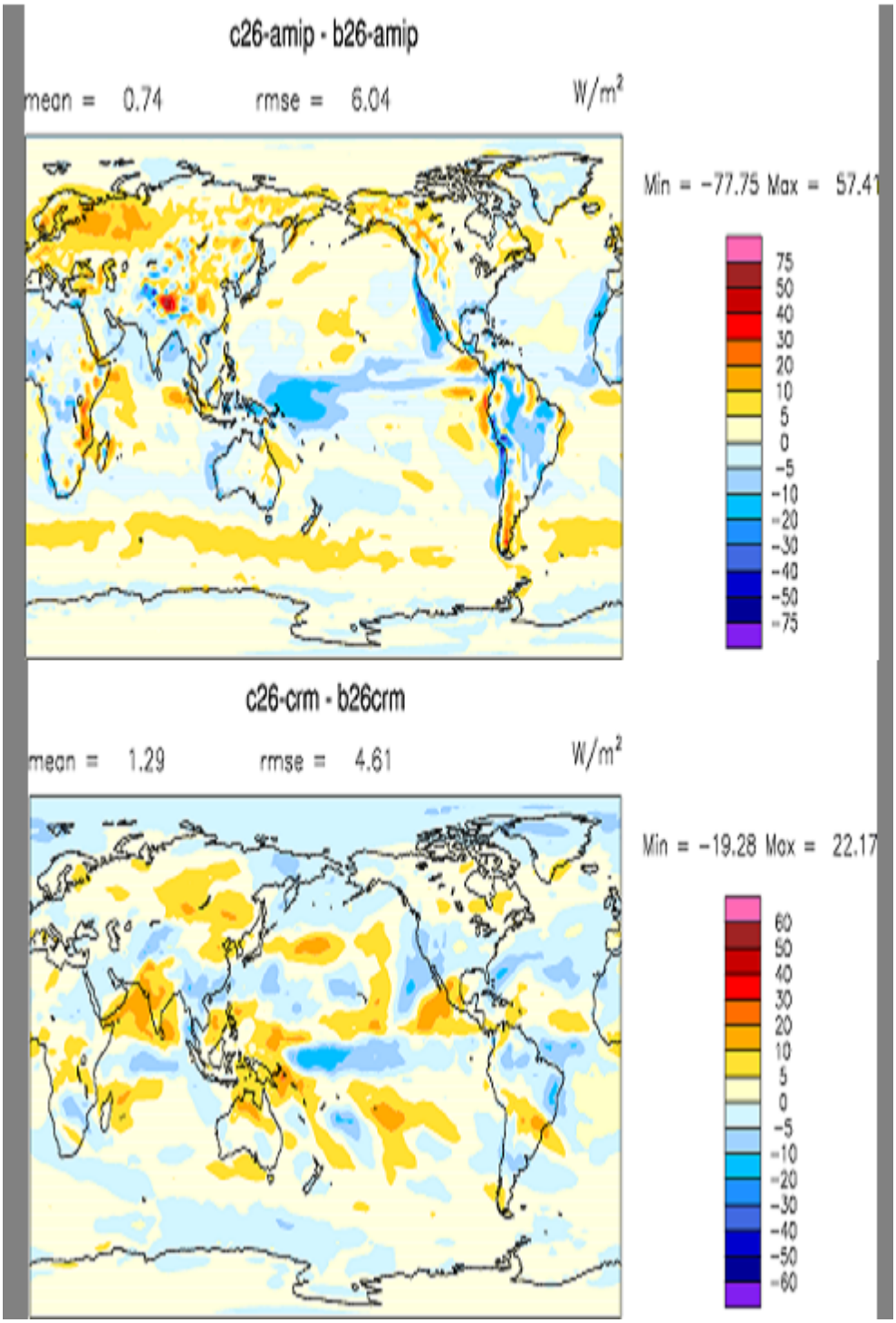

Figure 2.19: Resolution-dependence of annual-mean net longwave top of model flux (FLNT). Top: difference between c26 and b26 simulations. Bottom: difference between c26mmf and b26mmf simulations.

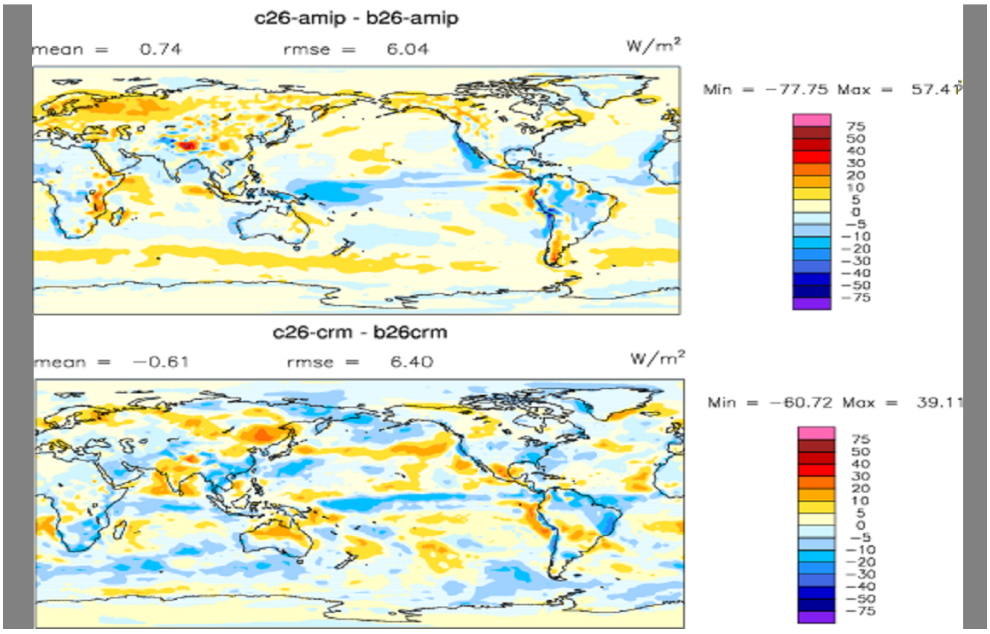

Figure 2.20: Same as Figure 2.3.1 above, except showing annual-mean net shortwave top-of-model flux. Compare to Figure 4 of Hack et al., [11].

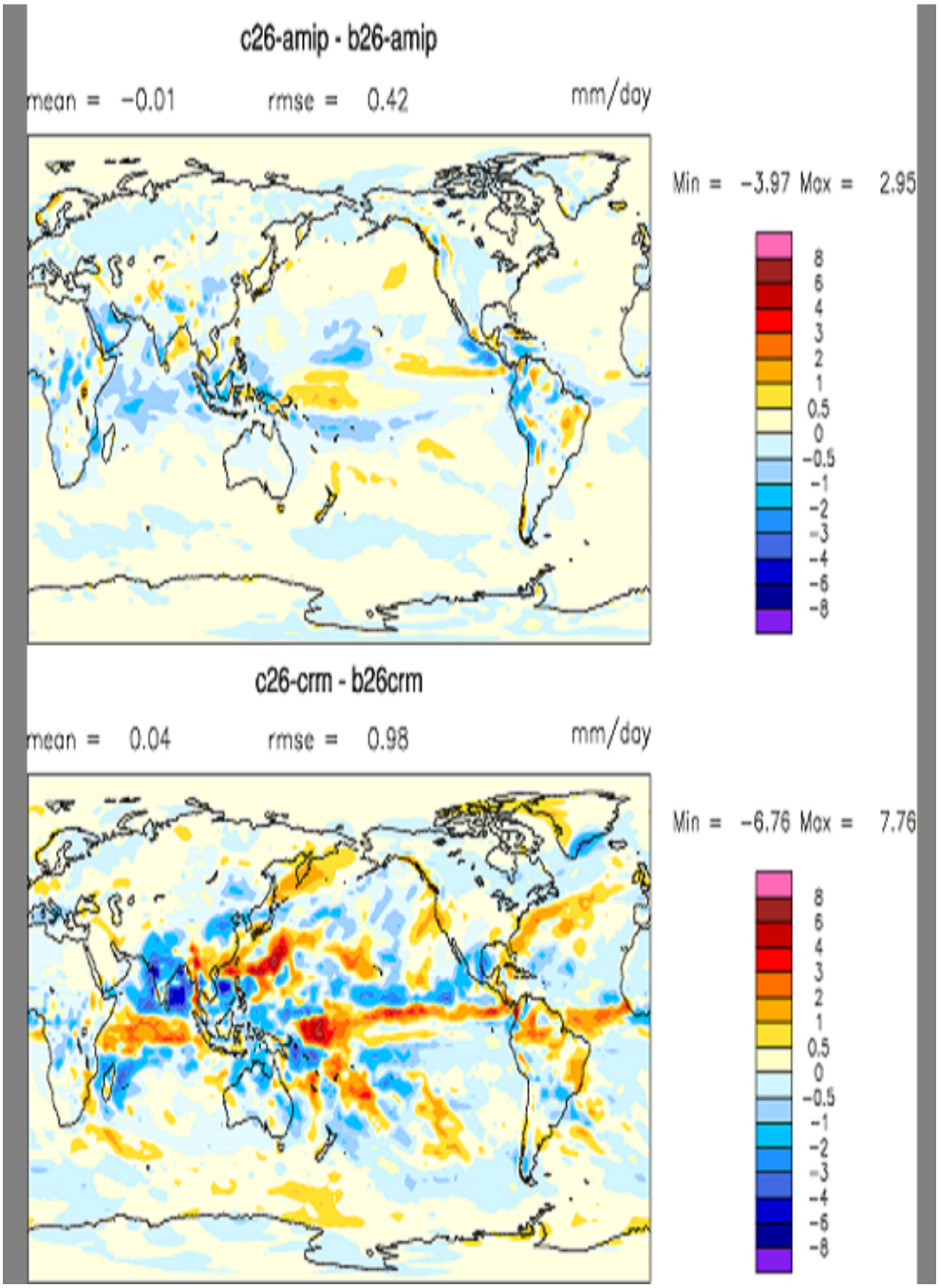

Figure 2.21: Resolution-dependence of precipitation in CAM3.

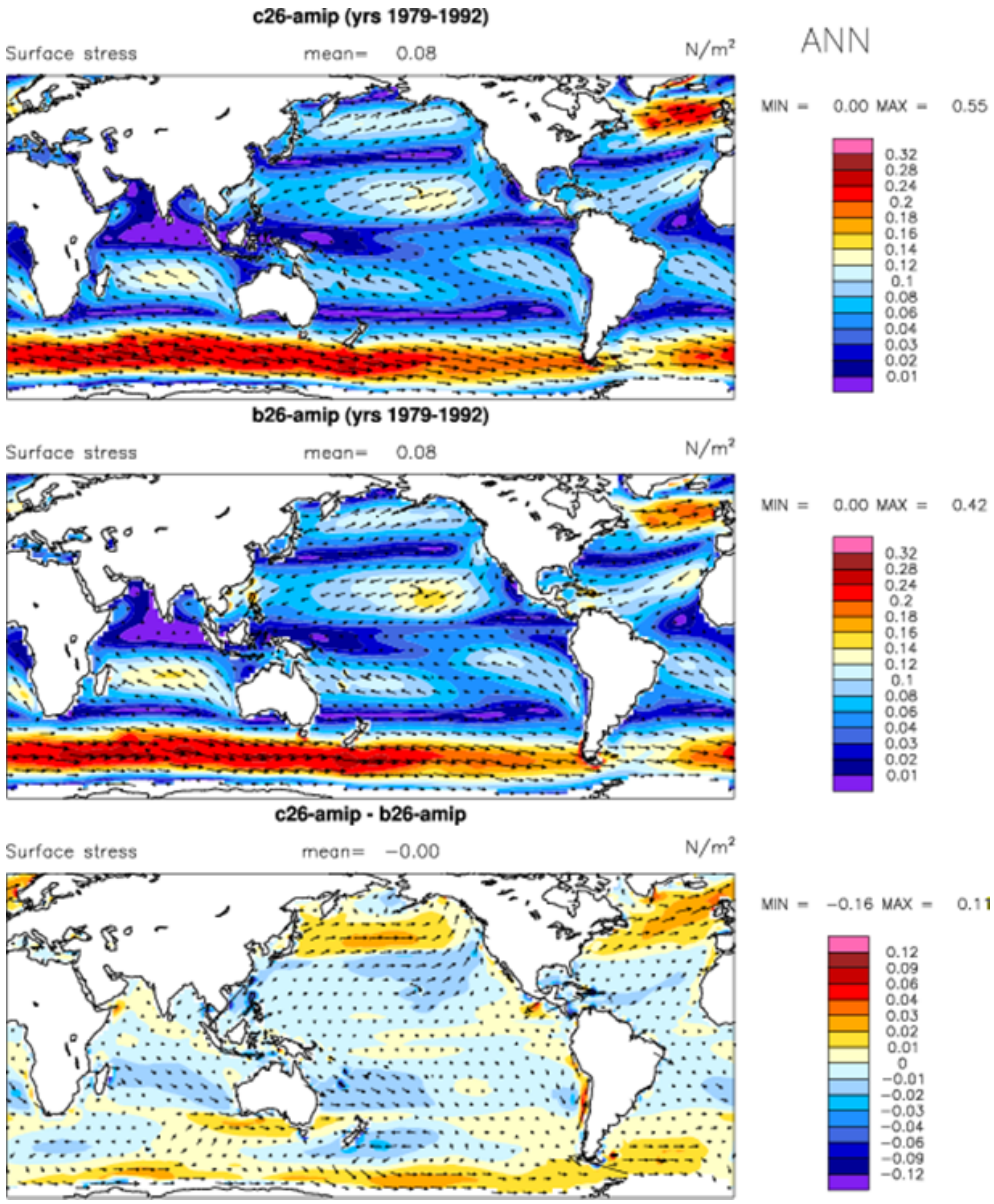

Figure 2.22: Annual mean surface wind stresses in c26 (top) and b26 (middle) simulations with CAM3, and their difference (bottom).

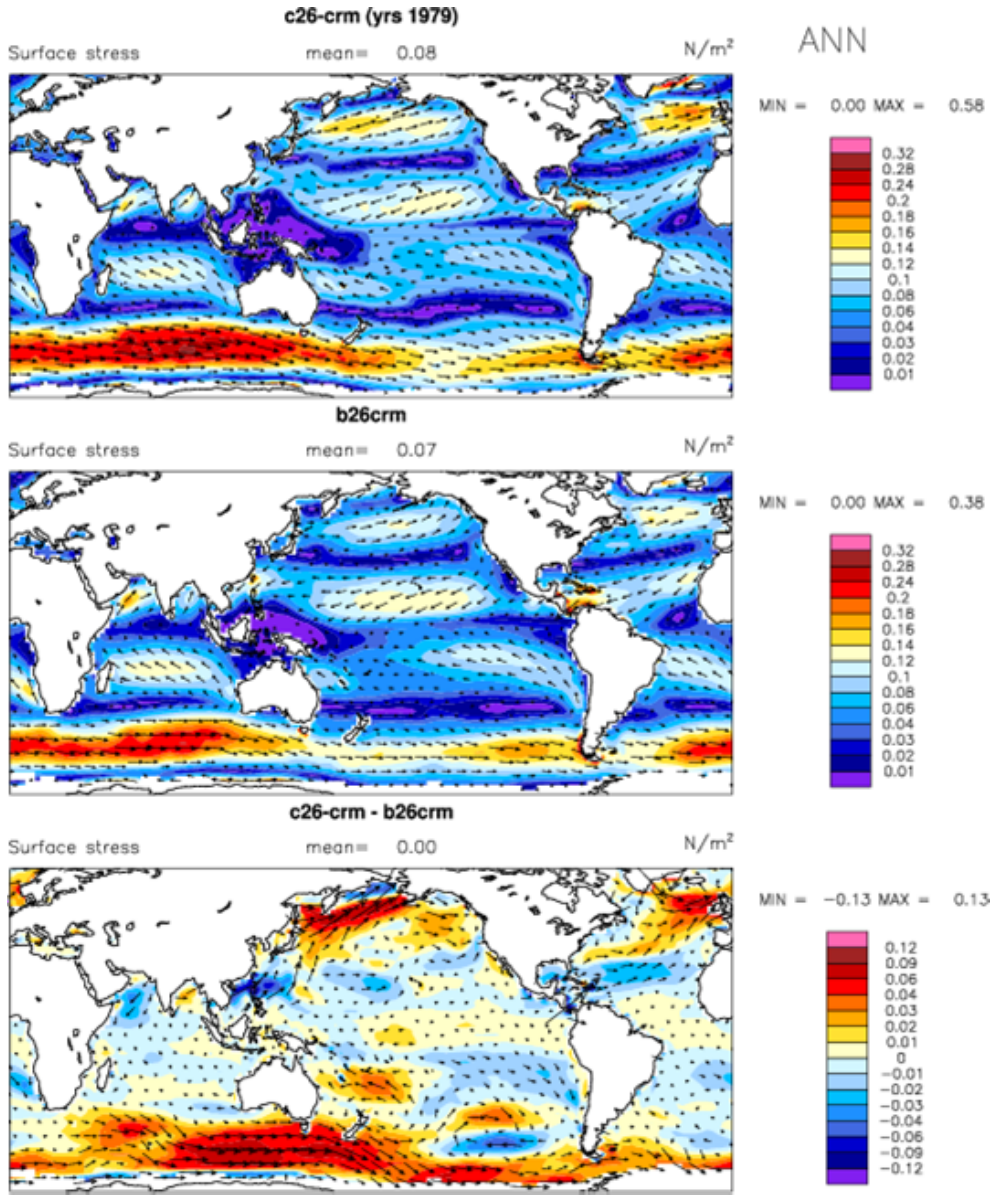

Figure 2.23: Same as Figure 2.3.1, except for c26mmf and b26mmf simulations.

2.3.2 Land Model and River Runoff Development

A number of activites have been pursued during this project in the development of the CLM3 and in pursuit of the goal of adding biogeochemical cycles to the CCSM.

The primary simulation target was to perform C4MIP simulations with the CASA' carbon model in the CCSM3 framework. This work started even before the IPCC configuration of the model was set and the CCSM3 code was released in June of 2004. Since much of the work required to perform this task overlapped with the efforts of Peter Thornton to do C4MIP simulations with the new CN (Carbon Nitrogen) model, the efforts and tasks contributed to his simulations as well. The SciDAC contributions to this effort are:

- Data cycling capabilities added to *csim* and *docn* to support BGC experiments,
- CASA' integration and vectorization,
- CN vectorization, and
- C4MIP Phase 1 simulations underway at ORNL.

The primary objective was to examine the simulations of the 20th century atmospheric CO_2 and the CO_2 fluxes at the land surface in the coupled atmosphere-terrestrial biosphere models. The terrestrial biosphere model was spun up to

- Equilibrate to near pre-industrial conditions defined as 1850 CO_2 using repeated cycles of the 1875-1899 SSTs,
- Force the model by two cycles of 1875-1899 SSTs, increasing CO_2 from 1850 to 1899.

For CLM-CN and CLM-CASA', the strategy for spin-up involves a series of CCSM3 runs in the F configuration (*cam, clm, csim-thermo, docn, cpl*) and the I configuration (*datm, clm, csim-thermo, docn, cpl*). See CSEG Project Plans for details (http://www.cgd.ucar.edu/cseg).

The status of this effort is given in the following bullets

- Coupling (Mariana Vertenstein, Jeff Lee, Rob Jacob): CO_2 forcing of land from atmosphere is tested and working. Net ecosystem exchange (NEE) (C flux from land to atmosphere) has also been tested and is working.

- CLM Modifications (Gordon Bonon, Mariana Vertenstein, Peter Thornton, Forrest Hoffman): The CN Vectorization is complete along with the integration of CASA' into the CCSM3. The soil water deficiencies of CLM3 that were affecting vegetation growth have been fixed. The addition of prescribed land cover (dynamic PFTs) is complete.

- Data Model Modifications (Mariana Vertenstein, Forrest Hoffman, Brian Kauffman): A special version of *datm* has been added in the BGC branch which reads only hourly data produced by CAM. The data cycling code has been integrated into *csim* and em docn and these modifications are available to collaborative partners who wish to perform their own BGC simulations with CCSM3.

- Scripts : The F and I BGC model configurations are tested and working with the B configuration being tested for a SciDAC reporting milestone (Q3FY05) .

- CLM-CN C4MIP spin-ups at NCAR (IBM) (Peter Thornton) .

- CLM-CASA' C4MIP spin-ups at ORNL (IBM) (Forrest Hoffman, Jasmin John, Inez Fung) .

- CCSM3-IBIS spin-ups at ORNL (IBM) (Forrest Hoffman, Art Mirin, Mac Post, David Erickson, Jon Foley): Evolved from LLNL/ORNL PCM-IBIS to coupling of CCSM3-IBIS.

Figures 2.24 and 2.25 show some of the early results from the CASA' simulations. The Net Primary Production (NPP) from the IBIS model configuration is shown in Figure 2.26.

The surface runoff and river flow data from the A1B scenario were captured from a downscaling run by Steve Ghan and Tim Shippert. This downscaling used the subgrid orography scheme and allows very high resolution results to be presented.

This result (Figure 2.27) shows a snapshot of the runoff difference between one month of a scenario simulation and an observed runoff climatology. Northern South American, in the Orinoco and part of the Amazon River basins, shows a considerable deficit in runoff compared to observations, as does Northeast Siberia.

Figure 2.28) shows the progression from the CCM3 atmosphere-land model, to CCSM2, and then to CCSM3. Observations for discharge and rainfall are also shown. The precipitation figure shows a progression in accuracy toward observed Xie-Arkin rainfall as the model went from CCM3 to

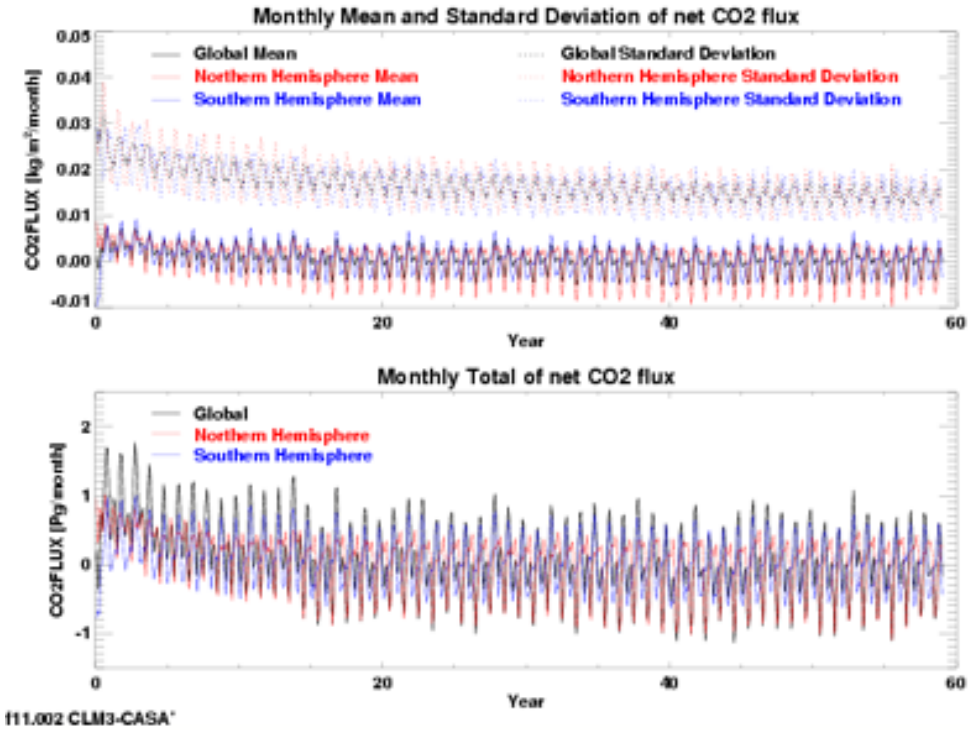

Figure 2.24: Monthly mean and standard deviation of net $C0_2$ flux from the land model (a) and monthly total net CO_2 flux from the land model using CLM3-CASA'.

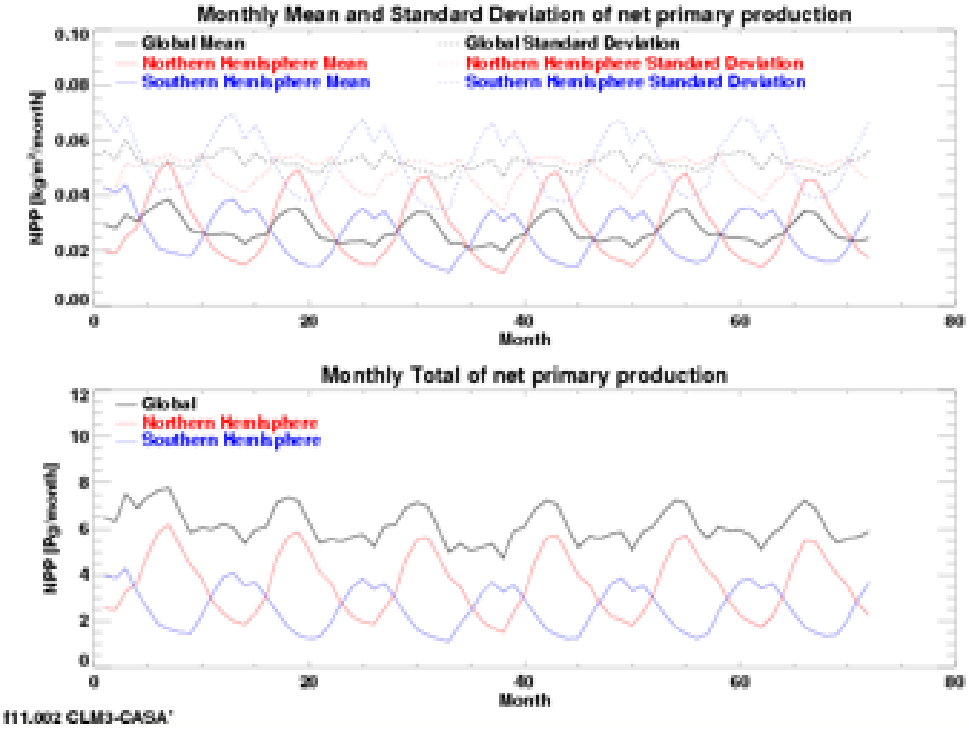

Figure 2.25: Net primary production (NPP) from CLM3-CASA' with the monthly mean and standard deviation (a) and monthly totals (b).

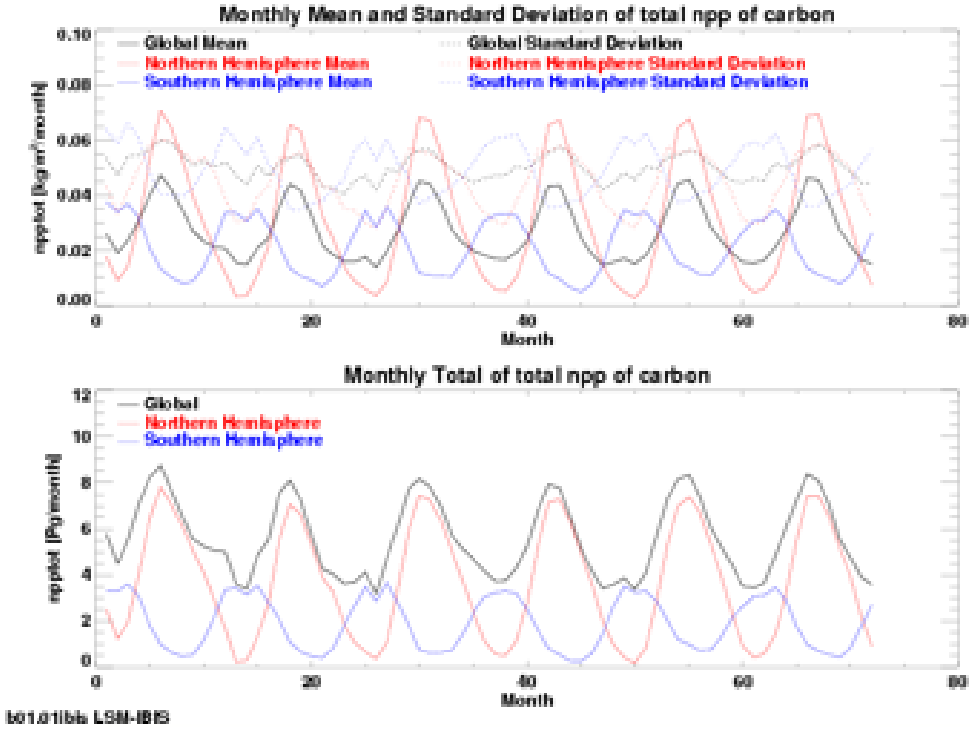

Figure 2.26: Net primary production (NPP) from LSM-IBIS with (a) the monthly mean and standard deviation and (b) monthly totals.

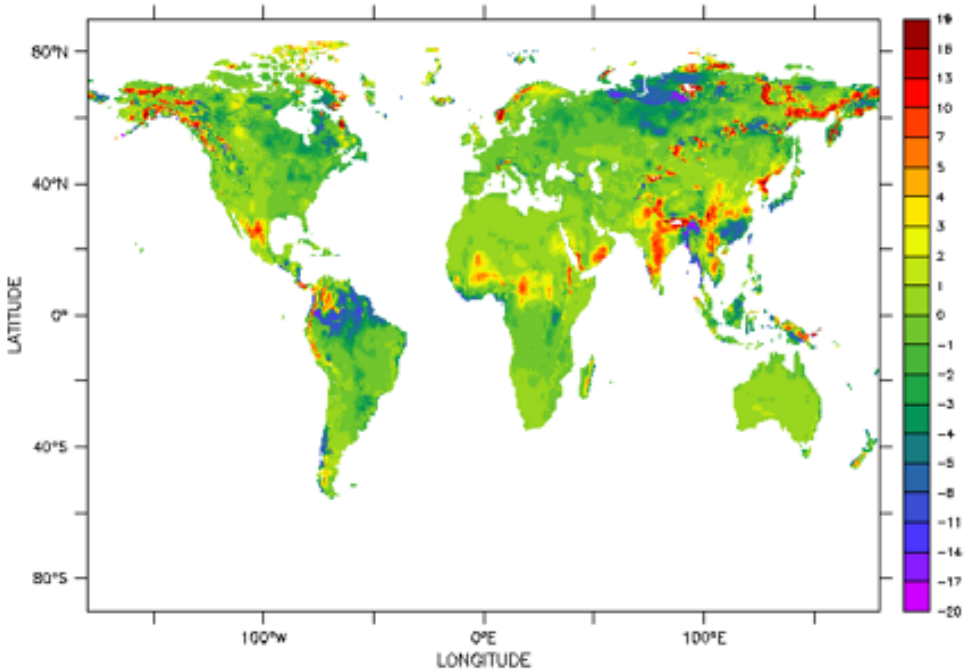

Figure 2.27: June surface runoff (mm/day) difference between A1B scenario (year 2000) with subgrid orography and observed runoff data.

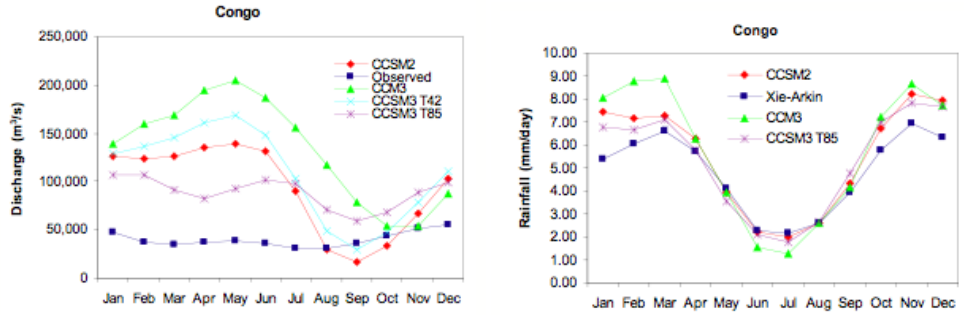

Figure 2.28: Congo River basin discharge and rainfall.

the current T85 CCSM3. This improved rainfall also contributes to an improvement in the river discharge. In each case, the discharge is significantly too high compared to observations, but the latest version comes closer than the others. Also notable is the seasonal timing of the observed Congo discharge is fairly flat across all months of the year. The T85 CCSM3 results line, while not as flat as observed, is flatter than previous results.

The plots in Figure 2.29) show the runoff from an A1B simulation using the subgrid orography parameterization by Steve Ghan. The details of the simulation are included in [77, 78]. Figure 2.29 is a 70-year average April and July runoff from the middle of the simulation period. It was generated to highlight how the high resolution subgrid orography scheme helps to capture more accurately the runoff generated in regions of high relief such as the Himalayas by producing better precipitation and snowfall results.

Figure 2.30 highlights the changes in overland flow in the Southeastern United States resulting from the A2 scenario. A2 is a high CO_2 loading scenario and the results are in the early part of the simulation (2000-2010), but a pattern is already emerging of a drier Southern region (less surface runoff) and wetter Northern region.

2.3.3 Ocean Model Development

While much of the POP 2.0 development was performance related as noted above, the 2.0 release of the code also contained a partial bottom cell option that permits the bottom grid cell to vary in thickness for a better representation of the ocean bottom topography. Support for tripole grids was included in this release. Similar to the present displaced pole grids, tripole grids shift polar singularities onto continents, but with more uniform grid spacing.

Ocean model development has shifted from POP itself to a new hybrid-vertical coordinate model, currently known as HYPOP. Until recently, ocean models were either z-coordinate Eulerian models like POP or isopycnal coordinate models like the Miami Isopycnal Coordinate Ocean Model (MICOM). The use of z-coordinate models, particularly for long climate integrations, results in too much diffusion of heat or other water mass properties into the deep abyssal ocean. Isopycnal models can better represent the deep ocean where flow follows isopycnal surfaces, but they can not resolve mixed layer properties because the mixed layer is of nearly constant density and is therefore represented by only one (or a few) isopycnal layers. The use of hybrid vertical coordinates attempts to get the best of both by representing the deep ocean using more Lagrangian coordinates (e.g. isopycnal coordinates)

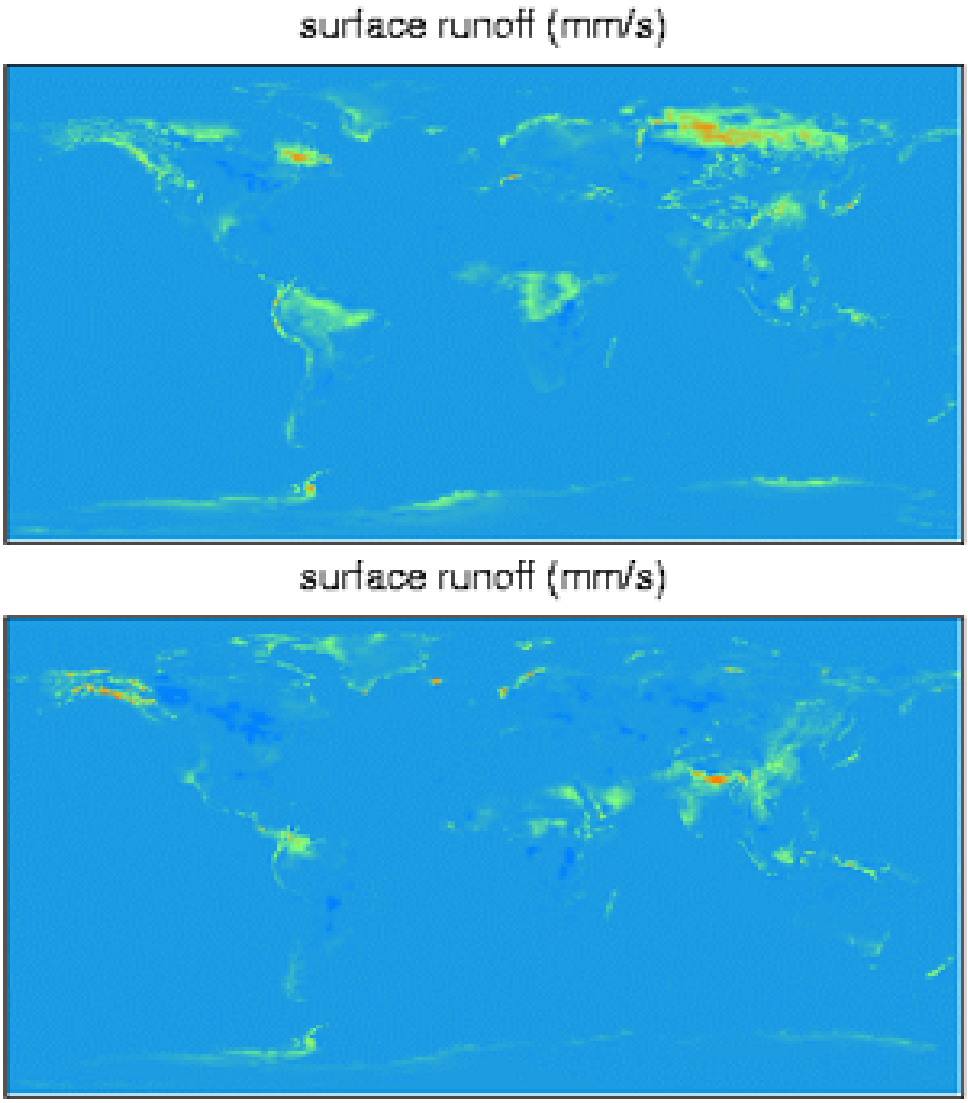

Figure 2.29: April and July runoff from A1B simulation using the subgrid orography scheme.

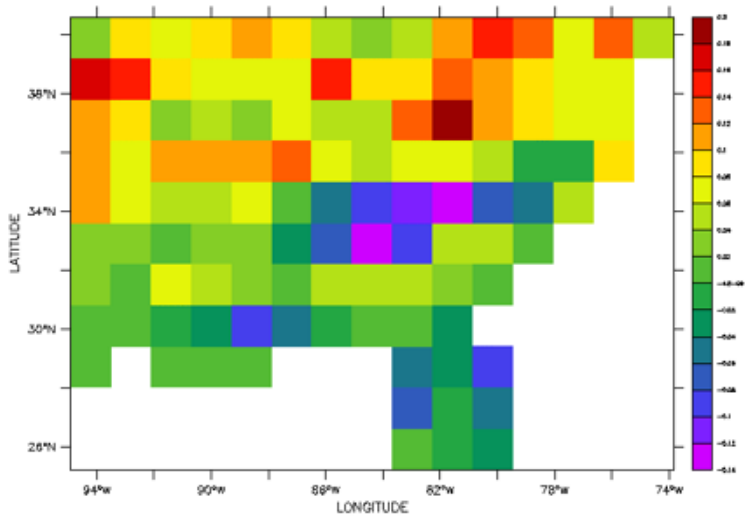

Figure 2.30: Southeast United States surface runoff difference (mm/day) between A2 IPCC simulation and control.

while retaining Eulerian (z-level) coordinates in the surface mixed layer.

For HYPOP, we have chosen to formulate the model using an Arbitrary Lagrangian-Eulerian (ALE) scheme. In an ALE scheme, the model is integrated forward as a Lagrangian model and is then periodically remapped to a chosen coordinate. So, for example, the deep ocean in HYPOP will typically remain Lagrangian while the surface Lagrangian surfaces are periodically remapped to Eulerian levels. ALE schemes are very flexible in the choice of vertical coordinates and many different choices can be attempted and tested.

In addition to the ALE scheme mentioned above, we planned to replace the current leap frog time stepping with more recently-developed forward-in-time schemes. In addition, we had planned to replace the implicit barotropic solver in the current POP formulation with an explicit subcycling scheme to avoid some of the performance bottlenecks due to the current implicit solver.

A prototype model was developed based on the ideas above, but unfortunately encountered several stability issues and we found it increasingly difficult to produce a working model. Development of a completely new model with so many new features was preventing the timely release of HYPOP. Instead, John Dukowicz introduced a new approach to a hybrid model that has many advantages over the current HYPOP model. In this new ap-

proach, the momentum equations remain in Eulerian (z-level) coordinates, while only the tracers utilize the ALE approach. Eulerian coordinates are a more natural coordinate for the momentum equations as the boundary conditions are formulated more cleanly and the pressure gradient force can be computed more accurately. In addition, all of the current POP code for the momentum equations, including the barotropic solver, can be maintained while only changing the tracer equations. This new approach requires only an interpolation of quantities between the tracer coordinates and momentum coordinates in a way that preserves energetic consistency. Such an interpolation has been developed and tested and we are currently implementing the new ideas. The resulting model will not only improve our simulation of the ocean but will also provide current POP users and developers with a more incremental path to a hybrid coordinate model.

2.3.4 Sea ice development

Improvements to the CICE model under both this SciDAC project and other DOE funding included a new ice transport scheme and an improved formulation of ridging processes. A new incremental remapping transport scheme was implemented in the CICE model [267]. In incremental remapping, velocities at cell corners are projected backward in time to compute a control volume that will contribute properties to each cell. Because the method is geometrically based, the control volumes can be computed once and reused for subsequent tracers or, in the case of CICE, the increased number of ice thickness categories that had been introduced. In addition, the scheme is conservative in all transported quantities. Improvements to the ridging scheme [95] were necessary to improve simulations in which there were large changes in ice thickness and ice strength that were creating instabilities in the ice dynamics in high resolution simulations.

Automatic Differentiation for Derived Sea Ice Parameters

The development of CCSM involves various parameterization schemes that employ a number of model parameter values with different scales of uncertainty. Many model parameters can be tuned to improve various aspects of the simulated climate. For example, the sea-ice model of CCSM includes numerous thermodynamic and dynamic parameters that control the computed seasonal sea ice conditions. In the POP ocean model, horizontal and vertical mixing coefficients govern the simulated ocean circulation. The purpose of this work is to enhance these CCSM components with objective parametric tuning schemes based on automatic differentiation (AD) techniques. This effort will result in the implementation of a broadly use-

ful method to make optimal use of climatological observation data to tune CCSM components.

The AD method is a technology to augment a computer program's functional calculations with derivative (or sensitivity) computation. Exploiting the chain rule of differential calculus, AD-processed code provides analytical derivatives in addition to a function calculation. The feasibility of applying AD to CCSM components was demonstrated with CICE. The AD-augmented CICE code (CICE.AD) enables computation of derivatives of any CICE output variables (seasonal sea-ice conditions) with respect to any given independent input model parameters. Derivative (or gradient) information produced by the CICE.AD code can be used in designing an optimized version of the CICE model.

The objective of this work is to provide tuned model parameter values based on robust sensitivity analysis that informs objective parameter tuning of CCSM components. Three main tasks are required to accomplish this goal: 1) implementation of objective derivative computation code using AD techniques, 2) implementation of a parameter tuning scheme using the AD-processed code, and 3) sensitivity and parameter tuning experiments for selected model parameters. This work was resumed during Q4 of FY06, with effort focused on the implementation of the serial and parallel versions of the CICE.AD code and preliminary testing of the CICE.AD code.

The CICE.AD code was created from the CICE code using the Tangent and Adjoint PENultimate Automatic Differentiation Engine (Tapenade; *http://www-sop.inria.fr/tropics*). Tapenade is a code transformation package developed by the French National Institute for Research in Computer Science and Control (INRIA). Given the Fortran90 CICE code, Tapenade successfully produced a portable Fortran90 CICE.AD code that allows the computation of partial derivatives of defined dependent and independent variables: ice conditions with respect to various thermodynamic and dynamic model input parameters.

Tapenade is still under development and supports most, but not all, of the Fortran90 standard. Lack of support for count, present, and dynamic memory allocation requires a preprocessing step to replace some Fortran90 commands with ones acceptable to Tapenade. Also, some type mismatch problems with the Fortran MOD intrinsic function calls were observed in processing the CICE code. Various netCDF calls are used in the CICE code to write restart and history files during simulation. Working as I/O statements, these netCDF routines are not directly related to the differentiation process. Based on a "black-box" approach, these netCDF routines were forced to bypass the differentiation process. The "black-box" mecha-

nism provided by Tapenade allows one to give user-defined differentiation information to Tapenade.

There are three main situations in which the user has to provide the detailed differentiation information to Tapnade: 1) a given routine is supplied only as object code or a compiled library, 2) a given routine's implementation language is not understood by Tapenade, or 3) the user prefers to differentiate certain routines by hand rather than invoke the AD procedure. In each of these cases, precise differentiation information can be supplied to Tapenade in two configuration files, one for the AD-independent routine information and one for the AD-related differentiation information. This "black-box" approach was used to provide user-defined differentiation information to ensure Tapenade handles properly the MPI library routines called by the CICE code. Correct communication of derivative variables between processors is an essential requirement for running the CICE.AD code on multiple processors. Based on this "black-box" approach, the netCDF and MPI routines called by the CICE code were successfully processed with Tapenade.

A coarse global grid system (3 degree) including both polar regions was used for the test and verification of the CICE.AD code. CICE.AD results were validated by comparison with those obtained using the divided differences (FD) method, which computes derivatives by dividing the response perturbation of the simulation to input parameter variation. Figure 2.31 shows the comparison of the results of the CICE.AD code and the divided difference results. The dependent and independent variables for the derivative computation are the ice volume per unit ice area and snow albedo, respectively. Two different step sizes were arbitrarily selected for the FD method. For a small step size (1.E-6), the FD And CICE.AD results match well. For a larger step size (1.E-4), however, the FD method shows significant truncation errors in the derivative calculation. This result shows that the CICE.AD code provides a more robust derivative computation scheme than the conventional FD method.

Preliminary sensitivity data at two representative polar locations (Fram Strait and Weddell sea) were computed using the CICE.AD code. Various thermodynamic and dynamic parameters were selected for the experiment. We computed sensitivities of averaged ice volume per unit area with respect to the selected parameters for the first week of January and July. These results indicate that albedo, thermal conductivity, ridging constant, ice and snow density, and prescribed maximum ice salinity have the strongest effect on the computed ice volume. In particular, sensitivity of ice volume with respect to the ice and snow albedos shows seasonality, being more pro-

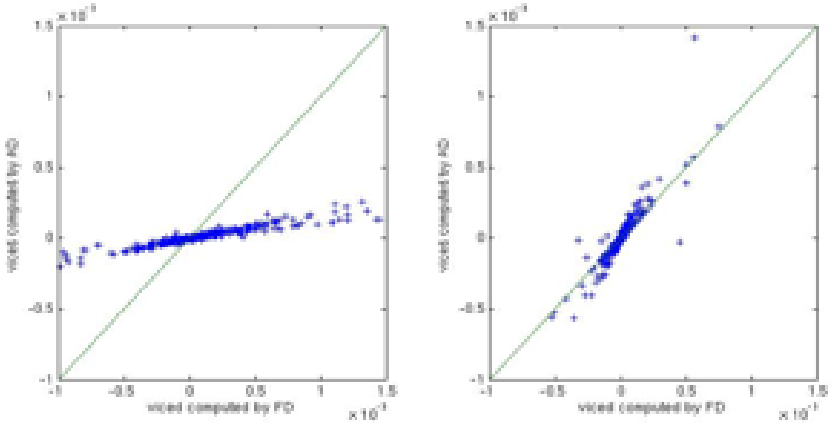

Figure 2.31: Comparison of AD and FD computed derivatives with the step size of 1.E-4 (left) and 1.6E-6 (right).

nounced during the melting season. Also, it is observed that the ocean drag coefficient strongly interacts with thermodynamic calculations.

2.4 Chemistry and BGC Model Developments

2.4.1 Interactive Chemistry in CAM3

Under SciDAC we incorporated full interactive tropospheric chemistry (including aerosols) into CAM3. For this purpose, we used the chemistry modules from the chemistry-transport model, MOZART (developed at NCAR, GFDL and MPI-Hamburg), and expanded the aerosols modules from MOZART to include ammonium nitrate. We also implemented a "fast" mechanism that is three times faster than the full mechanism based on the LLNL-IMPACT chemistry-transport model for millenial-scale simulations and are connecting the chemistry to aerosol microphysics and to ocean and land biogeochemistry as discussed below.

Comparison of fast mechanism model results with observations has shown that we simulate a realistic chemical state of the atmosphere in both gas-phase and aerosol chemistry. The overall conclusion is that the model performs similarly to the MOZART model. This model is now being used for assessing the roles of aerosols in driving changes in the chemistry and climate of the atmosphere. We have coupled our atmospheric chemistry capability with the ocean to analyze the role of interactive emissions of DMS, and a

parameterized calculation of droplet number to simulate the indirect effect of aerosols.

In support of the IPCC simulations done using the CCSM, we have simulated the evolution of ozone during the 20th century using a set of snapshot simulations (every 20 years between 1890 and 1990). Using our best estimates of ozone precursors emissions, we have found a tropospheric ozone burden increase of 71 Tg between 1890 and 1990, an increase of approximately 30%. When no anthropogenic emissions in 1890 are considered, this burden increase reaches 88 Tg. In addition, the ozone production in this study has increased rapidly until 1930 and after 1970. However the ozone production efficiency in the troposphere is shown to have decreased during the 20th century, making the troposphere less NO_x limited. Finally a decrease in the OH burden is estimated to be of the order of 8%, matched by a similar increase in the CO lifetime. In addition, we are leading an international modeling study to explore the role of nitrogen deposition as an agent for increase CO_2 uptake in the 21st century. Using results of nitrogen deposition from a set of 28 simulations from 6 different tropospheric chemistry models pertaining to present-day and 2100 conditions, we show that, under the assumed A2 scenario, the global annual average nitrogen deposition over land is expected to increase three-fold, mostly due to the increase in nitrogen emissions. This will create large areas where the annual average nitrogen deposition rate exceeds $1gN/m^2$. Using the results from all models, we have documented the strong linear relationship between models on the fraction of the nitrogen emissions that is deposited, regardless of the emissions (present-day or 2100). On average, approximately 70% of the emitted nitrogen is deposited over land. For present-day conditions, the results form this study suggest that the deposition over land ranges between 25 and 40 Tg(N)/year. By 2100, under the A2 scenario, the deposition over land is expected to range between 60 and 80 Tg(N)/year. Over forests, the deposition is expected to increase from 10 to 20 Tg(N)/year. This study was published in JGR-Atmospheres [178].

We have performed various simulations to evaluate the performance of the interactive chemistry (including bulk aerosols) in CAM3. In particular, we have performed a set of simulations that emphasize the sensitivity to aerosols emissions and have identified the strong negative relationship between the global amount of absorbing aerosols and the globally averaged latent heat flux (Fig. 2.4.1).

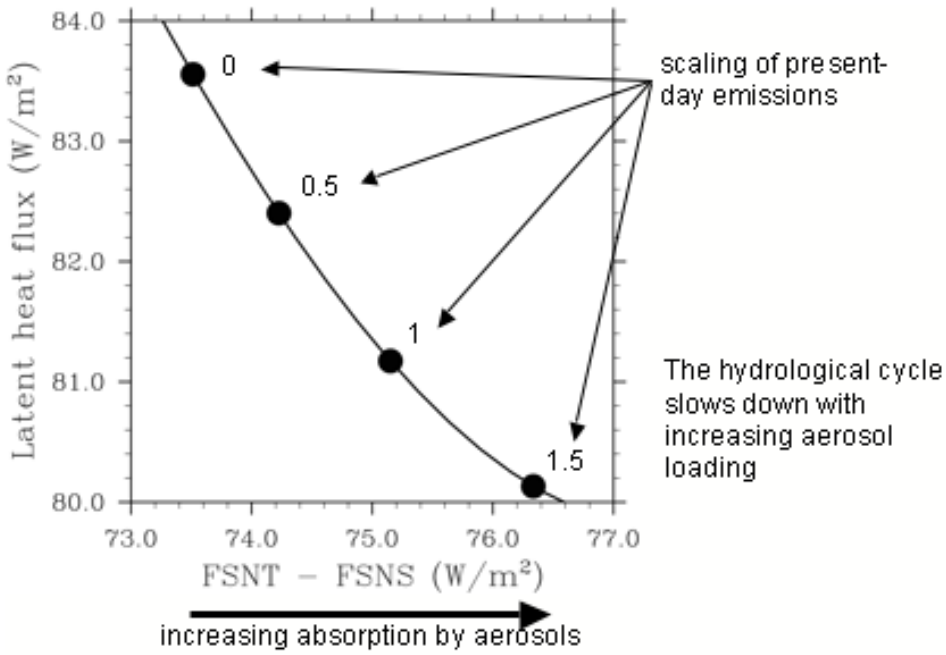

Figure 2.32: The CAM model shows a strong negative relationship between global aerosol emissions and the globally averaged latent heat flux.

2.4.2 Aerosol Dynamics for CAM

The treatment of aerosol direct and indirect effects in CAM is severely compromised by the use of prescribed particle size distributions. By prescribing particle size distributions, CAM cannot distinguish between particle sources that increase both particle number and volume (primary emissions), increase volume only (condensation), or effectively increase number only (nucleation). This weakness is particularly troublesome for treating indirect effects of aerosols, which depend strongly on particle number. Although treatments of aerosol dynamics using a sectional representation of the size distribution have been applied to a few global aerosol models, those treatments are too computationally demanding to permit the multi-decade simulations required for simulating global climate change. We therefore have begun to develop a computationally efficient treatment of aerosol dynamics for CAM. We started with an existing modal treatment that we developed for MIRAGE (the PNNL aerosol version of CAM [243]) and introduced a series of changes designed to reduce the computational burden of the aerosol dynamics in MIRAGE without significantly affecting the accuracy of predicted aerosol properties important for direct and indirect effects. These approximations include dropping the full prognostic treatment of both activated and interstitial aerosol particles, and using alternate numerical algorithms for computationally expensive modules such as coagulation and activation, and prescribing the width of each aerosol mode [79].

We are also in the process of adding a representation of the aerosols indirect effect to the interactive chemistry version of CAM3. Prognostic droplet number concentration [41] has been added to a branch of CAM3. Simulations with prognostic droplet number and prescribed aerosol show little impact of the scheme on the energy balance at the top of the atmosphere, so that little tuning is needed to apply the scheme to climate change simulations.

2.4.3 Fast Chemical Mechanism Development and Coupling to Oceanic DMS

We developed and implemented a fast ozone mechanism with interactive production of sulfate aerosols into the CAM model. This mechanism is 3 times faster than our full mechanism and realistically simulates the radiatively active species. We have now used this fast mechanism in around 200 years of simulations and are preparing the results for publication.

We developed our fast ozone mechanism by paring down our state-of-the-

art chemistry mechanism (TS2) from the LLNL-IMPACT off-line global atmospheric chemistry model [277], which includes $O_x, HO_y, NO_y, ClO_y, BrO_y$, and VOC chemistry for both the troposphere and stratosphere, in a way that realistically calculates ozone around the tropopause (where it produces the greatest radiative forcing). The compact mechanism (TS4) includes essential HO_x and NO_y reactions, is 4 times smaller and faster than our full mechanism (TS2), and covers both the troposphere and stratosphere.

We also incorporated a sulfur cycle into our fast mechanism that produces sulfate aerosols from anthropogenic and natural sulfur precursor species (SO_2, DMS). Our combined ozone-sulfur mechanism (TS6) runs about 3 times faster than our full mechanism in CAM.

We completed several multidecadal simulations with our fast ozone-sulfur mechanism (TS6) on-line in CAM and validated its ozone, OH, NO_x, and sulfate aerosol fields through comparison with observations, the full mechanism in CAM, and the LLNL-IMPACT off-line global atmospheric chemistry and aerosol model. Figures 2.33 and 2.34 show comparisons of ozone profiles and sulfate aerosol seasonal cycles respectively. The fast mechanism agrees well with the observations and the other models.

We have also been working on coupling DMS and CO_2 between the ocean and atmosphere in CCSM in collaboration with those in the SciDAC consortium and at NCAR involved with the coupler, ocean and ocean biogeochemistry, and land and land biogeochemistry. This included a demonstration implementation passing DMS through the CCSM coupler, writing the scientific and technical design documents, and now fully coupling the components together.

Because the direct coupling from chemistry to the atmospheric model is through radiation, we also need to check that the fast mechanism produces heating rates that are comparable to the full mechanism. To this end we have implemented short-wave and long-wave radiation packages into the LLNL-IMPACT model to allow comparison of the atmospheric chemistry simulations between the CAM and IMPACT models, and we see good agreement.

The development, implementation, and validation of this fast mechanism now provides a viable means of including interactive atmospheric chemistry and aerosols in expensive simulations, such as millenium scale and coupled biogeochemistry simulations.

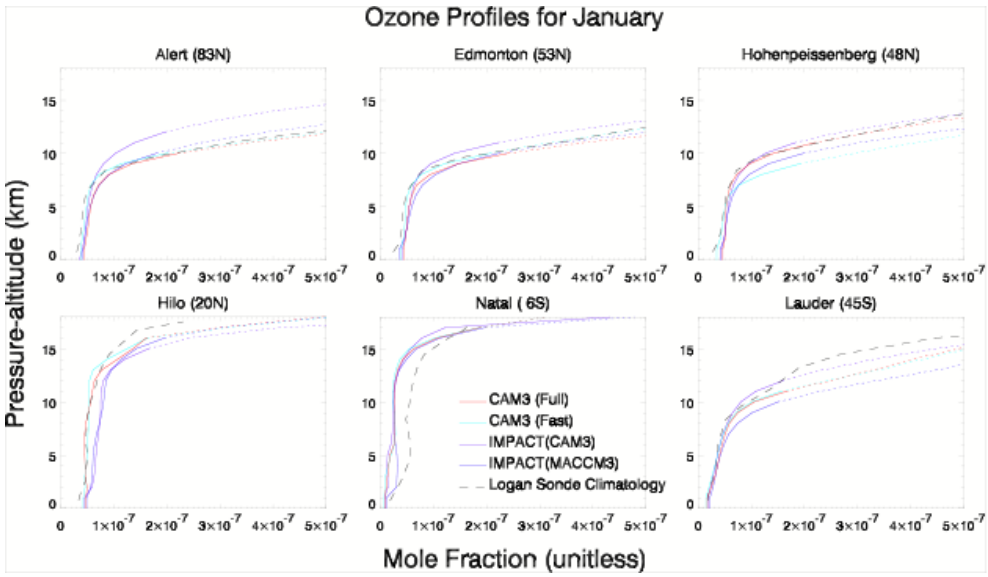

Figure 2.33: Comparison of ozone profiles at six ozonesonde locations for January. In each panel, the dashed line is the ozonesonde climatology; cyan and red are CAM with the fast and full mechanisms respectively; blue and purple are for the LLNL-IMPACT off-line model running with a full mechanism using meteorology from CAM and MACCM3.

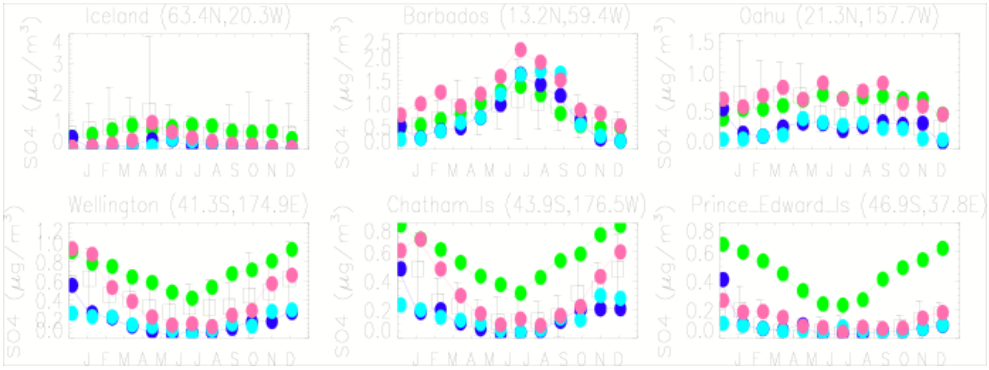

Figure 2.34: Comparison of monthly-mean sulfate aerosol concentrations at the surface for six ocean sites. In each panel, the observations are shown as boxes with error bars for the multi-year mean and standard deviation respectively; the green is a decadal mean for CAM with the full mechanism; the light and dark blues are two individual years for CAM with the fast mechanism; pink is for the LLNL-IMPACT off-line model running with the fast mechanism. Overall, the fast mechanism in CAM compares well. Note: the full mechanism in CAM has been improved since the last report in that its over-prediction of sulfate in the Southern ocean is much reduced, although it still over-predicts somewhat.

2.4.4 Biogeochemistry in the Ocean

As part of this project, an ocean ecosystem model and trace gas improvements were added to the POP model. These additions were validated using ocean-only simulations as well as the coupled simulation described below.

Carbon dioxide (CO_2) and dimethyl sulfide (DMS) were chosen as pilot species for an initial demonstration of capability, because they are relatively well understood and influence both CO_2 and aerosols in the atmospheric model. To predict these, an ocean ecosystem model of Moore, Doney and Lindsay was added to the POP model as well as a trace gas module developed under this project [70].

The design of sulfur cycle mechanisms was based on a Gabric [40] approach, but with bimolecular bacterial uptake appended as a smoothing device and plant volatile release rates optimized in inverse exercises to give agreement with the Kettle et al., [45] data base. The sulfur cycle in our model consists of a bins-and-time-constants scheme supplemented with removal terms accounting for regional shifts in ecology and photochemistry. Densities of DMS consuming bacteria are parameterized from the standard CCSM ecodynamics as a log-linear relation to plant nitrogen with a round value slope of one half. Phytoplankton are simultaneously the major producers of volatile sulfur, so that in steady state a proportionality is expected to the square root of photosynthetic biomass. Sulfur distributions are computed dynamically, however, so that time lags are permitted in blooming or transported systems. The effects have been apparent as filamentous structures in early POP biogeochemistry simulations conducted on eddy resolving grids. Bacterial uptake constants in our mechanism typically average one day and vary by less than a factor of two over most of the surface of the planet. Transfer upward from the mixed layer tends to require on the order of one week so that volatile sulfur remains under local biological control. We might expect that, as POP ecosystems build toward basin scale equilibria, dimethyl sulfide values will track plant densities and follow a square root law. Recent applications of CCSM ecodynamics to iron cycle studies involved runs of greater than twenty years duration intended to ensure stabilization of the total biota. In our experience with the same model, phytoplanktonic steady state was achieved at the eighty percent coverage level within three years, and only the Ross Sea and high Arctic remained depauperate over a decade.

In preparation for coupling to other components, the ocean circulation was spun up for ten years without the biogeochemical model, followed by eight years of ocean-only simulation with biogeochemistry. Marine ecody-

namic and geochemical quantities were initialized as in earlier applications emphasizing the iron cycle, with the exception of alkalinity and disolved inorganic carbon (DIC). Their distributions were taken from GLODAP data but were adjusted to represent the pre-industrial era. Atmospheric carbon dioxide partial pressure, on the other hand, was fixed (continually reset) to a relatively modern round value of 350 parts per million. Effectively, a step function perturbation was thus provided to the surface ocean chemistry system, but with the atmosphere behaving as a large storage unit under external control.

From a preindustrial state, surface seawater approached equilibrium at a rapid initial value of order 20 GtC/y, consistent with sharp gradients across the interfacial microlayer. The uptake then stabilized at 2-3 GtC/y, resembling the rate at which anthropogenic carbon currently penetrates the deep sea. The eight year preliminary run analyzed here is sufficient to generate a balanced sulfur cycle over almost the entire global ocean. It should be noted that while the plant production/bacterial uptake couple can be used to estimate concentrations, our mechanism treats many other established details of the surface ocean sulfur cycle. Examples include taxonomically varying Redfield signal to noise ratios, production of the intermediate species dimethyl sulfoniopropionate, its water column conversion due to lyase enzyme action, and photochemical degradation of DMS via nitrate and DOM photosensitization. As background, thermocline removal of 100 days was included during the final set of runs in order to prevent vertical recycling. The rate constant was tuned to reproduce available depth profiles.

To begin the analysis presented here we have considered initial, intermediate and final surface concentration distributions for the major carbon cycle components during the 8 year ocean-only spin up. Plots of time dependent, globally averaged fluxes have been examined as well. After several years of buildup, CO_2 partial pressures average close to the 350 ppm chemical equilibrium. Exceptions include minima a few tens of ppm lower and focused along major middle latitude frontal systems, which undergo rapid carbon fixation and are simultaneously in vertical communication with central ocean waters still in the preindustrial state. Residual peaks are observed at the equator. By the end of the 8 year period, DIC concentrations are up order tens of micromolar in the tropics and more in colder waters, consistent with expectations. Integrated flux from atmosphere to ocean begins at a level of 20 GtC/y as implied in the above arguments. It then falls to a value of 3 GtC/y well before the run terminates and decays only slowly. The final transport rate is slightly larger than the accepted contemporary central ocean penetration. This should not be surprising, however, since

the atmospheric introduction is a step function in the current configuration and should engender steep vertical DIC gradients. In the real global ocean, the anthropogenic buildup has accumulated steadily over many decades and recirculation can occur. Furthermore, cold water equilibria in our artificial start up scenarios are particularly rich in the inorganic carbon forms.

The standard ecodynamics model divides photosynthesizing organisms into classes of small noncoccolithophorids, the calcite secretors, diatoms and diazotrophs. We have summed their chlorophyll contents at key points during the 8 year ocean-only run and plotted constant longitude sections in the centers of the major ocean basins. Results were then compared with values obtained in analogous simulations employing coarse POP versions with the same ecology, and also with SeaWIFS remotely sensed color data. Latitudinal patterns are consistent across all runs and the climatology. However, the one degree ocean-only spin up gives concentrations which are between 10 and 50 percent higher than those obtained at three degrees in some of the gyre regions. Potential explanations include lingering effects of the primitive physical spin up strategy (from rest over a single decade). It is possible that central basin downwelling remains underdeveloped such that nutrient supplies are excessive. It also seems likely that, as the eddy admitting regime is approached in the horizontal, intense blooms driven by local vertical mixing begin to emerge. We have conducted several informal convergence tests upon the CCSM biogeochemistry model within POP and can report that similar changes are sometimes seen.

Changes in chlorophyll/biomass should have a minimal influence on dimethyl sulfide concentrations because of the square root dependence incorporated into its mechanism. Extra-microbial removal terms are usually secondary even in summation. Our sulfur cycling has traditionally been preoptimized through inverse calculations to give agreement with the Kettle concentration distribution. Chi-square normalization to the data base deviations demands a tight fit at low latitudes. In the tropics and subtropics, concentrations from the ocean only run segment are thus in strong agreement with the data. The log-linear relation to plant mass, however, tends to raise values along middle latitude fronts and the effect is not suppressed during inverse calculation because variability there is high.

Additionally, we examined time series for the globally integrated sea to air flux of volatile sulfur. Values declined during the run from roughly 35 teragrams per year (TgS/yr) to 32 TgS/yr. The increase is simply a reflection of the local approach to multiple ecodynamic steady states with DMS in pursuit. Rates lie at the high end or outside of the conventionally accepted range of 20-30 TgS/y, but the enhanced middle latitude concentrations con-

stitute an identifiable and sufficient reason. The problem is easily remedied for a given region via adjustment to plant release. Constraints on the implied intracellular kinetics are weak. We have shown in earlier work that sulfur species concentrations scale directly with the production constant so that any new setting may be readily computed. On the other hand, it will be difficult to establish accurate local and global fluxes simultaneously. The underlying issue here will be improvement of the gyre to frontal system reduced sulfur concentration ratio, which we are hoping to achieve through the introduction of a combination of

1. updated, taxonomically resolved S/N compositions,
2. determination of sulfur injections via true CCSM ecodynamic flow,
3. exertion of grazing pressure on specialist microbes which may comprise much of consumption, and
4. linkage of osmo-regulator production to nitrogen stress quotients.

Recycling of DMS buildup in the thermocline may also have contributed to the concentration and flux overages in some areas. We plan to include refined estimates of subeuphotic zone decay in future simulations.

At the end of the eight years of ocean-only calculation, a POP restart file with complete biogeochemistry was saved for use in the interactive CCSM experiment described below.

2.4.5 Prototype Coupling of Biogeochemistry for a First Generation Earth System Model

A fully coupled global climate and biogeochemical model configuration was recently assembled by this project and a run of a fully coupled biogeochemical code was initiated, completed and evaluated, satisfying a FY05 DOE/OMB deliverable. The CASA' terrestrial biogeochemistry module was coupled with the Community Land Model Version 3 (CLM3) and is a part of this model configuration. The POP ocean with attendant ocean ecosystem and trace gas modules was been coupled to the atmospheric climate model that simultaneously interacts with the terrestrial biosphere model. The fluxes of CO_2 and DMS between the ocean and land and the atmosphere were achieved via a modification to the coupler for tracer exchange. The spatial structure of DMS in the atmosphere reflects the input of DMS, passed through the coupler, emitted by the ocean sub-model and the seasonal cycle of the DMS system is reasonable. The distribution of CO_2 and

DMS in the atmosphere model reflects surface sources and sinks due to anthropogenic and natural sources and sinks in the ocean and the terrestrial biosphere.

This simulation represents the first fully coupled simulation of a physical ocean model (POP) that has an imbedded ocean biological ecosystem model with an atmosphere that is simultaneously coupled to a detailed model of continental biological and physical processes. The terrestrial biosphere, oceanic biosphere and the classically constructed physical climate system all interact and contribute to the simulated climate idealization. The biogeochemical and physical climate system is fully coupled in the sense that changes and trends in the biogeochemistry influence the physical climate at each time step and vice versa. While the model configuration is apparently stable so far in this simulation, a fully coupled spin up run is needed to determine if atmospheric CO_2 will stabilize, and a century-scale simulation is needed to evaluate climate and carbon cycle feedbacks.

Motivation for the Biogeochemical Coupling

The global climate system is strongly impacted by the details of, and feedbacks between, the various biogeochemical systems. A global biogeochemistry model has been constructed. We report the results of an initial run of the coupled biogeochemistry simulations. The results are divided into the four main components of the modeling infrastructure: land, ocean, atmosphere and coupler. Hereafter referred to as SciDAC-CCSM-BGC, this model configuration consists of the NCAR CCSM3 with the MOZART tropospheric chemistry model added to the CAM3, with the CASA' terrestrial biogeochemistry module added to the CLM3, and with the POP2, containing the Doney-Moore-Lindsay (DML) active ecosystem model and a trace gas model (Chu et al., [32]) replacing POP1.4. In addition to the physical climate represented by CCSM3, fluxes of carbon dioxide (CO_2) and dimethyl sulfide (DMS) are exchanged between the ocean and the atmosphere, CO_2 flux is also exchanged between the land and the atmosphere, and chemical constituent tracers are advected and chemically modified by the atmosphere in the SciDAC-CCSM-BGC model configuration.

A nine-year integration of the model was performed on the IBM Power 4 ("cheetah") at ORNL as a part of a project deliverable to demonstrate that the configuration would run and generate reasonable results. The finite-volume dynamical core was used for the coupled simulations. This is somewhat problematic, in that the CCSM does not have a documented physical climate in the coupled configuration using the finite-volume dynamical core for atmospheric dynamics. Further coupled experiments will need to establish this baseline control climate for the model in the standard configuration

without the biogeochemical components that were added here. In this way a meaningful relation between the biogeochemistry and the model climate can be documented.

The purpose of this exercise is first of all to demonstrate that all the modeling components and the software infrastructure are ready to accommodate the development of an earth system modeling capability that incorporates fully coupled biogeochemical cycles. A second objective is to obtain a first look at the stability and tendency of the carbon pools and chemical sources and sinks in the coupled configuration.

This study is preliminary to a more extensive development project. It should be noted that the climatology of the model has not been established or studied in what is reported here.

Land

The terrestrial model combines the biogeophysics of the CLM3 (Dickinson et al., [37]) with the Carnegie and Stanford Approach (CASA) biogeochemical model (Randerson et al., [50]) modified for use in global climate models. This modified biogeochemical module, called CASA', was formerly integrated into the Climate System Model Version 1.4 (CSM1.4) and used for a 1000-year simulation and a variety of climate change simulations that were recently described (Doney et al., [38]; Fung et al., [39]). CASA' simulates the life cycles of CLM3's plant functional types from carbon assimilation via photosynthesis, to mortality and decomposition, and the return of CO_2 to the atmosphere via microbial respiration. There are three vegetation (live) carbon pools and nine soil (dead) pools, and the rates of carbon transfer among the pools are climate sensitive. The carbon cycle is coupled to the water cycle via transpiration and to the energy cycle via dynamic leaf phenology which affects albedo. A terrestrial CO_2 fertilization effect is possible in the model because carbon assimilation via the Rubisco enzyme is limited by internal leaf CO_2 concentrations, eventually saturating at high CO_2 concentrations.

In the CASA' formulation, net primary productivity (NPP) is assumed to be 50% of gross primary production (GPP) as calculated by CLM3. NPP is allocated to the three live pools (leaf, wood, and root) with preferred allocation to roots under water-limited conditions and to leaves under light-limited conditions. Turnover times of the three live pools are specific to each plant functional type, and leaf mortality of deciduous trees includes cold-drought stress to cause leaf fall in one or two months. Leaf biomass is translated into prognostic leaf area indices (LAI) using specific leaf areas (SLA) so that LAI varies with climate. Excess carbon above the limits placed on LAI is added to litterfall.

For the nine dead carbon pools, leaf mortality contributes to metabolic and structure surface litter, root mortality contributes to metabolic and structure soil litter, and wood mortality contributes to coarse woody debris. The subsequent decomposition by microbes leads to transfer of carbon to the dead surface and soil microbial pools as well as to the slow and passive pools. A fraction of each carbon transfer is released to the atmosphere via microbial or heterotrophic respiration. The rates of transfer are climate sensitive and are functions of soil temperature and soil moisture averaged over the top 30 cm of soil. Before the fully coupled simulation was begun, the terrestrial and ocean carbon cycles were spun up independently of each other with a prescribed atmospheric CO_2 forcing of 350 ppm. The terrestrial carbon pools did not reach equilibrium before the fully coupled simulation was started; however, as will be shown, the atmospheric CO_2 concentration was quickly drawn down by the ocean and by the land. Because the nine-year integration of the fully coupled model is short compared to the turnover times of the terrestrial carbon pools, few conclusions can be drawn about the large scale behavior of the simulated climate or the feedbacks between the climate and the carbon cycle. Nevertheless, the fully coupled model ran adequately and produced reasonable results.

The land model with CASA' was spun up using an F-configuration run of CCSM3 with a fixed prescribed atmospheric CO_2 concentration of 350 ppm. In this configuration, used to avoid the computational expense of running the ocean model, the atmosphere and land models are active while the ocean component simply provides prescribed climatological sea surface temperatures (SSTs) to the atmosphere and the thermodynamic ice models uses prescribed climatological sea ice cover consistent with the SSTs. In order to more quickly reach equilibrium, initial terrestrial carbon pools for this spin-up run were taken from a partially spun-up F-configuration pre-industrial spin-up run which had a prescribed forcing of 285 ppm. The spin-up run used a T31 grid and was itself initialized from a spun-up version of the CSM1.4 implementation of CASA' (Doney et al., [38]; Fung et al., [39]).

When the fully coupled target simulation was to begin, the land model spin-up run had reached year 69; however, the carbon pools had not yet attained equilibrium. In particular, the wood and coarse woody debris pools were still increasing. While the target simulation was started with year 69 initial pool values, the spin-up run was continued until equilibrium was achieved. By year 200, all twelve pools individually appeared to reach equilibrium with the 350 ppm CO_2 atmospheric forcing. The Net Primary Production (NPP) averages about 93 Pg C/yr and Net Ecosystem Exchange (NEE) approaches an annual mean of zero as the carbon pools reach equi-

librium, Figure 2.35.

A nine-year integration of the SciDAC-CCSM-BGC model configuration with all active components was performed on the IBM Power 4 (cheetah). An initial month was run to generate all the files necessary to properly initialize the desired run. Terrestrial carbon pools were initialized to the year 69 values described above beginning in the second month. The fully coupled simulation was started with a contemporary global atmospheric CO_2 concentration of 355 ppm. With no fossil fuel emissions, but an active ocean ecosystem model and an active terrestrial biosphere only partially spun up, this concentration could not be maintained. Instead, the atmospheric CO_2 concentration, as shown both over land and globally in Figure 2.36, was about 342 ppm and continuing to fall at the end of the nine year simulation. This represents a net loss of 28 Pg C from the atmosphere in nine years. Values for the first month, shown here only for completeness, are not valid since the carbon pools and atmospheric CO_2 concentration were set at the beginning of the second month of the simulation.

Of this net loss, the terrestrial biosphere absorbed 16.23 Pg C from the atmosphere over the course of the entire integration; however, productivity began to drop as the atmospheric CO_2 concentration was reduced late in the simulation. As a result, the live carbon pools saw a net loss of 1.82 Pg C while the dead carbon pools experienced a net gain of 18.05 Pg C. Relative to the total amount of carbon stored in the biosphere, the changes are small. The most significant changes in live carbon occur in the Northern Amazon due to a drop in seasonal productivity. Correspondingly, the largest changes in dead carbon pools are increases in the same Northern Amazon region. Figure 2.37 shows the the concentration of CO_2 in the lowest level of the atmosphere model in the coupled simulation in July of the final year. The blue values show where the land model is taking up CO_2 from the atmosphere during the Northern hemisphere growing season. The red values reflect those regions where the land model terrestrial biosphere is releasing CO_2 due to respiration. Figure 2.38 shows the concentration of CO_2 in the lowest level of the atmosphere model in the coupled simulation in July of the final year. The blue values show where the land model is taking up CO_2 from the atmosphere during the Northern hemisphere growing season. The red values reflect those regions where the land model terrestrial biosphere is releasing CO_2 due to respiration. Figures 2.37 and 2.38 show a direct linking between the ocean-and-land-supplied CO_2 fluxes inside the coupler and the imprint on the 3-D atmospheric CO_2 distributions.

Ocean

The ocean was initialized with an 8-year ocean-only spinup described

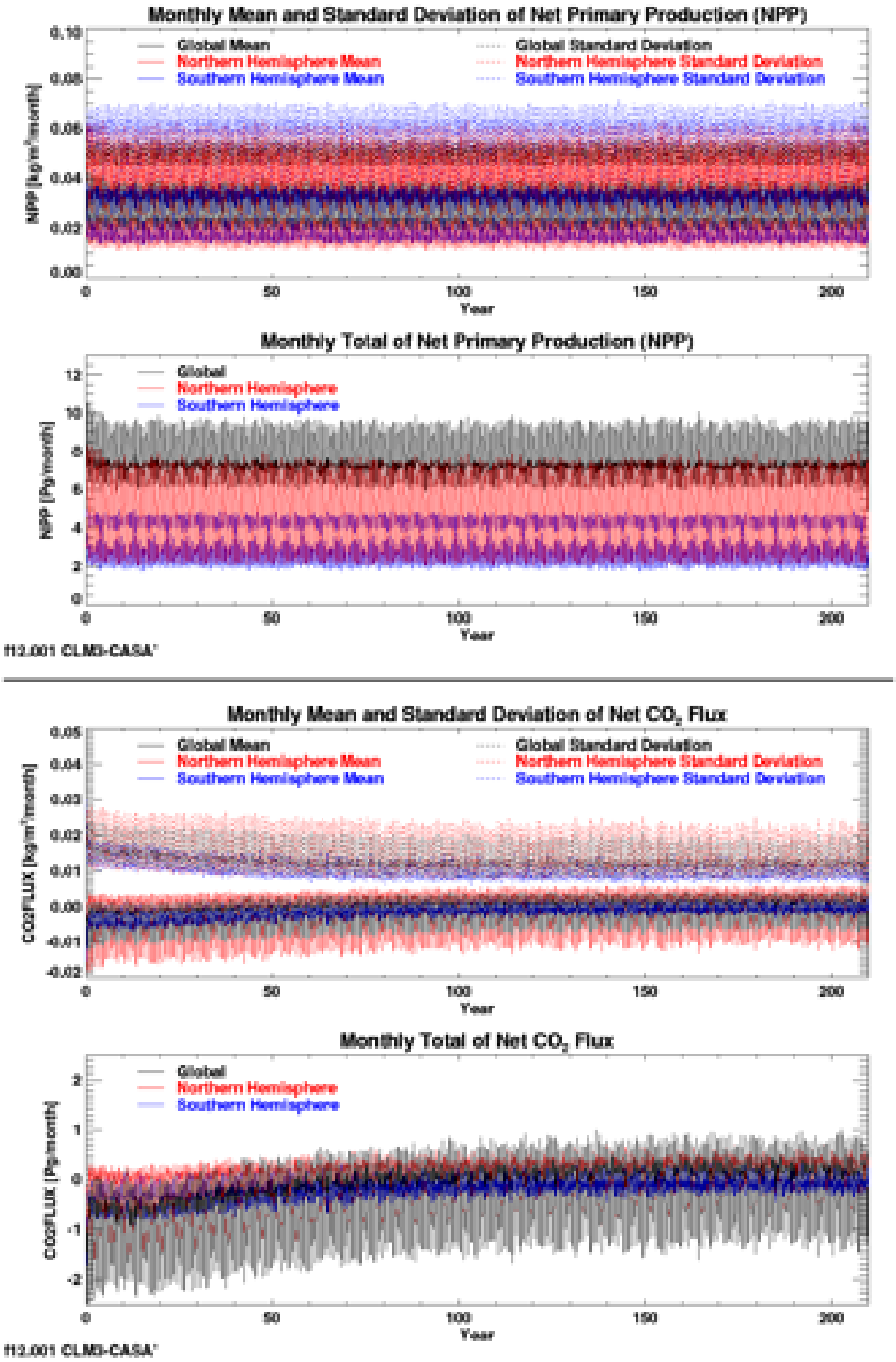

Figure 2.35: By year 200, all twelve pools individually appeared to reach equilibrium with the 350 ppm CO_2 atmospheric forcing. NPP averages about 93 Pg C/yr and NEE approaches an annual mean of zero as the carbon pools reach equilibrium.

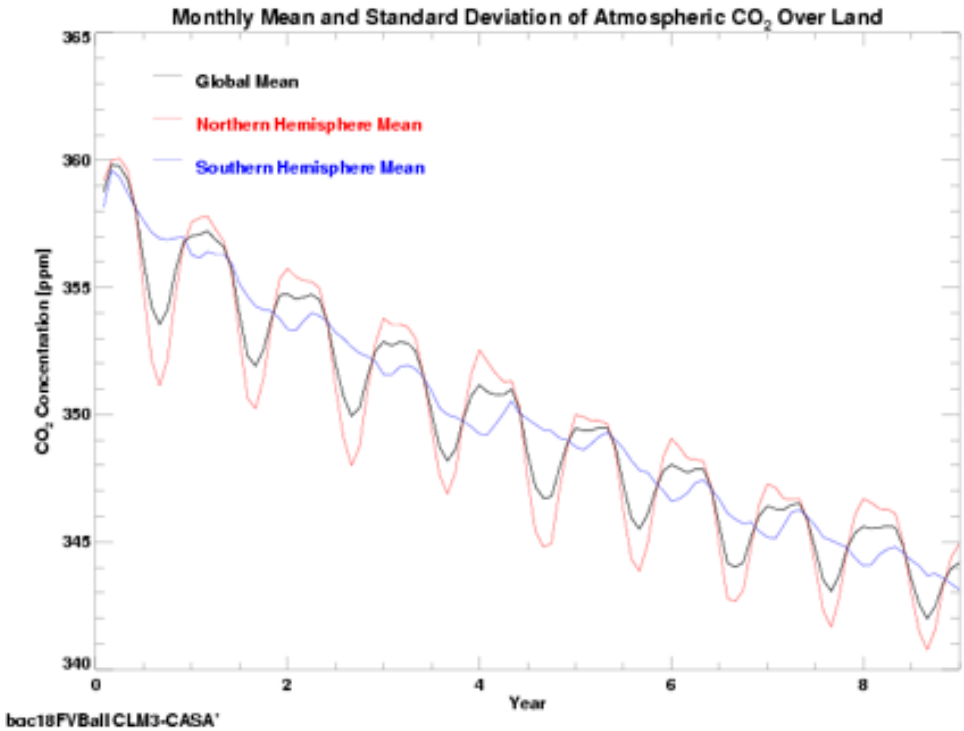

Figure 2.36: The atmospheric CO_2 concentration over land only and in the lowest layer of the atmosphere globally. The concentration dropped significantly from 355 ppm to about 342 ppm during the nine-year fully coupled simulation. This is equivalent to a net loss of about 28 Pg C from the atmosphere. Values for the first month, shown here only for completeness, are not valid since the carbon pools and atmospheric CO_2 concentration were set at the beginning of the second month of the simulation. This decrease in atmospheric mean CO_2 is consistent with the oceanic and terrestrial uptake of CO_2 in this model configuration where there is no anthropogenic CO_2 to replenish and impact the atmospheric CO_2 content.

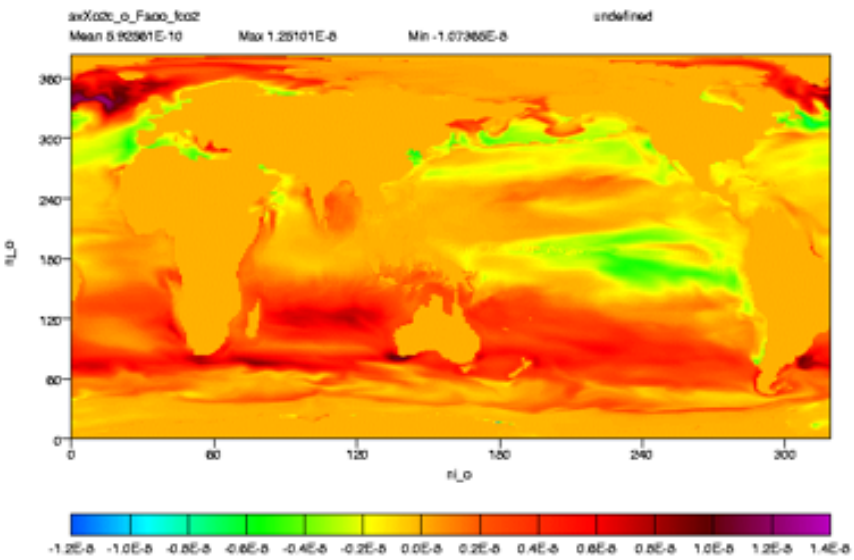

Figure 2.37: The flux of CO_2 between the ocean and the atmosphere as handled by the coupler. The red values show those regions where CO_2 is moving from the ocean to the atmosphere and the yellow to blue values show where the ocean is a sink of atmospheric CO_2 and CO_2 molecules are moving from the atmosphere to the ocean.

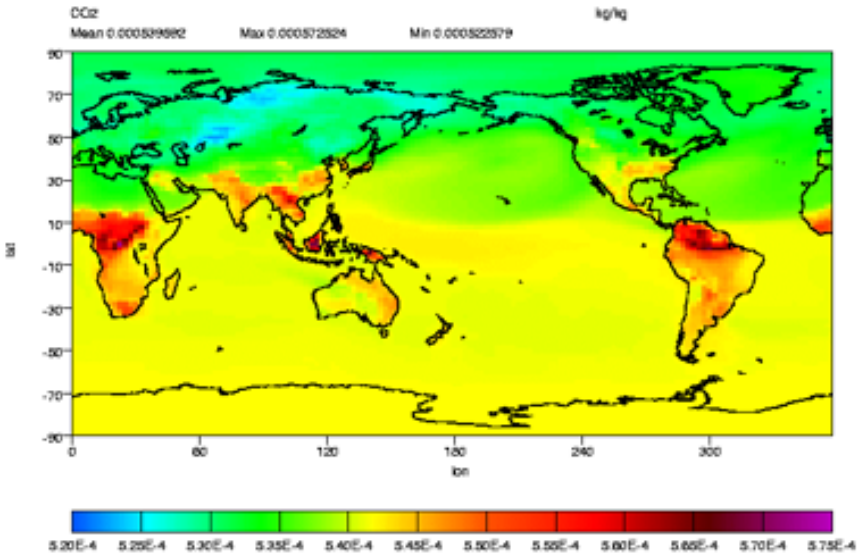

Figure 2.38: The concentration of CO_2 in the lowest level of the atmosphere model in the coupled simulation in July of the final year. The blue values show where the land model is taking up CO_2 from the atmosphere during the Northern hemisphere growing season. The red values reflect those regions where the land model terrestrial biosphere is releasing CO_2 due to respiration.

above. Carbon dioxide levels were released from resetting for the fully coupled simulation. Average fluxes across the interface remained steady. Liquid phase partial pressures and dissolved inorganic C levels were near the expected equilibria except in areas of strong biological activity or communication with preindustrial distributions at depth.

Dimethyl sulfide concentrations hovered near 2 nanomolar continually, under dynamic control of the simulated marine ecology and in broad agreement with available climatologies. Fluxes of the species into the troposphere are several tens of percent higher than the median of literature calculations. The surface ocean sulfur cycle model adopted had been optimized in a chi square sense to fit within tight tropical variability. Low latitude distributions and transfer were realistic, while the reduced sulfur generated by frontal systems was overpredicted somewhat. Mid-high latitude DMS fluxes are roughly 50% higher than observed since the ecosystem-DMS model was tuned for low latitudes.

For next generation CCSM chemistry runs, it is advocated that we work from more sophisticated physics initialization and from current distributions of alkalinity/inorganic carbon. Dimethyl sulfide production rates should be adjusted for regional flux studies, or else modulating influences should be included for the middle latitudes. In the medium term, research should proceed toward oxidation of gas phase sulfur into the aerosol and addition of other climate relevant gases to marine mixed layer geocycling. Ongoing research is work toward coupling of the chemistries of surface ocean and atmosphere in the CCSM. Specifically, dissolved trace gases relevant to climate are being passed from the POP, through the standard coupler interface and into the physics and photochemistry routines of the CAM. Carbon dioxide (CO_2) and dimethyl sulfide (DMS) were chosen as pilot species for an initial demonstration of capability, because they are relatively well understood and influential of the atmospheric state. Preparatory work has included

1. the porting of CCSM ecodynamics into version 2 of POP with its high performance blocked sub-sub domain structure,

2. development of a module for the emplacement of extra-CO_2 volatiles and their geocycling,

3. within this module the design of sulfur cycle mechanisms -typically based on a Gabric et al., (1999) approach,

4. construction of streamlined tropospheric photochemistry routines appropriate for the processing of sea-air transfer species,

5. simple flux tests with global integrations and comparison to observations, plus finally

6. general improvements to the user friendliness of algorithms for addition of species to the coupler.

Across these items, a coarse three degree resolution POP grid was often called upon in the interest of maintaining throughput.

The coupling experiments have begun in earnest based on these collective improvements to CCSM. A finer resolution one degree POP mesh was adopted during the interactive phase of the SciDAC research. Successful runs have yielded five year simulations of contemporary climate time reflecting certain detailed connections between surface marine geocycling and tropospheric chemistry. Samples from the complete computations are described below, primarily from the oceanic perspective but with reference to the other research components, in particular that of the atmospheric chemistry module. Nominal physical spin up of the POP model was conducted initially from a full resting state and extended for ten years. Standard monthly average climatological winds and temperature/salinity fluxes acted as driver fields. They were repeated annually. Under such conditions, major currents and the general circulation are expected to establish themselves to a depth of several hundred meters with approximate realism. Biogeochemical steady state conditions later attained in upper layers of the water column appear to be only weakly biased, so that the simple start up expedient has proven effective. More sophisticated techniques will, however, be recommended for detailed work to be conducted in the future.

A large number of cruise track measurements have become available for dimethyl sulfide since it was identified during the 1980s as a prominent teleconnector species in the global sulfate/albedo loop. The works have been reviewed exhaustively and interpolated (or extrapolated) into a mixed layer reduced sulfur climatology by Kettle et al., [45]. Broadly speaking, the DMS distribution is flat in the tropics and subtropics, averaging nearly two nanomolar with a standard deviation of about one in the same units. A narrow one nM peak follows the equator in the Eastern Pacific. The evenness of the pattern is remarkable given the complexity of geocycling involved, and may entail Gaian ramifications. Small maxima occur along some of the middle latitude fronts, concentrating in the Northern hemisphere. Moving to extreme polar waters, concentrations rise abruptly to order ten nanomolar, for reasons which remain somewhat obscure. Seasonality resembles that of plant biomass and so is weak in the tropics, bloom-triggered elsewhere.

Dimethyl sulfide was permitted to cross through the coupler into CAM photochemistry for reaction with oxidants such as the hydroxyl and nitrate radicals, and for generation of gas phase intermediates along the sequence leading to sulfate and nuclei. The influence of interactive sulfur fluxes on tropospheric concentration fields will be discussed elsewhere. The coupled run lasted 5 further years. We have once again adopted the expedient of examining concentration fields at the beginning, middle and end stages along with the plotting of planet-wide flux time series for both gases. We find that, on moving through the transition to interactive system modeling, neither the local values nor transfer rates make large jumps. The character of the ocean-only steady state is thus preserved. Annual cycles in the time series become less regular than they had been in the climatological forcing regime. This is likely a function of sudden introduction to model winds, which may differ appreciably from long term averages. Alterations to nutrient upwelling would be anticipated since material fluxes are controlled to some extent by the downward propagation of momentum. There is also the possibility that deviations from average precipitation and evaporation fields influence CO_2 partial pressures through dilution or concentration of alkalinity and the DIC. Strict charge neutrality and acid base requirements imposed by the seawater medium could well amplify such effects significantly. Specific biases of the CCSM including the well known double ITCZ feature are noteworthy in the biogeochemical surface fields but do not affect our major conclusions. Figure 2.39 shows the concentration of DMS in the surface level of the ocean as computed for July of years 7-9. The red values are the highest and reflect enhanced biological activity and increased DMS production in the surface ocean. Figure 2.40 shows the flux of DMS that is actually in the coupler. This is consistent with the concentration of DMS that is in the surface layer of the ocean in POP, Figure 2.39.

Agreement with climatologies and biophysically based hypotheses is in most cases encouraging. Simultaneously, however, new directions are indicated which might be explored in next generation work. Discrepancies are attributable to the simplicity and short duration of spin up, to the artificial nature of initial conditions or to known weaknesses in the sulfur cycle code. In most cases the fixes are easily conceived and have been discussed here. They include substitution of circulation equilibrated to the century scale, realistic/contemporary initial carbon distributions, and slight adjustments to the sulfur release rates. We thus advocate a continuation of the experiments with further enhancements to the nature of the chemical coupling. Connections with radiative transfer in CAM should be implemented. This will mean linkage of the atmospheric carbon distribution and its associated

marine uptake to greenhouse physics. Oxidation of sulfur within the troposphere should proceed through the formation of condensation nuclei to direct and indirect effects. The trace gas module is already being updated with a longer list of sea/air transfer species influential of the photo-aerosol chemistry tracked in CAM. New surface ocean geocycles include those of nitrous oxide, carbon monoxide, methane, straight chain nonmethane hydrocarbons and volatile organohalogens. Mixed layer carbonyl sulfide and isoprene mechanisms are in planning phases. Some or all of these species could be caused to pass through the coupler and into the gas phase in the near future. Improvements will also be made to latitudinal distributions computed for aqueous dimethyl sulfide, by enhancing sophistication of the existing sulfur cycle as described above.

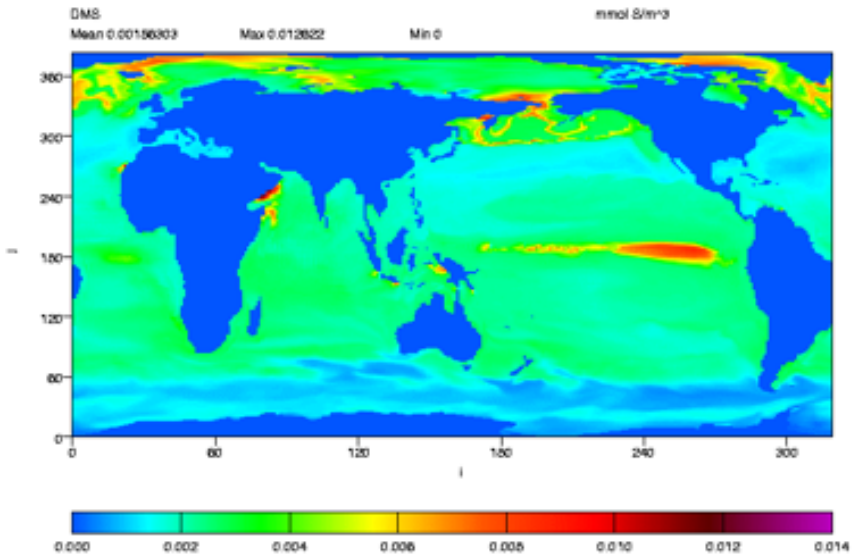

Figure 2.39: The concentration of DMS in the surface level of the ocean as computed for July of years 7-9. The red values are the highest and reflect enhanced biological activity and increased DMS production in the surface ocean.

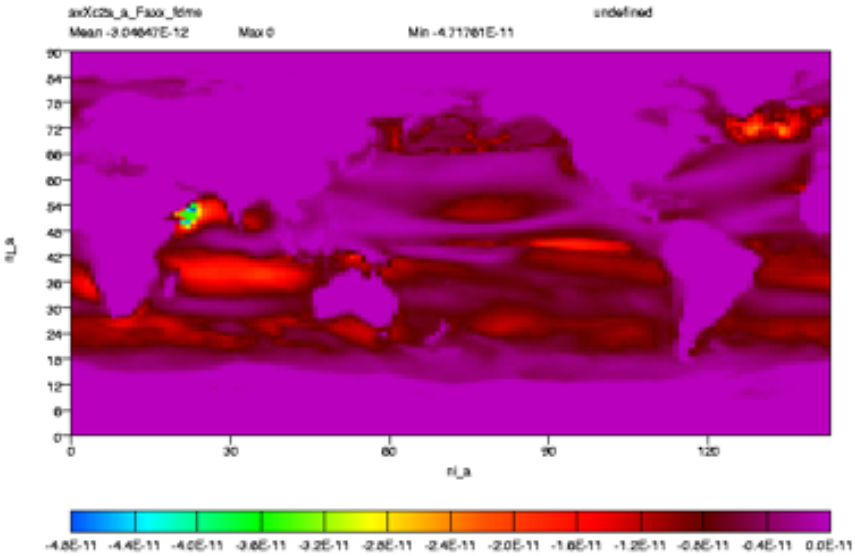

Figure 2.40: This figure shows the flux of DMS that is actually in the coupler. This is consistent with the concentration of DMS that is in the surface layer of the ocean in POP, Figure 2.39

Atmosphere The Community Atmosphere Model model with interactive chemistry (Lamarque et al., [46]) has been modified to use the interactively calculated oceanic DMS fluxes. The chemistry in CAM3 is based on the MOZART model that has been modified (Brasseur et al., 1998 [1]; Hauglustaine et al., 1998 [42]). To perform the atmospheric chemistry simulations, we use the CAM3 (Collins et al., [36]) coupled to the Model for Ozone and Related Tracers (MOZART) chemistry (Horowitz et al., [43]), including aerosols (Tie et al., [52], [53]).

MOZART has a representation of tropospheric chemistry with non-methane hydrocarbons (NMHCs) treated up to isoprene, toluene and monoterpenes. This chemical mechanism is an extension of the mechanism presented in Horowitz et al., [43]; changes include an updated terpene oxidation scheme and a better treatment of anthropogenic NMHCs. The MOZART aerosols have been extended from the work by (Tie et al., [52] 2005 [53]) to include a representation of ammonium nitrate that is dependent on the amount of sulfate present in the air mass following the parameterization of gas/aerosol partitioning by Metzger et al., [49]. In our model, we have included the uptake of N_2O_5, HO_2, NO_2, and NO_3 (Jacob, [44]) on aerosols. The effect of aerosols on photolysis rates is not included in this study. Because only the bulk mass is calculated, a log-normal distribution is assumed for all aerosols to calculate the surface area, using different mean radius and geometric standard deviation (Liao et al., [47]).

CAM3 with interactive chemistry simulates the evolution of the bulk aerosol mass of black or elemental carbon (EC, hydrophobic and hydrophilic), primary organic (POA, hydrophobic and hydrophilic), second organic ammonium (SOA, linked to the gas-phase chemistry through the oxidation of atmospheric NMHCs as in Chung and Seinfeld (2002) [33]), and ammonium nitrate (from NH_3 emissions), and sulfate aerosols (from SO_2 and DMS emissions). A description of sea-salt, updated from Tie et al., [53], is also included. Finally, a monthly-varying climatology of dust is used only for radiative calculations. In this study, the only way the chemistry affects the atmosphere is through the radiatively active gases and the direct effect of aerosols. The effects of the aerosols on the shortwave fluxes and heating rates are calculated following Collins et al., [35]. In addition, the radiative properties of ammonium nitrate are assumed to be identical to ammonium sulfate (Liao et al., [47]).

The DMS flux is interactively calculated in the ocean and is fluxed through the coupler into the bottom layer of CAM. The oxidation of DMS to SO_2 is based on published reaction rates and the model calculated OH concentration. The final step is the formation of sulfate from SO_2; this for-

mation occurs either in the gas-phase or in the liquid phase. Both formation paths are included in the model. As a general constraint on the performance of the atmospheric chemistry module, the mean lifetimes for years 2 to 9 of the simulation are 11.7 years for CH4 and 6.5 years for CH3CCl3, which are slightly longer than the observational estimates for the current atmosphere: 10-11 years for CH4, and 6.1 years ($\pm$ 0.1 year) for CH3CCl3. However, the model results are consistent with the chemistry run in an atmospheric only configuration (CAM) and are within the range of values from other state-of-the-science tropospheric chemistry models.

The primary focus of atmospheric chemistry and aerosols in this model is on the sulfur cycle, in particular the formation of sulfate aerosols from dimethyl sulfide emitted from the ocean biogeochemistry. The coupled model was run for nine years; we ignored the first year, during which the sulfur cycle will be affected by the initial conditions, so the following plots are for simulated years two to nine. Figure 2.41 shows a comparison of the simulated sulfate aerosols against observations at oceanic sites in the Eastern hemisphere. The mean concentration at these sites agrees fairly well at tropical sites, but poorly at the extratropical sites, reflecting the weakness of the DMS algorithm in the extratropics. Much better agreement between model and observations is seen for comparisons with land based observations on the east coast of the U.S., which are primarily affected by anthropogenicly emitted SO_2 (Figure 2.42). Figure 2.43 presents the global OH concentration in the atmospheric surface model level for July. The highest OH concentrations are in the mid-latitude Northern hemisphere reflecting the high flux of radiation during the summer period. The elevated concentrations in regions of anthropogenic influence are an indicator of active $HO_x - NO_x$ chemistry in polluted regions. Figure 2.44 shows the time series of atmospheric DMS and SO_4 for a site on the equator. The SO_4 concentrations track the atmospheric gas phase DMS reasonably well. Some divergences between the gas phase DMS concentrations and aerosol SO_4 is expected due to transport issues that occur on the time scales of the DMS and SO_4 residence times.

Overall the performance of the atmospheric chemistry portion of the calculation is encouraging. The residence time for CH_4 (11.6 years) is reasonable and the global supply of DMS related sulfate (32 Tg S/yr) is within the most recently published estimates. The spatial structure of the DMS fluxes are in good agreement with the most recently published global DMS flux simulation (Chu et al., [231]). The seasonal cycle of sulfate over land is in good agreement with observations.

Coupler

The DOE deliverable coincided with NCAR efforts to perform OCMIP

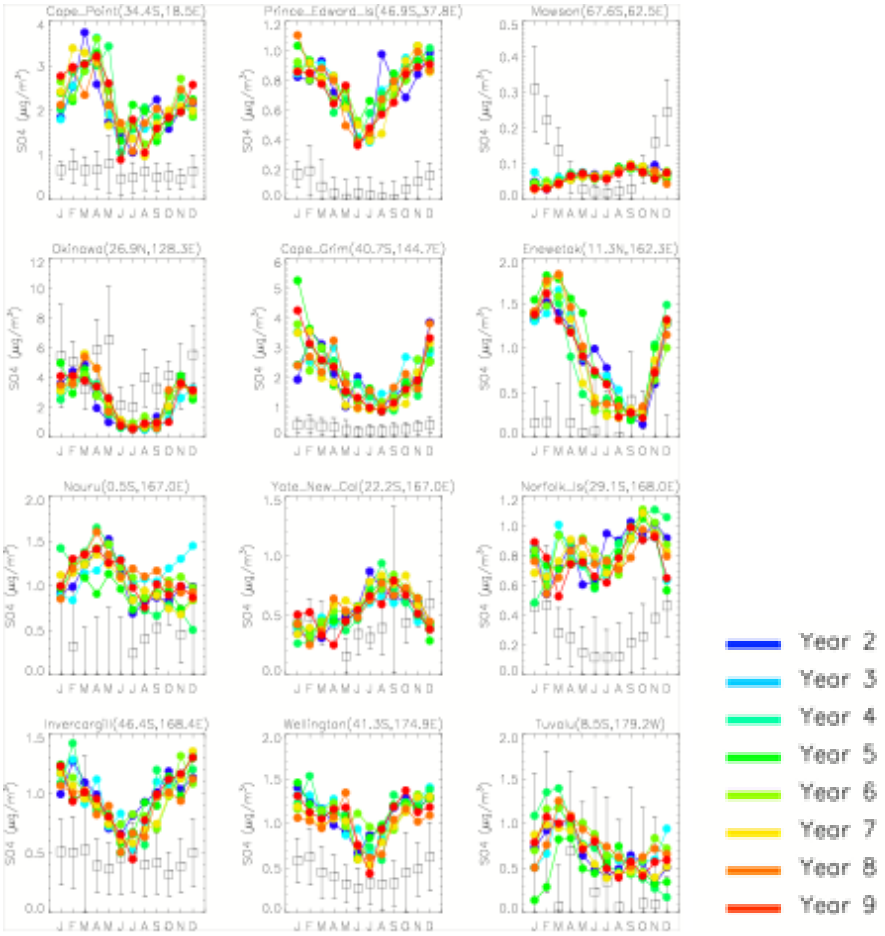

Figure 2.41: Comparison of the monthly-mean model SO_4 concentrations against surface observations made by the NOAA CMDL at oceanic sites in the Eastern hemisphere. The box and whiskers show the monthly mean and standard deviation of the observations.

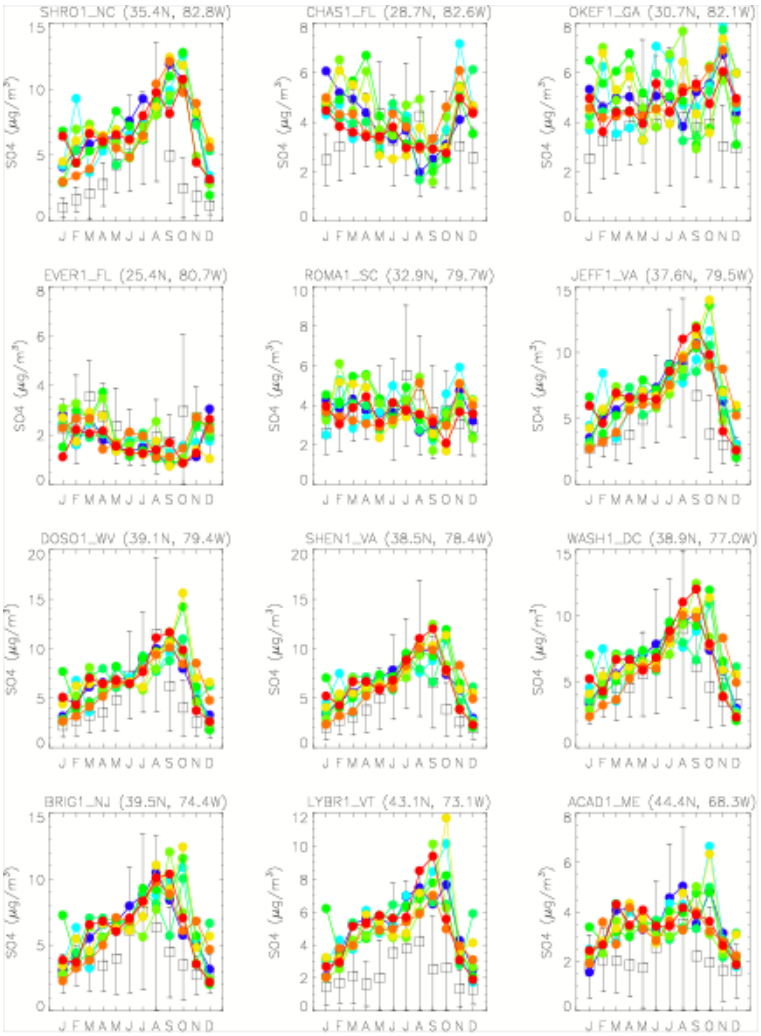

Figure 2.42: Comparison of the monthly-mean model SO_4 concentrations against surface observations made on the east coast of the USA by the IMPROVE network. The box and whiskers show the monthly mean and standard deviation of the observations.

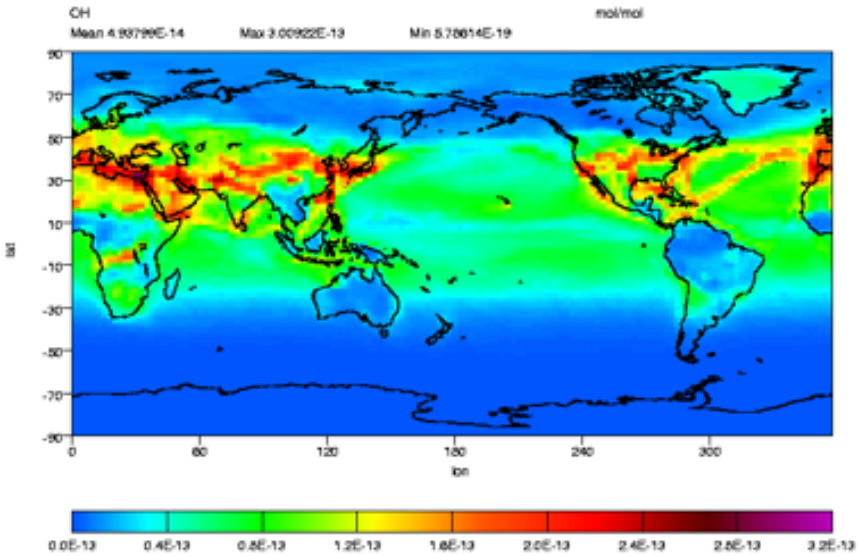

Figure 2.43: The map presents the global OH concentration in the atmospheric surface model level for July. The highest OH concentrations are in the mid-latitude Northern hemisphere reflecting the high flux of radiation during the summer period. The elevated concentrations in regions of anthropogenic influence is an indicator of active $HO_x - NO_x$ chemistry in polluted regions.

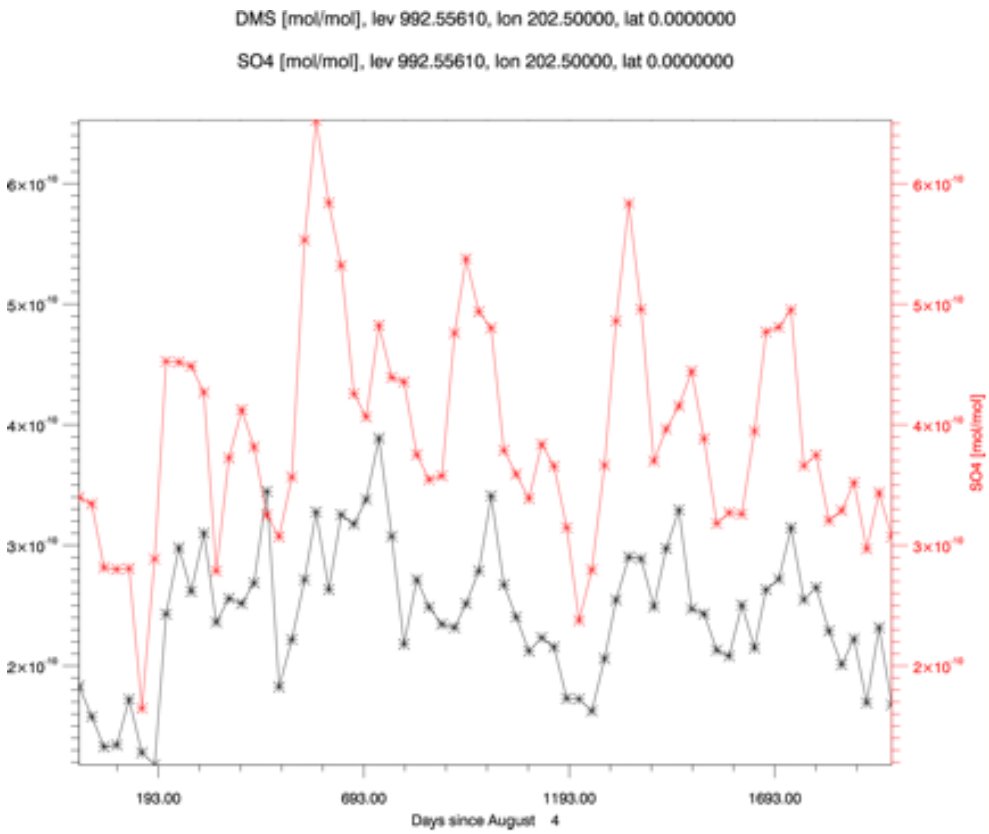

Figure 2.44: The time series of atmospheric DMS and SO_4 for a site on the equator in the Pacific. The SO_4 concentrations track the atmospheric gas phase DMS reasonably well.

simulations with CCSM3 and so SciDAC and NCAR scientists worked together to make it easier to add biogeochemistry fields to the data flowing through the CCSM coupler.

All the fields passed through the coupler are listed in a character string for each model-coupler pair and direction. Figure 2.45 shows the configuration of the present version of the coupler used in this simulation. These strings are contained in the *cpl_fields_mod.F90* module in the CCSM source code. Along with the strings are integer parameters indicating the location of each field in the string. For the released version of CCSM, CCSM3, adding a new field to the coupled data flow amounted to adding a new element to the appropriate character string and an integer parameter with the correct values. One flaw with this method was that the integer parameters and character strings could get out of sync and possibly introduce hard to find errors. The coupler-model interfaces were altered so that the integer indices were calculated at runtime from their position in the string using query functions from the Model Coupling Toolkit, the software underlying the CCSM coupler. The query functions made it possible to determine at runtime which fields were active (a return value of zero for the index indicates the field is not active) and this in turn allowed the model-coupler interfaces to support several different configurations of biogeochemistry tracers. The exact configuration is contained in new versions of the *cpl_fields_mod.F90* file such as *cpl_fields_mod.F90.CO2A* for passing CO_2 to the land and *cpl_fields_mod.F90.CO2B* for passing CO_2 to the land and calculating land-atmosphere CO_2 fluxes to the atmosphere. The choice of which configuration to use is made prior to building the CCSM executables. A design document governing these changes was prepared and is available at *http://climate.anl.gov/scidac/wiki/moin.cgi/CoupledClimateCarbon/DesignDocument* .

Predicted CO_2 at the lowest atmosphere level is passed to the coupler. The coupler passes the CO_2 value to the land and also maps it to the ocean grid and passes it to the ocean. The CO_2 tracer mapping uses the same bilinear interpolation weights as for other state variables in the coupled system. DMS tracer values are not passed from the atmosphere to the ocean. The ocean assumes the atmosphere value is zero in its DMS flux calculation.

The ocean passes calculated DMS and CO_2 fluxes back to the coupler which maps them to the atmosphere grid (using the conservative mapping weights of other fluxes) and passes them to the atmosphere along with a separate land-atmosphere CO_2 flux calculated by the land model. Figures 2.36-2.40 address the passing of DMS from the land, ocean and atmosphere

via the coupler. The merging of land and ocean CO_2 fluxes is performed in the atmosphere so that optional fossil fuel emissions read by the atmosphere can also be incorporated.

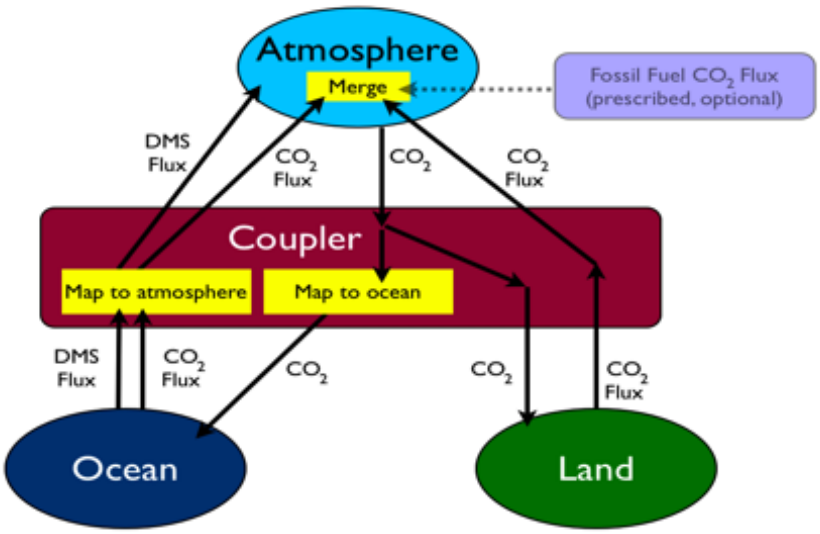

Figure 2.45: The mapping strategy as related to the coupler for the fluxes of CO_2 and DMS between the land, ocean and atmosphere system.

2.4.6 Conclusions

The fully coupled SciDAC-CCSM-BGC model configuration containing the MOZART tropospheric chemistry model, the CASA' terrestrial biogeochemistry model, and the Doney-Moore-Lindsay ocean ecosystem model and ocean trace gas model has completed a nine-year integration on the IBM Power 4 ("cheetah") at ORNL. The CASA' module was successfully coupled to CLM3 and appears to be producing reasonable results. Like most biogeochemistry models, CASA' requires a significant amount of simulated time for equilibrating carbon pools to any particular climate forcing. For the fully coupled run described here, the terrestrial carbon pools had not been completely spun up to an atmospheric CO_2 forcing of 350 ppm (or to the 355 ppm where the fully coupled simulation began); however, NPP was quickly reduced as the ocean and the land absorbed carbon from the

atmosphere. Fossil fuel emissions, estimated to be a source of 3 Pg C/yr to the atmosphere, were not included in the model.

As atmospheric CO_2 concentrations dropped from 355 ppm to about 342 ppm over the nine-year simulation, the terrestrial biosphere was a sink for a net total of 16.23 Pg C. Meanwhile, NPP dropped from 90 Pg C/yr to about 84 Pg C/yr primarily because of reduced CO_2 fertilization. The live carbon pools saw a net loss of 1.82 Pg C while the dead carbon pools experienced a net gain of 18.05 Pg C. The spatial structure of DMS in the atmosphere reflects the input of DMS, passed through the coupler, emitted by the ocean sub-model. The seasonal cycle of the DMS system is reasonable. The residence time of CH_4 in the model is about eleven years, which is 10% higher than presently thought. The distributions of atmospheric sulfate (SO_4), reflecting the oceanic DMS fluxes, is simulated reasonably well at low latitudes but is overestimated at mid-high latitudes. The distributions of atmospheric sulfate (SO_4), reflecting the oceanic DMS fluxes, is simulated reasonably well at low latitudes but is overestimated at mid-high latitudes.

A physical climate control run using the finite-volume dynamical core has not been made but is needed for comparison with the biogeochemical version of the model. Longer runs of the SciDAC-CCSM-BGC model configuration are needed to fully evaluate the simulated climate and the climate and biogeochemical feedbacks. In addition to spinning up the land and ocean ecosystems independently offline, the entire fully coupled model should be run for a considerable time to spin up the interacting land and ocean ecosystems together.

The SciDAC-CCSM-BGC model configuration lays the groundwork for a candidate Earth System Model and is expected to stimulate further development of coupled climate-biogeochemistry models. In future runs of the SciDAC-CCSM-BGC model configuration, fossil fuel emissions should be included. Additionally, a model of dust sources to the atmosphere and dust deposition into the ocean as well as a model of volatile organic compounds (VOCs) could be important to accurately simulating the radiation balance, the ocean ecosystem, and appropriate aerosol forcing.

Chapter 3

SPECIAL PUBLICATIONS

Significant new scientific insights were enabled by this project, many of which are published in articles in a special issue of the Journal of Climate edited by Bill Collins [5]. Among the conclusions are the attribution of warming in the latter part of the last century to greenhouse gas loading of the atmosphere. This conclusion was already made with the Parallel Climate Model (PCM) series models but has been reaffirmed in the more comprehensive CCSM3 model with better treatment of sulfate aerosols. Another conclusion is that the climate sensitivity of the model is higher than PCM but still lower than other models. The reasons for this are examined. Finally, we are involved with simulations that supplement the IPCC studies with highly resolved regional detail, downscaling and the inclusion of the carbon cycle and dynamic vegetation. The carbon experiments, referred to as the C4MIP, are quantifying the level of variability in climate due to land use patterns and changing, possibly collapsing, ecosystems.

A special issue of the International Journal of High Performance Computing and Applications appeared in the Fall 2005 issue. Many of the tasks supported by this project are described in this special issue. Articles describe the computational and software advances of the CCSM3, the performance portability of components, performance models, parallel algorithms, new numerical algorithms, new software toolkits and frameworks. The majority of articles in this special issue describe work conducted as part of this project. J. Drake (ORNL), P. Jones (LANL) and G. Carr (NCAR) are guest editors for this special issue. Dr. A. Patrinos, OBER Director, provided the preface.

Chapter 4

FUTURE PLANS

While much was accomplished over the past five years under SciDAC, much more needs to be done. A proposal to the follow-on SciDAC program was successful for FY07-FY12. Under this proposed effort, there will be a continued focus on biogeochemistry and aerosols. An interactive ice sheet model will also be added to address issues like Greenland melting and its climate impact. Work will continue on alternative algorithms and dynamical cores to improve both the fidelity and performance of the model. Software engineering and parallel algorithm development will focus on scalability for petascale systems that will likely employ over one hundred thousand processors.

Chapter 5

MANAGEMENT

In a collaboration such as this, which involves eight major research institutions, it is imperative that roles and responsibilities be clearly defined. Toward this end, a Management Plan (MP) was produced and reviewed by at least the lead investigator at each laboratory. The MP defined key topical areas in which this SciDAC project contributed to CCSM. Each DOE laboratory decided to which areas it was qualified to contribute and selected a "Topic Leader" in each such area to oversee that laboratory's activities and serve as a contact point in coordinating with other institutions in the Consortium. The PIs appointed one such Topic Leader to be the consortium Topic Coordinator; it was the responsibility of this person to coordinate activities among the six DOE laboratories and with the NCAR counterpart in the given topic area. We maintained frequent contact with the participating labs and with our colleagues at NCAR through weekly teleconference calls and periodic face-to-face meetings, typically arranged to coincide with the annual CCSM meeting or other CCSM working group meetings.

As part of the DOE SciDAC Program, the CCSM Consortium also worked collectively with parts of the whole SciDAC infrastructure development efforts, namely the ISICs and National Collaboratories (NCs). Coordination with the SciDAC ISICs and Collaboratories was also the responsibility of the PIs, but each coordinated task had a lead or contact designated. Collaborations were particularly important for the PERC center and the Earth System Grid collaboratory.

Collaboration with the NASA-funded Earth System Modeling Framework (ESMF) was maintained by contact with this effort through jointly funded investigators. Toward the end of the project, CCSM software engineers developed an evaluation plan for use of ESMF within CCSM.

Chapter 6

PERSONNEL SUMMARY

Researcher	Institution	Special Role	Expertise
John Drake	ORNL	PI, AMWG liason	algorithms for atm
Phil Jones	LANL	PI, OMWG liason	algorithms for ocn and ocn performance
David Erickson	ORNL	BGCWG liason	atm chemistry, carbon and sulfur cycle
Forrest Hoffman	ORNL	LMWG liason	land model, carbon cycle
Pat Worley	ORNL	SEWG liason	algorithms for atm and model performance
Marcia Branstetter	ORNL		river transport, hydrology
Bob Malone	LANL	PI, (retired)	algorithms for ocn
Scott Elliott	LANL		ocean biogeochemistry
Shou-Ping Chu	LANL		ocean biogeochemistry
Bill Lipscomb	LANL		ice model development
Mat Maltrud	LANL		ocean model development
Rob Jacob	ANL		coupler, MCT development
Jong Kim	ANL		automatic differentiation
Jay Larson	ANL		coupler, MCT development
Rob Loy	ANL		model performance
Steve Ghan	PNL		subgrid orography, atmos. chemistry
Timothy Shippert	PNL		subgrid orography
Philip Cameron-Smith	LLNL	ChemWG liason	atmospheric chemistry
Phil Duffy	LLNL		high-resolution atmosphere
Art Mirin	LLNL		FV core development, model
Chris Ding	LBNL		coupler, MPH development, ZioLib
Helen He	LBNL		coupler, single executable
Bill Collins	NCAR	SSC chair	CCSM Chief Scientist(2003-2005)
Peter Gent	NCAR	SSC chair	CCSM Chief Scientist(2005-2006)
Jeff Keihl	NCAR	SSC chair	CCSM Chief Scientist(2001-2003)
Warrren Washington	NCAR	CCWG co-chair	Climate change studies
Jean-Francios Lamarque	NCAR		atmospheric chemistry
Mariana Vertenstein	NCAR	SEWG co-chair	software engineering and land model
Jeff Lee	NCAR		software engineering
Wei Yu	NCAR		software engineering
Nancy Norton	NCAR		ocean model software engineering
Tony Craig	NCAR	CCSM architect	software engineering
Tom Henderson	NCAR	CAM architect	software engineering

Table 6.1: Personnel roles and responsibilities in the SciDAC CCSM Consortium.

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