SEWG 02-2003

Collaborative Design of the Community Climate System Model for Software Performance Portability

Sponsor: Department of Energy

Office of Biological and Environmental Research(OBER)

Scientific Discovery through Advanced Computing(SciDAC)

Principal Investigators

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Goals

- **Performance portability for CCSM**
- **Open software design process**
- **Layered architecture to insulate modeling**
- **Modern SWE practices**
- **Improvement of methods and models supporting more comprehensive coupled climate simulations**

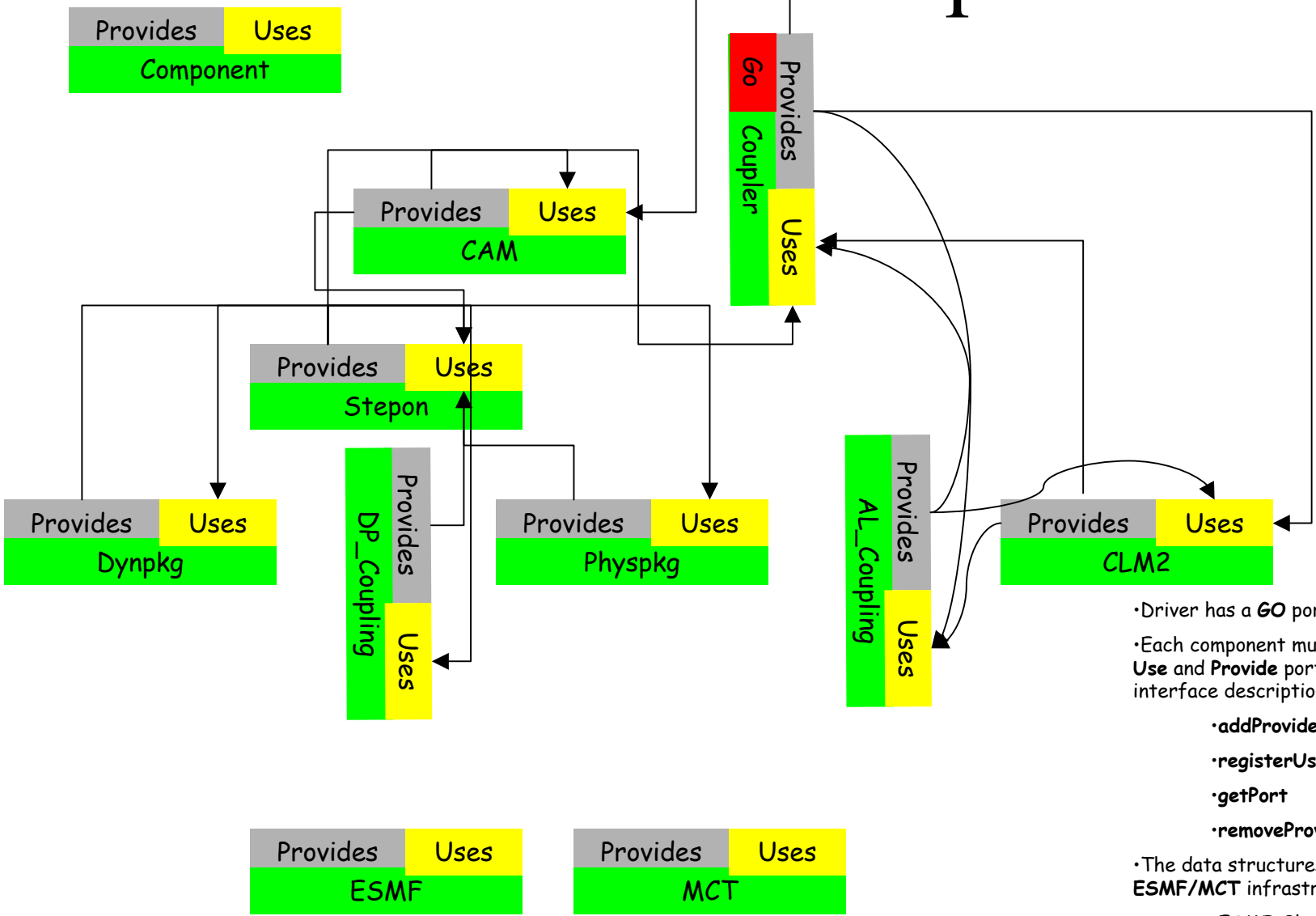
Tasks Accomplished

Milestone	Deliverable	Section
MCT software release	Expanded version of MCT1.0	4.1
MPH software release	MPH3.0 available	4.2
MLP Implementation of coupler CPL5	Performance study	3.3
Testing of new coupler CPL6	Performance study	4.1
2-D decomposition of DAO finite-volume dycore	Verified code in CAM2.0	2.1
Scaling of spectral dynamics, Physics chunking and load balancing	Verified code in CAM2.0.1	2.2
Load balancing of physics chunks	Verified code in CAM2.0.1	2.2
Subgrid precipitation parameterization tested	Simulation (publication)	2.3
Requirements document for POP drafted	Draft document in review	3.1
Cache-friendly chunking in POP2.0	Beta release of POP2.0	3.2
MLP implemented in POP	Alpha version of POP1.4.4	3.3
HYPOP tested in Lagrangian and Eulerian limits	Draft document in review	3.4
ZioLib software release	Performance study	5.1
Requirements document for land model	Published	6.1
CLM2.1/CAM interface improvements	Verified code in CAM2.0.2	6.1

Tasks Accomplished

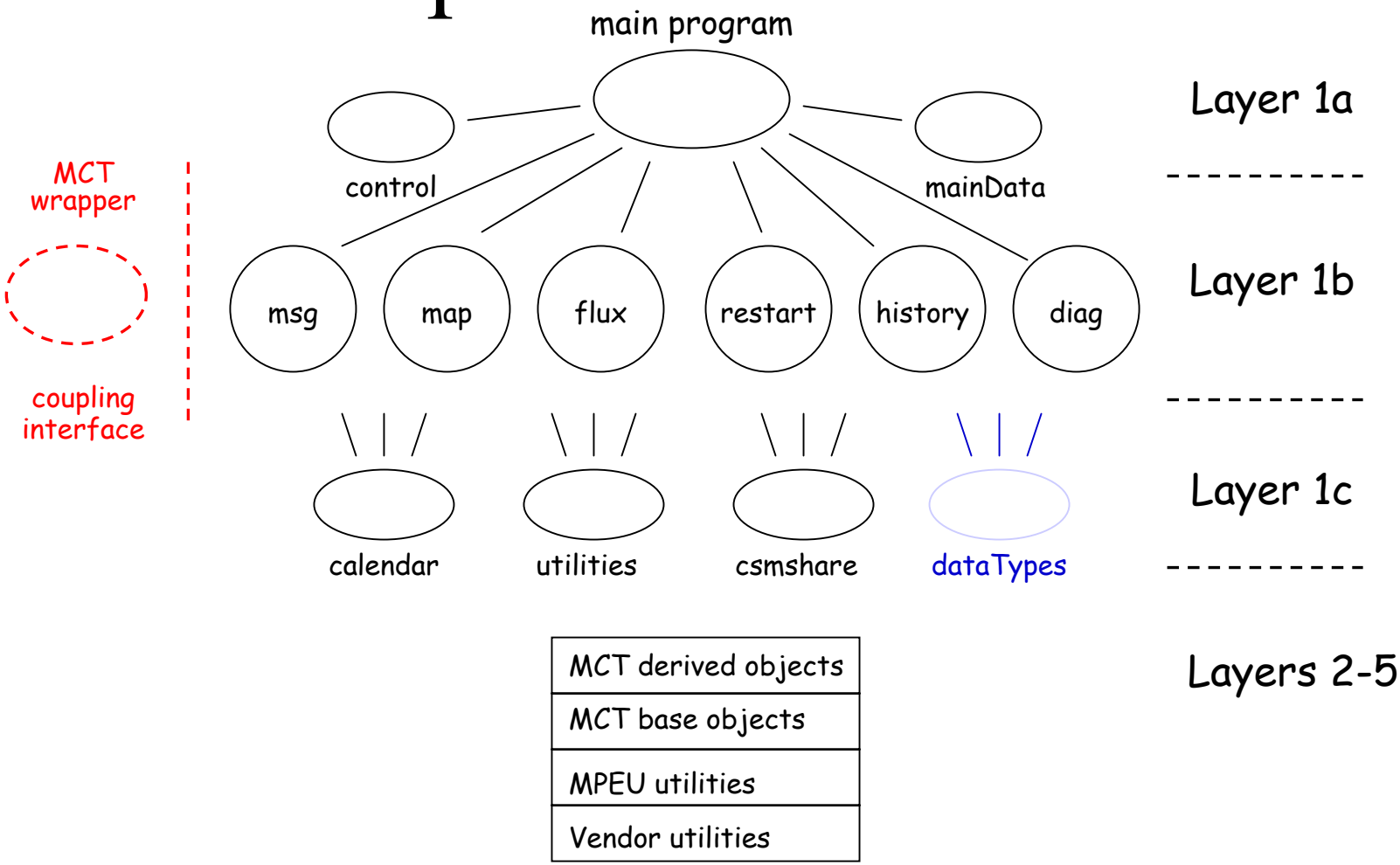
Small tropospheric Chemistry implemented	Simulation (publication)	7
WACCM configuration with FV implemented	Simulation (publication)	7
Ocean biogeochemistry modeled	Simulation (publication)	9.1
ESMF collaboration	Amended design document	9.2
PERC collaboration	AG Meeting	9.2
ESG collaboration	AG Meeting	9.2

CCA/ESMF Components



- Driver has a **GO** port
- Each component must register its **Use** and **Provide** ports via an interface description and
  - **addProvidesPort**
  - **registerUsesPort**
  - **getPort**
  - **removeProvidesPort**
- The data structures are from **ESMF/MCT** infrastrucutre
  - ESMF_PhysGrid
  - ESMF_DistGrid
  - ESMF_Field

Coupler Architecture



Coupler Development

- **Model Coupling Toolkit**
  - Release of MCT 1.0, November 2002
  - 12 new functions to retrieve subsets of data from MCT Attribute Vector and General Grid data types
  - additional communication functions for the GlobalSegMap
  - Rearranger module supports two forms of general data transfer between parallel components: between components that share no processors and between components that share all or a portion of their processor space
- **MPH3 (multi-processor handshaking) library for coupling component models**
  - ProTex was added, and a complete manual written
  - MPH2 used in CCSM2
  - MPH3 used in CSU coupled model development
- **CPL6 Development**
  - CPL6 datatypes (so-called bundles) built upon the basic datatype (attribute vector) defined in MCT
  - Initial timing of the message passing and mapping functions

MCT: Model Coupling Toolkit

Version 1.0 Released
14 November 2002

Major Attributes:

- *Maintains model decomposition descriptors (e.g., global to local indexing)*
- *Inter- and intra- component communications and parallel data transfer (routing)*
- *Flexible, extensible, indexible field storage*
- *Time averaging and accumulation*
- *Regridding (via sparse matrix vector multiply)*

→ *The MCT eases the construction of coupler computational cores and component-coupler interfaces.*

www-unix.mcs.anl.gov/mct

MPH: Multi-Component Handshaking Library

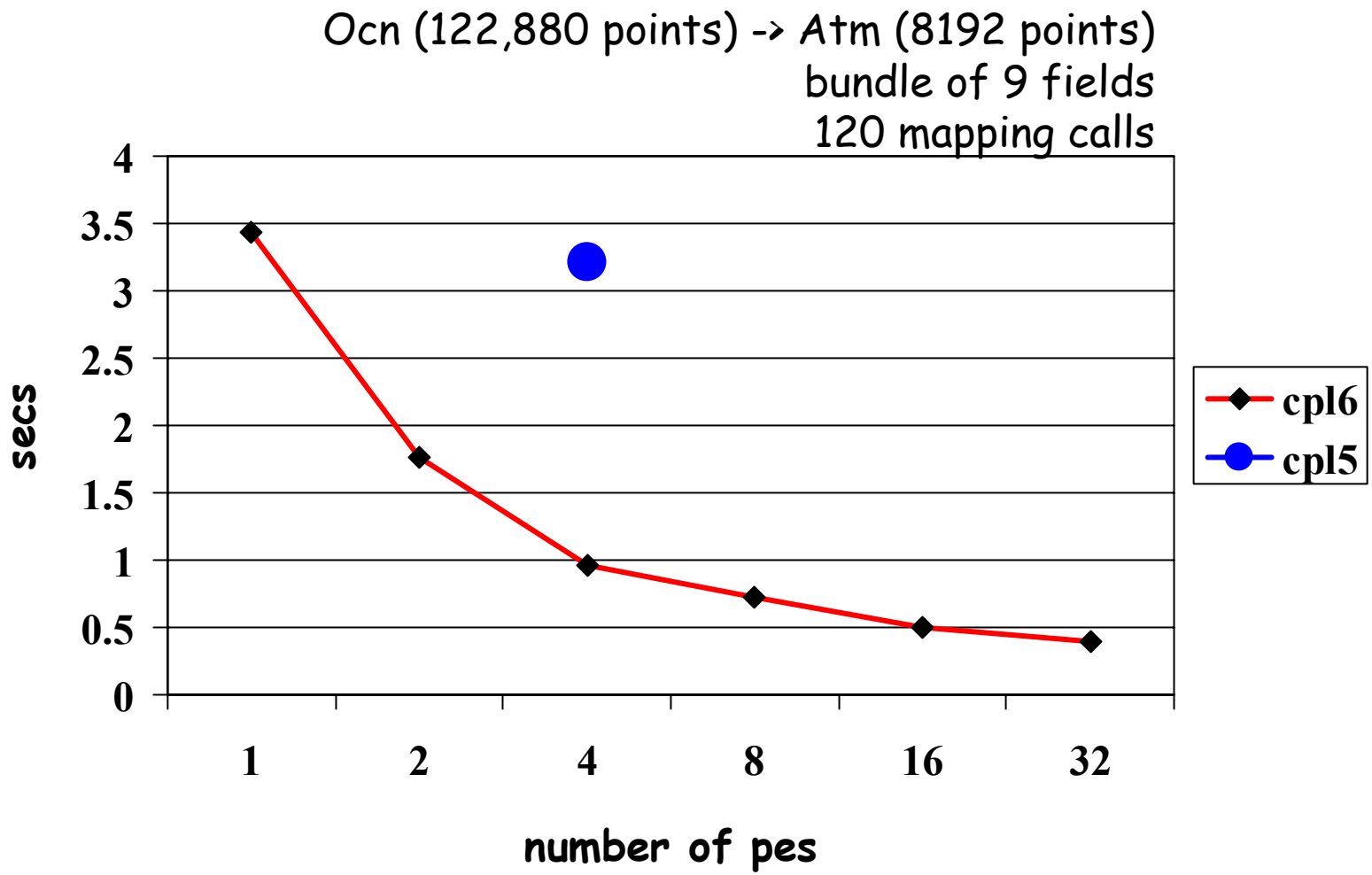
General Features:

- *Built on MPI*
- *Establishes MPI communicator for each component*
- *Performs component name registration*
- *Allows resource allocation for each component*
- *Supports different execution modes*

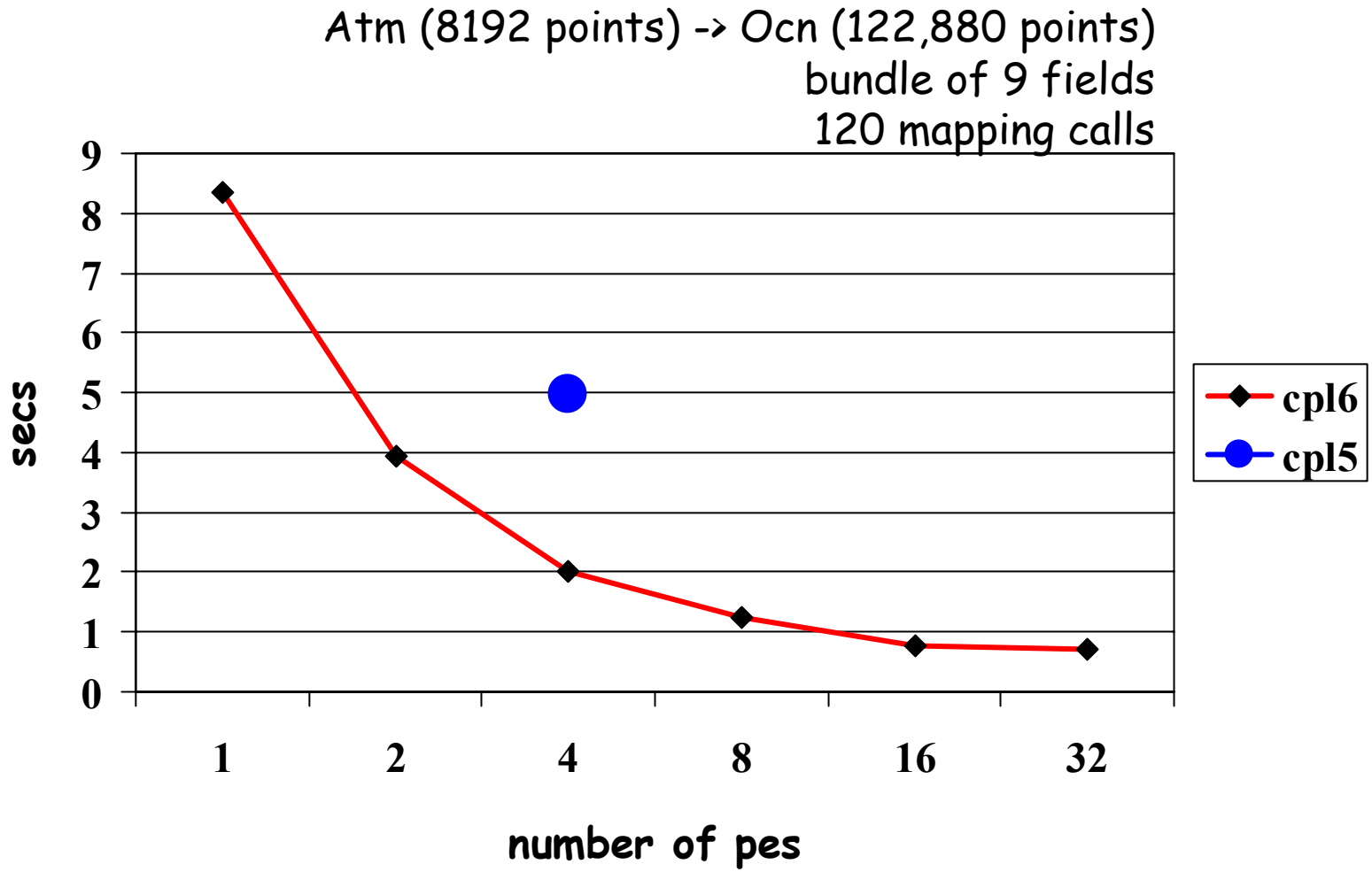
→ *MPH allows generalized communicator assignment, simplifying the component model communication and inter-component communication setup process.*

www.nersc.gov/research/SCG/acpi/MPH

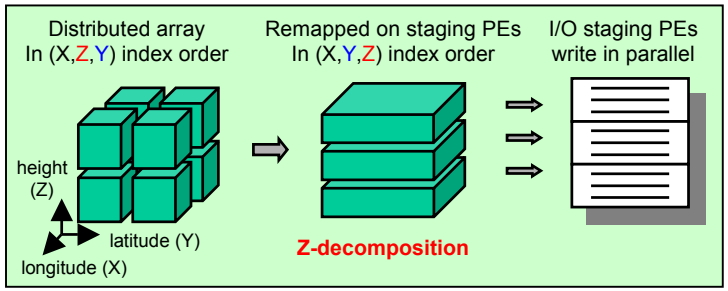
Mapping: ocn -> atm



Mapping: atm -> ocn

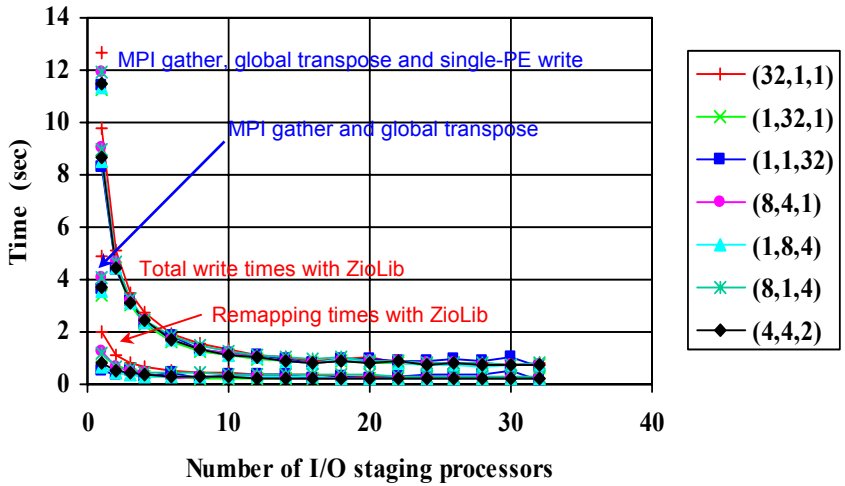


Parallel I/O



Parallel decompositions of ZioLib

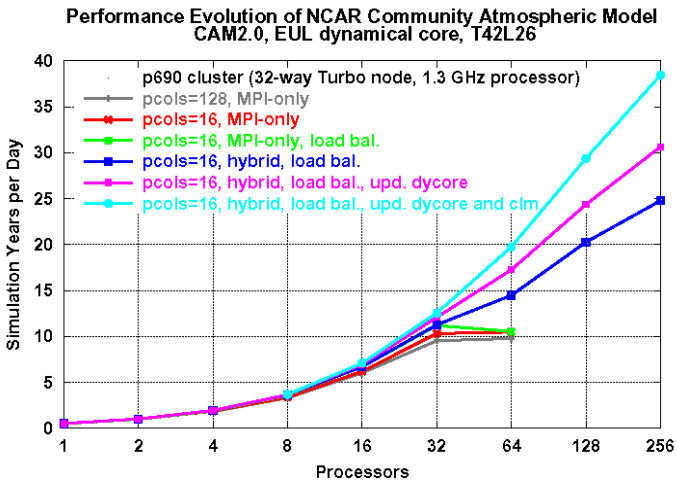
Parallel performance of Ziolib

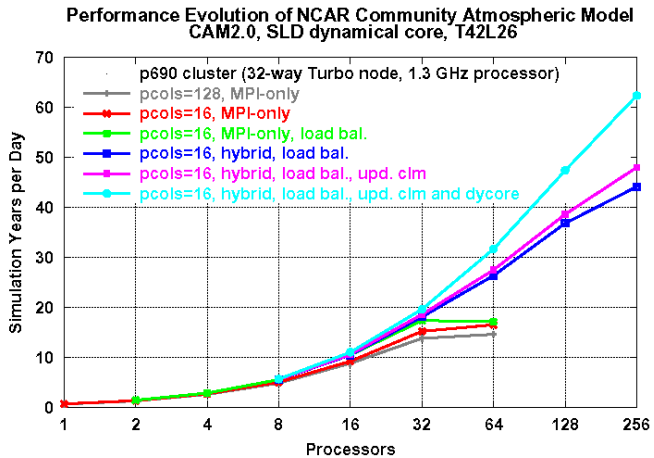


Parallel NetCDF in conjunction with SciDAC SDM Center

Evolution of Performance of the Community Atmospheric Model

- CAM2.0 Eulerian Spectral Model at T42L26
- ORNL IBM p690 and PSC Compag AlphaServer SC
- Hybrid MPI/OpenMP programming paradigm
- Cache friendly chunks, load balance, improved algorithms

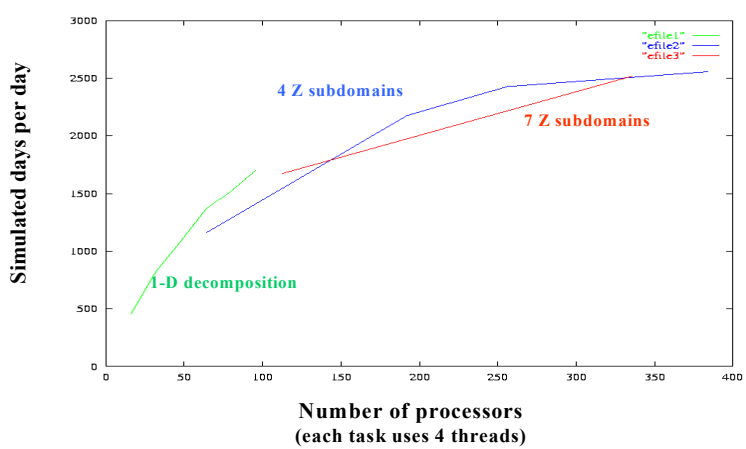




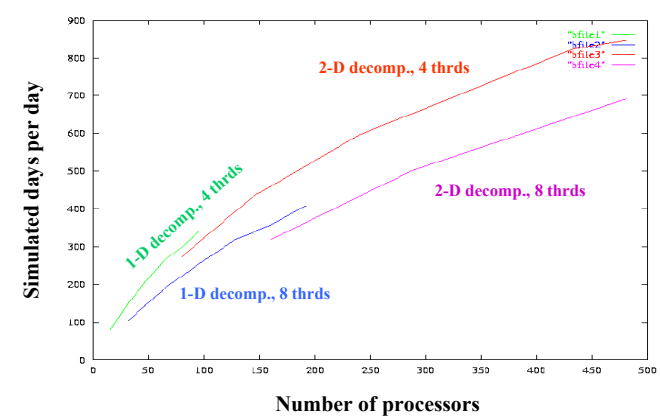
Performance of the CAM2 with FV Core

- FV Core on IBM NHII in lat-vert decomposition
- DAO's mod_comm replacing PILGRIM

Performance of CAM-2 with Finite-Volume Dycore at 2-deg x 2.5-deg x 26 levels

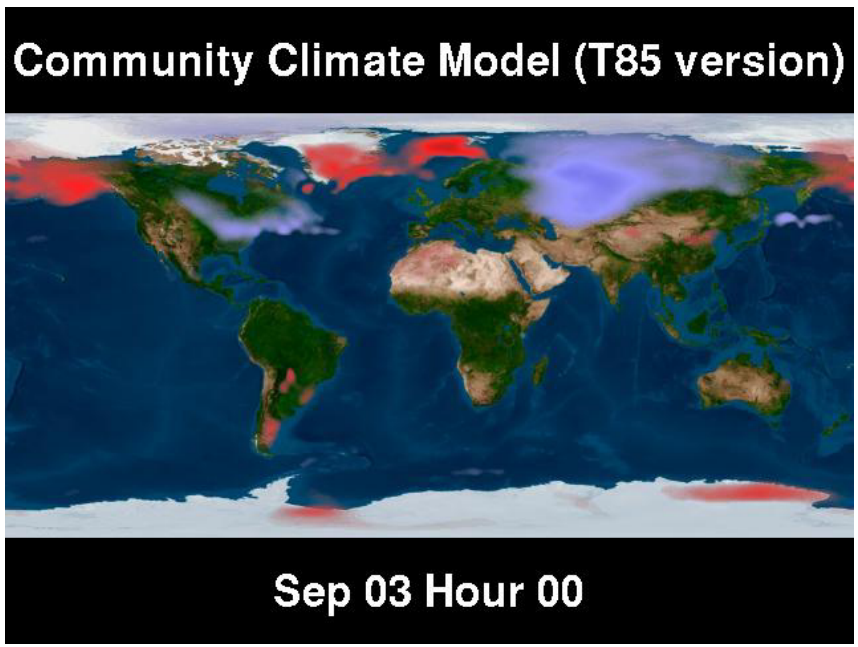


Performance of CAM-2 with Finite-Volume Dycore at 2-deg x 2.5-deg x 66 levels (WACCM Configuration)



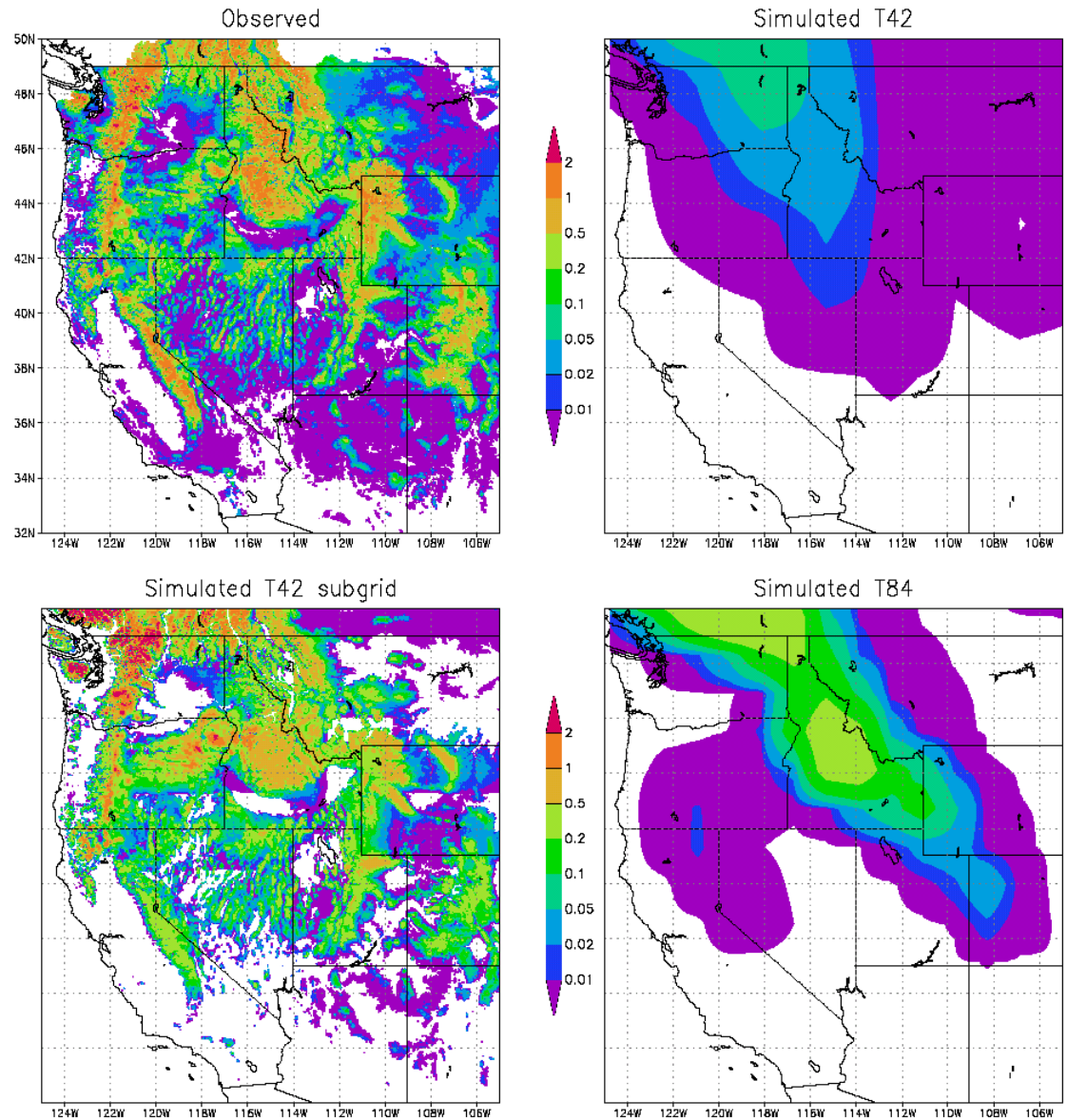
Atmospheric Model Resolution

- Increasing resolution to T85 (and beyond) in the operational model continues to be pursued. First coupled T85 study performed for CCSM workshop.
- Resolution studies at T170 planned. FV core resolution increased.



Subgrid Orography Scheme

- **Reproduces orographic signature without increasing dynamic resolution**
- **Realisitic precipitation, snowcover, runoff**
- **Month of March simulated with CCSM**



Land Surface Model and River Transport Model

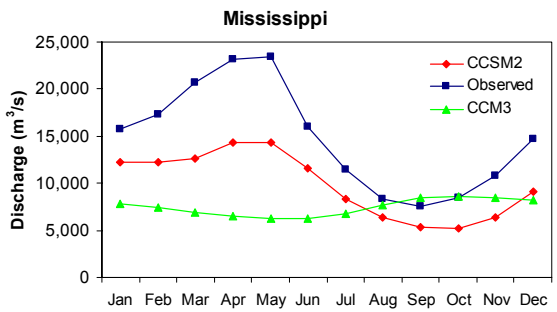
- Land Model Development Activity

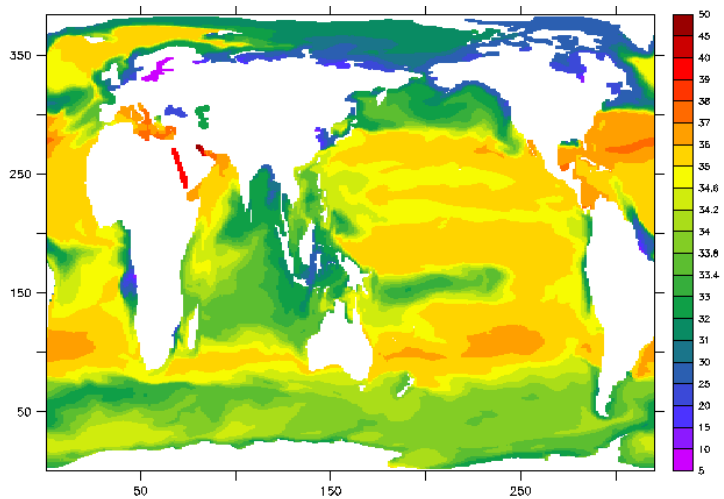
  Community Land Model (CLM) Requirements Document reviewed

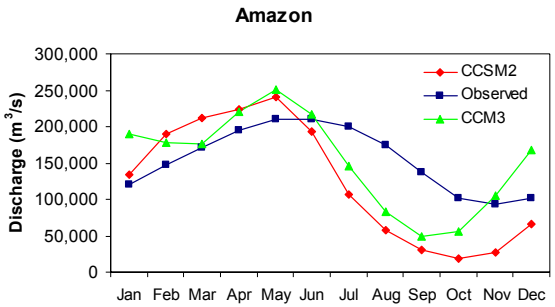
  – SciDAC software engineering is focused on the interface and reduction of gather/scatters; communications bottleneck removed

  – RTM is currently single processor -- designing parallel implementation and data structures

  – Analysis of runoff in control simulation. Effect on July ocean salinity.



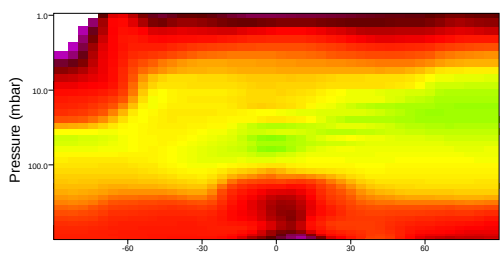




Atmospheric Chemistry

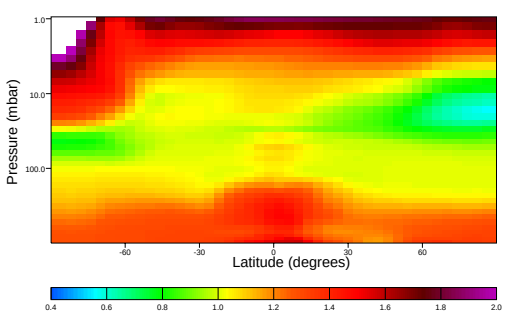
- Gas-phase chemistry with emissions, deposiiton, transport and photo-chemical reactions for 89 species.
- Experiments performed with 4x5 degree Fvcore – ozone concentration at 800hPa for selected stations (ppmv)
- Mechanism development with IMPACT
  - A) Small mechanism (TS4), using the ozone field it generates for photolysis rates.
  - B) Small mechanism (TS4), using an ozone climatology for photolysis rates.
  - C) Full mechanism (TS2), using the ozone field it generates for photolysis rates.

A)

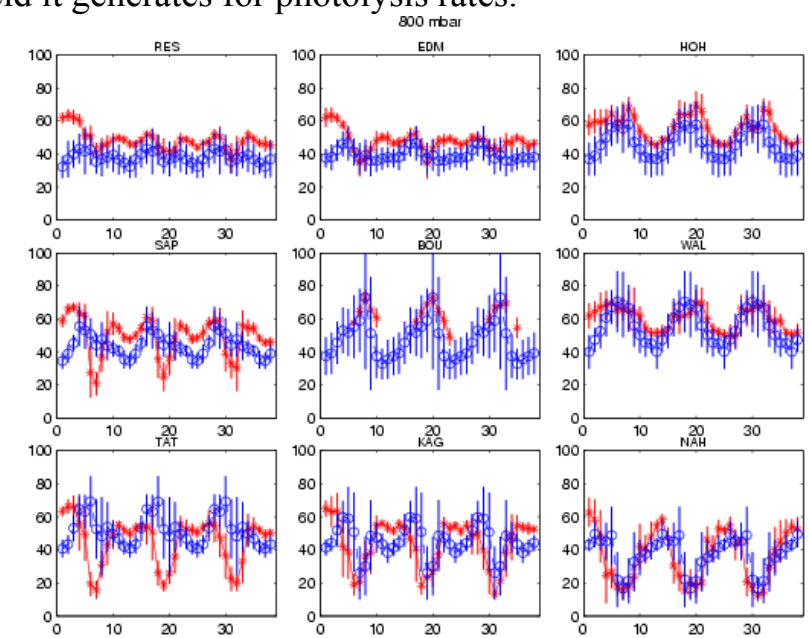


Zonal mean Ozone, Ratio A/C

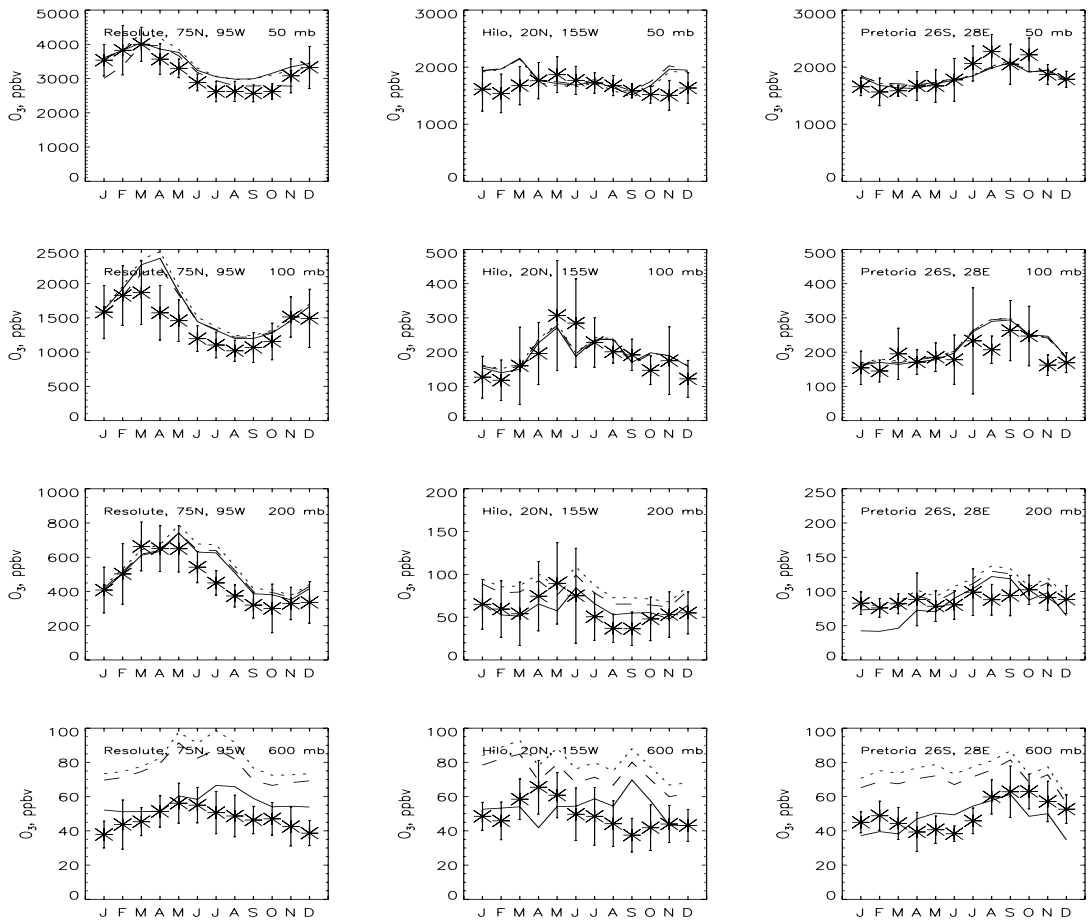
B)



Zonal mean Ozone, Ratio B/C



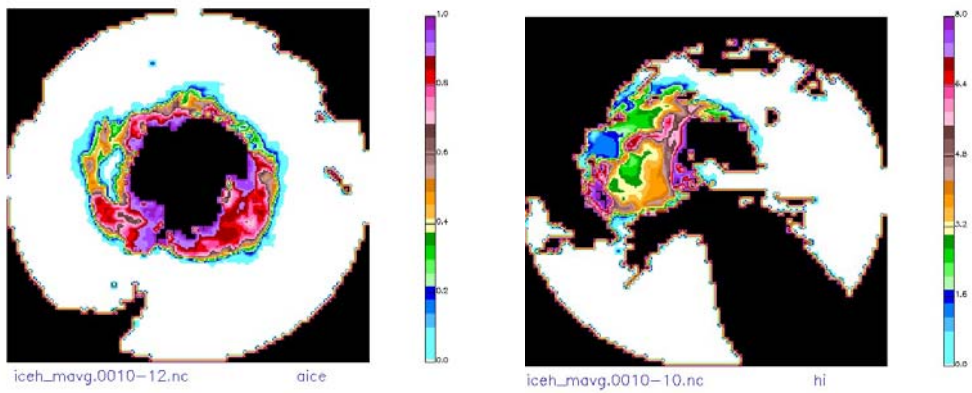
Chemistry Validation



Asterisks with error-bars are ozonesonde data. Solid line is full chemistry, dashed line is small chemistry using the climatology, and dotted line is small chemistry using its own ozone field

Sea Ice Model

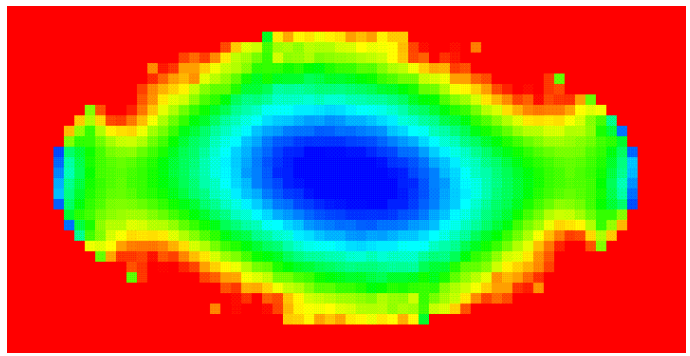
- **Incremental Remapping for Sea Ice and Ocean Transport**
  - Incremental remapping scheme that proved to be three times faster than MPDATA, total model speedup of about 30% --added to CCSM/CSIM
  - Cache and vector optimizations
  - CICE3.0 restructered for vector Community Sea Ice Model
- **Sensitivity analysis and parameter tuning test of the CICE code**
  - Automatic Differentiation (AD)-generated derivative code
  - Major modeling parameters that control the sea ice thickness computation were the ice-albedo constants, densities and emissivities of ice and snow, and salinity constant
  - Parameter tuning experiment with gradient information

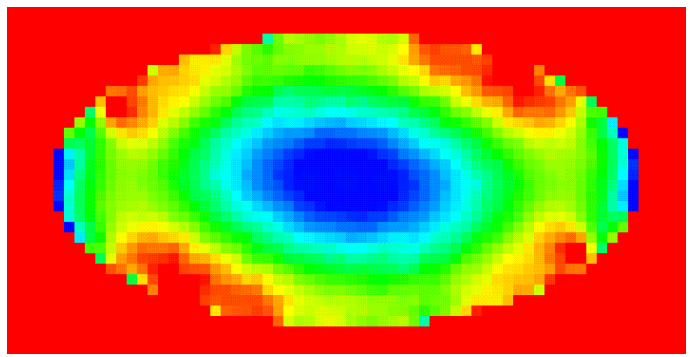


POP Ocean Model

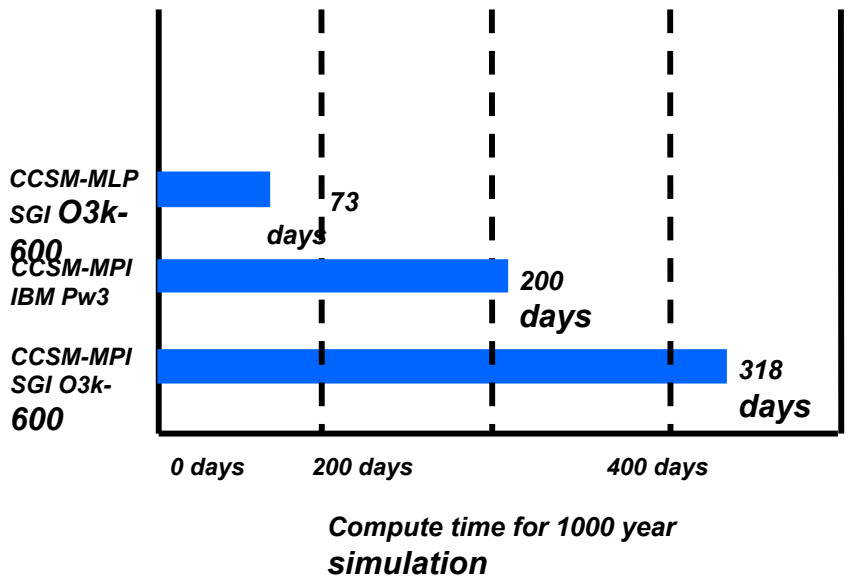
- **Software Engineering for POP and CICE**
  - Design and implementation for the new ocean model (HYPOP) and CICE in progress
- **Ocean Model Performance**
  - POP2: new design involves a decomposition of the computational domain into blocks that can be sized to fit into cache
  - On 1/10 degree, SGI (2x), IBM (1.25x), long vector gets 50% peak on Fujitsu
- **MLP in POP**
  - On 1/10 degree, SGI(2x)
- **HYPOP Model Development**
  - Treat purely Lagrangian dynamics of constant-mass layers as they inflate and deflate in regions intersecting bottom topography
  - Pressure gradient is split into a 'baroclinic' part that vanishes and a 'barotropic' part that does not vanish when the density is uniform
  - **Comparison of surface height in Lagrangian and Eulerian vertical after 400 baroclinic steps**

	old	new
Total	115s	55s
Baroclinic	93s	38s
Barotropic	9s	7s





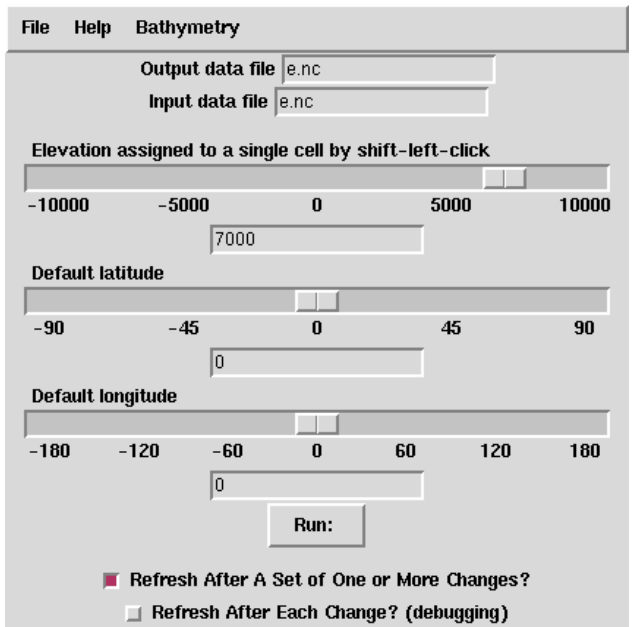
MLP version of CCSM

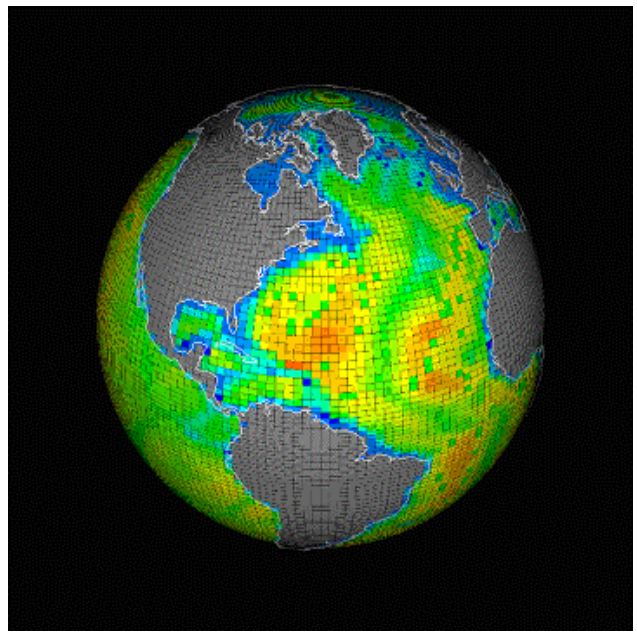


The first bar reflects the run time of CCSM 2 after its conversion to MLP-based inter-module communication. The second is the reported result for the original code on the Power3 cluster performed at NERSC. The third result is the original code as executed on the 600 MHZ Origin. Origin executions utilized 208 CPUs. The IBM execution utilized 128CPUs.

Ocean generic Grid Generator - gCubed

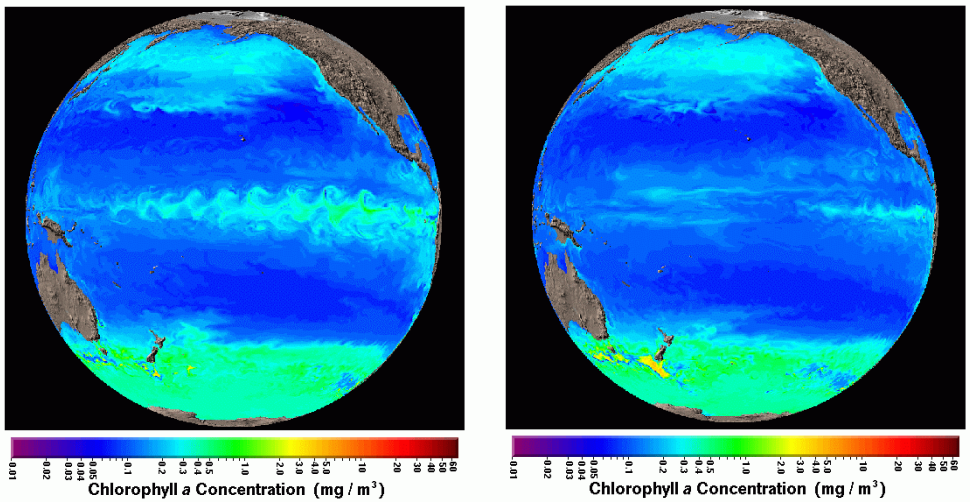
- GUI in Tcl/Tk
- Tripole grid supported

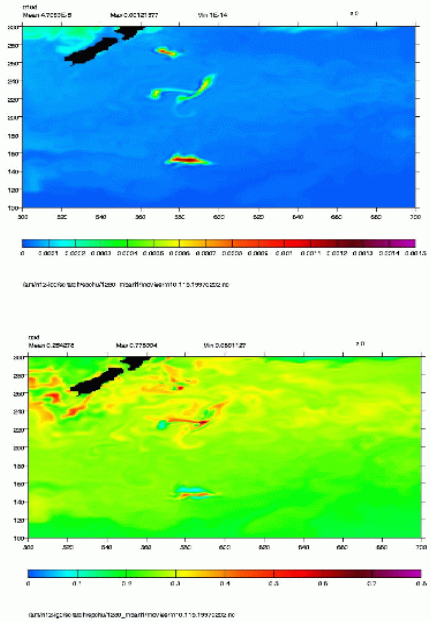




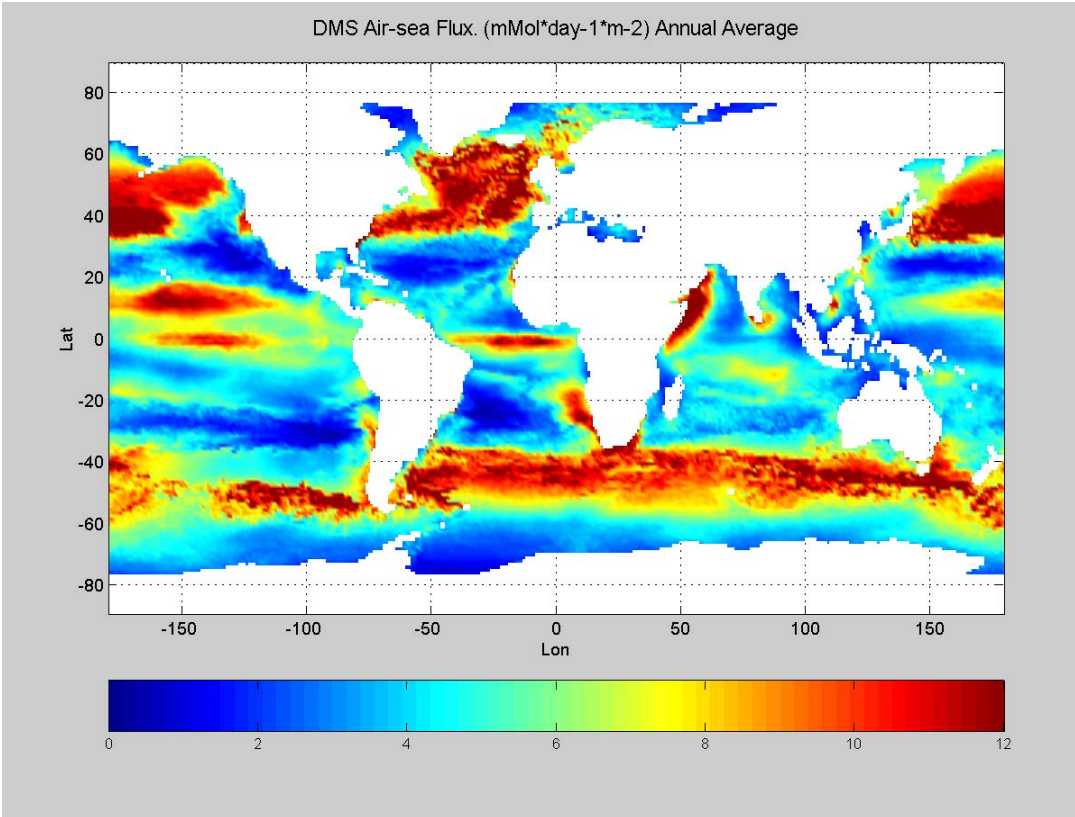
Ocean Biogeochemistry

- **Iron Enrichment in the Parallel Ocean Program**
- **Surface chlorophyll distributions in POP for 1996 La Niña and 1997 El Niño**





Global DMS Flux from the Ocean using POP



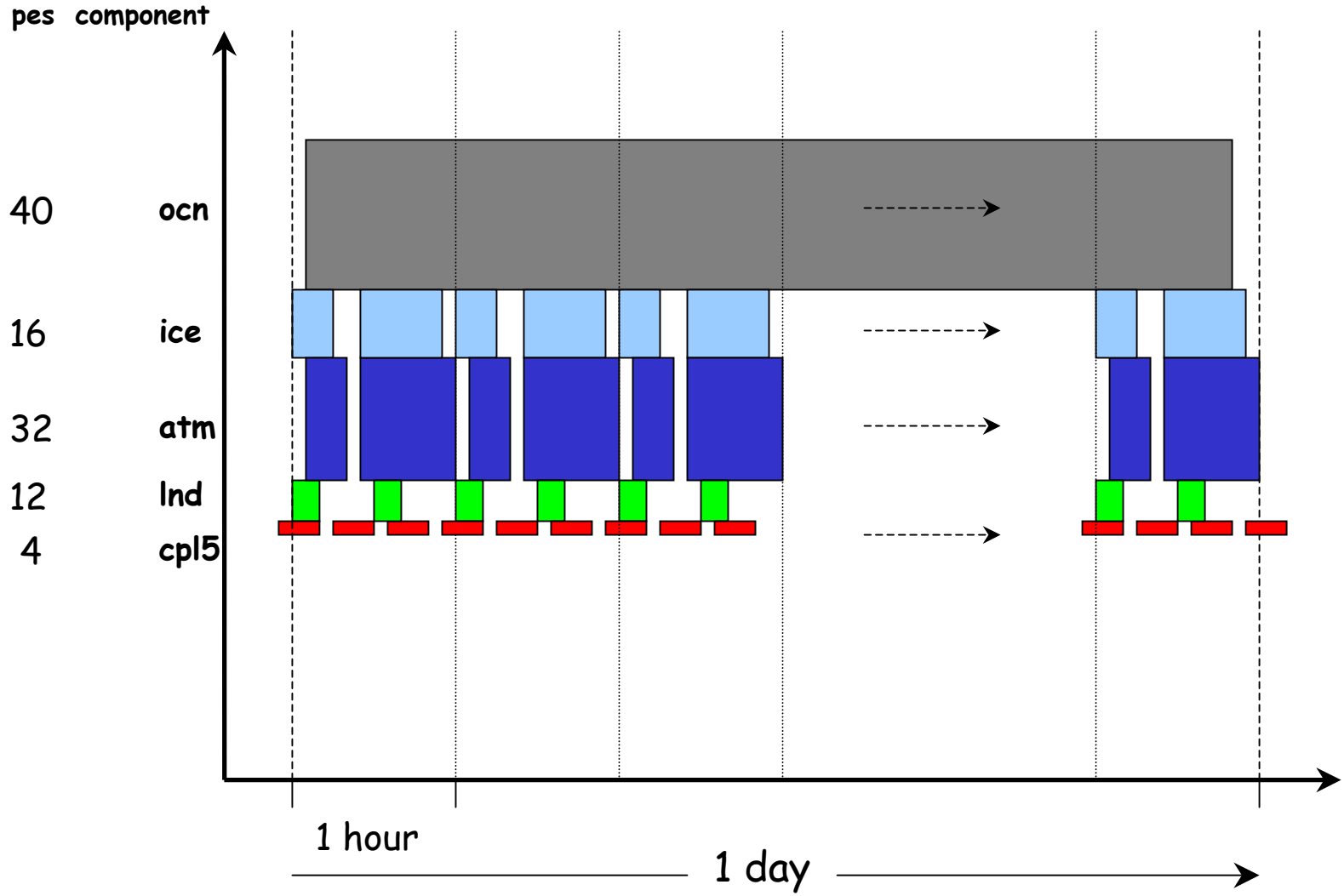
The global flux of DMS from the ocean to the atmosphere is shown as an annual mean. The globally integrated flux of DMS from the ocean to the atmosphere is 23.8 Tg S yr-1 .

Biogeochemistry

- Fine-resolution POP simulations
  - single phytoplankton-bin ecodynamics and embracing complete iron, nitrogen and sulfur cycles
  - carbon cycle has been added, diatoms segregated as separate tracer so silicon cycle also included
  - DMS distributions analyzed and improved
- CAM Analysis
  - global atmospheric methane and carbon monoxide (distributions and fluxes) from IMPACT
- Marine Aerosol-Gas Phase Interactions
  - (MAGPI) model extended to reactive bromine chemistry

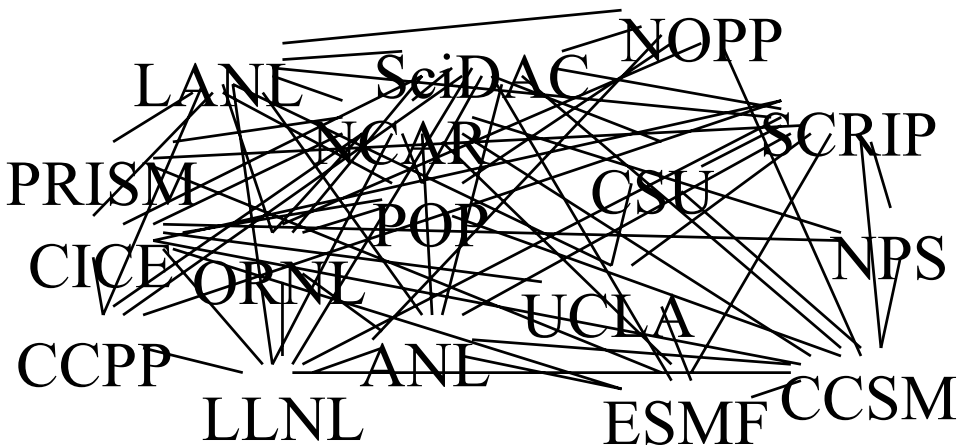
CCSM2.0 Configuration

(IBM Power3)



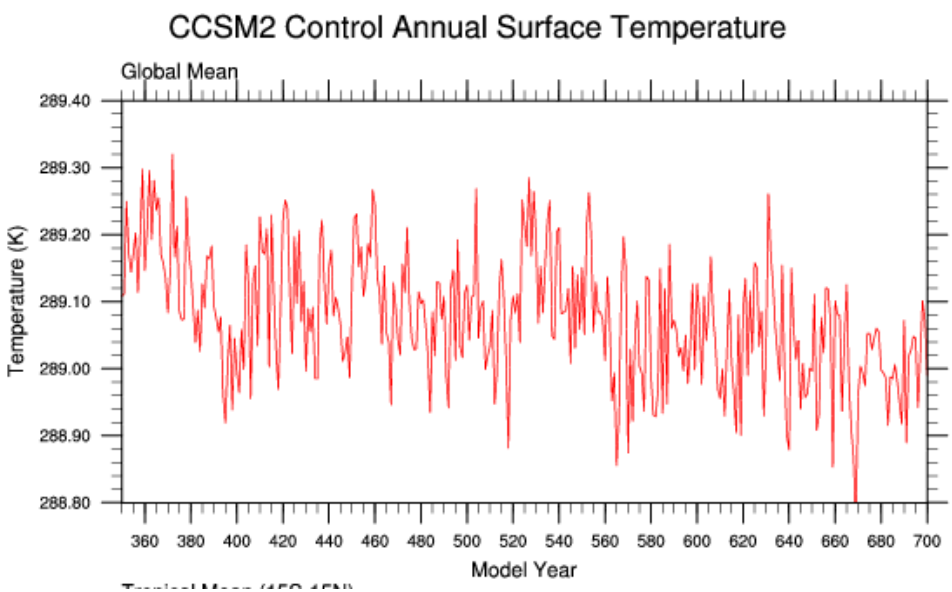
Coordination and Management

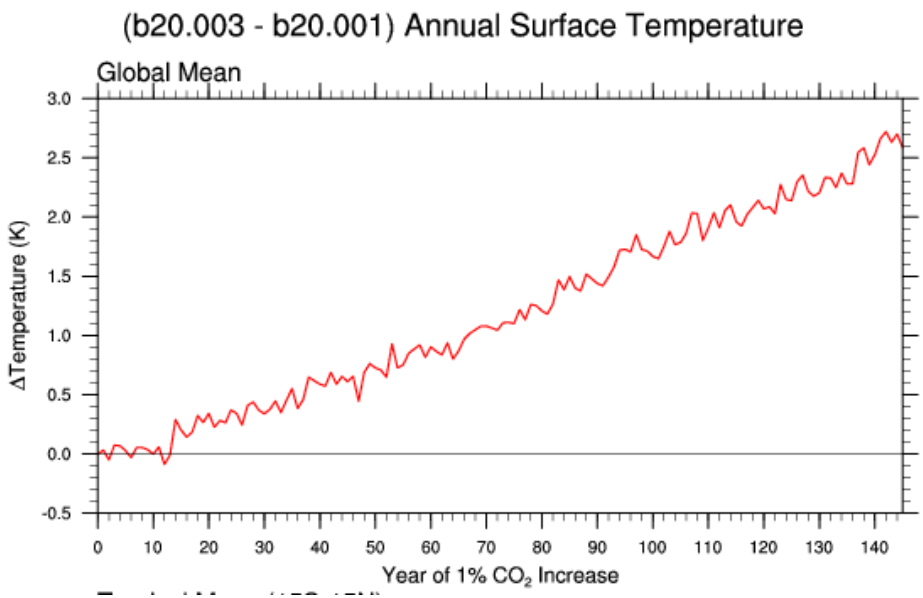
- **Management Plan**
- **Memorandum of Understanding between SciDAC and ESMF**
- **Coordination with SciDAC Integrated Software Infrastructure Centers and Collaboratories**
  - **PERC, ESG, SDM, TSTT, CCA, APDEC, TOPS, …**



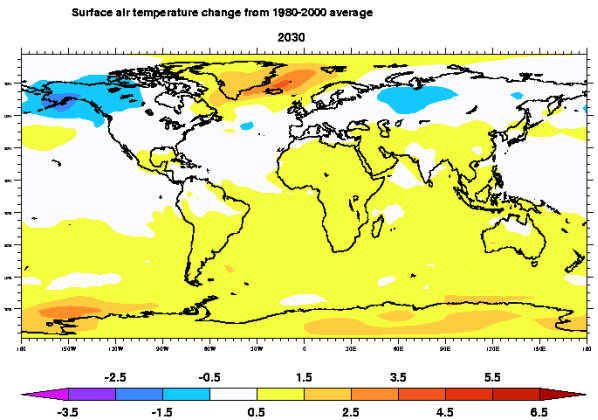
CCSM2 Coupled Simulations

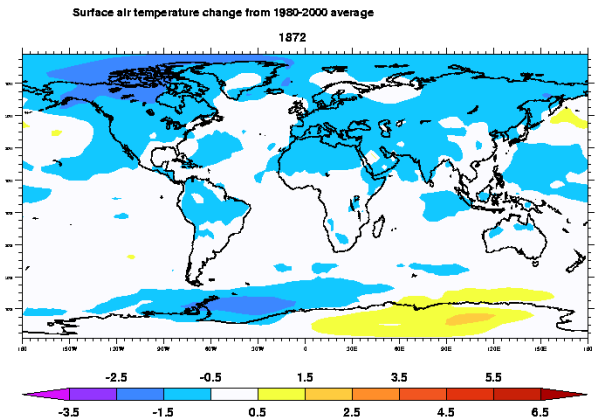
Coupled model released May 17, 2002

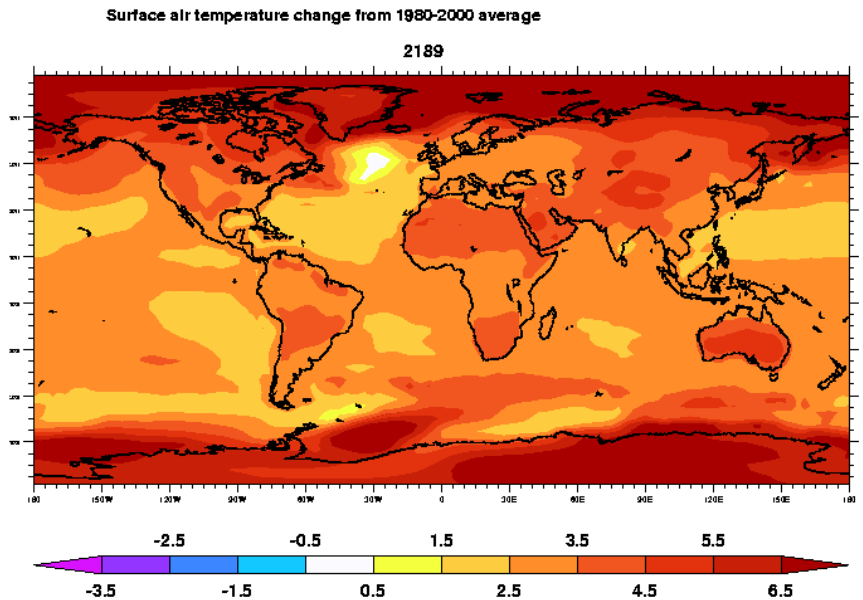




Simulation of Future Climates







Computing for this simulation was done
at DOE's National Energy Research Scientific Computing Center (NERSC)
at Lawrence Berkeley National Laboratory, NCAR and
Oak Ridge National Laboratory, Computer Science and Mathematics Division
managed by UT-Battelle, LLC for the U.S. Department of Energy under
Contract Number DE-AC05-00OR22725.

Credits
Animation and data management:
Michael Wehner/Lawrence Berkeley National Laboratory

Parallel Climate Model:
Warren Washington, Jerry Meehl, Julie Arblaster, Tom Bettge
and Gary Strand/National Center for Atmospheric Research

Visualization software
Dean Williams/Lawrence Livermore National Laboratory

The End

CAM and CLM2 Plans

- **Revisit architecture documents and bring into line with ESMF, CCA, etc.**
- **Block decomposition of dycores CAM, communicator interfaces**
- **Mod_comm for CAM**
- **CLM2 M-2-N coupling and Parallel RTM using MCT types and utilities**
- **Comprehensive performance portability/tuning**
- **Cache/vector optimizations**