High-resolution climate modeling with the Community Earth System Model

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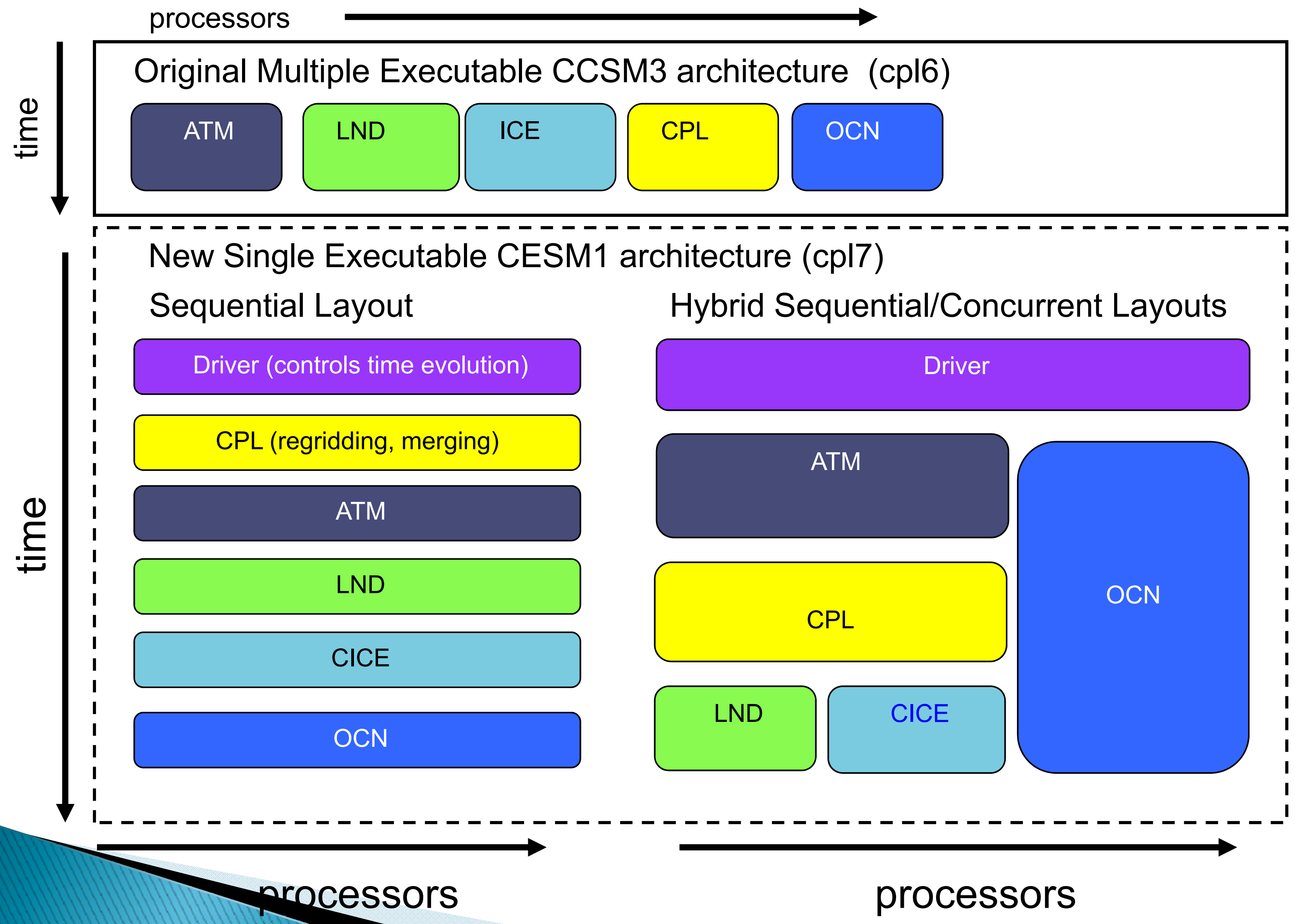
What is Community Earth System Model (CESM)?

- Consists of a set of 4->6 geo-components
  - ATM, OCN, LND, CICE, GLC, WAVE
  - Run on potentially different grids
  - Exchange boundary data with each other **via** coupler
    - hub and spoke architecture
- Large code base: >1.3M lines
  - Fortran 90 (mostly)
  - Developed over 20+ years
  - 200-300K lines are critically important
    - Communication, not computational kernels
- CESM is an interdisciplinary collaborative effort
  - DOE, NSF, NOAA, University Community
  - Applied Math, CS, software engineering, climate scientists

Evolution of CESM's Coupling Architecture



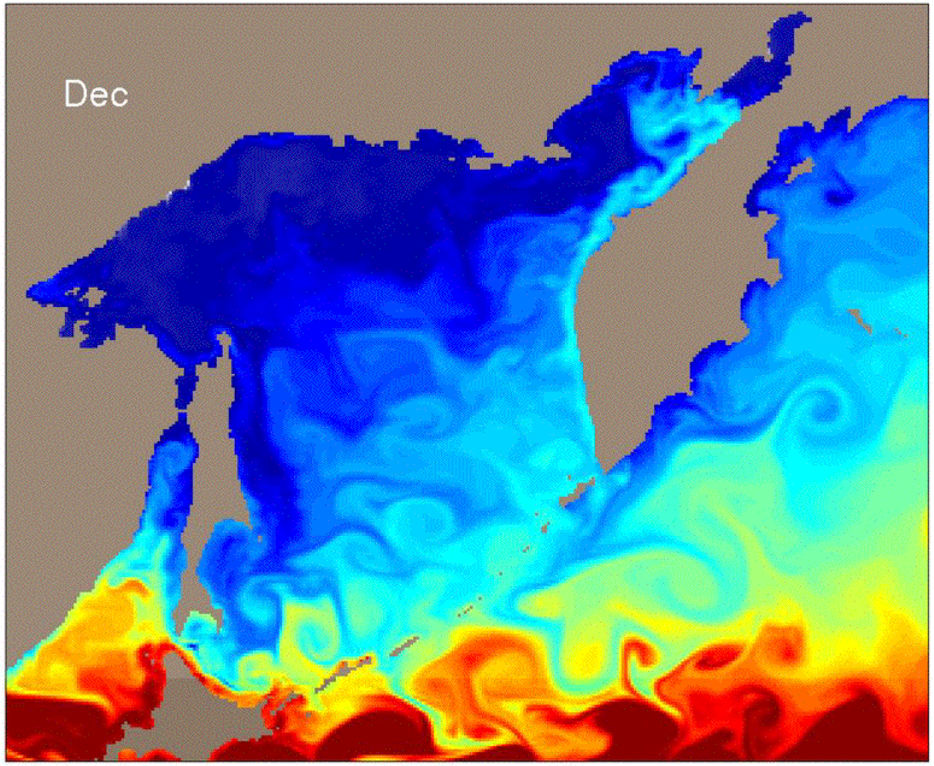
Outline

- Introduction
- High-resolution within CESM
- Spectral Element version of CAM (CAM-SE)
  - High-resolution
  - Moderate-resolution
- Parallel I/O
- Conclusions

High-Resolution effort

- Huge multi-year, multi-agency effort to enable and then optimize high-resolution climate capability
- Standard feature of release code
- Concerted effort to address scalability and robustness in entire code base

High-Resolution CCSM/CESM simulation



- NSF PetaApps project: Interactive Ensemble
  - 0.5° ATM, LND + 0.1° OCN, ICE
  - 155 year control run + several 50 year branches
  - Participants:
    - Kinter [PI], Stan (COLA)
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    - Bryan, Dennis, Loft, Vertenstein (NCAR)
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  - Teragrid Allocations
    - 35M SU (2009)
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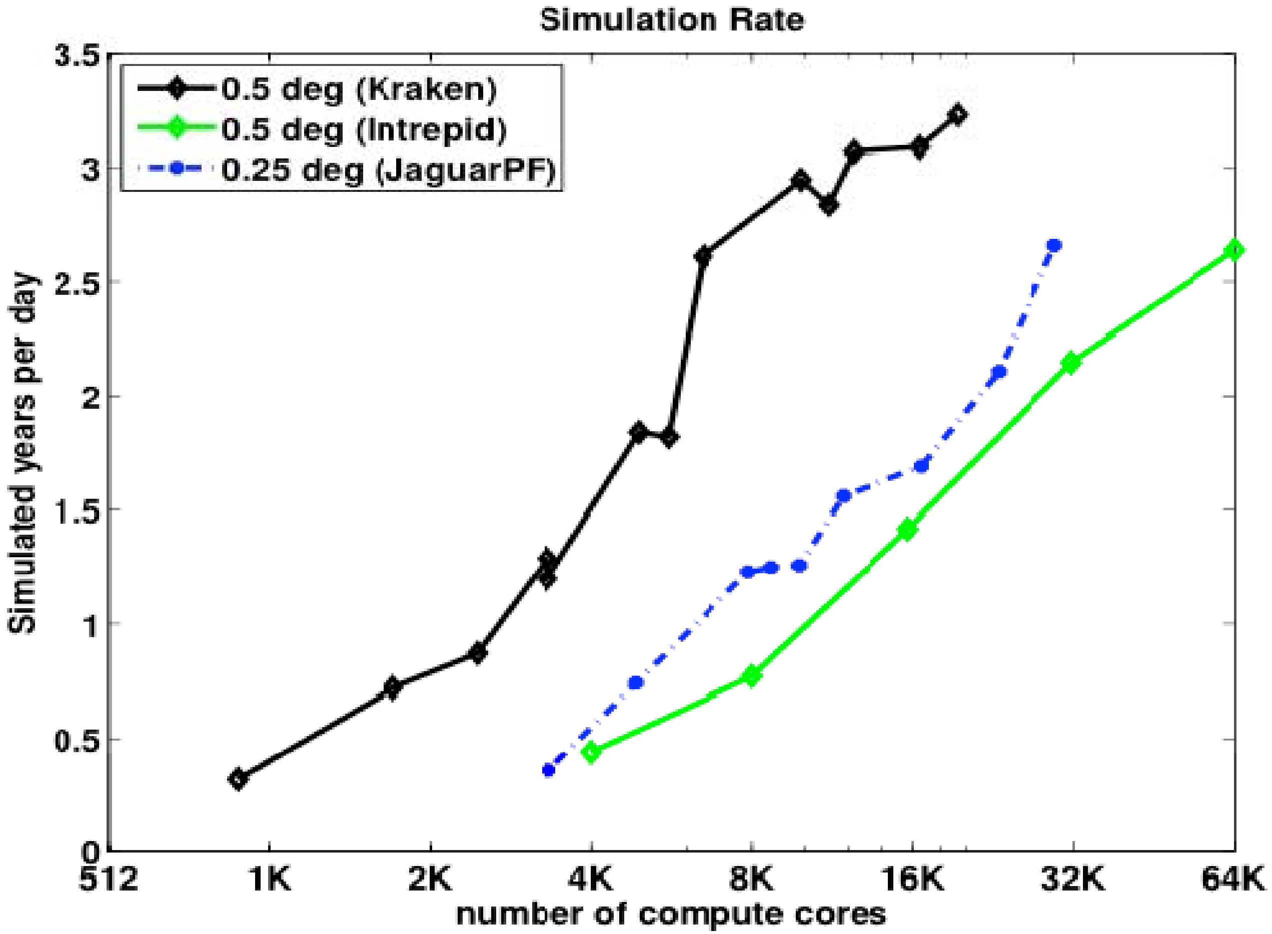
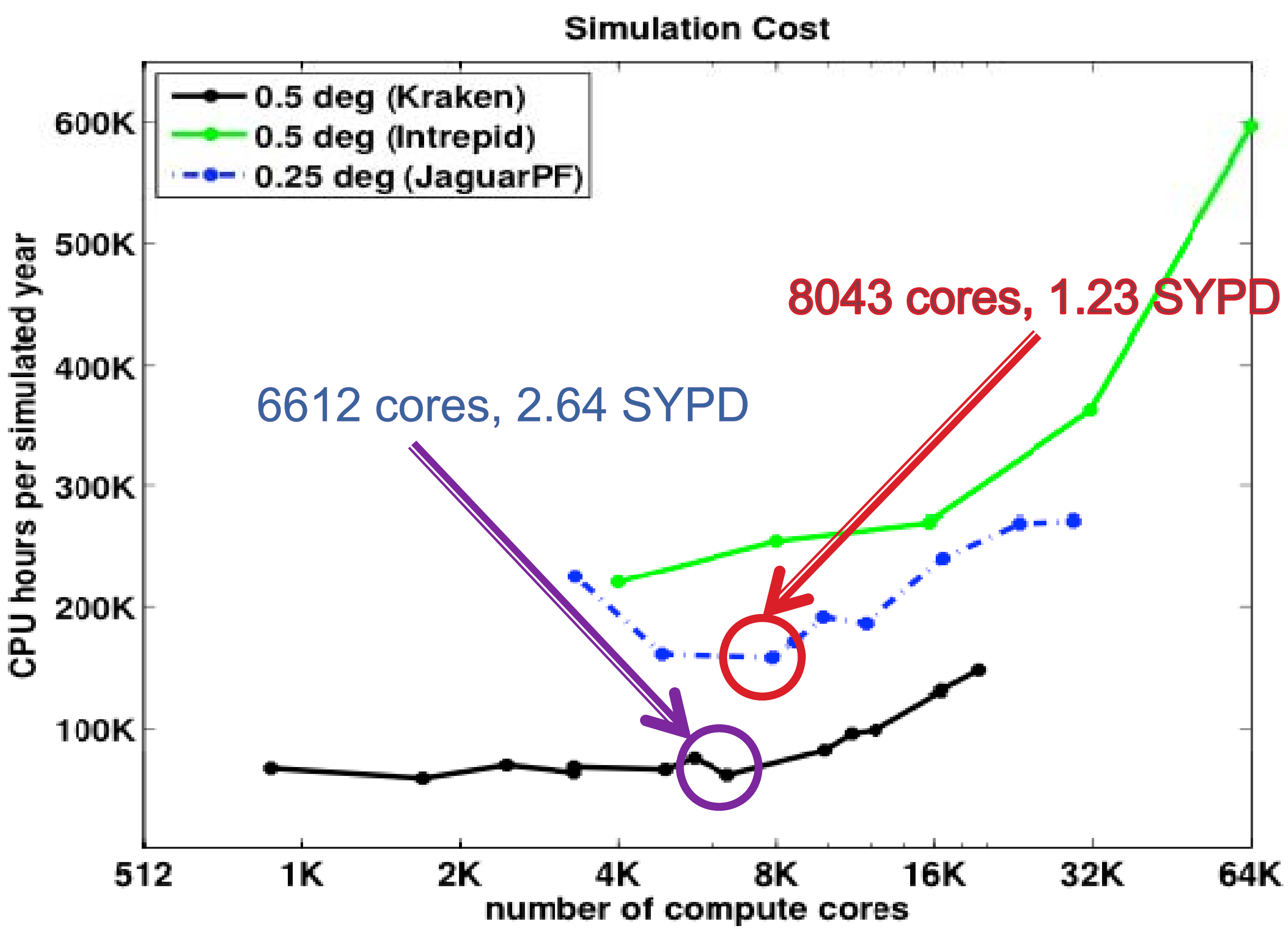
Simulation rate for high-resolution CESM (CAM-FV)



"Computational Performance of Ultra-High-Resolution Capability in the Community Earth System Model", IJPHCA [to appear]

Simulation cost for high-resolution CESM (CAM-FV)



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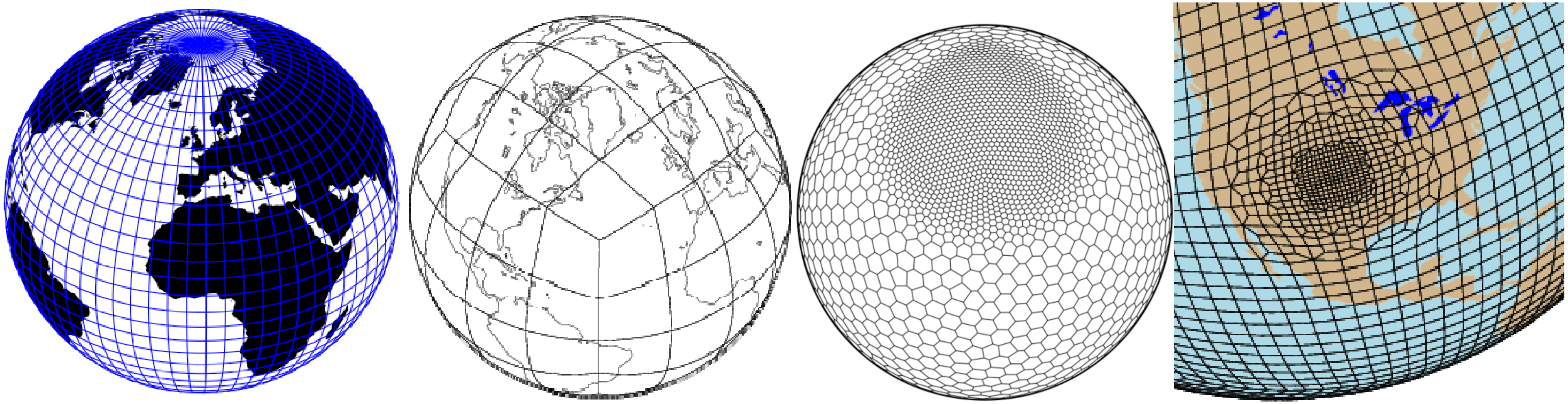
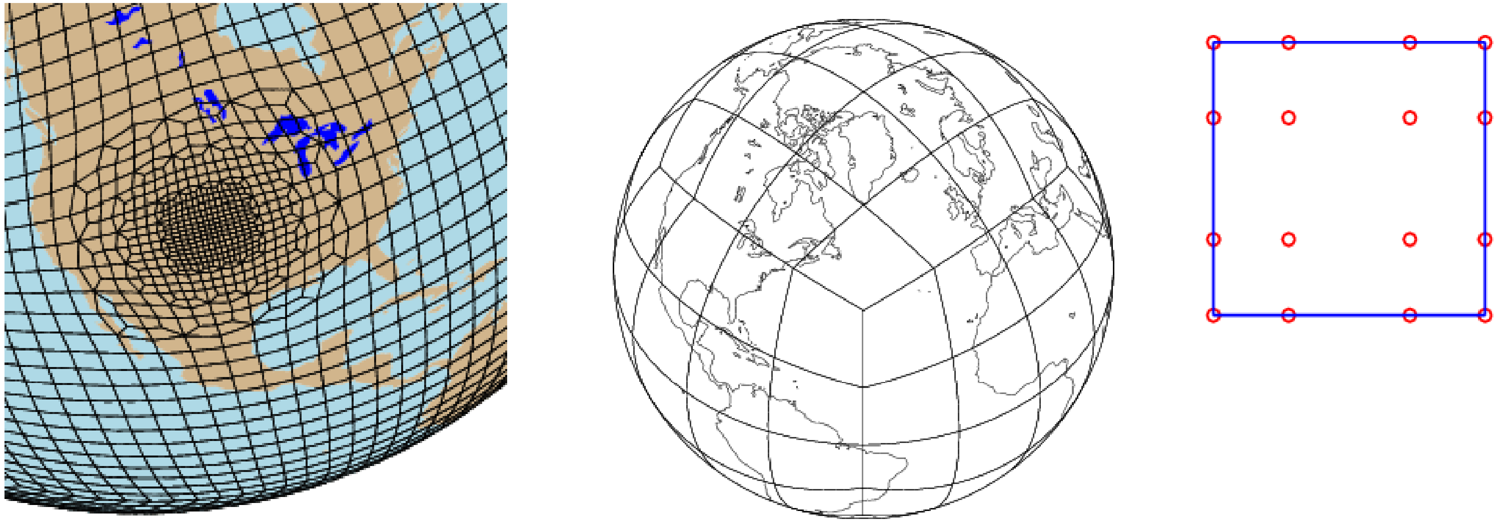
CAM Dynamical Cores

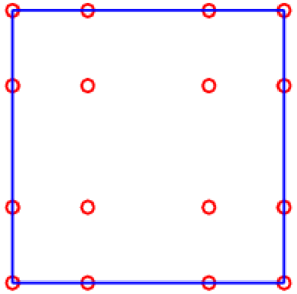


- CAM traditionally used lat/lon based dynamical core (spectral and FV)
  - Eliminated assumption in Physics enables: spectral element (SE), MPAS, FV3, MCORE/Chombo
- Naming conventions:
  - CAM{4,5}: Physics version
  - {FV,SE,MPAS,FV3,MCORE}: Dynamical core

Spectral Element Method



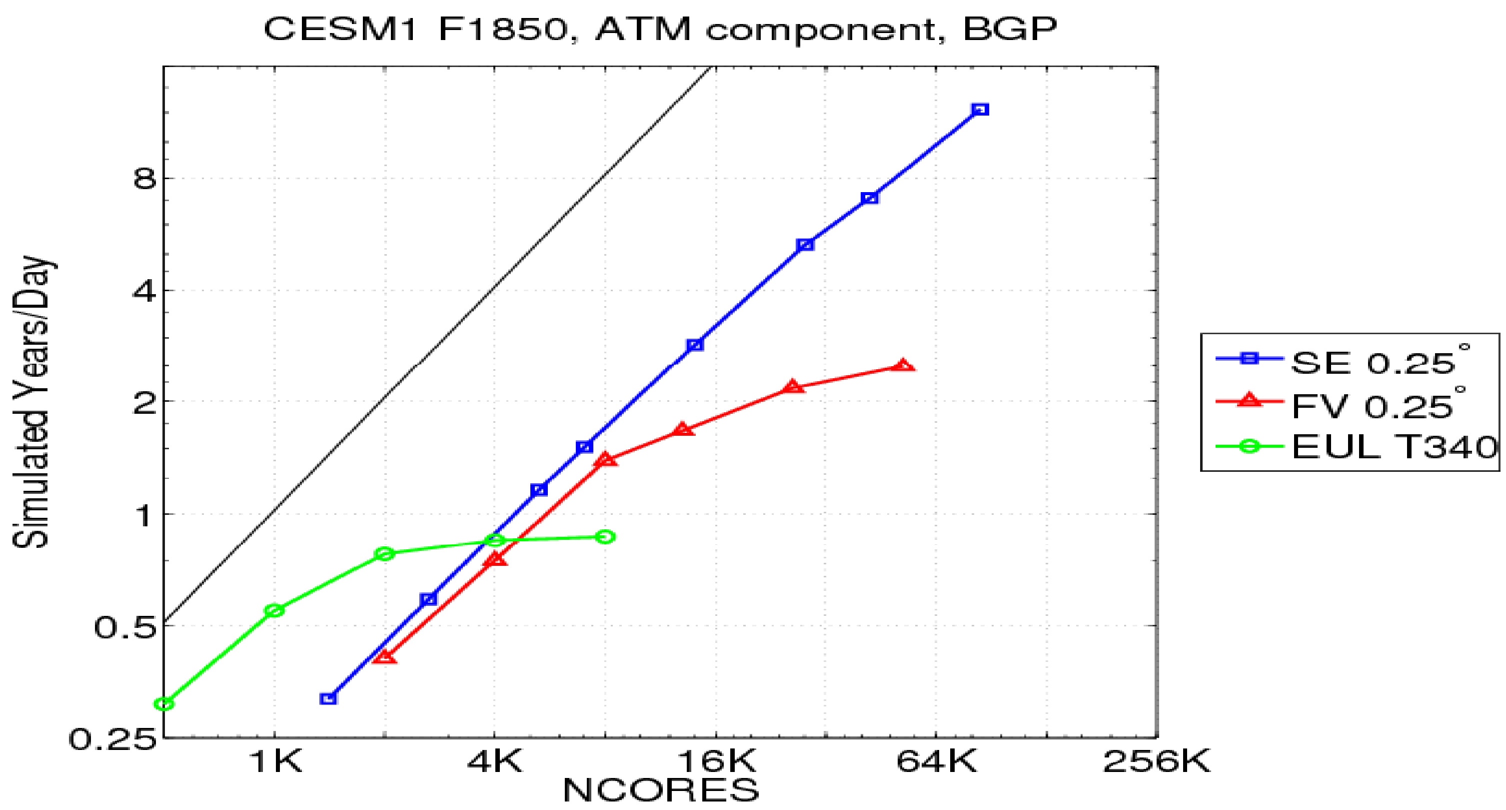
- Spectral Elements: A Continuous Galerkin Finite Element Method
  - Uses finite element grids made of quadrilateral elements
  - Galerkin formulation, with a Gauss-Lobatto quadrature based inner-product
  - Basis/test functions: degree *d* polynomials within each element, continuous across elements



Galerkin FE Approach Ideal for Modern Architectures

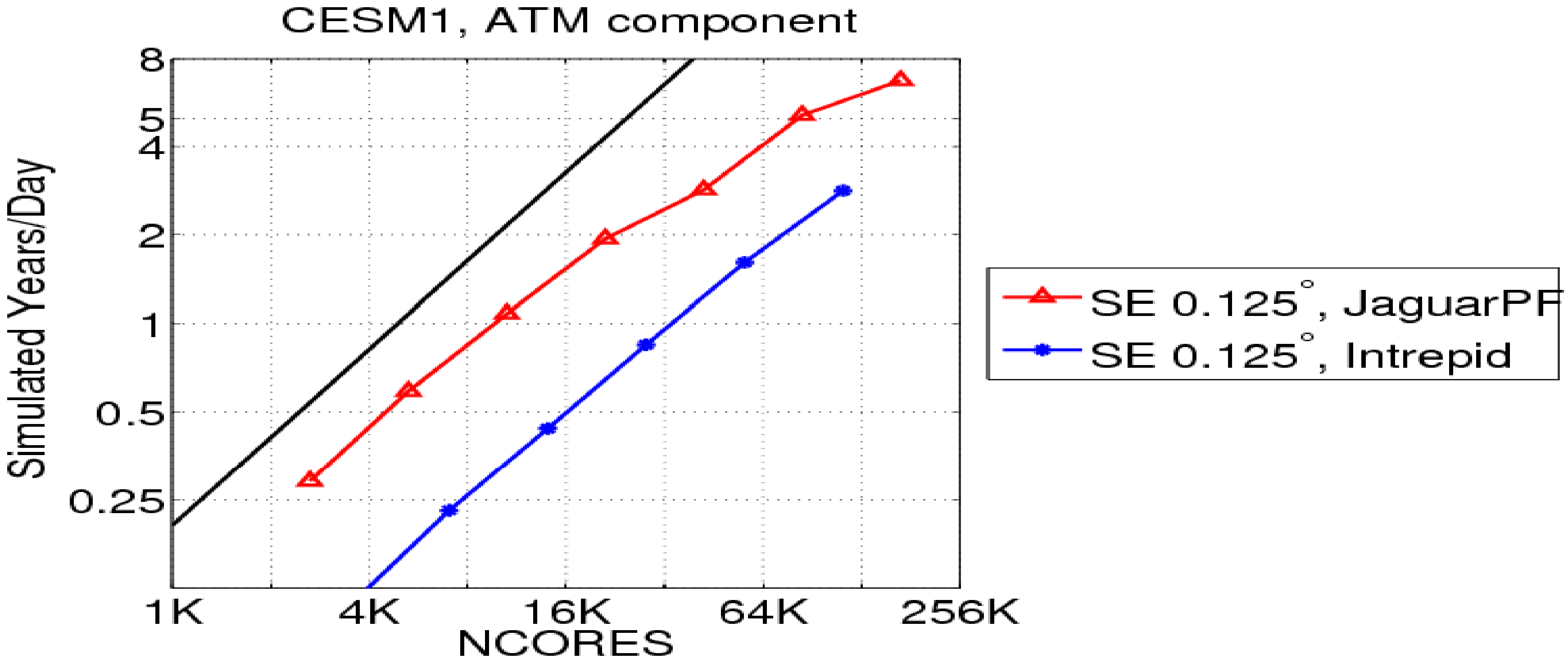
- Galerkin formulation of the equations leads to a 2 step solution procedure:
    - Step 1: All computations local to each element and on a tensor-product grid. Structured data with simple access patterns and arithmetically intensive operations: Extremely efficient on modern CPUs
    - Step 2: Apply inverse mass matrix (projection operator).
- All inter-element communication is embedded in Step 2, providing a clean decoupling of computation & communication.
    - Only a single routine has to be optimized for parallel computation.
    - Gordon Bell Awards: 2000 (best performance, NEK5000), 2001 (honorable mention, HOMME) , 2003 (best performance, SPECFEM3D)

CAM4 Scalability, ANL Intrepid ¼° (28km)



- Compare CAM with SE, FV and EUL (global spectral) dycores
- CAM-SE achieves near perfect scalability to 1 element per core (86,000 cores). Peak performance: 12.2 SYPD.
- Atmosphere only times. Full CESM runs ~50% slower because of other components

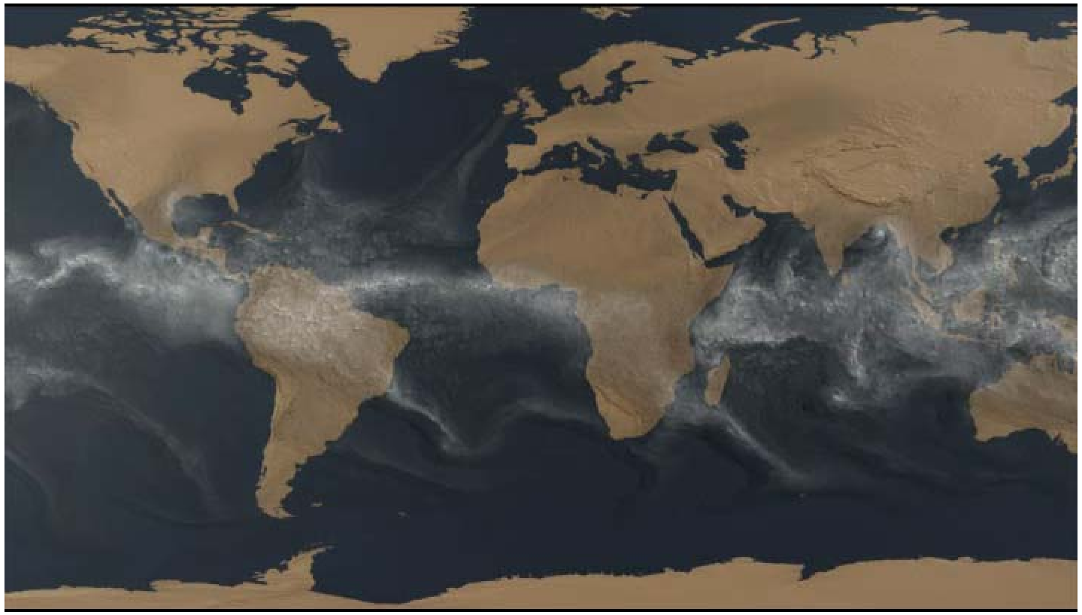
CAM-SE Scalability
Intrepid and JaguarPF 1/8° degree (14km)



- Excellent scaling to near full machine on both LCFs:
- Intrepid (4 cores/node): Excellent scalability, peak performance at 115K cores, 3 elements per core, 2.8 SYPD.
- JaguarPF (12 cores/node): Good scalability, peak performance at 172,800 cores (2 elements per core), 6.8 SYPD.

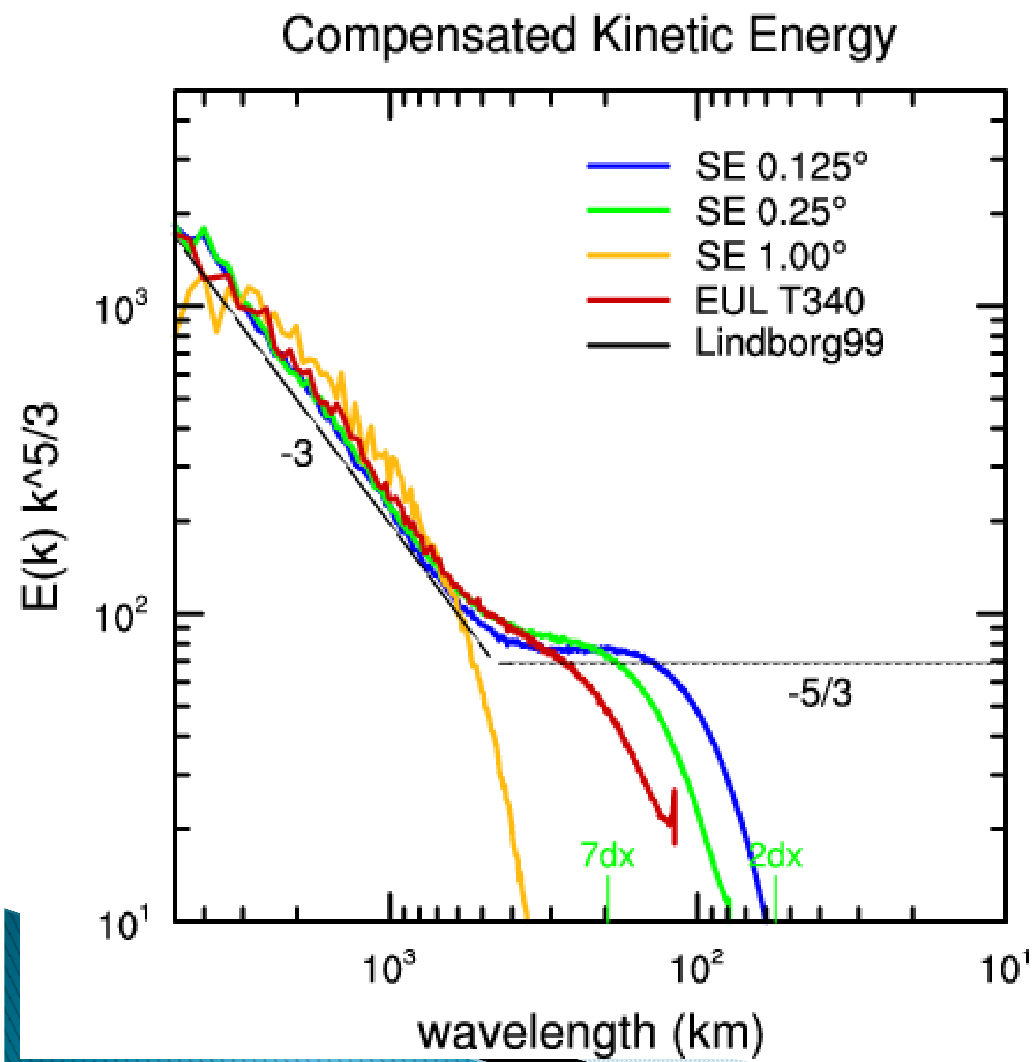
CAM4 1/8° (14km) Simulations

- CAM-SE 1/8° runs quickly and efficiently including I/O
- Excellent tropical cyclone activity
- Excellent KE spectra, with well captured -5/3 regime
- CAM4 climate suffers from physics resolution sensitivity issues.



Tropical cyclone activity at 1/8° resolution. Precipitable water animation from two months (Dec, Jan) of a 1 year simulation.

High Resolution Kinetic Energy



- CAM minimum resolution to resolve −5/3 regime: 1/8°
- CAM 1/8° departs from observations ~100km wavelength (50km grid scale).

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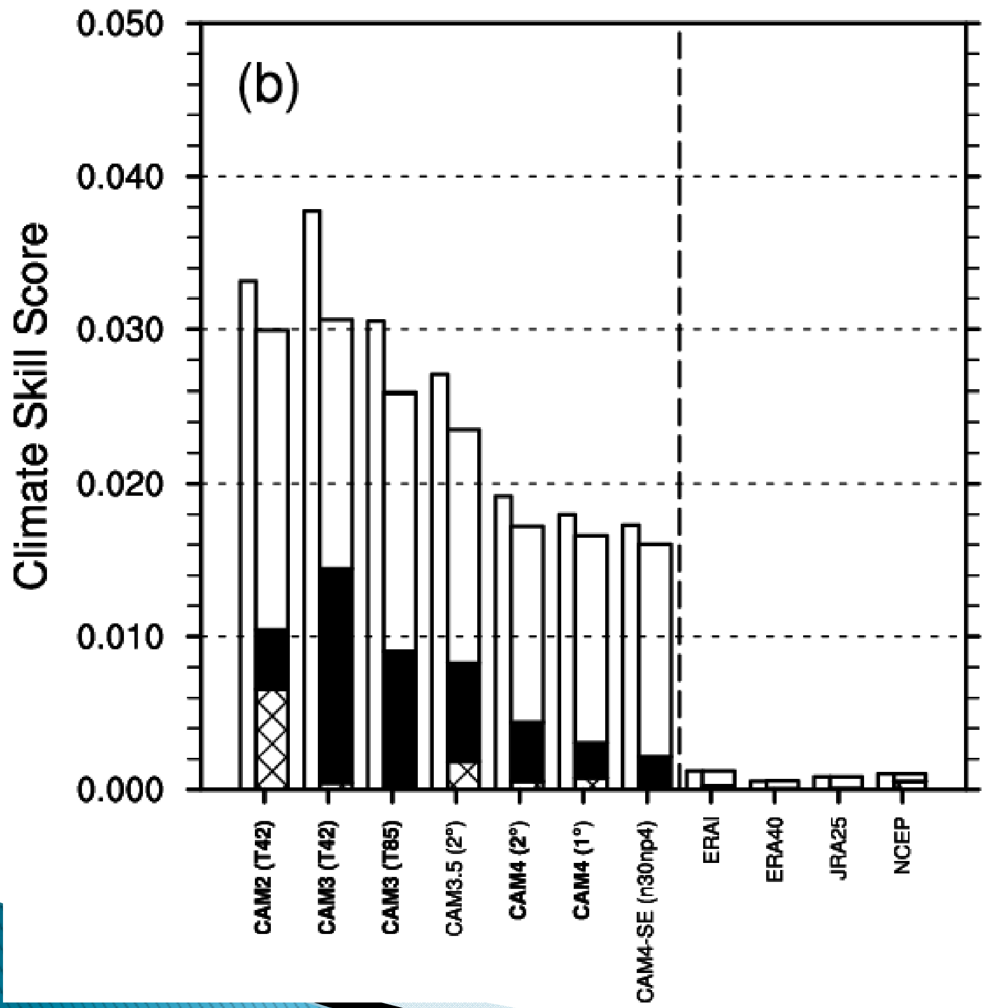
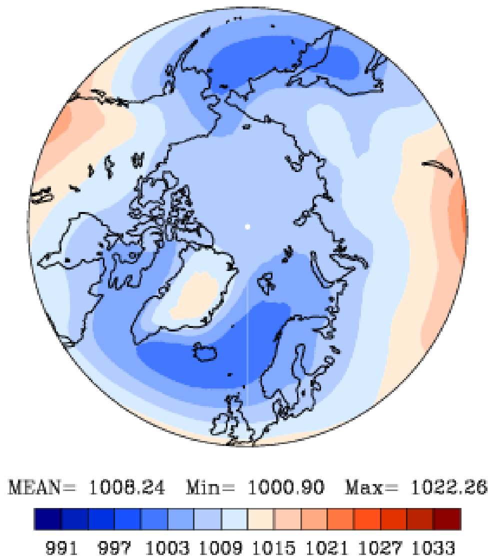
Improving Climate Skill
Resolution and Physics



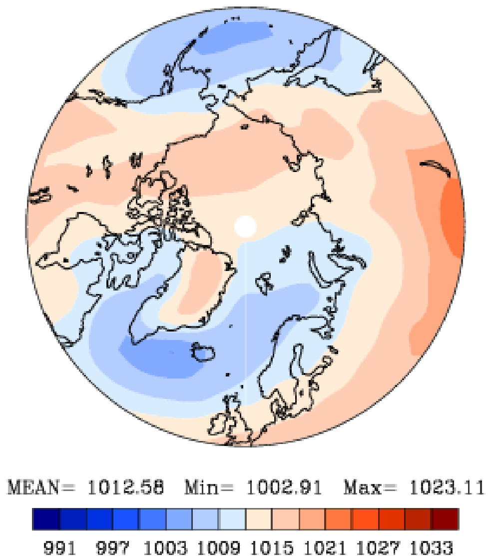
- CAM shows steady improvement as resolution is increased and physics improved
- 500mb geopotential height skill score (30-90N) DJF
- Mean square error from uncond. bias, cond. bias and phase error
- Source: Rich Neale (NCAR)

Sea Level Pressure

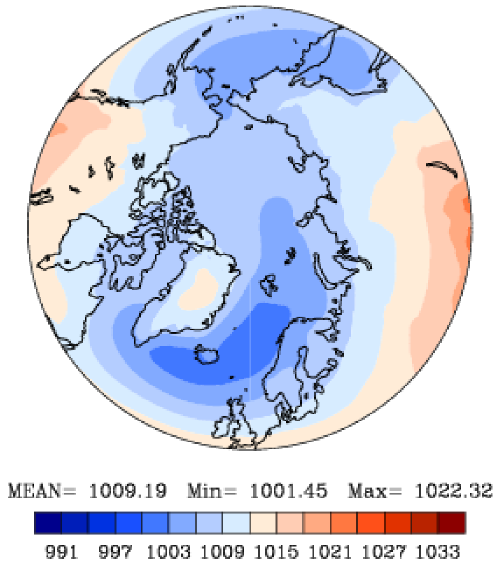
CAM4-SE 1°



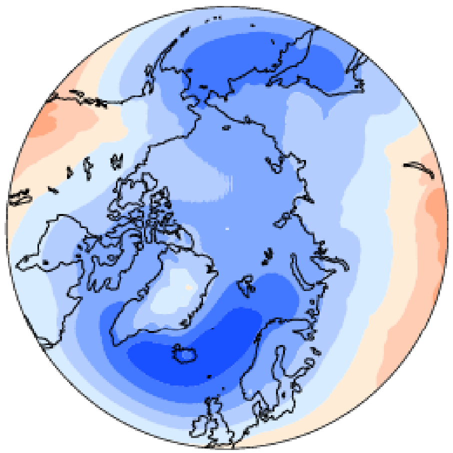
NCEP



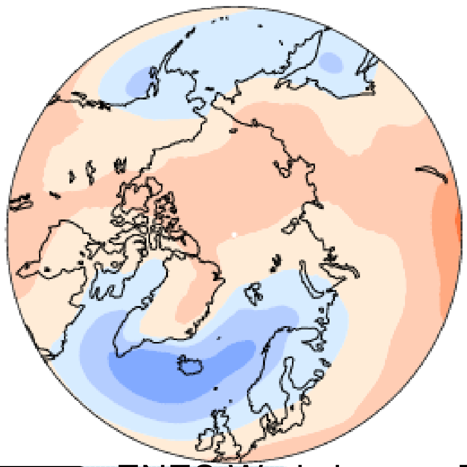
CAM4-FV 1°



CAM4-SE 1/4°



CAM5-SE 1°

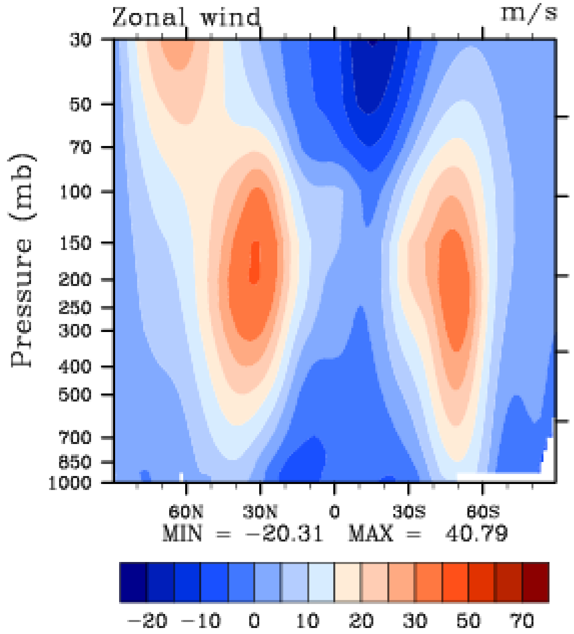


CAM has too strong of an Icelandic low, in both SE and FV

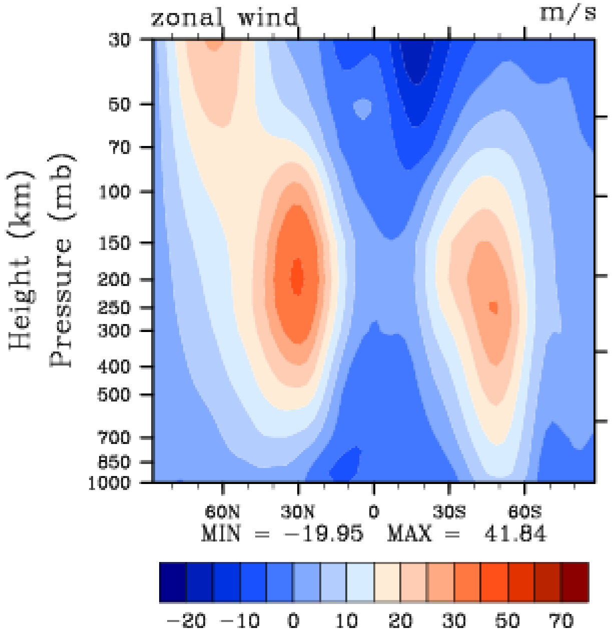
Icelandic low intensifies under mesh refinement, but is much improved with CAM5 physics

Zonal Mean Zonal Wind (DJF)

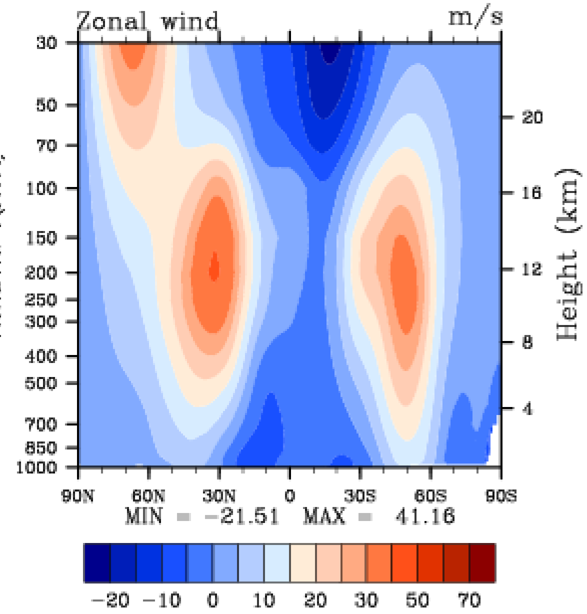
CAM4-SE 1°

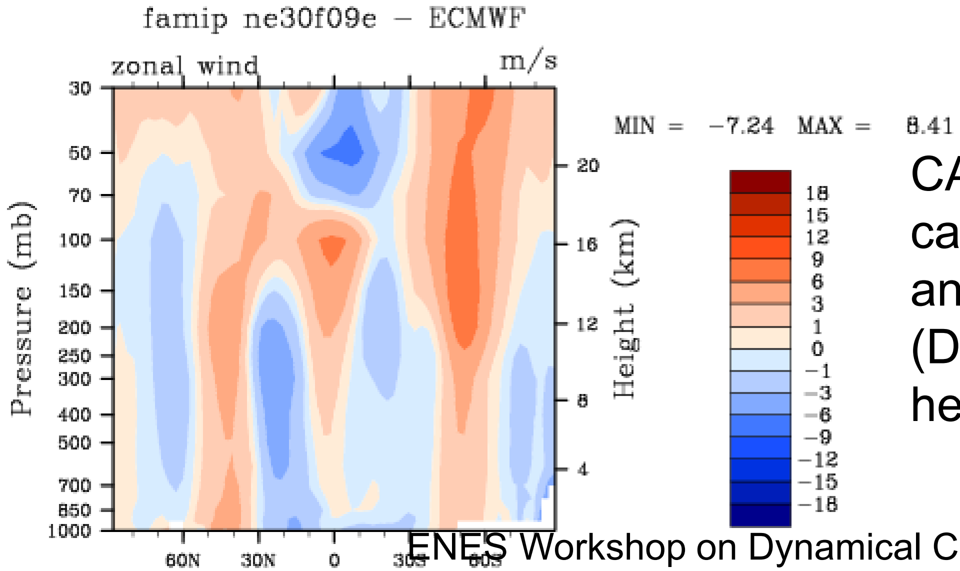


ECMWF



CAM4-FV 1°

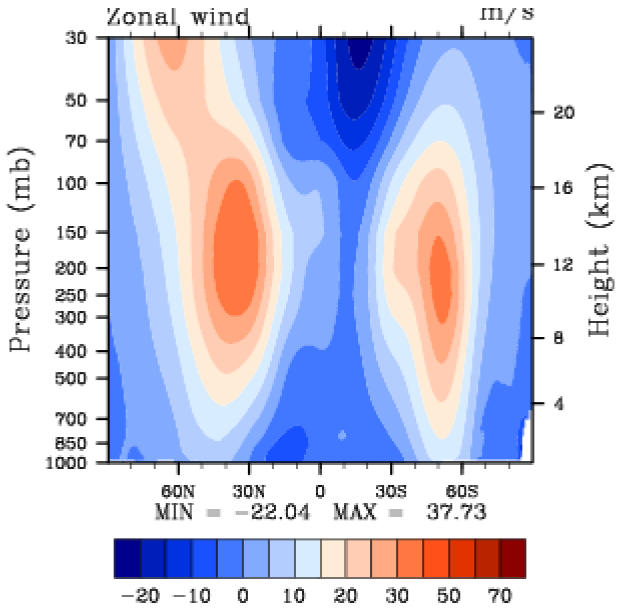




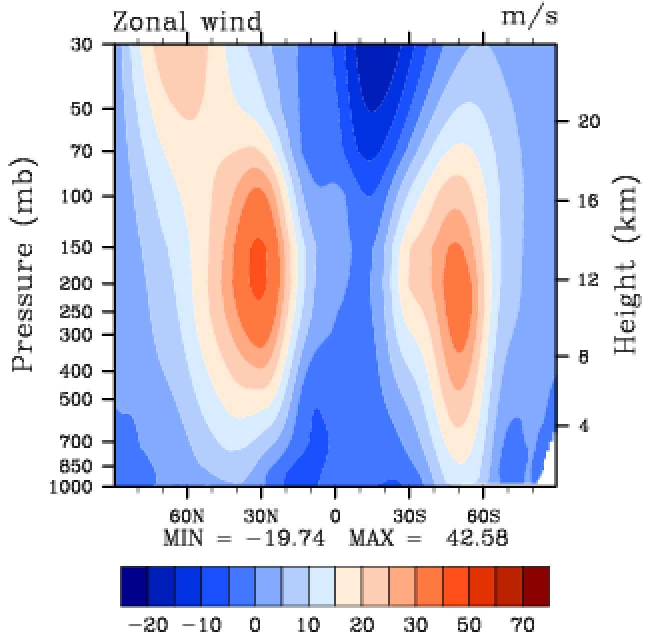
CAM does a good job capturing the southern (JJA) and northern hemisphere (DJF) polar jets. FV northern hemisphere jet is too strong

Zonal Mean Zonal Wind (DJF)

CAM4-SE 0.25°



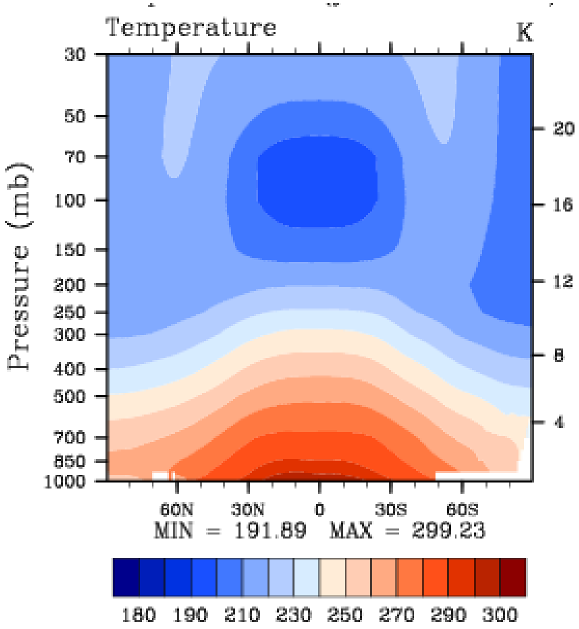
CAM5-SE 1°



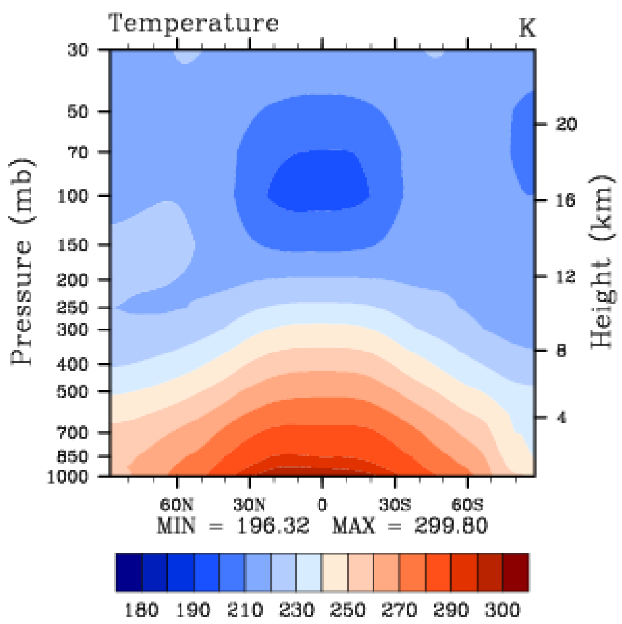
CAM-SE retains good polar jets at high resolution and with CAM5 physics

Zonal Mean Temperature

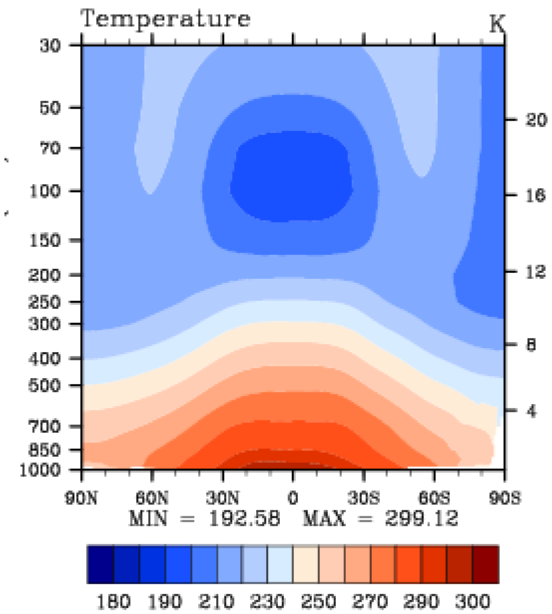
CAM4-SE 1°

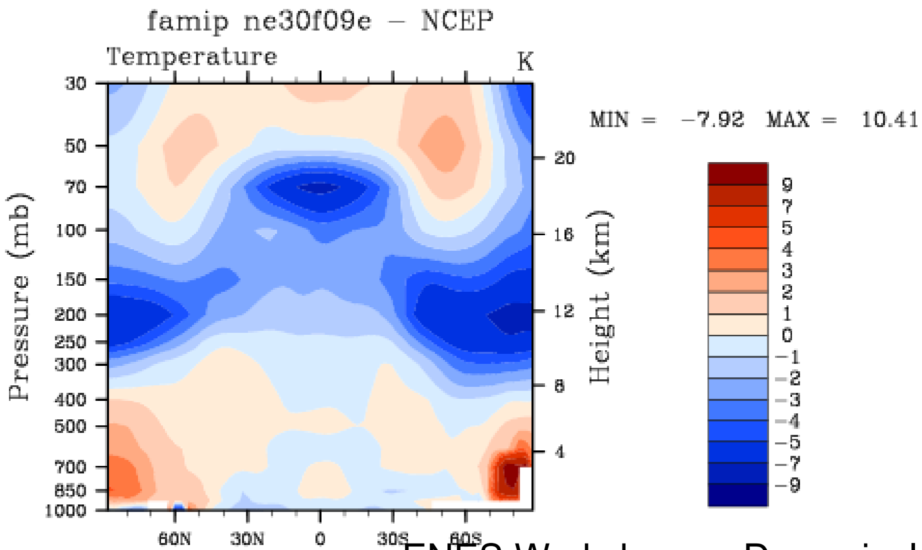


NCEP



CAM4-FV 1°

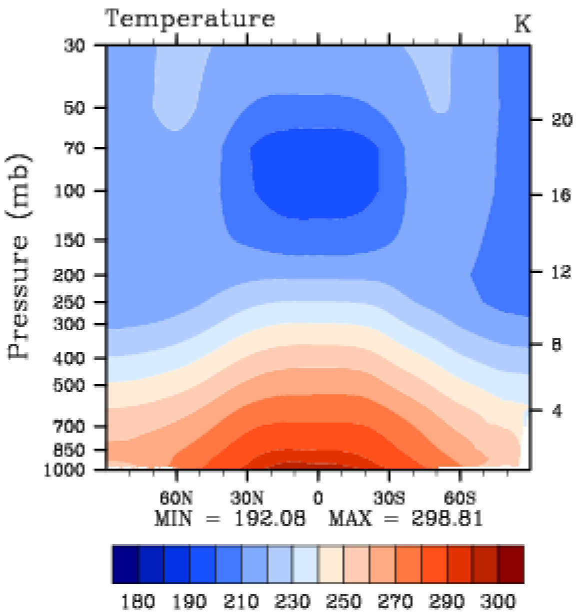




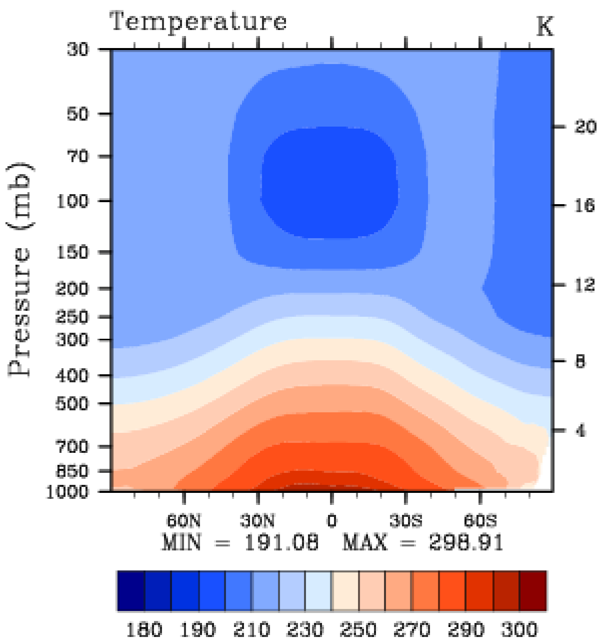
CAM has a long standing 200mb cold bias at the poles (both SE and FV)

Zonal Mean Temperature

CAM4-SE 0.25°



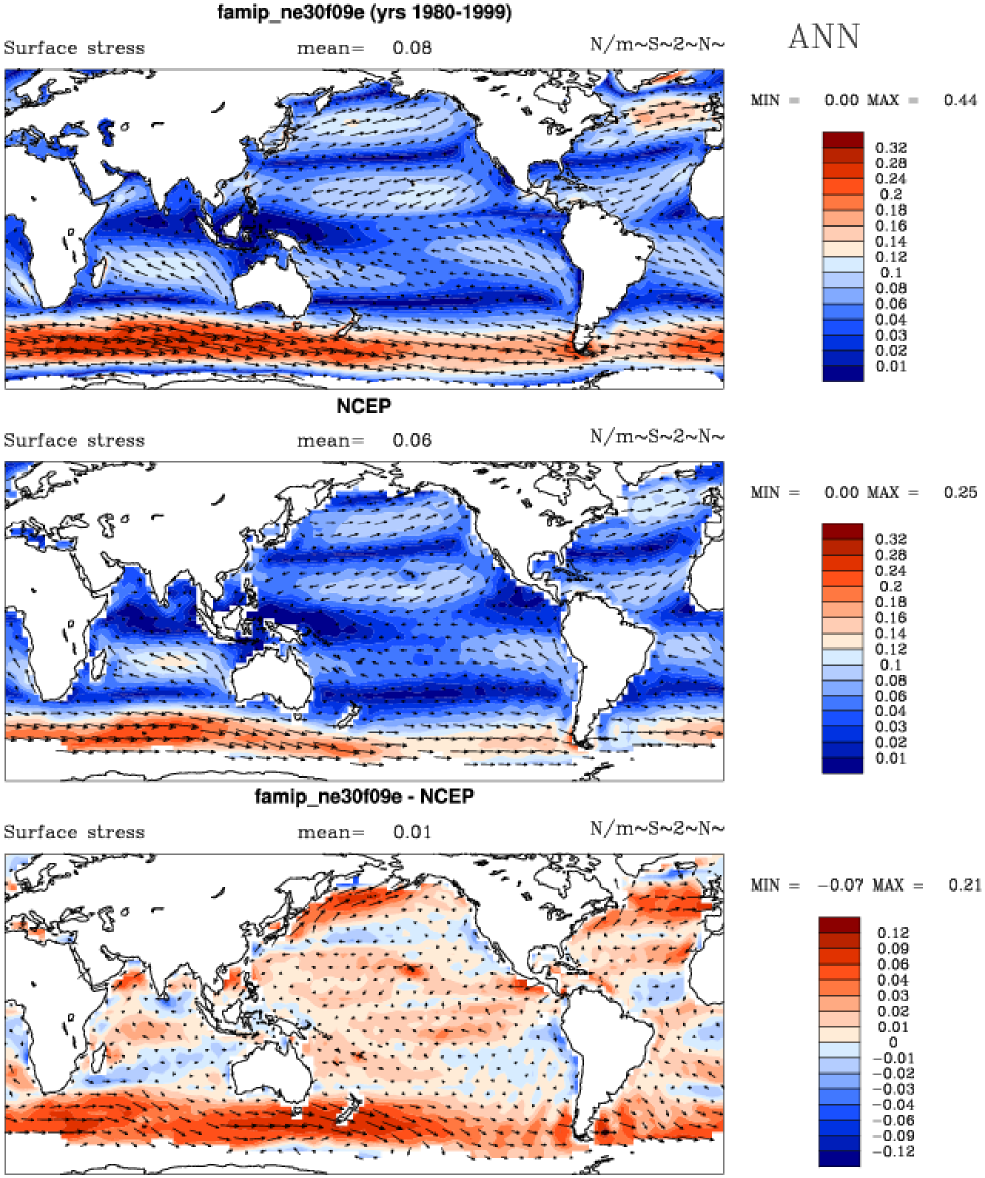
CAM5-SE 1°



Result is insensitive to increasing resolution (left) or CAM5 physics (right)

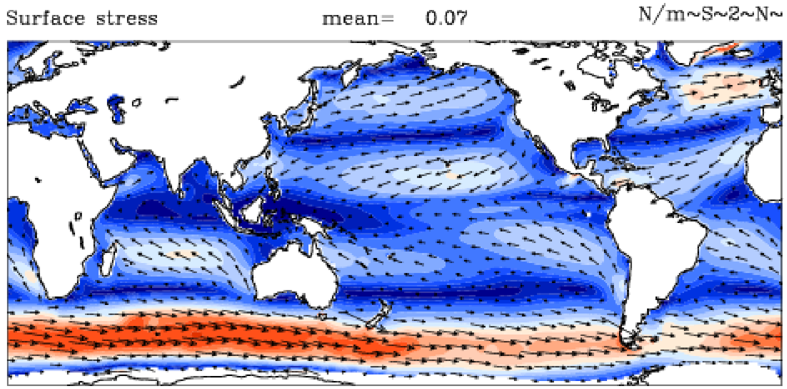
Surface Wind Stress (ocean)

CAM4-SE 1°



NCEP

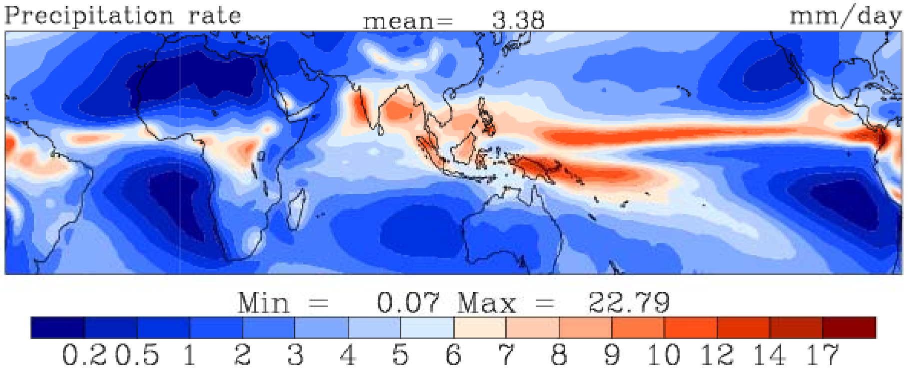
CAM4-FV 1°



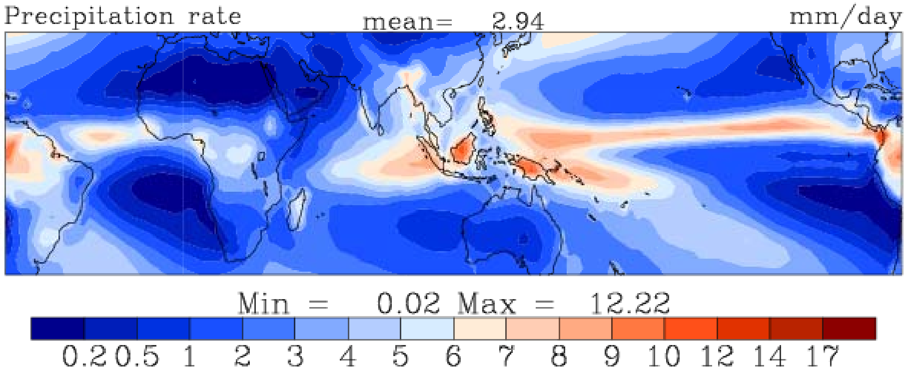
CAM wind stress is too strong (SE stronger than FV)

Tropical Precipitation Rate

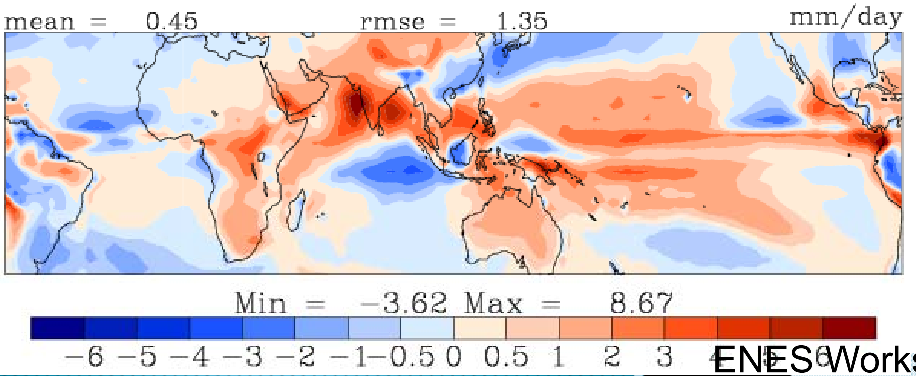
CAM4-SE 1°



GPCP



famip_ne30f09e - GPCP



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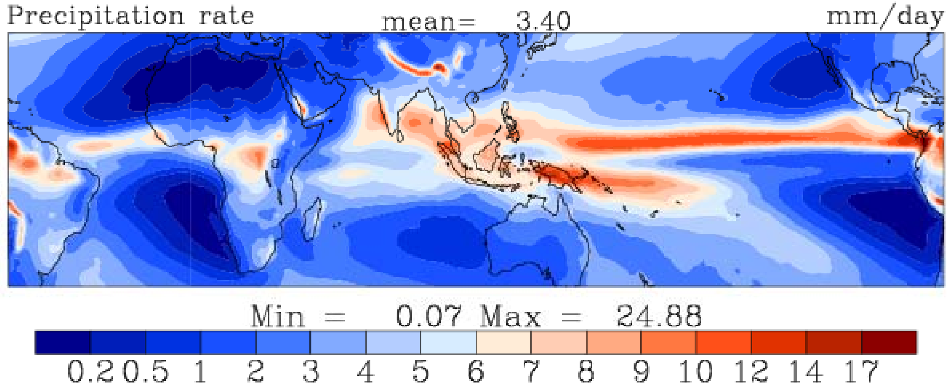

Large biases in both SE and FV

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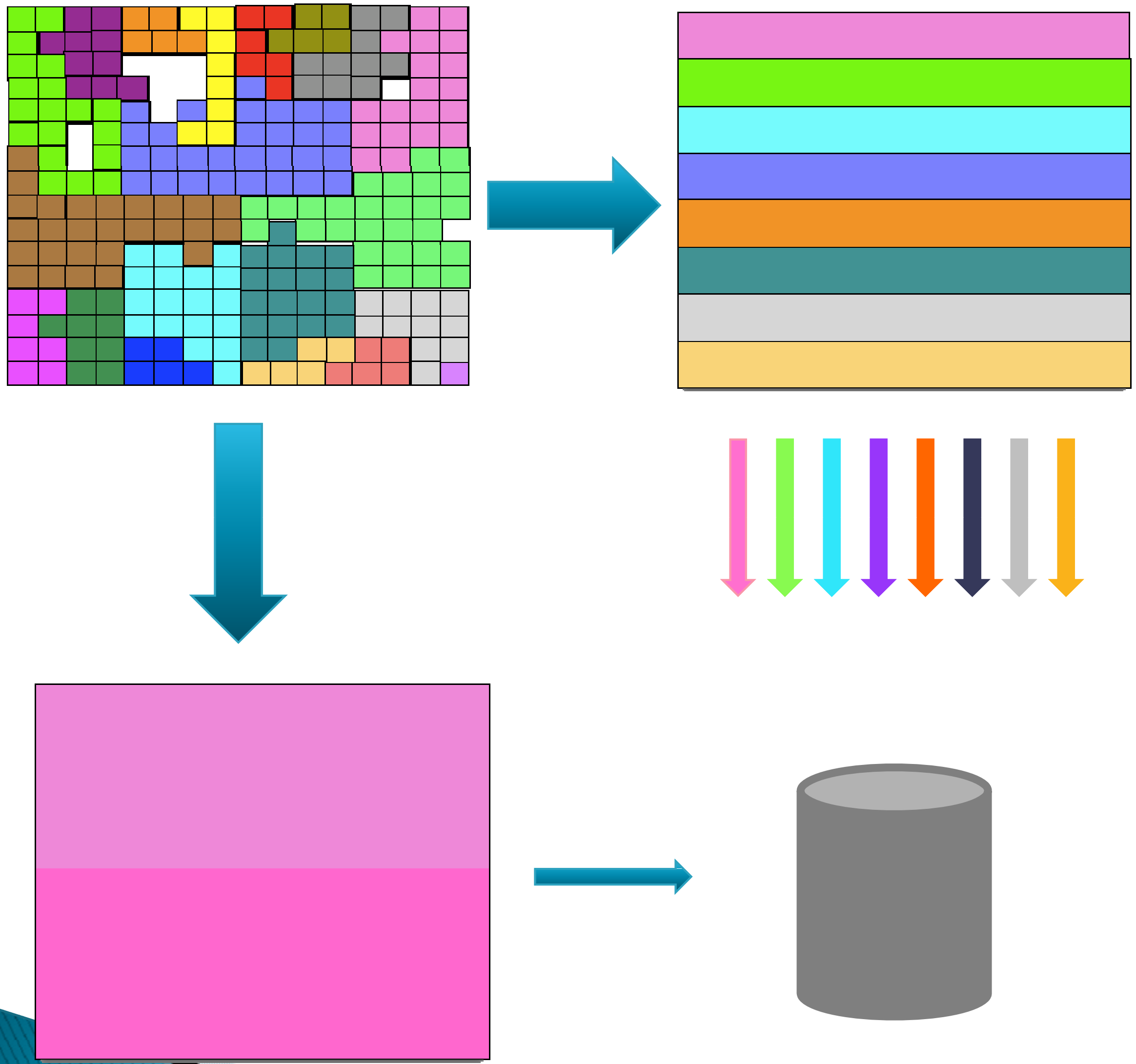
Parallel I/O (PIO) in CESM



Goals:

- Reduce memory usage
- Improve performance

Rearranges data from model decomp to I/O friendly decomp

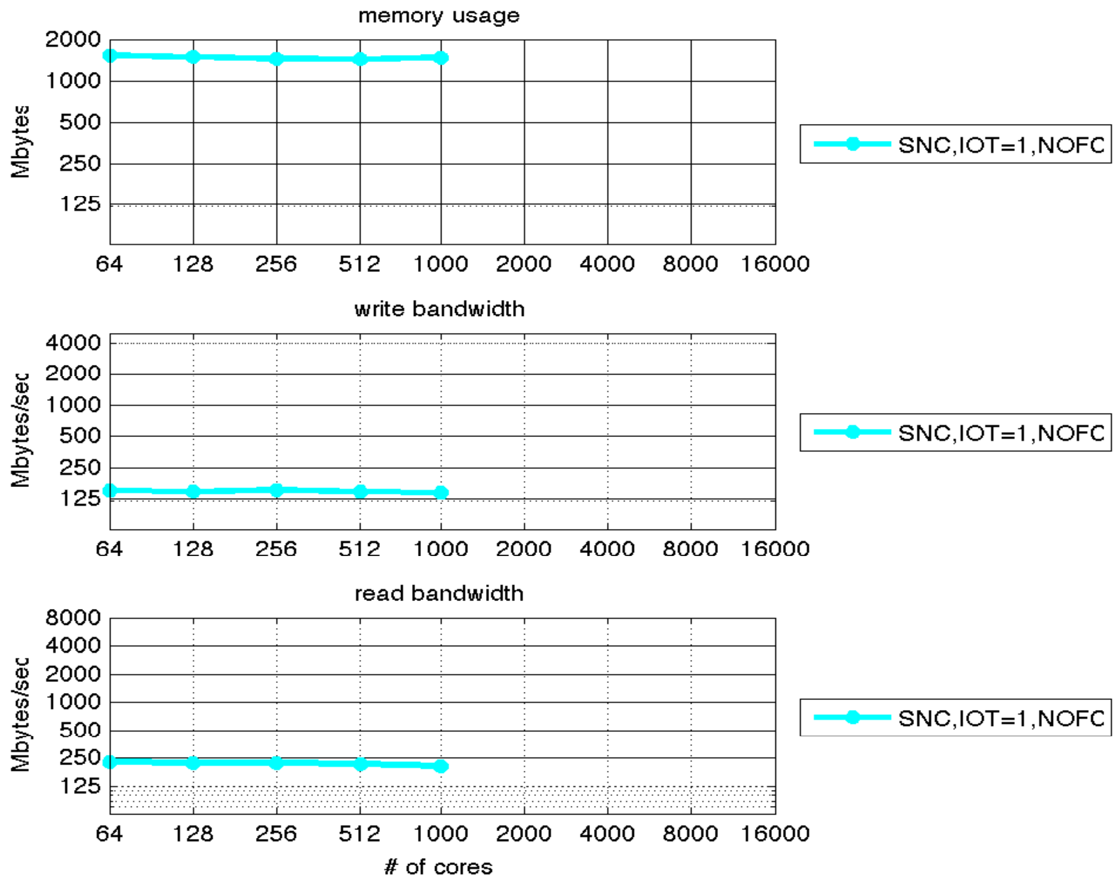
Interface between the model and the I/O library. Supports

- Binary
- NetCDF3 (serial netcdf)
- Parallel NetCDF (pnetcdf) (MPI/IO)
- NetCDF4

Implemented in *ALL* CESM components

Experimental setup

- Did we achieve our design goals?
- Impact of PIO features
  - Flow-control
  - Vary number of IO-tasks
  - Different general I/O backends
- Read/write 3D POP sized variable [3600x2400x40]
- 10 files, 10 variables per file, [max bandwidth]
- Using Kraken (Cray XT5) + Lustre filesystem
  - Used 16 of 336 OST


memory usage
2000
1000
500
250
125
Mbytes
64
128
256
512
1000
2000
4000
8000
16000
SNC,IOT=1,NOFC
write bandwidth
4000
2000
1000
500
250
125
Mbytes/sec
64
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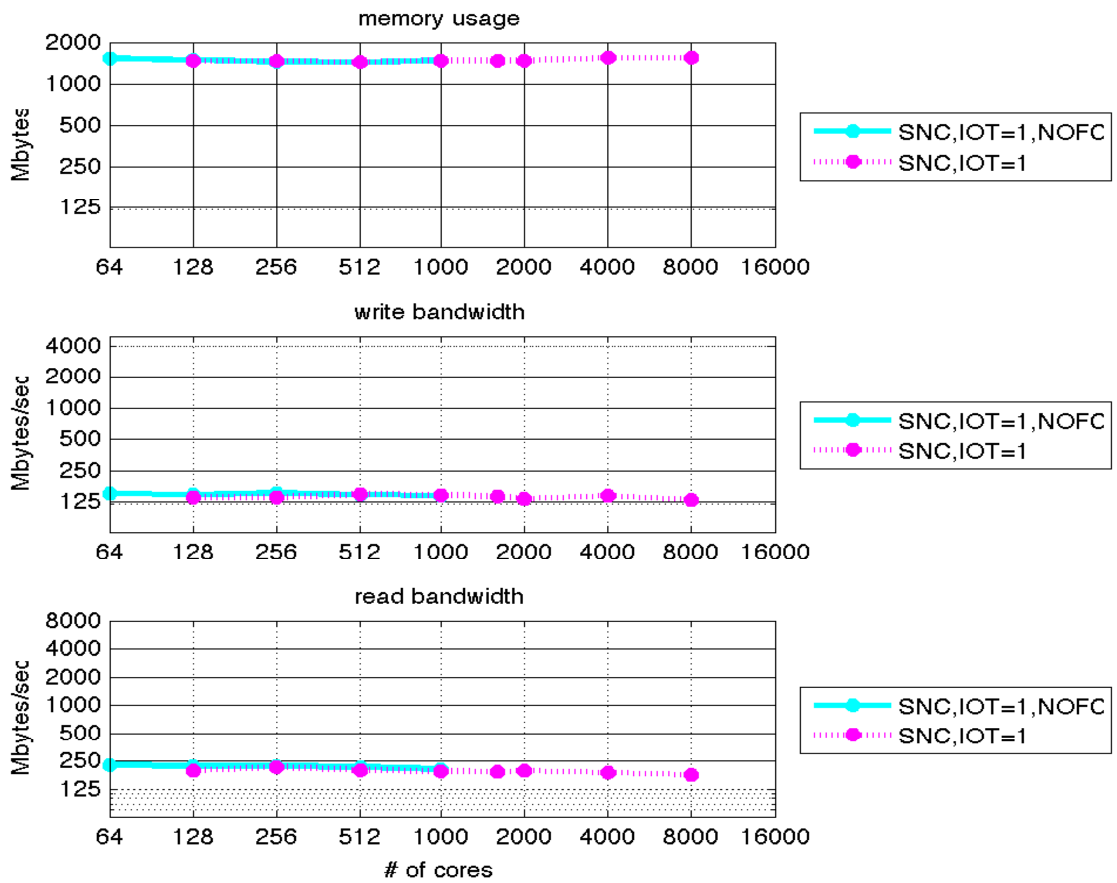
# of cores
SNC,IOT=1,NOFC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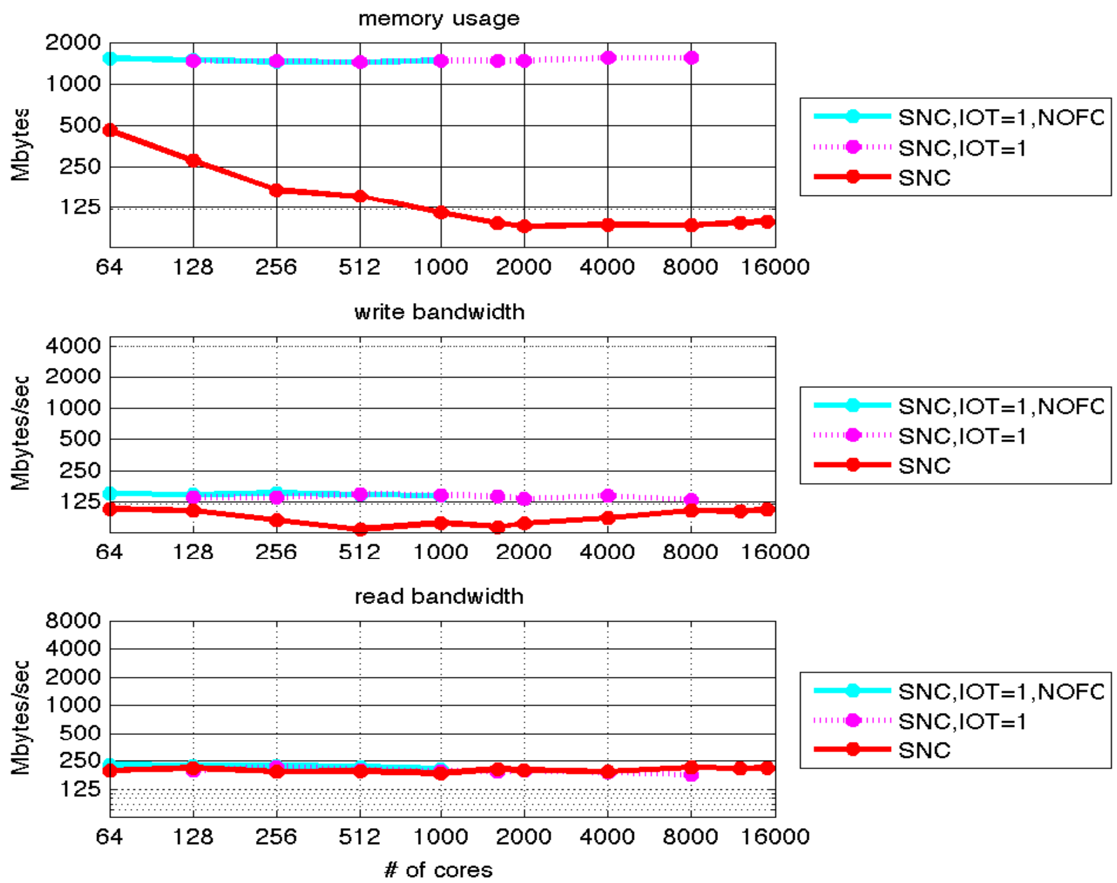
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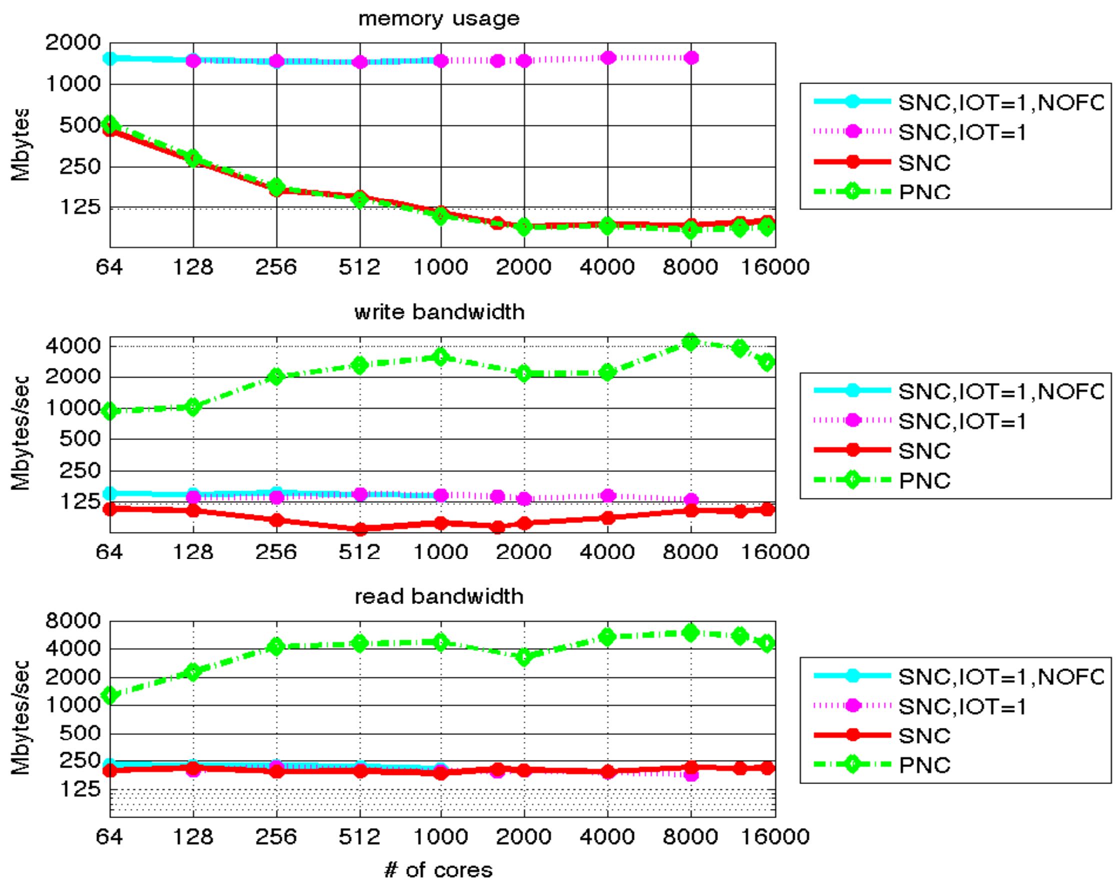
SNC



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PNC
write bandwidth
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Conclusions

- CESM now has High-resolution capability
  - OCN, ICE, ATM
- CAM-SE enables high-resolution ATM capability
  - Scalability to 170K cores
  - CAM5 improves sea-level pressure
  - SE has similar or better results versus FV
- Parallel I/O present in all models
  - Reduces per MPI task memory usage
  - Improves bandwidth
  - Necessary for certain simulations

Acknowledgements

- NCAR:
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  - F. Bryan
  - T. Craig
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  - K. Lindsay
  - N. Norton
  - M. Vertenstein
- COLA:
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  - C. Stan
- U. Miami
  - B. Kirtman
- U.C. Berkeley
  - W. Collins
  - K. Yelick (NERSC)
- U. Washington
  - C. Bitz

- NICS:
  - M. Fahey
  - P. Kovatch
- ANL:
  - R. Jacob
  - R. Loy
- LANL:
  - E. Hunke
  - P. Jones
  - M. Maltrud
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    - DE-PS02-07ER07-06 [SciDAC]
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    - Cooperative Grant NSF01
    - OCI-0749206 [PetaApps]
    - CNS-0421498
    - CNS-0420873
    - CNS-0420985
- Computer Allocations:
  - TeraGrid TRAC @ NICS
  - DOE INCITE @ NERSC
  - LLNL Grand Challenge
- Thanks for Assistance:
  - Cray, NICS, and NERSC

and many more…

Questions?

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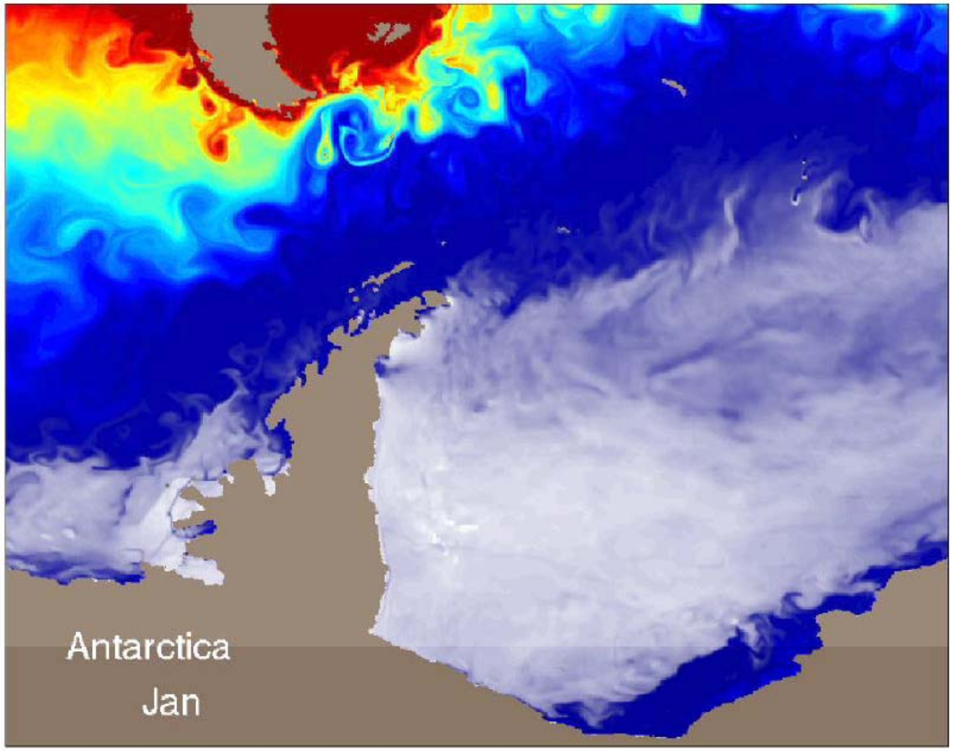

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    - Collins, Yelick (Berkley)
    - Bryan, Dennis, Loft, Vertenstein (NCAR)
    - Bitz (U of Washington)
  - Teragrid Allocations
    - 35M SU (2009)
    - 28M SU (2011)
  - 155 year control run + several 50 year branches

High-Resolution CCSM/CESM

- LLNL Grand Challenge project
  - 0.25° ATM, LND + 0.1° OCN, ICE
  - Participants:
    - Bader [PI] , McClean, Ivanova, Boyle (LLNL)
    - Bryan, Dennis, Vertenstein, Craig, Norton (NCAR)
    - Jones (LANL)
    - Worley (ORNL)
    - Jacob (ANL)
  - 20 year run

- NSF PetaApps project: Interactive Ensemble
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How do we analyze high-resolution climate data faster?

John Dennis, Matthew Woitaszek (NCAR)
Taleena Sines* (Frostburg State)

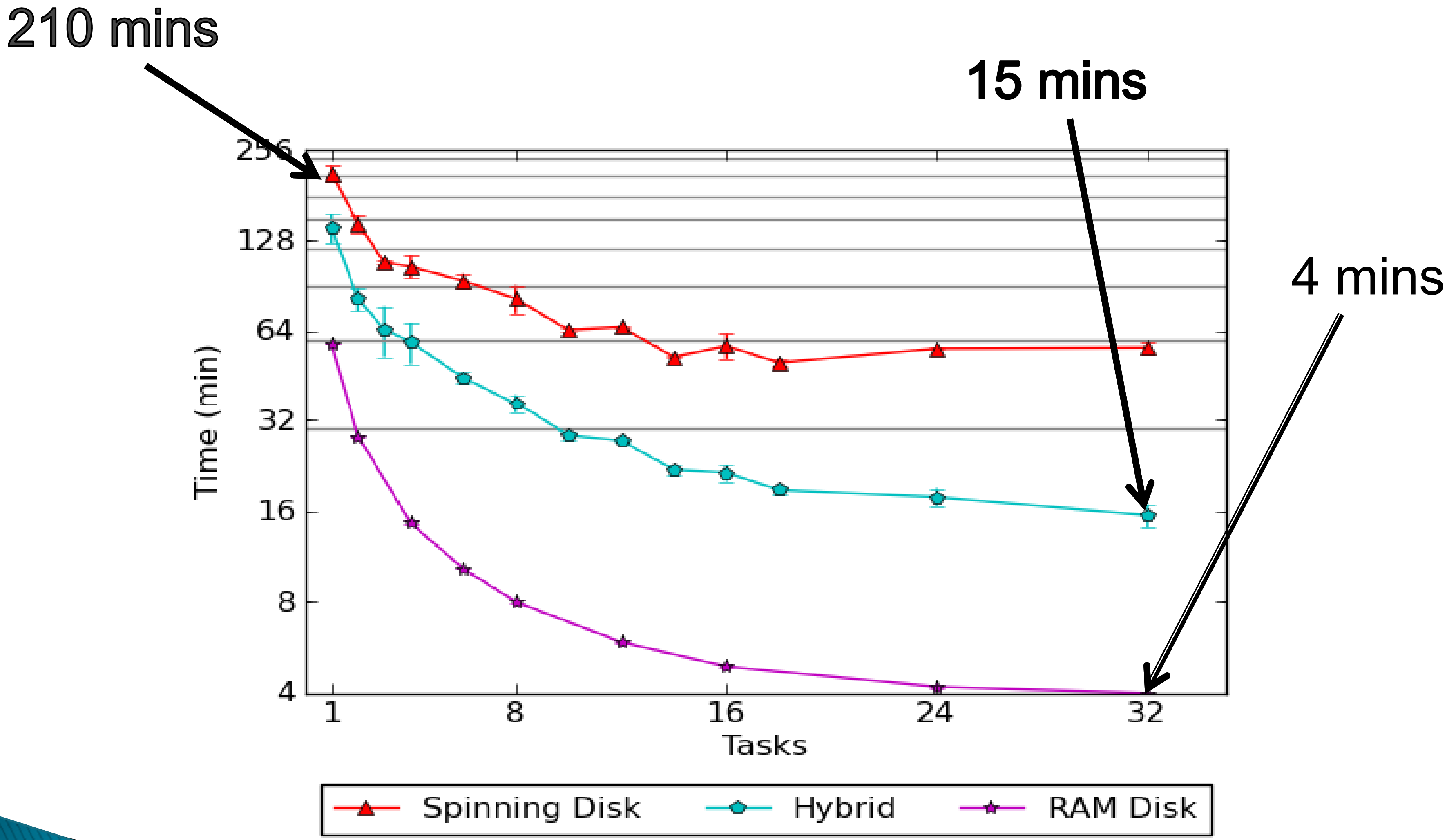
"Parallel high-resolution climate data analysis using Swift", Linux Clusters [under review]

* SIParCS Intern

Parallelizing diagnostics

- Used Swift a workflow language (UC/ANL)
  - Parallel scripting language
  - Data dependency driven
- Examine performance on several data-intensive architectures
  - Flash memory: Dash (SDSC)
  - SGI UV: Nautilus (NICS)
  - Large memory node: Polynya (NCAR)
    - 32 cores
    - 1 TB ram [512 GB memory/ 512 GB ramdisk]
    - 120 TB GPFS file-system (old hardware)

Polynya: 0.5°/10yr



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    - Cooperative Grant NSF01
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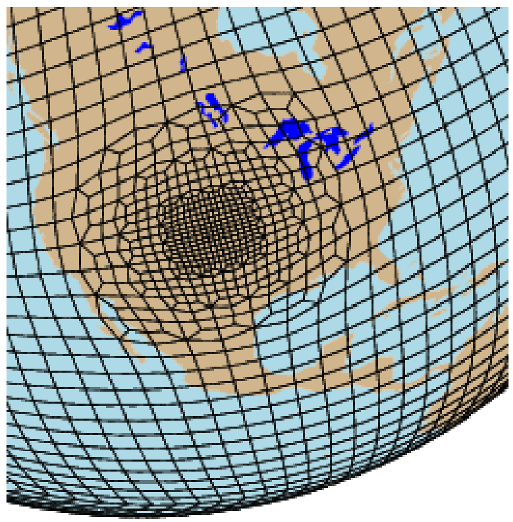
    - CNS-0420873
    - CNS-0420985
- Computer Allocations:
  - TeraGrid TRAC @ NICS
  - DOE INCITE @ NERSC
  - LLNL Grand Challenge
- Thanks for Assistance:
  - Cray, NICS, and NERSC

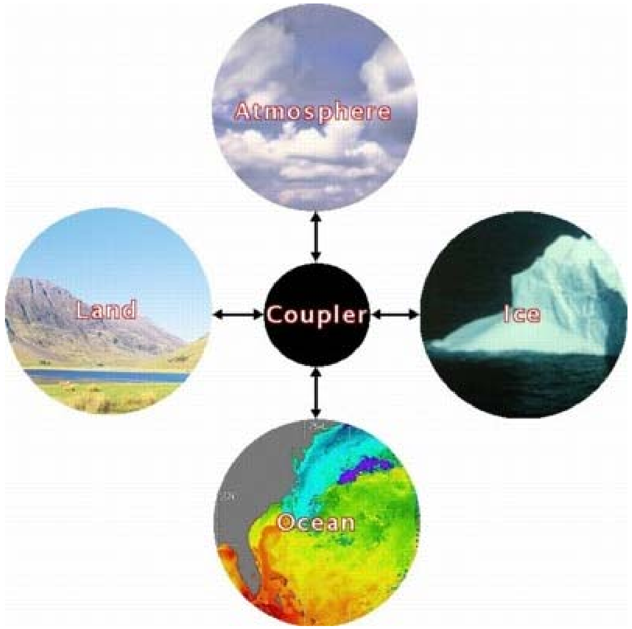
and many more…

Spectral Element Method

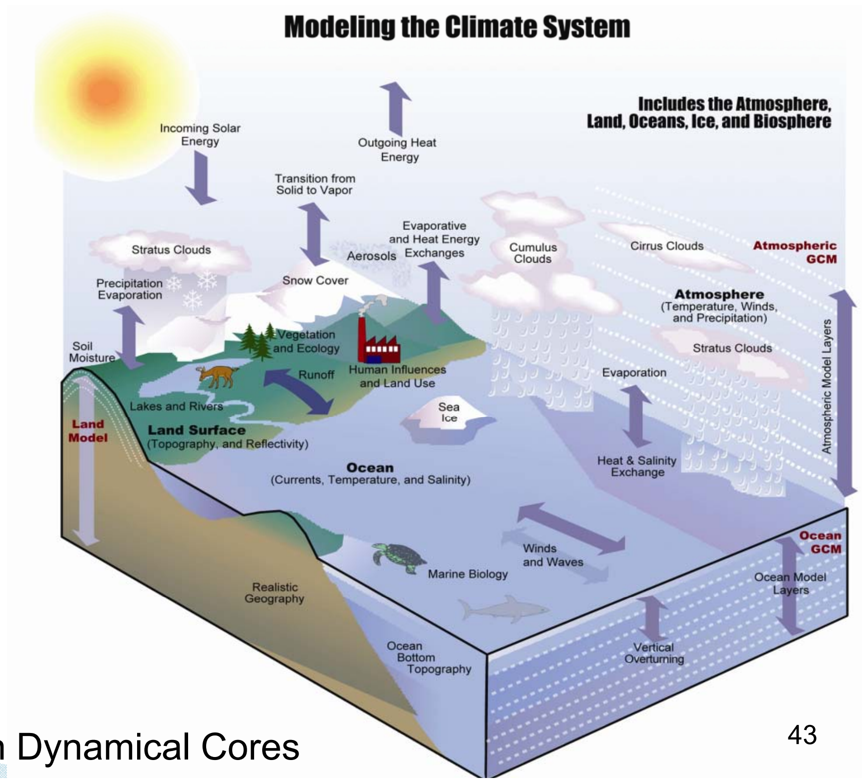
- High-order (4th) discretization
- Mimetic/compatible numerics:
  - Discretization preserves adjoint properties of div, grad and curl operators
  - Discrete versions (element level) of Stokes and Divergence theorem
  - Result: excellent local conservation, even for equations not written in conservation form: mass, energy, 2D PV.
- All properties preserved on unstructured grids



The Community Earth System Model (CESM)



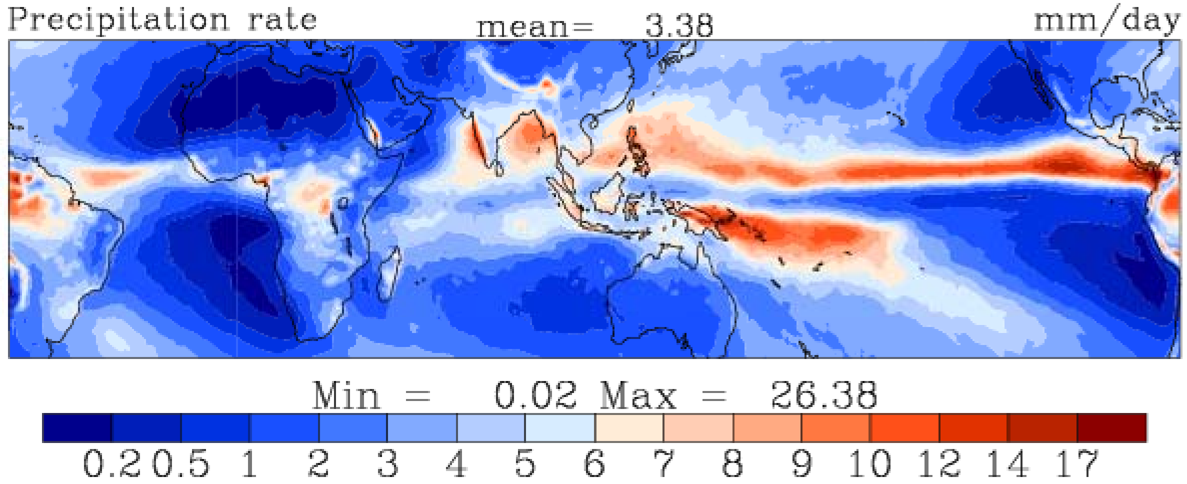
- IPCC-class model:
  - Seasonal and interannual variability in the climate
  - Explore the history of Earth's climate
  - Estimate future of environment for policy formulation
  - Contribute to assessments
- Developed by NCAR, National Labs and Universities.
- CESM1 released summer, 2010: Higher resolution and increasing complexity:



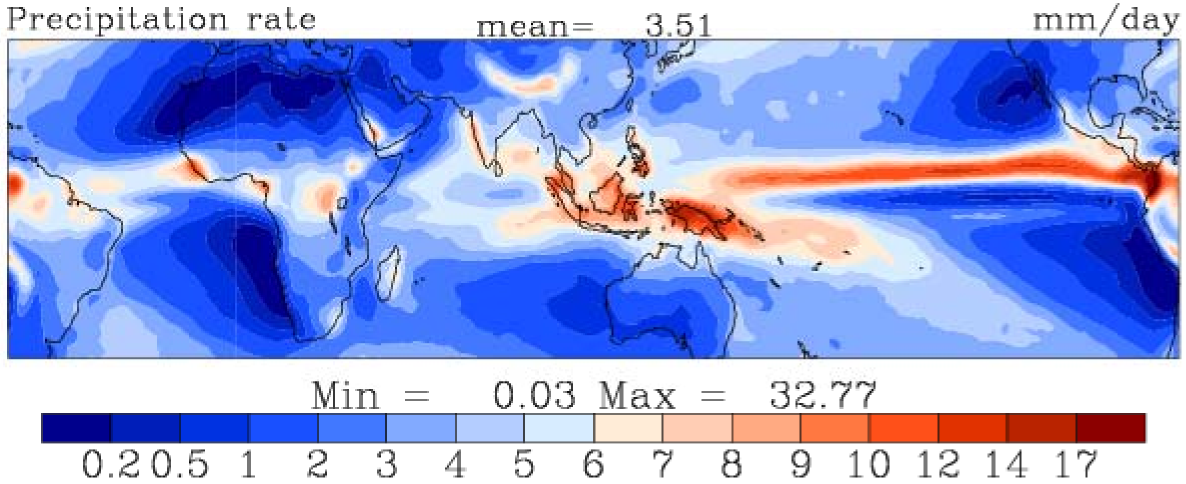
•CAM: Community Atmosphere Model
•CAM-SE: CAM with the spectral element dynamical core from HOMME
•HOMME: High Order Method Modeling Environment

Tropical Precipitation Rate

CAM4-SE 0.25°



CAM5-SE 1°



Pushing the boundaries of what is possible: lessons learned from century-long, high-resolution climate simulations

Richard D. Loft*
Computational and Information Systems Laboratory
National Center for Atmospheric Research**
Boulder, CO

*Thanks to Drs. M. Vertenstein, J. Dennis. and P. Worley

**NCAR is sponsored by the National Science Foundation

Community Earth System Model: Key Ingredients for Success

- CESM's flexible software architecture
- Community governance model
- Engineered for scalability performance
- Coevolution of models and cyberinfrastructure
- Interdisciplinary workforce development

Management Structure

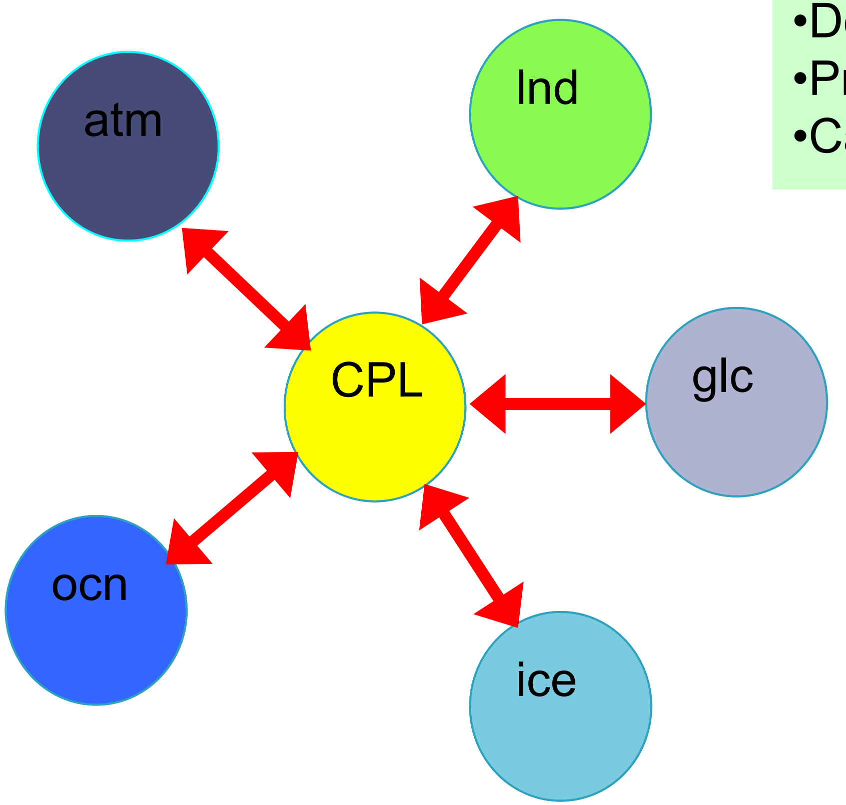
- The Need for a Scientific Steering Committee
  - Provides Oversight and Coordination
  - Provides Scientific Vision
  - Decisions of Resource Allocations
- The Importance of Working Groups
  - Where the Work Really Gets Done
- The Purpose of an Advisory Board
  - Composed of People of Breadth
  - Advises Program Managers
  - Advises Steering Committee

Test, Validation, Tuning

- Validation applies to specific:
  - Platform, Compiler, CESM version
- Functionality tests: build, startup, exact restart
- Validation:
  - perturbation growth test (few days)
  - 200 year simulation
- Component Load Balancing

  $t_{ocn} \sim t_{atm} + t_{ice} + t_{cpl}$
- Production

CESM1 "Hub and Spoke" Coupling Architecture



Atm -> Coupler

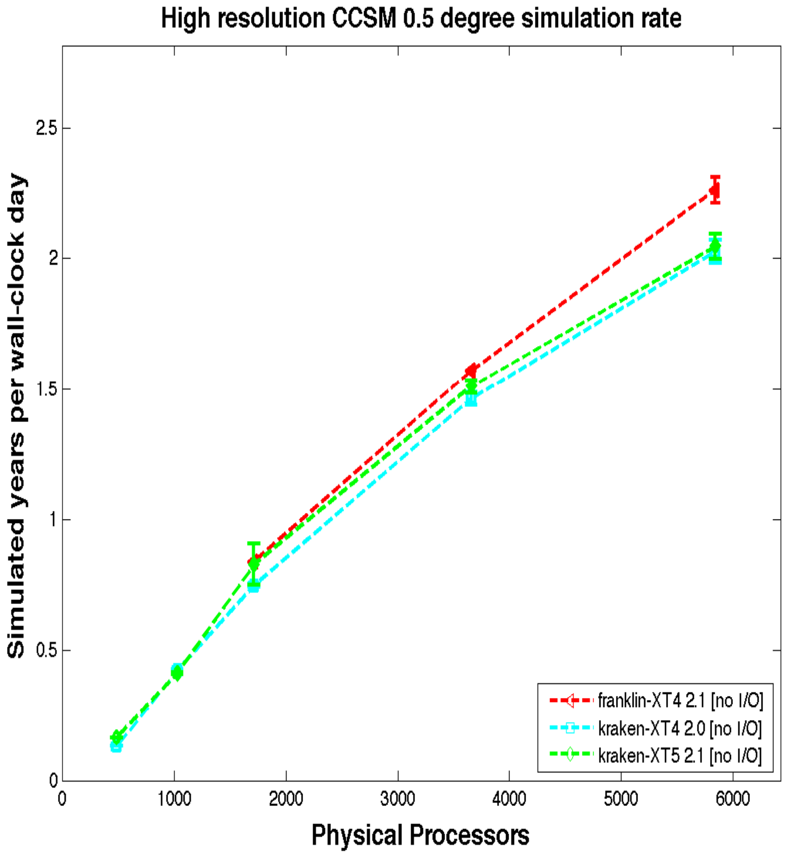
- Bottom level temperature, pressure,wind…
- Downward Shortwave (vis, nir)
- Precipitation
- Carbon and Dust fluxes

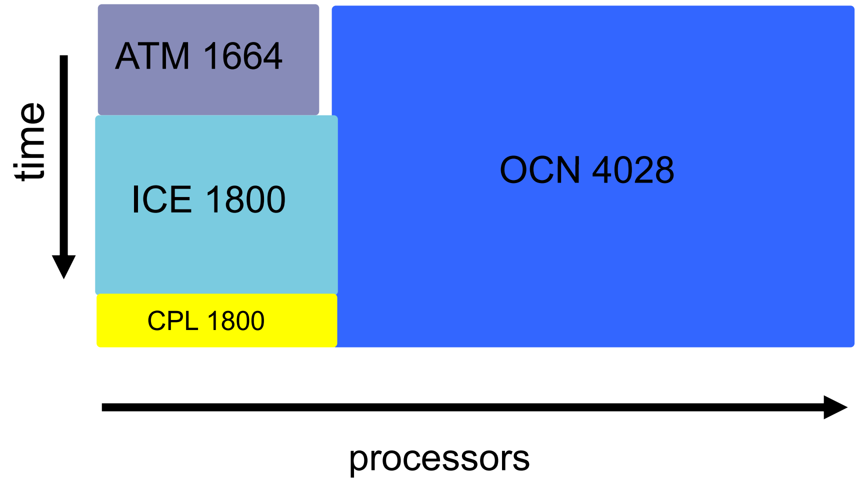
Coupler -> Atm

(merged from lnd, ice and ocn)

- Latent, sensible heat fluxes
- Surfaces Stresses
- Upward long wave
- Evaporative water flux
- Surface Albedos

CCSM 50 km ATM/LND x 10 km (OCN/CICE) Scalability on Cray XT systems





1.9 years/day on 5844 cores
with I/O
on kraken hex-core XT5

$$t_{ocn} \sim t_{atm} + t_{ice} + t_{cpl}$$

(Courtesy of John Dennis)

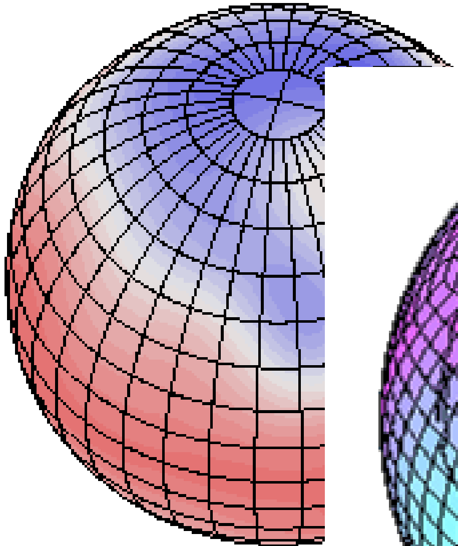
Important Ingredients (and problems) for High Resolution Climate Modeling

- Scalable Algorithms
  - Free from coordinate singularities with local numerics
  - Effective Mesh Partitioning e.g. via Space Filling Curves
  - Global solvers are problematic
- Component coupling infrastructure
  - Coupler allows algorithmic autonomy and flexibility
  - Scalability of regridding algorithms
- Expression of parallelism
  - CAM, CLM, CICE, OCN all use hybrid MPI and OpenMP
  - What about accelerators? (GPU's, MIC)
- Memory footprint
  - Memory scalability of all components - parallel I/O
  - Scientist keep adding physical variables

History: a succession of ever finer, quasi-uniform computational grids based on Platonic solids, using scalable mathematical methods

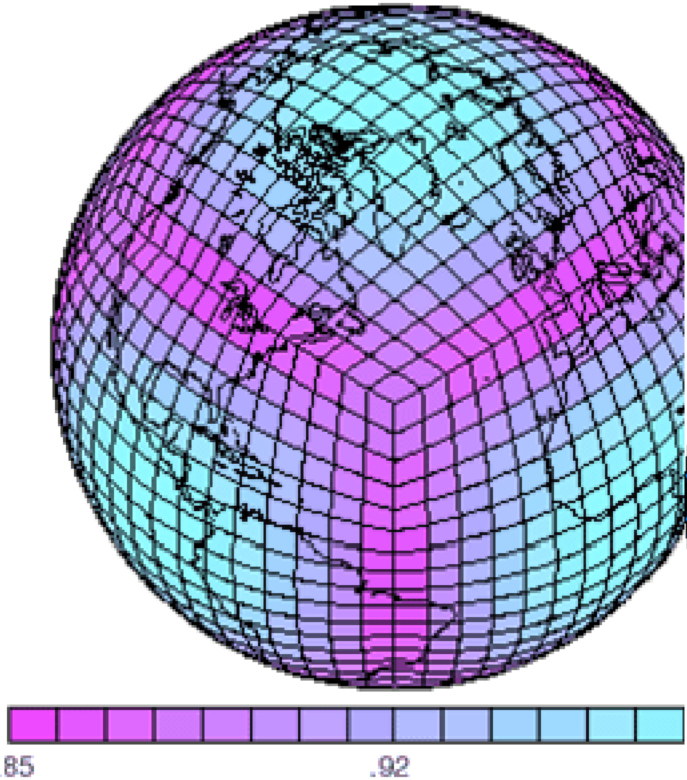
Spherical Harmonics

$Y^l_m(\theta,\varphi)$



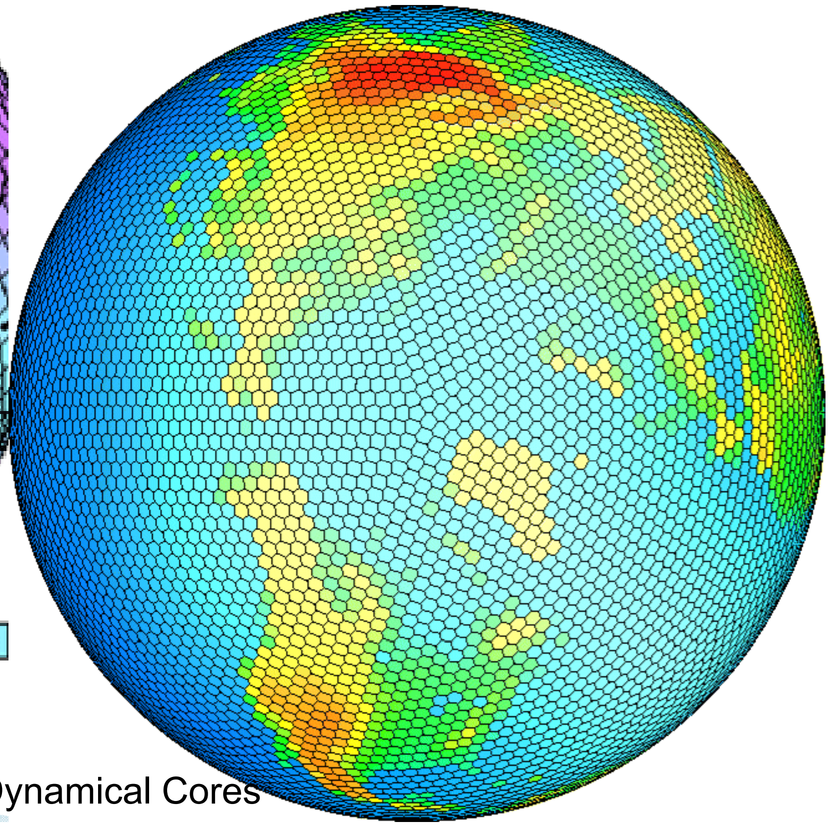
$$\mathcal{M}^k_{ij} = \int_{\mathsf{D}^k} \ell^k_i(x)\ell^k_j(x)\,dx, \quad \mathcal{S}^k_{ij} = \int_{\mathsf{D}^k} \ell^k_i(x)\frac{d\ell^k_j}{dx}\,dx$$

Spectral Elements



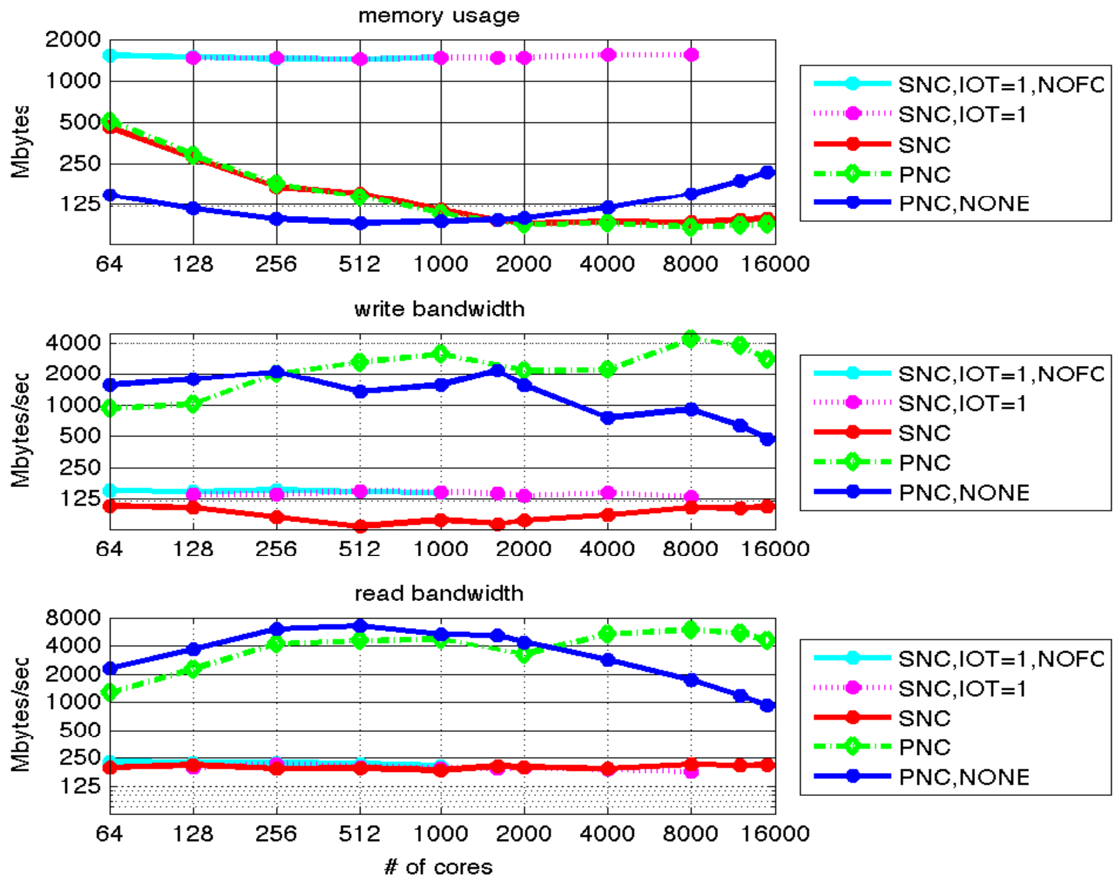
$$\frac{d\bar{\rho}_i}{dt} + \frac{1}{\Delta x_i}\left[f_{i+\frac{1}{2}} - f_{i-\frac{1}{2}}\right] = 0$$

Finite Volume Methods



The NCAR-Wyoming Supercomputing Center is Coming Online

Key Point: Petascale facilities and resources are required to develop high-resolution community models


memory usage
Mbytes
2000
1000
500
250
125
64
128
256
512
1000
2000
4000
8000
16000
SNC,IOT=1,NOFC
SNC,IOT=1
SNC
PNC
PNC,NONE
write bandwidth
Mbytes/sec
4000
2000
1000
500
250
125
read bandwidth
8000
# of cores

"Yellowstone" at a Glance

NWSC's First High Performance Computing Resource

- Compute Nodes
  - Processor: 2.6 GHz Intel Sandy Bridge EP processors
  - Node: dual socket; 32 GB memory; 2 GB/core
  - 4,662 nodes, 74,592 cores total – 1.552 PFLOPs peak
  - 149.2 TB total memory
- High-Performance Interconnect
  - Mellanox FDR14 InfiniBand full fat-tree
  - 13.6 GB/sec bidirectional bw/node
  - <2.5 usec latency (worst case)
  - 31.7 TB/sec bisection bandwidth
- Central File System
  - 2012: 11 PB
  - 2014: 16.4 PB
  - Bandwidth: 100 GB/sec

CESM Science Opportunities

Yellowstone Allocation Request Timeline

- Accelerated Scientific Discovery
  - *Deadline: January 13, 2012*
  - 2- to 3-month, large-scale activities, with NSF support
- Climate Simulation Laboratory
  - Large-scale, climate-related projects, support from any agency
  - *Deadline: February 15, 2012*
- Large University requests
  - Twice per year. *Next deadline: March 26, 2012*
  - Must have NSF award in atmospheric, related science
- Wyoming-NCAR requests
  - Once per year. *Next deadline: March 2012*
  - Work may be across the geosciences, any funding agency support
  - Requires Wyoming collaboration. Targeting EPSCoR state collaborators.
- *http://www2.cisl.ucar.edu/docs/allocations*

Summer Internships in Parallel Computational Science: Students work in NCAR's Supercomputing Lab with mentors on challenging R&D projects

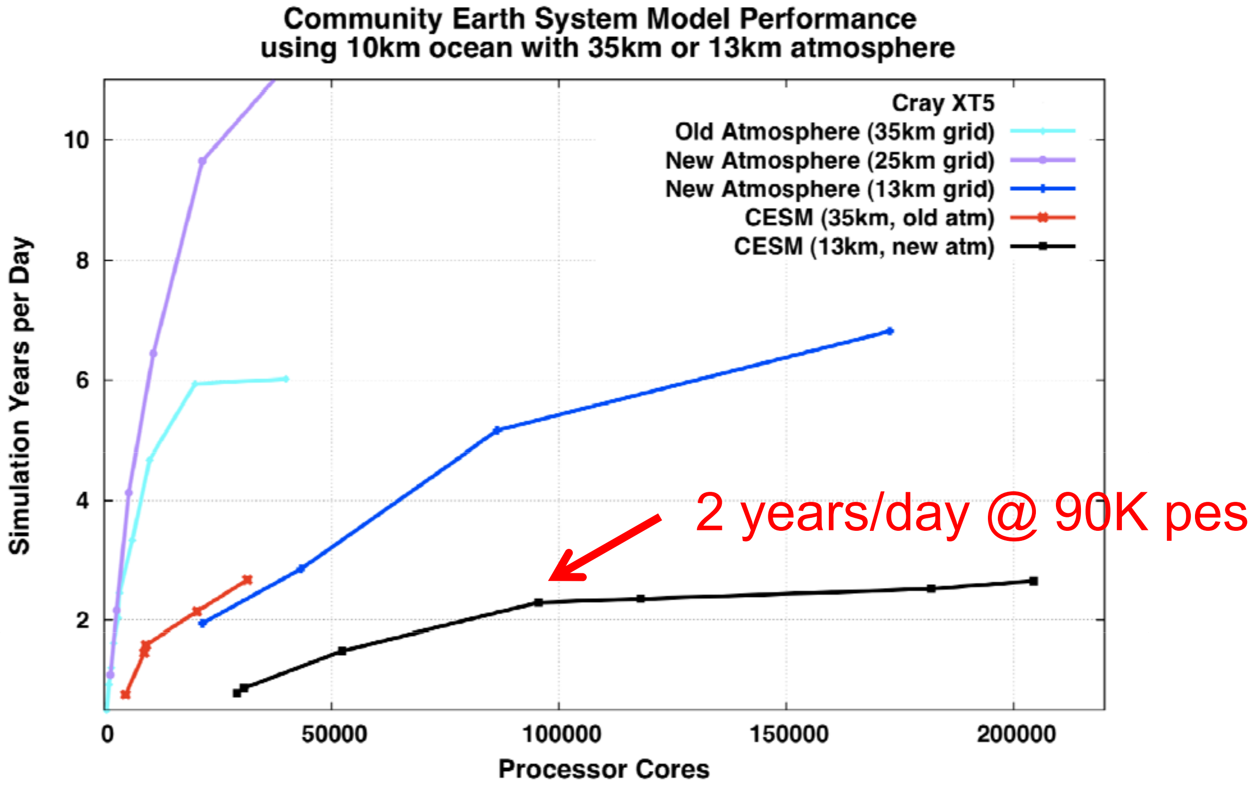
SIParCS Class of 2011

- 11-week Summer internship program
  - May 21 – August 3, 2012
- Open to:
  - Upper division undergrads
  - Graduate students
- In Disciplines such as:
  - Computer Science and Software Engineering
  - Mechanical Engineering
  - Applied Math and Statistics
  - Earth System Science
- Support:
  - Travel, Housing, Per diem
  - 11 weeks salary
  - Conference travel and Publication costs
- Number of interns selected:
  - Typically 15-20

http://www.cisl.ucar.edu/siparcs

CESM Computational Performance

(courtesy of Pat Worley)



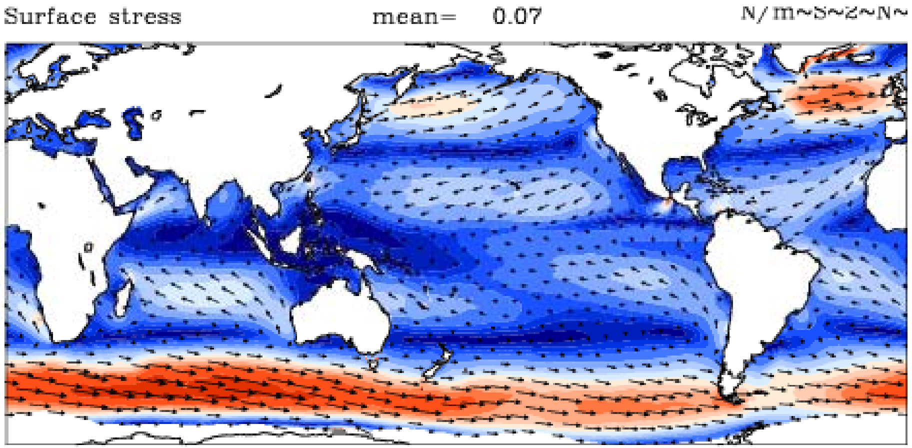
For 13km ATM / 10 km OCN/ICE, CESM performance is not constrained by ATM

Spectral element-based atmospheric dynamics permits scalable CESM performance at high resolution.

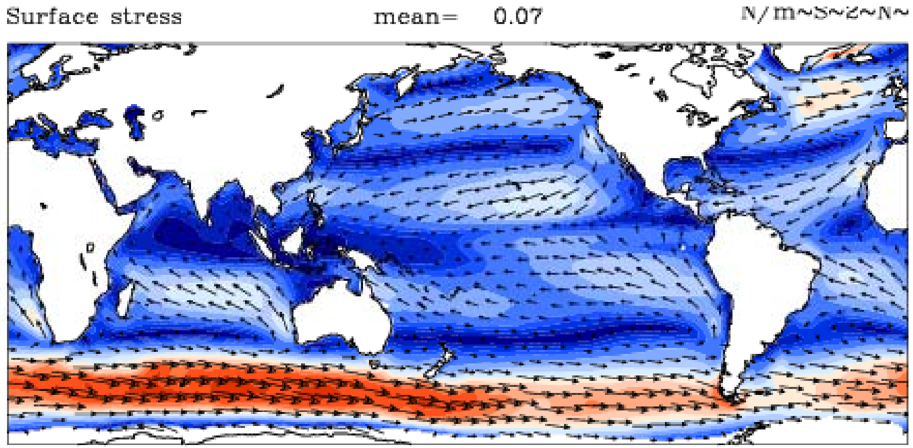
Questions?

Surface Wind Stress (ocean)

CAM4-SE 0.25°



CAM5-SE 1°



Questions?

dennis@ucar.edu

Q2: What impact does PGAS languages have on complexity and performance?

Andy Stone*, Michelle Strout (CSU)