Spectral Elements

CSRF FY05 Completing Projects Review

October 18, 2:30pm

PI: Bill Spotz, 1433

PM: Jennifer Nelson, 1430

Mark Taylor, Mark Boslough

1433

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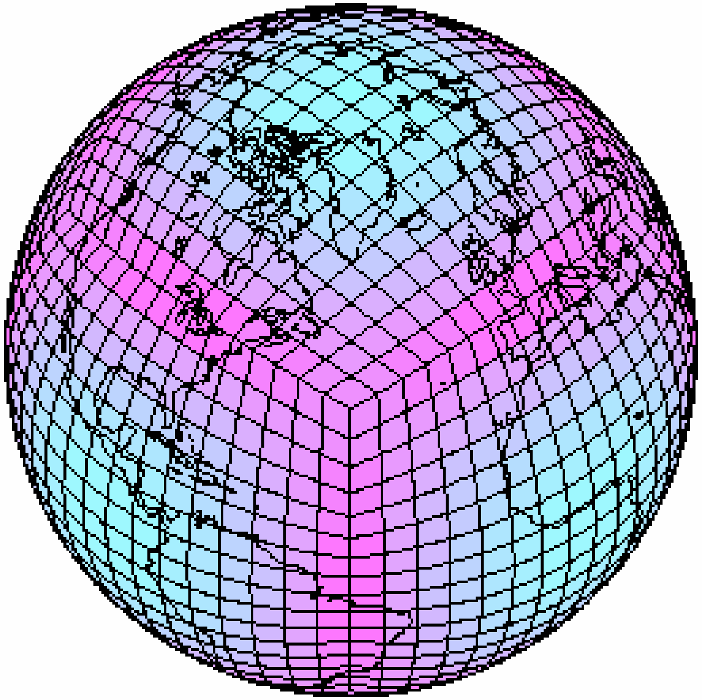
A Little Background…

- Interest in getting Sandia into the climate modeling community
- I proposed working with spectral element model
  - Highly scalable research code
  - Collaboration with NCAR
- For CSRF, stressed Dual Use capabilities of spectral elements
- LDRD the following year
  - Independence of projects
  - Dual Use the conceptual dividing line

SEAM: Spectral Element Atmosphere Model



- Atmospheric global circulation model (GCM)
  - NCAR/DOE CHAMMP
- Quadrilateral spectral elements in horizontal
- Finite differences in vertical
- Cubed sphere, 2D domain decomposition
- 6 transforms between spherical and local cartesian coordinates
  - No pole problem
  - Edge conditions
- 2001 Gordon Bell Honorable Mention

SEAM: A Little History

- Developed in 1996 at NCAR (Taylor, Tribbia, Iskandarani)
- Taylor left NCAR for LANL in 1998
- Tribbia, Fournier, Wang continued work w/SEAM
- Loft, Thomas wrote new SEAM (later HOMME)
- SEAM(2) wins Gordon Bell Honorable Mention (2001, stacked shallow water)
- Sandia begins collaboration in 2003
  - Stacked shallow water → full 3D primitive eqns
  - Explicit time stepping → semi-implicit
  - Pushed high-resolution, HPC capabilities
  - Physics integration
- LDRD in 2004
- Sandia hires Taylor, 2004

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Collaborators

- National Center for Atmospheric Research
  - Steve Thomas
  - Joe Tribbia
  - Rich Loft
  - Amik St-Cyr
  - Jim Edwards
  - Henry Tufo (joint w/CU Boulder)
- Naval Research Laboratories
  - Frank Giraldo (Monterrey)
  - Alan Wallcraft (Stennis)
- Oak Ridge National Laboratory
  - John Drake
- Los Alamos National Laboratory
  - Phil Jones
  - Beth Wingate
- University of New Mexico
  - Tim Warburton (now at Rice)
  - Dagoberto Justo
  - Joe Galewsky

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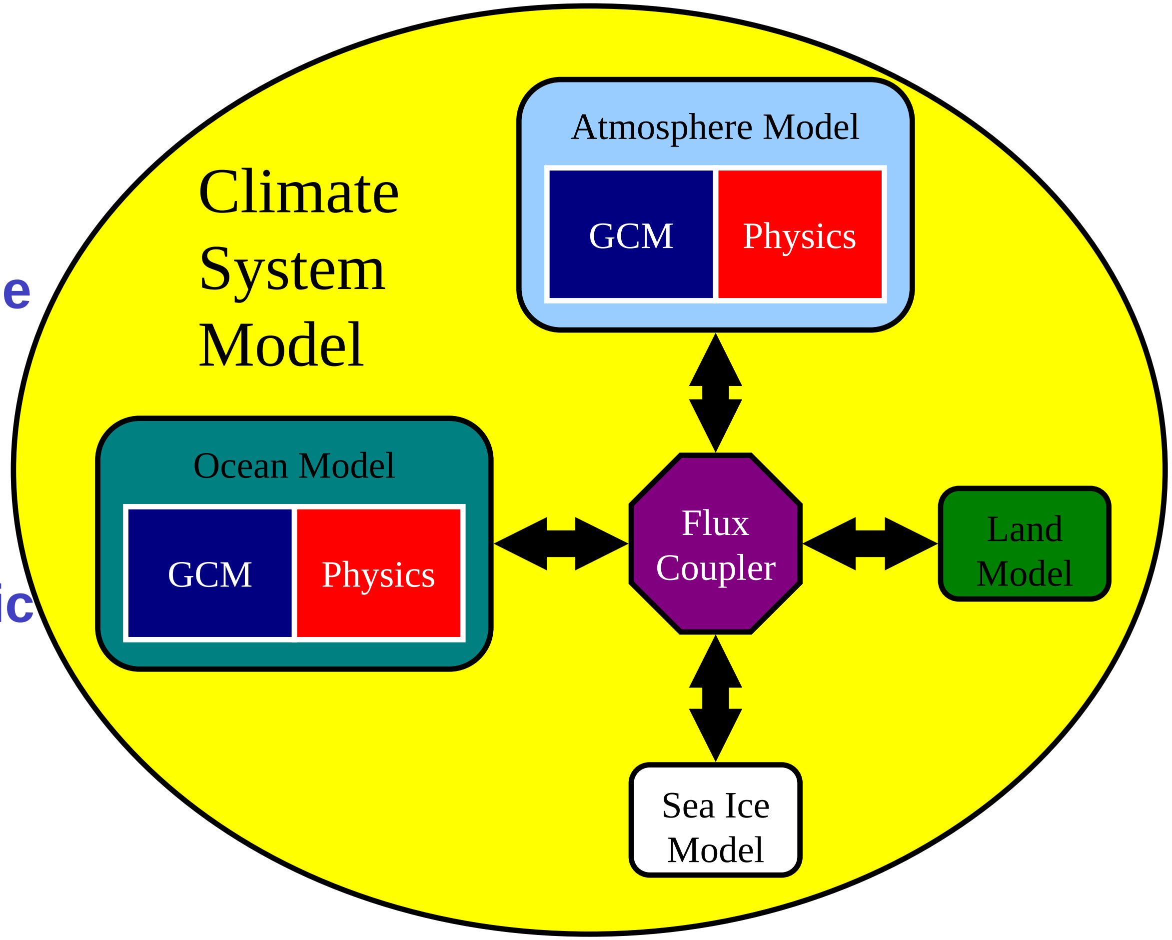
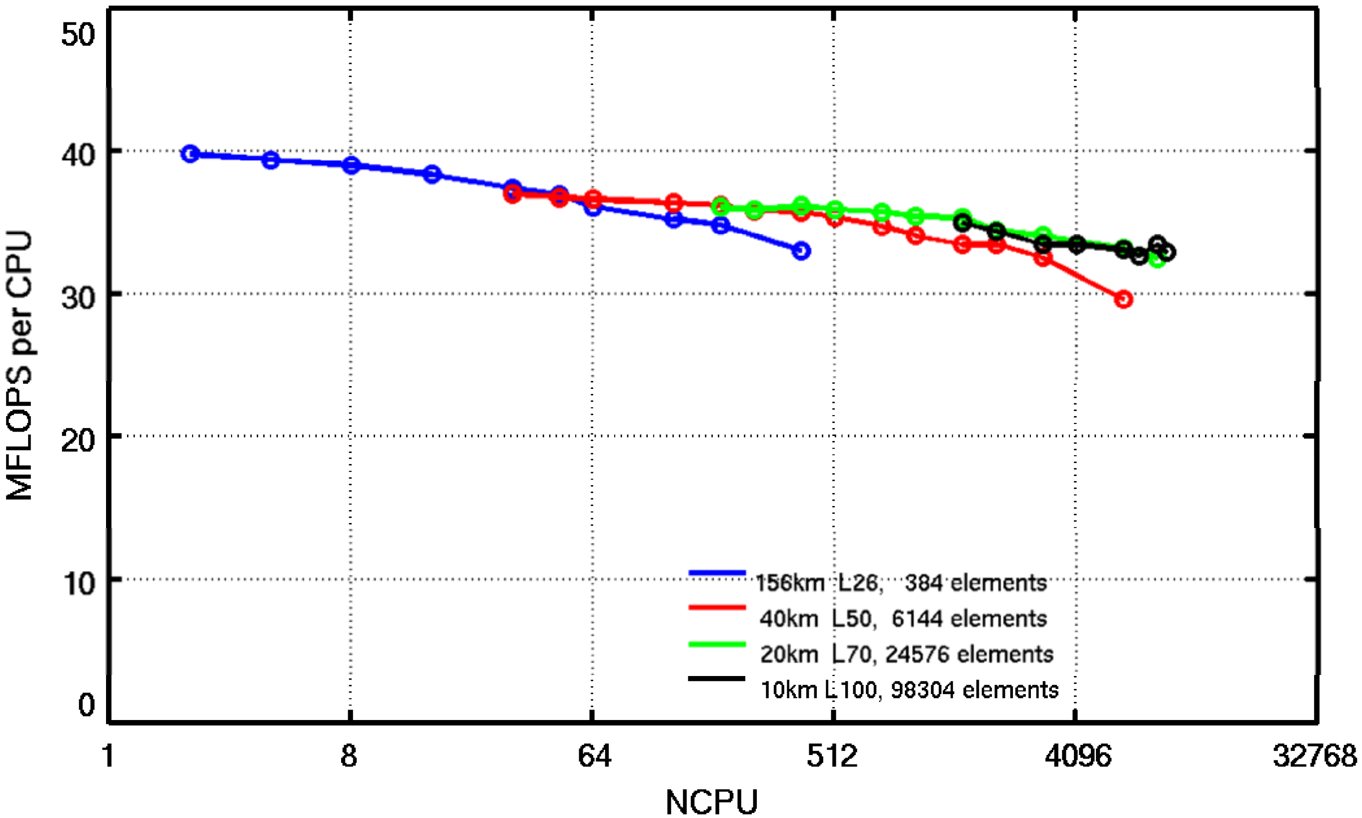
Where SEAM Fits in Climate Modeling

- Community Climate System Model (CCSM)
- Managed by NCAR
- Funding sources include SciDAC
- Atmosphere model is most computationally intense
- Community Atmospheric Model (CAM):
  - Spectral Transform
  - Finite Volume
  - Spectral Element?



How Well Does SEAM Scale?

Janus



Spotz, "Performance Results and Analysis of the Spectral Element Method on the Sphere at Sandia," presented at the *2004 Workshop for the Solution of PDEs on the Sphere*, Yokohama, Japan, July 21, 2004.

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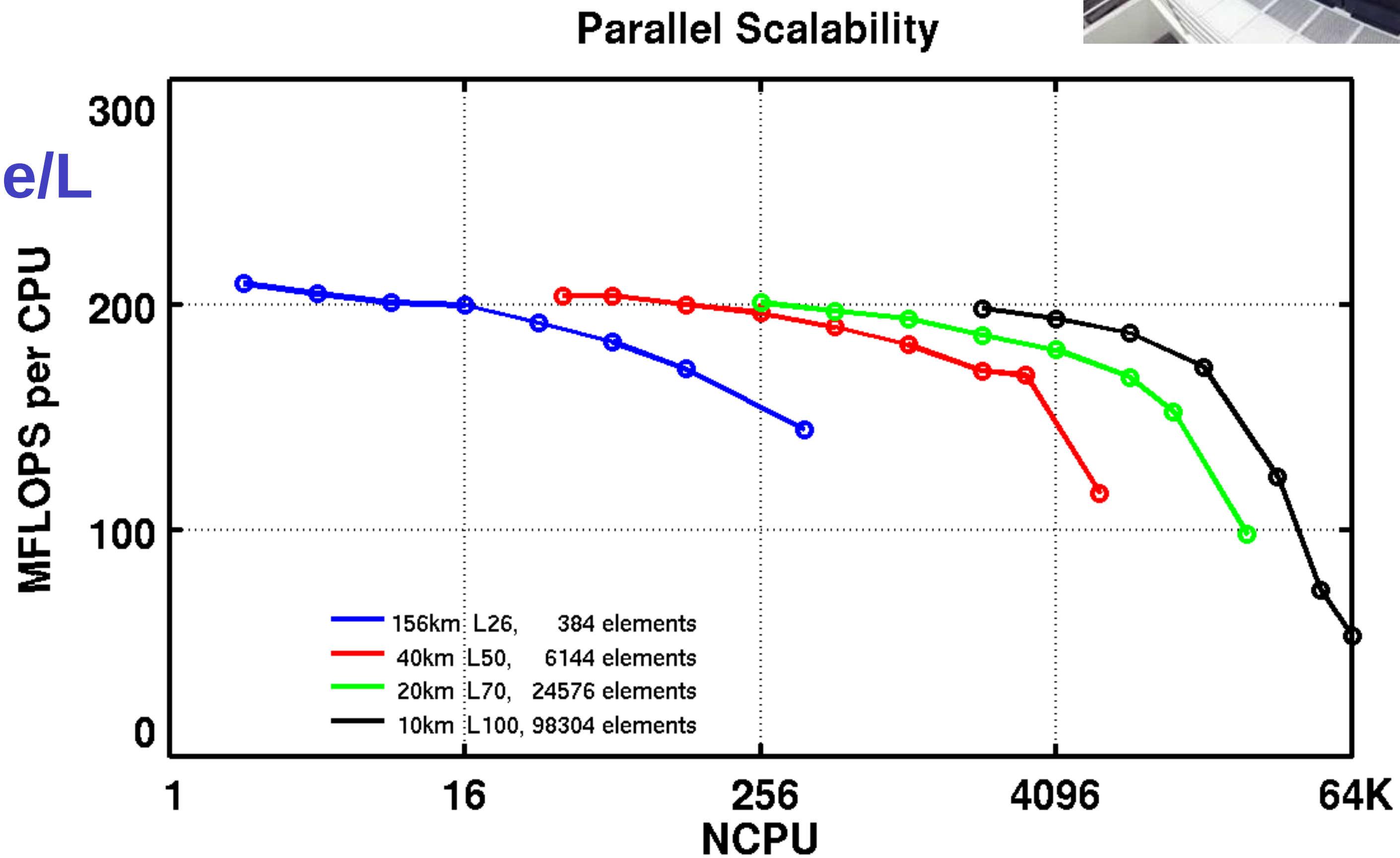
How Well Does SEAM Scale?

BlueGene/L



Dennis, Fournier, Spotz, St.-Cyr, Taylor, Thomas, Tufo, "High Resolution Mesh Convergence Properties and Parallel Efficiency of a Spectral Element Atmospheric Dynamical Core," *Int. J. High Perform. Comp. Appl.* special issue on Climate Modeling Algorithms and Software Practice

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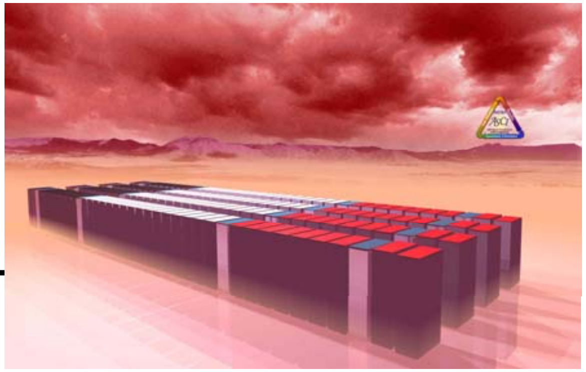
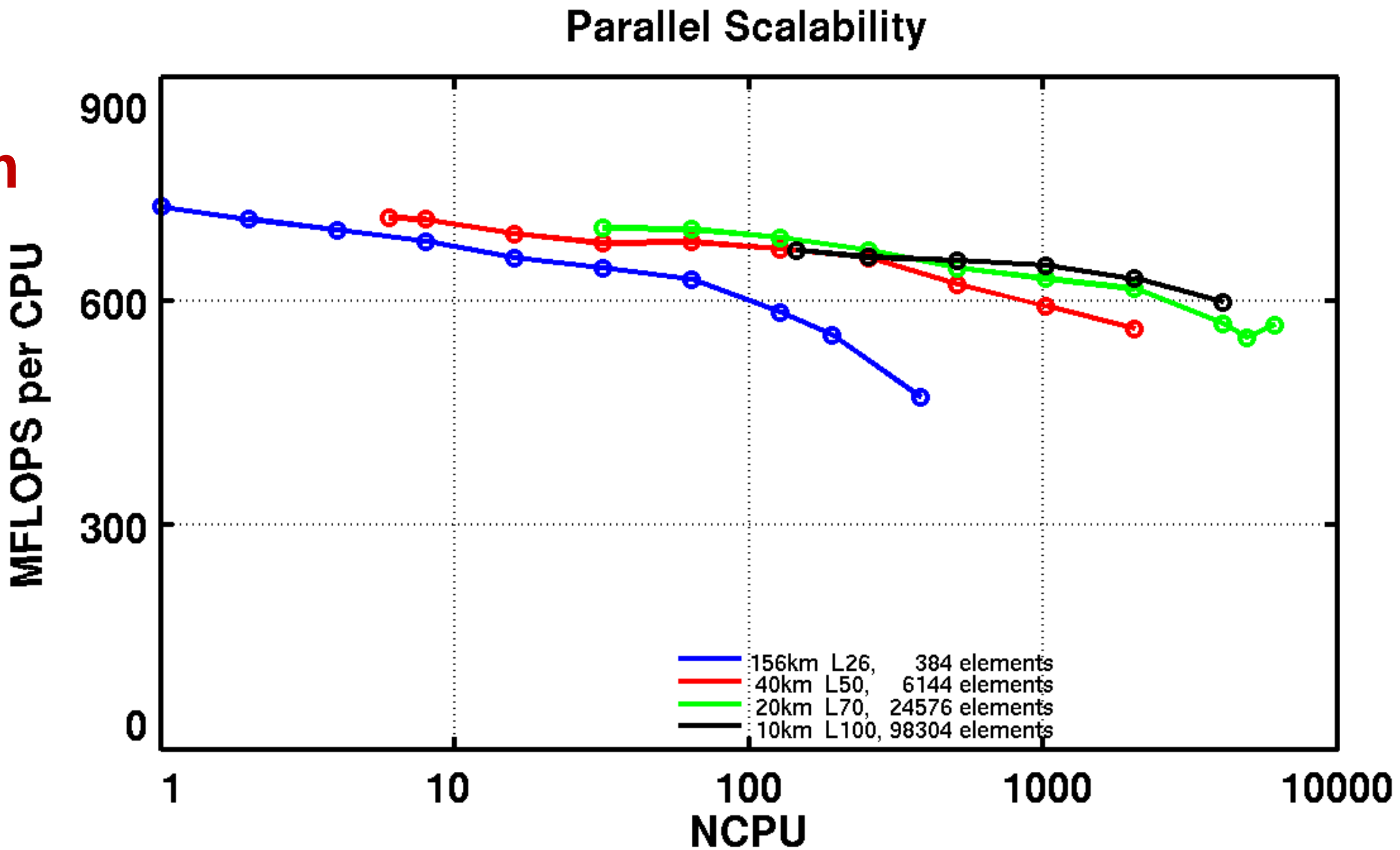
How Well Does SEAM Scale?



Red Storm



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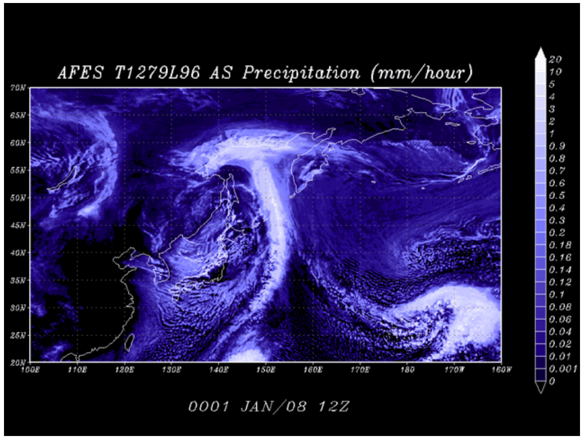
Goal: Compete with Japanese Earth Simulator

- **Atmosphere For Earth Simulator (AFES)**
  - Global spectral model (spherical harmonics: Legendre transforms, all-to-all transpositions)
  - Full physics
  - 10km (24TF) 57 sim days/day



- **Red Storm (SEAM)**
  - Spectral elements: local computations and communications
  - Aquaplanet (reduced physics)
  - 40km (3TF) 7-30 sim years/day
  - 10km (5TF) 32-128 sim days/day

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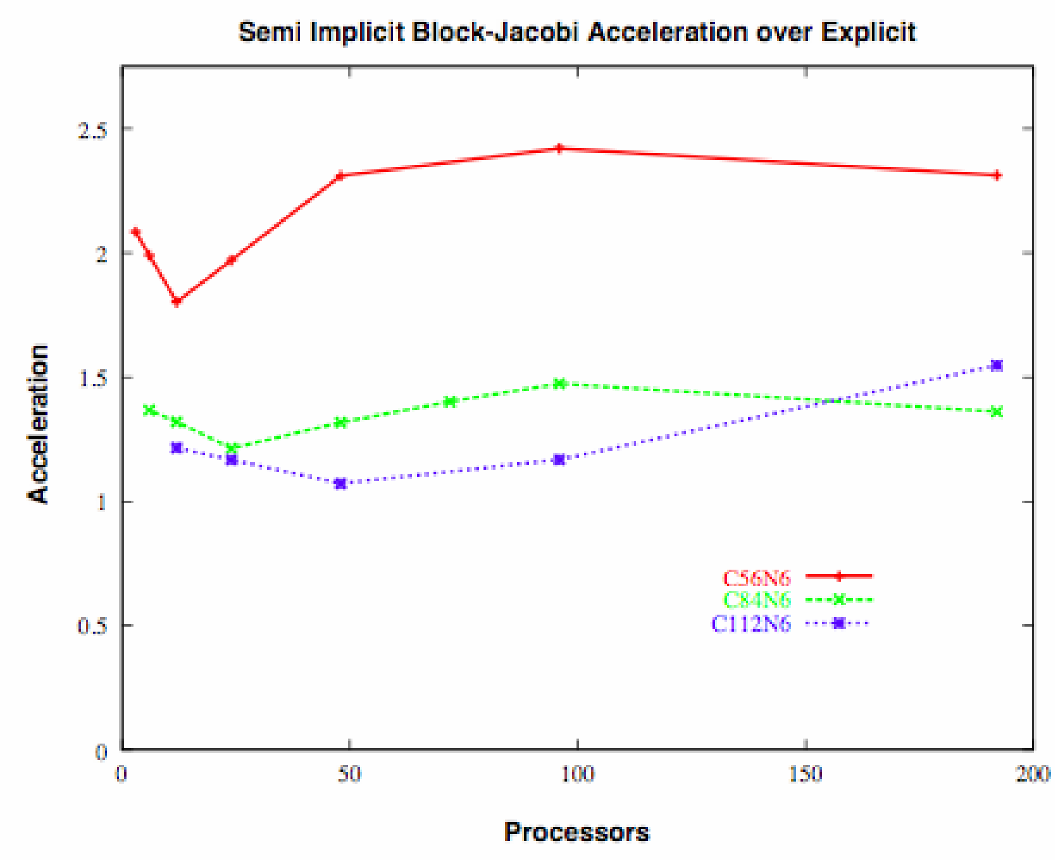
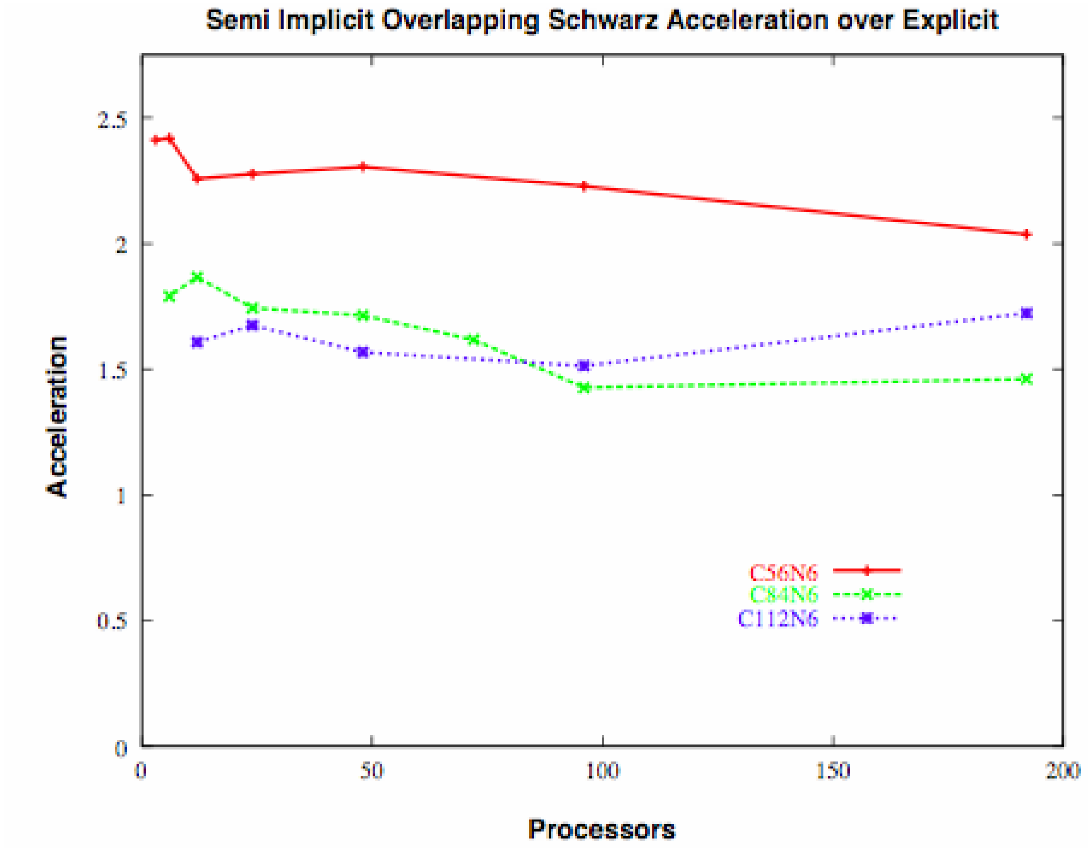
Why the Range of Integration Rates?

- Explicit vs. Semi-implicit time stepping
- Explicit (lower bound):
  - Small Δt for stability
  - Efficient numerical kernel
- Semi-implicit (upper bound…):
  - Larger Δt for stability (~x8)
  - Helmholtz solve: communication required every iteration
  - How many iterations?
- Dual use research question: what is the best algebraic preconditioner for spectral elements?
- Related question: what is the best integration rate we can obtain?

Block Jacobi



Overlapping Schwarz



Current Semi-Implicit Scheme

- 3D primitive equations
- Hydrostatic assumption
- Loosely coupled “stack” of shallow water equations
- Eigenmode decomposition in vertical direction (split semi-implicit)
  - For L levels, this is an L x L eigensystem
  - Results in L independent 2D systems to solve
  - Most energy & linear system solver work occurs in lowest eigenmodes
  - Decomposition is pre-processing step
  - Transforms: physical space ⇔ eigenspace
  - Quantity of interest: post-spinup average iterations for each eigenmode (function of resolution)

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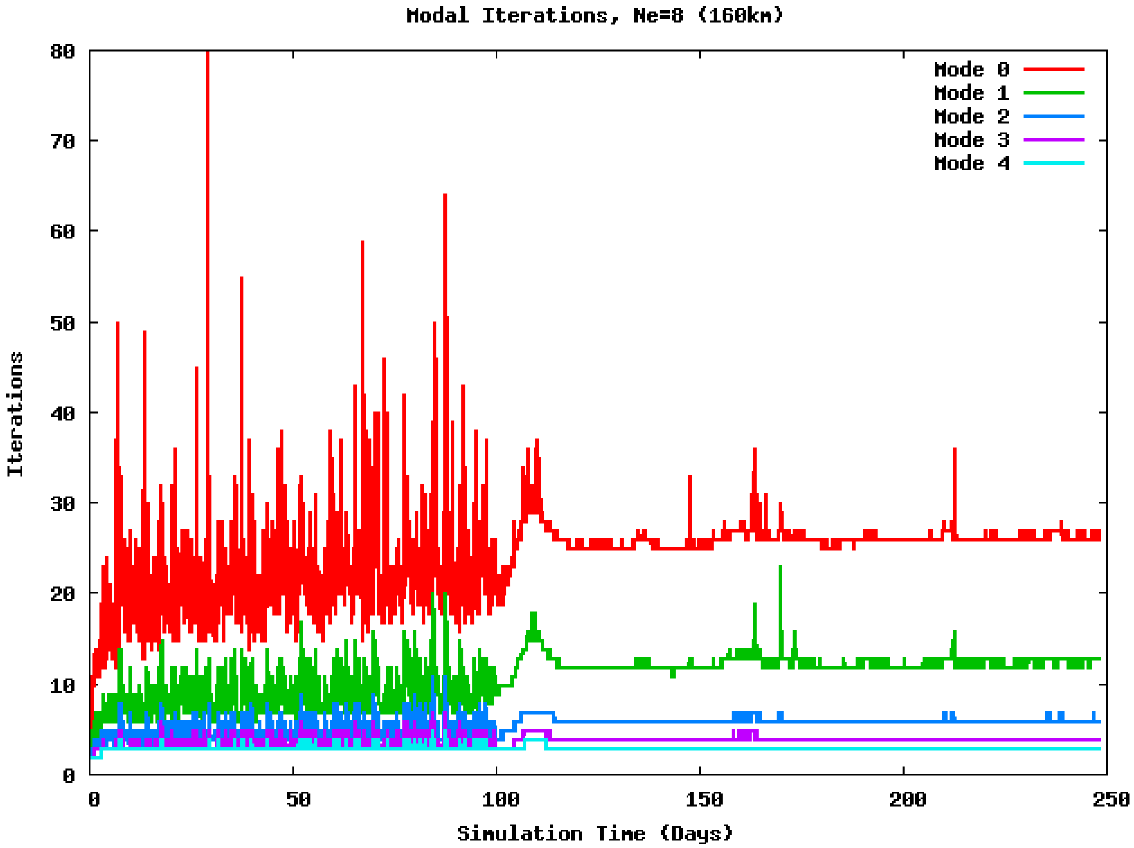
SEAM Split Semi-Implicit Iterations



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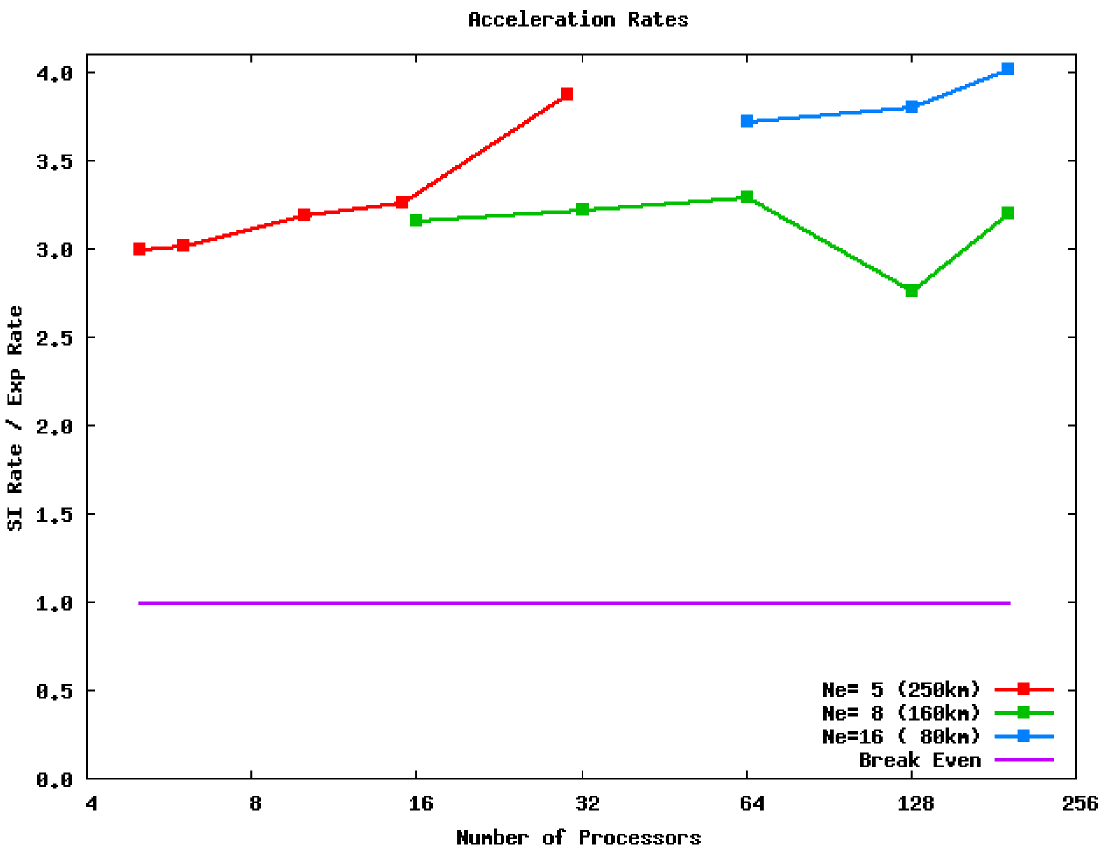
SEAM Split Semi-Implicit Acceleration



Issues

- Some fail-to-converges seen
- Unexplained iteration profiles
- Overlapping Schwarz implementation
- Higher resolutions
- Higher processor counts

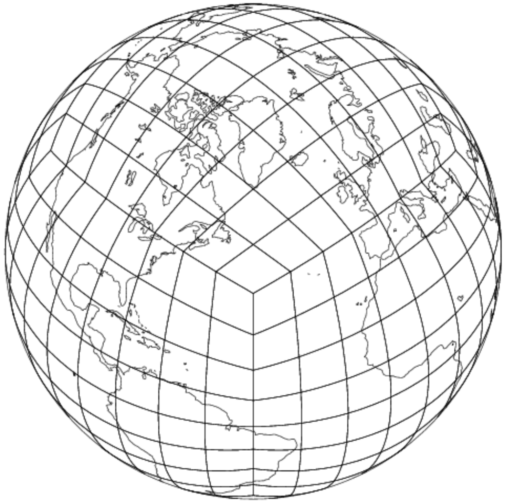
Using Trilinos to Study Preconditioners

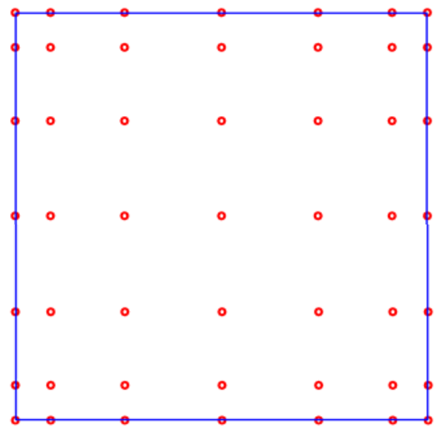
- SEAM is written in FORTRAN 90
- Trilinos is written in C++
- Interfacing F77 and C is a pain . . . interfacing F90 and C++ is excruciating
- Possible solutions:
  - SIDL/Babel
  - Python (using swig and f2py)
    - Python is an “off-line” solution
    - Winning preconditioner must be re-coded for SEAM
    - Advantages…

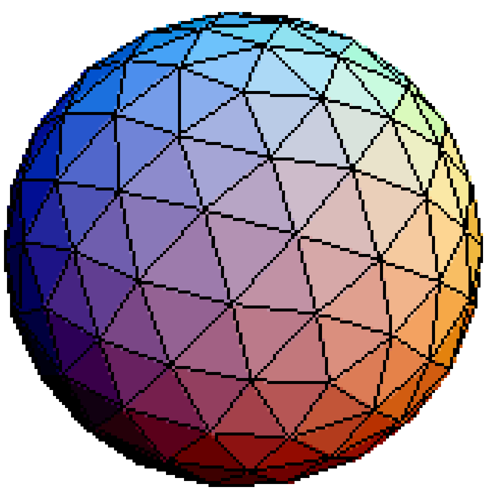
Spin-off Enabling Technology: PyTrilinos

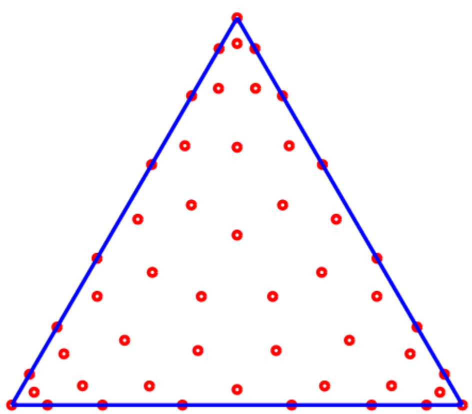
- **Python interface to selected Trilinos packages:**
  - **Epetra, EpetraExt, NOX (with Alfred Lorber)**
- **Mike Heroux has been very supportive**
- **In addition to "gluing," it facilitates rapid prototyping, enhances testing capabilities, and expands Trilinos user base**
- **Recruited Trilinos developers to wrap packages:**
  - **Eric Phipps: NOX, LOCA; Marzio Sala: AztecOO, IFPACK, ML, Amesos, TriUtils; Heidi Thornquist: Anasazi**
- **First appeared in Trilinos Release 5.0 with 3 packages; 10 packages in Trilinos Release 6.0**
- **Presentation at 2005 Scientific Python Conference at Cal Tech**
- **Sala, Spotz, Heroux, "PyTrilinos: High-Performance Distributed-Memory Solvers for Python," submitted to *ACM TOMS*.**

Spectral Elements in Triangles









- **Quadrilateral spectral elements**
  - **Choice of tensor-product Gauss-Lobatto points for nodal basis and quadrature leads to diagonal mass matrix and excellent interpolation properties**
- **Triangular spectral elements**
  - **Choice of nodal grid points is much more complicated . . . hard to get good interpolation and quadrature simultaneously**
- **Taylor: perform numerical optimization to look for suitable points**
- Taylor, Wingate, Bos, "A New Cardinal Function Algorithm for Computing Multivariate Quadrature Points," accepted by *SIAM J. Numer. Anal.*

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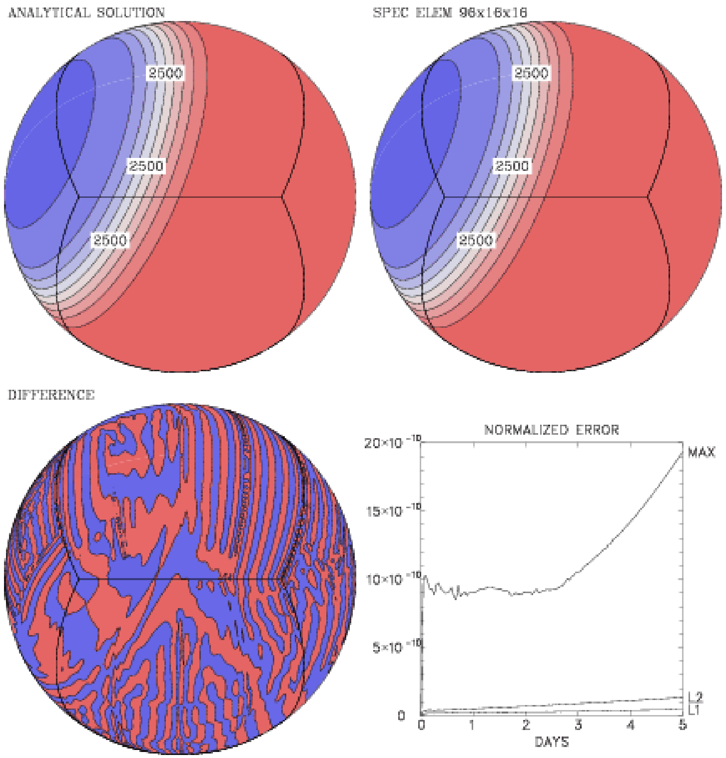
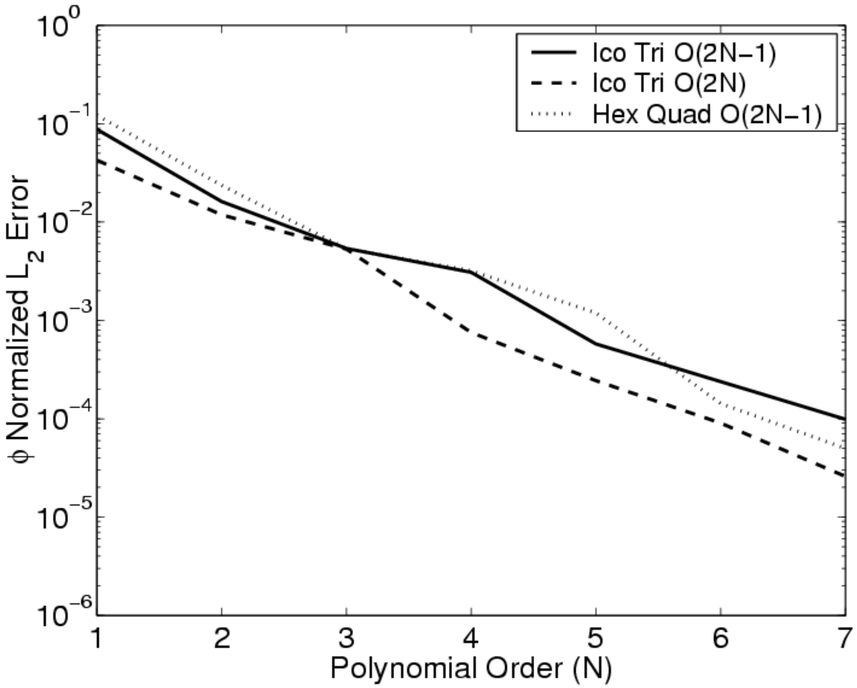
Triangular Spectral Element Results





Giraldo, Warburton, Taylor, "A Triangle-Based Spectral Element Method with Diagonal Mass Matrix," invited paper in preparation for *J. Eng. Mech.* special issue on spectral interpolation and applications.

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Programmatics

- Sandia climate mission: "depth" and "breadth"
- Successful funding acquisitions
  - LDRD (SEAM - Spotz)
  - LDRD (Conflict Modeling - Boslough)
  - ASC (High-performance ocean modeling)
  - CSRF (Red Storm Demonstration run)
- Other attempts
  - MICS (Multiscale climate - w/Los Alamos)
  - LDRD (Infrasound - Taylor)
  - CCPP (Advancements to SEAM - Spotz, Taylor)
  - NASA (Superparameterization - Debenedictis)
- Pending opportunities
  - Strategic Adaptation to Climate Change (Backus)
  - SciDAC (SEAM, Parameterizations - Spotz, Taylor)

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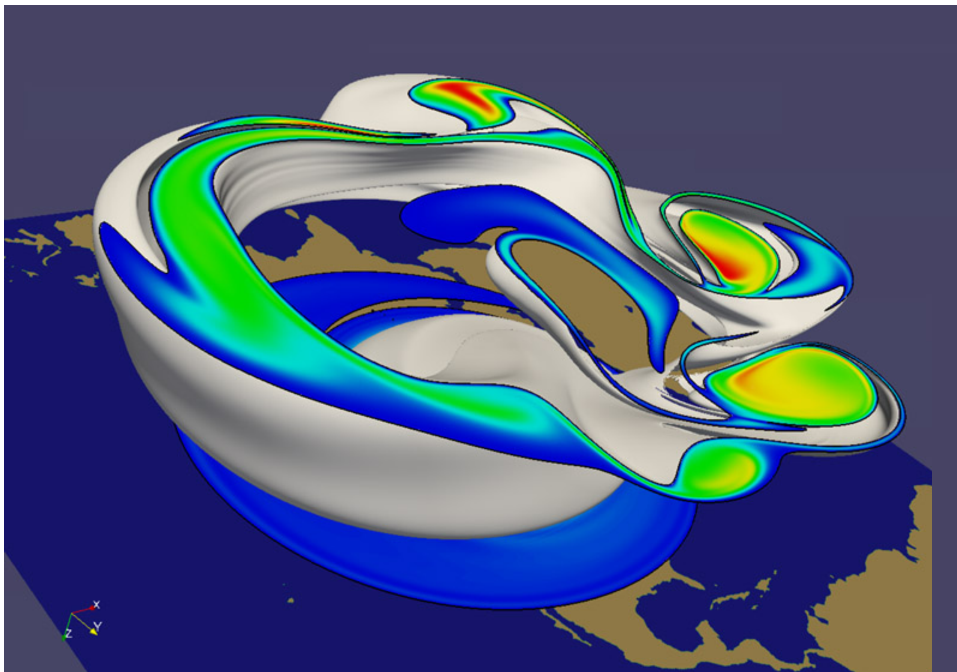
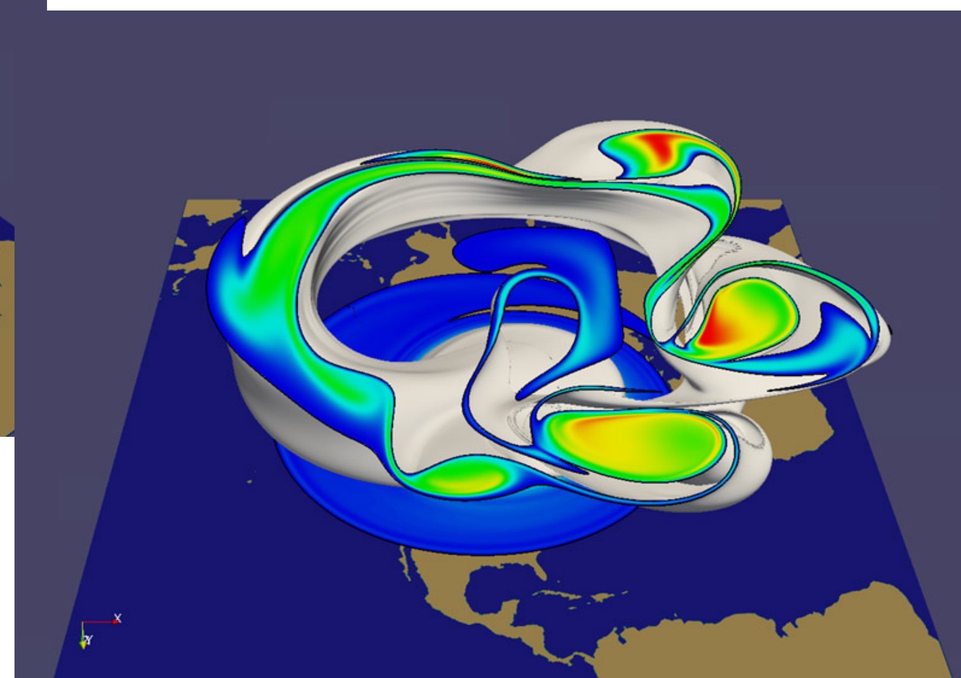
Red Storm Demonstration Run

- Polar vortex problem: Strong circumpolar jet that traps air over the poles
- Numerical Statistics
  - 13km grid spacing, 300 levels in the vertical (1 billion grid points)
  - Integrated for 288,000 time steps using 7200 CPUs for 36 hours
  - Produced 1TB of data

Red Storm Demonstration Run



Isosurface and contours of potential vorticity over north pole



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