Spectral Elements

CSRF FY05 Completing Projects Review

October 18, 2:30pm

PI: Bill Spotz, 1433
PM: Jennifer Nelson, 1430

Mark Taylor, Mark Boslough
1433

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.
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
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
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?

BlueGene/L

Parallel Scalability

MFLOPS per CPU

1
16
256
4096
64K

How Well Does SEAM Scale?

Parallel Scalability

Red Storm

MFLOPS per CPU

NCPU

- 156km L26, 384 elements
- 40km L50, 6144 elements
- 20km L70, 24576 elements
- 10km L100, 98304 elements
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
Why the Range of Integration Rates?

- Explicit vs. Semi-implicit time stepping
- Explicit (lower bound):
  - Small $\Delta t$ for stability
  - Efficient numerical kernel
- Semi-implicit (upper bound...):
  - Larger $\Delta t$ 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

Semi Implicit Block-Jacobi Acceleration over Explicit

Acceleration vs. Processors

- C56N6
- C84N6
- C112N6
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 \( L \times L \) 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)
SEAM Split Semi-Implicit Iterations

Modal Iterations, N_e=8 (180km)

Simulation Time (Days)

Iterations

Mode 0
Mode 1
Mode 2
Mode 3
Mode 4
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

Triangular Spectral Element Results

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)
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