Computational Mathematics at the Oak Ridge National Laboratory

Presented by

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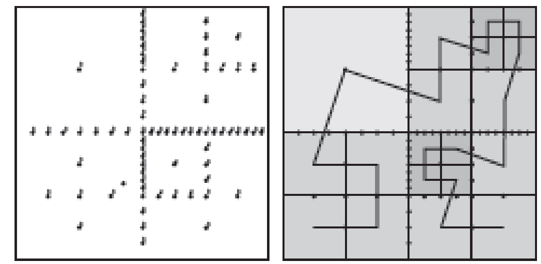
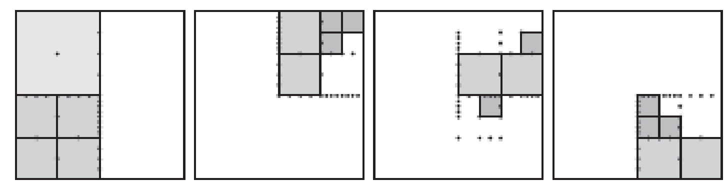
Extending adaptive sparse grids for stochastic collocation to hybrid architectures

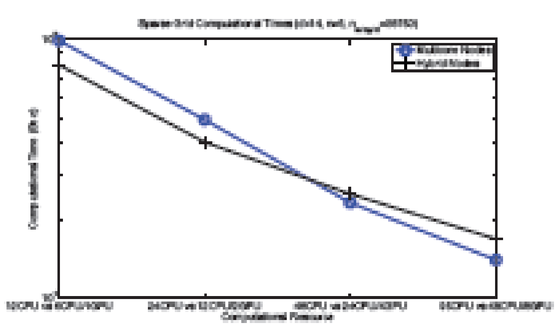
- Motivation
- Very large scale uncertainty quantification (UQ) of realistic problems require 'curse of dimensionality' limiting methods, such as sparse grids, and scalable UQ methods, such as stochastic collocation.
- Growing high-performance computing to the exascale will require high flop/watt computing devices, and next generation architectures are adopting these devices in hybrid CPU/GPU systems.



2D unbounded adapted sparse grid using five subspace levels. Left: each point indexed with subspace level used. Right: domains of the respective highest level and a generalized SFC used for decomposition.



Domain decomposition of above adaptive sparse grid to four nodes and/or thread blocks based on a generalized SFC.

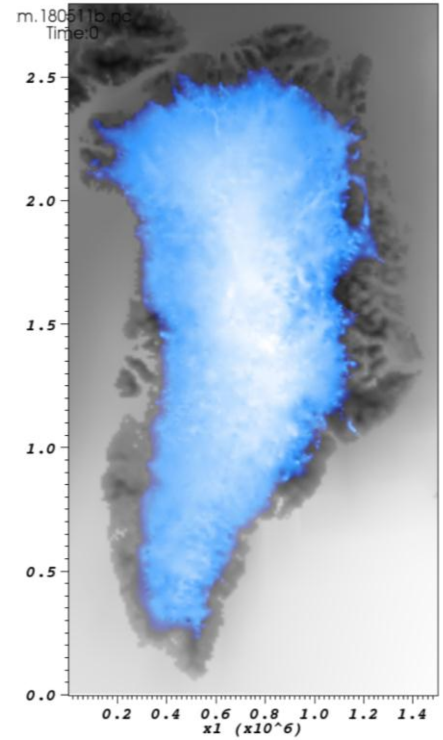


Strong scaling of sparse grid construction on the hybrid test cluster. MPI only vs. hybrid MPI/CUDA parallelization.

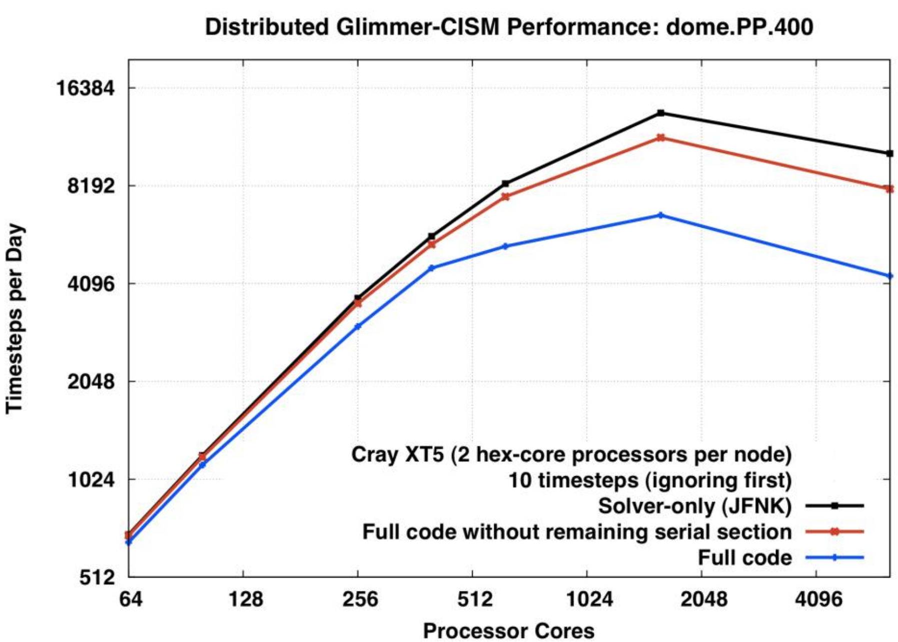
Results

- Built an adaptive sparse grid library for stochastic collocation
- Extended this library so that parallel sparse grids can be scalable on small hybrid test clusters.

Recent Progress to develop a scalable, efficient, and accurate Community Ice Sheet Model



- Newton-Krylov (JFNK) method is now used to solve higher-order velocity model
- For equivalent test cases evaluated, JFNK is ~2-3.5 times faster than Picard for a given # processors
- Existing Picard solver in CISM is reused as a physics based preconditioner
- Lemieux et al. (2011) J. Comp. Phys. 230:6531-6545



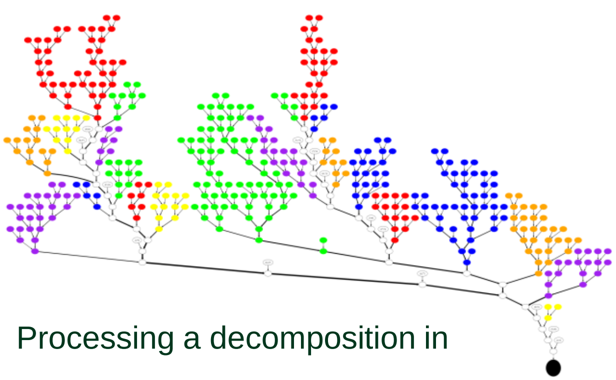
JFNK solver scaling/performance

- Scales to 1600 processors for 1.6M grid point problem
- Parallel velocity solve implemented in version 2.0, now in CESM repo
- Next steps: scalable preconditioner, i/o, CFL limited thickness advection
- Evans et al (2011) Int. J. High Perf. App. (submitted)

Scalable Graph Decompositions & Algorithms to Support the Analysis of Petascale Data

Objectives

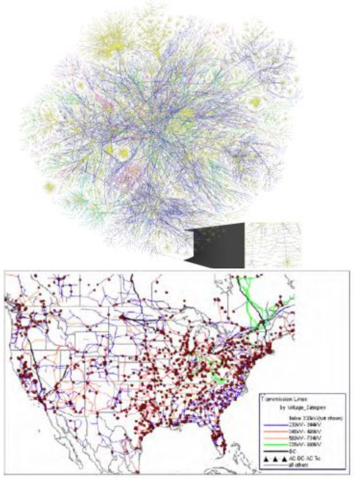
- Demonstrate viability of graph decomposition-based algorithms for large combinatorial optimization problems
- Exploit parallelism to enable dynamic programming (DP) speed-up
- Provide computational evidence that exponential worst-case running times predicted in theory are not realized in practice



Processing a decomposition in parallel using subtrees

Impact

- Provide computationally efficient alternative method for solving discrete optimization problems
- Enable optimal solutions on graphs with width an order of magnitude larger than previously believed possible
- Crucial new strategies for memory reduction in DP tables



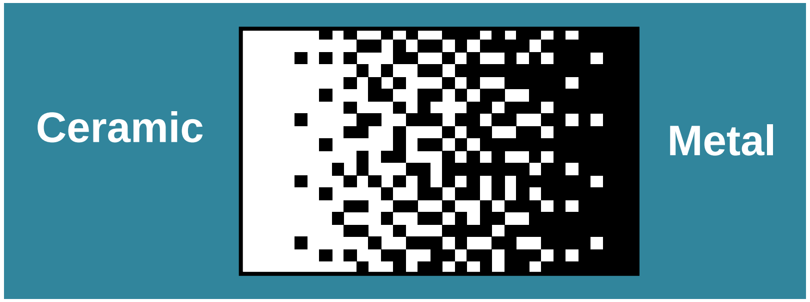
Accomplishments

- Developed efficient software library to generate tree decompositions and provide framework for running TD-based dynamic programming algorithms
- Using maximum weighted independent set as a prototypical dynamic programming application, solved problems on graphs with width > 400
- Fixed parameter tractability-type scaling enables exact solutions on graphs with over a million nodes
- Working parallel implementation using MPI and pthreads

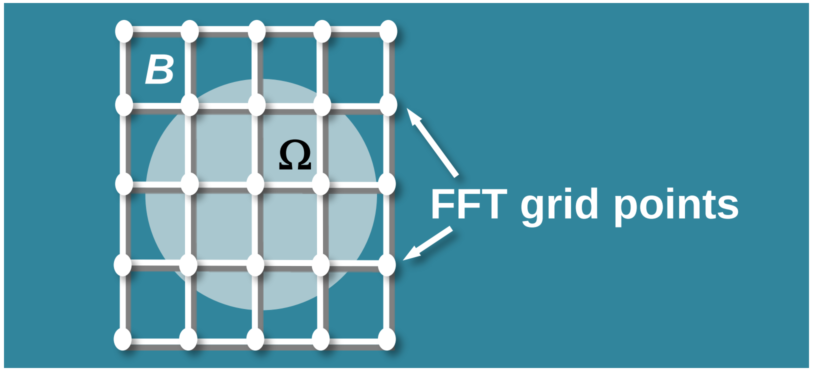
Contacts: Blair Sullivan, Chris Groer and Dinesh Weerapurage

Boundary integral modeling of functionally graded materials (FGMs)

- FGM applications
  - Biomedical
  - Thermal barrier coatings
  - Sensors
- Recent results
  - Derived elasticity Green's Function for 2- and 3-dimensional (2D and 3D) exponentially graded materials
  - Implemented in Galerkin and collocation boundary integral codes in 3 dimensions
- Fast solution of boundary integral equations
  - General framework using pre-corrected Fast Fourier Transform
  - Treatment of singular and hyper-singular equations
  - Applications in modeling electrospray process, crack propagation, and fiber composite materials

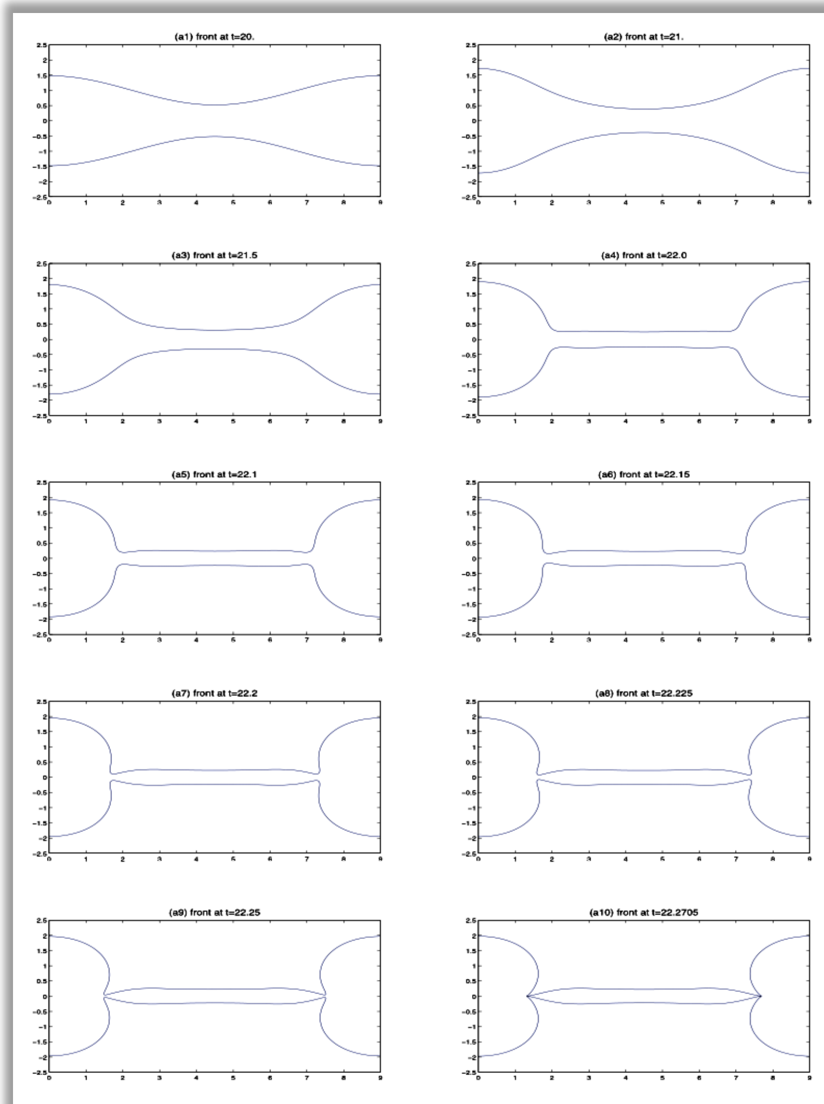


K. S. Ravichandran, *Materials Science and Engineering* **A201 (1995)** 269–276



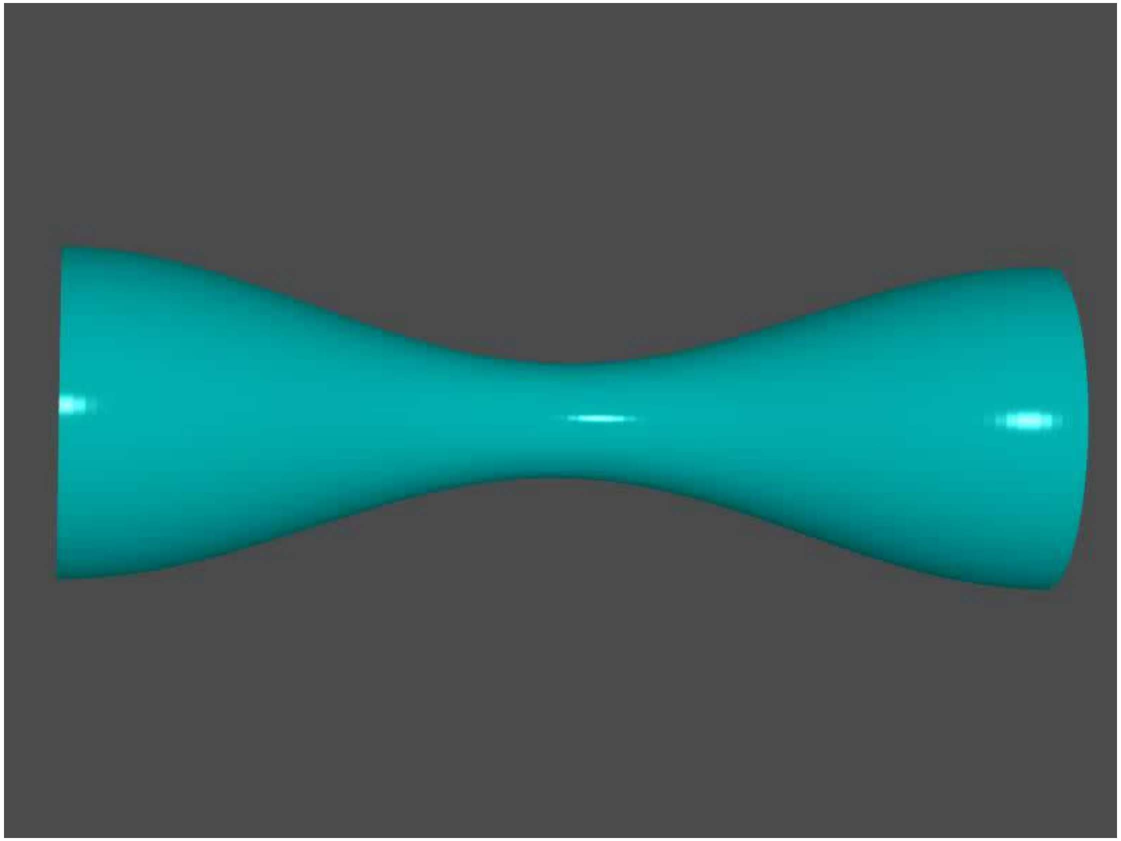
Numerical simulation of the Rayleigh-Taylor instability

- Combined level set and boundary integral methods to model the motion and eventual pinch-off of an inviscid fluid column
- Advanced level set methods are employed to propagate the free surface, and topological changes
- The simulation results at and after pinch-off are in excellent agreement with theoretical scaling laws

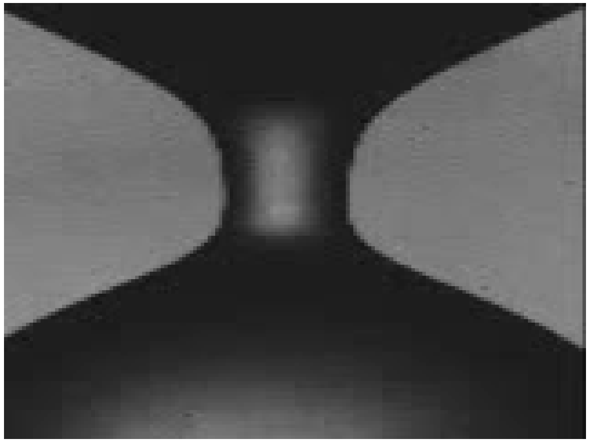


Time snapshots of the fluid column approaching pinch-off at time $t = t_p$

Numerical simulation of the Rayleigh-Taylor instability



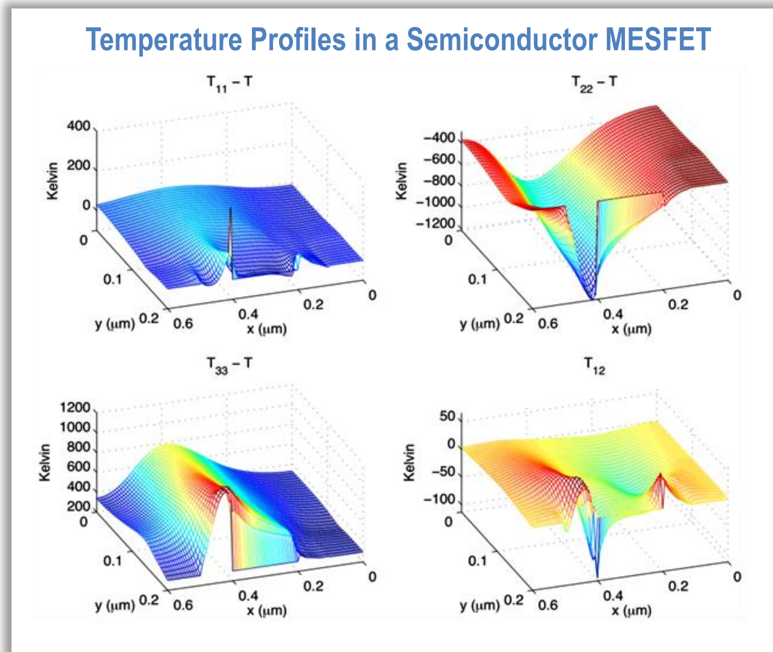
Video from simulation of pinch-off

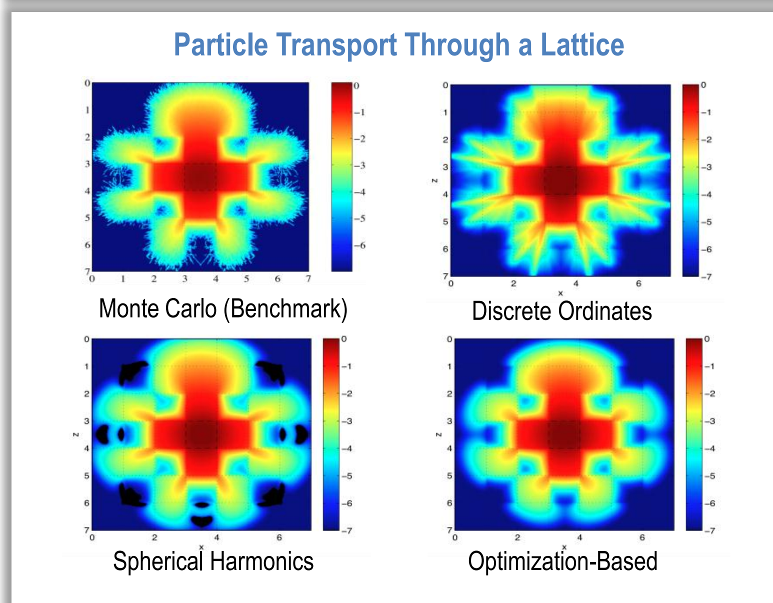


Video from experiment showing pinch-off

Optimization-based closures for kinetic equations

- Objective: Reduce the microscopic, kinetic description of complex many-particle systems while maintaining an accurate description of the macroscopic dynamics
- Approach
  - Approximate unresolved, microscopic dynamics via the solution of a physically motivated, convex optimization problem
  - Incorporate optimization-based approximations into partial differential equation (PDE) solvers
  - Invest in parallel implementations that take advantage of the spatially local structure
- Applications
  - Gas dynamics
  - Collisional plasmas
  - Electron transport in semiconductors
  - Neutrino transport in astrophysics
  - Photon transport in inertial confinement fusion

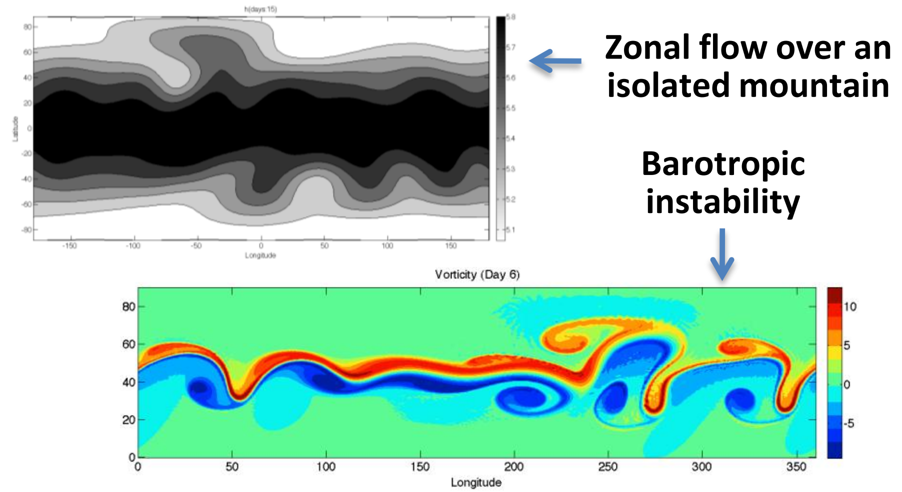




Time acceleration methods for shallow water equation on the cubed sphere

Time acceleration motivation

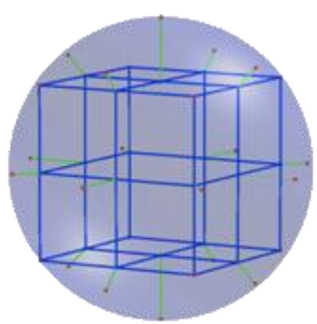
- Without it, climate simulation will hit the time-step barrier
- Dramatically improve accuracy of highly coupled models
- Dramatically accelerate spin-up of new simulations
- Potentially revolutionize climate simulation and other application areas with long time integration



Multiwavelet discontinuous Galerkin method with four levels, polynomial order k=3, and time-step 16X accelerated over the RKDG method (time step is 22.5 min)

Multiwavelet discontinuous Galerkin (DG)

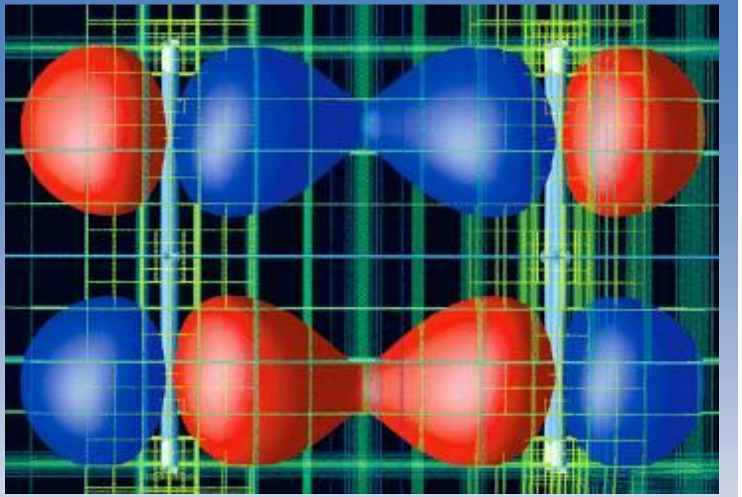
- Adaptive DG hierarchical structure that improves computational speed through error truncation and fast pre-conditioner estimation
- Direct methods for hp-adaptivity
- Enhanced time integration
- Scalable on cubed-sphere geometry



Cubed-sphere geometry, in which the singularity problems at the pole are avoided by transforming and computing the dynamics to the six sides of the cube

MADNESS: multiresolution analysis for integro-differential equations and Ψ-PDE

- Developed 3D multiwavelet, low separation rank approximation, and high-order panel singular value approximations for static and time-dependent Schrodinger's equation (Hartree-Fock and density functional theory) in chemistry and nuclear physics
- Approximated d-D functions and operators using discontinuous basis with compact support and dictionaries that scales as log(d). Developing fast O(N) real analysis-based algorithms to approximate functions and operators to arbitrary but finite precision
- Computed some of the most accurate energies and energy levels for small molecules to date
- Obtained positive initial results for 6D, 2-body Schrodinger's equations
- Scales to thousands of cores on Cray and IBM BG/L



A molecular orbital of the benzene dimer computed using the multiresolution solver MADNESS in a multiwavelet basis and low separation rank approximation. Note the adaptive refinement, which automatically adjusts to guarantee precision

Fully implicit extended magneto-hydrodynamic (MHD) algorithms

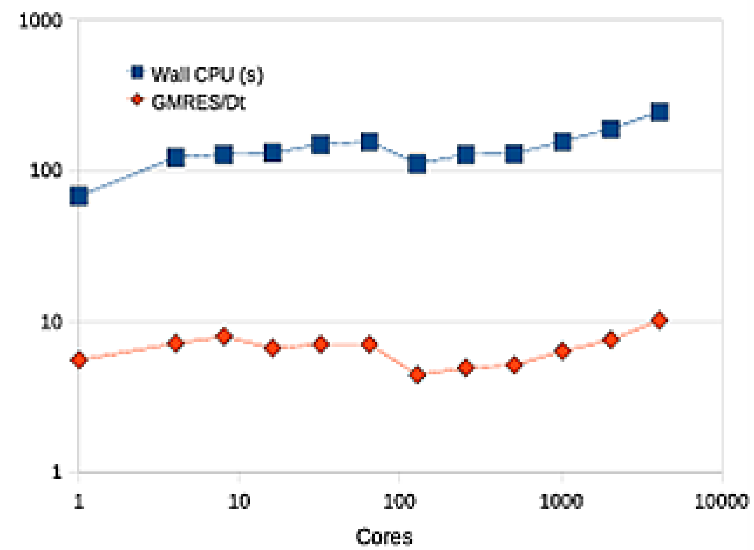
L. Chacon, ORNL

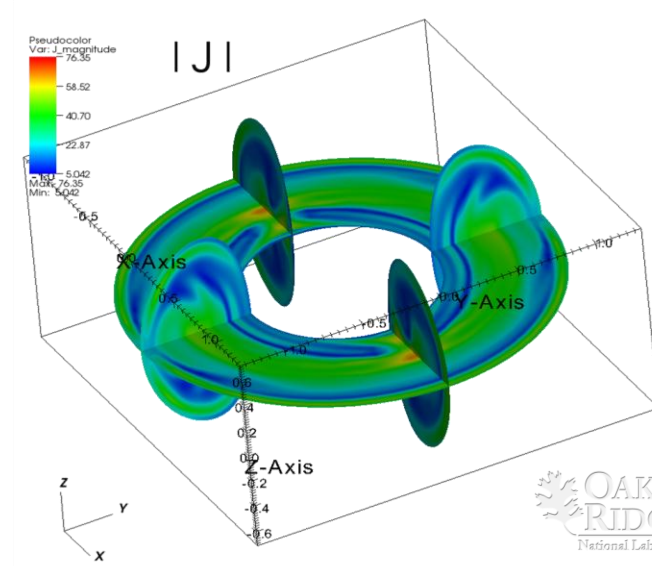
- **Relevance:** first-of-its-kind fully implicit scalable MHD code, based on Newton-Krylov solver technology
- **Applications:** fusion, astrophysics, magnetospheric physics
- **Features:**
  - Algorithmically scalable. Key: physics-based preconditioning
  - Massively parallel, excellent parallel scaling
- **Publications:**

L. Chacón, “Scalable solvers for 3D magnetohydrodynamics,” *J. Physics: Conf. Series* **125,** 012041 (2008)

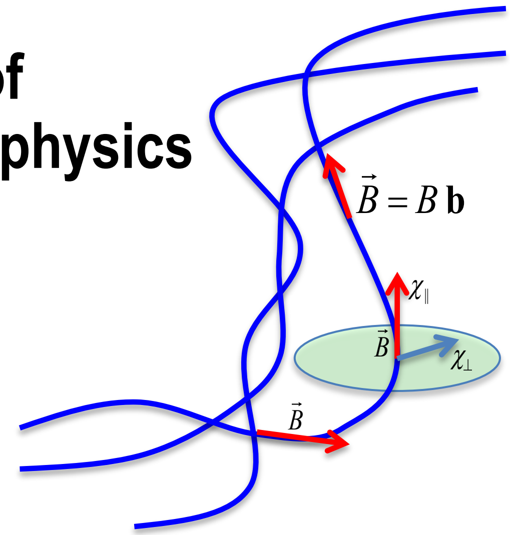
L. Chacón, “An optimal, parallel, fully implicit Newton-Krylov solver for three-dimensional visco-resistive magnetohydrodynamics,” *Phys. Plasmas* **15,** 056103 (2008)

L. Chacón, "A non-staggered, conservative, solenoidal, finite-volume scheme for 3D implicit extended magnetohydrodynamics in curvilinear geometries," *Comput. Phys. Comm.* **163 (3),** 143-171 (2004)





A novel method to compute heat transport in plasmas with general magnetic fields



- Transport in magnetized plasmas is a problem of fundamental interest to control fusion and astrophysics

$$\partial_t T - \nabla \cdot \left[\chi_\parallel \mathbf{b}\mathbf{b} \cdot \nabla T + \chi_\perp \left(\mathbf{I} - \mathbf{b}\mathbf{b}\right) \cdot \nabla T\right] = S$$

- This is a very challenging problem because
  - Extreme anisotropy, in fusion plasmas
  - Magnetic field line chaos $\chi_\parallel / \chi_\perp \sim 10^{10}$
  - Nonlocal (free streaming) transport

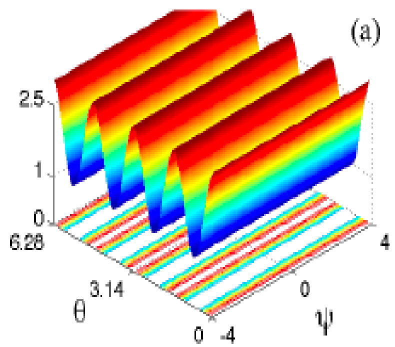
$$\mathbf{q} = \chi_\parallel \int \frac{T(s+z) - T(s-z)}{z^\alpha} dz$$

- We have proposed a novel method to solve this problem in the case $\chi_\perp = 0$ for local and nonlocal transport in general magnetic fields
- By construction the method preserves transport barriers, is positive definite and algorithmically scalable and parallel

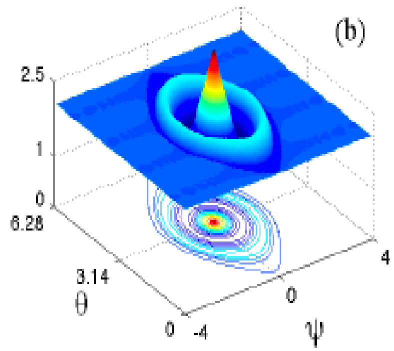
D. del-Castillo-Negrete and L. Chacon, submitted to *Phys. Rev. Letters* (2010).

Applications of the method

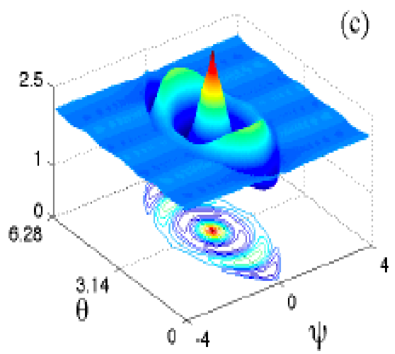
Temperature Flattening in Magnetic Islands



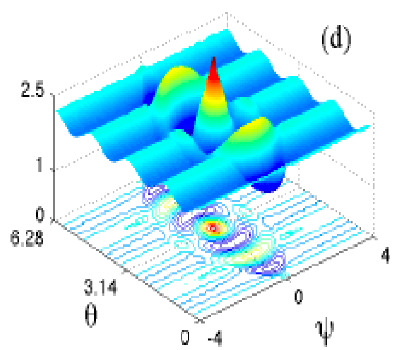
Initial Condition



Final State



Local

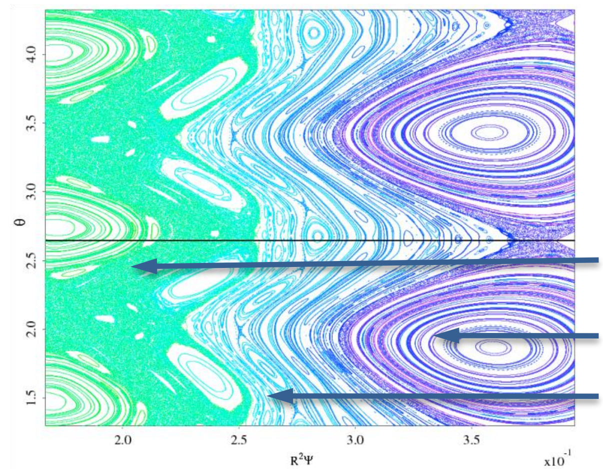


Nonlocal

Contact: Diego del-Castillo-Negrete, 865-574-1127, delcastillod@ornl.gov
Luis Chacon, 865-574-1309, chaconl@ornl.gov
Funding sources: DOE Office of Fusion Energy, and OASCR
Resources: ORNL Fusion Energy Division

Fractal Temperature Profiles in Chaotic Fields

Poincare Plot of a Chaotic Magnetic Field



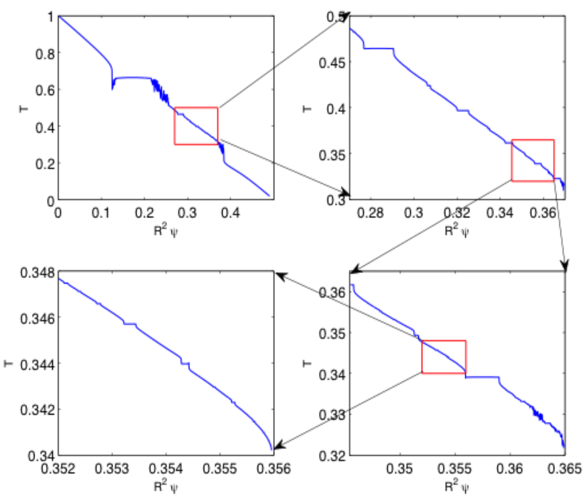
In the presence of perturbations, the magnetic field topology in confined fusion plasmas exhibits a fractal mixture of:

Chaotic orbits

Islands

Barriers

Fractal Radial Temperature Profile



Numerical solution of the parallel transport problem in the chaotic magnetic field above

The clockwise successive zooms reveal a fractal radial staircase dependence caused by the fractal structure of the magnetic field topology

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