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


Ceramic
Metal

FFT grid points

B
Ω
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 experiment showing pinch-off

Video from simulation of 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 (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

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)

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 $\Psi$-PDE

- Developed 3D multiwavelet, low separation rank approximation, and high-order panel singular value approximations for static and time-dependent Schrödinger’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 Schrödinger’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.
Scalable graph decomposition

- Tree and branch decompositions provide a framework for dynamic programming solutions to NP-hard problems on graphs
- Offer the potential for new data parallel algorithms on large graphs
- Current progress is serial C++ code for generating tree and branch decompositions and running dynamic programming
- Future work will focus on parallelization, applications in computational biology and operations research

- A branch decomposition (left) of the graph (above) where dynamic programming can be run on different colored sub-trees in parallel
- The dynamic programming at a node requires access to only a small part of the original graph and information about the child nodes
Fully implicit extended magnetohydrodynamic (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**:
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

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

- 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

- 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

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

- Chaotic orbits
- Islands
- Barriers

Numerical solution of the parallel transport problem in the chaotic magnetic field above reveals a fractal radial staircase dependence caused by the fractal structure of the magnetic field topology.

Applications of the method

Temperature Flattening in Magnetic Islands

Fractal Temperature Profiles in Chaotic Fields

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