Computational Mathematics at the Oak Ridge National Laboratory

Presented by

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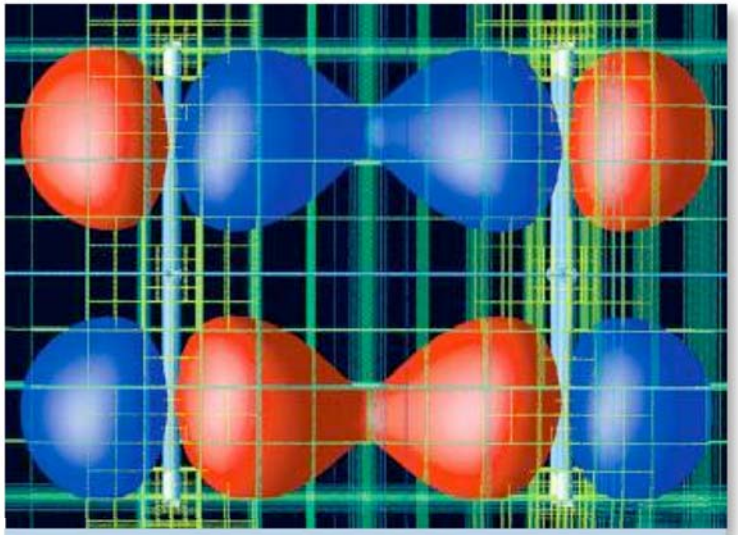
Computational Mathematics
Computer Science and Mathematics Division

SC07

OAK RIDGE National Laboratory

Development of multiresolution analysis for integro-differential equations and Ψ-PDE

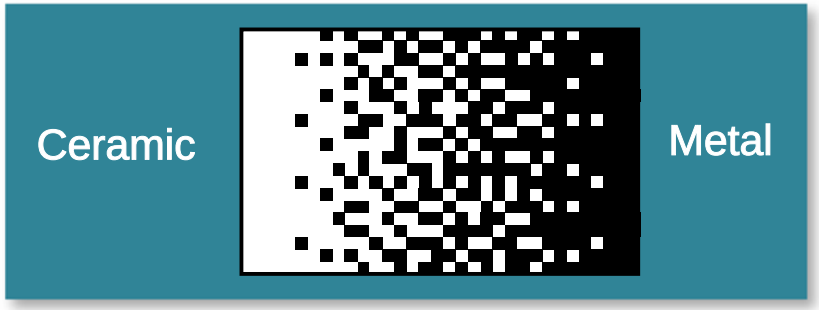
- Developed 3-D multiwavelet, low separation rank approximation, and high-order panel singular value approximations for Schrodinger's equation (Hartree-Fock and density functional theory).
- Approximated n-D functions and operators using compact basis and dictionaries. Developing real analysis-based 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 6-D, 2-body Schrodinger's equations.



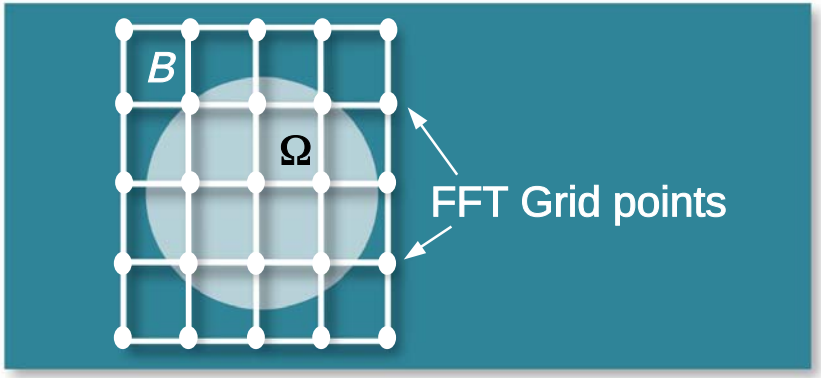
A molecular orbital of the benzene dimer computed using the multiresolution solver MADNESS in a multiwavelet basis and low separation rank approximation. Note the adaptive refinement, which automatically adjusts to guarantee precision.

Boundary integral modeling of functionally graded materials (FGMs)

- FGM applications
  - Biomedical
  - Thermal barrier coatings
  - Sensors
- Recent results
  - Derived elasticity Green's Function for 2-D and 3-D exponentially graded materials
  - Implemented in Galerkin and collocation boundary integral codes in 3-D
- 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

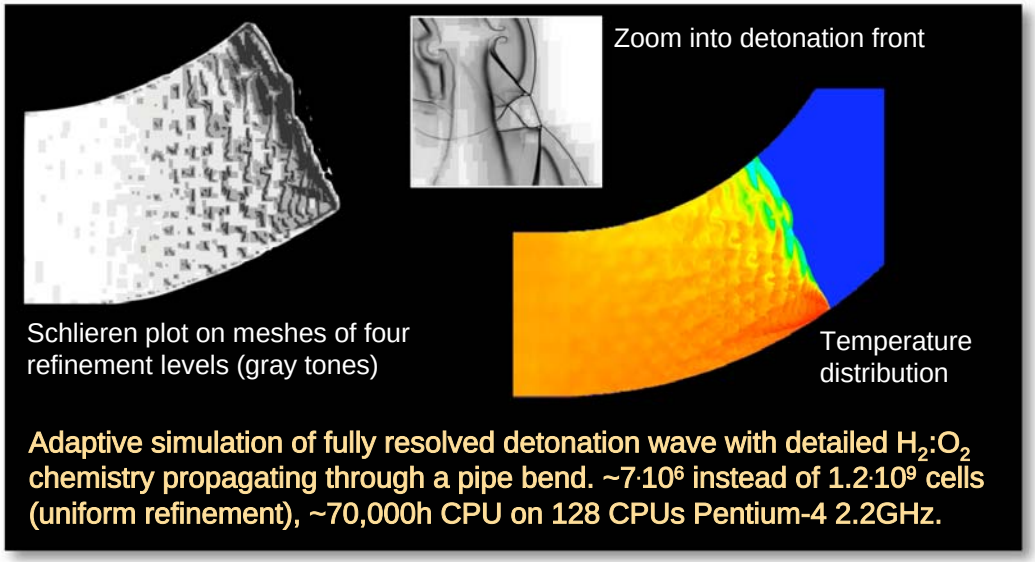


K. S. Ravichandran, Materials Science and Engineering A201 (1995) 269-276

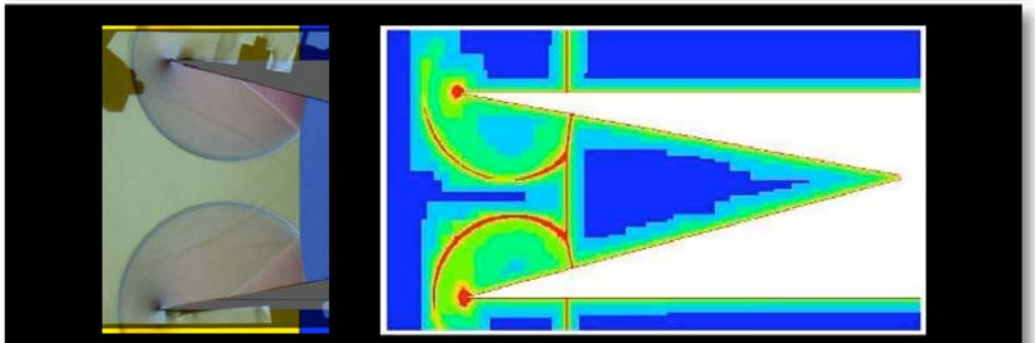


Large-scale parallel Cartesian structured adaptive mesh refinement

- High-resolution simulation of detonation and shock wave phenomena with second-order finite volume schemes
- Cartesian method with dynamically adaptive structured mesh refinement and complex boundary embedding via an implicit geometry representation approach
- Rigorous domain decomposition parallelization with automatic re-balancing based on generalized space-filling curves



Adaptive simulation of fully resolved detonation wave with detailed H_2:O_2 chemistry propagating through a pipe bend. ~$7 \cdot 10^6$ instead of $1.2 \cdot 10^9$ cells (uniform refinement), ~70,000h CPU on 128 CPUs Pentium-4 2.2GHz.



Mach 1.51 shock wave with two von Neumann triple points traveling into a converging wedge. Left: density contours overlaying schlieren photo (experiment by C. Bond, Caltech); right: simulation with four additional levels by D. Hill (Caltech).

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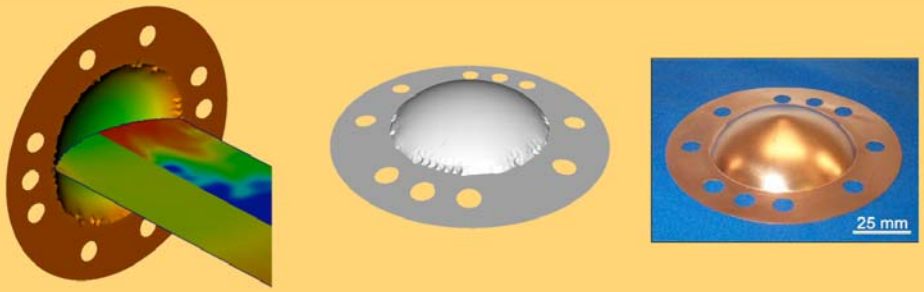
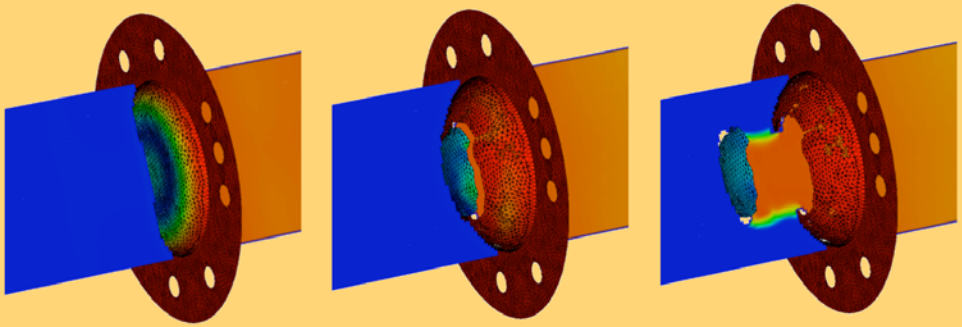
Fluid-structure interaction simulation of trans- and supersonic wave impact

- Partitioned approach for loosely coupled fluid-structure interaction simulation between shock-capturing Eulerian finite volume solvers and Lagrangian finite element structure mechanics solvers.
- Cartesian computational fluid dynamics methods with dynamically adaptive mesh refinement and on-the-fly embedding of interchangeable coupled solid mechanics solvers. All components parallelized for distributed memory machines.



Viscoplastic plate deformation. Simulation 1.62 ms after piston impact at shocktube end and plate after simulation and experiment.

Piston-induced waterhammer impact on thin copper plates simulated with three-dimensional two-component Riemann solver based on stiffened gas equation of state. Thin-shell finite element solver by F. Cirak (U Cambridge); experiment: V.S. Deshpande (U Cambridge).



Simulation with plate fracture. The fluid density in the mid-plane visualizes the water splash. The solid mesh displays the velocity in direction of the tube axis.

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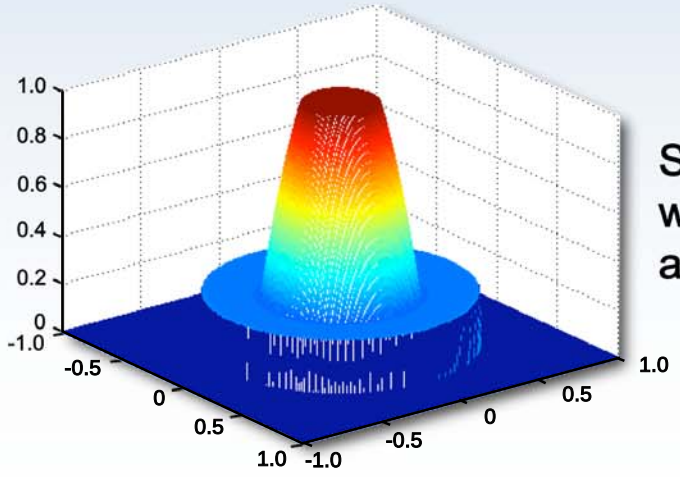
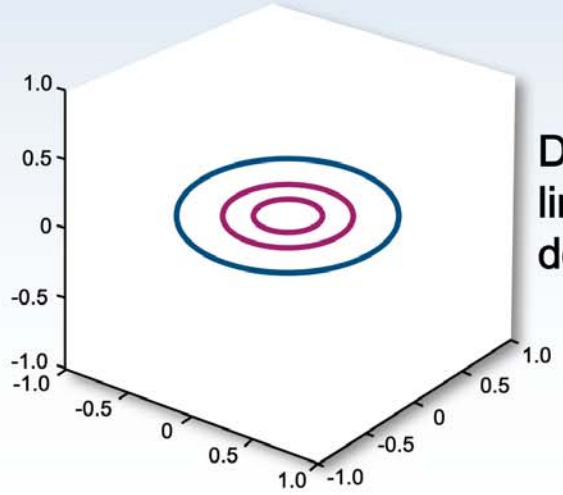
Limiting of discontinuous Galerkin methods for hyperbolic systems

- The discontinuous Galerkin computational strengths are
  - Capacity for complex geometries,
  - Treatment of boundary conditions,
  - High-order accuracy,
  - Adaptable parallel capacity.
- Essential to retaining accuracy in this method is the application of limiting techniques in regions of discontinuities and singularities.

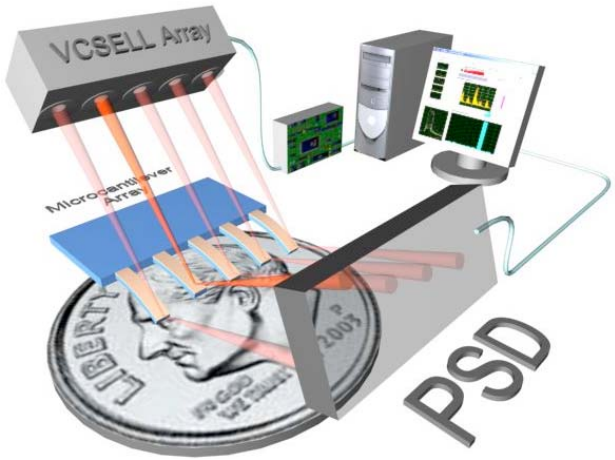


Solution of wave equation at t=1

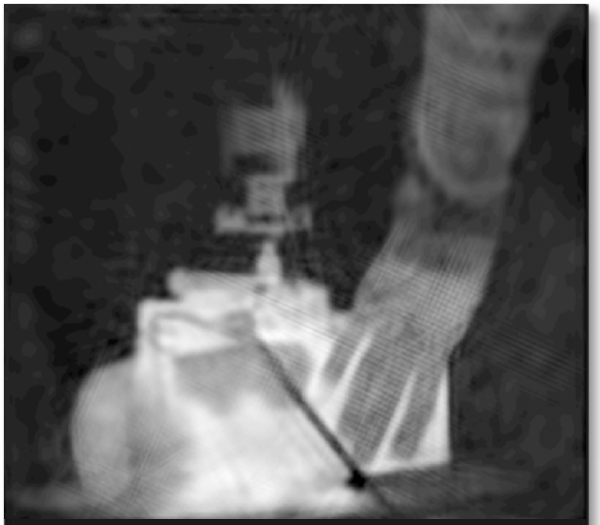


Detected limiting domains

Feature extraction and classification of multidimensional signals

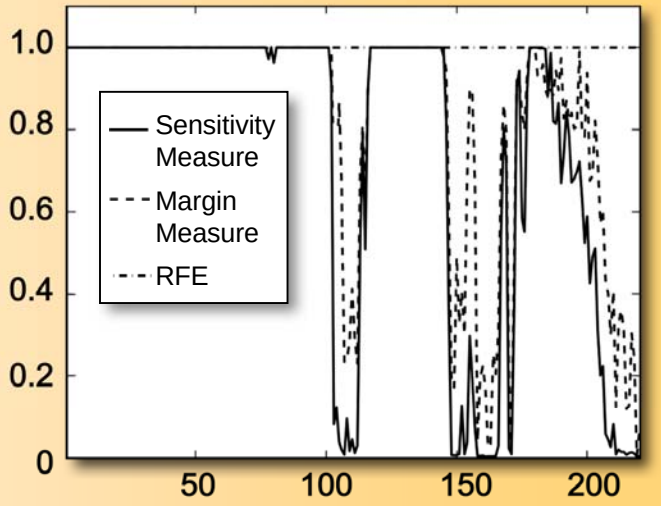


The detection and identification of chemical and biological agents have been significantly augmented by coupling the feature extraction abilities of ICA to functionalized nanomechanical sensor arrays.



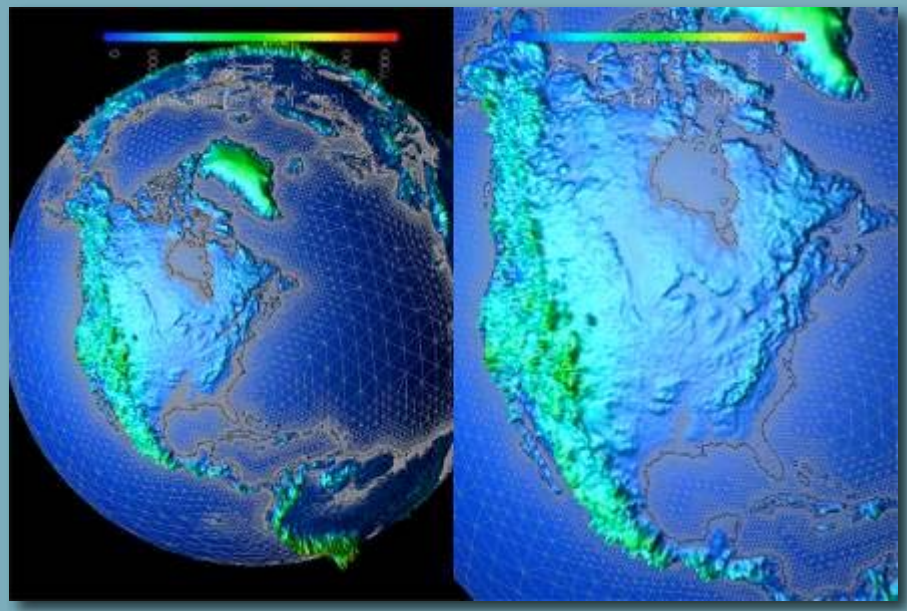
Images obtained with an uncooled MEMS infrared system can be enhanced using a curvelet-based inpainting restoration method.

Data-driven knowledge discovery of important bands in classification of hyperspectral images is achieved by the development of an Embedded Feature Selection Support Vector Machine.



Adaptive shallow atmosphere simulation

- Orography field plays a fundamental role in shallow-atmosphere fluid flow simulations.
- The orography surface gradient is a dominant momentum driving force in climate modeling.
- hp-adaptive meshing method is used to approximate high-resolution (rough) data fields.
- h-adaptive meshes are refined in large gradient regions and coarse or small gradients.
- p-adaptive method of high polynomial degree is used on regions where data are approximated satisfactorily.



hp-adaptive elevation approximation of GLOBE data (zoom-in on North America)

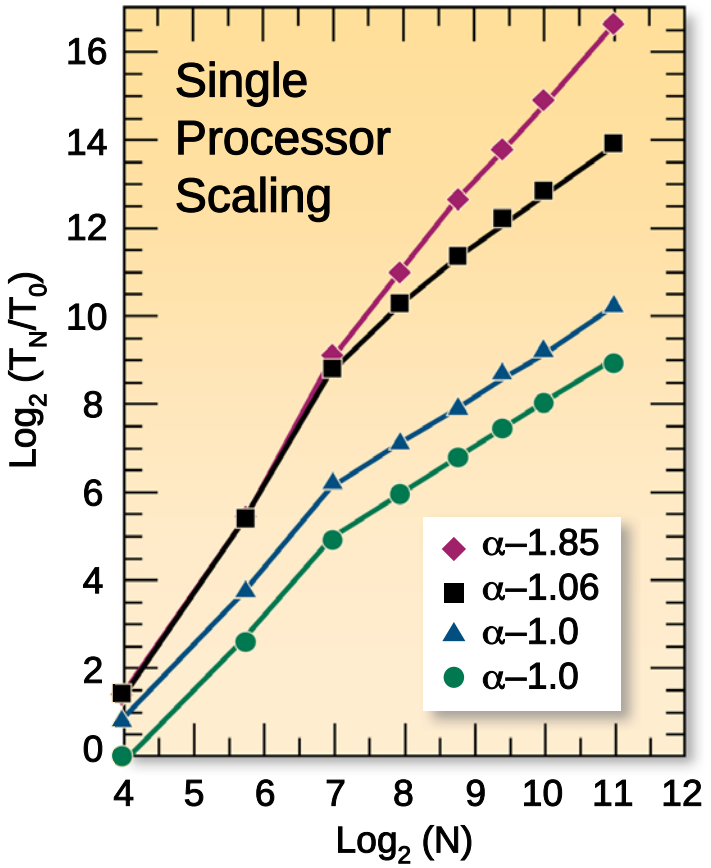
- Solution singularities at the poles can be resolved via hp adaptivity.
- The method provides an accurate representation of landscape data at much lower storage cost.

New large-scale first principles electronic structure code

- Formulation produces a sparse matrix representation:
  - 2-D case has tridiagonal structure with a few distant elements due to periodicity.
  - 3-D case has scattered elements, mainly due to mapping 3-D structure onto a matrix (2-D).
- It requires block diagonals of the inverse of $\tau(\varepsilon)$ matrix:
  - Block diagonals represent the site $\tau(\varepsilon)$ matrix and are needed to calculate the Green's function for each atomic site.
- We have developed preconditioned non-symmetric sparse iterative methods that take advantage of our sparsity pattern to calculate only $\tau^{ii}(\varepsilon)$:
  - Transpose free quasi-minimal residual method preconditioners: Jacobi, ILU, etc.
- We have also incorporated direct sparse matrix methods based on SuperLU.
- New full potential and forces being developed:
  - Discontinuous Galerkin and local discontinuous Galerkin approaches combined with preconditioned iterative techniques.
  - 2-D code is currently being tested; 3-D code is under development.

New electronic structure method

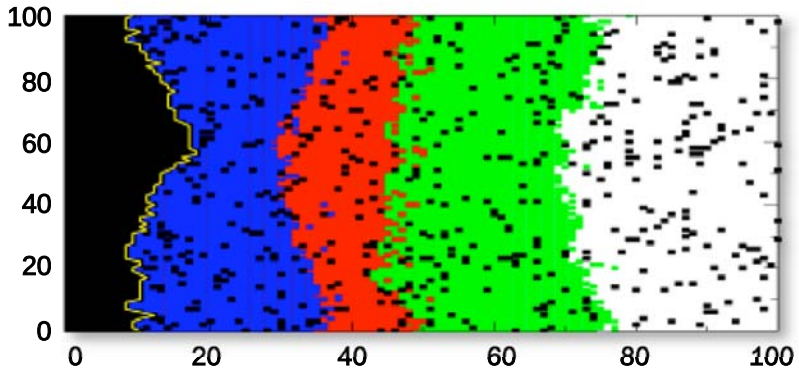
- Performs large-scale first principles simulations for chemistry, materials science, and condensed matter physics.
- Is capable of treating hundreds of thousands of atoms or more.
- Scales nearly linearly with increasing system size.
- Is capable of treating
  - highly parallel,
  - disorder beyond mean-field theory,
  - non-local coherent potential.
- Mathematically based approach is more accurate than previous methods based on ad-hoc assumption.
- Single code contains LSMS, KKR-CPA, Scr-LSMS and Scr-KKR-CPA.

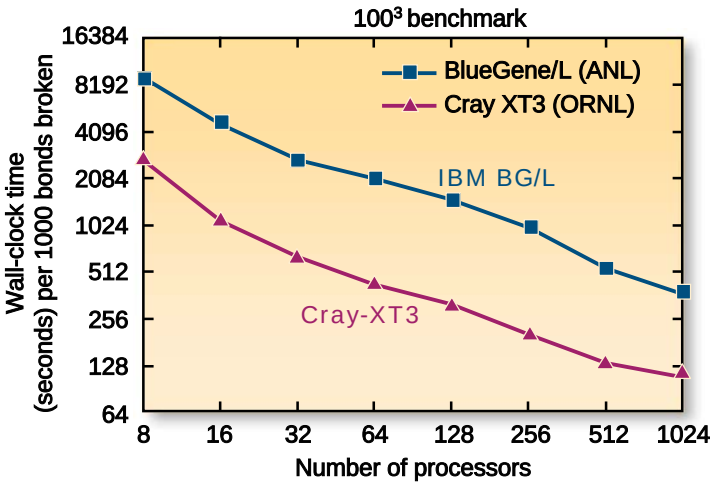


Fracture of 3-D cubic lattice system

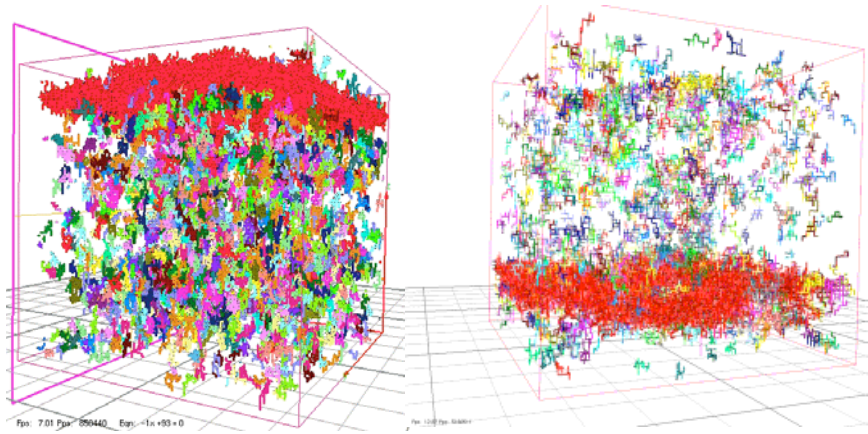
Motivation

- What are the size effects and scaling laws of fracture of disordered materials?
- What are the signatures of approach to failure?
- What is the relation between toughness and crack surface roughness?
- How can the fracture surfaces of materials as different as metallic alloys and glass, for example, be so similar?
- CPU ~ O($L^{6.5}$) in L x L x L cubic lattice.
- Recycling Krylov subspace in 3-D.



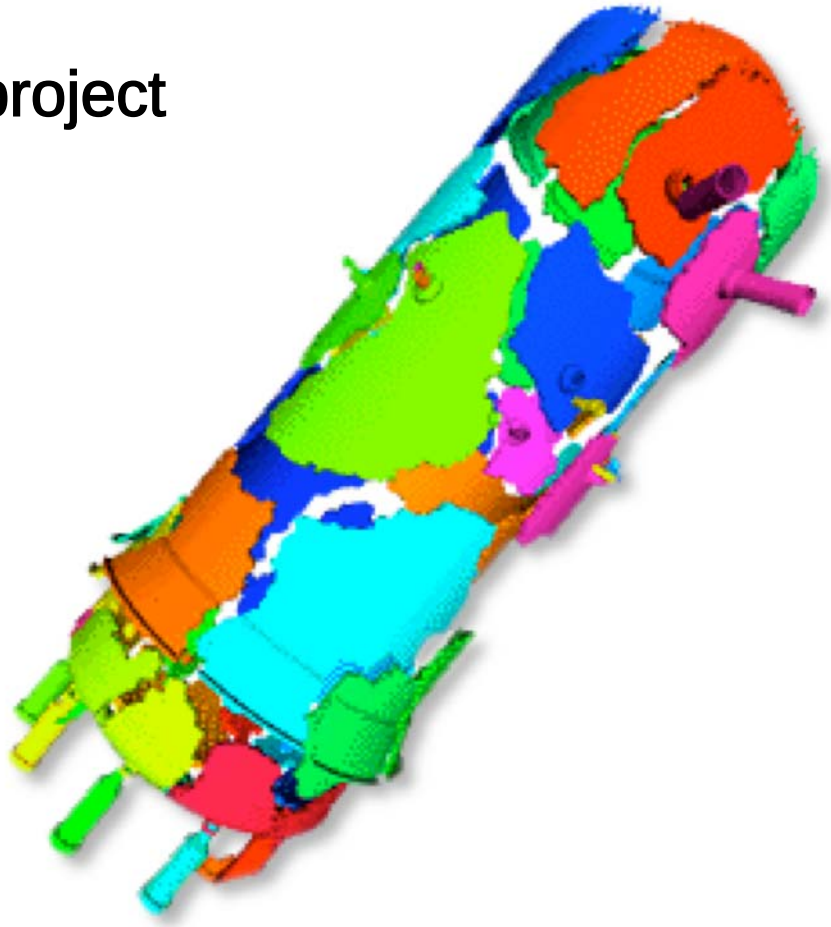


L	Processors	Time
L = 64	128	3 hr
L = 100	1024	12 hr
L = 128	1024	3 days



Adventure system

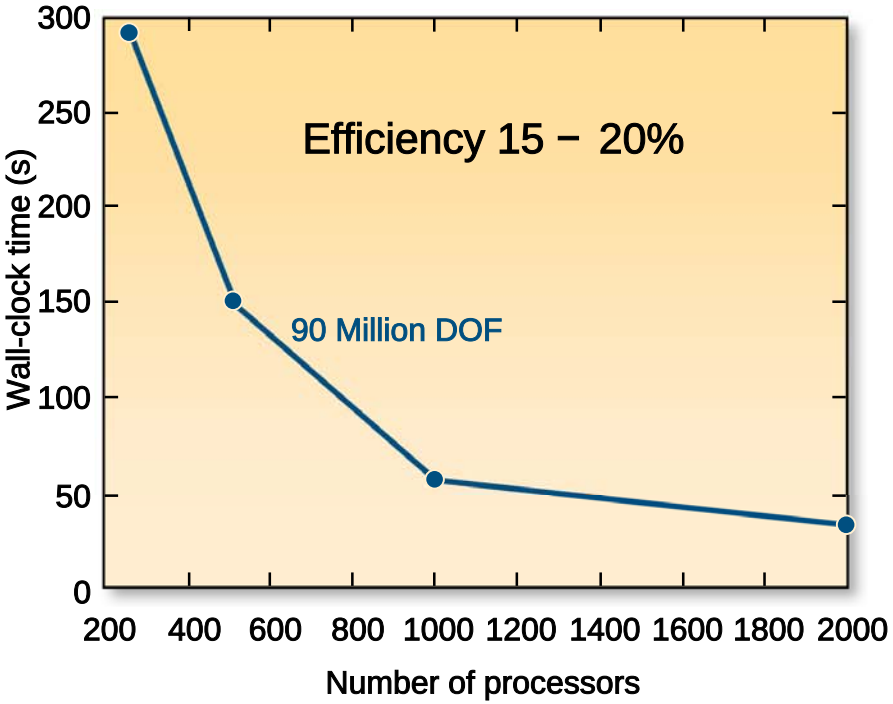
- General-purpose system for large-scale analysis
  - Thermal, fluid, solid, electro-magnetics
- Developed for Earth Simulator project
- Employs a hierarchical domain decomposition method (HDDM) to efficiently utilize massively parallel computer resources
  - Partition problem into non-overlapping sub-domains
  - Analyze sub-domains (fine problem)
  - Enforce compatibility between sub-domains (coarse problem)

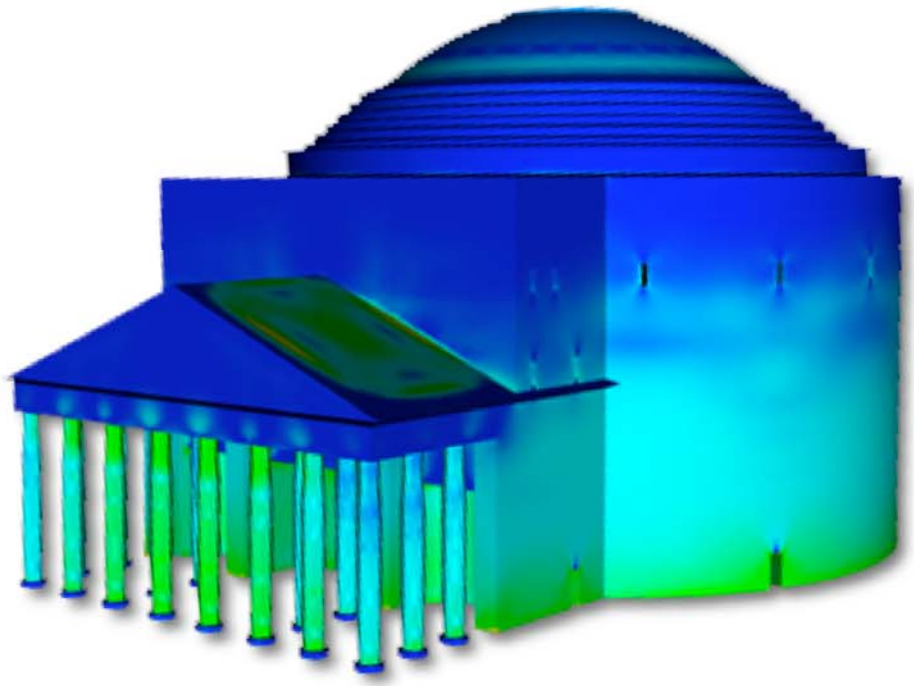


http://adventure.q.t.u-tokyo.ac.jp/

ADVENTURE on NCCS systems

- Test problem: Static stress analysis of Pantheon
- 90 million (DOF) on Cray XT4
- Scaling up to 2000 cores





An eigensolver with low-rank updates for spin-fermion models

- Monte Carlo simulations of colossal magnetoresistance (CMR) effect on lattice systems require the calculation of all eigenvalues of the Hamiltonian matrix at each step to determine acceptability of a proposed change. The Hamiltonian matrix undergoes a low rank modification if the change is accepted.
- A technique used in "divide-and-conquer" eigensolver was adapted to update spectrum under low rank modification.
- Infrequent recalculation of entire spectrum was still required.
- The incremental update was an order of magnitude faster than complete eigen decomposition at each step.

Matrix size	Time of update algorithm	Time LAPACK zheev('N')
288	0.34 s	0.55 s
800	2.5 s	18.5 s
1152	9.7 s	64 s
2048	32 s	365 s

Time for 10 steps of simulation

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