Adaptive Meshing with Zero Projection Error

Jeff Erickson, Shuo-Heng Chung and Shripad Thite, Department of Computer Science
Jayandran Palaniappan, Reza Abedi and Robert B. Haber, Theoretical & Applied Mechanics

Objective
Adaptive meshing is crucial for resolving multiple length and time scales in transient numerical simulations. When implemented as an instantaneous operation in space, it introduces projection error as the solution is transferred from the old to new mesh. This limits solution accuracy, the primary goal of adaptive analysis. Global remeshing can hinder parallel execution. We seek new techniques that circumvent these problems.

Approach
We adapt unstructured spacetime meshes using strictly local remeshing operations to avoid serial bottlenecks in parallel codes. We implement the common remeshing operations (edge flips, vertex deletion, smoothing, etc.) within spacetime elements to improve element quality while eliminating all solution projections and associated errors. This preserves the element-wise conservation properties of spacetime discontinuous Galerkin methods.

Impact
Our adaptive method offers improved performance and accuracy, especially for models with extremely sensitive energetics, as are common in simulations of materials microstructure.

Center for Process Simulation and Design (UIUC), http://www.cpsd.uiuc.edu/.
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Analysis of Velocity Singularity in Dynamic Cohesive Fracture

Morgan Hawker and Robert Haber, Department of Theoretical & Applied Mechanics

Objective
Dynamic fracture along interfaces describes certain forms of material failure as well as the mechanics of earthquakes at much larger length scales. We study numerically the dynamics of fracture using a cohesive damage model. We discovered unexpected singular velocity response at cohesive crack tips; we seek a deeper understanding of this phenomenon.

Approach
We embed a cohesive failure model within an elastodynamic spacetime discontinuous Galerkin (SDG) model. Adaptive analysis techniques guarantee very high-resolution solutions. Post-simulation analysis reveals singular response with the same form as in classical, non-cohesive fracture, possibly with non-singular core.

Impact
The discovery of the crack-tip velocity singularity suggests a fundamental rethinking of the physics of dynamic fracture that can lead to improved understanding and prediction of materials failure under dynamic loads and of geological fractures along fault lines in earthquakes.

Center for Process Simulation and Design (UIUC), http://www.cpsd.uiuc.edu/.
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Hyperbolic Heat Conduction and Thermomechanical Response

Scott Miller and Robert B. Haber, Department of Theoretical & Applied Mechanics
Brent Kraczek and Duane Johnson, Department of Materials Science & Engineering

Objective

The parabolic Fourier heat equation, although useful in many situations, implies infinite propagation speed and is ineffective at the very small length and time scales associated with nanoscale systems. We seek an effective numerical implementation of hyperbolic thermal and thermomechanical models to avoid these problems.

Approach


Impact

This high-resolution model can be applied to pulsed lasers in corneal surgery, nanotechnology (e.g., CPU overheating, phase-change data storage, micromachining of thin films with pulsed lasers), and thermomechanical dynamic fracture. A similar method can model the dynamics of phase transitions (generalized Cahn-Hilliard equation applied to shape memory alloys), biotransport as well as chemisorption and hydrogen storage.
Interactive Point-Based Rendering of High-Order Tetrahedral Data

Yuan Zhou and Michael Garland, Department of Computer Science

Objective

Spacetime discontinuous Galerkin simulations produce high-order solutions defined over tens of millions of tetrahedra in potentially non-conforming meshes. Existing rendering methods cannot achieve interactive frame rates when visualizing such extensive data sets. Our goal is to render these data interactively without sacrificing accuracy or quality.

Approach

We use an interactive point-based rendering system accelerated by GPUs (Graphics Processing Units). We adaptively sample tetrahedra in streaming fashion, decimating points at run time according to importance to fit the GPU memory limits. The memory consumption is independent of the input size. Our order-independent point rendering method can render on the order of 20 million tetrahedra at interactive rates. Our approach is about 200 times faster than the widely-used ray casting method, with no loss in fidelity.

Impact

This work provides a powerful tool for interactively visualizing high-order solutions with sharp, shock-like features. It naturally extends to general nonlinear conservation laws and should prove valuable in fluid dynamics, earthquake simulation, seismic petroleum exploration and nondestructive methods for detecting internal flaws in metal castings and weldments. Our fast rendering method can also be used to visualize 3D data in space only, as in medical imaging.
Parallelizing Adaptive Spacetime Finite Element Simulations

S. Chakravorty, A. Becker, R. Blake, and L. V. Kale, Department of Computer Science

Objective
Shock waves drive many forms of material failure and transformation. Parallelizing shock simulations will allow scientists to get results faster and study problems at a scale that was impossible on desktop computers.

Approach
We have tied the serial program into ParFUM, a framework for parallel finite element programs developed at the University of Illinois. This framework handles the communication and synchronization needed to divide the mesh among hundreds or thousands of processors. This approach is more scalable than previous techniques which kept a master mesh on one processor and farmed work out to other processors.

Impact
On a desktop workstation, spacetime finite element simulations can take days or weeks. By running these simulations on supercomputers, scientists can get results that used to take days in minutes. This means that they can study problems so large that they would be impossible to do on a desktop machine.
Promoting Cross-Disciplinary Researchers and Communities

1Robert Haber, 2,3Duane Johnson, 3Brent Kraczek
Departments of 1 Mechanical Science & Engineering 2 Materials Science & Engineering, 3 Physics

Interdisciplinary Research and Graduate Education
This project is an interdisciplinary effort that involves faculty in applied mechanics (R. Haber, J. Dantzig), mathematics (R. Jerrard, J. Sullivan), computer science (J. Erickson, M. Garland, L. Kale) and Physics and Materials Science (D. Johnson, N. Goldenfeld). In addition to fostering new faculty collaborations, the project is training a new generation of scientists in cross-disciplinary research and software development. Graduate students participate in weekly team meetings and in several cases are co-advised by faculty in different departments. Many of our research accomplishments could not have been realized within a conventional single-discipline research environment. We also leveraged research across CPSD and the Materials Computation Center.

Building Interdisciplinary Research Communities
CPSD has taken a leadership role in promoting and organizing the emerging research specialty of Atomistic-to-Continuum Coupling (AtCC). This important new topic draws on expertise from the physics, mathematics, applied mechanics and materials science communities. Profs. Haber and Johnson organized highly successful minisymposia on AtCC at the 8th U.S. National Congress on Computational Mechanics, Austin, TX, July 2005 and the 7th World Congress on Computational Mechanics, Los Angeles, CA, July 2006. Both events drew leading researchers working on ATCC from diverse fields, with participants from the U.S. and Europe as well as from academia and the U.S. national labs.
Renormalization group methods for multiscale materials pattern formation

Faculty: Nigel Goldenfeld (Physics), Jon Dantzig (MechSE)
Students and Post docs: B. Athreya, P. Chan, Z. Huang

Research
The goal of this project is to develop multiscale methods for simulating the development of materials microstructure. Our approach is based upon a continuum representation of atomic density, obeying diffusive dynamics. During the course of this project we have developed analytical methods to describe the coarse-grained dynamics of the atomic density. In the last year, these equations have been solved by implementing adaptive mesh refinement, enabling a thousand-fold increase in speed compared to a atomic-scale resolved simulation.

Broader Impacts
The work described herein was performed by an interdisciplinary team of mechanical engineers and theoretical physicists. Three students have been associated with this project, including one who has graduated and moved to industry. Our project has educated mechanical engineers in renormalization techniques, and physicists in adaptive mesh refinement techniques.

In the lower image, we show a portion of a grain boundary between two misoriented crystals. The sequence of images shows the multiscale resolution, finally resolving the dislocation array comprising the grain boundary. This work shows enables the solution of problems in materials science, seamlessly integrating length scales from nanoscopic to mesoscopic.

Center for Process Simulation and Design (UIUC), http://www.cpsd.uiuc.edu/.
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**Time and spacetime finite elements for coupled atomistic-continuum dynamics**

*1Robert Haber, 2Duane Johnson, 3Brent Kraczek*

*Departments of 1Mechanical Science & Engineering, 2Materials Science & Engineering, 3Physics*

**Objective**

Computer simulations are a major part of analysis, prediction and design of structural, electronic, energy and bio-medical materials. Traditionally, simulations are based on either atomistic or continuum mathematical models. We are developing methods that leverage the strengths of each within a consistent mathematical framework.

**Approach**

For the continuum and coupled models, we use spacetime discontinuous Galerkin formulation with coupling derived from balance of momentum and energy. For atomistic models we use high-order time finite element methods. For the same cost (number of force evaluations), our method has energy error at machine precision and clearly outperforms the standard velocity-Verlet algorithm (see figure). The accuracy of atomic trajectories also improves significantly.

**Impact**

Our new time-stepping scheme significantly improves the efficiency and reliability of atomistic simulations of materials, and should be useful in astronomy and other fields. By leveraging the strengths of continuum and atomistic methods we may address larger complex systems, such as nano-scale and biological structures and energy devices.
Tracking Evolving Discontinuities in Spacetime Solutions

Jayandran Palaniappan and Robert B. Haber, Department of Theoretical & Applied Mechanics
Shuo-Heng Chung and Shripad Thite, Department of Computer Science

Objective
Evolving surfaces of discontinuity arise in continuum physics as shocks, moving phase boundaries, cracks and dislocations; their discrete representation is one of the most challenging problems in computational science. Conventional methods use expensive grid refinement and error-inducing stabilization to capture these features. We seek more effective finite element methods that explicitly track the trajectories of singular surfaces.

Approach
Adaptive meshing aligns spacetime element faces with solution-dependent trajectories of singular surfaces; our discontinuous Galerkin model admits solution discontinuities and enforces necessary jump conditions. Spacetime smoothing and Delaunay edge flips ensure mesh quality.

Impact
Our adaptive spacetime discontinuous Galerkin approach provides more robust tracking capabilities and more accurate solutions with substantial cost reductions. These techniques can be used to model evolving microstructures, to predict the paths of dynamic fractures and to model vascular and cellular mechanics in biomedical applications.