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Spacetime Discontinuous Galerkin Methods: Applications to Molecular Dynamics and Thermomechanical Response

Robert Haber

Professor of Theoretical and Applied Mechanics, University of Illinois at Urbana-Champaign

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Abstract:

The first part of this talk introduces spacetime discontinuous Galerkin (SDG) finite element methods, a novel paradigm for high-resolution, multiscale simulation in computational mechanics. We begin with an invariant spacetime formulation of classical mechanics using the tools of differential forms and the exterior calculus on manifolds. Straightforward Galerkin projections generate finite element methods with element-wise balance properties on spacetime grids, with suitable jump conditions for problems with shocks and other discontinuities. If the spacetime mesh satisfies a causality constraint, then mesh generation and the finite element solution can be interleaved in a patch-by-patch procedure with linear complexity in the number of elements. An adaptive spacetime meshing scheme produces unstructured spacetime grids with refinement ratios as large as 10^6 on a serial processor. However, the algorithm has a natural parallel structure, so even stronger mesh grading is possible on parallel systems. The second part of the talk focuses on a pair of applications that are currently under development. The first involves new time integration algorithms for molecular dynamics and schemes for atomistic-to-continuum coupling; the second is a hyperbolic thermomechanical model based on the Maxwell-Cattaneo-Vernotte conduction model that is suitable for thermal simulation at very small length and time scales (e.g., a pulsed laser impinging on a thin film). We discuss prospects for approximating classical parabolic diffusion models (such as Fourier conduction) with the hyperbolic model and for adaptively switching between parabolic and hyperbolic models in multiscale simulations.

Speaker's Bio:

Robert B. Haber is Professor of Theoretical & Applied Mechanics at the University of Illinois at Urbana-Champaign; he directs the Center for Process Simulation & Design, a multidisciplinary research center with primary funding from the NSF Information Technology Research (ITR) program. He received the Bachelors degree in Architecture from Cornell University in 1977 and the Ph.D. degree in Civil Engineering in 1980, also from Cornell. He is a fellow of both the International and the U.S. Associations for Computational Mechanics.

