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Discontinuous Galerkin Methods in Materials Modeling

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Hyperbolic PDEs and Conservation Laws in Materials Modeling

Hyperbolic systems play an important role in continuum models of materials systems. Examples include:

- shock wave propagation in solids
- evolution equations for state variables in inelastic constitutive models (porosity, dislocation density, etc.)
- Hamilton-Jacobi level set models for interface kinetics

Hyperbolic systems are among the most difficult problems for numerical simulation. Their solutions exhibit shocks (or discontinuities) that are difficult to capture on numerical grids. Available numerical methods are imperfect, and the search for better methods is an active area of research.

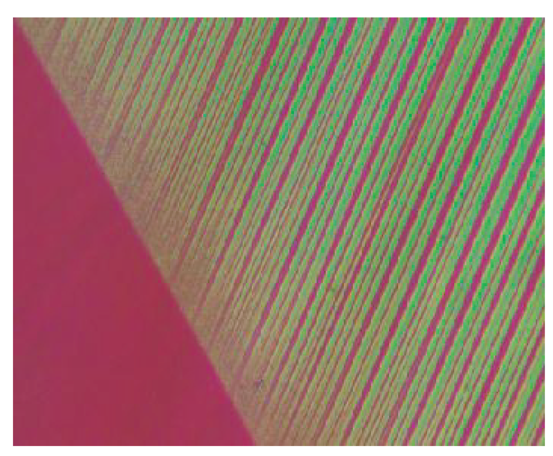

Figure 1: Martensite–Austenite phase boundary (Credit: Thomas Shield, University of Minnesota)

We are developing a new analysis technique, spacetime discontinuous Galerkin (SDG) finite element methods, to address this class of problems. SDG methods offer a number of desirable features:

- exact balance on every element
- no global oscillations due to shocks
- $O(N)$ complexity on causal grids
- supports nonconforming, hp-adaptive spacetime meshes
- rich parallel structure, modest communication requirements
- track moving boundaries and interfaces

This poster reports progress in formulating and implementing new SDG methods for elastodynamics and describes on-going work to apply them in multiscale modeling of materials microstructures.

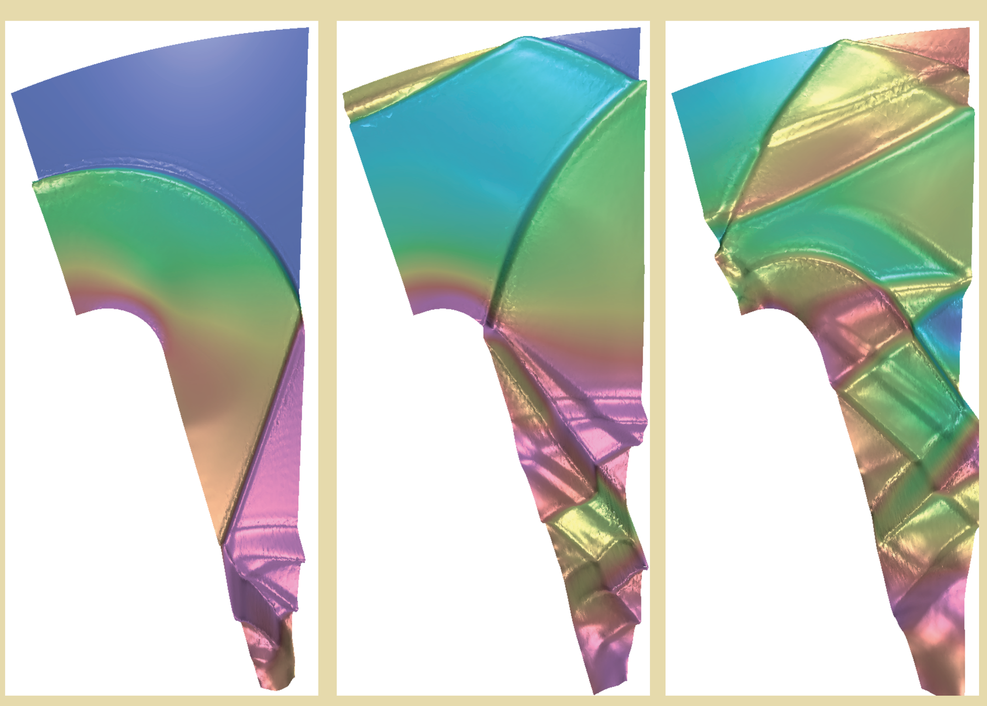

Figure 2: Shock wave propagation in a star-shaped rocket grain

SDG Finite Element Model

The distinguishing features of the SDG finite element method are:

- inter-element discontinuous basis
- direct spacetime model (in lieu of time-marching in semi-discrete methods)

These lead to several advantages when the method is implemented on causal grids.

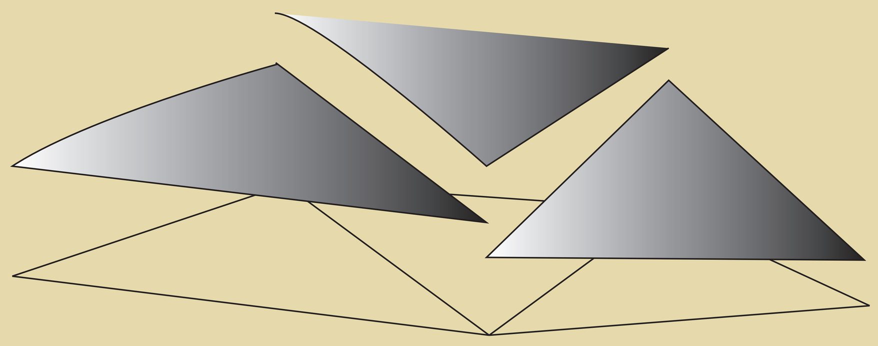

Figure 3: Discontinuous Galerkin finite element basis functions

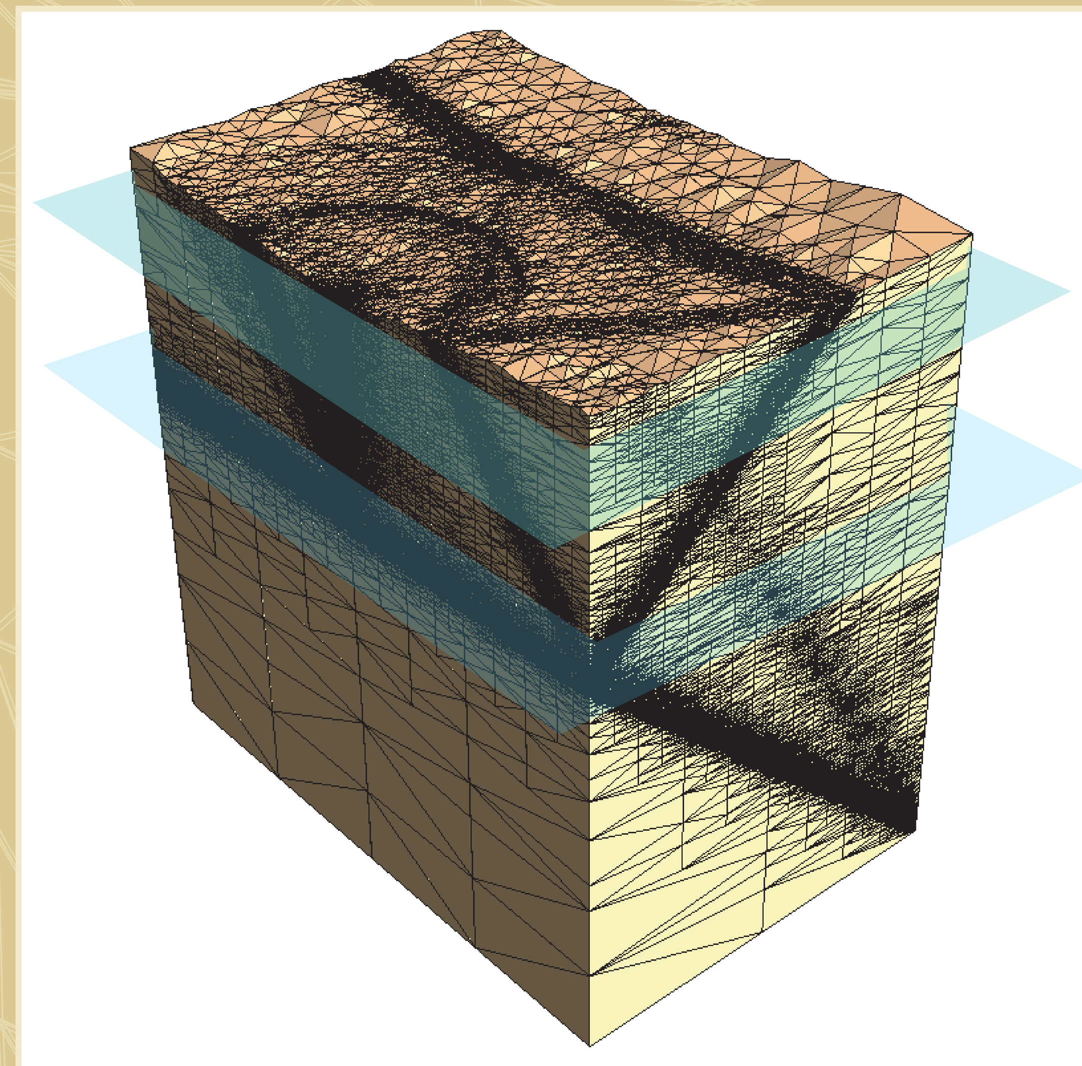

Figure 7: Unstructured spacetime mesh showing adaptive refinement for crack-tip scattering problem. The trajectories of the main shock front, Rayleigh waves, as well as scattered dilatational and shear waves are evident.

Tent Pitcher: Constructing and Solving Adaptive Spacetime Grids

Our solution relies on a novel spacetime meshing algorithm called "*Tent Pitcher*". Given a space mesh M and a target time T, Tent Pitcher constructs an unstructured mesh on the spacetime domain $M \times [0,T]$ using a local advancing front method. The advancing front is a *terrain* in spacetime, initially the space mesh M at time $t = 0$. Tent Pitcher repeatedly chooses a vertex of the front, advances that vertex forward in time to create a "tent", solves the PDE within that tent, and finally updates the front.

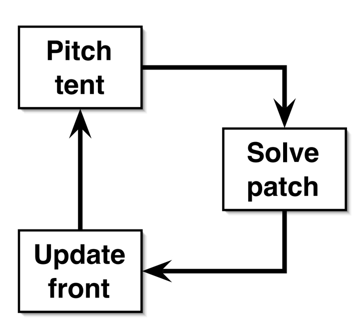

Figure 4: Tent Pitcher solution strategy

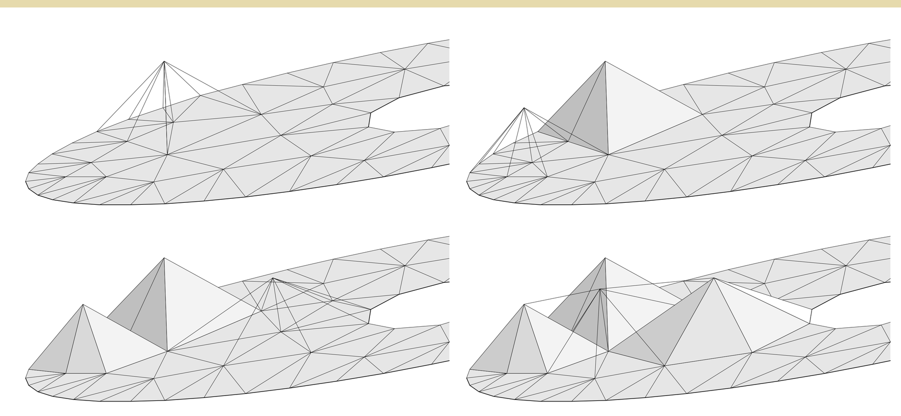

Figure 5: Pitching tents in spacetime

The height of each tent is limited in two ways. The *causality* constraint limits the slope of each facet to be less than the inverse of the local wave speed. This constraint ensures that the solution within each tent depends only on the solutions within previous tents. A more technical *progress* constraint ensures that our algorithm makes significant forward progress at every iteration.

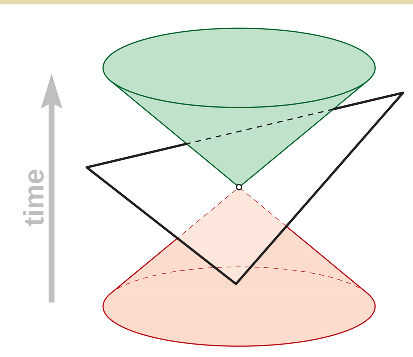

Figure 6: Causality constraint: facet separates domains of influence and dependence

We also refine or coarsen the front in response to a posteriori error estimates returned by our spacetime DG solver. If the error within a patch is too large, we refine the front using *newest-vertex refinement*.

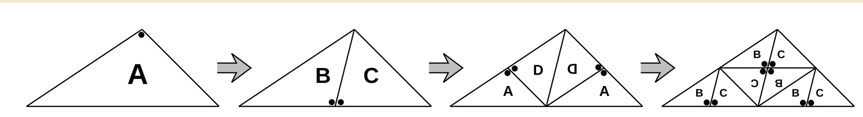

Figure 8: Newest-vertex refinement strategy

By refining the front, we reduce the size of future spacetime elements. If the error within a patch is below some threshold, we attempt to undo earlier refinements. Adaptivity allows us to track shocks and other subtle features of the evolving solution. Our method creates non-conforming spacetime meshes; fortunately, these are supported by our spacetime DG methods.

Our technique has three key advantages:

- *Adaptive*: The size and duration of each spacetime element depends only on the local spatial geometry and the complexity of the local solution.
- *Fast*: We solve a small system of equations for each tent, instead of one huge system for each time step, so our total solution time is only linear in the number of spacetime elements.
- *Flexible*: Tents with no causal relationship can be pitched and solved in any order, or in parallel (cf. parallel solution method)