NNSA Laboratory Directed Research & Development

Innovation Advancing Nuclear Security

High-Order Finite Elements Improve Lagrangian Hydrodynamics Simulations

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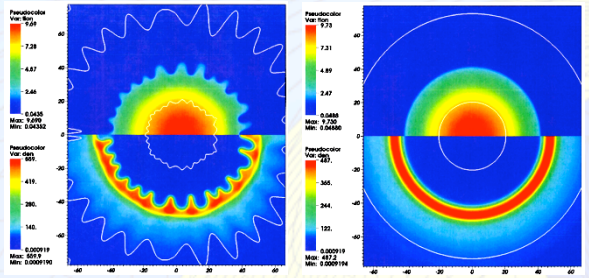
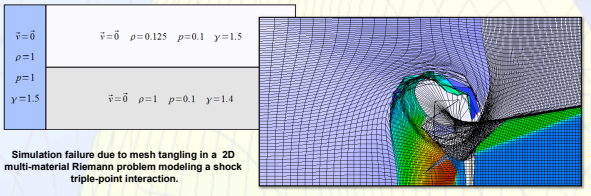
Multi-physics simulation challenges

Next-generation numerical algorithms are needed to enable higher-quality computational multi-physics simulations.

In the absence of underground nuclear testing, computer simulation has become a cornerstone of the stockpile stewardship effort. *Reliable shock hydrodynamics simulations* are of critical importance to the NNSA simulation code efforts and applications such as the National Ignition Facility (NIF). Current Lagrangian hydrodynamics algorithms have a number of long-standing numerical issues that can *reduce the predictive capabilities* of our large-scale multi-physics codes, including: lack of *symmetry preservation* and total *energy conservation*, the handling of *artificial viscosity* in multiple dimensions, and the presence of hourglass instabilities leading to *mesh tangling*.



NIF point-design capsule implosion at the onset of ignition in a physically perturbed capsule (left) and an unperturbed capsule (right). For designers to make decisions based on simulation results, it is imperative that the code can preserve symmetry at a level sufficient to distinguish numerical from physical perturbations. Such calculations on unstructured multi-block meshes are very challenging due to the high compression rate and hydrodynamic instabilities.

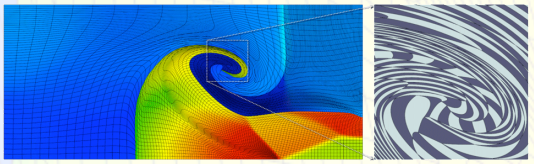


Simulation failure due to mesh tangling in a 2D multi-material Riemann problem modeling a shock triple-point interaction.

A new computational approach

We are developing a general high-order curvilinear finite element framework for Lagrangian hydrodynamics.

To address the above deficiencies, we are developing new numerical methods for Lagrangian hydrodynamics based on *high-order finite element* field representations, *curvilinear zone* geometries, *tensor artificial viscosity*, and *high-order time stepping* algorithms. Although this approach can be viewed as a high-order generalization of current methods, it has a number of advantages over them, such as *increased accuracy and robustness* on unstructured grids and *significant improvement in symmetry preservation*.



Curvilinear finite elements use additional degrees of freedom to more accurately represent deformations and avoid mesh tangling. *Naturally developing high aspect ratio curvilinear zones are impossible to represent with straight edges.*

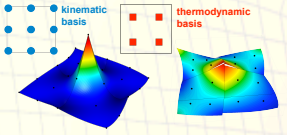
The framework utilizes a *pointwise mass conservation principle* and its computational kernel is the locally FLOP-intensive evaluation of a *generalized corner force matrix*.

Semi-discrete finite element method

Momentum Conservation: $\mathbf{M_v}\frac{d\mathbf{v}}{dt} = -\mathbf{F}\cdot\mathbf{1}$

Energy Conservation: $\mathbf{M_e}\frac{de}{dt} = \mathbf{F}^T\cdot\mathbf{v}$

Equation of Motion: $\frac{d\mathbf{x}}{dt} = \mathbf{v}$

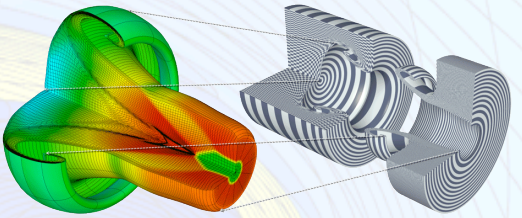


The semi-discrete finite element method can be defined in terms of the kinematic and thermodynamic mass matrices, Mv and Me, and the mixed generalized corner force matrix F. For example, our default discretization scheme uses finite element functions corresponding to *bi-quadratic kinematic fields* and *discontinuous bi-linear thermodynamic variables*.

Promising numerical results

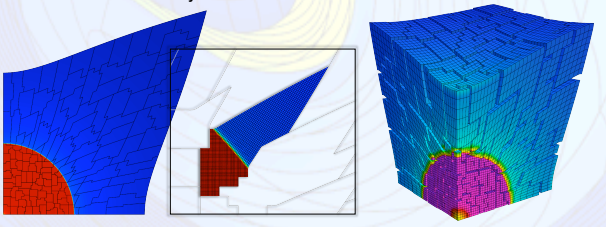
Our numerical methods have a number of practical advantages over traditional algorithms.

The new discretization methods were implemented in the recently developed research code BLAST, *http://www.llnl.gov/casc/blast*. The results from an extensive set of 2D, 3D and axisymmetric test problems demonstrate a number of practical advantages, including: *exact total energy conservation* by construction, *significant reduction in mesh imprinting*, increased *robustness and symmetry preservation* on unstructured and distorted grids, and the ability to *resolve shocks and thermodynamics gradients within a zone*.



Revolved 3D density and the curvilinear mesh computed in the axisymmetric version of the triple-point problem. The curvilinear approach maintains robust performance in axisymmetric simulations, leading to *one of the few known algorithms that supports both symmetry preservation and exact total energy conservation in cylindrical geometry.*

The new high-order algorithms are *ideally suited for parallel and exascale multi-core/GPU architectures* due to their locally FLOP-intensive nature.

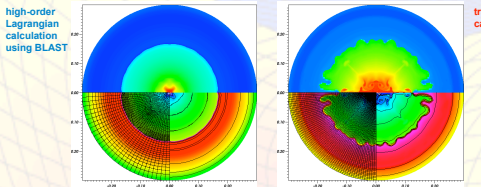


Parallel partitioning and single-zone shock resolution for the Noh implosion test problem in 2D (left) and 3D (right) on 128 processors. Computations dominate communications even with small problem sizes per processor.

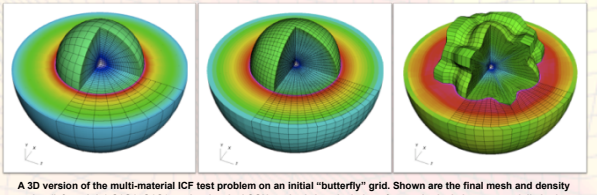
Why is this important for our nation?

High-order finite elements are a promising new technology for next-generation simulation capabilities.

Computer simulations are proving essential for stockpile stewardship. The technology developed in this research project has *overcome a number of long-standing numerical challenges* that are limiting the currently used simulation algorithms. The improved accuracy and robustness lead the way to *increased predictive capabilities* and to more reliable inertial confinement fusion (ICF) simulations in current and *future exascale simulation codes*.



A multi-material axisymmetric ICF test problem on an initial 2D "butterfly" grid. Shown are the final mesh, density and internal energy for the finite element (left) and a classical (right) method. The jets on the right are purely numerical.



A 3D version of the multi-material ICF test problem on an initial "butterfly" grid. Shown are the final mesh and density using (left to right) Q2Q1, Q1Q0, and a classical SGH method. Any deviations from spherical shape, especially in the material interface shown on top are purely numerical.

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