A Virtual Test Facility for Simulating Detonation-induced Response of Solid Materials

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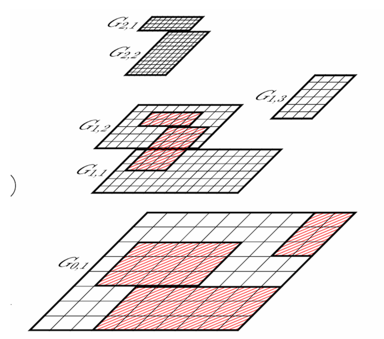
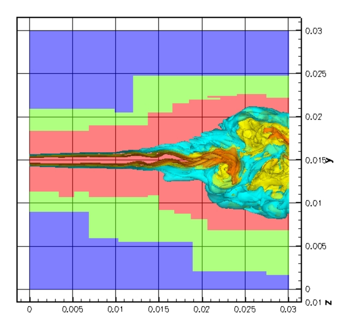
Abstract. The fluid-structure interaction simulation of detonation- and shock-wave-loaded solid structures requires numerical methods that can cope with large deformations as well as topology changes (fracture and fragmentation). We present a robust level-set-based approach that combines two finite element solvers with an Eulerian Cartesian fluid solver framework with dynamic mesh adaptation. As application examples, we show the deformation of a tantalum cylinder from the combustion of an enclosed load of the high explosive HMX and the rupture of thin aluminum tubes due to the passage of a gaseous detonation wave in an ethylene-oxygen mixture.

Amroc fluid solver frame work



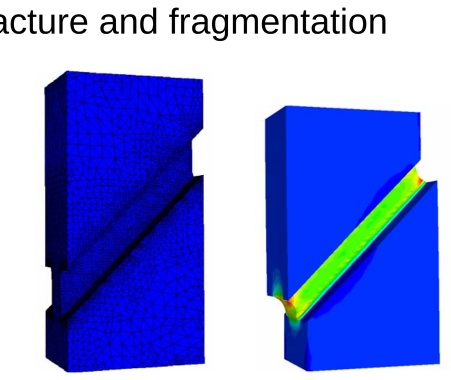
- Encapsulates dynamic mesh adaptation and parallelization to the fluid solver developer
  - Numerical scheme only for single block necessary
- Available 3d patch solvers:
  - WENO-TCD LES upwind scheme for turbulence simulations
  - Riemann-solver-based MUSCL schemes for simplified and detailed chemistry
- Implementation of Berger-Collela SAMR algorithm coupled to generic ghost-fluid implementation for multiple level sets
- Conservative correction for purely Cartesian problems



Right: LES of turbulent jet with WENO-TCD patch solver .

Adlib finite element solver

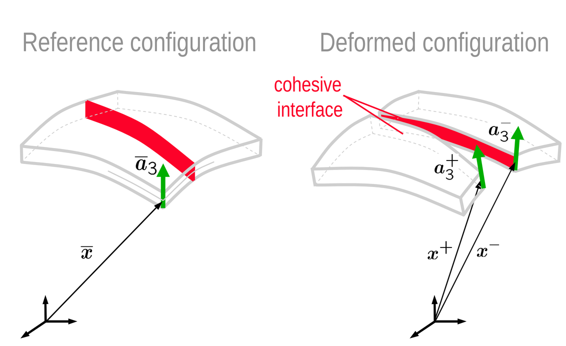
- Hexahedral solver in 3d
- Parallel explicit dynamics
- Solid modeling
- Fully scalable unstructured parallel meshing
- Thermo-mechanical coupling and multi-physics model
- Extensive constitutive library
  - single and polycrystal plasticity
  - ab-initio equation of state
- shock physics, artificial viscosity
- Contact
- Fracture and fragmentation



Simulation of shear compression experiment performed with Adlib.

SFC finite element solver

- Tetrahedral thin-shell solver in 3d
- Subdivision shell finite elements
  - Stretching and bending resistance
  - Large deformations
- Parallel explicit shell dynamics
  - Fully scalable communications
- Geometric modeling capabilities
- Access to a number of constitutive models
  - Adlib models as well as own implementations
- Parallel contact
- Fracture and fragmentation with cohesive interface elements

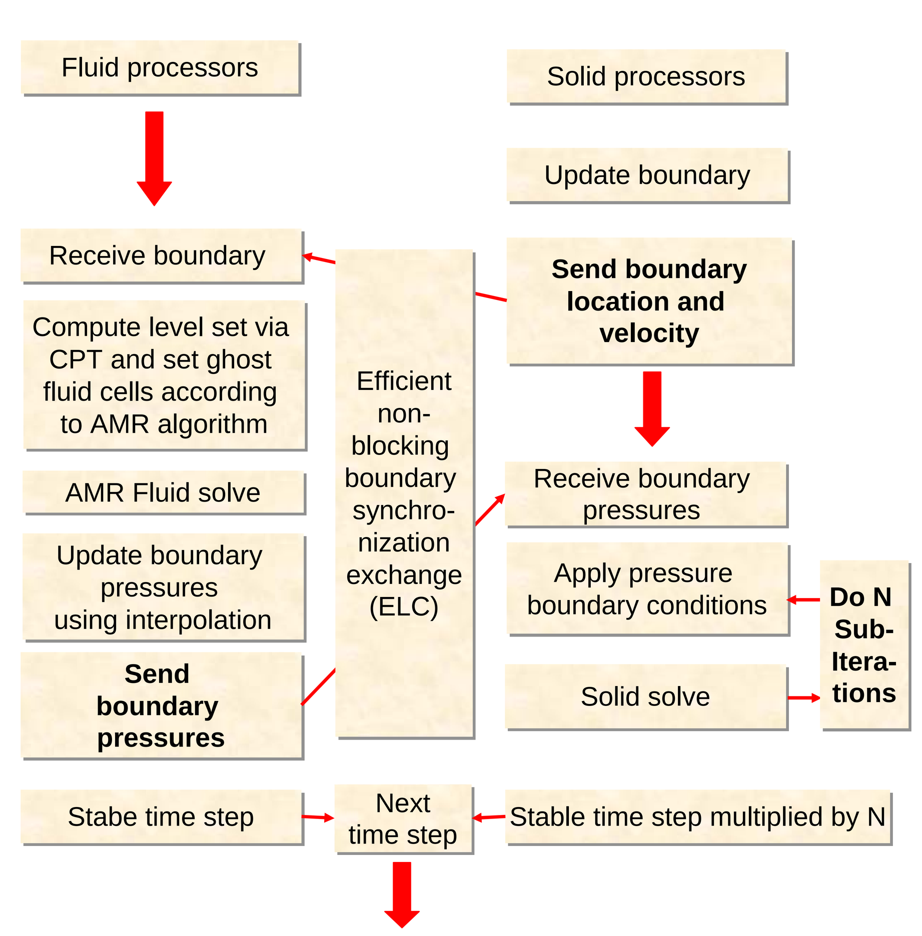


Fractured thin-shell kinematics used in SFC.

Fluid-Structure coupling

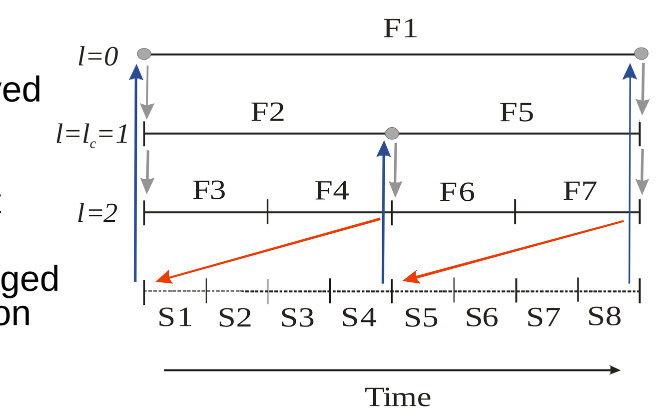
- Coupling of Euler equations for compressible flow to Lagrangian structure mechanics
- Compatibility conditions between inviscid fluid and solid at a slip interface
  - Continuity of normal velocity
    $u^S_n = u^F_n$
  - Continuity of normal stresses
    $\sigma^S_{nn} = -p^F$
  - No shear stresses
    $\sigma^S_{n\tau} = \sigma^S_{n\omega} = 0$
- Interpolation operations with solid surface mesh
  - Mirrored fluid density and velocity values $\mathbf{u}^F$ into ghost cells
  - Solid velocity values $\mathbf{u}^S$ on facets
  - Fluid pressure values in surface points (nodes or face centroids)

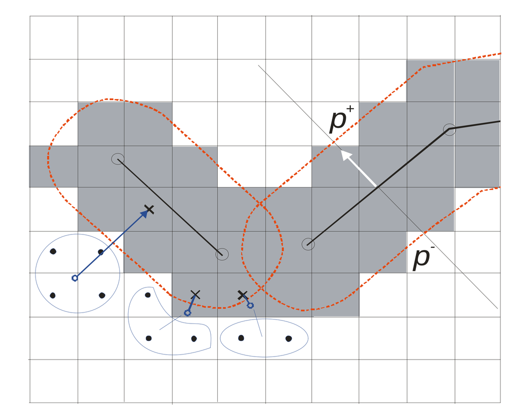
Right: Coupling algorithm: data exchange between dedicated fluid and solid processors.



Coupling of Eulerian SAMR to non-adaptive Lagrangian FEM

Exploit SAMR time step refinement for effective coupling to solid solver
  - Lagrangian simulation is called only at level $l_c < l_{max}$
  - SAMR refines solid boundary at least at level l_c
  - One additional level reserved to resolve ambiguities in GFM (e.g. thin structures)
- Nevertheless: Inserting sub-steps accommodates for time step reduction from the solid solver within an SAMR cycle
- Communication strategy
  - Updated boundary info from solid solver must be received (blue arrow) before regridding operation (gray dots and arrows)
  - Boundary data is sent to solid (red arrow) when highest level available
- Inter-solver communication (point-to-point or globally) managed on the fly by current SAMR partition bounding box information by Eulerian-Lagragian-Coupling module (ELC)



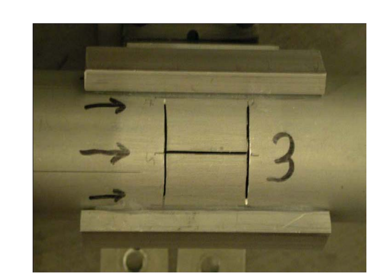


Treatment of lower-dimensional thin-shells

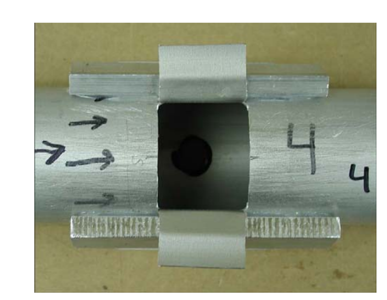
- Thin boundary structures require "thickening"
- Unsigned distance level set function ϕ
- Treat cells with $0<\phi<d$ as ghost fluid cells (gray)
- Leaving j unmodified ensures correctness of $\nabla\phi$
- Refinement criterion based on ϕ ensures reliable mesh adaptation
- Use face normal in shell element to evaluate in $\Delta p = p^+ - p^-$

Fracture induced by detonations in gases

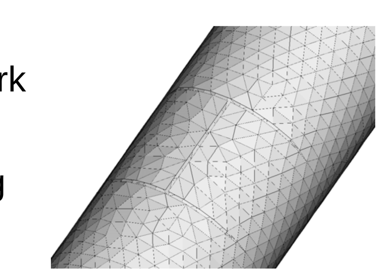
Motivation: Validate VTF for complex fluid-structure interaction problem
- Interaction of detonation, ductile deformation, fracture
- Modeling of ethylene-oxygen detonation with constant volume burn detonation model



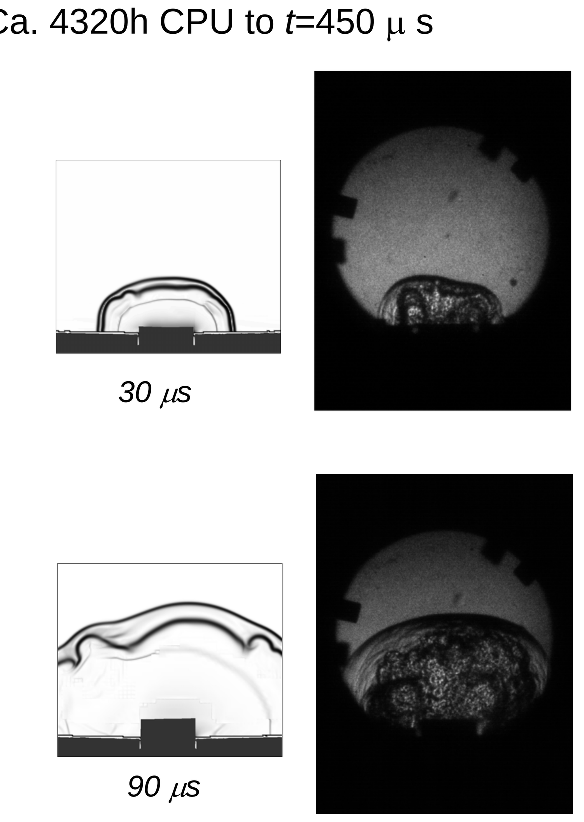
Elastic-plastic validation – Tube with flaps



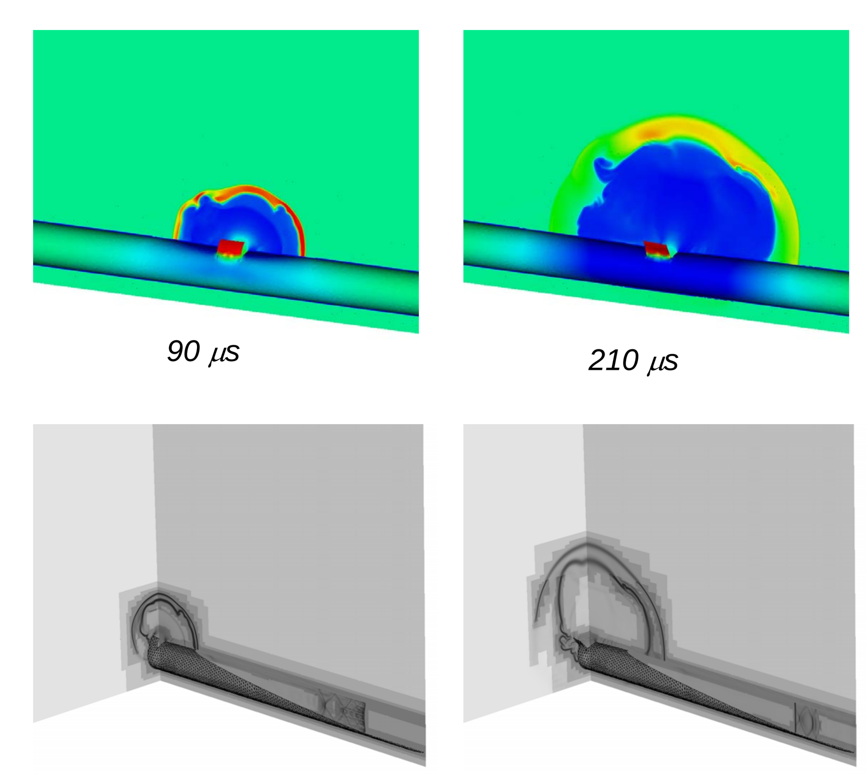
Fluid
- Constant volume burn model with γ=1.24, P_{CJ} =3.3 MPa, D_{CJ}=2376 m/s
- AMR base level: 104x80x242, 3 additional levels, factors 2,2,4
- Approx. 40M cells instead of 7,930M cells (uniform)
- Tube and detonation fully refined
- Thickening of 2d mesh: 0.81mm on both sides (real thickness on both sides 0.445mm)
- 16 nodes 2.2 GHz AMD Opteron quad processor, PCI-X 4x Infiniband network



Solid - SFC
- Aluminum, J2 plasticity with hardening, rate sensitivity, and thermal softening from Adlib material library
- Mesh: 8577 nodes, 17056 elements
- 16+2 nodes 2.2 GHz AMD Opteron quad processor, PCI-X 4x Infiniband network
- Ca. 4320h CPU to t=450 μ s



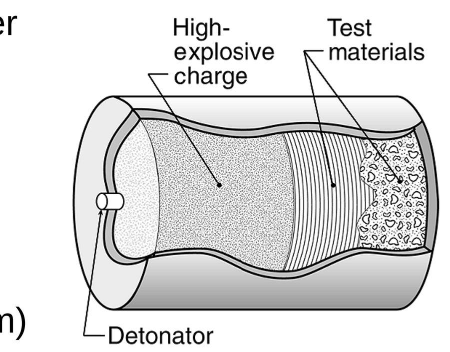
Comparison of simulated and experimental schlieren images for tube with flaps.



Top: Color plot of fluid density and solid displacements in y-direction. Bottom: schlieren images of density on refinement levels show the dynamic mesh adaptation in the fluid domain.

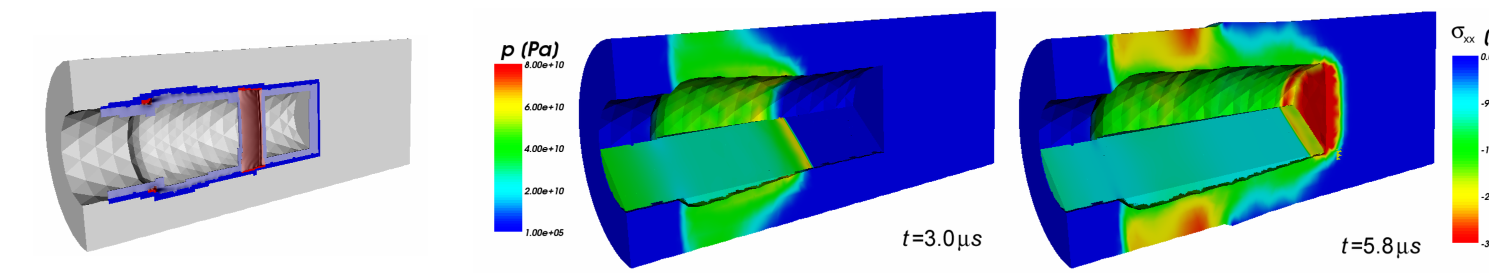
Large deformation from detonations in solids

Planar CJ detonation in HMX impinges on Tantalum cylinder



Fluid
- Modeling of a resolved detonation in high explosive HMX ($C_4H_8N_8O_8$) with one-step reaction model
- SAMR base mesh 60x60x120, two additional levels with factors 2, 4 to resolve detonation wave
- Coupling level l_c=1
- Fluid simulation uses <10M cells instead of 221M (uniform)

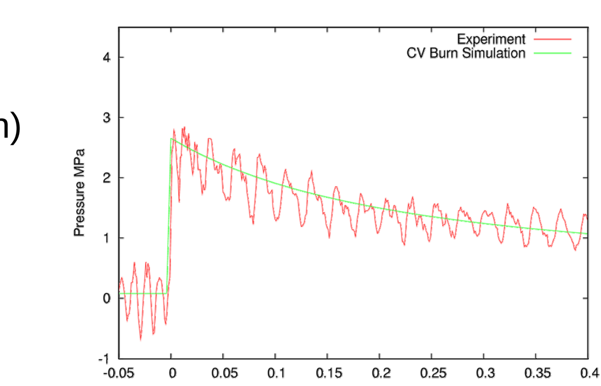
Solid - Adlib
- Tantalum material model: J2 flow theory with Vinet's thermal equation fitted to the ab-initio data of R.E. Cohen and O. Gülseren
- Polyconvex deviatoric stress (polyconvexity is known to guarantee existence of solutions)
- Artificial viscosity for oscillation damping around dilatation and shear waves
- Adlib mesh with 56k elements
- ~500h CPU with 14 fluid and 2 solid processes on ALC at LLNL

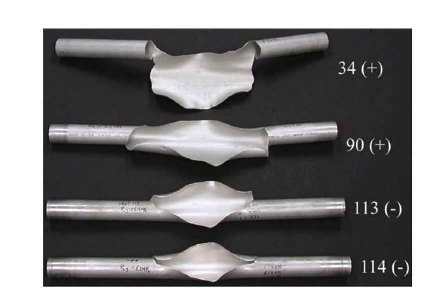


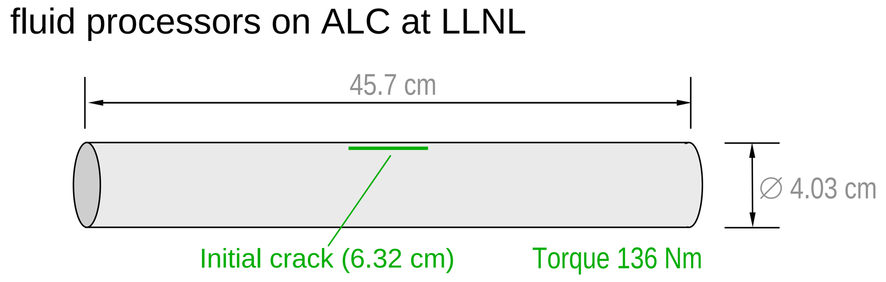
VTF validation runs – Tube with fracture and fragmentation

Fluid
- CV burn model with γ=1.24, P_{CJ} =6.1 MPa, D_{CJ}=2402 m/s (Right: flow field before specimen)
- 40x40x725 cells unigrid

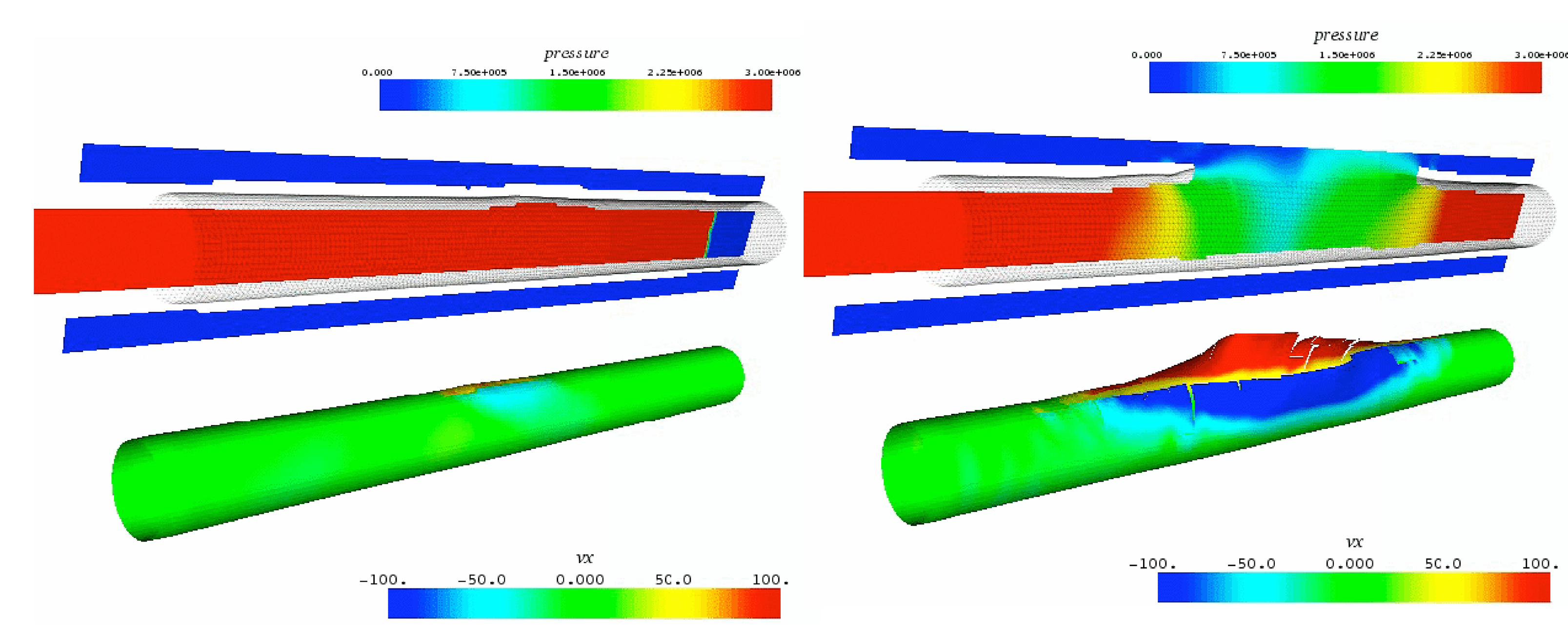
Solid - SFC
- Material model for cohesive interface: linearly decreasing envelope
- Shell mesh: 206208 nodes
- 972h CPU with 33 shell and 21 fluid processors on ALC at LLNL







Top: Specimen geometry. Left: Typical experimental rupture patterns.



Conclusions. A highly integrated C++ framework for fluid-structure interaction has been developed. It uses components in Fortran 77/90 (patch solvers) and C (bulk material models). The approach is tailored to high-speed events (detonations, shock waves) with large material deformation and strongly coupled response. Three-dimensional fluid-structure interaction simulations with arbitrary topology evolutions allowing for fracture and fragmentation are possible. Dynamic mesh adaptation can be used in the fluid to decrease the computational costs significantly. Scalable MPI parallelization for all components allows the effective utilization of the ASC machines to achieve results in minimal real time. Further information is available under http://www.cacr.caltech.edu/asc.

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