Multiscale models: development and integrated validation

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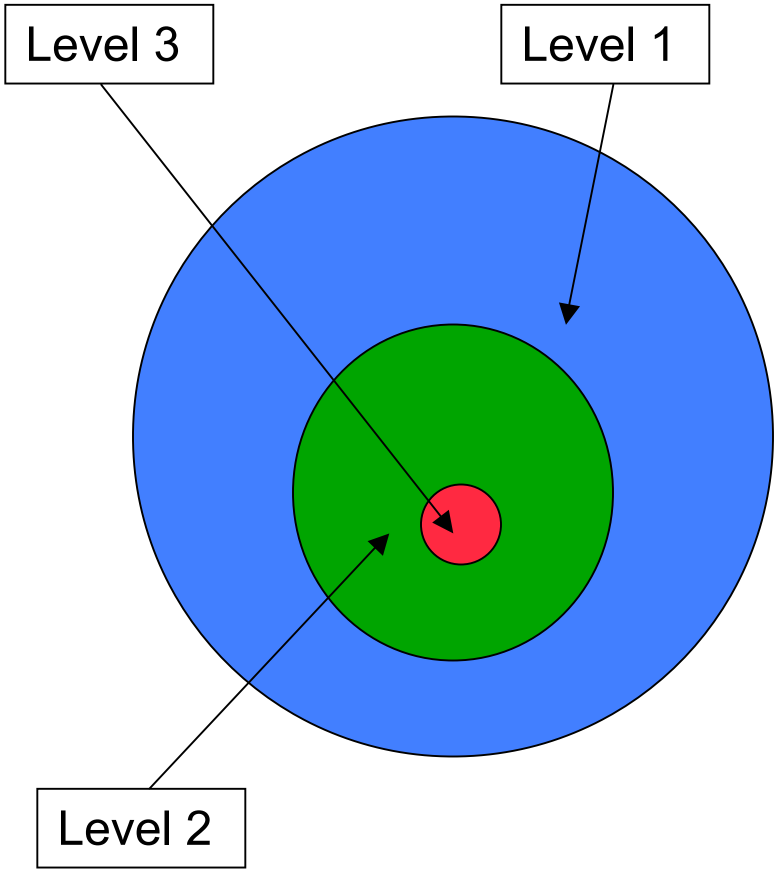
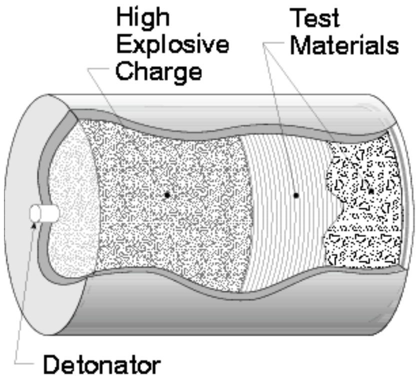
Levels of modeling

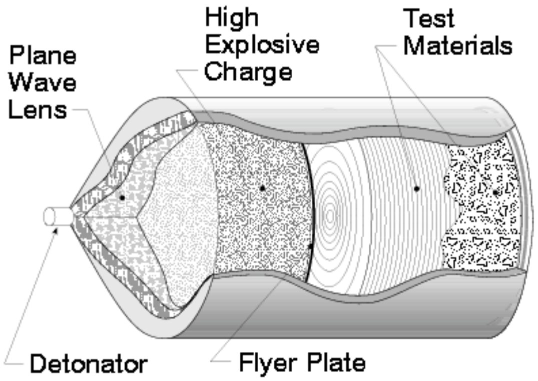
- Level 3
  - *Model typically has empirical origin*
  - *Model parameters fit to experiment*
  - *One choice of parameters may not fit a whole suite of experiments*
  - *Can be used to reproduce specific experiments*
  - *Can be used to explore small perturbations*
  - *Typically not predictive*
- Level 2
  - *Model form is based on physical understanding or universality*
  - *Parameters obtained from well diagnosed experiment*
  - *One choice of parameters can fit a whole suite of experiments*
  - *Model is typically predictive provided excursions from region of validity are not too large*
  - *No self consistent assessment that model validity has been violated*
- Level 1
  - *Model based on "first principles"*
  - *Model parameters computed from lower level hierarchy*
  - *Can perform self-consistent assessment of model validity*
  - *Predictive by definition*



Caltech/ASC virtual shock physics facility

- Explore full dynamic response of target materials to wide range of loadings
  - *compressive*
  - *tensional*
  - *shear*
- Loading generated by
  - *high velocity impact - strong shock waves*
  - *detonation of high explosive*
- Facilitate full three dimensional simulation
- Validate these computations against experiment

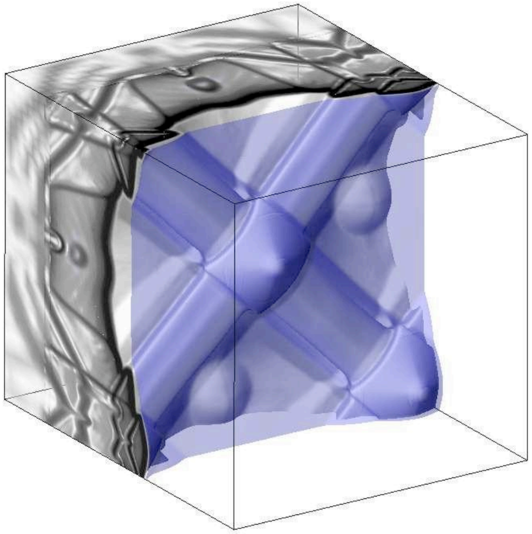


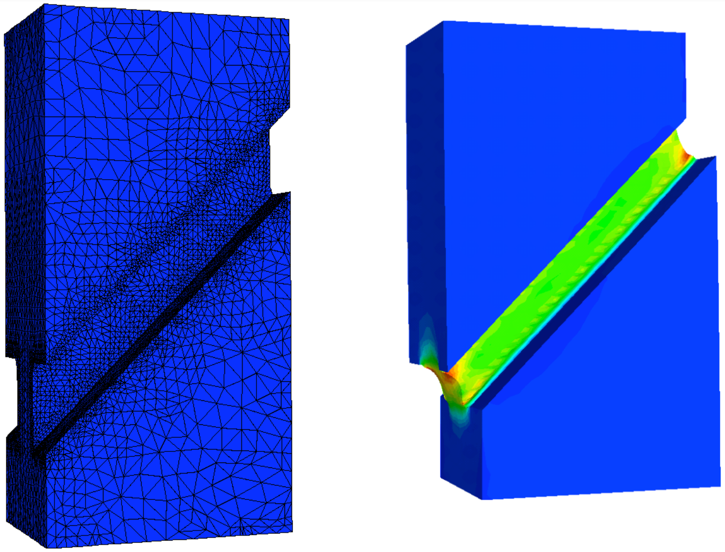


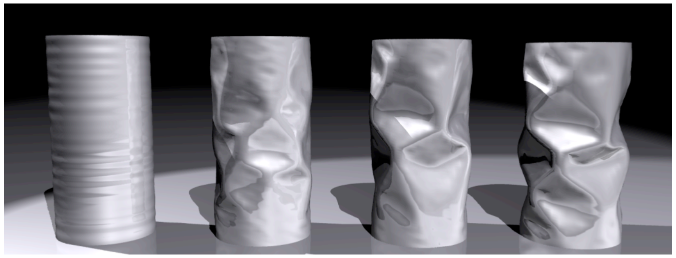
Role of high performance computation

- Computation has had a profound role in shock compression investigations
  - *Continuum mechanics*
  - *First principles simulation*
- Massive parallelism offered the hope of exploring three dimensional response
- If faithful computational capability can be developed, computation can play as important a role as experimentation

VTF simulation capabilities



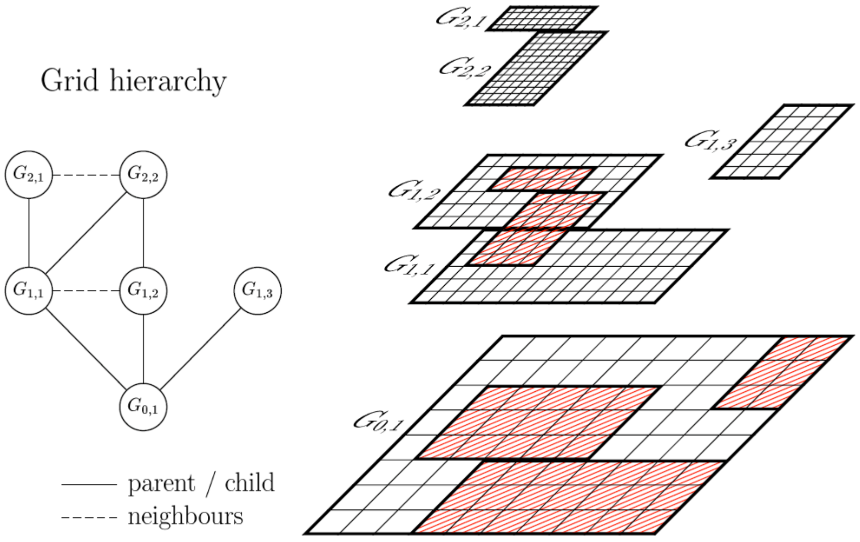


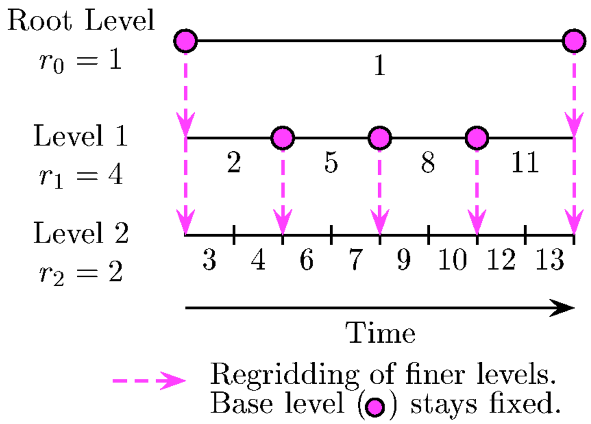


- Computational engines
  - *CFD*
  - *Solid mechanics*
- Fluid-solid coupling capability
- Optional Python based control and staging infrastructure

Adaptive mesh refinement (AMR)

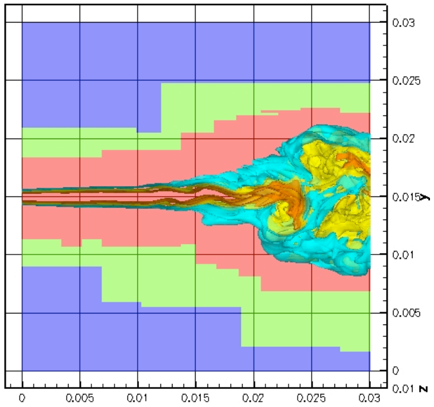
- Generic implementation of Berger-Collela SAMR algorithm
- Conservative correction
- Refined subgrids overlay coarser ones
- Computational decoupling of subgrids by using ghost cells
- Refinement in space *and* time
- Block-based data structures
- Cells without mark are refined
- Cluster-algorithm necessary
- Efficient cache-reuse / vectorization possible
- Explicit finite volume scheme only for single rectangular grid necessary



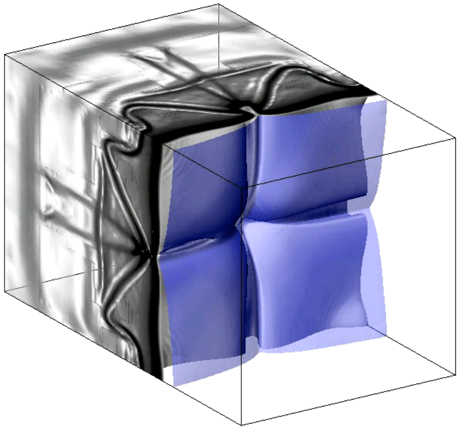


Fluid solvers

- AMROC encapsulates dynamic mesh adaptation and parallelization to the fluid solver developer
  - *Numerical scheme only for single block necessary*
  - *Efficient cache re-use and vectorization possible*
- Extended Clawpack with for full and one-step chemistry in Fortran 77 (R.Deiterding)
  - *Riemann solvers and flux vector splitting schemes with positivity preservation*
  - *In full production status: Used for several PhD thesis and research especially at GALCIT*
- WENO-TCD scheme with optional LES and chemical reaction capability in Fortran 90 (D.Hill, C.Pantano)
- Riemann solver for gas-dynamics with chemistry in C++ (P.Hung)



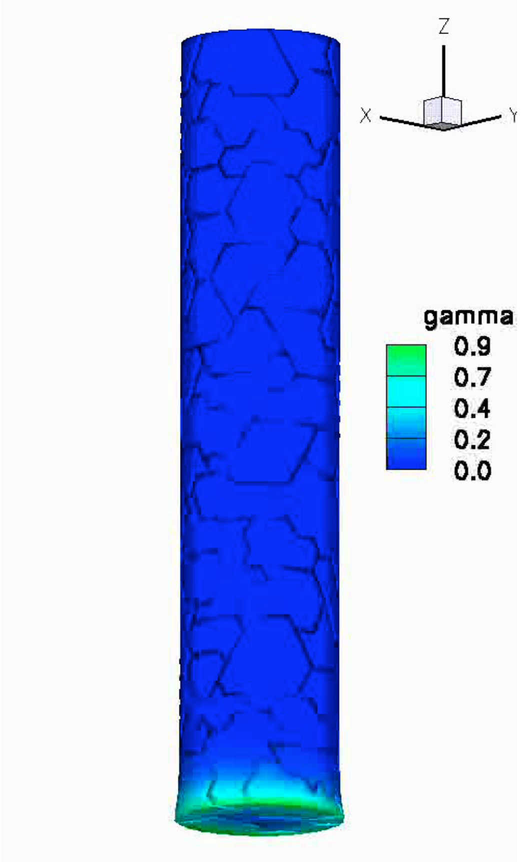
LES of turbulent hydrogen jet



Hydrogen and ethylene detonation structure simulations

Solid mechanics solvers: adlib

- Parallel explicit dynamics
- Fully scalable communications
- Solid modeling
- Fully scalable unstructured parallel meshing
- Thermomechanical coupling and multiphysics models
  - *Extensive constitutive library*
    - *single and polycrystal plasticity*
    - *ab initio EOS*
    - *shock physics, artificial viscocity*
- Contact
- Fracture and fragmentation
- Coupling to other solvers



Taylor impact test on polycrystalline Tantalum

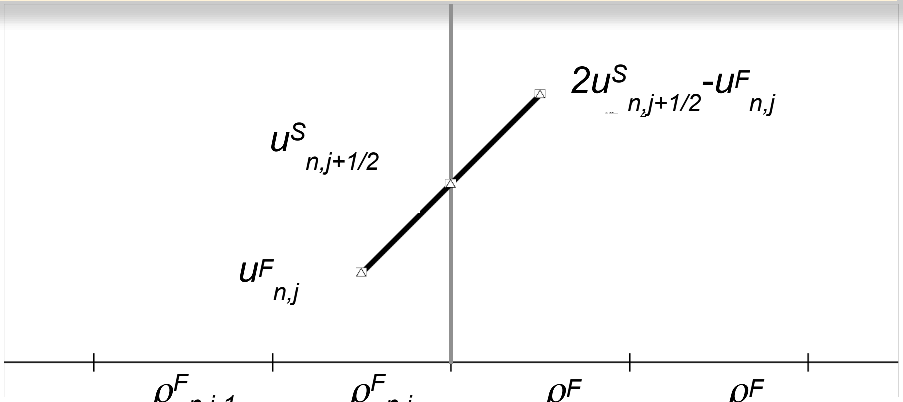
Solid mechanics solvers: sfc

- 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

Explosively driven inflation of an airbag

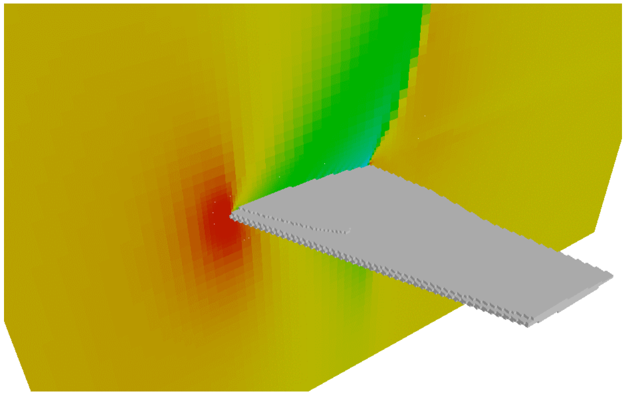
Fluid-solid coupling: Ghost fluid method

- Incorporate complex moving boundary/ interfaces into a Cartesian solver (extension of work by R.Fedkiw and T.Aslam)
- Implicit boundary representation via distance function φ, normal $n=r\varphi / |r\varphi|$
- Treat an interface as a moving rigid wall
- Method diffuses boundary and is therefore not conservative
- Higher resolution at embedded boundary required than with first-order unstructured scheme
- Problems sensitive to boundary interaction require thorough convergence studies
- Appropriate level-set-based refinement criteria are available to cure deficiencies



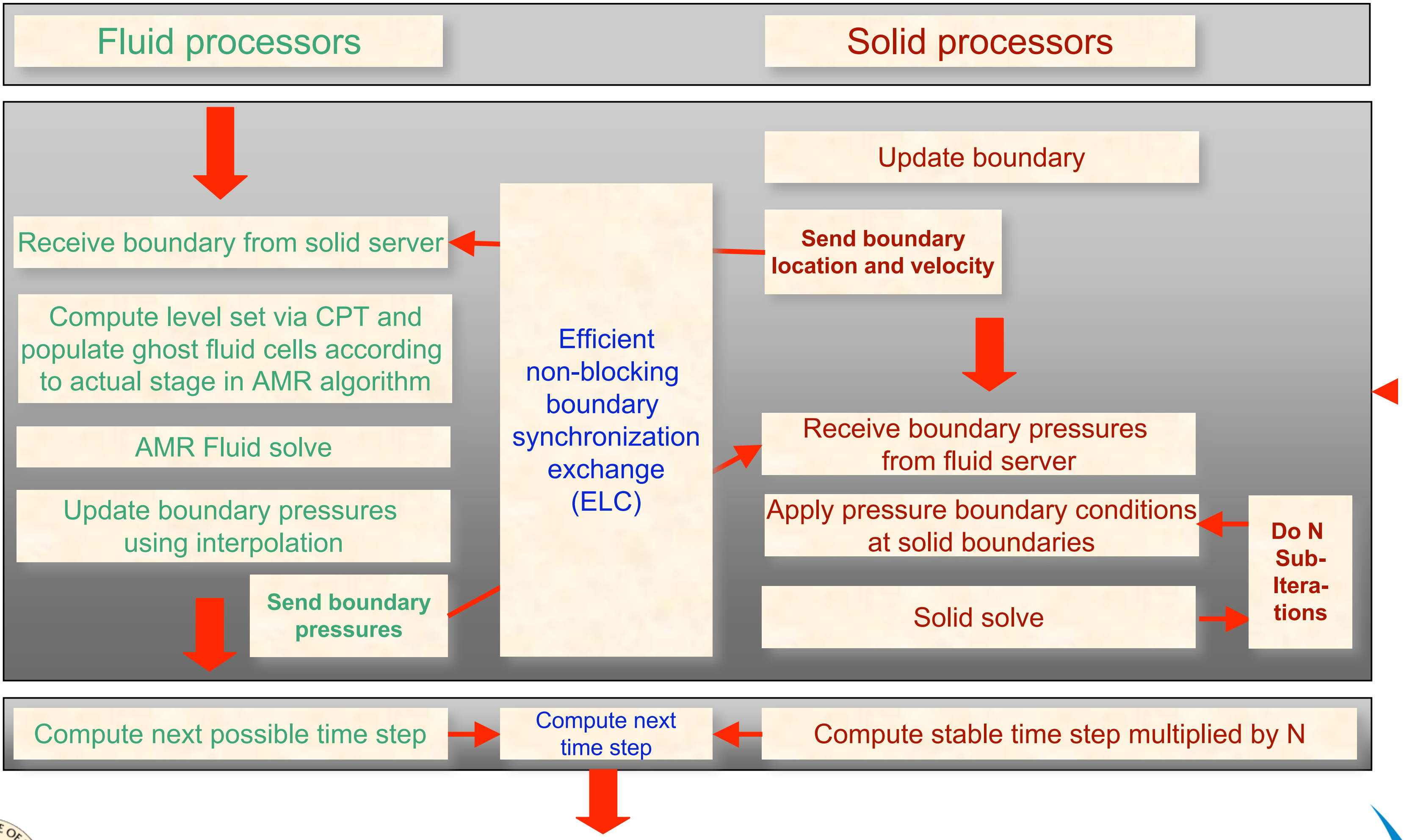
$\rho^F_{n,j-1}$	$\rho^F_{n,j}$	$\rho^F_{n,j}$	$\rho^F_{n,j-1}$
$u^F_{n,j-1}$	$u^F_{n,j}$	$2u^S_{n,j+1/2}-u^F_{n,j}$	$2u^S_{n,j+1/2}-u^F_{n,j-1}$
$u^F_{t,j-1}$	$u^F_{t,j}$	$u^F_{t,j}$	$u^F_{t,j-1}$
$p^F_{n,j-1}$	$p^F_{n,j}$	$p^F_{n,j}$	$p^F_{n,j-1}$

Velocity: $\mathbf{u}^F_{Gh}=2((\mathbf{u}^S-\mathbf{u}^F_M)\cdot \mathbf{n})\,\mathbf{n} + \mathbf{u}^F_M$



Left: Pressure field around an Onera M6 wing (angle of attack 3.06°) in Mach-0.8395 flow. Test simulation with Euler equations. Highest two SAMR levels not shown.

Time step flow chart



Fluid processors

Solid processors

Receive boundary from solid server

Compute level set via CPT and populate ghost fluid cells according to actual stage in AMR algorithm

AMR Fluid solve

Update boundary pressures using interpolation

Send boundary pressures

Efficient non-blocking boundary synchronization exchange (ELC)

Update boundary

Send boundary location and velocity

Receive boundary pressures from fluid server

Apply pressure boundary conditions at solid boundaries

Solid solve

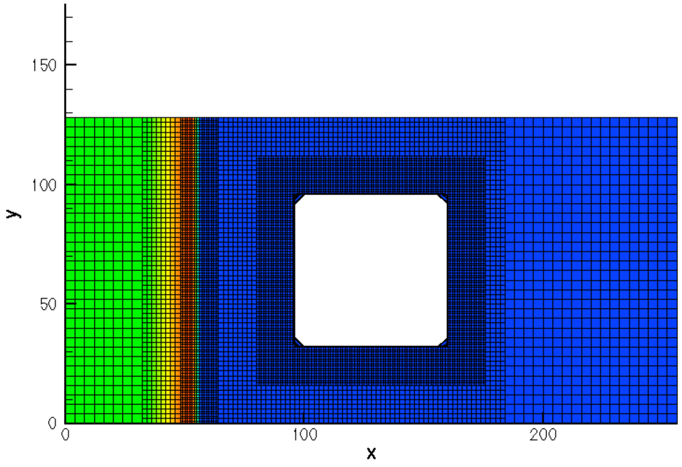
Do N Sub-Itera-tions

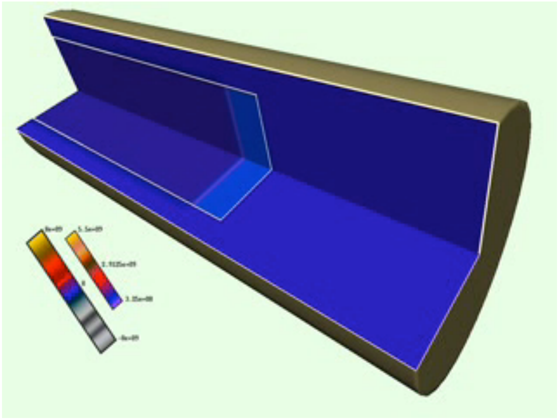
Compute next possible time step

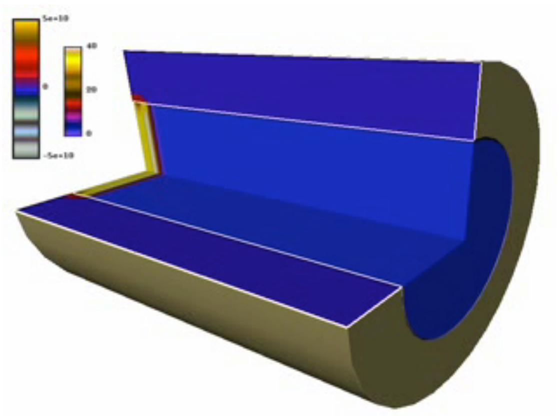
Compute next time step

Compute stable time step multiplied by N

Integrated simulation: 2-D coupled detonation with elastic shell



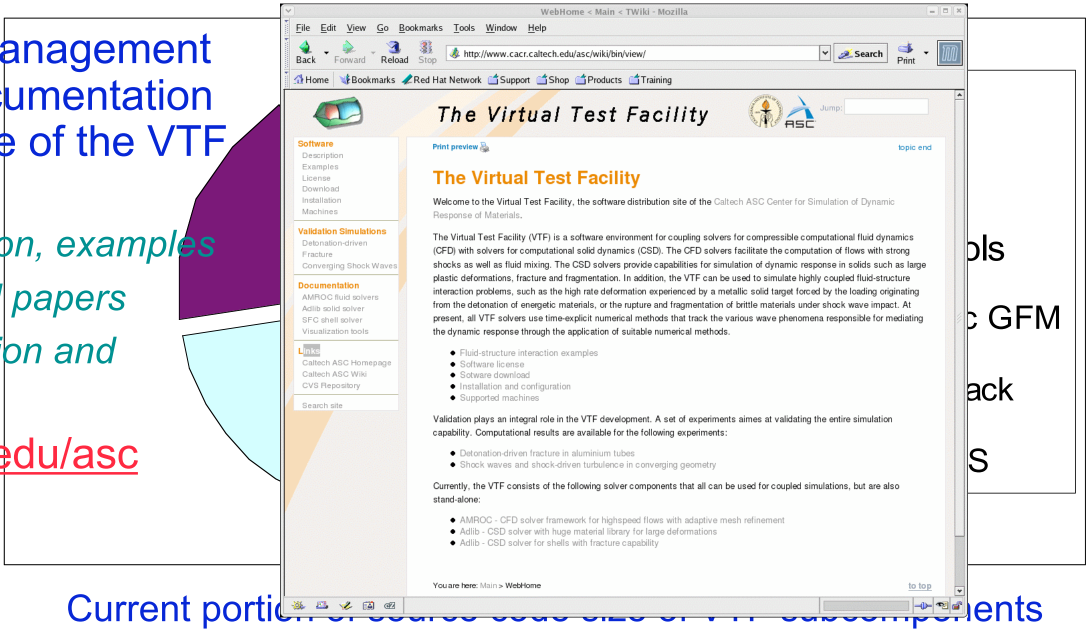




VTF Software statistics

- Language: object-oriented C++ with components in C, F77, F90. Size ~12MB
- ~430,000 lines of source code (ANSI)
- autoconf/ automake environment with full support for all ASC platforms

- Use an online content management system to create the documentation necessary for the release of the VTF software
  - *Installation, configuration, examples*
  - *Scientific and technical papers*
  - *Archival of key simulation and experimental results*
- http://www.cacr.caltech.edu/asc



The Virtual Test Facility

Welcome to the Virtual Test Facility, the software distribution site of the Caltech ASC Center for Simulation of Dynamic Response of Materials.

The Virtual Test Facility (VTF) is a software environment for coupling solvers for compressible computational fluid dynamics (CFD) with solvers for computational solid dynamics (CSD). The CFD solvers facilitate the computation of flows with strong shocks as well as fluid mixing. The CSD solvers provide capabilities for simulation of dynamic response in solids such as large plastic deformations, fracture and fragmentation. In addition, the VTF can be used to simulate highly coupled fluid-structure interaction problems, such as the high rate deformation experienced by a metallic solid target forced by the loading originating from the detonation of energetic materials, or the rupture and fragmentation of brittle materials under shock wave impact. At present, all VTF solvers use time-explicit numerical methods that track the various wave phenomena responsible for mediating the dynamic response through the application of suitable numerical methods.

- Fluid-structure interaction examples
- Software license
- Sotware download
- Installation and configuration
- Supported machines

Validation plays an integral role in the VTF development. A set of experiments aimes at validating the entire simulation capability. Computational results are available for the following experiments:

- Detonation-driven fracture in aluminium tubes
- Shock waves and shock-driven turbulence in converging geometry

Currently, the VTF consists of the following solver components that all can be used for coupled simulations, but are also stand-alone:

- AMROC - CFD solver framework for highspeed flows with adaptive mesh refinement
- Adlib - CSD solver with huge material library for large deformations
- Adlib - CSD solver for shells with fracture capability

You are here: Main > WebHome

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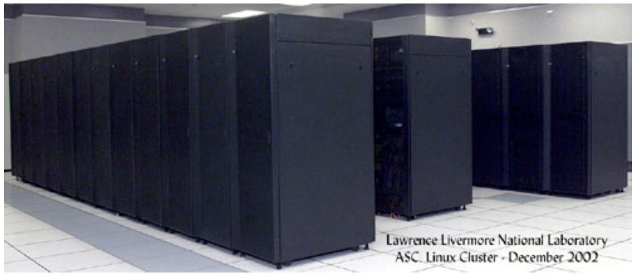
Current portion of source code size of VTF subcomponents

ASC platform specifics

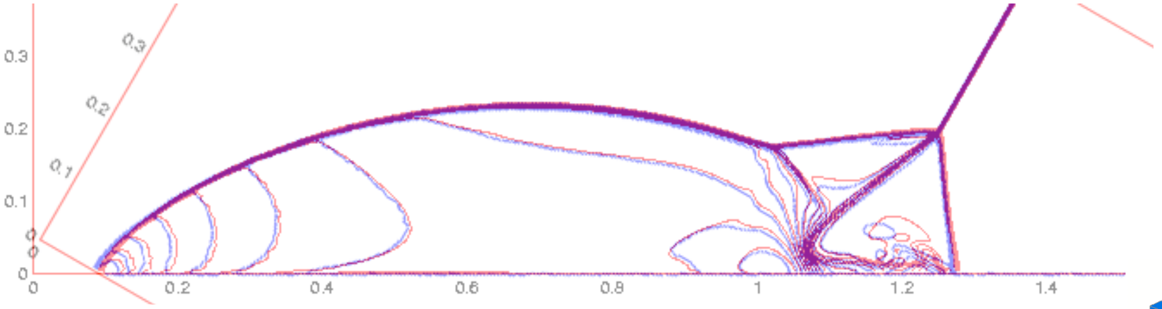
- LLNL’s Digital Linux cluster (Thunder)
  - *1024 node SMP, 1.4 GHz Itanium-2 (4 CPUs/node)*
  - *22.9 GB memory/node*
  - *~ 151 TB global parallel file system*

- LANL’s HP/Compaq Alphaserver ES45 (QSC)
  - *256 node SMP, 1.25 GHz Alpha EV6 (4 CPUs/node)*
  - *16 GB memory/node*
  - *~ 12 TB global file system*
  - *Quadrics network interconnect (QsNet)*
    - *2 mus latency*
    - *300 MB/sec bandwidth*

- LLNL’s Linux cluster (ALC)
  - *1920 processors, (2.4GHz Pentium 4)*
  - *4 GB memory/node*
  - *176 TB global parallel file system*
  - *Lustre file system*

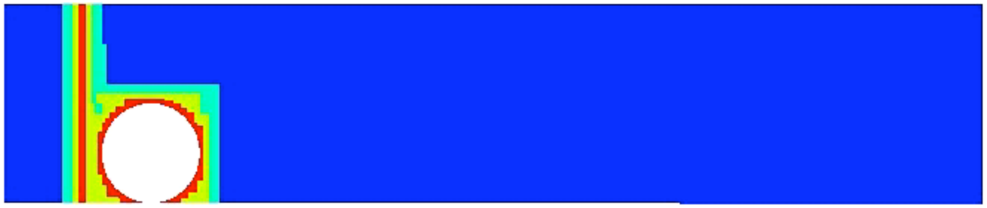


Verification of the VTF software



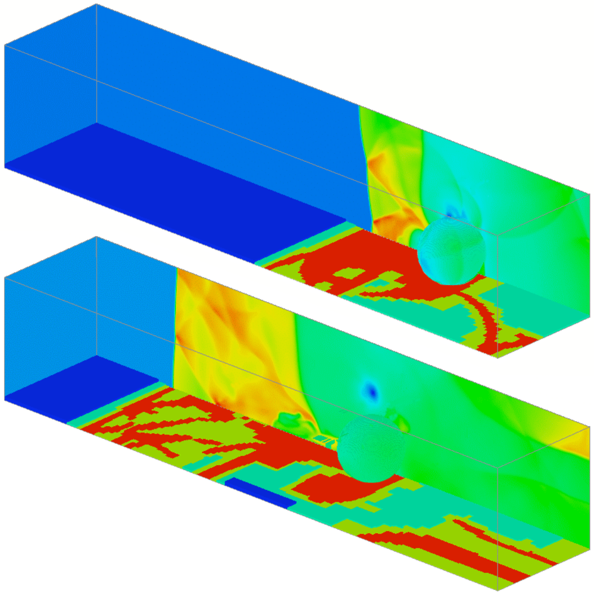
Overlay of two simulation of a Mach reflection on 800x400 grids with GFM (shown rotated) and 2nd order accurate scheme (initial conditions rotated)

Schlieren plot of density



3 additional refinement levels

Lift-up of a solid body in 2D and 3D when being hit by Mach 3 shock wave, Falcovitz et al. (1997)



Extension to 3D, color plot of density

- 640h CPU on Pentium-4 2.2GHz
- AMR base grid 150x30x30, 3 additional levels all with factor 2

Validation approach: coupling experiment to simulation

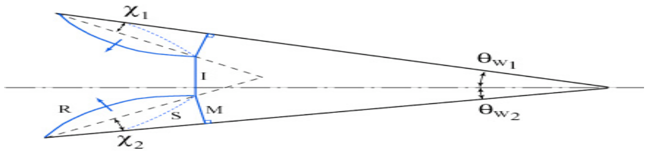
- Validating experiments / simulations
  - *Converging shock waves in fluids and solids*
  - *Detonation driven fracture*
  - *Shock dynamics of polycrystals*
  - *Brittle fracture*
- Integrated simulations
  - *Direct linkage with experiments*
  - *Validation-simulation-modeling reinforce one another*
  - *VTF solvers used in both stand-alone and coupled modes*

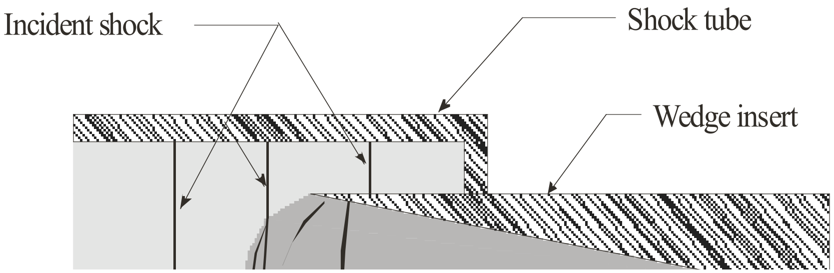
Why in-house experiments?

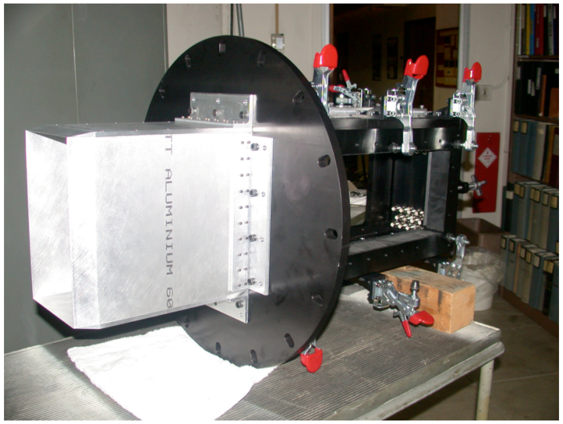
- Want to design well-instrumented benchmark experiments
    - *High level of temporal and spatial resolution*
- Ensure experimental results can be interpreted from the observational point of view
- Experimental results can be used to sharpen simulations and vice versa
- Provide real but reasonable challenges to simulation

Shock focusing and fluid instability in converging geometry

- Motivation
  - *Converging geometry essential component in high energy density physics*
- Expected validation data
  - *Mixing layer growth*
  - *Shock stability*
- Simulation and modeling needs
  - *Solid-fluid coupling (static)*
  - *Shock capturing methods*
  - *LES/SGS turbulence modeling*
- VTF elements
  - *AMR fluid solver*
  - *Solid-fluid coupling*
  - *New algorithms for shock-turbulence interaction*
  - *Multiscale modeling of turbulent mixing*

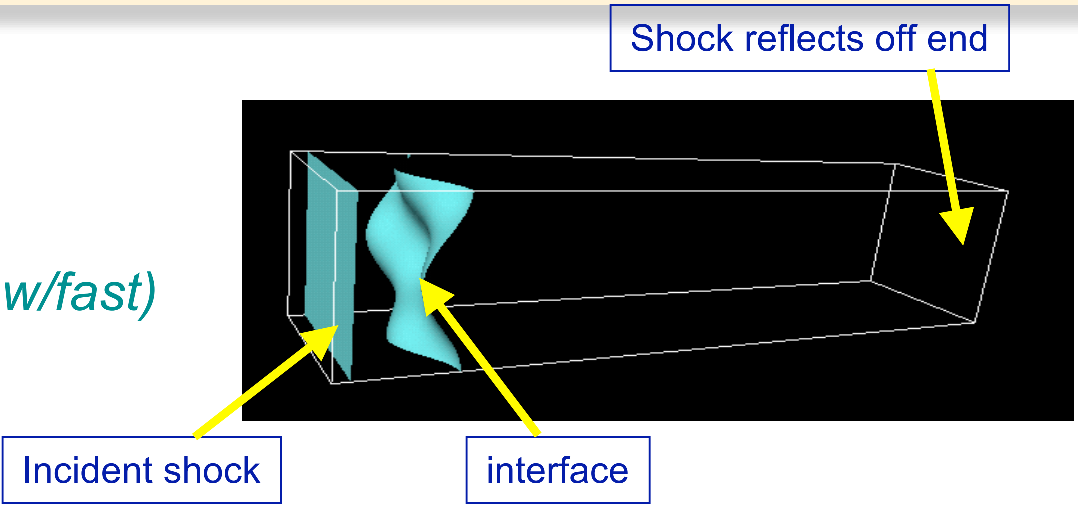


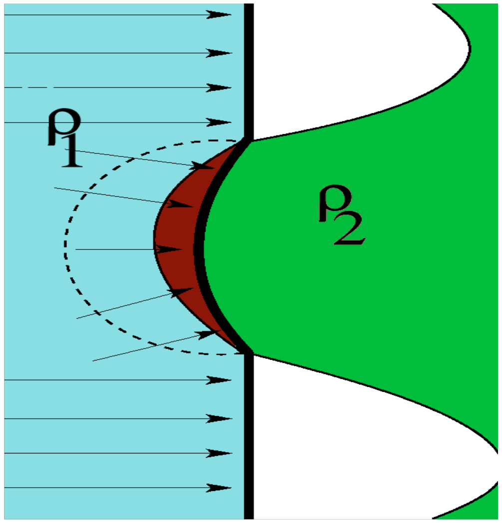




Richtmyer-Meshkov instability: a canonical example of compressible turbulence and mixing

- Strong shocks
- Density ratios
  - *heavy to light (slow/fast)*
  - *Light to heavy (fast/slow)*

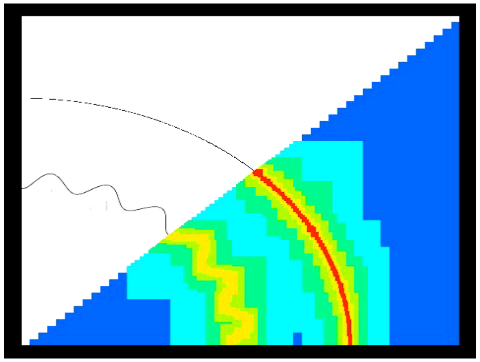


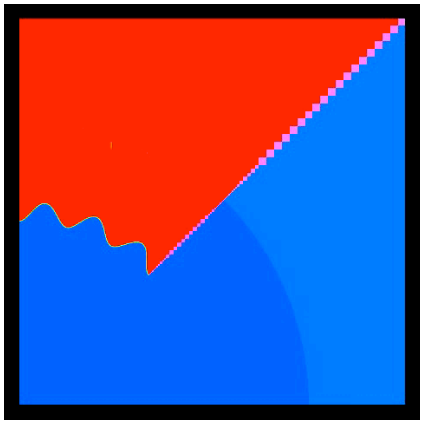


The interaction of a shock wave with a density gradient produces vorticity and then turbulence and mixing

Cylindrical R-M instability with AMROC

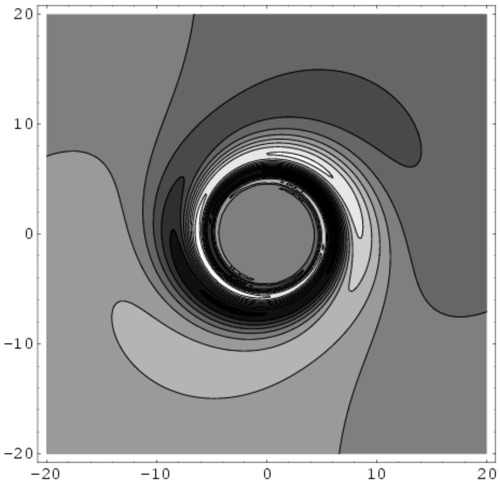
- Passage of the shock results in vorticity deposition by means of baroclinic generation
- Euler simulation
- Initial density interface ; sinusoidal perturbation corresponding to n = 24 on circle



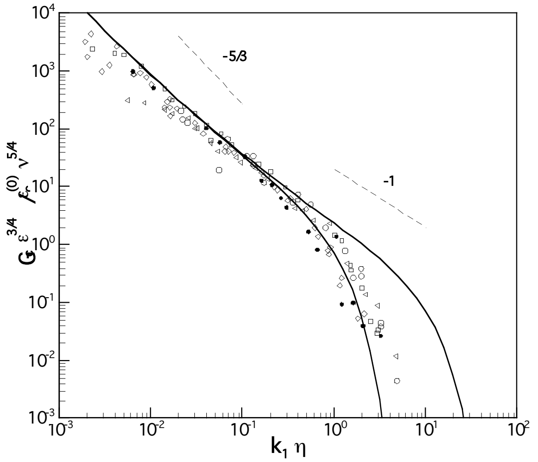


DNS of these flows is not possible – modeling is required

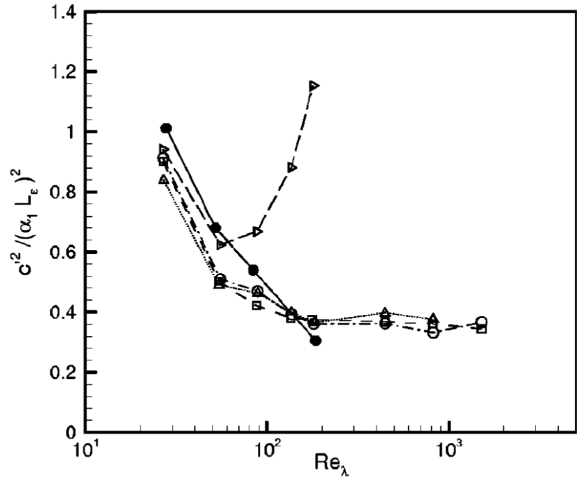
A multiscale approach to modeling of compressible turbulent mixing



Vortex mixing a scalar field



Obukhov-Corrsin/Batchelor scalar spectrum (Pullin, Lundgren)

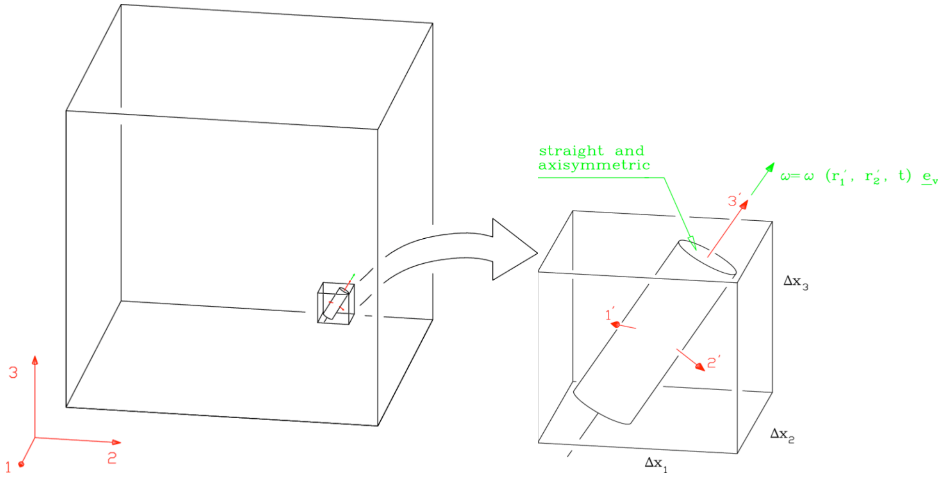


LES of scalar mixing
Pullin (2000)

Mixing transition
(Dimotakis 2000)

LES with stretched-vortex SGS model

- Structure-based approach
- Subgrid motion represented by nearly axisymmetric vortex tube within each cell.
- Align vortices depending on large scale vorticity, rate of strain
- Plug-in model: ease of implementation
- Subgrid stresses are:



$$T_{ij} = K\ (\delta_{ij} - e_i\, e_j)\,,$$

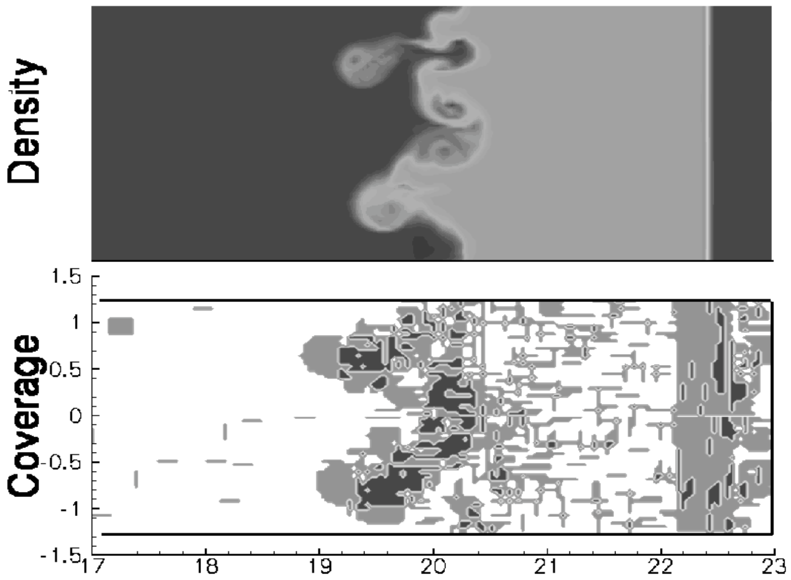
$$K = \int_{k_c}^{\infty} E(k)\, dk.$$

- Model parameters estimated locally by matching local resolved flow 2’nd-order velocity structure function to local subgrid estimate
- Subgrid strucure axes aligned with both resolved vorticity and eigenvector of principal resolved rate-of-strain
  - *Highly UnResolved Turbulence Simulation (HURTS)*

Hybrid WENO-TCDS algorithm: LES and strong shocks

- Numerical methods for shock-capturing and LES “orthogonal”.
- Our solution: hybrid technique: blending Weighted Essentially Non-Oscillatory (WENO) scheme with Tuned Centered-Difference (TCD) stencil.
- WENO in regions of very-large density ratio (Shocks)
  - *But WENO is not suitable for LES in smooth regions away from shocks.*
  - *Upwinding strategy is too dissipative*
- TCD stencil in smooth regions away from shocks
  - *Low numerical dissipation (centered method)*
  - *optimized for minimum resolved-scale discretization error in LES (Ghosal, 1996)*
  - *5- or 7-point stencil trades off formal order of accuracy for small dispersion errors*
- Target WENO stencil = TCD stencil
- In practice, target TCD stencil not always achieved; switch is used based on acceptable WENO smoothness measure
- Hybrid method designed for LES in presence of strong shocks

WENO-TCDS coverage



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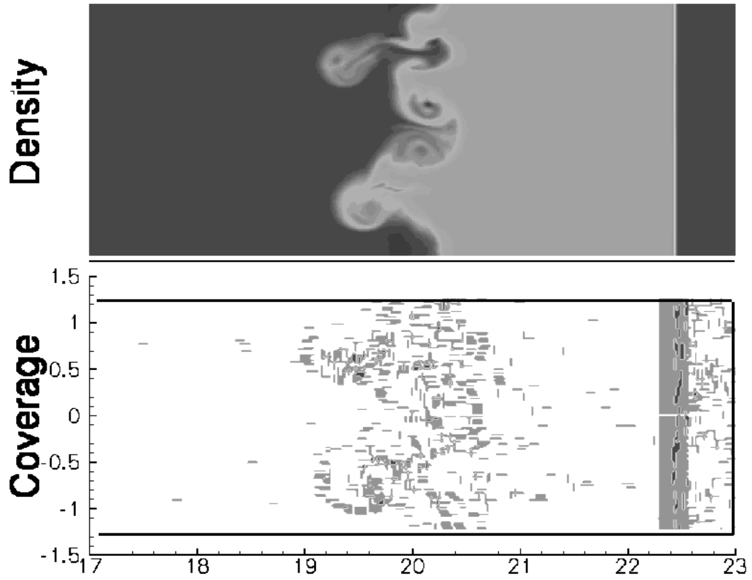
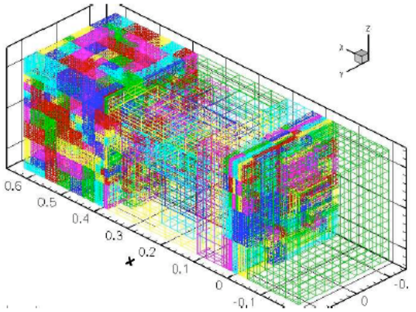


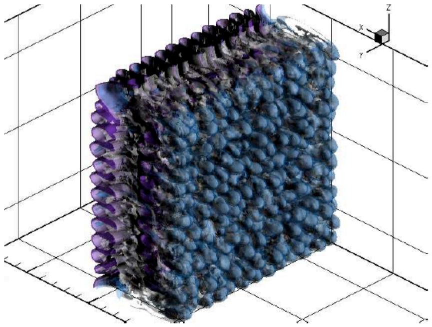
1024x128

VTF simulation of Richtmyer-Meshkov instability

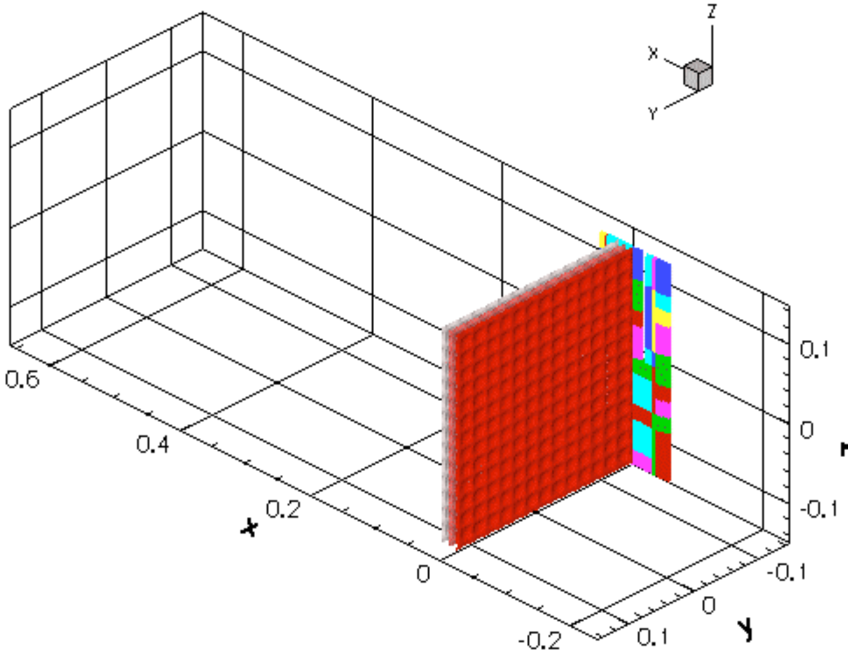
- Vetter & Sturtevant (1995) RMI with reshock off end wall
- Air/SF_6, Mach=1.5
- 3 levels of refinement

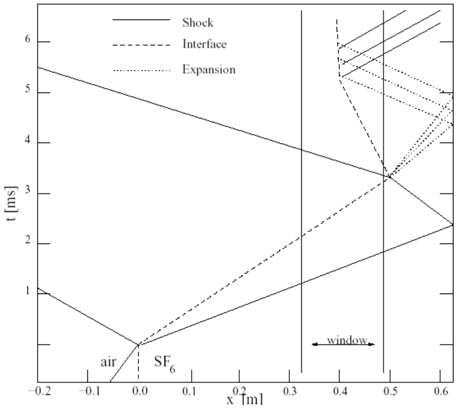


Mesh at one time

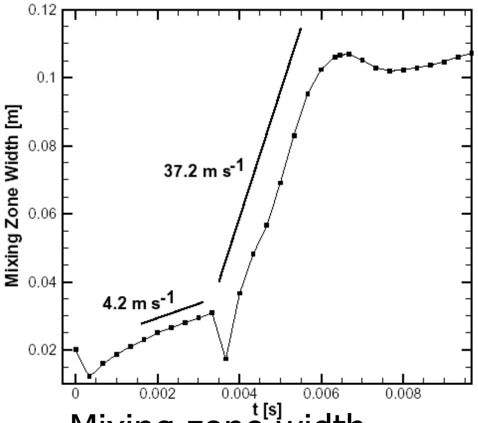


Interface at one time





Wave diagram

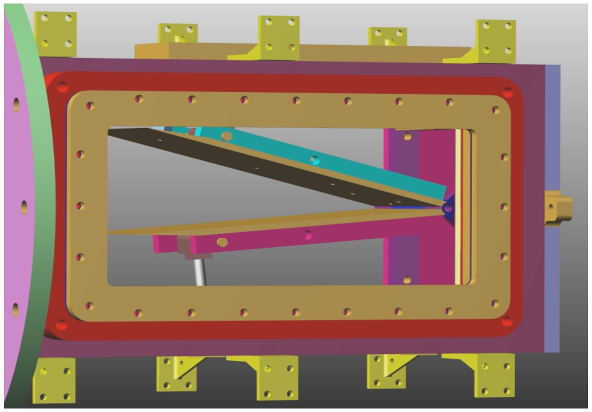


Mixing zone width

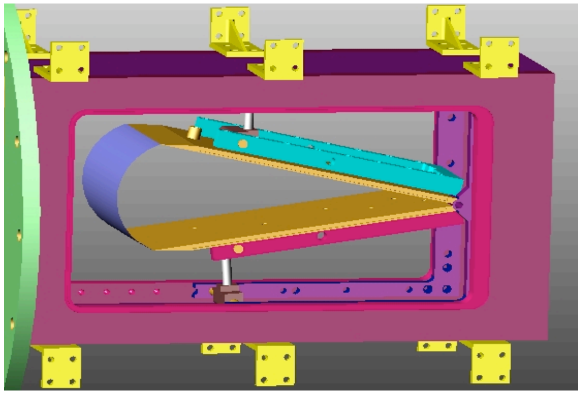
The converging shock experiment

Counts # of membranes

- Phase-0 (no membrane):
  - *Study of shock reflection, wave interaction, and compressible turbulence*
  - *Hinge plates can be set at angles between* 10º - 15º.
  - *Provides proof-of-concept for many experimental components as well as a valuable environment for the first set of validation tests*
- Phase-1:
  - *Shock refraction to produce converging shock*
  - *Hinge plates fitted with suitably shaped membrane*
  - *Test section and driven test gas mixtures must have different* W *and* γ *to achieve finite-amplitude wave cancellation.*
- Phase-2:
  - *Second circular membrane for study of interface instabilities (RMI) in converging flow*

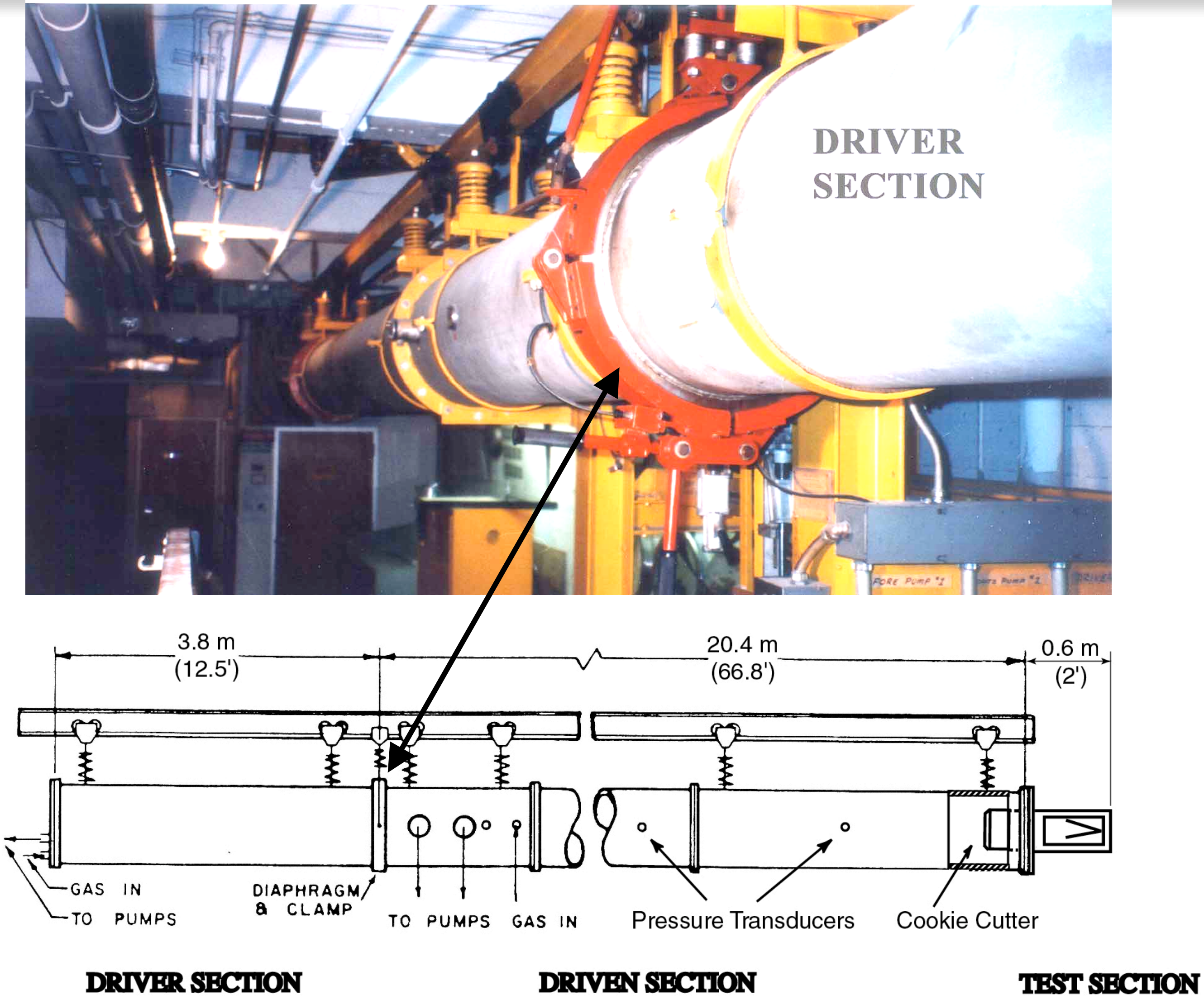


Phase 0

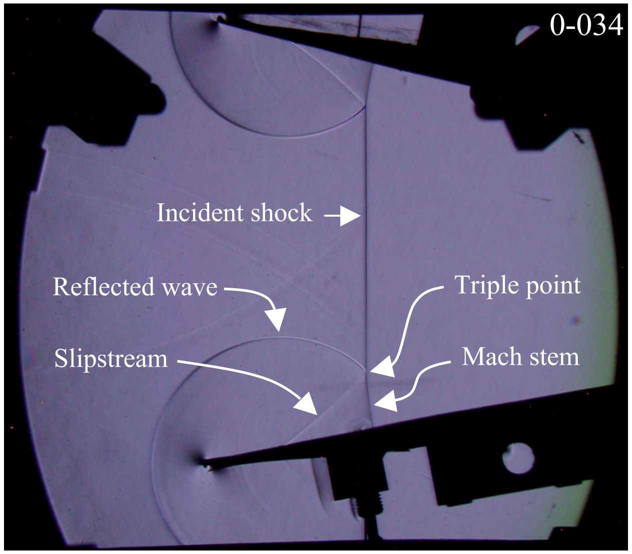


Phase 1

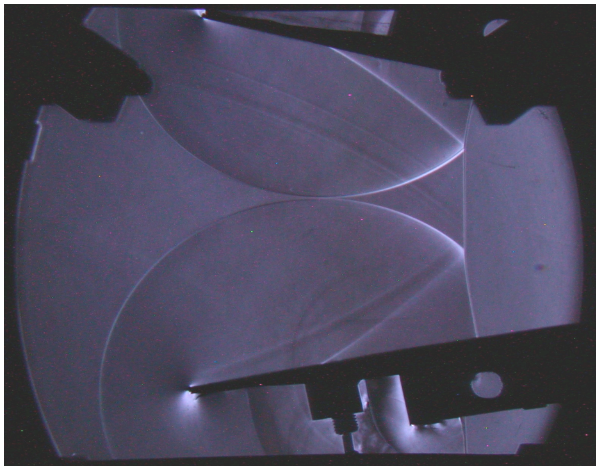
Experimental facility — *GALCIT 17" shock-tube*



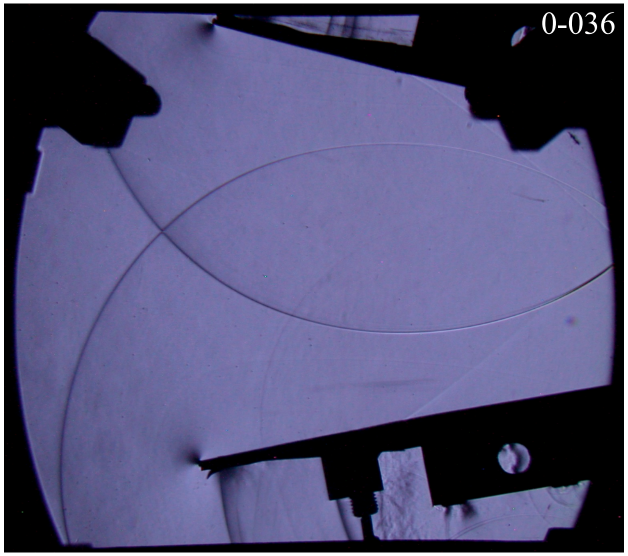
Phase-0 — *Experimental data*: $M_s \cong 1.5$



$M_s = 1.514 \pm 0.007$
$U_s = 531 \pm 2$ m/s



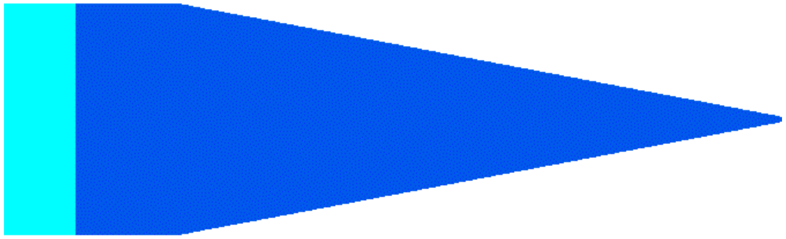
$M_s = 1.503 \pm 0.007$
$U_s = 527 \pm 2$ m/s



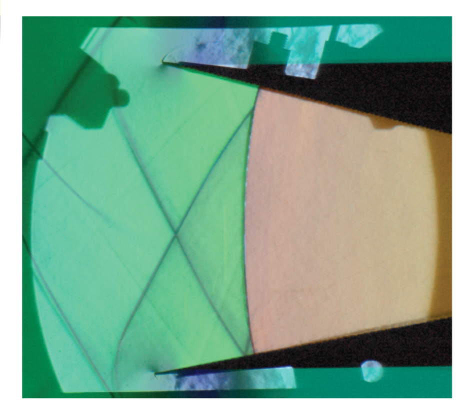
$M_s = 1.502 \pm 0.007$
$U_s = 527 \pm 2$ m/s

- Mach reflection pattern as expected for the experimental geometry and angles
- Schlieren images show:
  - *Incident planar shock*: $U_s \cong 0.53$ mm/μs
  - *Triple point*
  - *Mach stem*
  - *Reflected wave*
  - *Slipstream (shear layer)*
- Thin (laminar) boundary layers behind shock
  - *High-Re flow behind Mach-stem shock*
  - $\chi_2 \cong 17.5° \pm 0.2°$
- Also discernible:
  - *Portion of incident shock propagating outside hinge-plate assembly*
  - *Small disturbance from small opening on bottom plate used to inject helium to tune schlieren system*

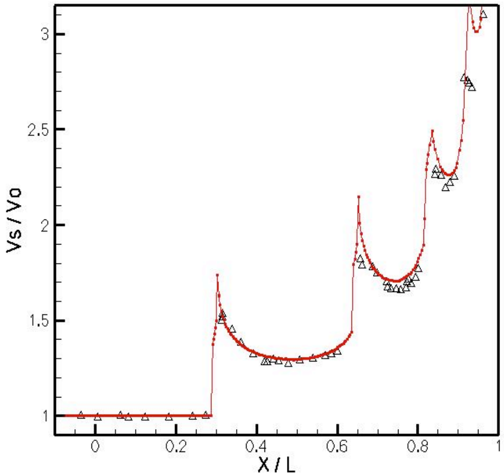
VTF converging shock validation



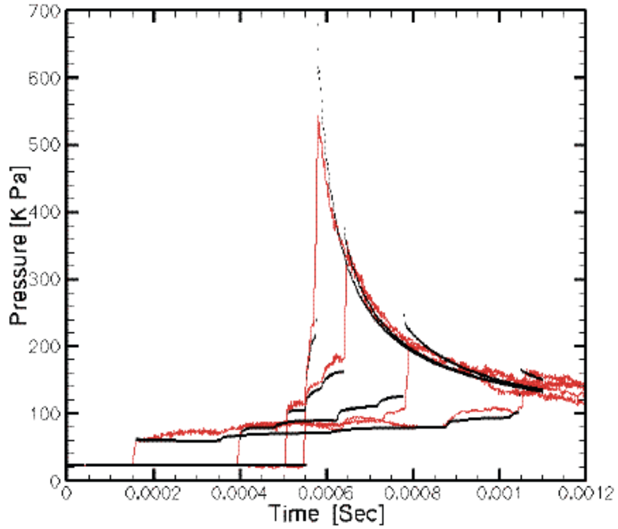
VTF simulation of conical converging shock



Overlay of experimental Schlieren and simulation

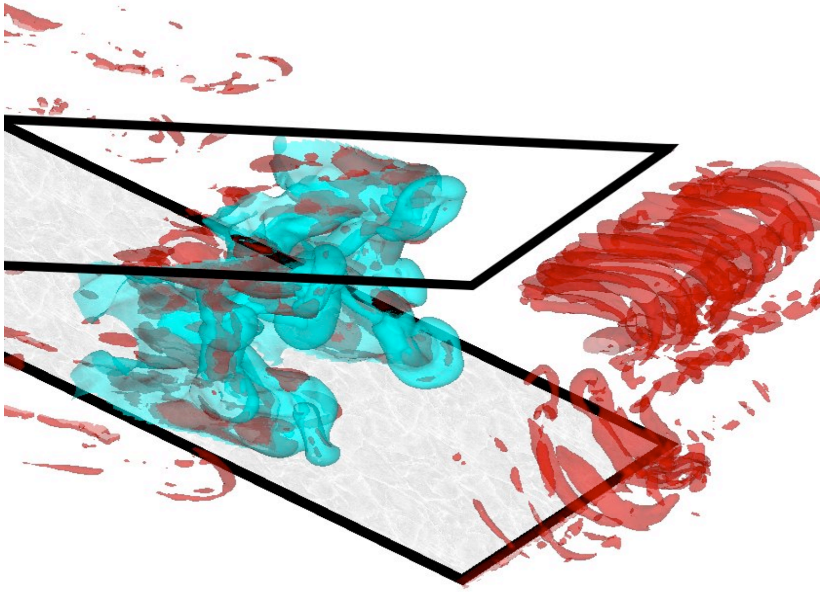


Comparison with experiment of Setchel et al

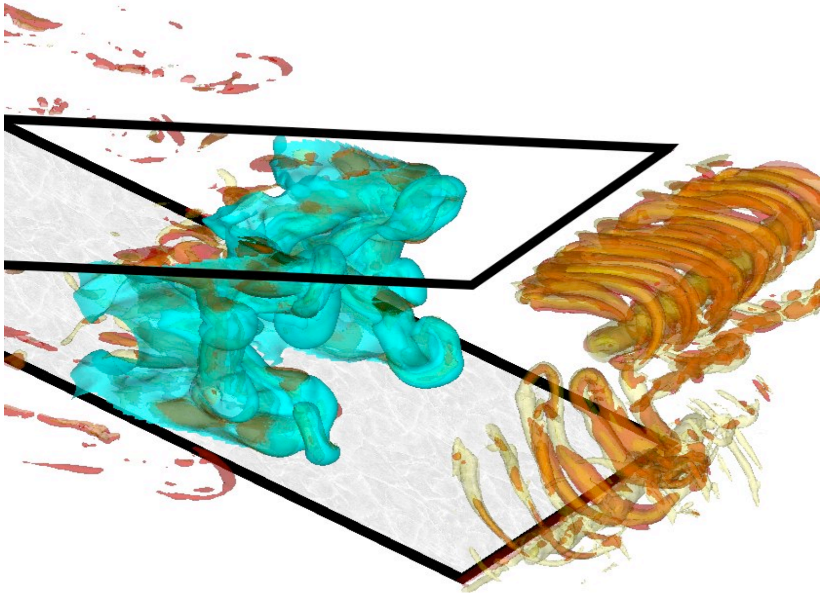


Comparison of pressure trace data

The next step: validation of turbulent R-M instability

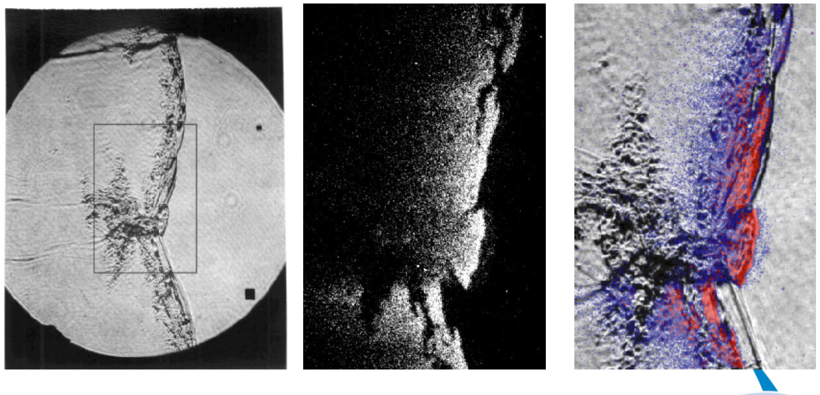


Mixing interface and SGS activity



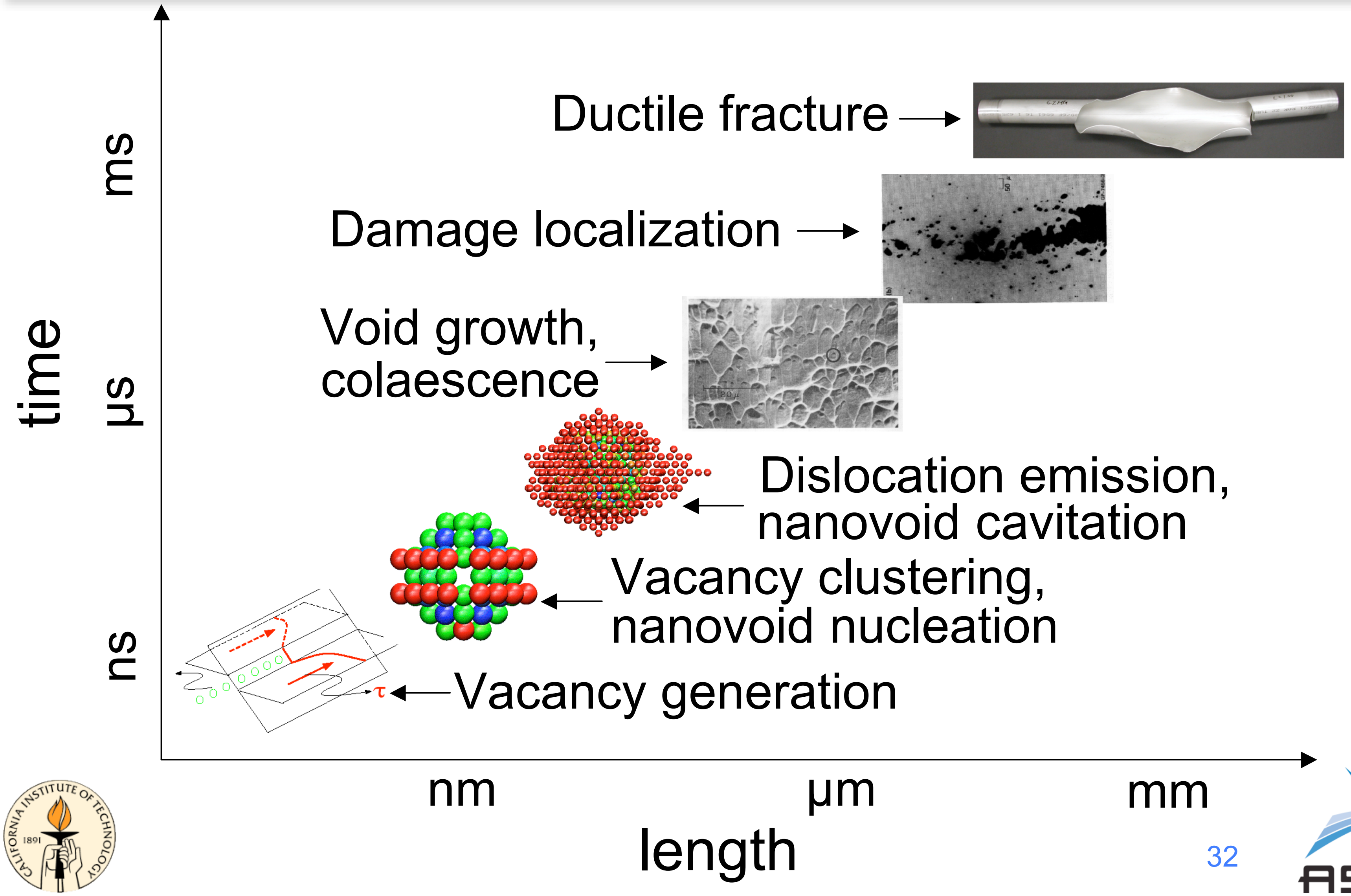
Vorticity and SGS activity

Detonation driven fracture



- Motivation
  - *Interaction of detonation, ductile deformation, fracture*
- Expected validation data
  - *Stress history of cylinder*
  - *Crack propagation history*
  - *Species concentration and detonation fine structure*
- Simulation and modeling needs
  - *Modeling of gas phase detonation with complex chemistry*
  - *Multiscale modeling of ductile deformation and rupture*
- VTF elements
  - *AMR fluid mechanics*
  - *Reduced chemistry modeling for combustion*
  - *Solid-fluid coupling algorithm*
  - *Shell elements with cohesive capability for fracture*
  - *Multiscale model of ductility*

Ductile fracture lengthscale hierarchy



Ductile fracture

Damage localization

Void growth,
colaescence

Dislocation emission,
nanovoid cavitation

Vacancy clustering,
nanovoid nucleation

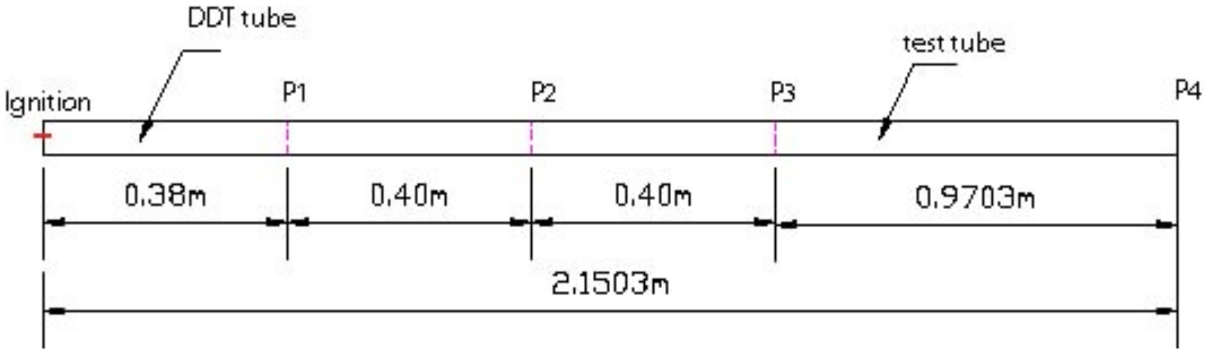
Vacancy generation

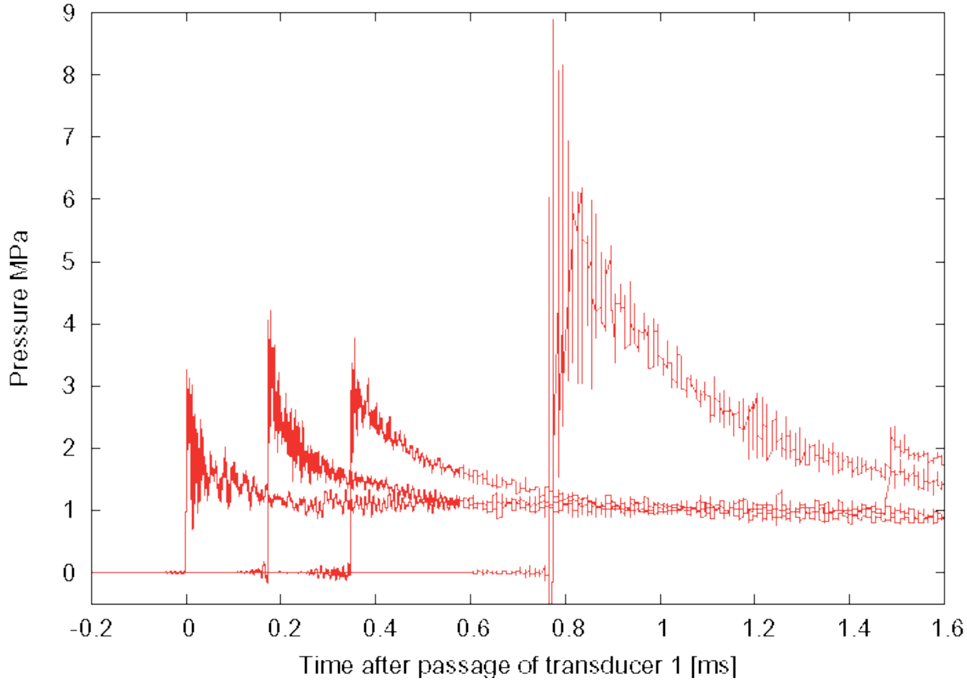
Detonation modeling

- Modeling of detonation with constant volume burn detonation model by C. Mader (1979)
  - *Equation of state for Euler equations:* $p = (\gamma-1)(\rho e - \rho Y q0)$
  - *No explicit source term, but linear enforcing of CJ state*
  - *Model eliminates von Neumann state completely, but detonation velocity is always correct, independent of the resolution*
- Verification of CV burn model with one-step reaction model
  - *Arrhenius kinetics:* $kf(T) = k \exp(-EA/RT)$
  - *Chosen parameters: EA=25,000 J/mol, k=20,000,000 1/s*

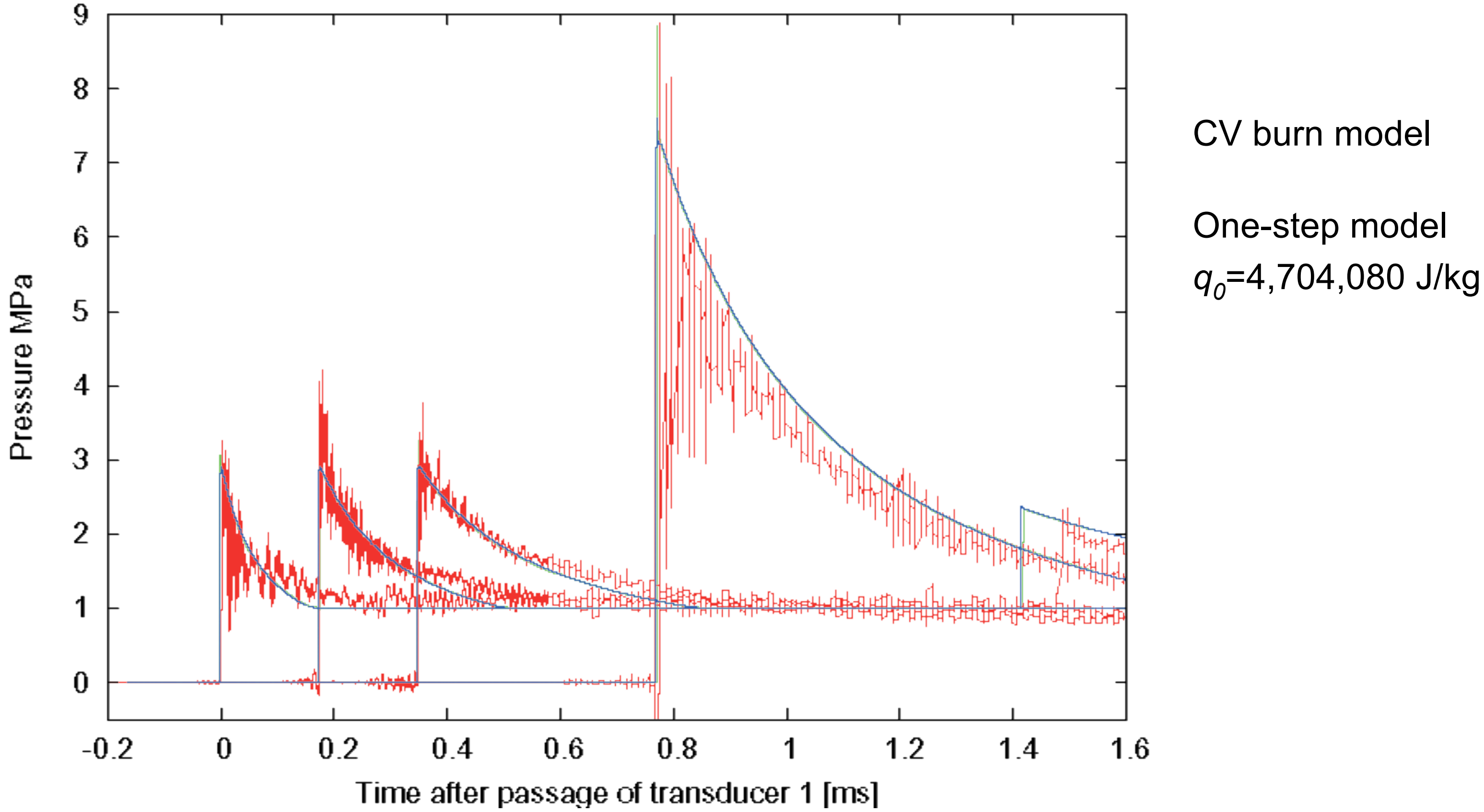
CV burn model verification and validation

- Experimental configuration with 4 pressure transducers
- Test tube closed at upper (different to detonation-driven fracture experiments)
- p_0=100kPa
- u_{det}= 2291.7 m/s (measured), u_{CJ}=2376 m/s
- Detonation propagation from left to right
- Right graphic: pressure traces at P1, P2, P3, P4 (from left to right)





CV burn model verification and validation: γ=1.24



- Excellent agreement between CV burn model and one-step reaction model results for incident detonation wave
- Discrepancy for propagation velocity of reflected, non-reactive shock wave between simulations and experiment

- p_0=100kPa
- u_{det}= 2291.7 m/s (adjusted to experimentally measured velocity)
- γ=1.24 (value at CJ point)

Coupled Fracture Simulation - Shot 136

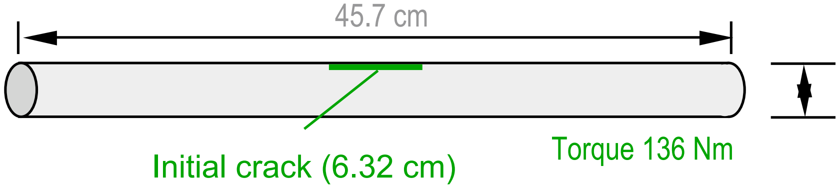
- C2 H4+3 O2 CJ detonation for p0=180kPa drives tube fracture
- Motivation: Full configuration

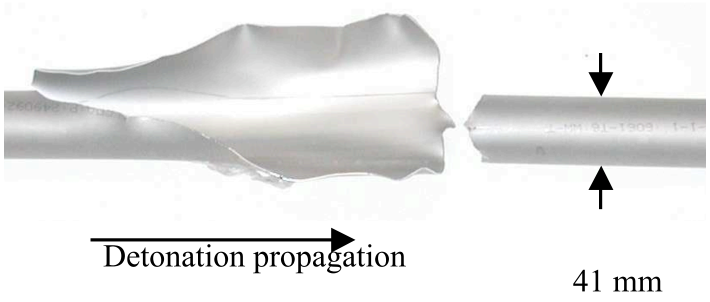
Fluid

- Constant volume burn model
- 40x40x725 cells unigrid

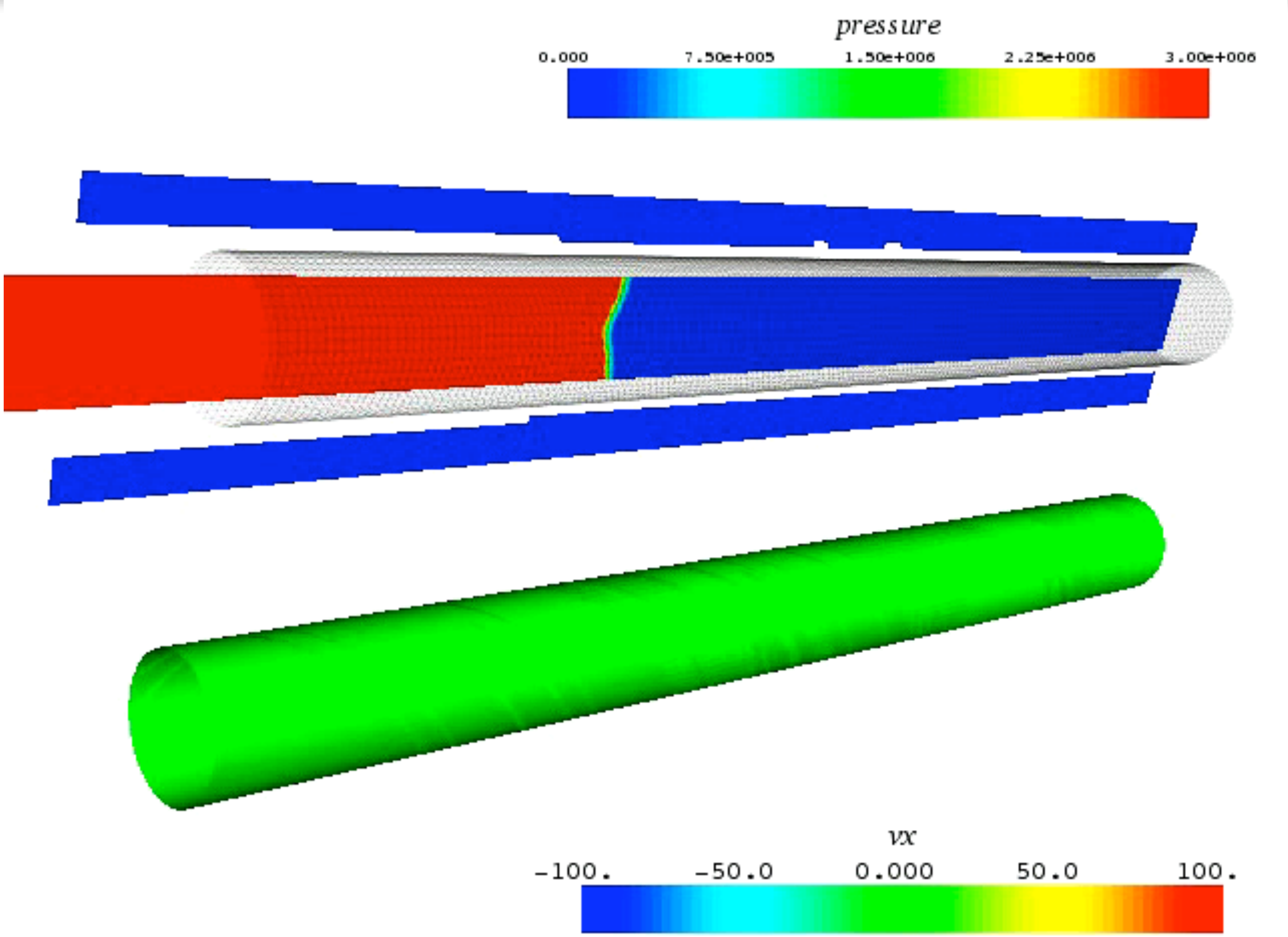
Solid

- Aluminum, J2 plasticity with hardening, rate sensitivity, and thermal softening
- Material model for cohesive interface: Linearly decreasing envelope
- Mesh: 206208 nodes
- 27 nodes ALC with 33 shell and 21 fluid processors
- Ca. 972h CPU





Coupled Fracture Simulation - Shot 136

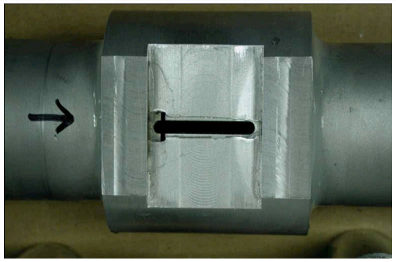


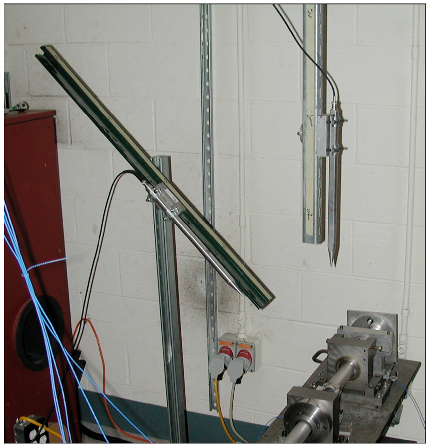
Fluid solver validation - venting event

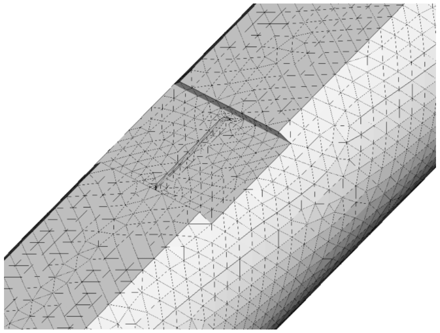
- $C_2 H_4 + 3 O_2$ CJ detonation for p0=100kPa expands into the open through fixed slot
- External transducers to pick up venting pressure
- Motivation:
  - *Validate 3D fluid solver with detonation model*

Simulation

- 2nd order upwind finite volume scheme, dimensional splitting
- AMR base level: 108x114x242, 4 additional levels, refinement factor 2,2,2,2
- Approx. $6 \cdot 10^6$ cells used in fluid on average instead of $12.2 \cdot 10^9$ (uniform)
  - *Tube and detonation fully refined*
  - *No refinement for $z<0$ (to approximate Taylor wave)*
  - *No maximal refinement for $x>0.1125m$, $y>0.1125m$, $z<0.37m$, $z>0.52m$*
- Solid mesh: 28279 nodes, 56562 elements
- 16 nodes 2.2 GHz AMD Opteron quad processor, Infiniband network, ca. 3300h CPU to t=3000 μs



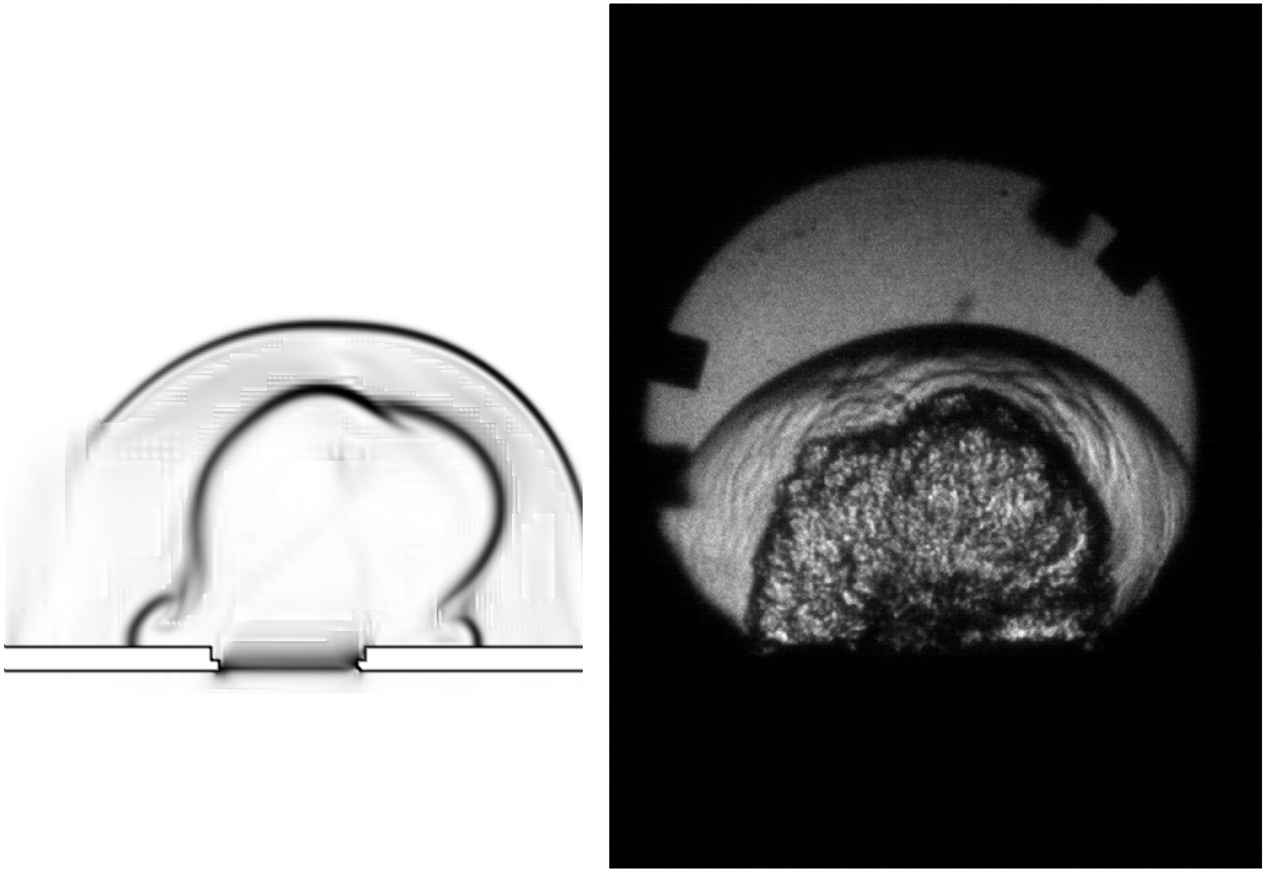




Venting event – computational results

Schlieren plot of flow through slot

Venting event – computational results



Comparison of simulated and experimental results at t=60μs

Fluid-structure interaction validation – tube with flaps

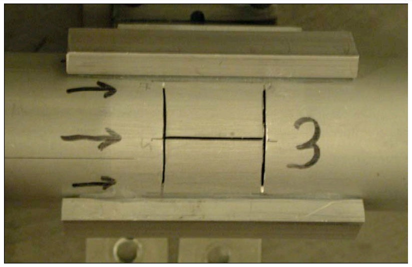
- $C_2 H_4 + 3 O_2$ CJ detonation for p0=100kPa drives plastic opening of pre-cut flaps
- Motivation:
  - *Validate fluid-structure interaction method*
  - *Validate material model in plastic regime*

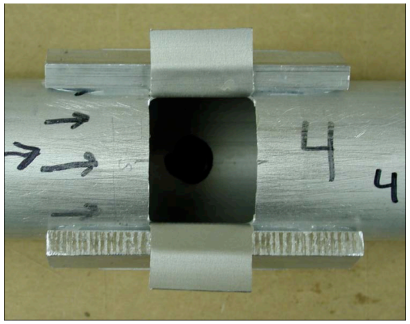
Fluid

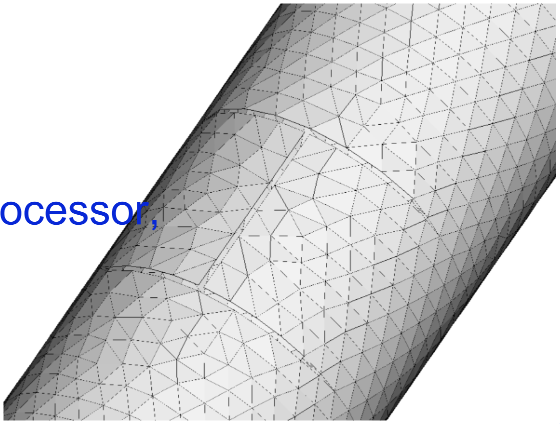
- Constant volume burn model
- AMR base level: 104x80x242, 3 additional levels, factors 2,2,4
- Approx. $4 \cdot 10^7$ cells instead of $7.9 \cdot 10^9$ cells (uniform)
- Tube and detonation fully refined
- Thickening of 2d mesh: 0.81mm on both sides (real thickness on both sides 0.445mm)

Solid

- Aluminum, J2 plasticity with hardening, rate sensitivity, and thermal softening
- 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 μs





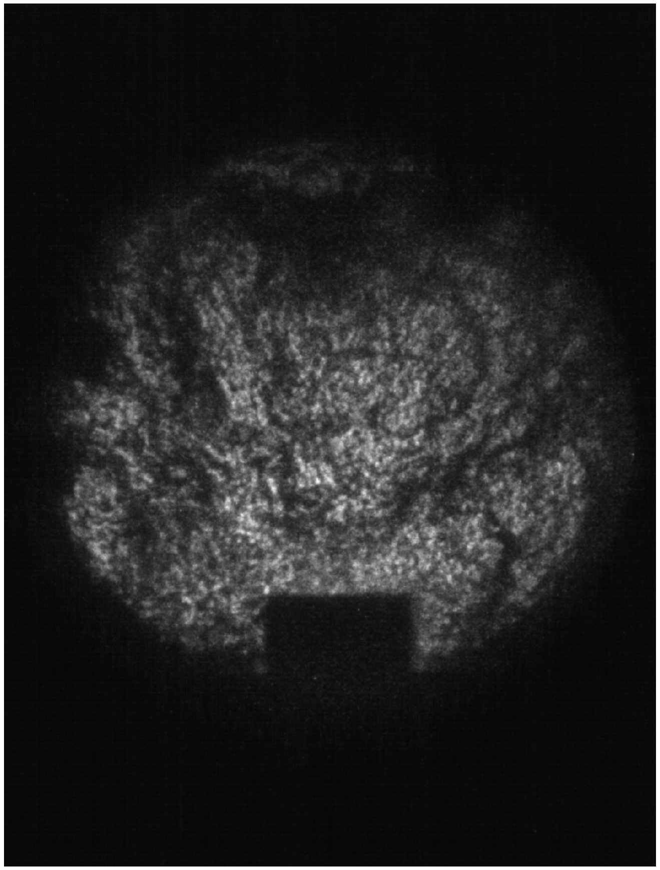


Tube with flaps – computational results

Schlieren plot of flow and shadow of deforming solid mesh

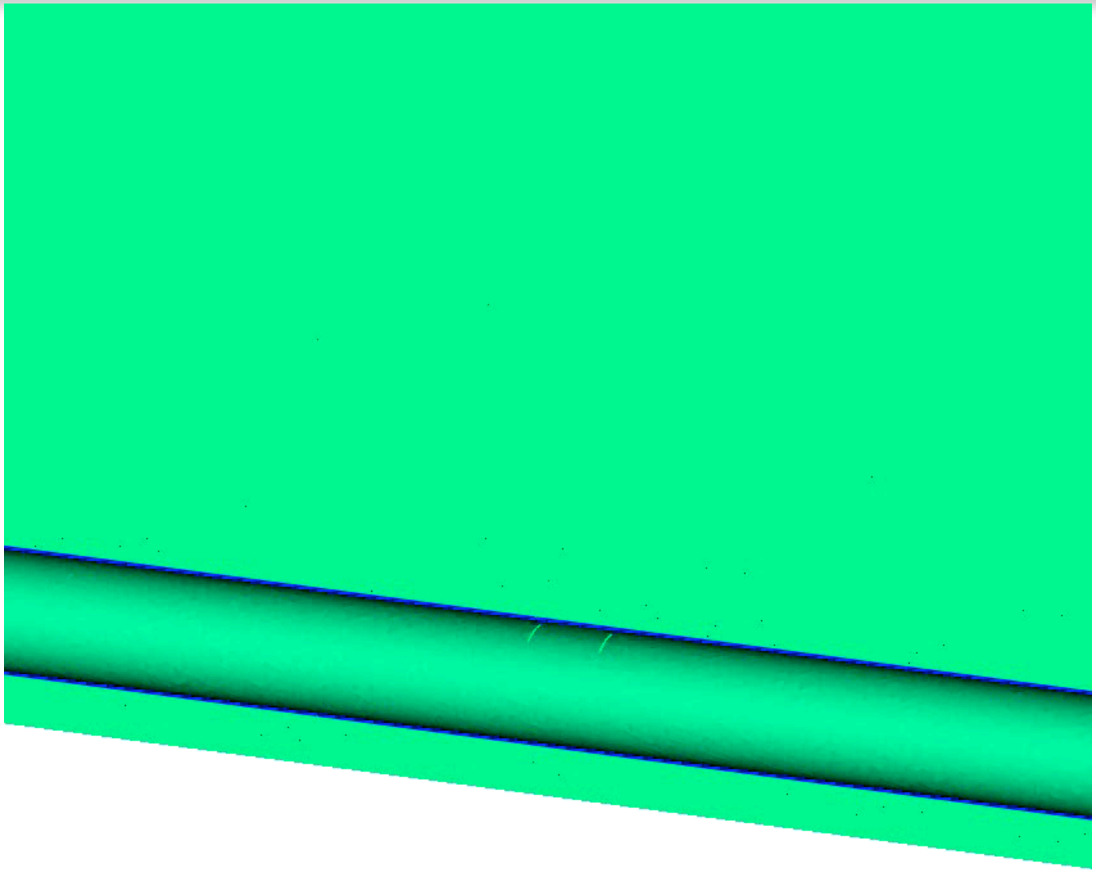
Tube with flaps – computational results

Simulated results at t=[illegible]μs



Experimental results at t=[illegible]μs

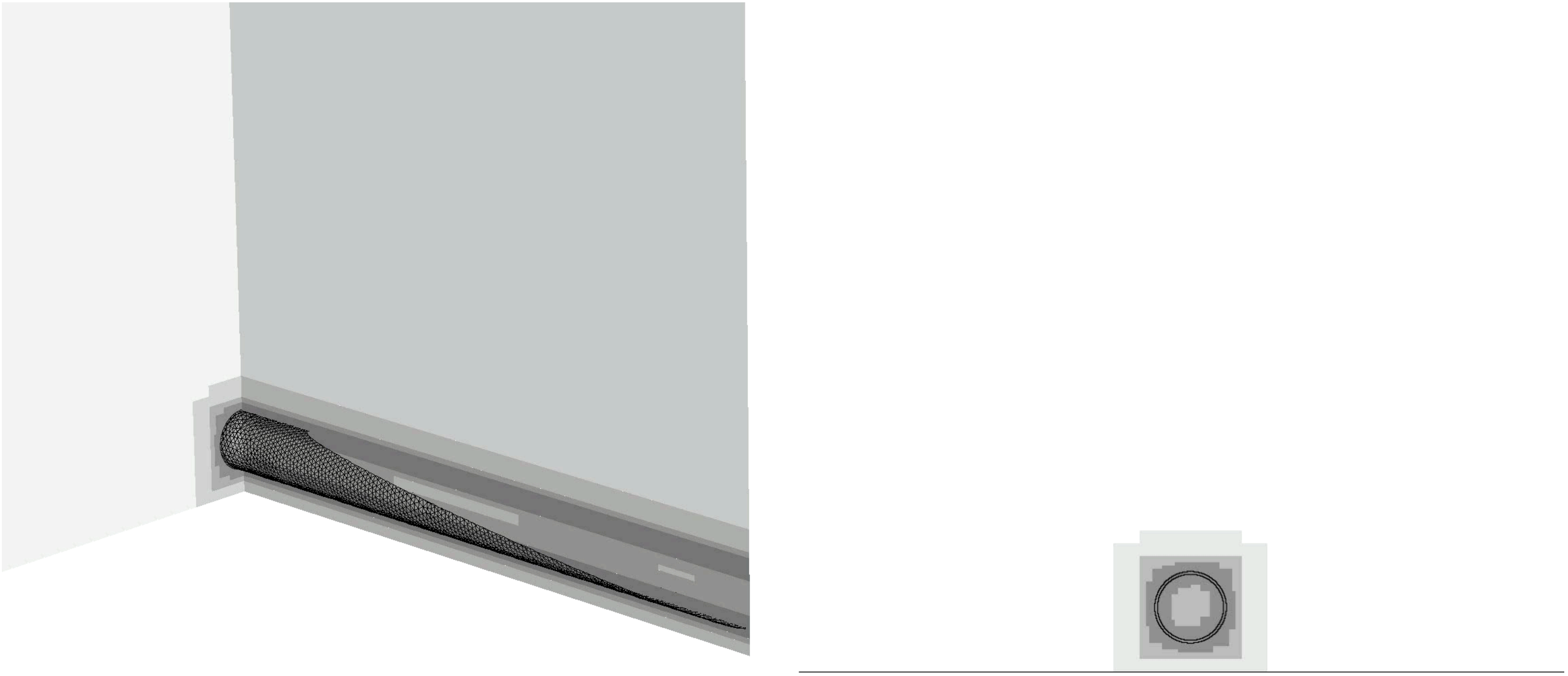
Tube with flaps – computational results



Fluid density and displacement in y-direction in solid

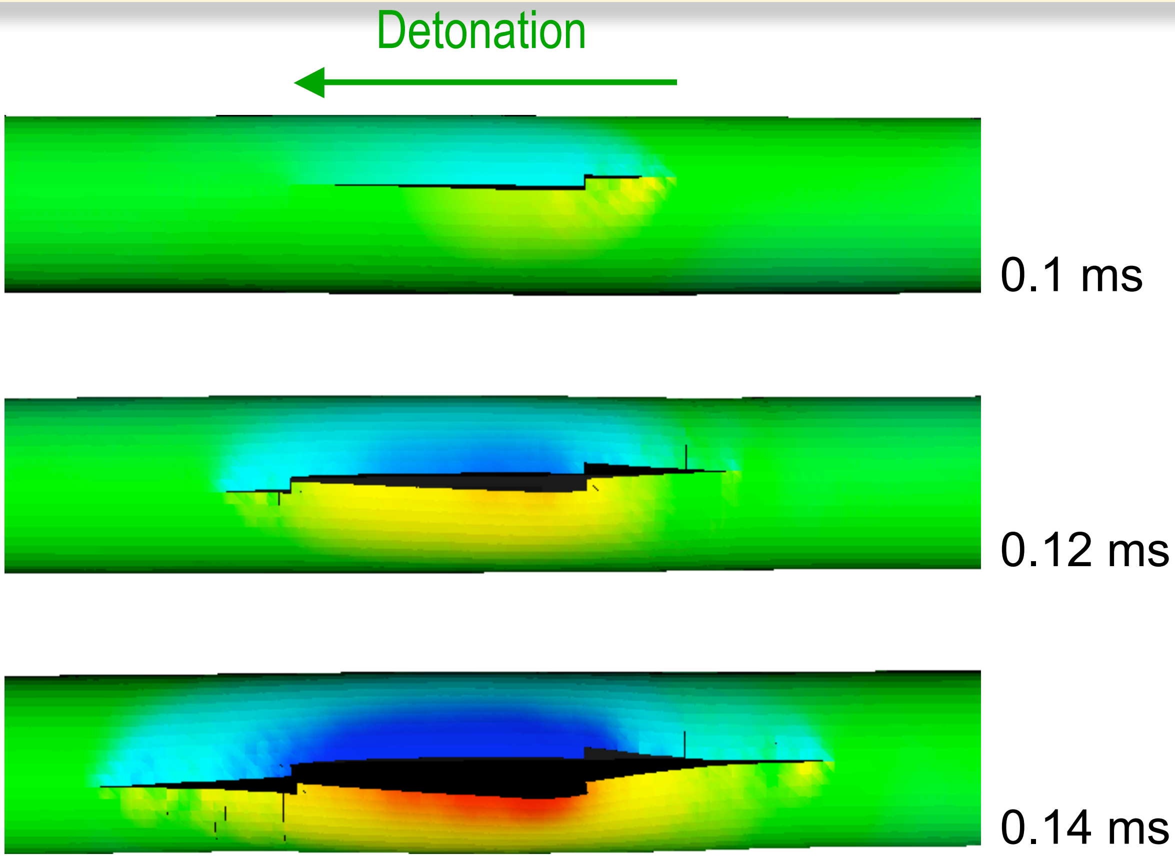
- *Excellent agreement for flow field and flap deformation between coupled simulation and experiments for t<300 μs*
- *For t>300 μs the plastic solid material deformation is incorrect (swing back of flaps is qualitatively wrong, cf. movie)*

Tube with flaps – fluid mesh adaptation



Schlieren plot of fluid density on refinement levels

Simulation of crack propagation remains a challenge



- *Crack path in qualitative agreement with the experiment*
- *Crack speeds are ~2-3 x higher than experimentally observed*
- *Fragmentation of fracturing material is incorrect*

Summary and conclusions

- Multiscale modeling as a promising approach towards predictive simulation
  - *Fluid mechanics*
  - *Solid mechanics*
  - *Solid-fluid coupling*
- Integration of validation and simulation
  - *Simulation contributes to the design of experiments*
  - *Iterative improvement of modeling and experiment*
  - *Role of high performance computation*
    - *High resolution diagnosis of multiscale models*
    - *Validation of multiscale models at macroscale*
- Many open questions remain
  - *Can we develop multiscale models for engineering applications?*
  - *What are the computational requirements?*
  - *What is the right computational paradigm?*
  - *Are there intrinsic limits to prediction?*
  - *If so can we rigorously bound effects that are not resolved?*