Towards simulation of detonation-induced shell dynamics with the Virtual Test Facility

Ralf Deiterding, Fehmi Cirak, Dan Meiron
Caltech

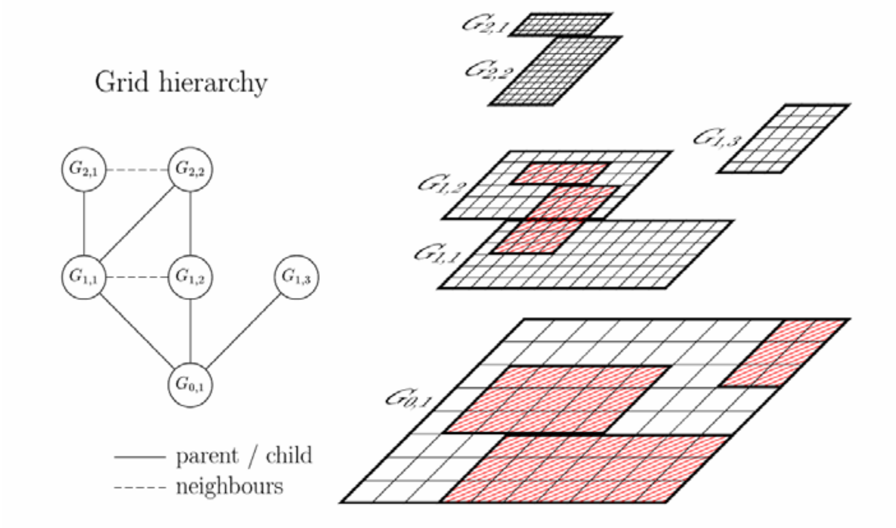
Comref 2005, Heidelberg
Jan. 27, 2005

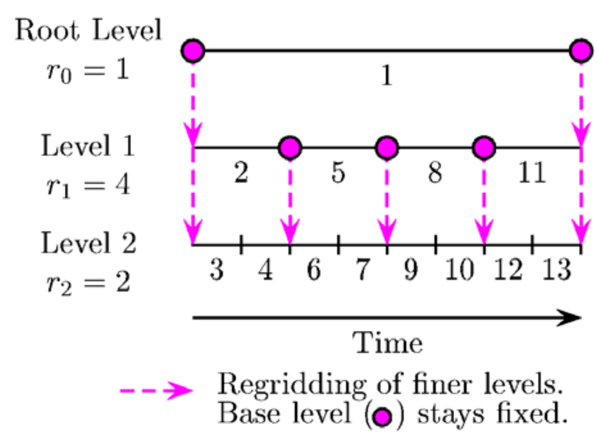
Outline of presentation

- Detonation simulation
  - *Governing equations*
  - *A reliable Roe-type upwind scheme*
  - *Validation via cellular structure simulation in 2D and 3D*
  - *Work mostly supported by German priority research program “Analysis und Numerik von Erhaltungsgleichungen”*
  - *R. Deiterding, **Parallel adaptive simulation of multi-dimensional detonation structure**, PhD thesis, BTU Cottbus, 2003. → http://www.cacr.caltech.edu/~ralf*
- Structured Adaptive Mesh Refinement (SAMR)
- Moving embedded complex boundaries
  - *Ghost fluid method*
  - *Validation*
- Fluid-structure coupling
  - *Efficient level-set construction*
  - *Incorporation of coupling scheme into SAMR*
  - *Outline of implementation*
- Detonation-induced dynamic shell response
  - *Preliminary elastic investigation*

Structured AMR- AMROC

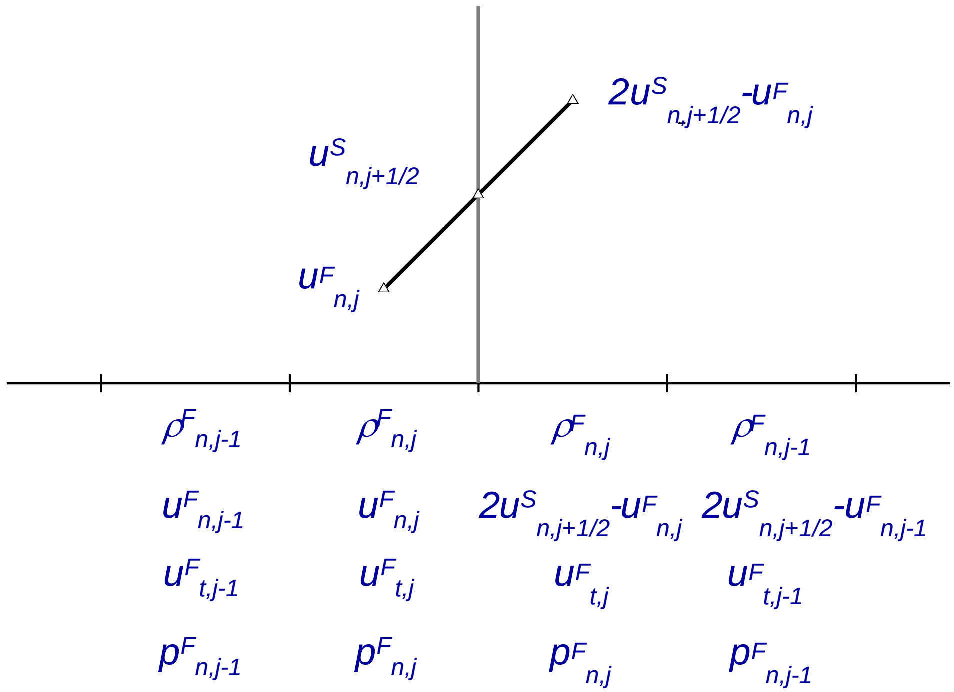
- Framework for dynamically adaptive structured finite volume schemes
  - *http://amroc.sourceforge.net*
- Provides Berger-Collela AMR
  - *Hierarchical multi-level approach*
  - *Time step refinement*
  - *Conservative correction at coarse-fine interface available*
- Provides ghost fluid method
  - *Multiple level set functions possible*
  - *Fully integrated into AMR algorithm*
  - *Solid-fluid coupling implemented as specialization of general method*
- Hierarchical data structures
  - *Refined blocks overlay coarser ones*
  - *Parallelization capsulated*
  - *Rigorous domain decomposition*
- Numerical scheme only for single block necessary
  - *Cache re-use and vectorization possible*



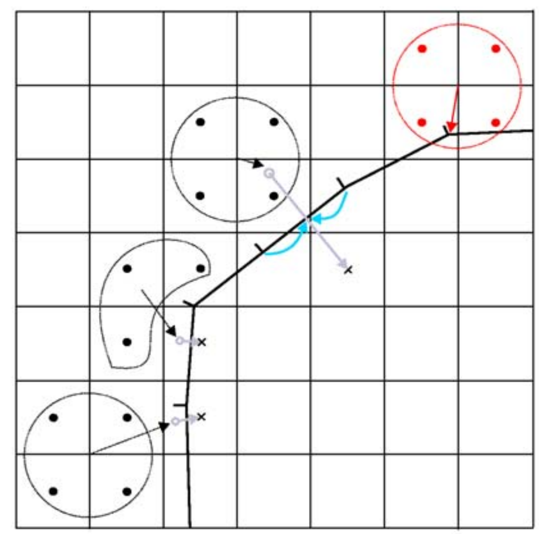


Ghost fluid method

- 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 $n = \nabla\varphi / |\nabla\varphi|$
- Treat an interface as a moving rigid wall



- Interpolation operations – e.g. with solid surface mesh
  - *Mirrored fluid density and velocity values $\mathbf{u}^F_M$ into ghost cells*
  - *Solid velocity values $\mathbf{u}^S$ on facets*
  - *Fluid pressure values in surface points (nodes or face centroids)*

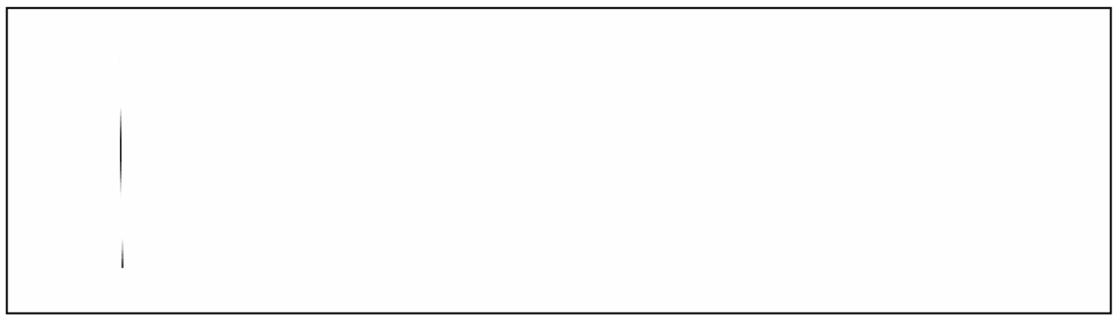


Vector velocity construction for rigid slip wall: $\mathbf{u}^F_{Gh} = 2((\mathbf{u}^S - \mathbf{u}^F_M) \cdot \mathbf{n})\, \mathbf{n} + \mathbf{u}^F_M$

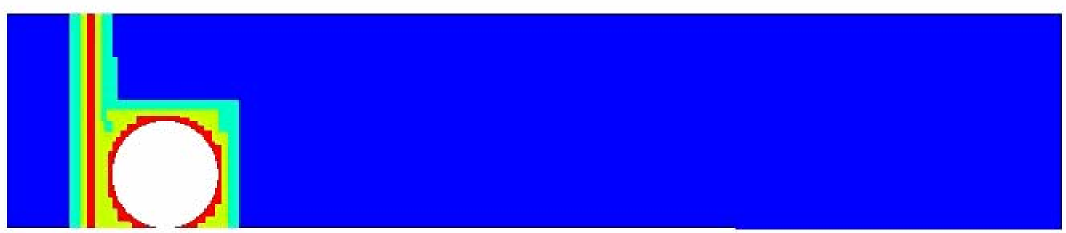
Verification test for GFM

- Lift-up of solid body in 2D when being hit by Mach 3 shock wave

- Falcovitz et al., **A two-dimensional conservation laws scheme for compressible flows with moving boundaries,** JCP, 138 (1997) 83.
- H. Forrer, M. Berger, **Flow simulations on Cartesian grids involving complex moving geometries flows**, Int. Ser. Num. Math. 129, Birkhaeuser, Basel 1 (1998) 315.
- Arienti et al., **A level set approach to Eulerian-Lagrangian coupling**, JCP, 185 (2003) 213.



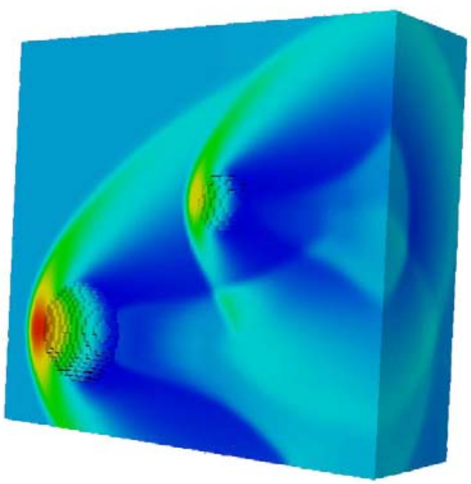
Schlieren plot of density

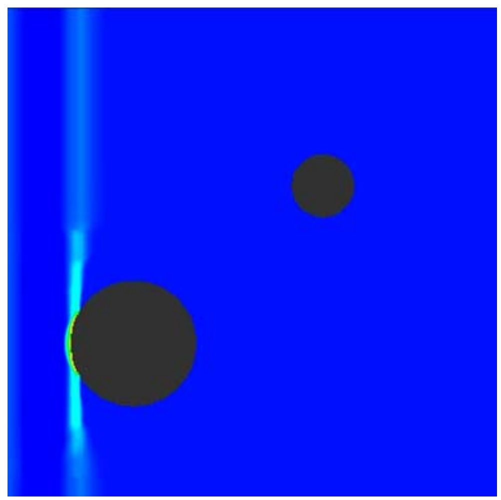


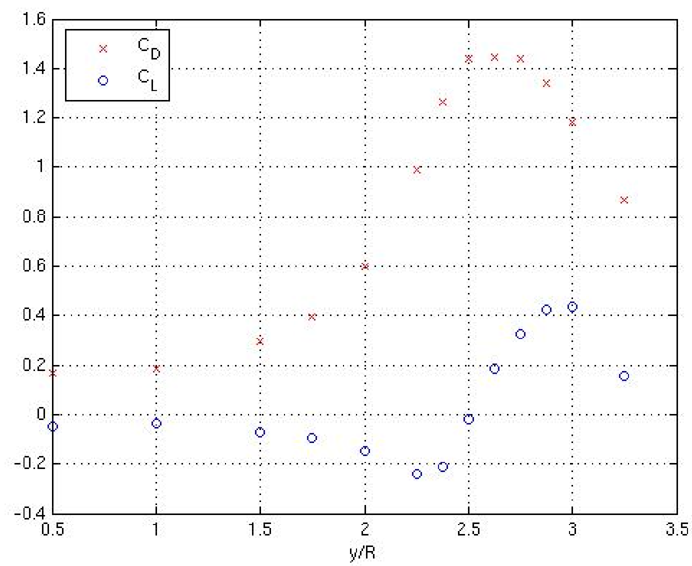
3 additional refinement levels

Validation case for GFM

- Drag and lift on two static spheres in due to Mach 10 shock
- Full 3D calculations, without AMR up to 36M cells, typical run 2000h CPU SP4
- Stuart Laurence, **Proximal Bodies in Hypersonic Flow,** PhD thesis, Galcit, Caltech, 2006.







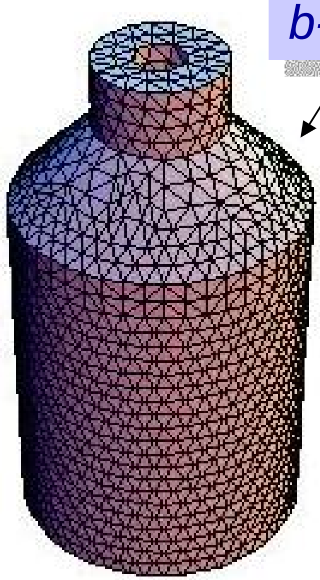
Drag coefficient C_d on first sphere:

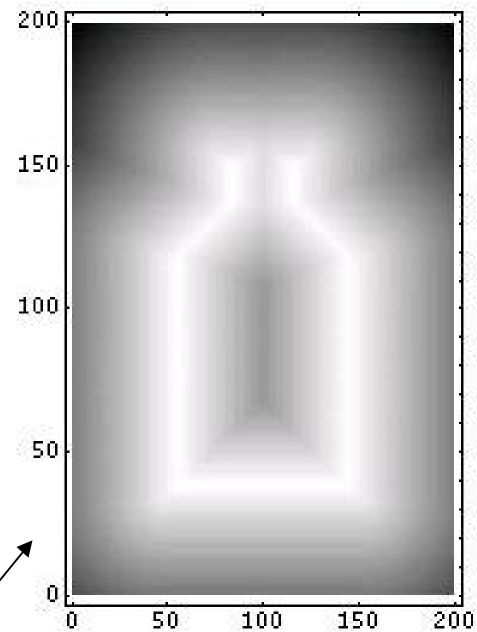
$C_d = F_D / (0.5\, \rho\, u^2\, \pi\, r^2) = 0.8785$

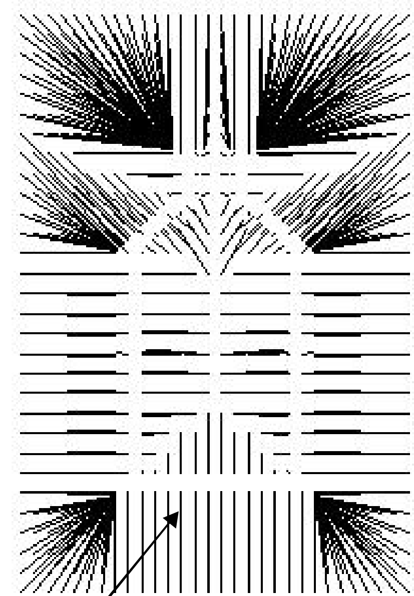
Force coefficients on second sphere

Implicit representations of complex surfaces

- FEM Solid Solver
  - *Explicit representation of the solid boundary, b-rep*
  - *Triangular faceted surface.*
- Cartesian FV Solver
  - *Implicit level set representation.*
  - *need closest point on the surface at each grid point..*



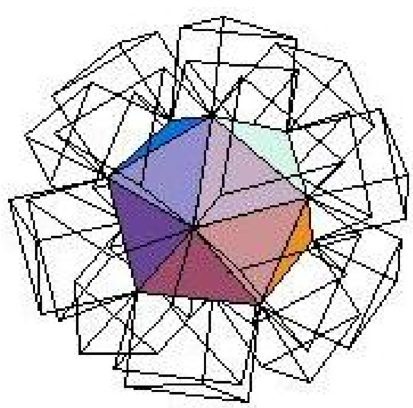




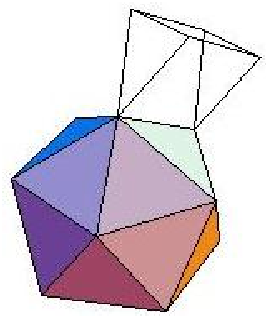
→ Closest point transform algorithm (CPT) by S. Mauch

CPT in linear time

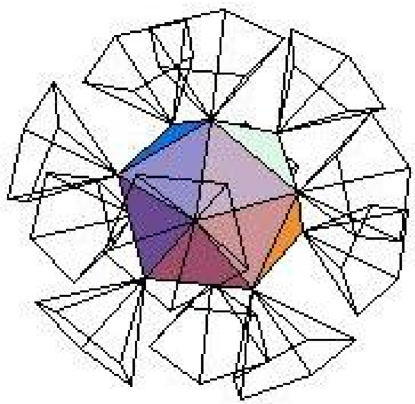
- Problem reduction by evaluation only within specified max. distance
- The characteristic / scan conversion algorithm.
  - *For each face/edge/vertex.*
    - *Scan convert the polyhedron.*
    - *Find distance, closest point to that primitive for the scan converted points.*
- Computational complexity.
  - *O(m) to build the b-rep and the polyhedra.*
  - *O(n) to scan convert the polyhedra and compute the distance, etc.*



Face Polyhedra

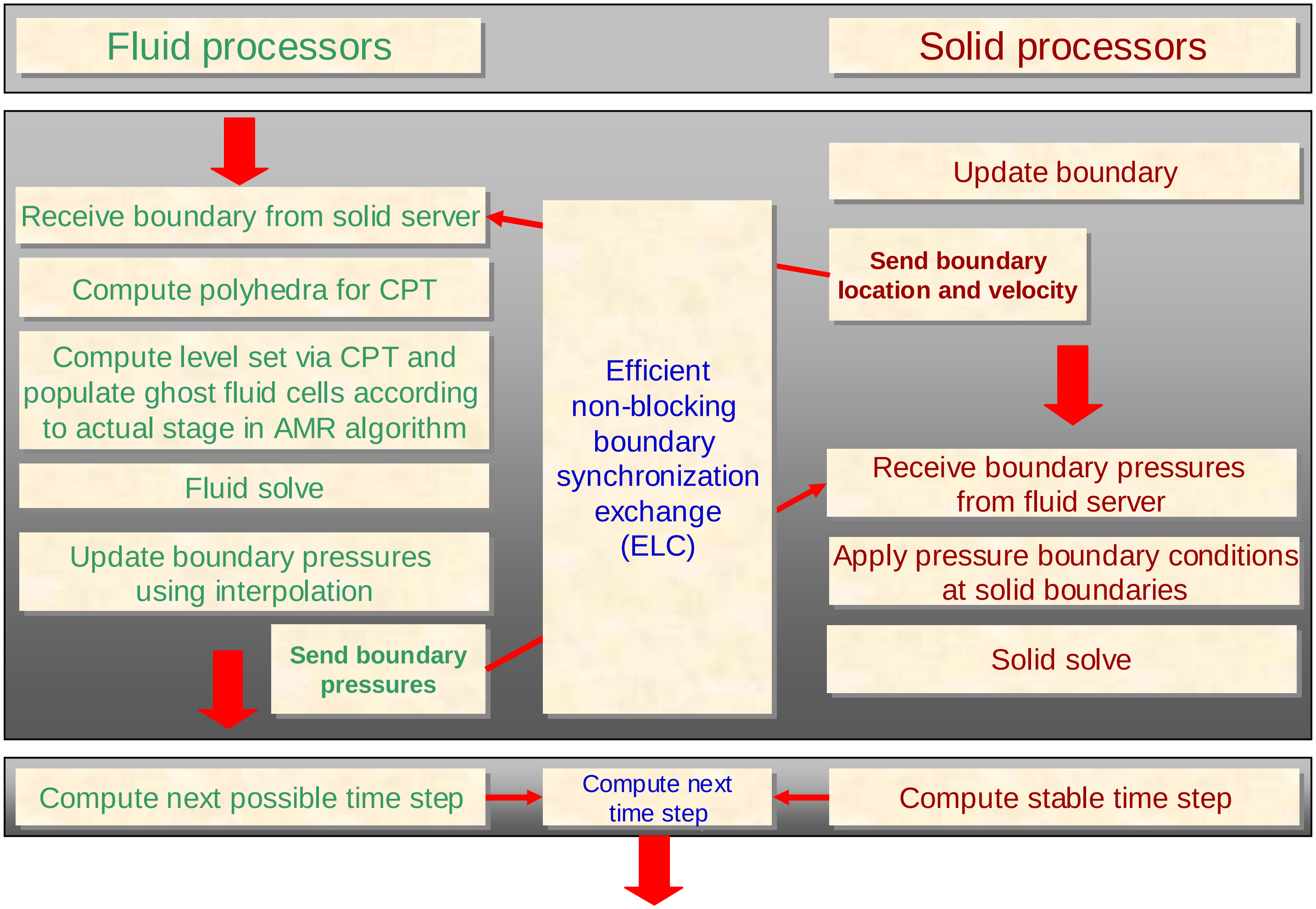


Edge Polyhedra



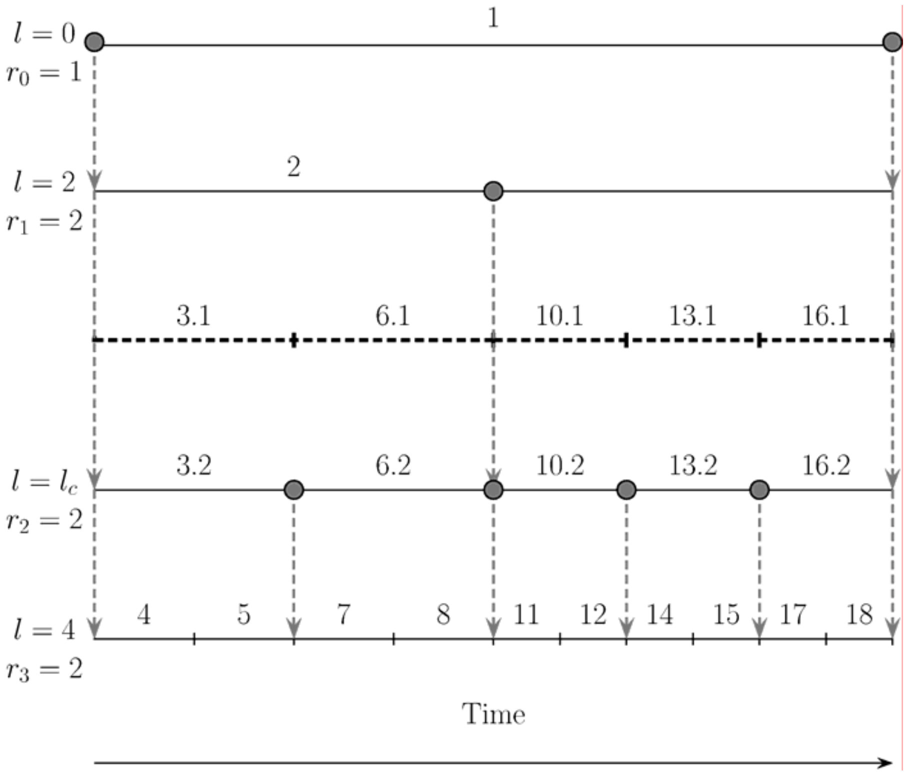
Vertex Polyhedra

Coupled simulation – time splitting approach

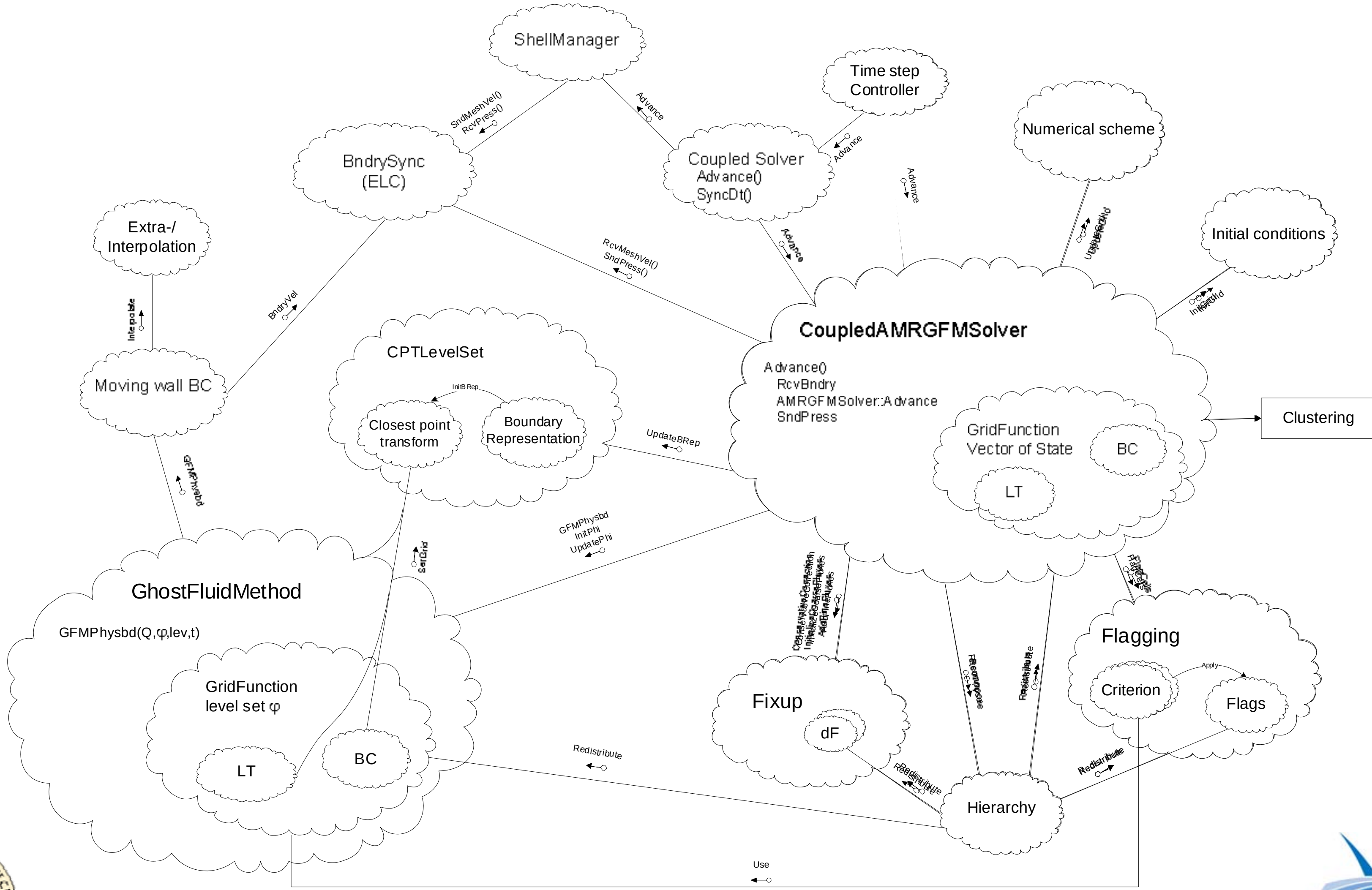


Time step control in coupled simulation

- Eulerian AMR + non-adaptive Lagrangian FEM scheme
  - *Exploit AMR time step refinement for effective coupling*
  - *Lagrangian simulation is called only at level $l_c < l_{max}$*
  - *AMR refines solid boundary at least at level l_c*
  - *One additional level reserved to resolve ambiguities in GFM (e.g. thin structures)*
  - *Inserting sub-steps accommodates for time step reduction from the solid solver <u>within</u> an AMR cycle*
  - *Updated boundary info from solid solver must be received before regridding operation (grey dots left)*

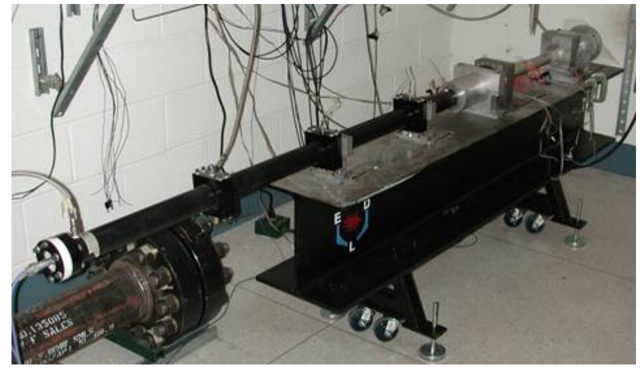


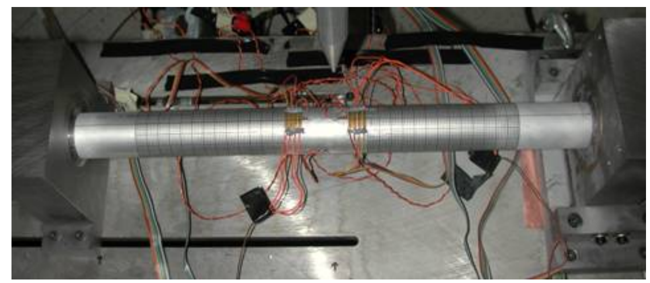
AMROC with GFM in VTF

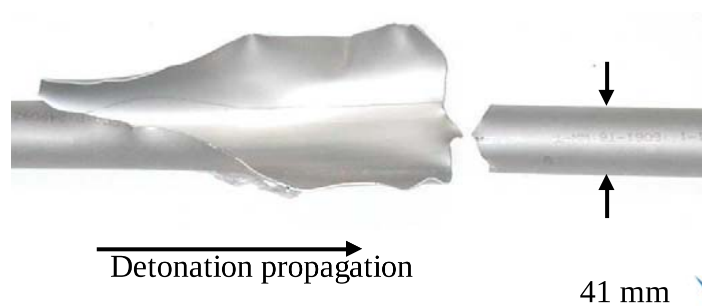


Detonation driven fracture

- Experiments by T. Chao, J.E. Shepherd
- Motivation
  - *Interaction of detonation, ductile deformation, fracture*
- Expected validation data
  - *Stress history of cylinder*
  - *Crack propagation history*
  - *Species concentration and detonation fine structure*
- Modeling needs
  - *Modeling of gas phase detonation*
  - *Multiscale modeling of ductile deformation and rupture*
- Test specimen: Al 6061
  - *Young's modulus 69GPa, density 2780 kg/m^3*
  - *Poisson ratio 0.33*
  - *Tube length 0.610m, outer diameter 41.28mm*
  - *Wall thickness 0.80mm*
- Detonation: Stoichiometric Ethylene and Oxygen
  - *Internal pressure 80 kPa*
  - *CJ pressure 2.6MPa*
  - *CJ velocity 2365m/s*

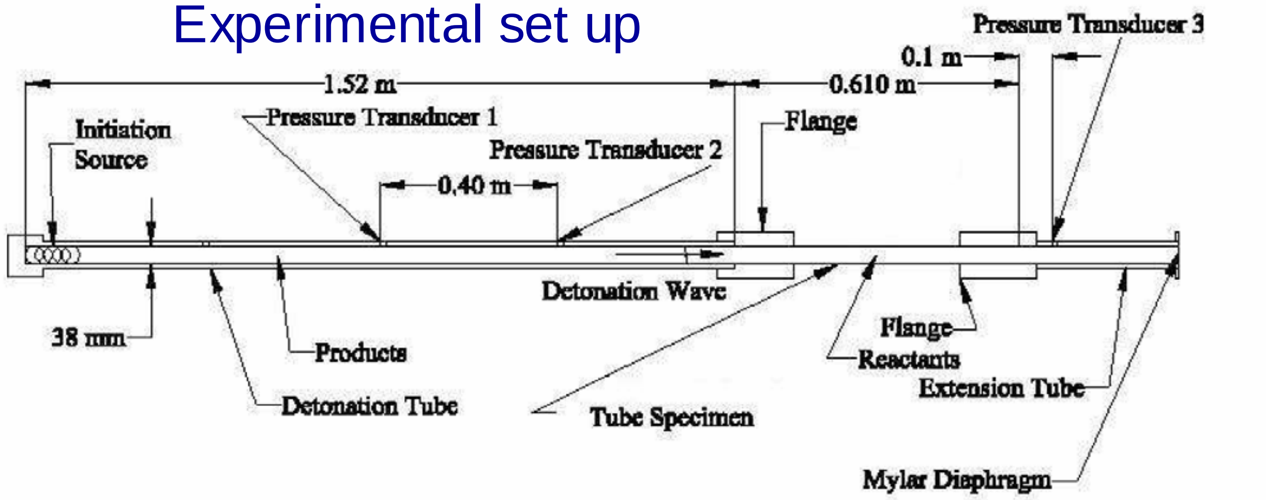




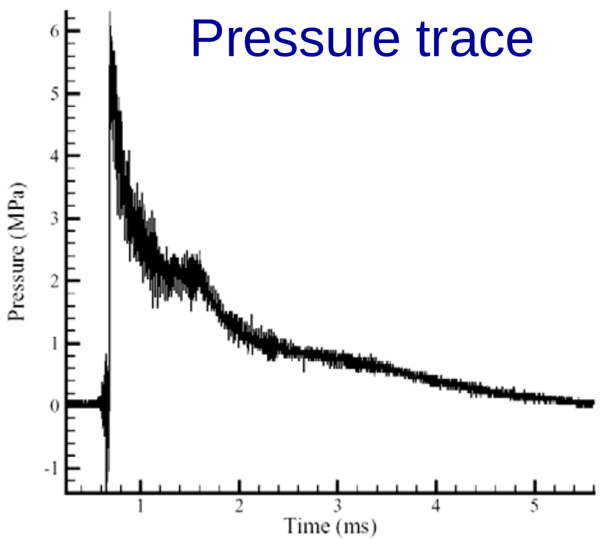


Initial investigation in elastic regime

Experimental set up



Pressure trace



Shell response

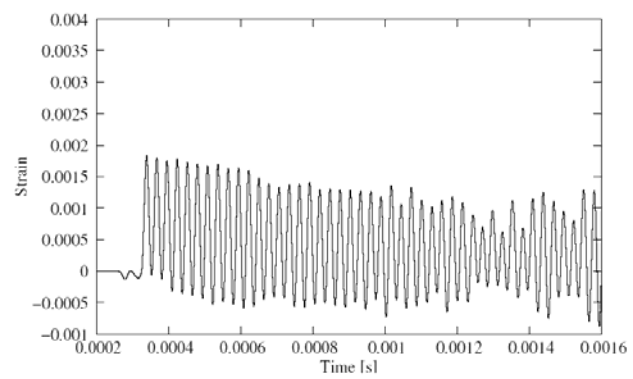


Figure 7: Circumferential strain at strain gage two.

Detonation modeling

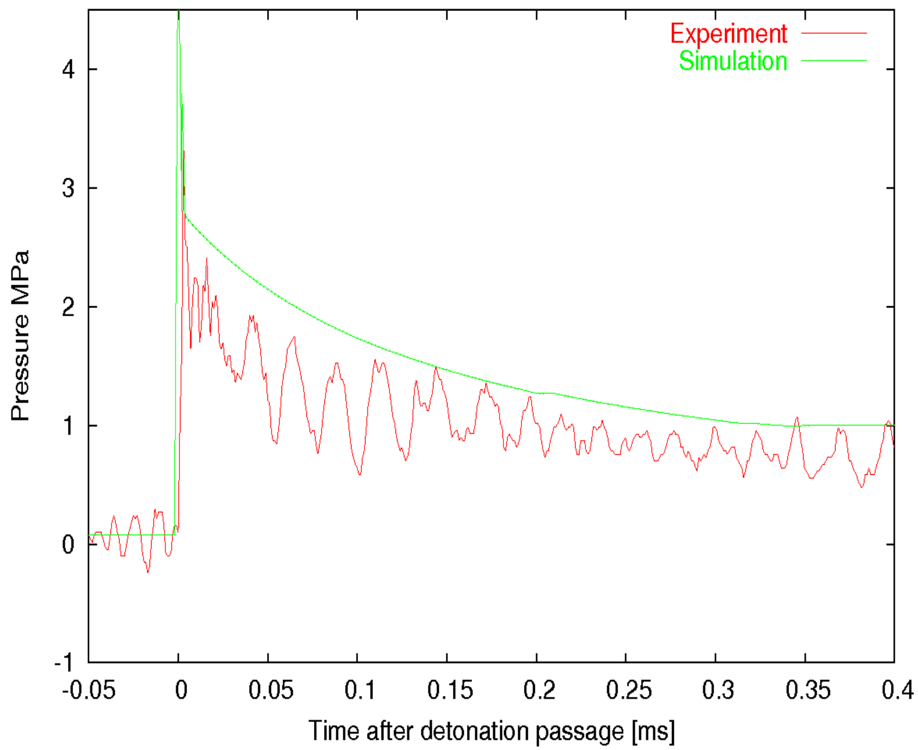
- Modeling of ethylene-oxygen detonation with one-step reaction model
  - *Arrhenius kinetics:* $k^f(T) = k \exp(-E_A/RT)$
  - *Equation of state for Euler equations:* $p = (\gamma-1)(\rho e - \rho(1-Z) q_0)$
  - *Adjust parameters to match CJ and vN state of* $C_2 H_4+3 O_2$ *CJ detonation at* p_0=0.8 MPa *and* T_0=295 K *as close as possible*
  - *Chosen parameters:* q_0=5,518,350 J/kg, E_A=25,000 J/mol, k=20,000,000 1/s

	GRI 3.0	Model
u_{det}	2363.2 m/s	2636.7 m/s
p_0	0.8 MPa	0.8 MPa
ρ_0	1.01 kg/m^3	1.01 kg/m^3
γ_0	1.338	1.240
p_{vN}	51.25 MPa	50.39 MPa
ρ_{vN}	9.46 kg/m^3	8.14 kg/m^3
p_{CJ}	26.81 MPa	25.59 MPa
ρ_{CJ}	1.91 kg/m^3	1.80 kg/m^3
γ_{CJ}	1.240	1.240
$\Delta_{1/2}$	~0.03 mm	~0.03 mm

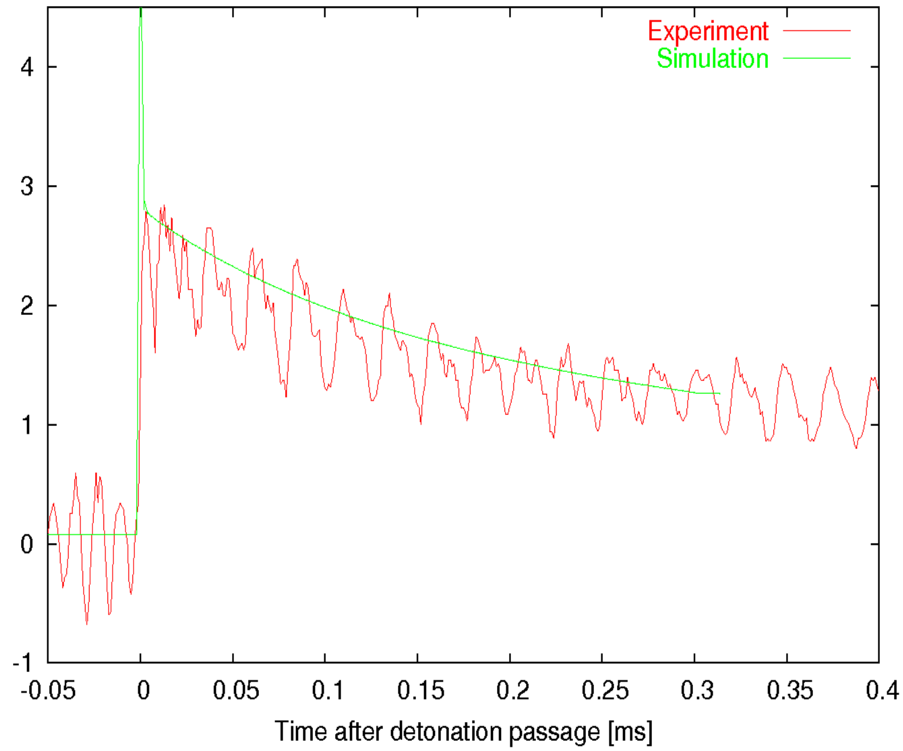
- 1D Simulation
  - 2 m *domain to approximate Taylor wave correctly*
  - *Direct thermal ignition at x*=0 m
  - *AMROC calculation with 4000 cells, 3 additional levels with factor 4*
  - ~ 4 cells within $\Delta_{1/2}$ (minimally possible resolution)
  - Compute time ~ 1 h

Detonation modeling- Validation

Transducer 1 – 0.8 m

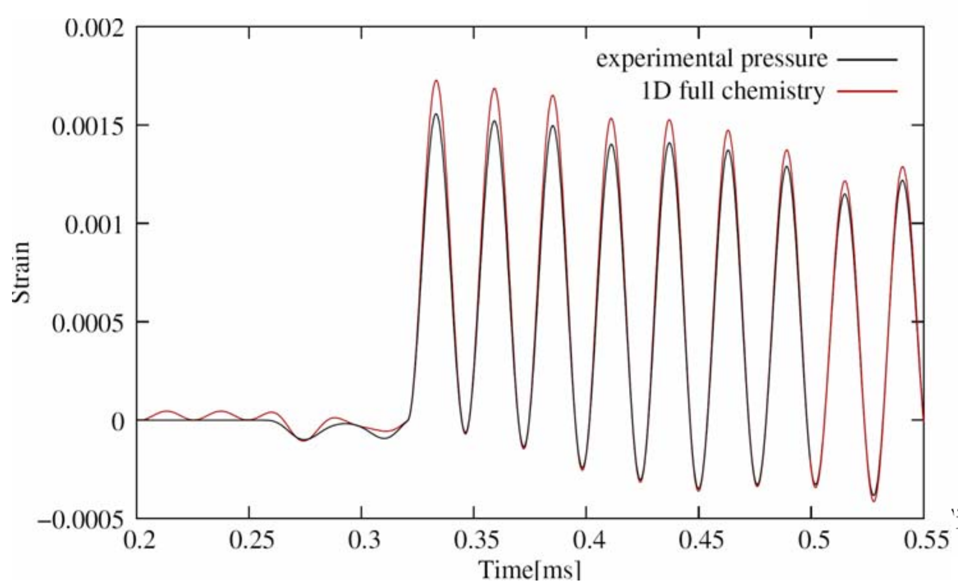


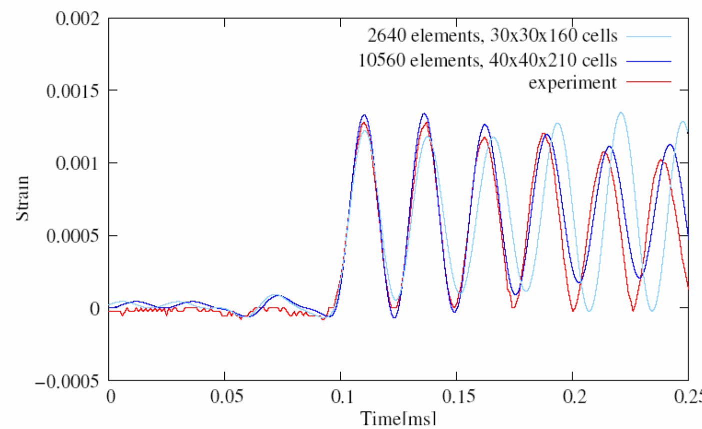
Transducer 2 – 1.2 m



- *Direct ignition in simulation leads to an earlier development of CJ detonation than in experiment, but both pressure traces converge*
- *In tube specimen with x>1.52 m CJ state should have been fully reached*
- *Computational results are appropriate model for pressure loading*

Shell reponse under prescribed pressure

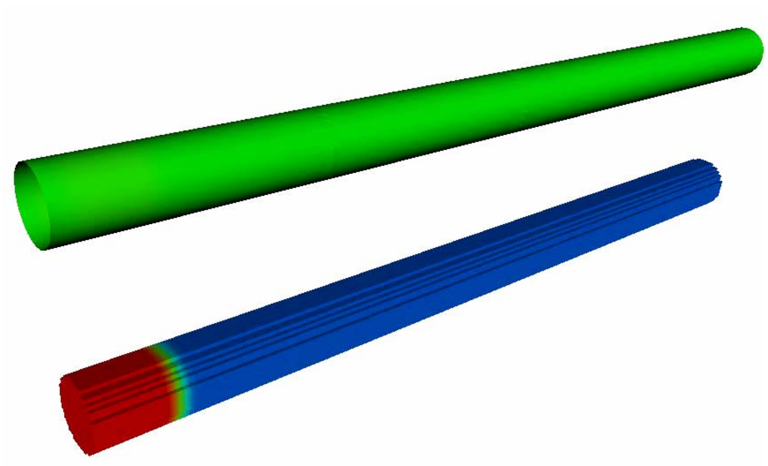




Rough verfication of convergence towards experimental results

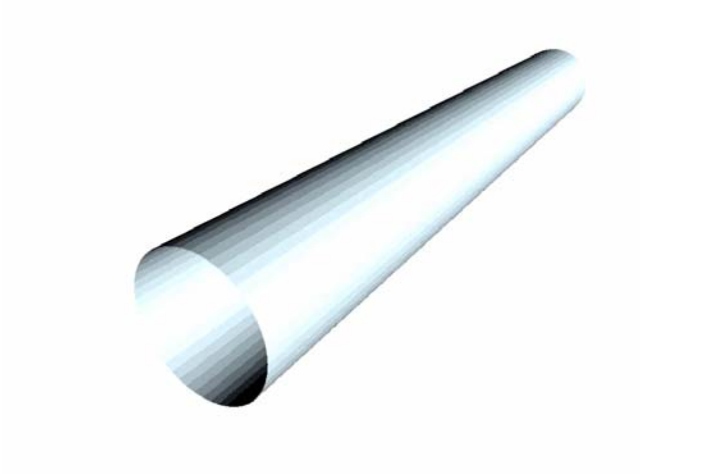
- Use of 1-D detonation pressure leads to excellent agreement in phase length experiment and shell simulation
- Taylor wave drives oscillation, not von Neumann pressure, already very good agreement, if <u>average</u> pressure is prescribed via appropriate shock
- Further work to assess steadiness of detonation in experiment
- Next step is to redo strain gauge measurements

Tests towards fully coupled simulations

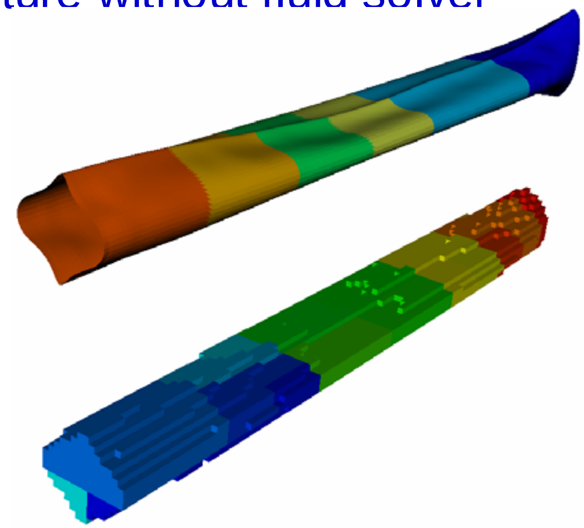


Coupled simulation in elastic regime

- *<u>Average</u> pressure of 1D simulation prescribed by a pure shock wave solution of <u>non-reactive</u> Euler equations*
- *Shock speed chosen to equal detonation velocity*



Fracture without fluid solver

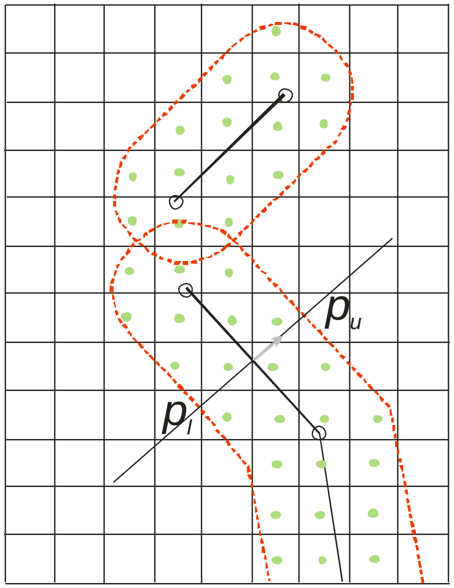


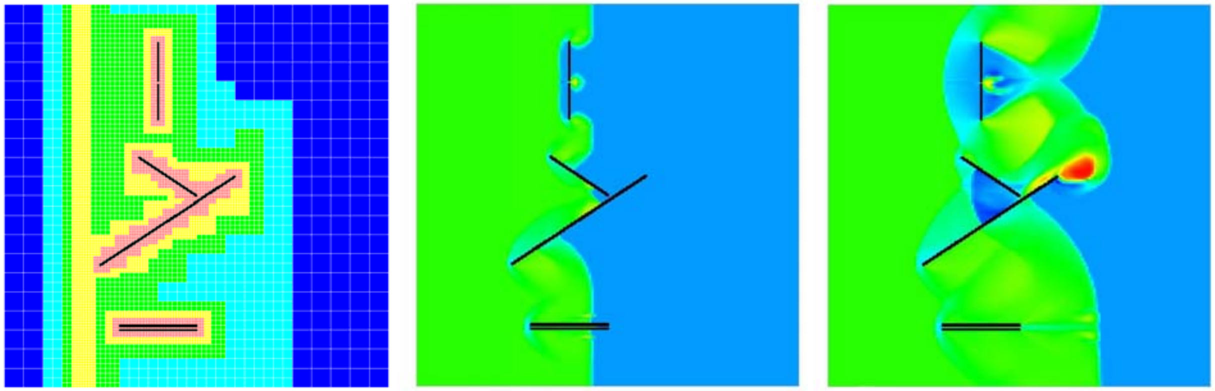
Coupled simulation with large deformation in plastic regime

Treatment of shells/thin structures

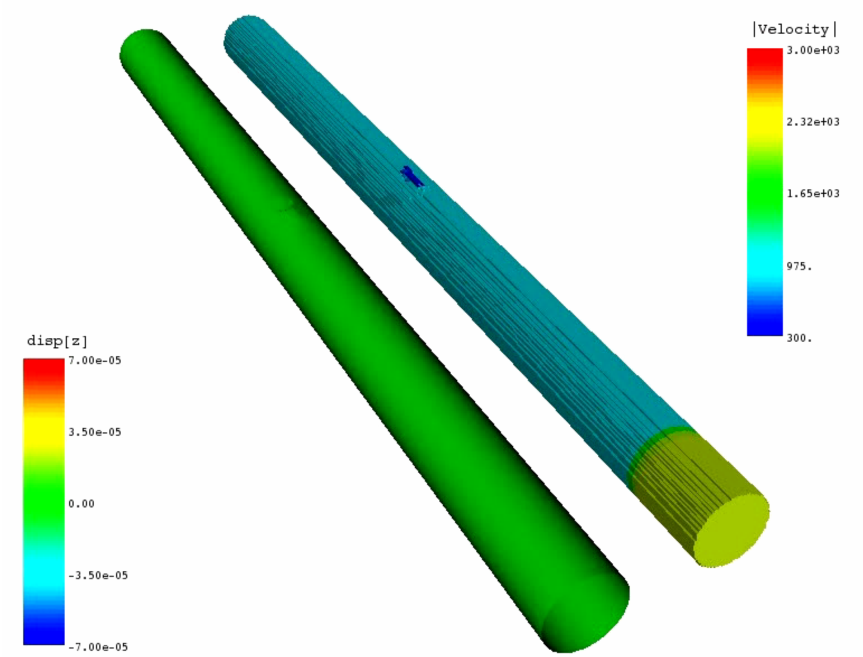
- Thin boundary structures or lower-dimensional shells require artificial "thickening" to apply ghost fluid method
  - *Unsigned distance level set function* φ
  - *Treat cells with* $0<\varphi<d$ *as ghost fluid cells (indicated by green dots)*
  - *Leaving* φ *unmodified ensures correctness of* $\nabla\varphi$
  - *Refinement criterion based on* φ *ensures reliable mesh adaptation*
  - *Use face normal in shell element to evaluate in* $\Delta p = p_u - p_l$

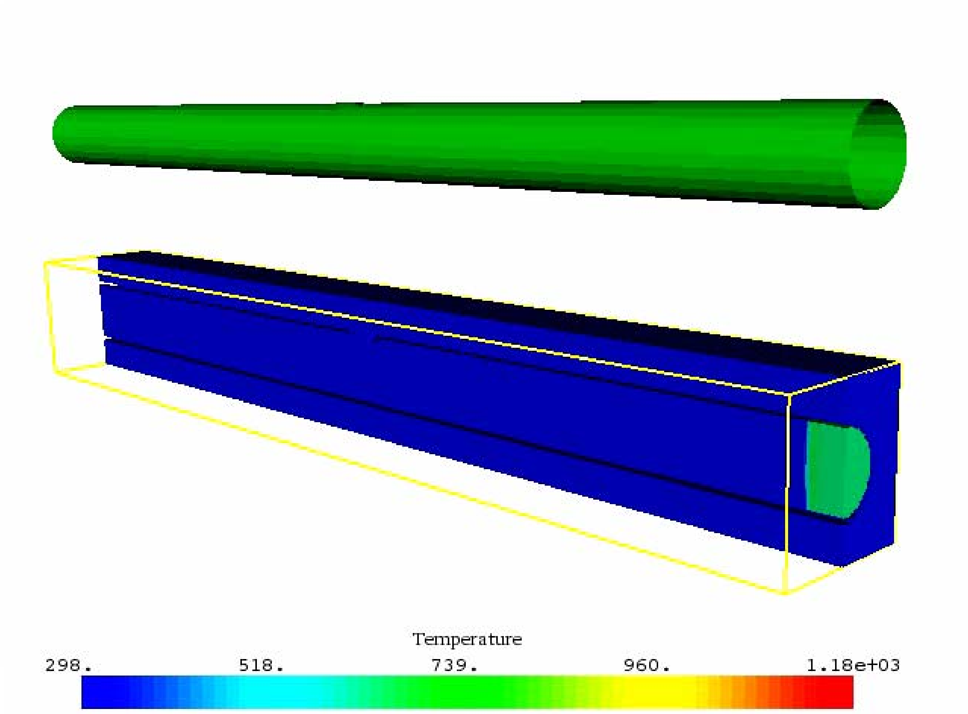
- about ~10^7 cells required to capture correct wall thickness in fracturing tube experiment with this technique (2-3 ghost cells within wall, uniform spatial discretization)





Coupled simulations for thin shells





- *Average pressure of 1D simulation prescribed by a pure shock wave solution of non-reactive Euler equations with shock speed chosen to equal detonation velocity*

- *Test calculation with thermally perfect Euler equations and detailed reaction (H_2-O_2)*
- *Detonation with suitable peak pressure will be initiated due to shock wave reflection*

Performance of coupled thin shell code

- Coupled simulation with standard Euler equations (Roe+MUSCL, dimensional splitting)
- AMR base mesh 40x40x80, 2 additional levels with refinement factor 2, ~3,000,000 cells.
- Modeled tube thickness 0.0017 mm, (2x thicker than in experiment).
- Solid Mesh: ~ 5,000 elements.
- Calculation run on 26 fluid CPUs, 6 solid CPUs P4: ~4.5h real time

Task	%
Fluid dynamics	31.3
Boundary setting	22.3
Interpolation	5.9
Recomposition	6.8
GFM Extra-/Interpolation	10.9
Locating GFM cells	5.5
GFM Various	3.0
Receive shell data	4.3
Closest point transform	2.6
Node velocity assignment	2.2
Construct nodal pressure	1.5
Misc	3.7

Conclusions and outlook

- Detonation simulation
  - *Fully resolved detonation structure simulations for basic phenomena in 3D possible for smaller detailed reaction systems*
  - *Combination of mixed explicit-implicit time-discretization with parallel SAMR and reliable higher order scheme*
- Cartesian scheme for complex embedded boundaries
  - *Accurate results can be obtained by supplementing GFM with SAMR*
  - *With well developed auxiliary algorithms an implicit geometry representation can be highly efficient*
  - *Future goal: Extend implementation from diffused boundary method GFM to accurate boundary scheme based on*

$$V_j^{n+1}\mathbf{Q}_j^{n+1} = V_j^n\mathbf{Q}_j^n - \Delta t\left(A_{j+1/2}^{n+1/2}\,\mathbf{F}(\mathbf{Q},j) - A_{j-1/2}^{n-1/2}\,\mathbf{F}(\mathbf{Q},j-1)\right)$$

- Detonation-induced fracturing tube
  - *Fully coupled AMR simulations with fracture using GFM with thin shell technique*
  - *Detonation model to propagate three-dimensional Ethylen-Oxygen detonation with CJ velocity*
  - *Redo experiments with mixture that allows direct simulation, e.g. Hydrogen-Oxygen*