Topics in immersed boundary and contact methods: current LLNL projects and research

FEM@LLNL

Mike Puso, Paul Tsuji, Ben Liu, Jerome Solberg, Kenneth Weiss, Tony Degroot, Steve Wopschal, Ed Zywicz, Carly Spangler, Eric Chin, Mike Owens, Bob, Ferencz, Randy Settgast, et. al.

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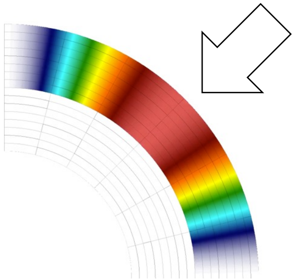
Lawrence Livermore National Laboratory

Current LLNL efforts in computational modeling of interfaces

Mechanics interfaces come in many forms, both physical and computational e.g. contact/impact, fracture/crack interfaces, immersed boundary, embedded interfaces

Contact

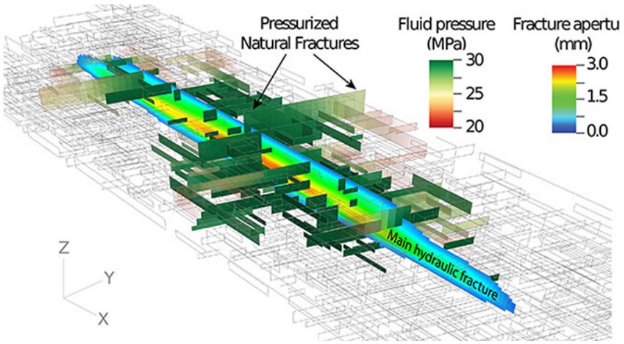
- Tribol: Develop a modern software library for modeling contact interface physics (Wopschall)
  - Higher order discretization methods (MFEM)
  - Initial implementations in Blast, Diablo, ALE3D and Smith
- Smith: Next Gen Engineering Code (Bramwell)
  - Implement MFEM & Tribol into an Engineering Multiphysics code
  - Focus on optimization
- Diablo: Engineering production code (Solberg)
- ALE3D: Physics production code (Liu)



Cubic mesh result from Blast (K. Weiss)

Fracture:

- GEOS: Computational Geoscience (Settgast)
  - Hydraulic Fracture
  - Cohesive zones in contact with interstitial fluid



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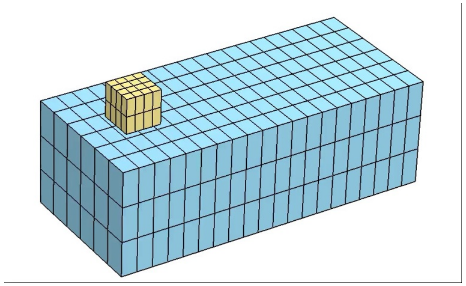

Tribol-Diablo result

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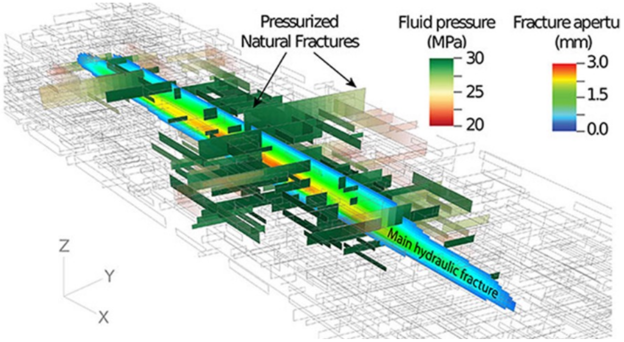

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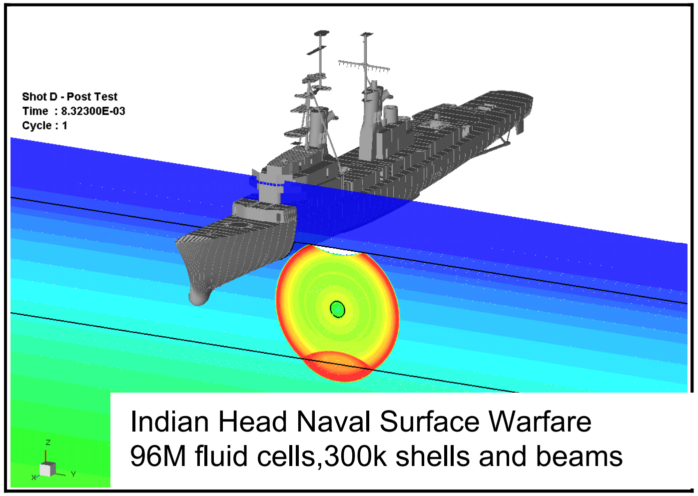
Immersed Boundary

- DYSMAS: Couples Paradyn-Gemini (Zywicz, McGrath)
  - Finite Volume Fluid, Structural Shell
- FEusion: Couples ALE3D-Paradyn-Spheral (Liu, Tsuji, Degroot, Owens, Me)
  - Cut cell technology in background
  - Lagrange Multiplier coupling
- LDRD: Displaced Boundary Coupling (Tomov)
  - Focus on high order elements
  - Nitsche method coupling (Scovazzi)

DYSMAS
(Indian Head Naval Surface Warfare)



Indian Head Naval Surface Warfare
96M fluid cells,300k shells and beams

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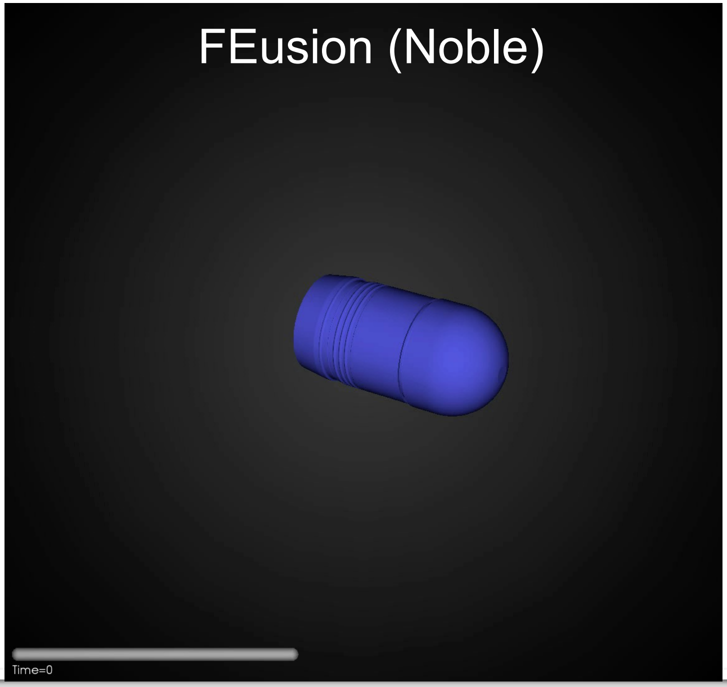

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Outline:

Tractions enforce displacement or velocity constraints at boundary
3 Flavors: Penalty, Nitsche/Interior Penalty Method, Lagrange Multipliers

- FEusion Immersed Boundary
  - Approach
    - Lagrange Multiplier Coupling
    - Advection
    - Extension to SPH
  - V&V
- Symmetric (Two Pass) Mortar Contact
  - Approach
    - Obviates bias of standard mortar contact
    - Stabilized Lagrange Multiplier Method
  - V&V
- Structure Preserving Time Integration
  - Approach
    - Lagrange multipier contact enforcement
    - Provable stability for large deformation kinematics
    - Exactly conserves linear and angular momentum
  - V&V

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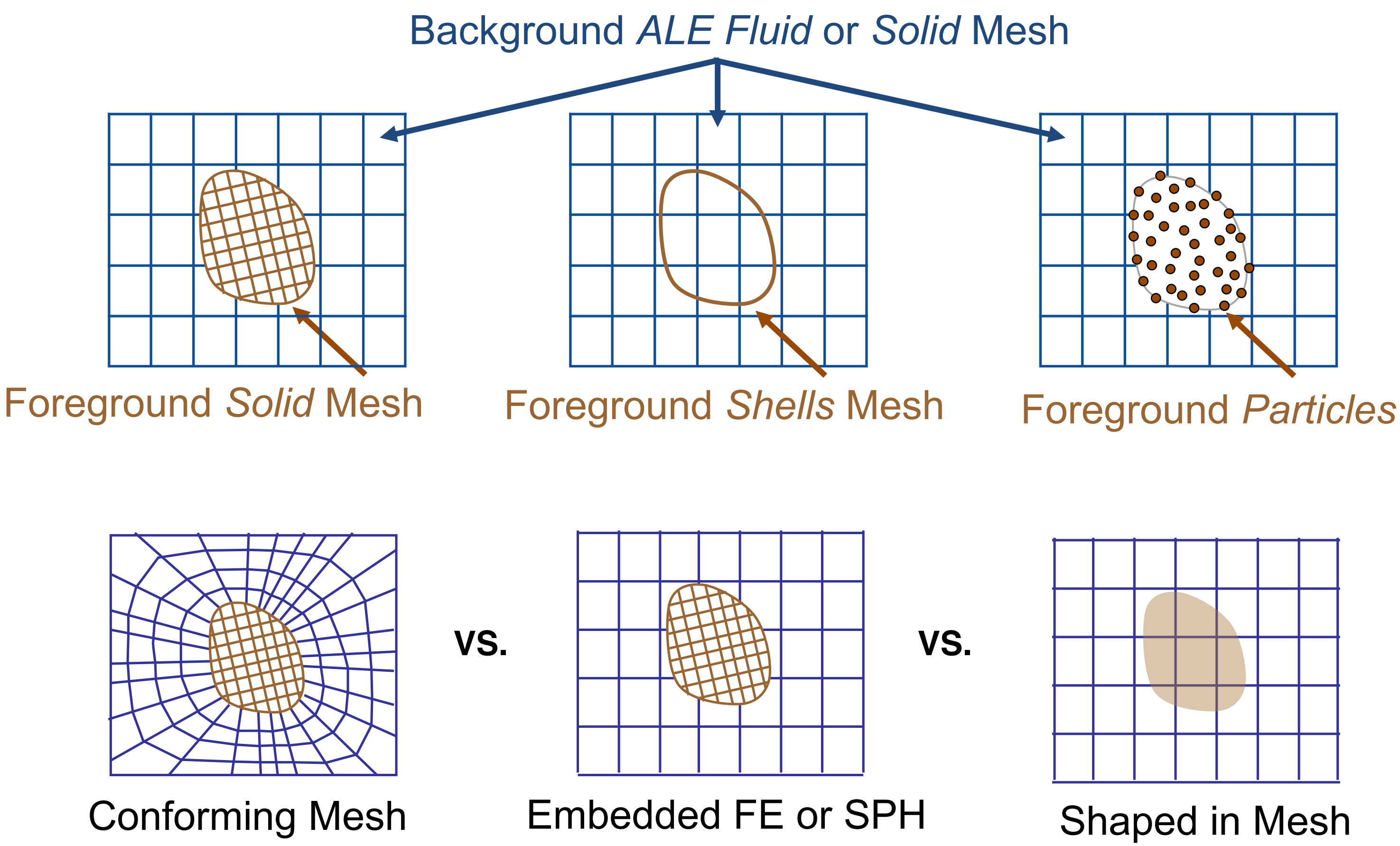
Immersed Boundary methods couple overlapping discretizations



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Many Previous Works: to name a few

- Existing *Immersed boundary* methods
  - *CEL method* (W.F. Noh, 1964)
  - *Immersed boundary methods* (C.S. Peskin 1977, 2002)
  - *Immersed finite element methods* (W.K. Liu 2004)
  - *Overset grid methods* (Steger 1983)
  - *Zapotec material insertion method* (Bessette 2002)
    - Sandia code couples CTH and Pronto
  - *LS-Dyna, ABAQUS* (commercial codes)
  - *Fictitious domain methods* (Glowinski 1991, 2001)
  - *Nitsche's Method* (Hansbo and Hansbo, 2003)
  - *Ghost Fluid methods* (Fedikew et. al. 1999)
    - *DYSMAS* Gemini-PARADYN (Luton et. al. 2003)
  - *FIVER* (Farhat et. al. 2012)
  - *Shifted Boundary* (Scovazzi et. al. 2017)

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Approach

Algorithmic Design

- No restriction to penalized constraints
- Good estimate for explicit stable time step

Mathematical Issues

- Stability of Lagrange multiplier space => pressures
- Solvability => condition number
- Stability of time integrator => estimate stable time step

Time Splitting ALE

- Lagrange Step: modified for constraint
- Advection Step: restrict flow

M. Puso, E. Kokko, R. Settgast and B. Liu "An embedded mesh method using piecewise constant multipliers with stabilization: mathematical and numerical aspects" *International Journal for Numerical Methods*, 104, pp. 697-720, (2015).

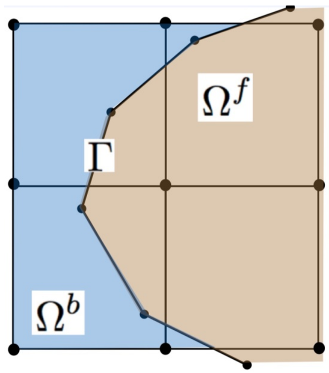
M. Puso, J. Sanders, R. Settgast, and B. Liu "An Embedded Mesh Method in a Multiple Material ALE", *Computer Methods in Applied Mechanics and Engineering* (15) 245-246, pp.273-289, (2012).

Mathematical Details: Lagrange Step

Stability of Multipliers

- Consider equations of motion *i.e.* $F = Ma$

$$M^b a^b + K^b u^b + B^{bT}\lambda = 0$$
$$M^f a^f + K^b u^f + B^{fT}\lambda = 0$$
$$B^b v^b + B^f v^f = 0$$



Solution to EOM

- Central difference $a_n = (v_{n+1/2} - v_{n-1/2})/\Delta t$

$$\begin{bmatrix} M^b & 0 & B^{bT} \\ 0 & M^f & B^{fT} \\ B^b & B^f & -\bar{C}^{-1}/\Delta t \end{bmatrix} \begin{Bmatrix} v^b_{n+1/2} \\ v^f_{n+1/2} \\ \lambda\Delta t \end{Bmatrix} = \begin{Bmatrix} -K^b u^b_n + M^b v^b_{n-1/2} \\ -K^f u^f_n + M^f v^f_{n-1/2} \\ 0 \end{Bmatrix}$$

$$H = \Delta t^2 \left(B^b {M^b}^{-1} {B^b}^T + B^f {M^f}^{-1} {B^f}^T\right) + \bar{C}^{-1} \qquad H\lambda = f \qquad s_{con} = \frac{\lambda^{eig}_{max}(H)}{\lambda^{eig}_{min}(H)} =$$ constant independent of *h*

Stability in Time

- Central difference scheme leads to following recursion

$$a_n^T A a_n + v_n^T K v_n \leq a_0^T A a_0 + v_0^T K v_0$$

- Recursion bounds a_n and v_n when $K \geq 0 \;\; A > 0$ $\quad A = M + \frac{\Delta t}{2} C - \frac{\Delta t^2}{4} K$

$$\Delta t \leq \frac{2}{\omega_c} \quad \text{where} \quad \omega_c^2 = \sup_u \frac{u^T K u}{u^T M u}$$

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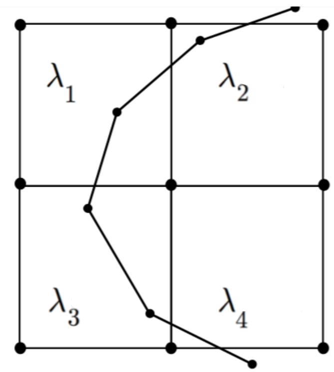

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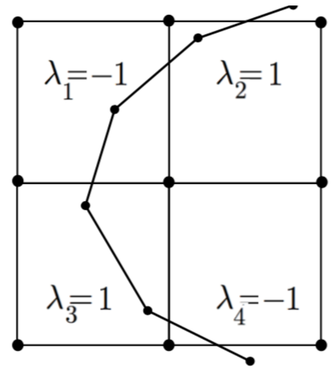

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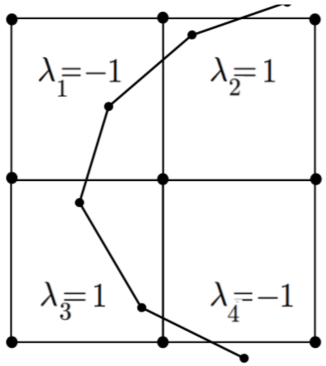

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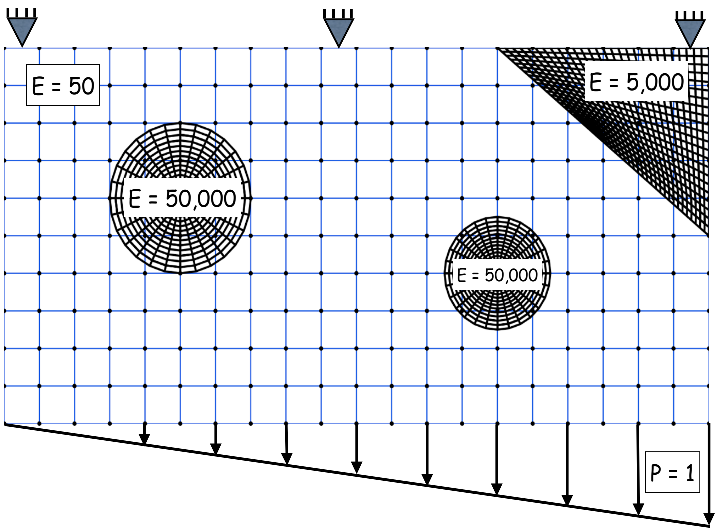
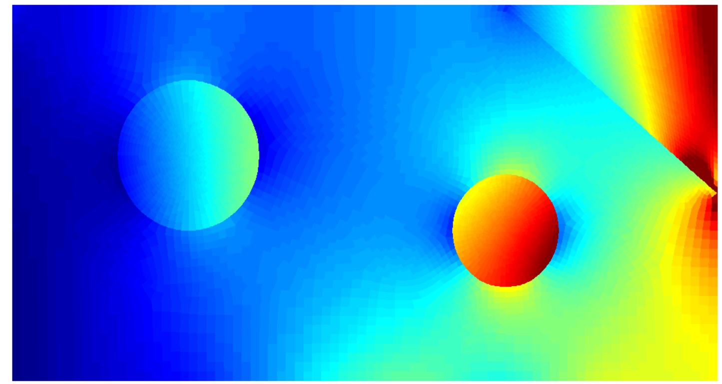
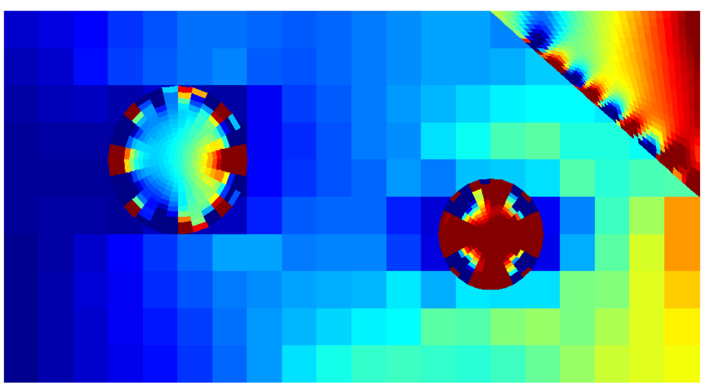
Multipliers on background mesh: 2D Lagrange result

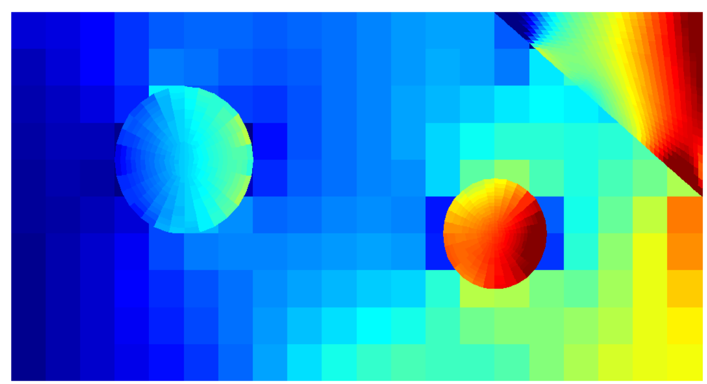




conforming



foreground



background

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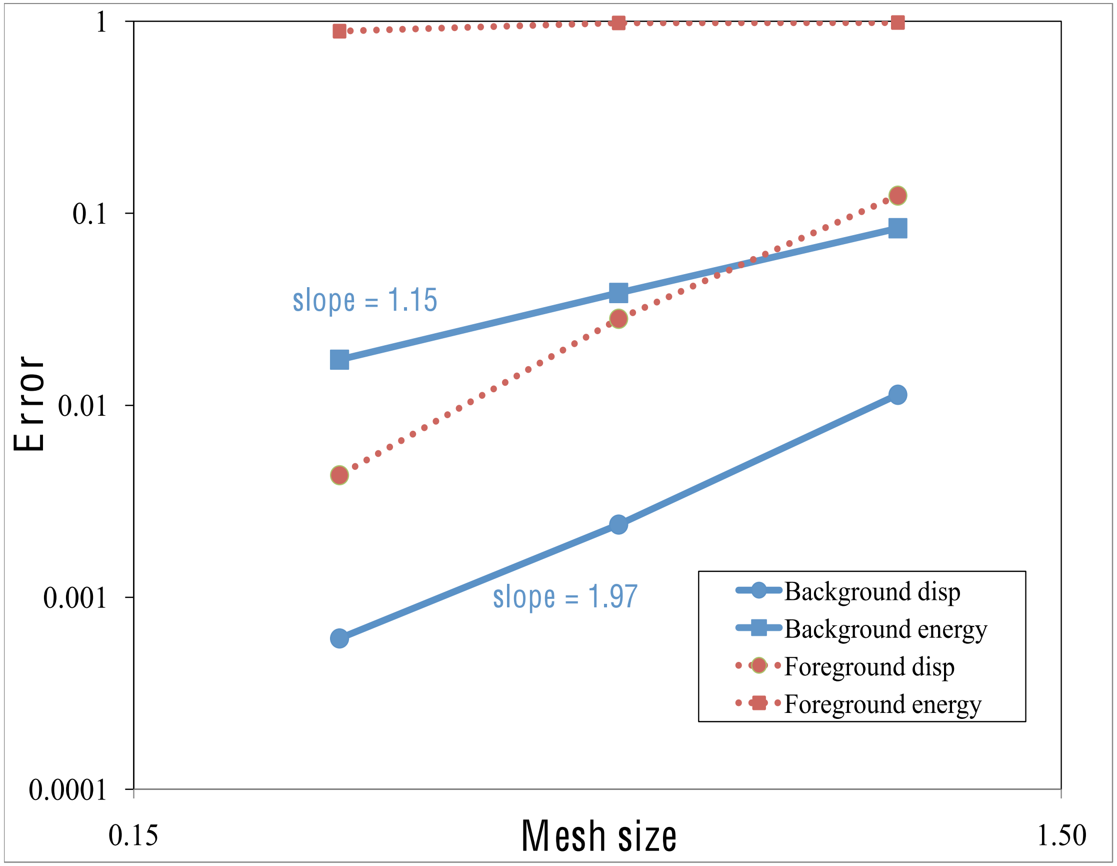

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ALE implementation: with foreground Lagrange Mesh

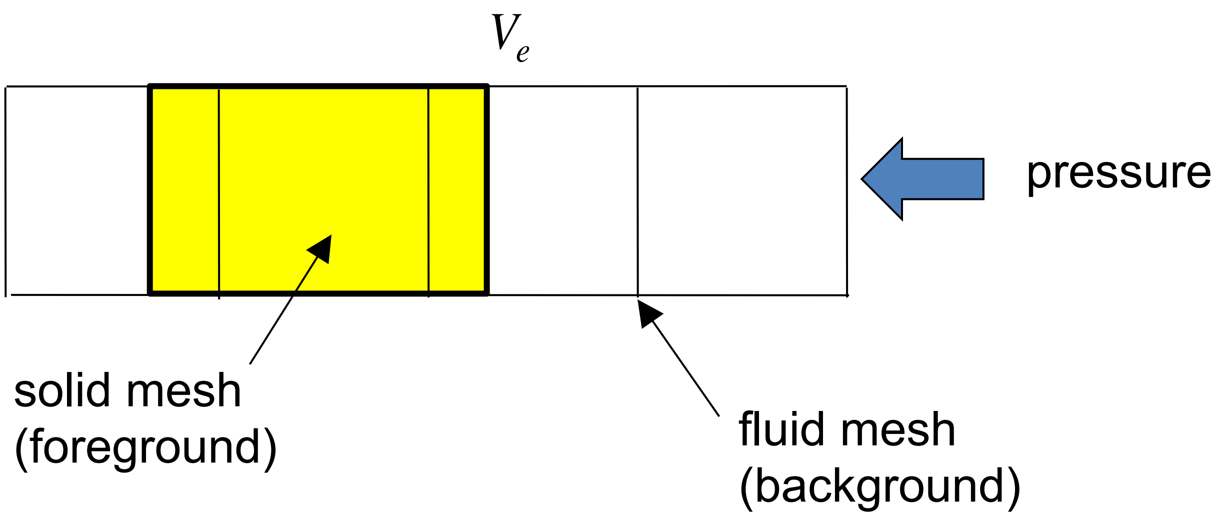
- Use central difference explicit 2 step ALE approach

Load step

Lagrange step

Advection remap step

Advance time step $t_n \rightarrow t_{n+1}$



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ALE implementation: with foreground Lagrange Mesh

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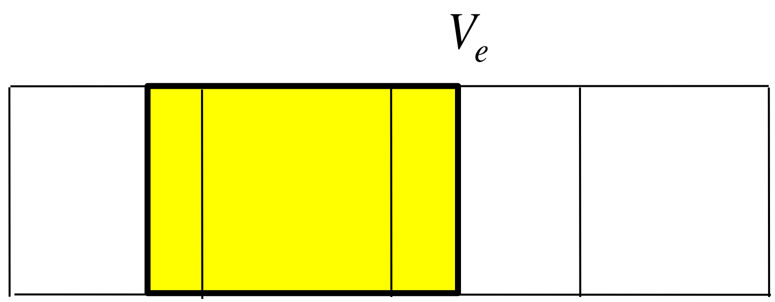
  - Load step
  - Lagrange step (velocity constraints applied)
  - Advection remap step
  - Advance time step $t_n \rightarrow t_{n+1}$



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ALE implementation: with foreground Lagrange Mesh

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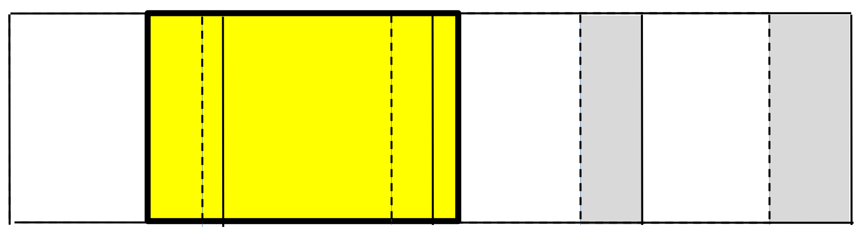
Load step

Lagrange step

Advection remap step (yields volume flux)

Advance time step $t_n \rightarrow t_{n+1}$

$V_e + \Delta V_e^R$



$\Delta V_e^L = 0$ ΔV_e^R

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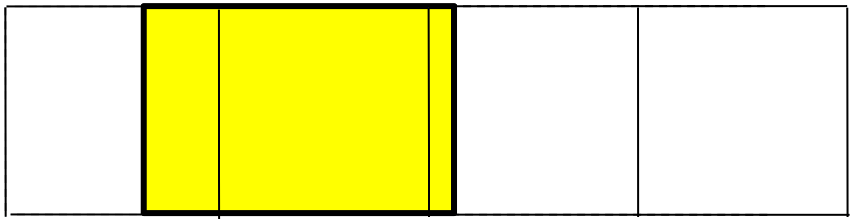
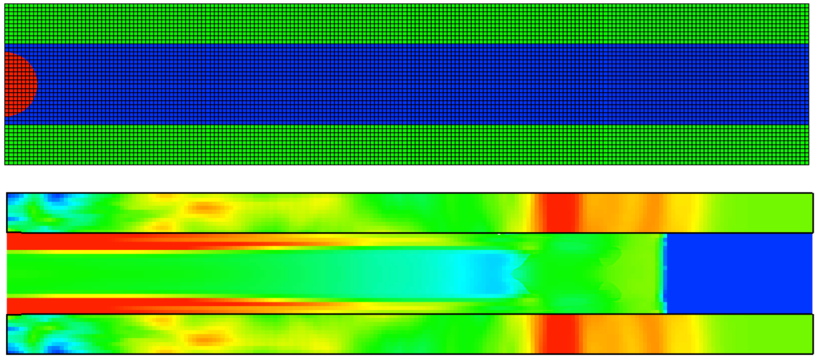
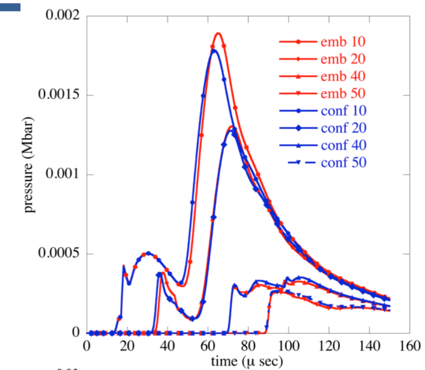


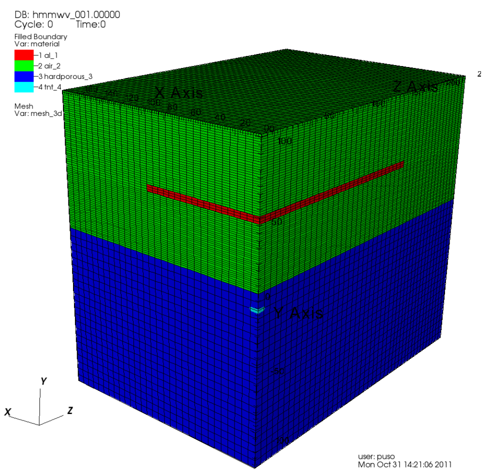
Verification/Validation: Conforming vs Immersed

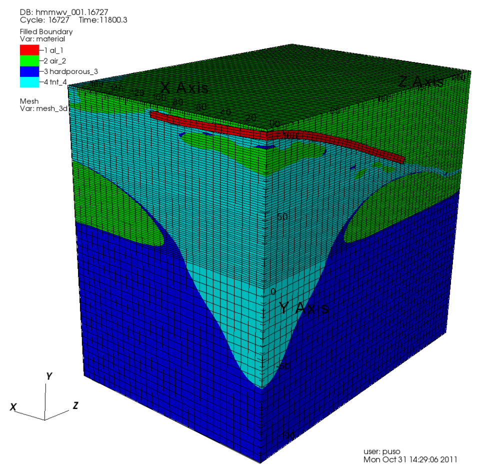
Shock Tube

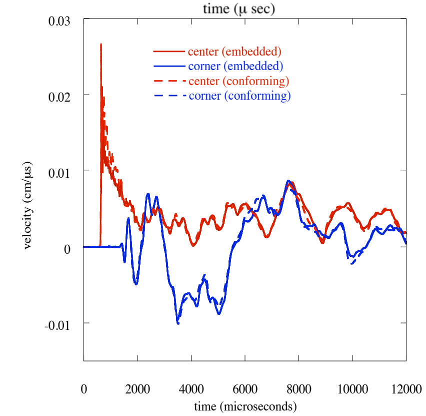




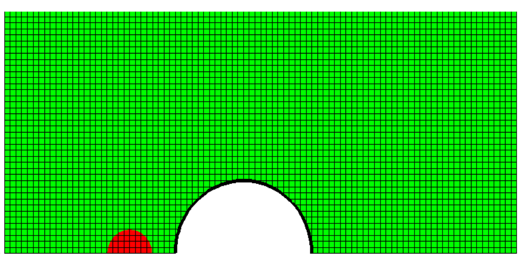
Buried Mine

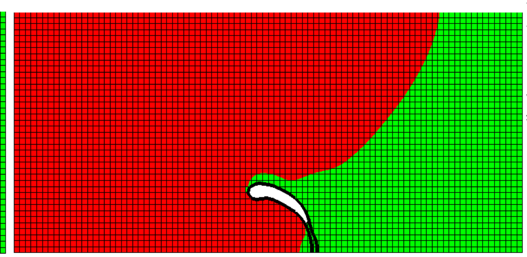


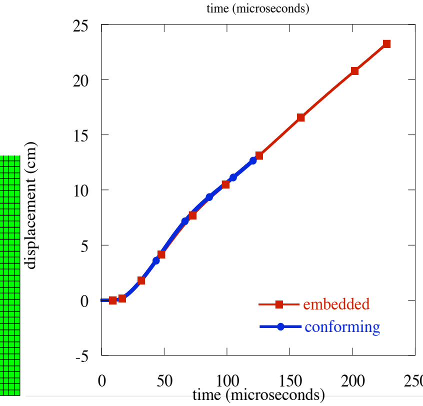




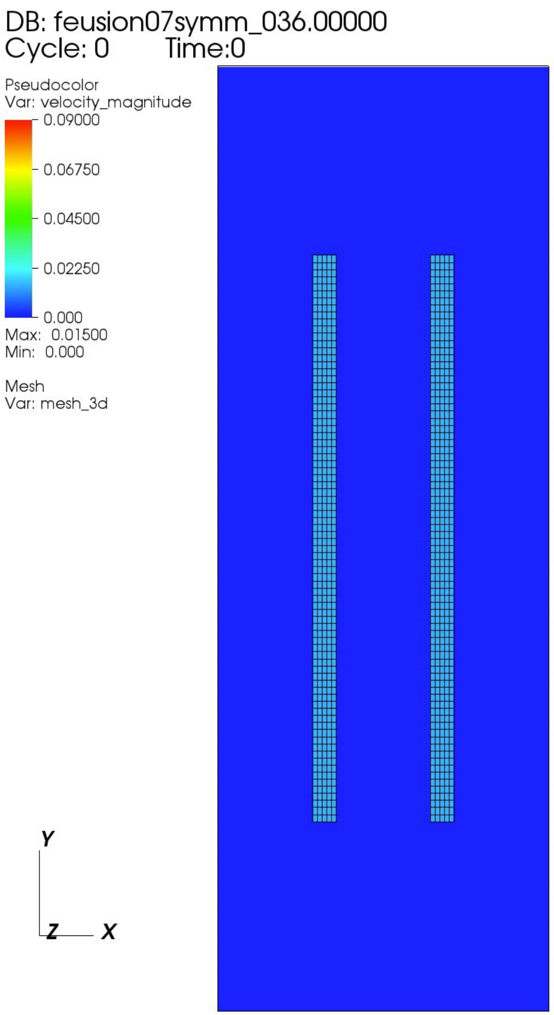
Shell Pipe

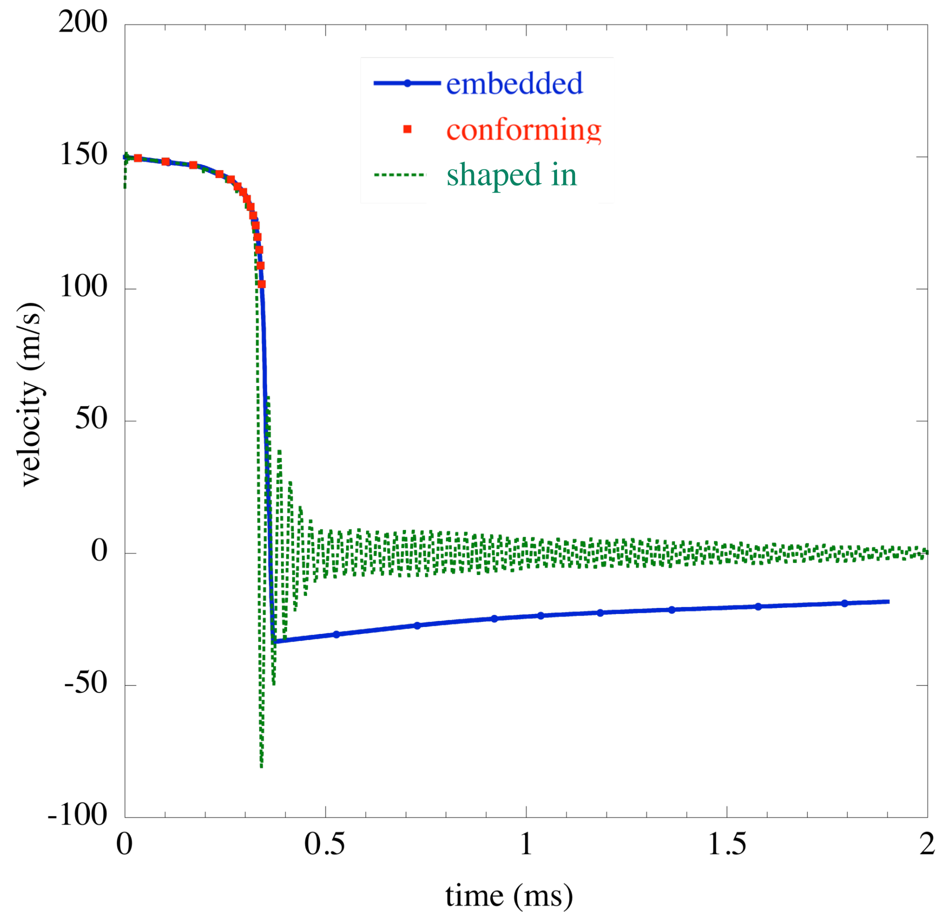






Impacting Plates: contact





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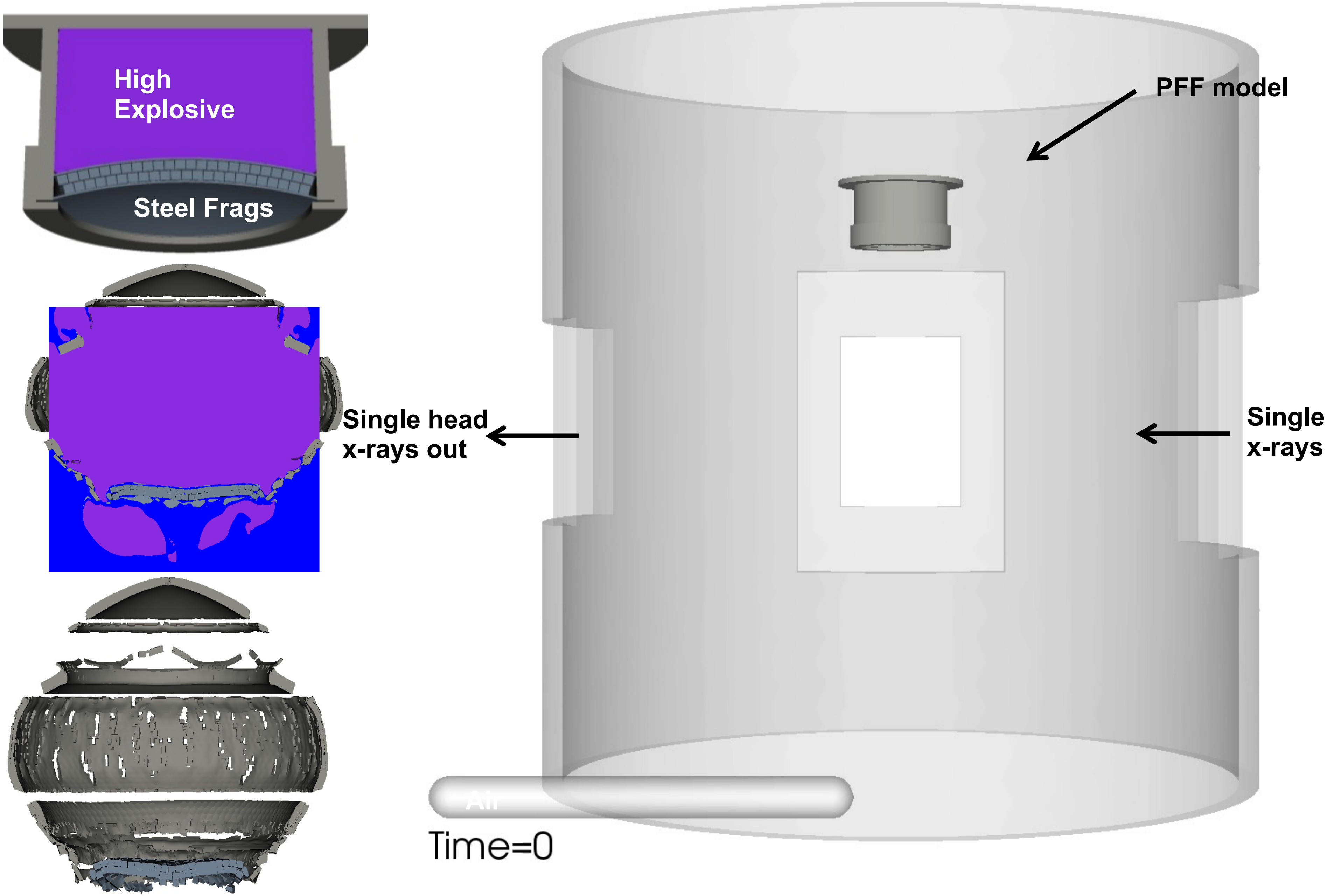
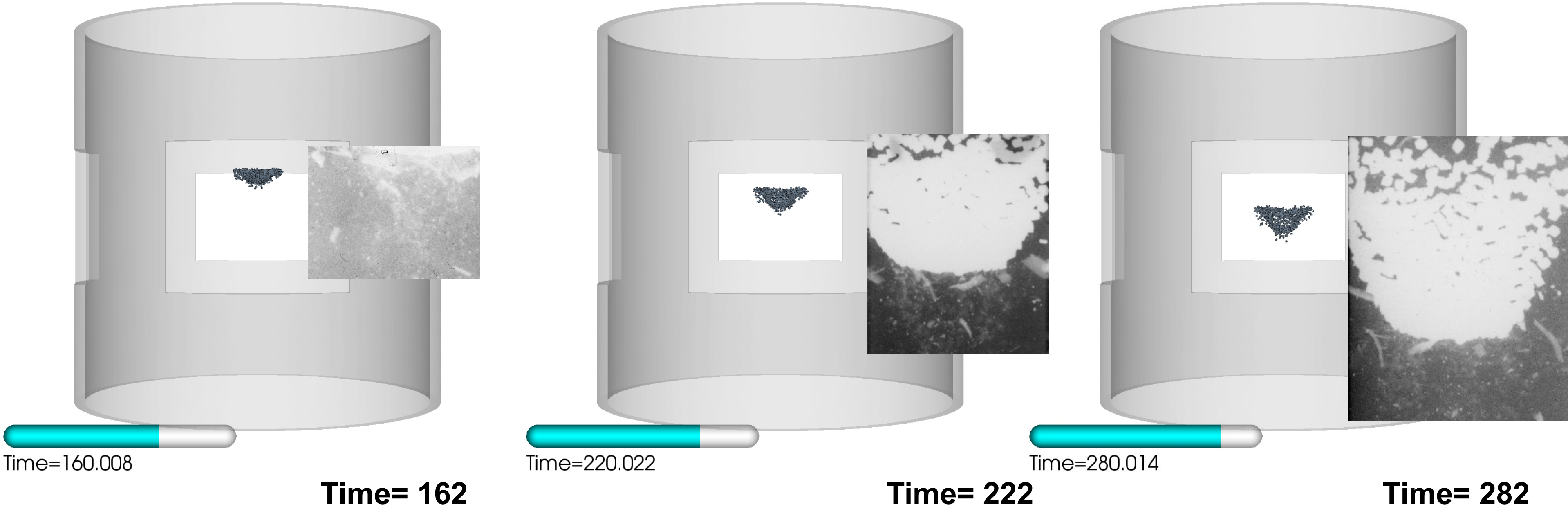
Experimental validation of Pre-Formed Frags weapon (Christensen)



Computed fragment distributions and velocities agree well with the collected data (cluster) (Christensen)



Simulated velocities and displacements within 1% of experimental results for times considered

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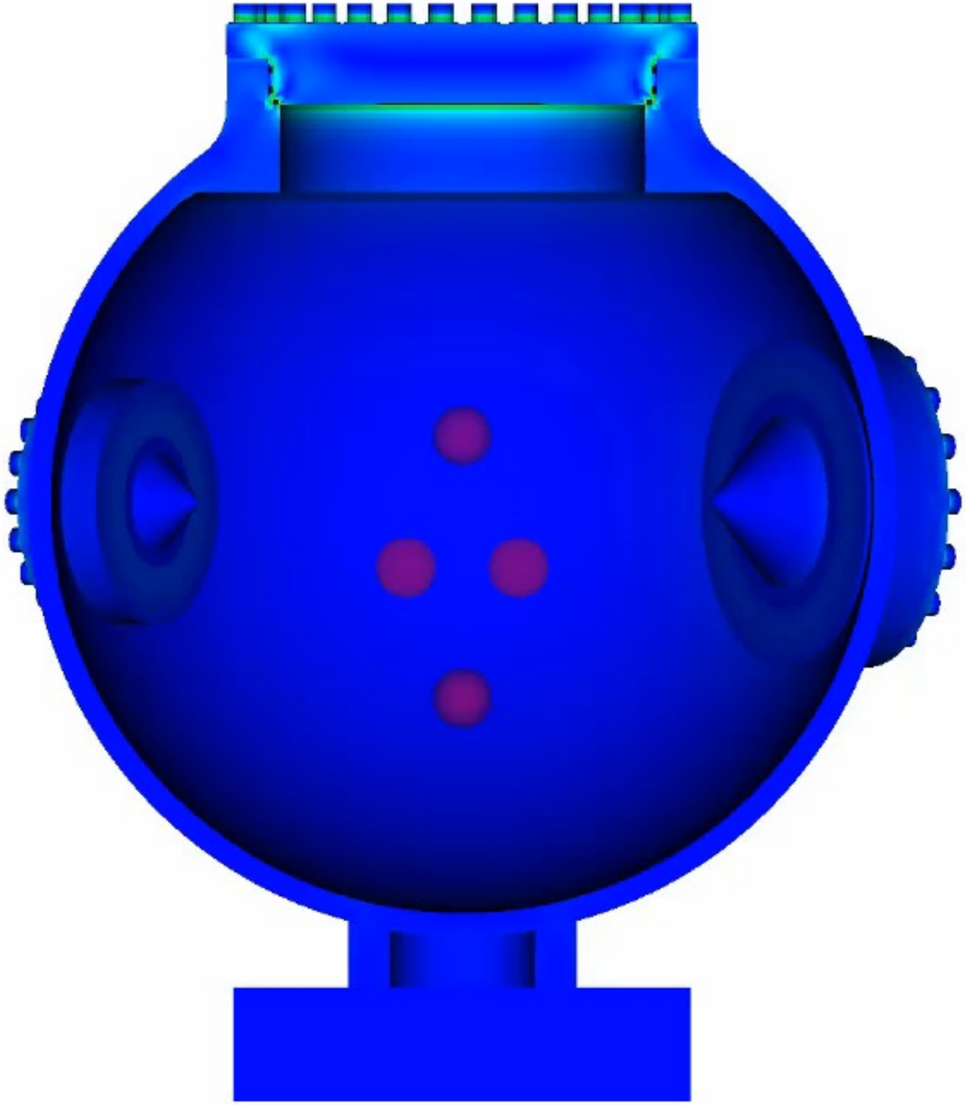
Nimble Vessel Analysis (Lam)



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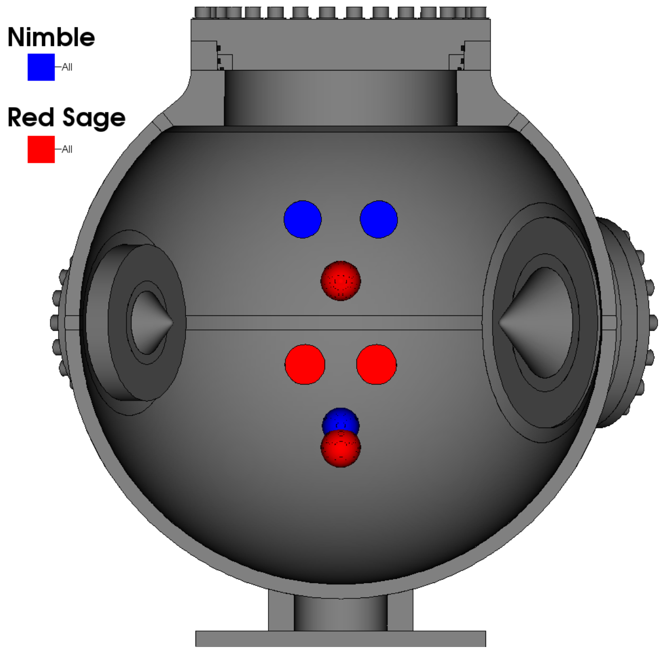
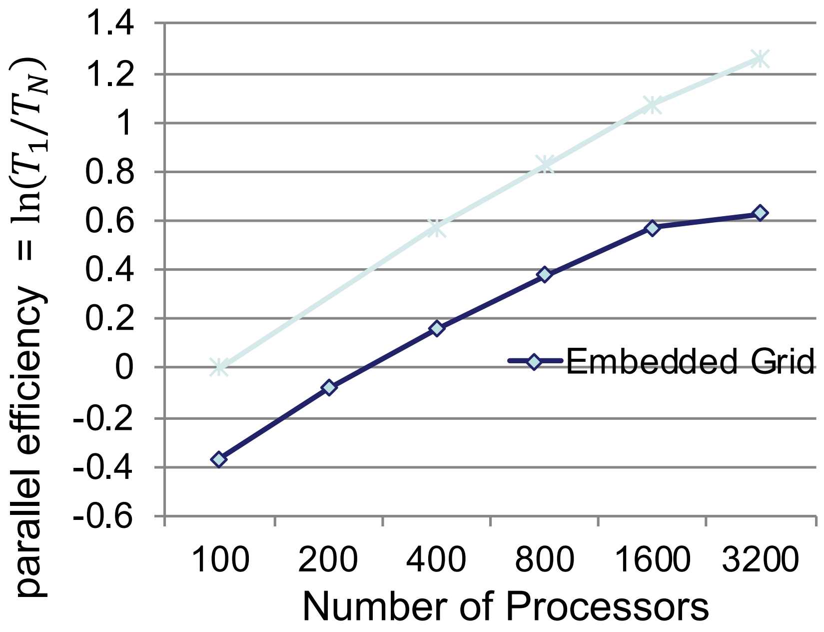
Vessel Analysis: parallel (strong) scaling study





360 degree model:
1.1 million zones foreground solid mesh
121,757 mortar contact segments
29 million zones background ALE mesh

Dominant costs:

1. Computational geometry embedded mesh
2. Contact
3. PLIC Interface reconstruction for multiphase fluids

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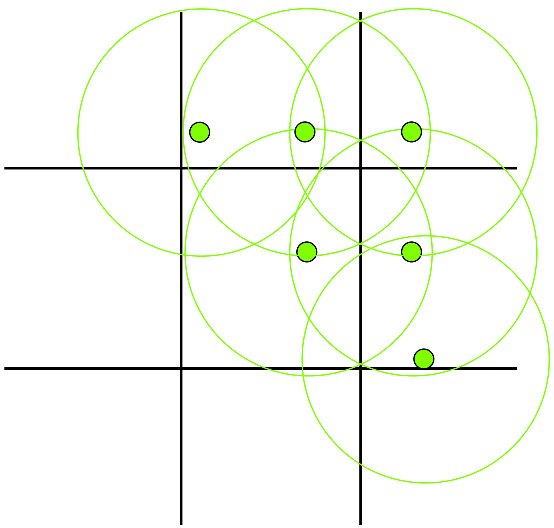
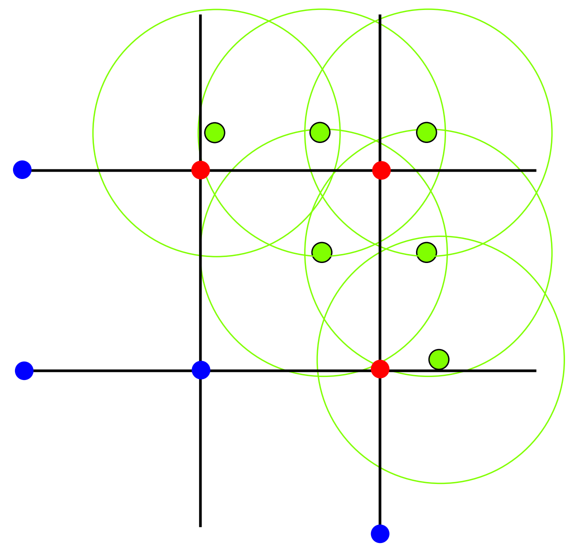
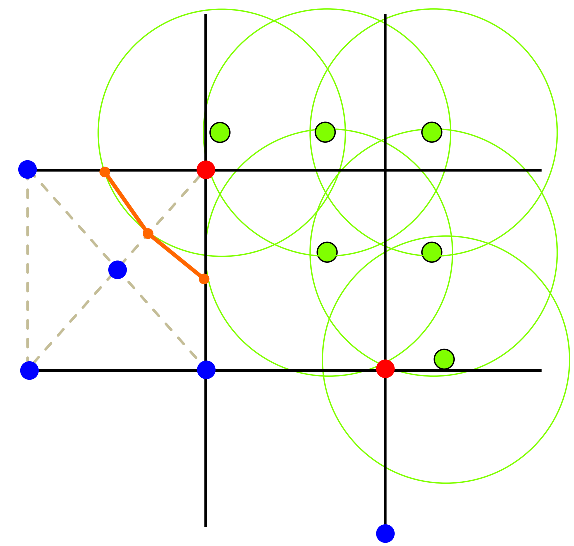
SPH Coupling Compute closed surface with level set like approach



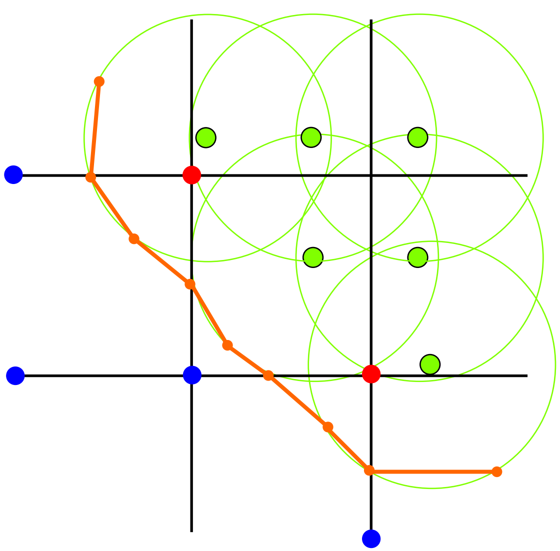
Foreground Particles overlapping Background Mesh



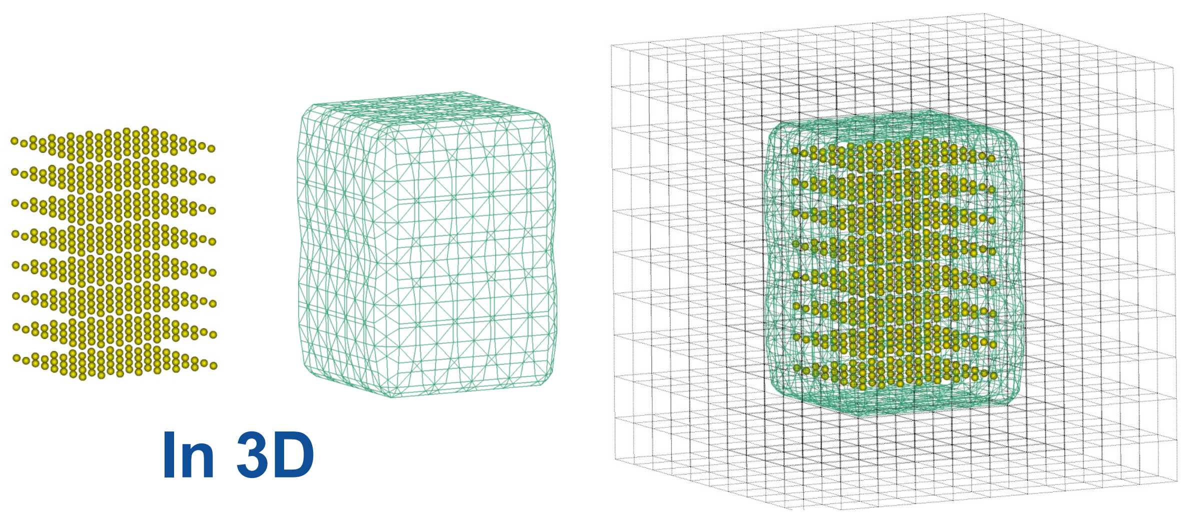
Identify exterior cut edges



Add triangles to cell, connect dots



Repeat in each cell to get surface



In 3D

Tsuji, P; Puso, MA; Spangler, CW; Owen, JM; Goto, D; Orzechowski, T. “Embedded smoothed particle hydrodynamics” *COMPUT METHOD APPL MECH ENG*, **366**, (2020).

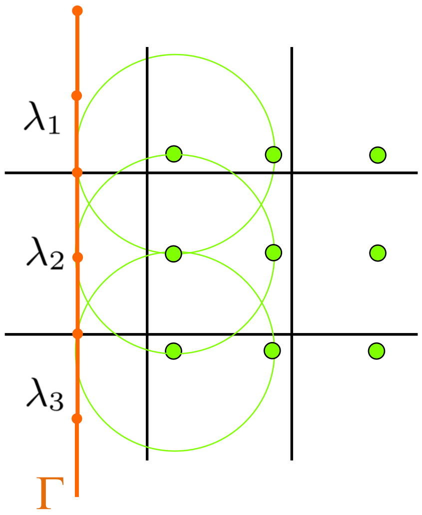
Couple particles to background

SPH EOM's $\Leftrightarrow$ FEM using nodal integration

$$m_i \mathbf{a}_i + (B^f \lambda)_i = \sum_{j=1}^{N} m_i m_j \left(\frac{\boldsymbol{\sigma}_i}{\rho_i^2} + \frac{\boldsymbol{\sigma}_j}{\rho_j^2} \right) \cdot \nabla W_{ij}$$

Consider EOM's

$$\begin{aligned} M^b a^b + B^{b\,T} \lambda &= F^b \\ M^f a^f + B^{f\,T} \lambda &= F^f \\ B^b v^b + B^f v^f - \bar{C}^{-1} \lambda &= 0 \end{aligned}$$



Background interface force

$$B^{bT} \lambda \Rightarrow \int_\Gamma \phi_A^b(x) \lambda(x)\, d\Gamma = \sum_e \lambda_e \int_{\Gamma_e} \phi_A^b(x)\, d\Gamma$$

Foreground interface force

$$B^{fT} \lambda \Rightarrow \int_\Gamma \tilde{W}_i(x) \lambda(x)\, d\Gamma = \sum_e \lambda_e \int_{\Gamma_e} \tilde{W}_i(x)\, d\Gamma \quad \tilde{W}_i(x) = \frac{W_i(x)}{\sum_j W_j(x)}$$

Couple particles to background

SPH EOM's ⇔ FEM using nodal integration

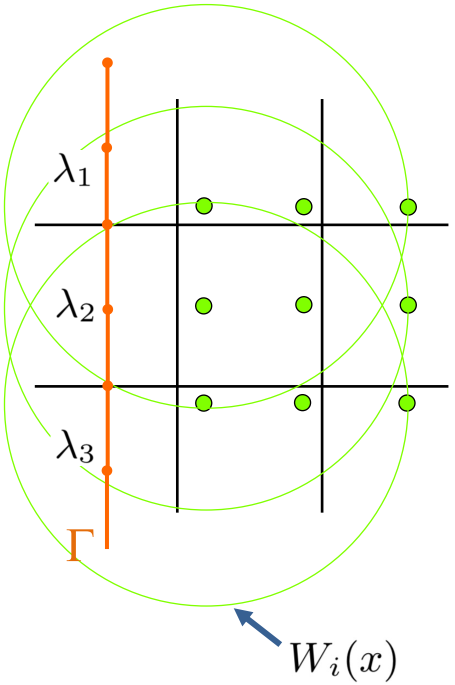
$$m_i \mathbf{a}_i + (B^f \lambda)_i = \sum_{j=1}^{N} m_i m_j \left(\frac{\boldsymbol{\sigma}_i}{\rho_i^2} + \frac{\boldsymbol{\sigma}_j}{\rho_j^2} \right) \cdot \nabla W_{ij}$$

Consider EOM's

$$M^b a^b + B^{b\,T} \lambda = F^b$$

$$M^f a^f + B^{f\,T} \lambda = F^f$$

$$B^b v^b + B^f v^f - \bar{C}^{-1} \lambda = 0$$



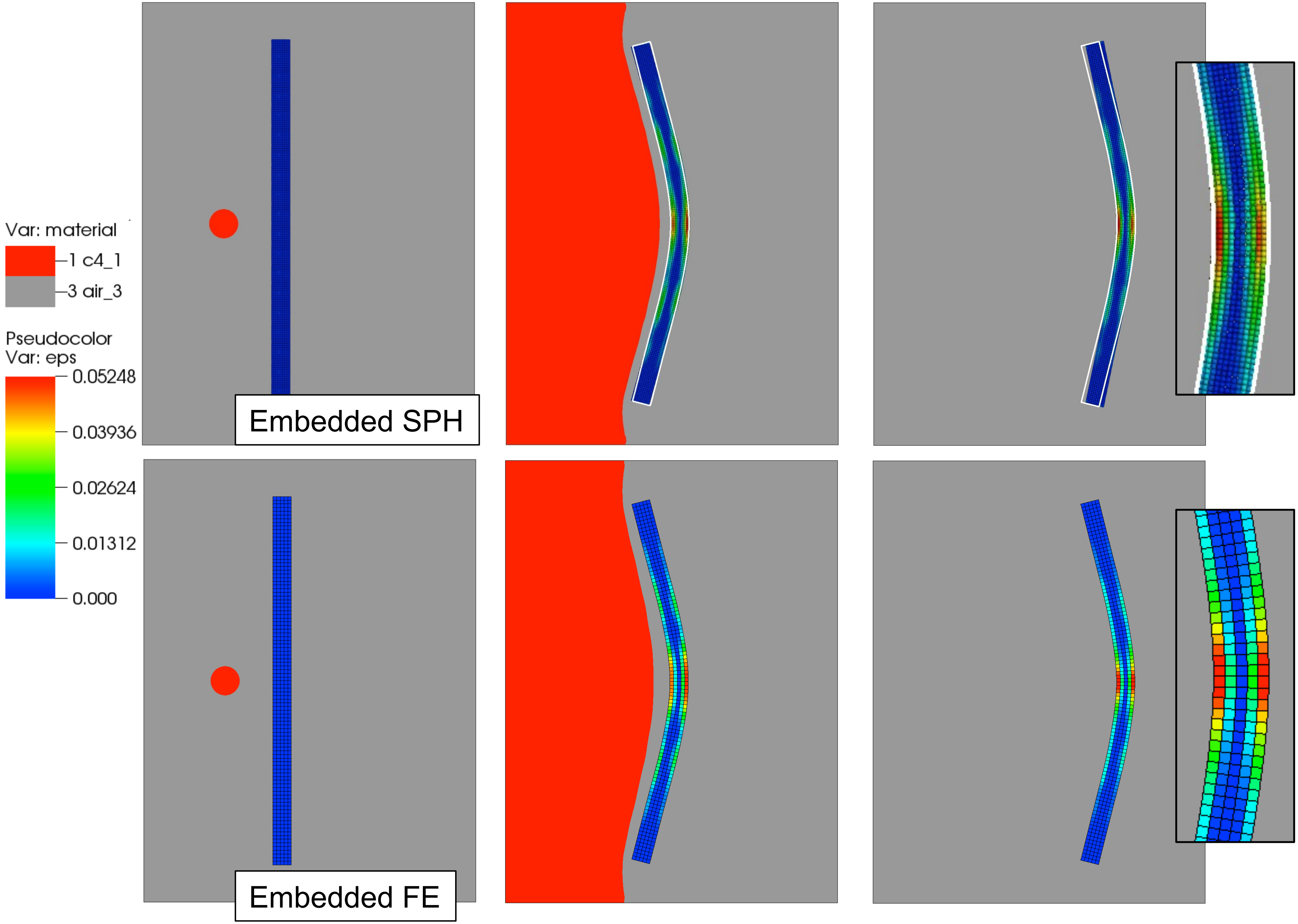
Background interface force

$$B^{bT} \lambda \Rightarrow \int_\Gamma \phi_A^b(x) \lambda(x)\, d\Gamma = \sum_e \lambda_e \int_{\Gamma_e} \phi_A^b(x)\, d\Gamma$$

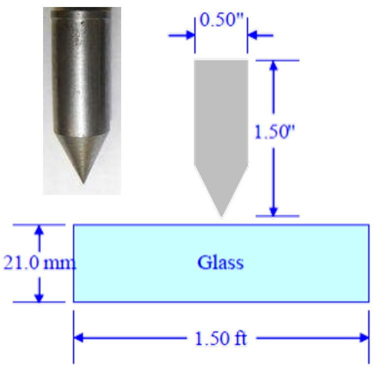
Foreground interface force

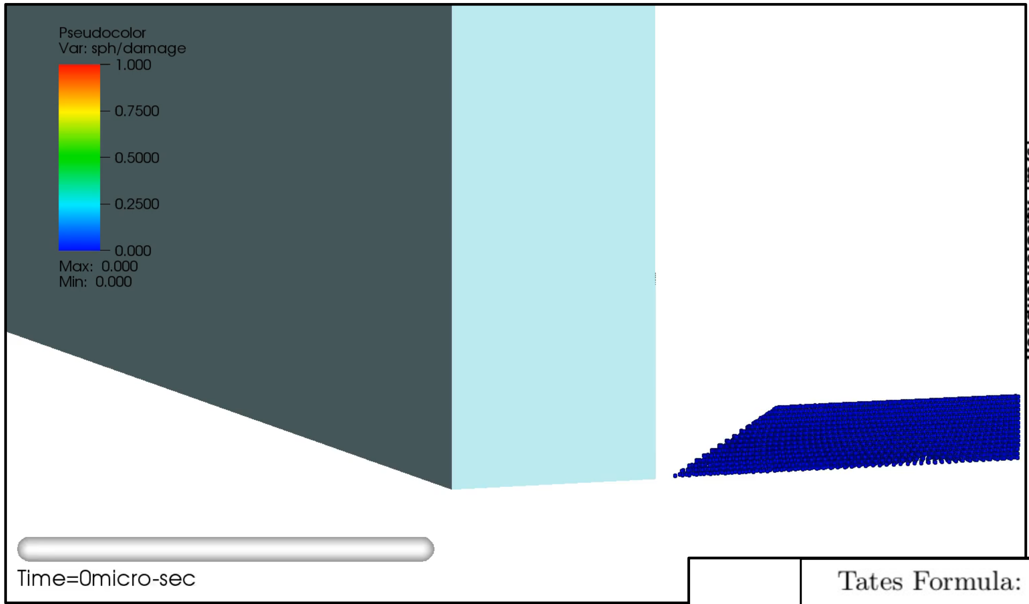
$$B^{fT} \lambda \Rightarrow \int_\Gamma \tilde{W}_i(x) \lambda(x)\, d\Gamma = \sum_e \lambda_e \int_{\Gamma_e} \tilde{W}_i(x)\, d\Gamma \qquad \tilde{W}_i(x) = \frac{W_i(x)}{\sum_j W_j(x)}$$

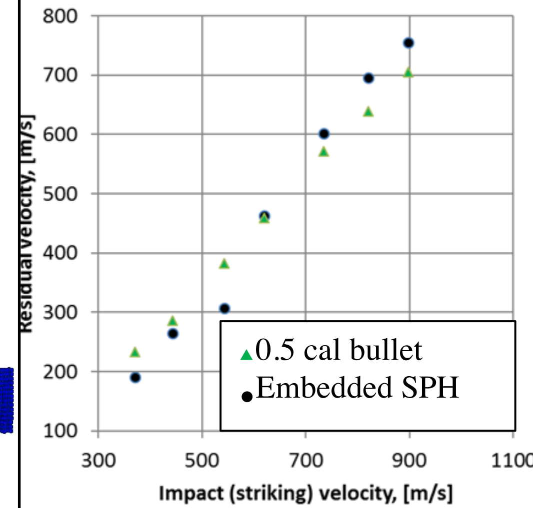
Embedded SPH vs Embedded FE

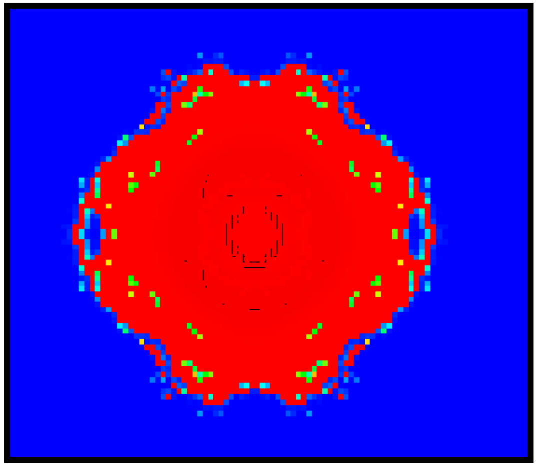


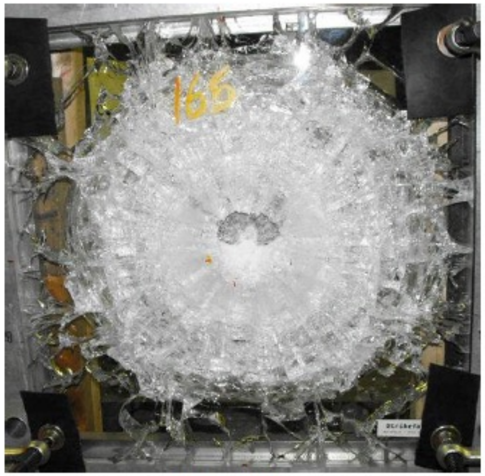
Validation: penetrators (Spangler)







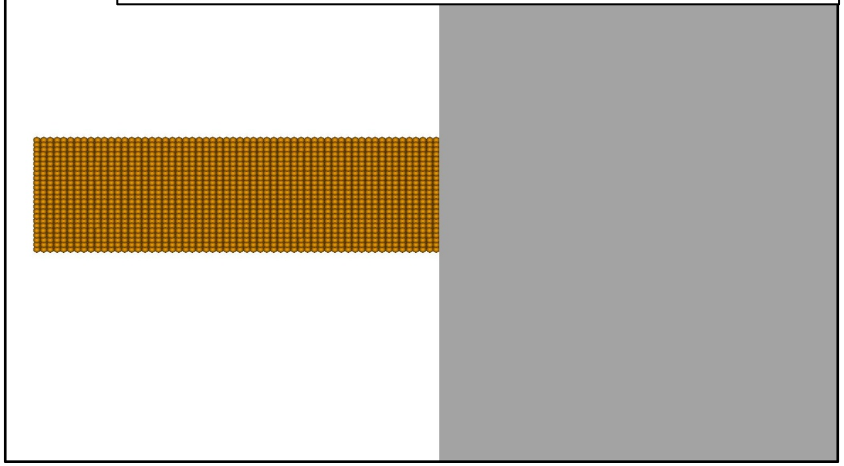




(a) $V_s = 911$ m/s

$$\text{Tates Formula: depth} = L\sqrt{\rho_{pen}/\rho_{target}} = 1.73\ \text{cm}$$

$$\text{Embedded SPH: depth} = 1.65\ \text{cm}$$



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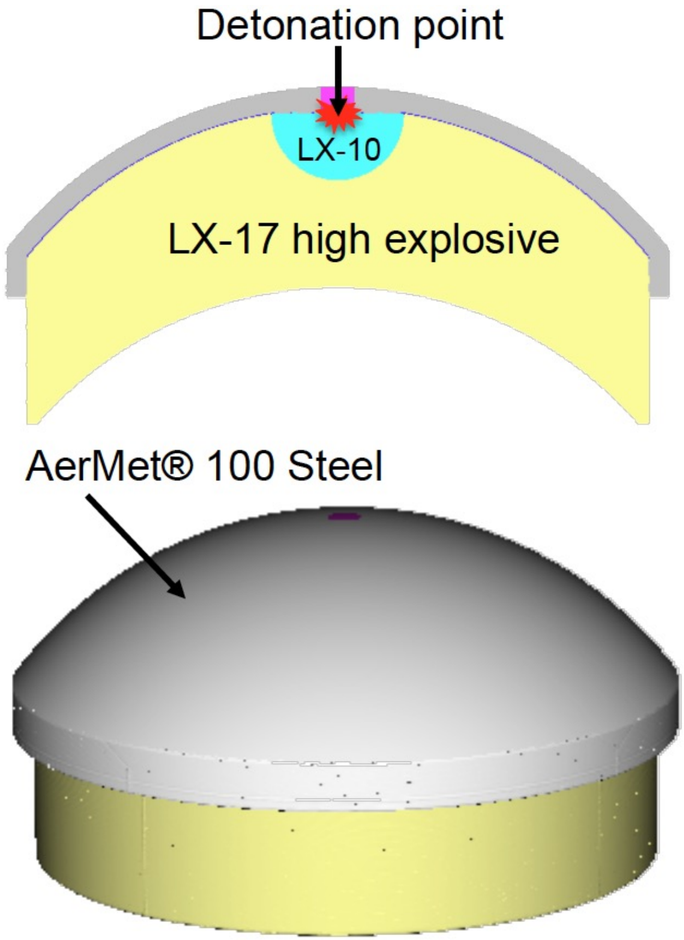
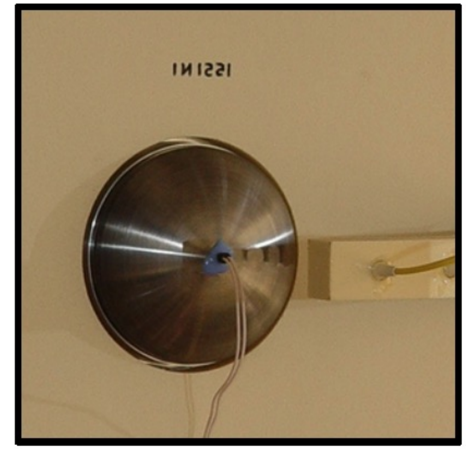
Validation: AerMet steel cylinder & hubcap exp. (Tsuji)





Cylinder test geometry

Hemispherical shell test geometry (“hubcap”)

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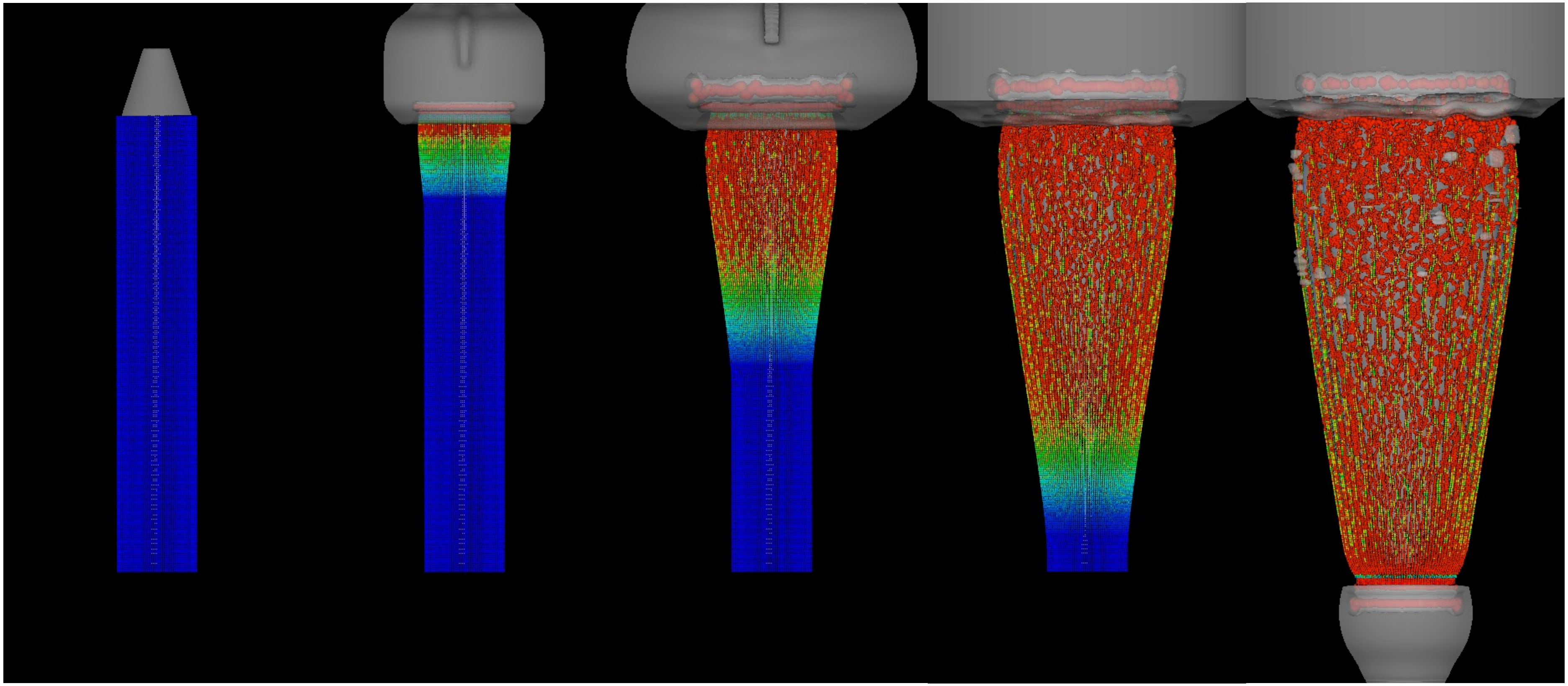
Validation: Damage evolution with Embedded SPH



0 µs | 10 µs | 20 µs | 30 µs | 40 µs

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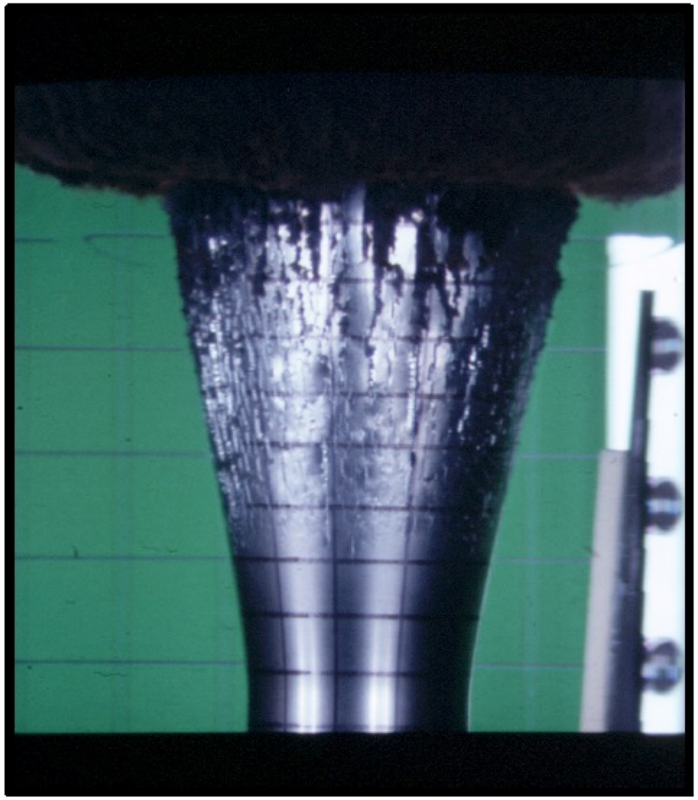
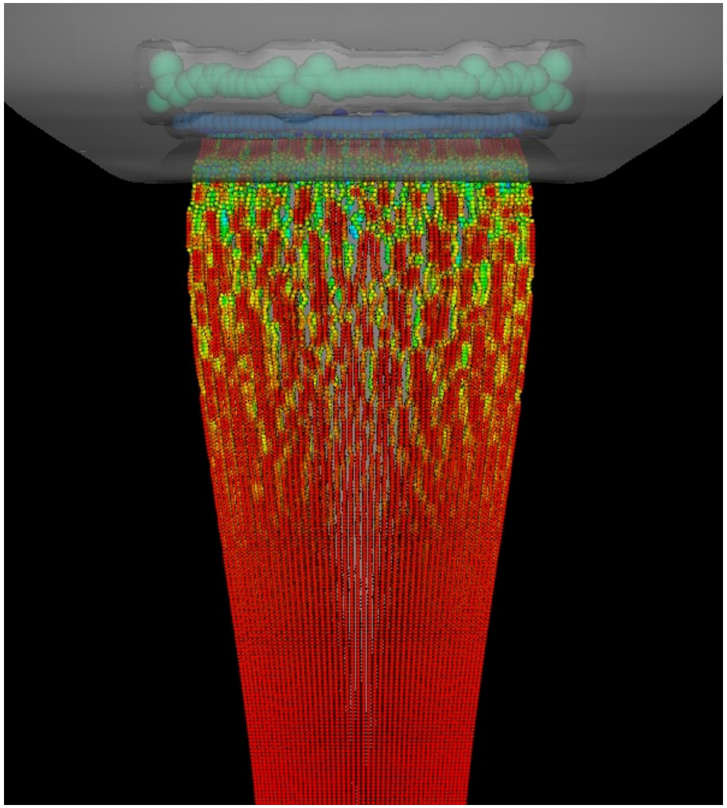
High speed camera image of the cylinder is compared to FEusion/SPH



High speed images at t = 21 μs



Density at 21 μs

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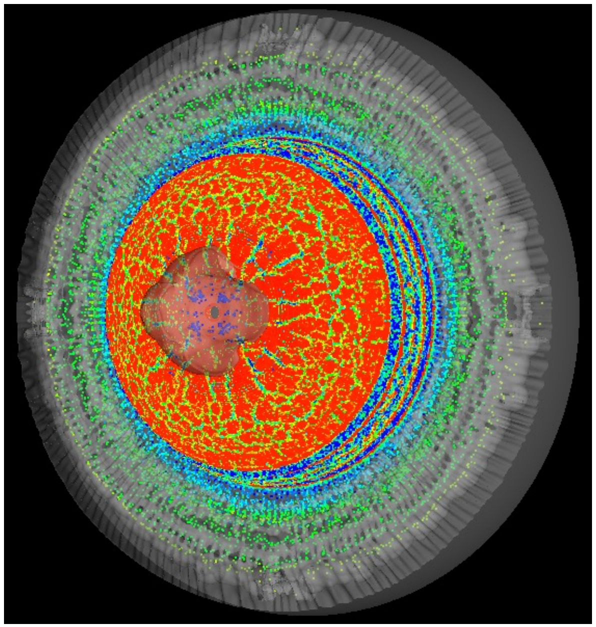
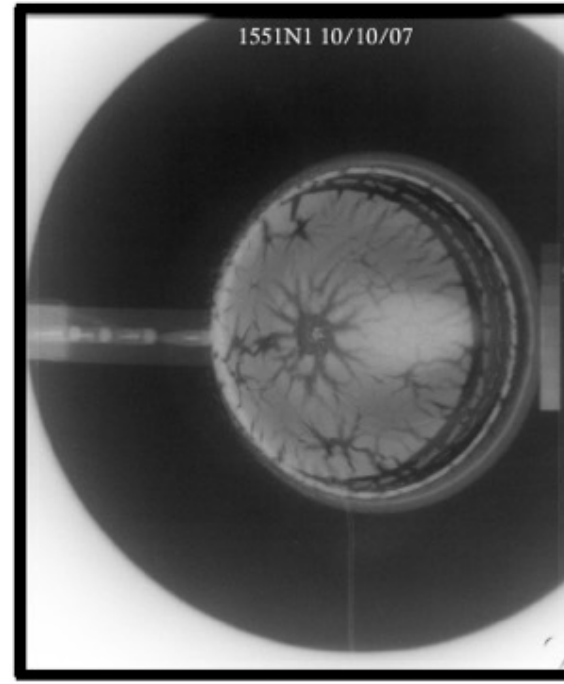
Hubcap simulation with Embedded SPH



Density at 22 μs

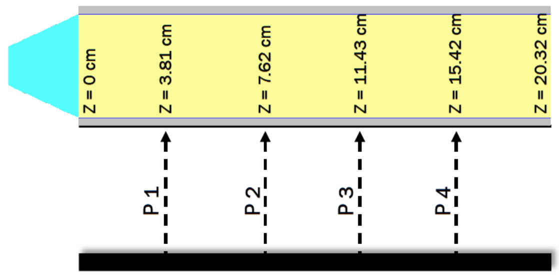
Post Processor Simulated Radiograph at 22 μs

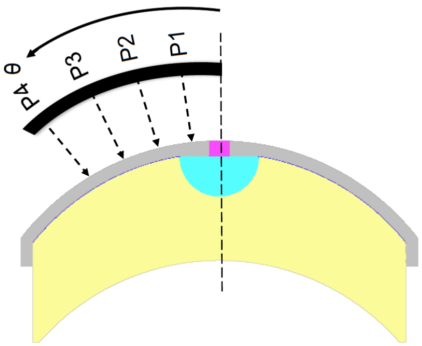


Real Radiograph at 22 μs

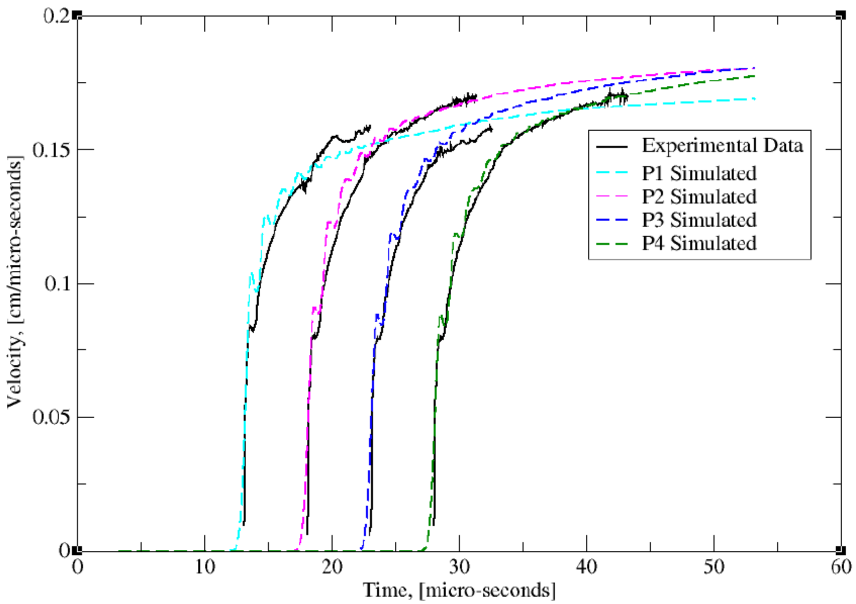
Validation: AerMet steel cylinder & hubcap experiments

Probe locations for cylinder and hubcap

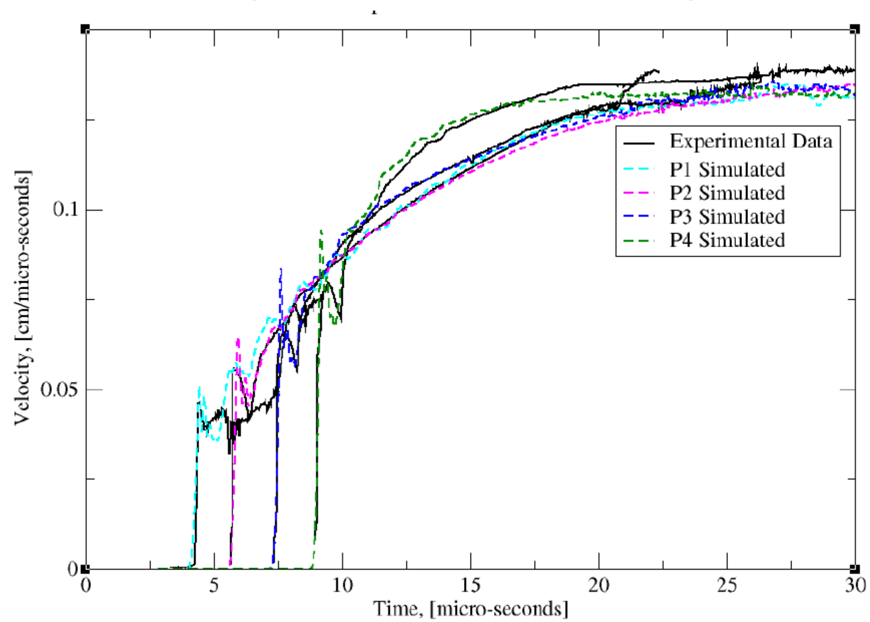




Cylinder: Embedded FE vs Experiment



Hubcap: Embedded FE vs Experiment



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Validation: AerMet steel cylinder & hubcap experiments

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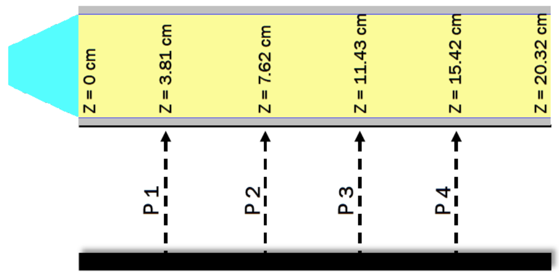
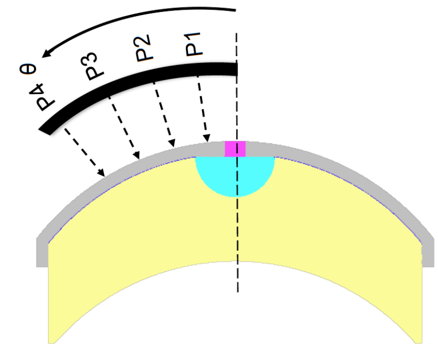
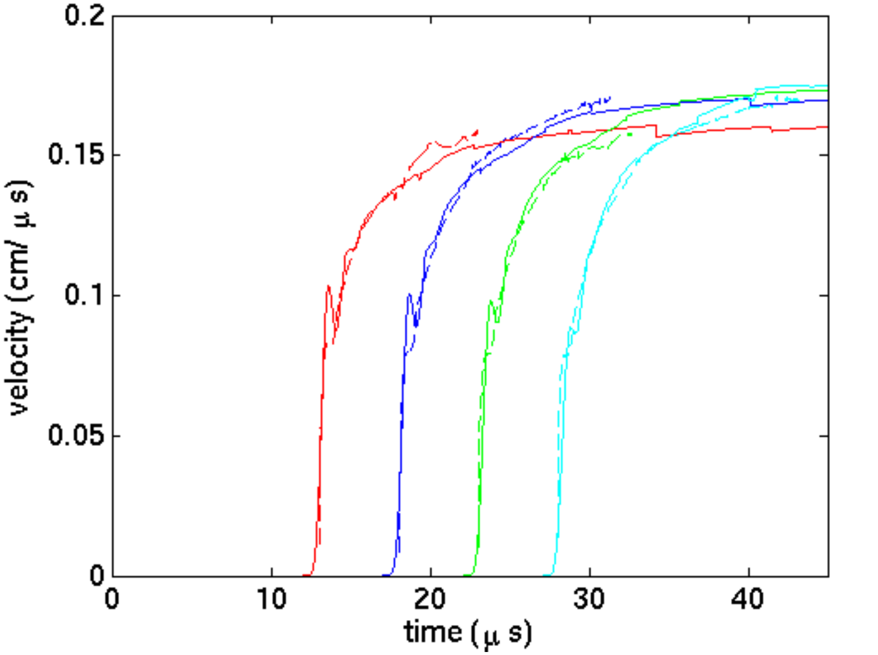
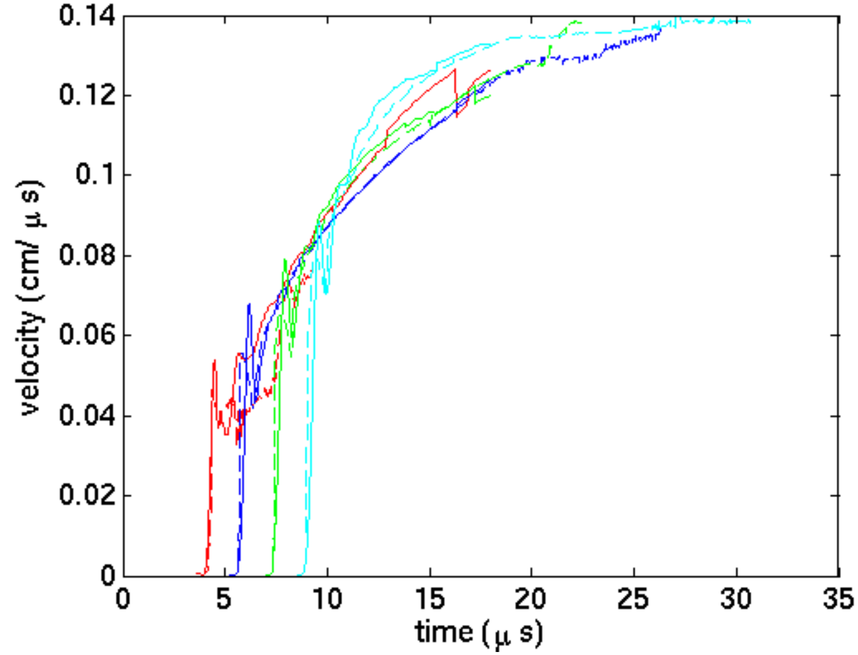




Cylinder: Embedded SPH vs Experiment



Hubcap: Embedded SPH vs Experiment



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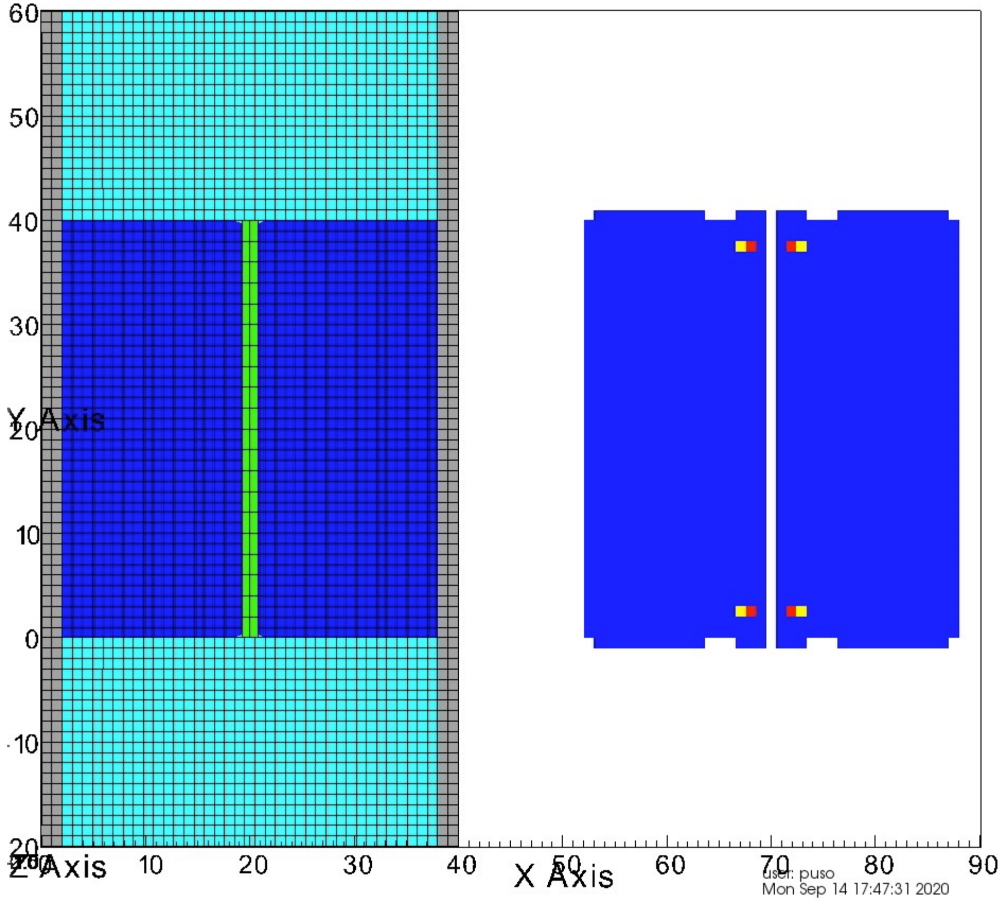
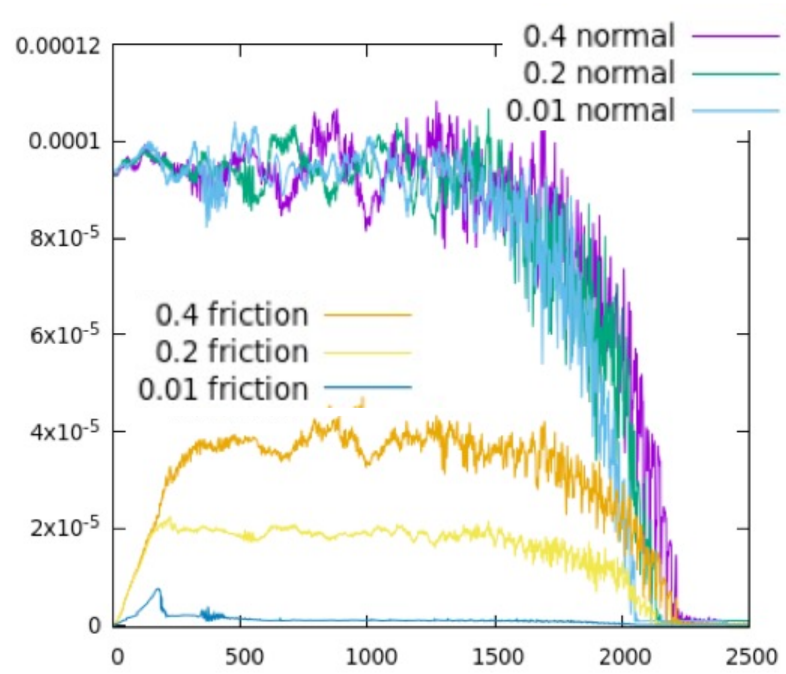
Current Work: Unilateral contact and friction

Friction important for bar pull out, penetration μ = 0.4, 0.2, 0.01





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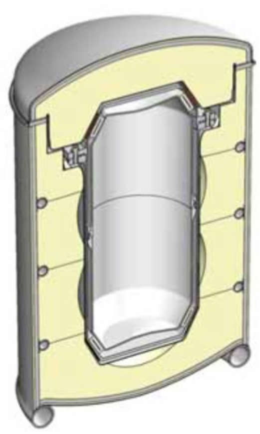
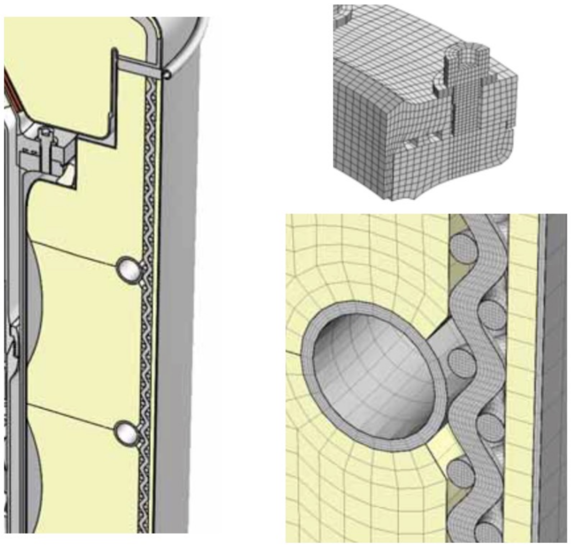
Contact Problems

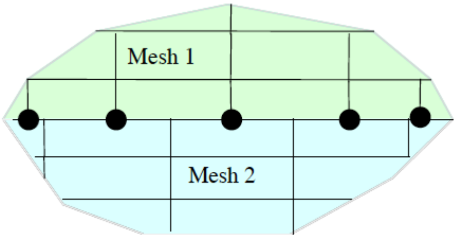
- *Many* engineering problems are contact dominated
- Different forms of constraint enforcement:



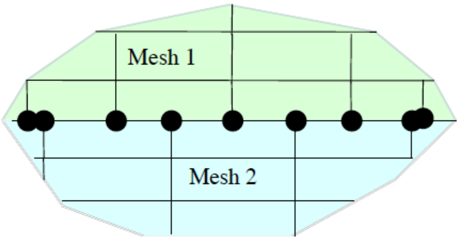
Shipping Container
Courtesy T. DePiero & S. Densberger



node to surface (n-s)

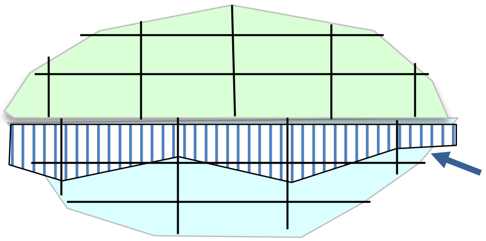


single pass (inaccurate)



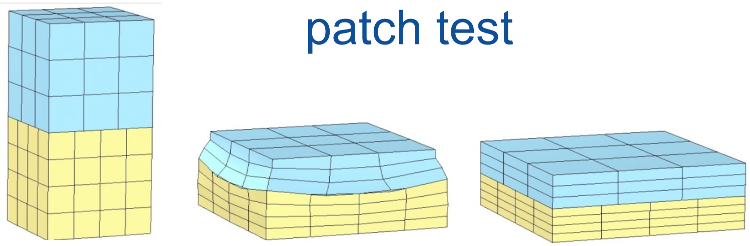
double pass (locks)

surface to surface (s-s)



e.g. mortar (piecewise linear)

patch test

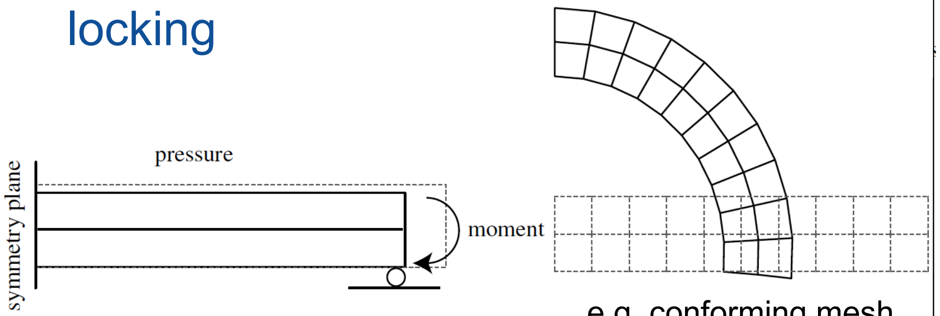


uniaxial compression

single pass n-s (bad)

surface to surface (good)

locking



overlapped beams

e.g. conforming mesh

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Contact Problems

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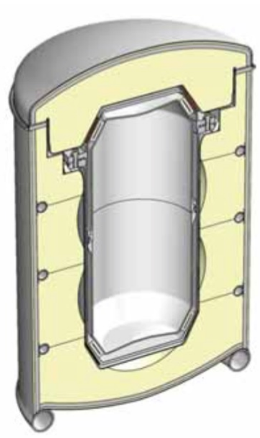
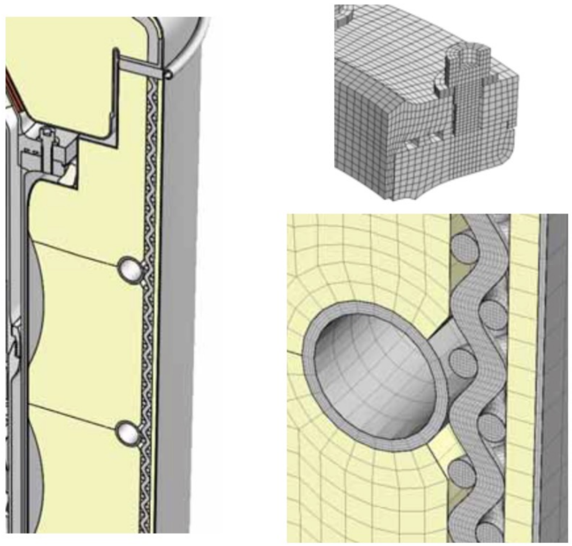
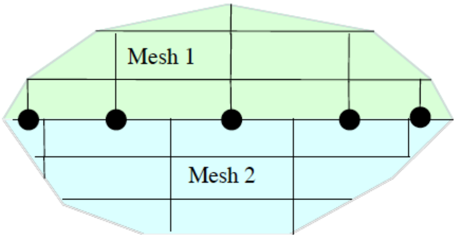
- Different forms of constraint enforcement:



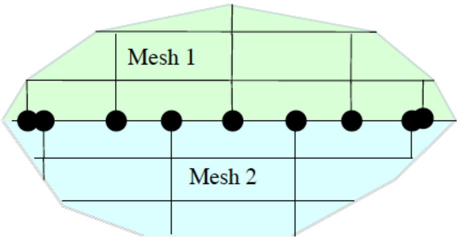
Shipping Container
Courtesy T. DePiero & S. Densberger



node to surface (n-s)

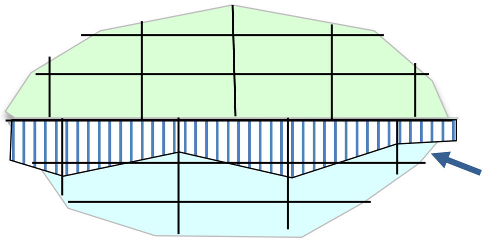


single pass (inaccurate)



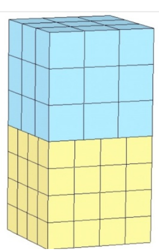
double pass (locks)

surface to surface (s-s)

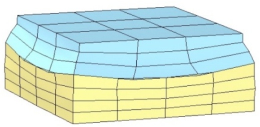


e.g. mortar (piecewise linear)

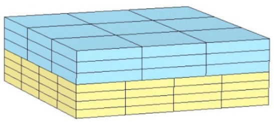
patch test



uniaxial compression

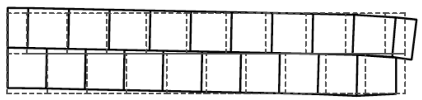


single pass n-s (bad)

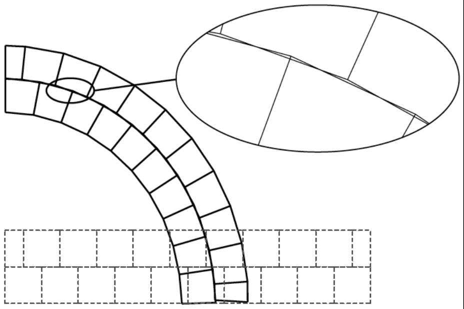


surface to surface (good)

locking



double pass n-s (locks!)



mortar s-s

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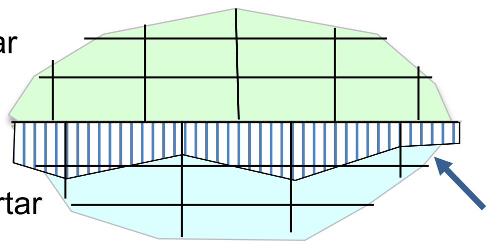
Surface to Surface options:

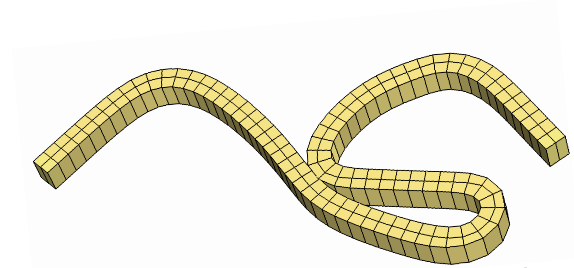
- Standard mortar approach is biased: requires choice of *mortar* and *non-mortar* sides

mortar side



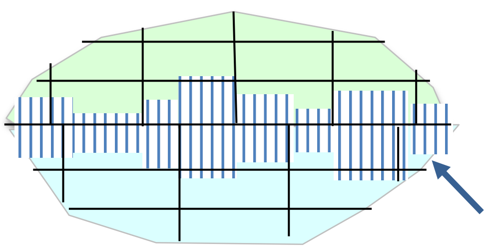
non-mortar side

Piecewise linear field based on on ***nodes***

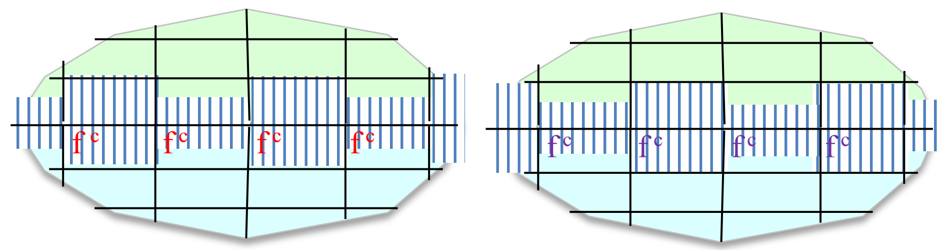


Problem: biased contact doesn't work

- Segment based approaches not biased but not stable (kinda okay for penalty method)

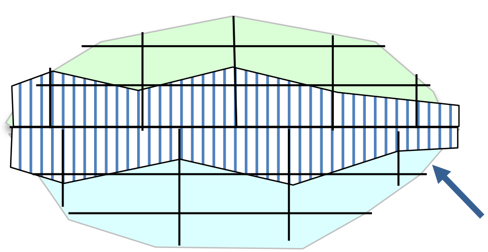


Piecewise constant field based on ***segments***

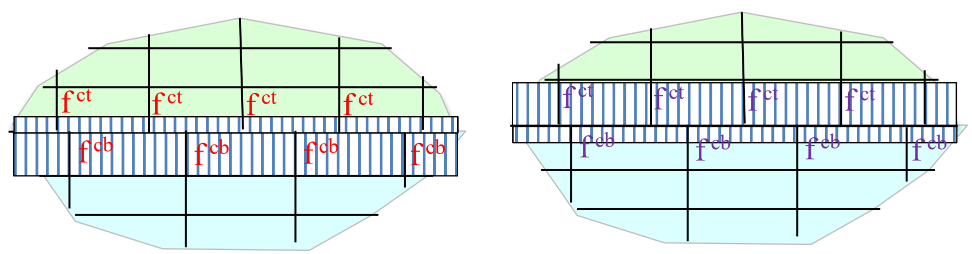


Problem: uncontrolled pressure mode $f^c = f^c$ with symmetry

- Two pass mortar approach not biased also not stable



Piecewise linear field based on on ***nodes***



Problem: uncontrolled pressure mode $f_c = f_c$ with symmetry

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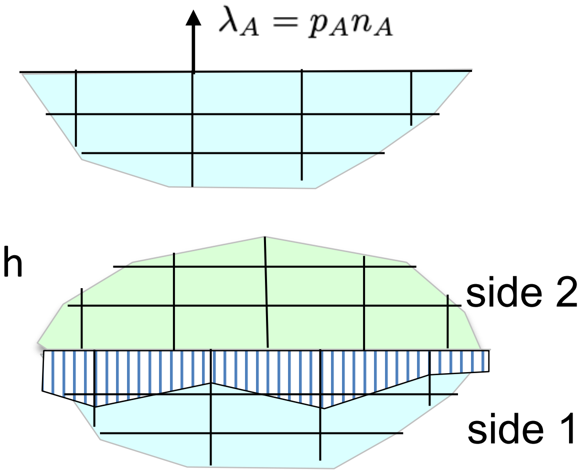
Surface to surface formulation

- Definitions $\varphi_A \equiv \text{FE shape function at node A}$

trial functions $u_h = \sum_A \varphi_A u_A \quad \lambda_h = \sum_A \varphi_A \lambda_A$

test functions $v_h = \sum_A \varphi_A v_A \quad \mu_h = \sum_A \varphi_A \mu_A$



- Consider "abstract"BVP for *mortar* surface-to-surface approach

$$\begin{aligned} a(u_h, v_h) + b(\lambda_h, v_h) &= \langle f, v_h \rangle \\ b(\mu_h, u_h) &= 0 \end{aligned}$$

strain energy $a(u_h, v_h) = \int_\Omega \varepsilon(v_h) C \varepsilon(u_h) d\Omega \qquad \varepsilon(u_h) = 1/2(\nabla u_h + \nabla^T u_h)$

constraints $b_h(\mu_h, u_h) = \int_\Gamma \mu_h^1 (u_h^1 - u_h^2) \cdot d\Gamma \Rightarrow \mu_A^1 \int_\Gamma \varphi_A^1 (u_h^1 - u_h^2) \cdot d\Gamma$

contact force $b_h(\lambda_h, v_h) = \int_\Gamma \lambda_h^1 (v_h^1 - v_h^2) \cdot d\Gamma \Rightarrow v_B^1 \cdot \int_\Gamma \lambda_h^1 \varphi_B^1 d\Gamma - v_C^2 \cdot \int_\Gamma \lambda_h^1 \varphi_C^1 d\Gamma$

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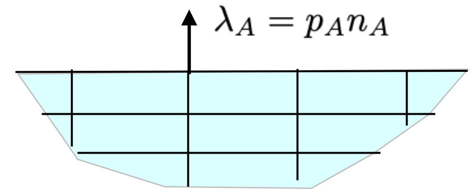
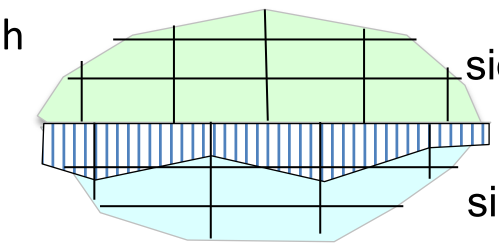


- Consider "abstract" BVP for *mortar* surface-to-surface approach



$$
\begin{aligned}
a(u_h, v_h) + b(\lambda_h, v_h) &= \langle f, v_h \rangle \\
b(\mu_h, u_h) &= 0
\end{aligned}
$$

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constraints $b_h(\mu_h, u_h) = \int_\Gamma \mu_h^1 (u_h^1 - u_h^2) \cdot d\Gamma \quad \Rightarrow \quad g_A = n_A \cdot \int_\Gamma \varphi_A^1 (u_h^1 - u_h^2) d\Gamma \geq 0$

contact force $b_h(\lambda_h, v_h) = \int_\Gamma \lambda_h^1 (v_h^1 - v_h^2) \cdot d\Gamma \quad \Rightarrow \quad v_B^1 \cdot \int_\Gamma \lambda_h^1 \varphi_B^1 d\Gamma - v_C^2 \cdot \int_\Gamma \lambda_h^1 \varphi_C^2 d\Gamma$

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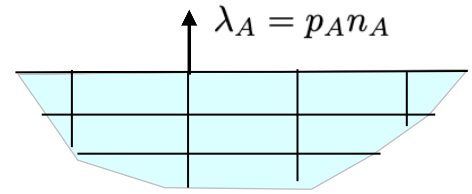

trial functions $u_h = \sum_A \varphi_A u_A \quad \lambda_h = \sum_A \varphi_A \lambda_A$

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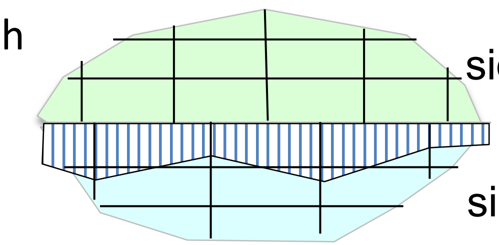
- Consider "abstract" BVP for *mortar* surface-to-surface approach



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\begin{aligned}
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contact force $b_h(\lambda_h, v_h) = \int_\Gamma \lambda_h^1 (v_h^1 - v_h^2) \cdot d\Gamma \;\Rightarrow\; f_B^{c1} = \int_\Gamma \lambda_h^1 \varphi_B^1 d\Gamma \quad f_C^{c2} = -\int_\Gamma \lambda_h^1 \varphi_C^2 d\Gamma$

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Surface to surface formulations

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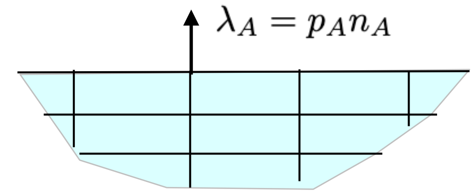
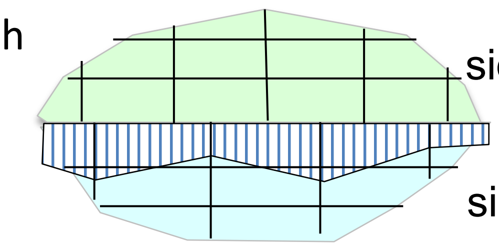


- Consider "abstract" BVP for *mortar* surface-to-surface approach



$$\begin{aligned} a(u_h, v_h) + b(\lambda_h, v_h) &= \langle f, v_h \rangle \\ b(\mu_h, u_h) &= 0 \end{aligned}$$

$$\text{strain energy} \quad a(u_h, v_h) = \int_\Omega \varepsilon(v_h) C \varepsilon(u_h) d\Omega \qquad \varepsilon(u_h) = 1/2(\nabla u_h + \nabla^T u_h)$$

$$\text{constraints} \quad b_h(\mu_h, u_h) = \int_\Gamma \mu_h^1 (u_h^1 - u_h^2) \cdot d\Gamma \quad \Rightarrow \quad g_A = \int_\Gamma \varphi_A^1 (u_h^1 - u_h^2) \cdot d\Gamma \geq 0$$

$$\text{contact force} \quad b_h(\lambda_h, v_h) = \int_\Gamma \lambda_h^1 (v_h^1 - v_h^2) \cdot d\Gamma \quad \Rightarrow \quad f_B^{c1} = \int_\Gamma \lambda_h^1 \varphi_B^1 d\Gamma \quad f_C^{c2} = -\int_\Gamma \lambda_h^1 \varphi_C^2 d\Gamma$$

$$\begin{bmatrix} K^1 & 0 & B^{1T} \\ 0 & K^2 & B^{2T} \\ B^1 & B^1 & 0 \end{bmatrix} \begin{Bmatrix} u^1 \\ u^2 \\ \lambda \end{Bmatrix} = \begin{Bmatrix} F^1 \\ F^2 \\ 0 \end{Bmatrix}$$

no "modes" with standard mortar using $\lambda = \lambda^1$

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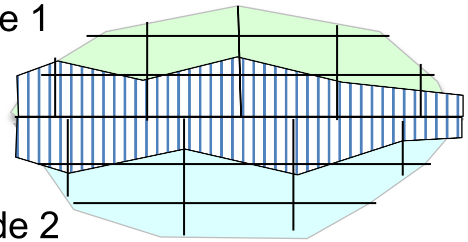
Stabilized two pass mortar approach

$$a(u_h, v_h) + b(\lambda_h, v_h) = \langle f, v \rangle$$
$$b(\mu_h, u_h) - j(\mu_h, \lambda_h) = 0$$

$$b(\lambda_h, v_h) = \frac{1}{2}\int_{\Gamma^c} (\lambda_h^1 - \lambda_h^2) \cdot (v_h^1 - v_h^2)\, d\Gamma$$

$$j(\mu_h, \lambda_h) = \frac{\gamma h}{2}\int_{\Gamma^c} (\mu_h^1 + \mu_h^2) \cdot (\lambda_h^1 + \lambda_h^2)\, d\Gamma$$



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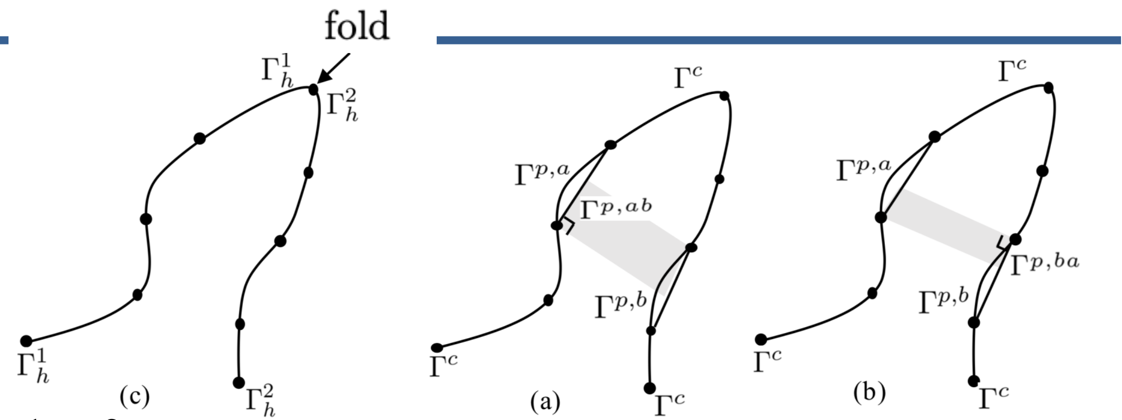
Stabilized approach: implementation

$$a(u_h, v_h) + b(\lambda_h, v_h) = \langle f, v \rangle$$
$$b(\mu_h, u_h) - j(\mu_h, \lambda_h) = 0$$

$$b(\lambda_h, v_h) = \frac{1}{2} \int_{\Gamma^c} (\lambda_h^1 - \lambda_h^2) \cdot (v_h^1 - v_h^2)\, d\Gamma$$

$$j(\mu_h, \lambda_h) = \frac{\gamma h}{2} \int_{\Gamma^c} (\mu_h^1 + \mu_h^2) \cdot (\lambda_h^1 + \lambda_h^2)\, d\Gamma$$



Implementation is really "agnostic" of side 1 or 2

$$b(\lambda_h, u_h) = \frac{1}{2} \sum_{p=1}^{\#\text{of pairs}} \left(\int_{\Gamma^{p,ab}} \lambda_h^{p,a} \cdot (u^{p,a} - u^{p,b})\, d\Gamma + \int_{\Gamma^{p,ba}} \lambda_h^{p,b} \cdot (u^{p,b} - u^{p,a})\, d\Gamma \right)$$

$$j(\mu_h, \lambda_h) = \frac{h}{2} \sum_{p=1}^{\#\text{of pairs}} \gamma^p \Big(\underbrace{\int_{\Gamma^{p,ab}} \mu_h^{p,a} \cdot (\lambda^{p,a} + \lambda^{p,b})\, d\Gamma}_{\Gamma^{p,ab}} + \underbrace{\int_{\Gamma^{p,ba}} \mu_h^{p,b} \cdot (\lambda^{p,b} + \lambda^{p,a})\, d\Gamma}_{\Gamma^{p,ba}} \Big)$$

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Stabilized approach: inf-sup

$$a(u_h, v_h) + b(\lambda_h, v_h) = \langle f, v \rangle$$
$$b(\mu_h, u_h) - j(\mu_h, \lambda_h) = 0$$

$$b(\lambda_h, v_h) = \frac{1}{2} \int_{\Gamma^c} (\lambda_h^1 - \lambda_h^2) \cdot (v_h^1 - v_h^2) \, d\Gamma$$
$$j(\mu_h, \lambda_h) = \frac{\gamma h}{2} \int_{\Gamma^c} (\mu_h^1 + \mu_h^2) \cdot (\lambda_h^1 + \lambda_h^2) \, d\Gamma$$

Stability: weak form $\mathcal{B}$ must satisfy inf-sup (BNB) conditions:

$$\mathcal{B}((u_h, \lambda_h), (v_h, \mu_h)) = a(u_h, v_h) + b(\lambda_h, v_h) + b(\mu_h, u_h) - j(\mu_h, \lambda_h)$$

$$\inf_{(u_h, \lambda_h)} \sup_{(v_h, \mu_h)} \frac{\mathcal{B}((u_h, \lambda_h), (v_h, \mu_h))}{|||u_h, \lambda_h|||, |||v_h, \mu_h)|||} \geq c$$

For some suitable norm $|||\cdot, \cdot|||$, so what is this?

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Stabilized approach: what norm?

$$a(u_h, v_h) + b(\lambda_h, v_h) = \langle f, v \rangle$$
$$b(\mu_h, u_h) - j(\mu_h, \lambda_h) = 0$$

$$b(\lambda_h, v_h) = \frac{1}{2} \int_{\Gamma^c} (\lambda_h^1 - \lambda_h^2) \cdot (v_h^1 - v_h^2)\, d\Gamma$$
$$j(\mu_h, \lambda_h) = \frac{\gamma h}{2} \int_{\Gamma^c} (\mu_h^1 + \mu_h^2) \cdot (\lambda_h^1 + \lambda_h^2)\, d\Gamma$$

Stability: weak form $\mathcal{B}$ must satisfy inf-sup (BNB) conditions:

$$\mathcal{B}((u_h, \lambda_h), (v_h, \mu_h)) = a(u_h, v_h) + b(\lambda_h, v_h) + b(\mu_h, u_h) - j(\mu_h, \lambda_h)$$

$$\inf_{(u_h,\lambda_h)} \sup_{(v_h,\mu_h)} \frac{\mathcal{B}((u_h, \lambda_h), (v_h, \mu_h))}{|||u_h, \lambda_h|||, |||v_h, \mu_h)|||} \geq c$$

For some suitable norm $|||\cdot, \cdot|||$, so what is this? It's a norm which gives an upper bound i.e.

$$\mathcal{B}((u_h, \lambda_h), (v_h, \mu_h)) \leq M |||u_h, \lambda_h||| \, |||v_h, \mu_h|||$$

$$|||u_h, \lambda_h|||^2 = \sum_{i=1}^{2} (\|u_h^i\|_1^2 + \|\lambda_h^i\|_{-1/2,h}^2 + \|\pi^i[u_h]\|_{1/2,h}^2) \qquad [u_h] = (u_h^1 - u_h^2)$$

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Stabilized approach: mesh dependent norms

$$\mathcal{B}((u_h,\lambda_h),(v_h,\mu_h)) = a(u_h,v_h) + b(\lambda_h,v_h) + b(\mu_h,u_h) - j(\mu_h,\lambda_h)$$

Stability: weak form $\mathcal{B}$ must satisfy inf-sup condition: $\inf_{(u_h,\lambda_h)} \sup_{(v_h,\mu_h)} \frac{\mathcal{B}((u_h,\lambda_h),(v_h,\mu_h))}{\|\!|u_h,\lambda_h|\!\|, \|\!|v_h,\mu_h)|\!\|} \geq c$

$$\mathcal{B}((u_h,\lambda_h),(v_h,\mu_h)) \leq M\|\!|u_h,\lambda_h|\!\|\|\!|v_h,\mu_h|\!\|$$

$$\|\!|u_h,\lambda_h|\!\|^2 = \sum_{i=1}^{2}(\|u_h^i\|_1^2 + \|\lambda_h^i\|_{-1/2,h}^2 + \|\pi^i[u_h]\|_{1/2,h}^2) \qquad [u_h] = (u_h^1 - u_h^2)$$

where we use the following mesh dependent norms $\int_\Gamma \mu_h u_h \, d\Gamma \leq \|\mu_h\|_{-1/2,h}\|u_h\|_{1/2,h}$

$$\|\mu_h\|_{-1/2,h}^2 = h\int_\Gamma \mu_h \cdot \mu_h \, d\Gamma \qquad \|u_h\|_{1/2,h}^2 = \frac{1}{h}\int_\Gamma u_h \cdot u_h \, d\Gamma$$

and π^i is the $L_2(\Gamma^i)$ projection

$$\forall \mu_A^i \quad \mu_A^i \int_{\Gamma^c} \varphi_A^i (v - \pi^i v)\, d\Gamma = 0$$

$$\pi^i v(x) = \varphi_A^i(x)(M_{AB}^i)^{-1}\int_{\Gamma^c} \varphi_B^i \, v \, d\Gamma \quad \text{where} \quad M_{AB}^i = \int_{\Gamma^c} \varphi_A^i \varphi_B^i \, d\Gamma, \quad x \in \Gamma^c$$

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Stabilized approach: test function ansatz

$$\mathcal{B}((u_h, \lambda_h), (v_h, \mu_h)) = a(u_h, v_h) + b(\lambda_h, v_h) + b(\mu_h, u_h) - j(\mu_h, \lambda_h)$$

Stability: weak form $\mathcal{B}$ must satisfy inf-sup condition: $\inf_{(u_h,\lambda_h)} \sup_{(v_h,\mu_h)} \frac{\mathcal{B}((u_h, \lambda_h), (v_h, \mu_h))}{|||u_h, \lambda_h|||, |||v_h, \mu_h)|||} \geq c$

$$b(\lambda_h, v_h) = \frac{1}{2} \int_{\Gamma^c} (\lambda_h^1 - \lambda_h^2) \cdot (v_h^1 - v_h^2) \, d\Gamma$$

$$j(\mu_h, \lambda_h) = \frac{\gamma h}{2} \int_{\Gamma^c} (\mu_h^1 + \mu_h^2) \cdot (\lambda_h^1 + \lambda_h^2) \, d\Gamma$$

$$b(\mu_h, u_h) = \frac{1}{2} \int_{\Gamma^c} (\mu_h^1 - \mu_h^2) \cdot (u_h^1 - u_h^2) \, d\Gamma = \frac{1}{2} \int_{\Gamma^c} (\mu_h^1 \cdot \pi^1[u_h] - \mu_h^2 \cdot \pi^2[u_h]) \, d\Gamma$$

using the following test functions we can prove inf-sup

$$v_h^1(x) = u_h^1(x) + \beta h \lambda_h^1(x) \qquad x \in \Omega_h^1, \qquad \mu_h^1(x) = +\frac{\alpha}{h}\pi^1[u_h](x) - \lambda_h^1(x) \quad x \in \Gamma_h^1$$

$$v_h^2(x) = u_h^2(x) + \beta h \lambda_h^2(x) \qquad x \in \Omega_h^2, \qquad \mu_h^2(x) = -\frac{\alpha}{h}\pi^2[u_h](x) - \lambda_h^2(x) \quad x \in \Gamma_h^2$$

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Stabilized approach: test function ansatz

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$$b(\lambda_h,v_h) = \frac{1}{2}\int_{\Gamma^c}(\lambda_h^1-\lambda_h^2)\cdot(v_h^1-v_h^2)\,d\Gamma$$

$$j(\mu_h,\lambda_h) = \frac{\gamma h}{2}\int_{\Gamma^c}(\mu_h^1+\mu_h^2)\cdot(\lambda_h^1+\lambda_h^2)\,d\Gamma$$

$$b(\mu_h,u_h) = \frac{1}{2}\int_{\Gamma^c}(\mu_h^1-\mu_h^2)\cdot(u_h^1-u_h^2)\,d\Gamma = \frac{1}{2}\int_{\Gamma^c}(\mu_h^1\cdot\pi^1[u_h]-\mu_h^2\cdot\pi^2[u_h])\,d\Gamma$$

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$$b(\lambda_h,v_h) = \frac{1}{2}\int_{\Gamma^c}(\lambda_h^1-\lambda_h^2)\cdot(v_h^1-v_h^2)\,d\Gamma \Rightarrow \boxed{\frac{\beta h}{2}\int_{\Gamma^c}(\lambda_h^1-\lambda_h^2)\cdot(\lambda_h^1-\lambda_h^2)\,d\Gamma}$$

$$j(\mu_h,\lambda_h) = \frac{\gamma h}{2}\int_{\Gamma^c}(\mu_h^1+\mu_h^2)\cdot(\lambda_h^1+\lambda_h^2)\,d\Gamma$$

$$b(\mu_h,u_h) = \frac{1}{2}\int_{\Gamma^c}(\mu_h^1-\mu_h^2)\cdot(u_h^1-u_h^2)\,d\Gamma = \frac{1}{2}\int_{\Gamma^c}(\mu_h^1\cdot\pi^1[u_h]-\mu_h^2\cdot\pi^2[u_h])\,d\Gamma$$

using the following test functions we can prove inf-sup

$$v_h^1(x) = u_h^1(x) + \boxed{\beta h\lambda_h^1(x)} \quad x\in\Omega_h^1, \qquad \mu_h^1(x) = +\frac{\alpha}{h}\pi^1[u_h](x) - \lambda_h^1(x) \quad x\in\Gamma_h^1$$

$$v_h^2(x) = u_h^2(x) + \boxed{\beta h\lambda_h^2(x)} \quad x\in\Omega_h^2, \qquad \mu_h^2(x) = -\frac{\alpha}{h}\pi^2[u_h](x) - \lambda_h^2(x) \quad x\in\Gamma_h^2$$

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Stabilized approach: test function ansatz

$$\mathcal{B}((u_h,\lambda_h),(v_h,\mu_h)) = a(u_h,v_h) + b(\lambda_h,v_h) + b(\mu_h,u_h) - j(\mu_h,\lambda_h)$$

$$b(\lambda_h,v_h) = \frac{1}{2}\int_{\Gamma^c}(\lambda_h^1-\lambda_h^2)\cdot(v_h^1-v_h^2)\,d\Gamma$$

$$j(\mu_h,\lambda_h) = \frac{\gamma h}{2}\int_{\Gamma^c}(\mu_h^1+\mu_h^2)\cdot(\lambda_h^1+\lambda_h^2)\,d\Gamma$$

$$b(\mu_h,u_h) = \frac{1}{2}\int_{\Gamma^c}(\mu_h^1-\mu_h^2)\cdot(u_h^1-u_h^2)\,d\Gamma = \frac{1}{2}\int_{\Gamma^c}(\mu_h^1\cdot\pi^1[u_h]-\mu_h^2\cdot\pi^2[u_h])\,d\Gamma \quad \Rightarrow \quad \boxed{\frac{\alpha}{2}(\|\pi^1[u_h]\|^2_{1/2,h}+\|\pi^2[u_h]\|^2)_{1/2,h}}$$

using the following test functions we can prove inf-sup

$$v_h^1(x) = u_h^1(x) + \beta h\lambda_h^1(x) \qquad x\in\Omega_h^1, \qquad \mu_h^1(x) = \boxed{+\frac{\alpha}{h}\pi^1[u_h](x)} - \lambda_h^1(x) \quad x\in\Gamma_h^1$$

$$v_h^2(x) = u_h^2(x) + \beta h\lambda_h^2(x) \qquad x\in\Omega_h^2, \qquad \mu_h^2(x) = \boxed{-\frac{\alpha}{h}\pi^2[u_h](x)} - \lambda_h^2(x) \quad x\in\Gamma_h^2$$

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$$j(\mu_h,\lambda_h) = \frac{\gamma h}{2}\int_{\Gamma^c}(\mu_h^1 + \mu_h^2)\cdot(\lambda_h^1 + \lambda_h^2)\,d\Gamma \Rightarrow \boxed{\frac{\gamma h}{2}\int_{\Gamma^c}(\lambda_h^1 + \lambda_h^2)\cdot(\lambda_h^1 + \lambda_h^2)\,d\Gamma}$$

$$b(\mu_h,u_h) = \frac{1}{2}\int_{\Gamma^c}(\mu_h^1 - \mu_h^2)\cdot(u_h^1 - u_h^2)\,d\Gamma = \frac{1}{2}\int_{\Gamma^c}(\mu_h^1\cdot\pi^1[u_h] - \mu_h^2\cdot\pi^2[u_h])\,d\Gamma$$

using the following test functions we can prove inf-sup

$$v_h^1(x) = u_h^1(x) + \beta h\lambda_h^1(x) \qquad x\in\Omega_h^1, \qquad \mu_h^1(x) = +\frac{\alpha}{h}\pi^1[u_h](x) - \boxed{\lambda_h^1(x)} \quad x\in\Gamma_h^1$$

$$v_h^2(x) = u_h^2(x) + \beta h\lambda_h^2(x) \qquad x\in\Omega_h^2, \qquad \mu_h^2(x) = -\frac{\alpha}{h}\pi^2[u_h](x) - \boxed{\lambda_h^2(x)} \quad x\in\Gamma_h^2$$

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a-priori error estimate

Consider exact solution (u, λ) and approximate FE solution (u_h, λ_h) , compute error

$$
\begin{aligned}
|||u - u_h, \lambda - \lambda_h||| \leq & |||u - v_h, \lambda - \mu_h||| + |||u_h - v_h, \lambda_h - \mu_h||| \\
\leq & |||u - v_h, \lambda - \mu_h||| + \\
& \frac{1}{c} \sup_{(w_h, \rho_h)} \frac{\mathcal{B}((u_h - v_h, \lambda_h - \mu_h), (w_h, \rho_h))}{|||w_h, \rho_h|||}
\end{aligned}
$$

Triangle inequality

Using Galerkin orthogonality

Remember, if $a(u_h, v_h) =< f, v_h > \forall v_h$ then $a(u - u_h, v_h) = 0$ and $a(u_h, v_h) = a(u, v_h)$

$$|||u - u_h, \lambda - \lambda_h||| \leq (1 + \frac{M}{c}) |||u - v_h, \lambda - \mu_h|||$$

Using the mesh dependent estimates $\min_{v_h \in V_h} \|u - v_h\| \leq Ch^2 \|u\|_2$ $\quad \min_{v_h \in V_h} \|u - v_h\|_1 \leq Ch \|u\|_2$

$$\min_{v_h \in V_h} \|u - v_h\|_{1/2,h} \leq Ch \|u\|_2 \qquad \min_{\lambda_h \in M_h} \|\lambda - \lambda_h\|_{1/2,h} \leq Ch \|\lambda\|_{-1/2}$$

Leads to $|||u - u_h, \lambda - \lambda_h||| \leq Ch(\|u\|_2 + \|\lambda\|_{-1/2})$

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KKT Conditions

$$a(u_h, v_h) + b(\lambda_h, v_h) = \langle f, v \rangle$$
$$b(\mu_h, u_h) - j(\mu_h, \lambda_h) = 0$$

Leads to matrix set of equations

$$\begin{bmatrix} A & -B^T \\ -B & -J \end{bmatrix} \begin{Bmatrix} u \\ \lambda \end{Bmatrix} = \begin{Bmatrix} F \\ 0 \end{Bmatrix}$$

which also motivations scaling for γ

$$(BA^{-1}B^T + J)\lambda = -BA^{-1}F \qquad \gamma = \frac{\alpha}{E}$$

Which comes from minimization of this energy functional

$$\mathcal{L}(u, \lambda) = \frac{1}{2} u \cdot Au + \frac{1}{2} \lambda \cdot J\lambda - u \cdot F - (Bu + J\lambda)\lambda$$

which is *not* canonical form of KKT

If we let $J\mu = J\lambda$, then the following Lagrangian *is* in canonical form *and* equivalent to above

$$\mathcal{L}(u, \mu, \lambda) = \underbrace{\frac{1}{2} u \cdot Au + \frac{1}{2} \mu \cdot J\mu - u \cdot F}_{f(u,\mu)} - \underbrace{(Bu + J\mu)}_{g(u,\mu)}\lambda \qquad g(u,\mu) \geq 0 \quad \lambda \geq 0 \quad \lambda g(u,\mu) = 0$$

$$\begin{bmatrix} A & 0 & -B^T \\ 0 & J & -J \\ -B & -J & 0 \end{bmatrix} \begin{Bmatrix} u \\ \mu \\ \lambda \end{Bmatrix} = \begin{Bmatrix} F \\ 0 \\ 0 \end{Bmatrix}$$

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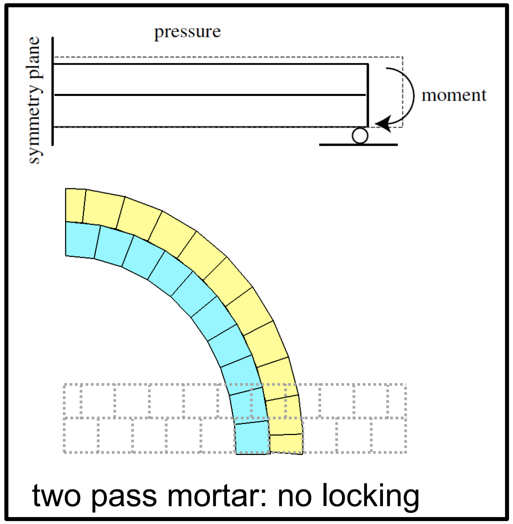
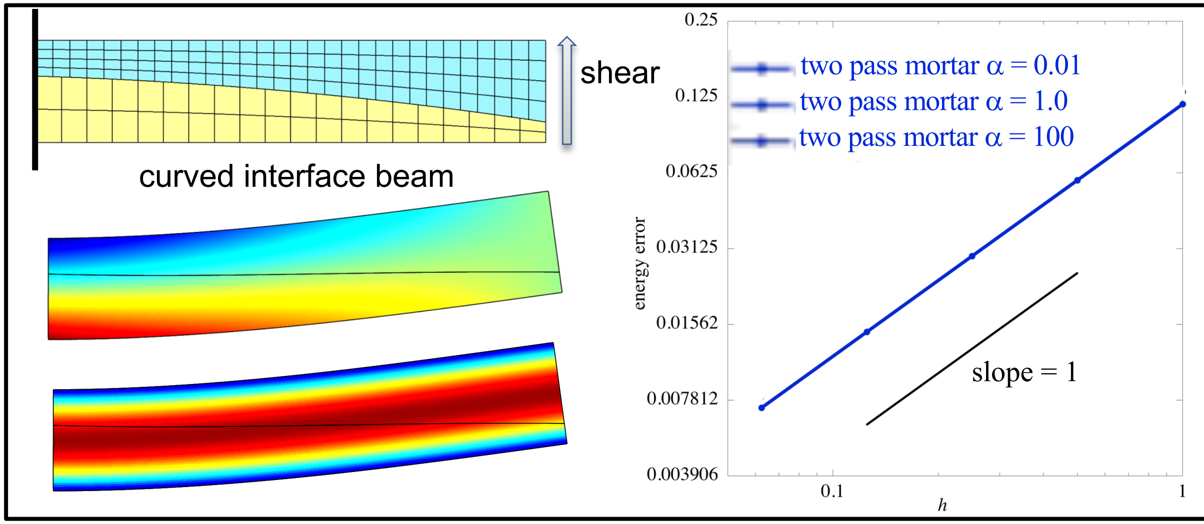
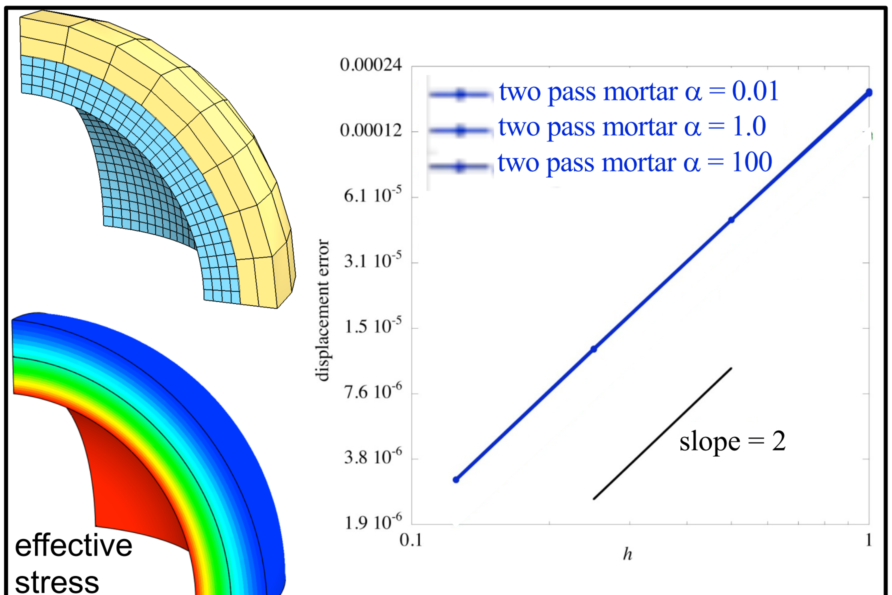
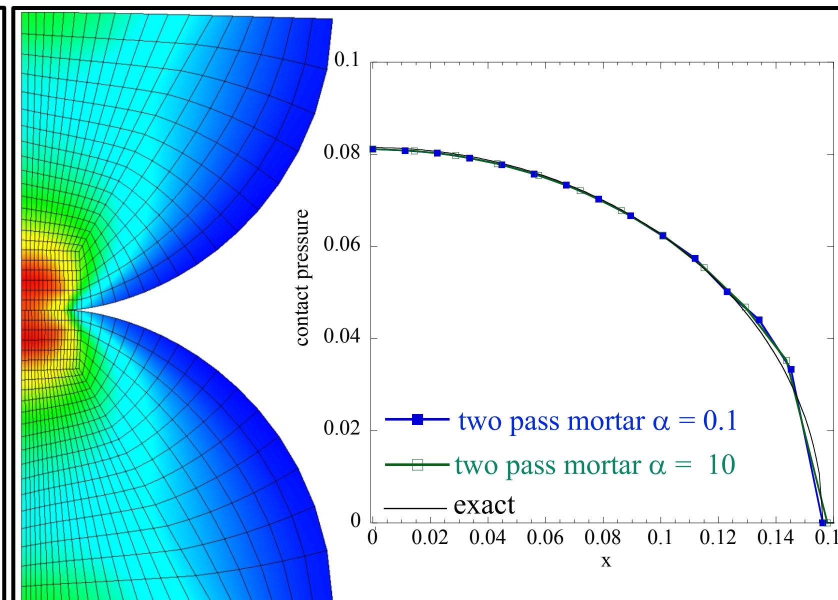
Results:









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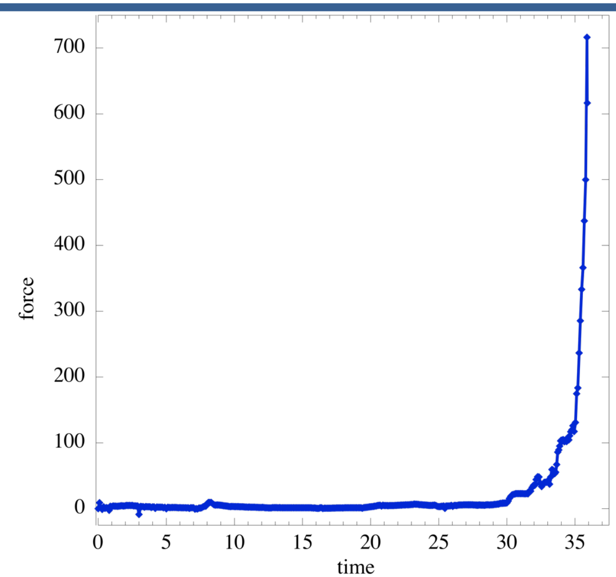
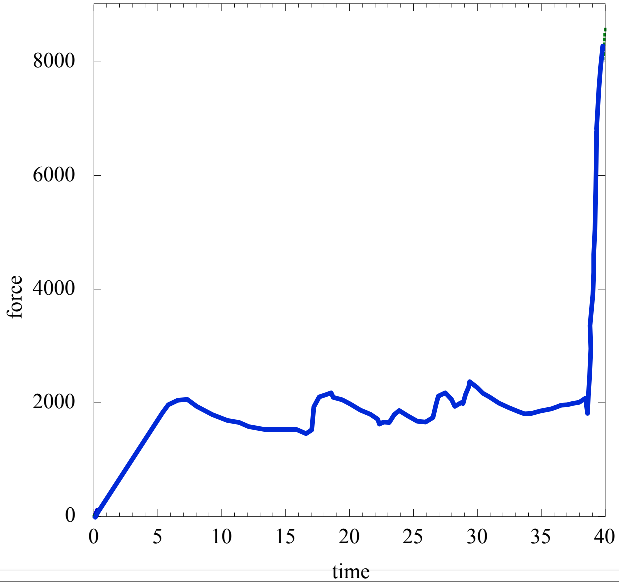
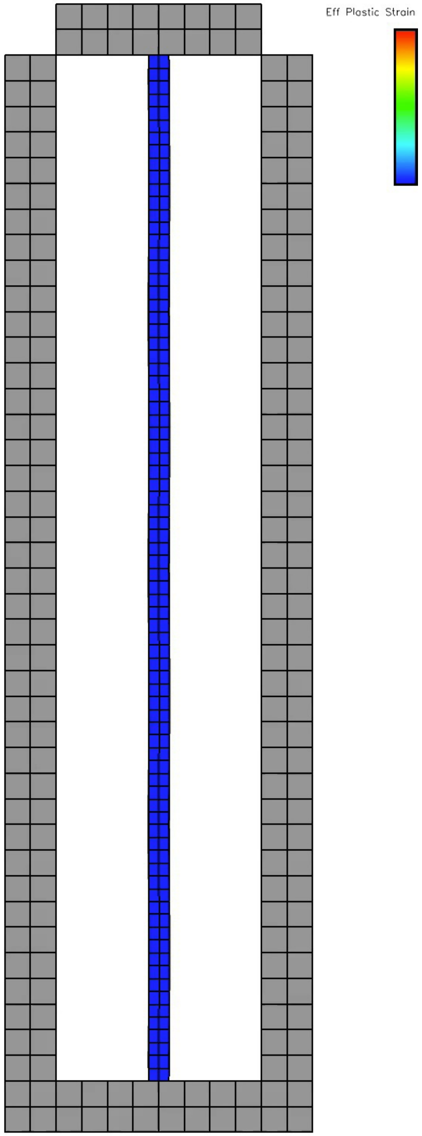
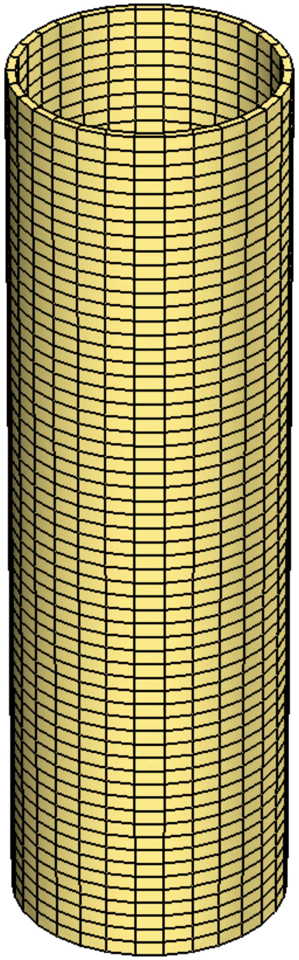
Self Contact: rod and cylinder buckling



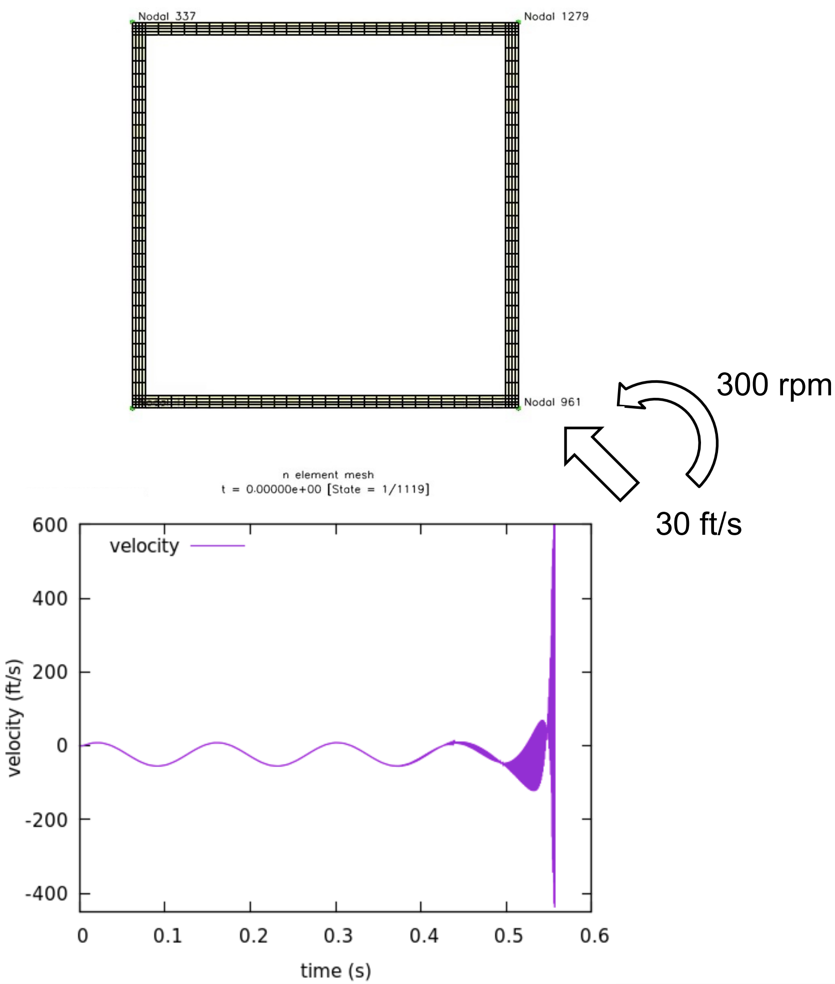


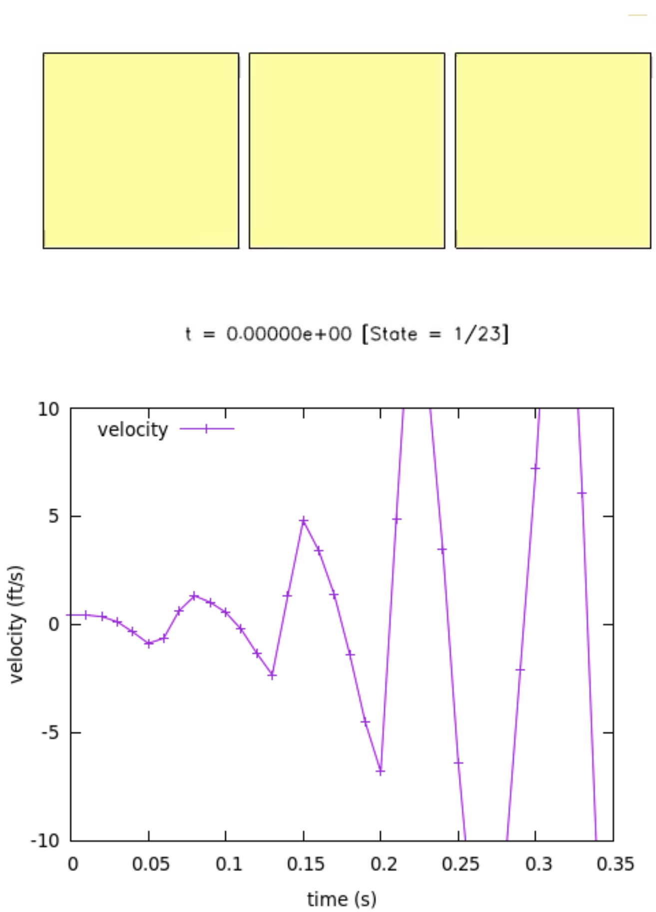




Many implicit time integrators are *unstable* for nonlinear problems

- Consider Trapezoid rule (Newmark's method $\gamma = 0.5$, $\beta = 0.25$) for large rotations or contact





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National Nuclear Security Administration

Structure preserving time integration w/ contact

- 2nd order schemes that conserve *discrete* forms of energy/momentum or are symplectic: **good for long time events**

$$\text{equations of motion:} \quad M_{AB}(v_B^{n+1} - v_B^n)/\Delta t + f_A^{(int)n+1/2} - f_A^{(c)n+1/2} = 0$$

$$\text{midstep time integrator:} \quad (x_A^{n+1} - x_A^n) = \frac{1}{2}(v_A^{n+1} + v_A^n)\Delta t$$

$$\frac{1}{2}v_A^{n+1} M_{AB} v_B^{n+1} - \frac{1}{2} v_A^n M_{AB} v_B^n + (x_A^{n+1} - x_A^n) \cdot f_A^{(int)n+1/2} = (x_A^{(n+1)} - x_A^n) \cdot f_A^{(c)n+1/2})$$

$$f_A^{(int)n+1/2} = \int_\Omega F_{n+1/2} S_{n+1/2} \nabla \varphi_A \, d\Omega \qquad \text{e.g.} \quad S_{n+1/2} = C\frac{1}{2}(E_{n+1} + E_n)$$

$F \equiv$ Deformation Gradient, $\quad E \equiv$ Green Strain

Conservation: get classical results when $f^c = 0$

$$\text{linear momentum:} \quad L_{n+1} - L_n = M_{AB}(v_B^{n+1} - v_B^n) = 0$$

$$\text{angular momentum:} \quad J_{n+1} - J_n = x_A^{n+1} \times M_{AB} v_B^{n+1} - x_A^n \times M_{AB} v_B^n = 0$$

$$\text{energy:} \quad \mathcal{E}_{n+1} - \mathcal{E}_n = (T_{n+1} + U_{n+1}) - (T_n + U_n) = 0$$

$$T_n = \frac{1}{2} v_A^n M_{AB} v_B^n \quad U_n = \frac{1}{2}\int_\Omega E_n C E_n \, d\Omega$$

$\mathcal{E}(t) = \text{constant} \geq 0 \ \forall t$ bounds displacements and velocities $\Rightarrow$ B stability

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Structure preserving time integration w/ contact

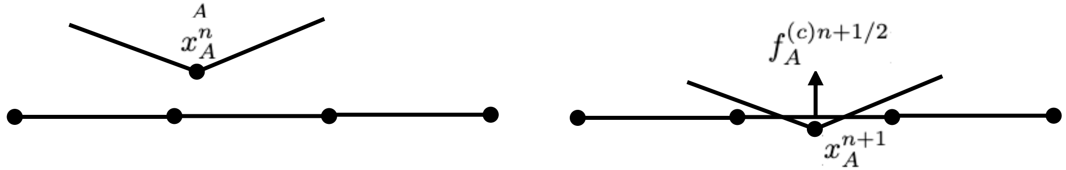
- Stability and momentum conservation requirements for contact force

$$f_A^{(c)n+1/2} = G_{BA}^{n+1/2}\lambda_B^{n+1/2} \qquad \lambda_B^{n+1/2} \geq 0 \qquad g_A^{n+1/2} = \int_\Gamma \varphi_A n_A \cdot (x_h^1(t_{n+1/2}) - x_h^2(t_{n+1/2}) d\Gamma \;= G_{AB}^{n+1/2} x_B^{n+1/2} \geq 0$$

$$\text{linear momentum:} \quad \sum_A f_A^c = \sum_{A,B} G_{BA}\lambda_B = 0 \quad \text{result of segment projection scheme}$$

$$\text{angular momentum:} \quad \sum_A x_A \times f_A^c = x_A \times \sum_{A,B} G_{BA}\lambda_B = 0 \quad \text{result of choice of contact normal } n_A$$

$$\text{energy:} \quad \sum_A (x_A^{n+1} - x_A^n) \cdot f_A^{(c)n+1/2} = -\kappa_A \leq 0$$



3 Step Process

Step 1: Solve for $v_B^{n+1}, \lambda_B^{n+1/2}$ from EOM $\quad M_{AB}(v_B^{n+1} - v_B^n)/\Delta t + f_A^{(int)n+1/2} - G_{BA}^{(c)n+1/2}\lambda_B^{n+1/2} = 0$

Step 2: Using v_B^{n+1}, compute velocity update $\bar{v}_B^{n+1}$

Enforce gap velocity constraint $\quad \dot{g}_A = G_{AB}\bar{v}_B^{n+1} = 0$ to avoid contact chatter and provide dissipation

$$M_{AB}(\bar{v}_B^{n+1} - v_B^{n+1}) + G_{BA}\bar{\lambda}_B^{n+1} = 0$$
$$G_{AB}\bar{v}_b^{n+1} = 0$$

using the identity $\bar{v}_A^{n+1} = 1/2(\bar{v}_A^{n+1} + v_A^{n+1}) + 1/2(\bar{v}_A^{n+1} - v_A^{n+1})$ can show update is strictly dissipative

$$\bar{v}_A^{n+1} \cdot (M_{AB}(\bar{v}_B^{n+1} - v_B^n) + G_{BA}\bar{\lambda}_B^{n+1}) = 0$$

$$\frac{1}{2}\bar{v}_A^{n+1} M_{AB}\bar{v}_B^{n+1} = \frac{1}{2}v_A^{n+1} M_{AB} v_B^{n+1} - \frac{1}{2}(\bar{v}_A^{n+1} - v_A^{n+1}) M_{AB}(\bar{v}_B^{n+1} - v_B^{n+1}) \qquad \Rightarrow \mathcal{E}_{n+1} \leq \mathcal{E}_n$$

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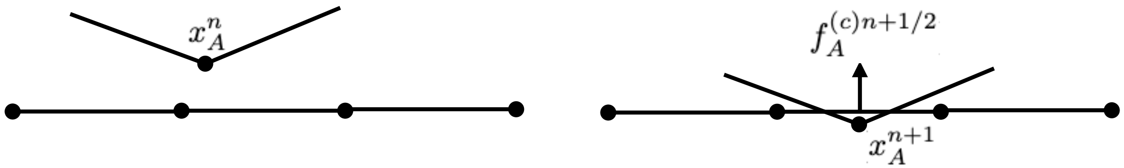
Structure preserving time integration w/ contact

- Can return dissipated energy upon contact release

initial gap dissipation: $\sum_A (x_A^{n+1} - x_A^n) \cdot f_A^{(c)n+1/2} = -\kappa_A \leq 0$



plastic impact dissipation: $\bar{\kappa}_A$

$$\frac{1}{2}\bar{v}_A^{n+1} M_{AB} \bar{v}_B^{n+1} - \frac{1}{2} v_A^{n+1} M_{AB} v_B^{n+1} = \frac{1}{2}(\bar{v}_A^{n+1} - v_A^{n+1}) M_{AB} (\bar{v}_B^{n+1} - v_B^{n+1})$$
$$= \sum_A -\bar{\kappa}_A \leq 0$$

$$\bar{\kappa}_A = \sum_B v_B^{n+1} \cdot G_{AB} \bar{\lambda}_A$$

Step 3: total dissipation: $\bar{\bar{\kappa}}_A = \kappa_A + \bar{\kappa}_A$ can be returned upon contact release i.e. $\lambda_A^{n+1/2} = 0$

$$M_{AB} \bar{\bar{v}}_B^{n+1} - M_{AB} \bar{v}_B^{n+1} = f_A^{rel} \alpha^2 \qquad f_A^{rel} = G_{CA} \bar{\bar{\kappa}}_C \qquad \alpha = 2 \sum_A \bar{\bar{\kappa}}_A / \sum_{AB} f_A^{rel} M_{AB}^{-1} f_B^{rel}$$

can show

$$\bar{\bar{v}}_A^{n+1} M_{AB} \bar{\bar{v}}_B^{n+1} - \bar{v}_A^{n+1} M_{AB} \bar{v}_B^{n+1} = \sum_A \bar{\bar{\kappa}}_A$$

Now using $\bar{\bar{v}}_A^{n+1}$ energy is conserved i.e. $\mathcal{E}_{n+1} = \mathcal{E}_n$ and set $v_A^{n+1} = \bar{\bar{v}}_A^{n+1}$ for next time step

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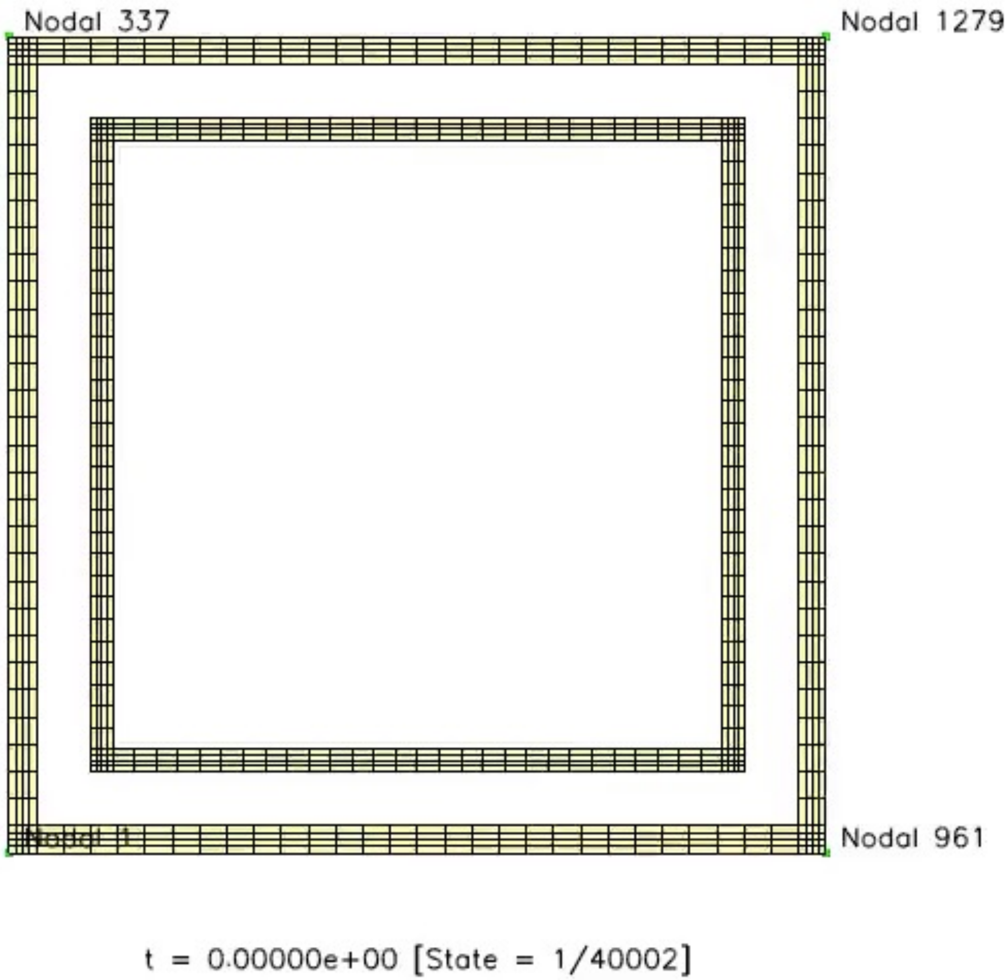
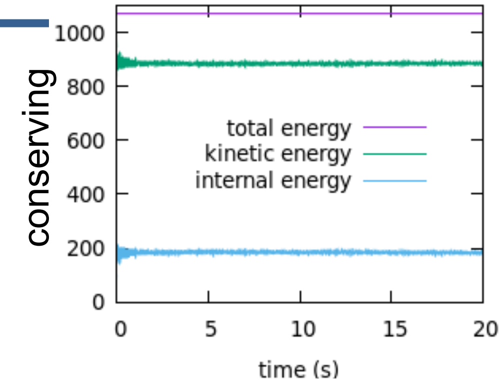
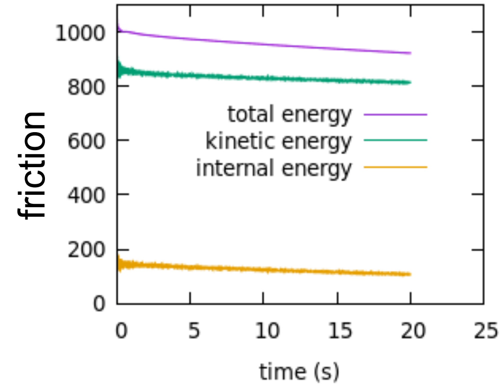
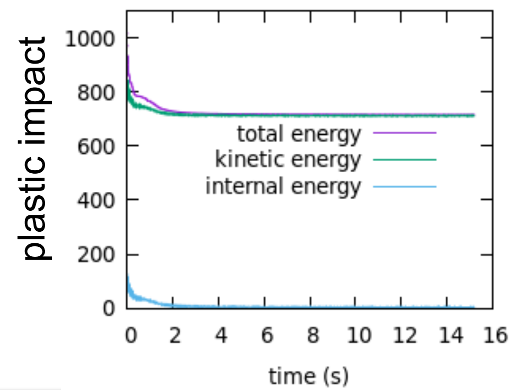
Structure preserving time integration w/ contact

- Large rotation w/ contact









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Structure preserving time integration w/ contact

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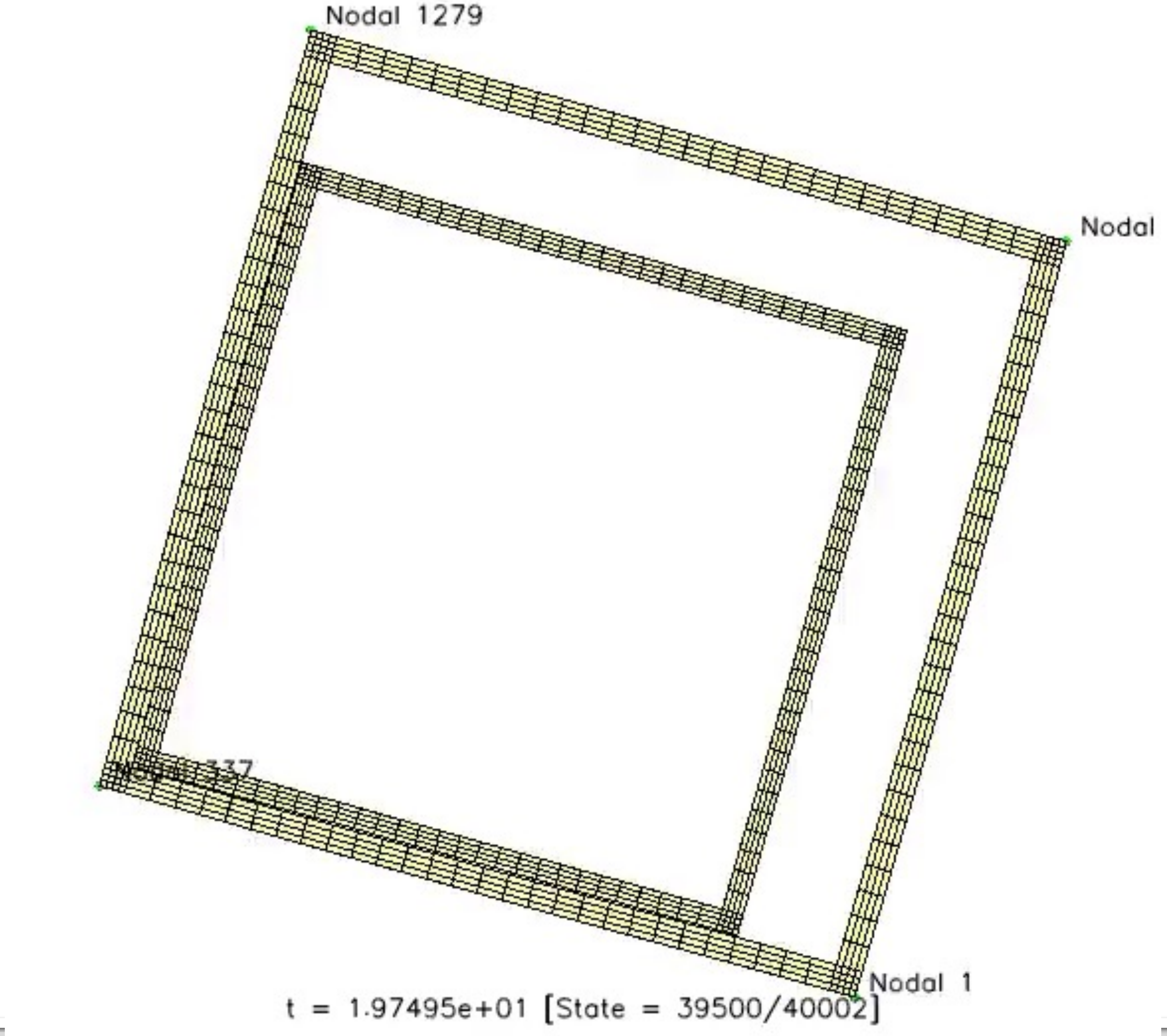

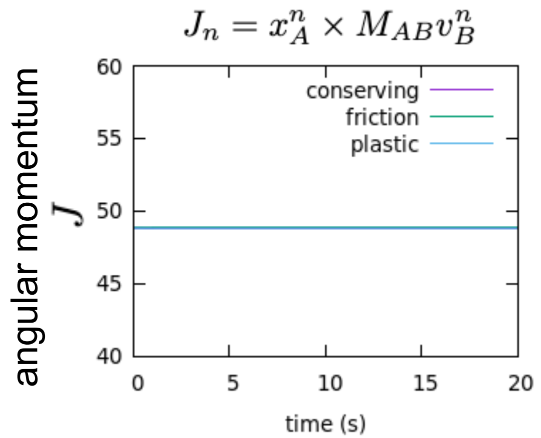

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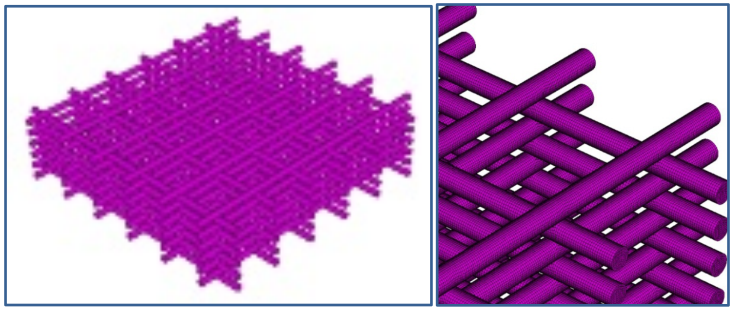
Summary and current projects

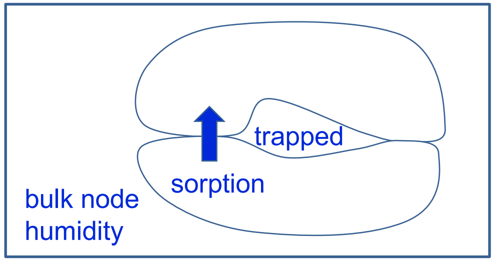
- Develop immersed FE, ALE and SPH methods using Lagrange multipliers with stabilization
- Stabilized two pass mortar contact
- Structure preserving time integration for contact
- GPU ports of immersed boundary FE & Tribol mortar contact (Tsuji, Dayton, Liu, Robertson, Stillman) (Wopshal, Weiss, Liu, Chin)
- Domain decomposition with Slide World (Liu, Chin, Weiss)
- Topology optimization with contact with LIDO, Smith, Diablo



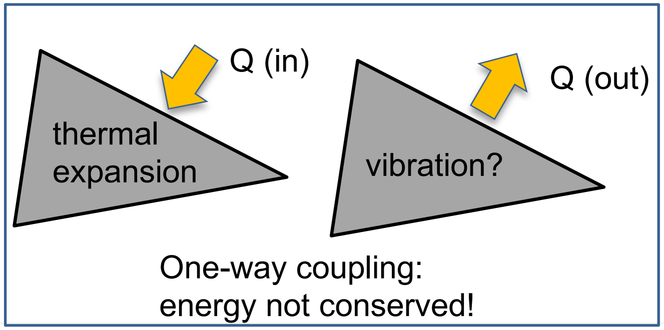
optimize nylon layups (Weisgraber)

Fernandez, F; Puso, MA; Solberg, J; Tortorelli, DA. "Topology optimization of multiple deformable bodies in contact with large deformations" *COMPUT METHOD APPL MECH ENG*, **371**, (2020).

- Scalable methods for contact with optimization. Better regularization techniques for semi-smooth Newton and interior point methods using AMG (Petra)
- Fluid sorption across interfaces, diffusion-thermal-structural (Castonguay, MDG)



- Multicomponent ROM's with contact (MDG)
- Adaptive meshing with contact (MDG)
- Two-way thermal-mechanical contact with Joule-Gough effect (MDG)



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