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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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)

Fracture:

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

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Outline:

Traction 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 multiplier contact enforcement
    - Provable stability for large deformation kinematics
    - Exactly conserves linear and angular momentum
  - V&V
Immersed Boundary methods couple overlapping discretizations

Background *ALE Fluid* or *Solid* Mesh

Foreground *Solid* Mesh

Foreground *Shells* Mesh

Foreground *Particles*

VS.

Conforming Mesh

Embedded FE or SPH

Shaped in Mesh
Many Previous Works: to name a few

- Existing *Immersed boundary* methods
  - *CEL method* (W.F. Noh, 1964)
  - *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)
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


Mathematical Details: Lagrange Step

- Consider equations of motion i.e. $F = Ma$
  
  $$M^b a^b + K^b u^b + B^{bT} \lambda = 0$$
  $$M^f a^f + K^b u^f + B^{fT} \lambda = 0$$
  $$B^b v^b + B^f v^f = 0$$

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

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

$$H = \Delta t^2 (B^b M^{-1} B^{bT} + B^f M^{-1} B^{fT}) + \bar{C}^{-1}$$

- 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 $K \geq 0$ $A > 0$ $A = M + \frac{\Delta t}{2} C - \frac{\Delta t^2}{4} K$ $\Delta t \leq \frac{2}{\omega_c}$ where $\omega_c^2 = \sup_u \frac{u^T K u}{u^T M u}$
Mathematical Details: Lagrange Step

- Consider equations of motion \( i.e. F = Ma \)

\[
\begin{align*}
M^b a^b + K^b u^b + B^{bT} \lambda &= 0 \\
M^f a^f + K^b u^f + B^{fT} \lambda &= 0 \\
B^b v^b + B^f v^f &= 0
\end{align*}
\]

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

\[
\begin{bmatrix}
M^b & 0 & B^{bT} \\
0 & M^f & B^{fT} \\
B^b & B^f & -\overline{C}^{-1}/\Delta t
\end{bmatrix}
\begin{bmatrix}
v_{n+1/2}^b \\
v_{n+1/2}^f \\
\lambda \Delta t
\end{bmatrix}
= \begin{bmatrix}
-K^b u_n^b + M^b v_{n-1/2}^b \\
-K^f u_n^f + M^f v_{n-1/2}^f \\
0
\end{bmatrix}
\]

\[
H = \Delta t^2 (B^b M^{b^{-1}} B^{bT} + B^f M^{f^{-1}} B^{fT}) + \overline{C}^{-1} \quad H \lambda = f 
\]

\[
s_{\text{con}} = \frac{\lambda^{\text{eig}}_{\max}(H)}{\lambda^{\text{eig}}_{\min}(H)} = \text{constant independent of } h
\]

- 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 \( K \geq 0 \), \( A > 0 \)

\[
A = M + \frac{\Delta t}{2} C - \frac{\Delta t^2}{4} K
\]

\[
\Delta t \leq \frac{2}{\omega_c} \quad \text{where} \quad \omega_c^2 = \sup_u \frac{u^T K u}{u^T M u}
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  \bar{C}^{-1} = J + \frac{1}{\alpha} I
  \]

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\begin{bmatrix}
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B^b & B^f & -\bar{C}^{-1}/\Delta t
\end{bmatrix}
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v_{n+1/2}^f \\
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0
\end{bmatrix}
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\begin{align*}
\begin{array}{c}
a_n^T A a_n + v_n^T K v_n \\ a_0^T A a_0 + v_0^T K v_0
\end{array}
\leq \begin{array}{c}
\Delta t^2 C + \frac{\Delta t^2}{4} K
\end{array}
\]

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

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\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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-K^b u^f_n + M^f v^f_{n-1/2} \\
0
\end{bmatrix}
\]

\[Ma_n + C v_{n+1/2} + K d_n = 0 \quad C = \begin{bmatrix}
B^{bT} \bar{C} B^b \\
B^{fT} \bar{C} B^f
\end{bmatrix}
\]

• Central difference scheme leads to following recursion
\[
a^T_n A a_n + v^T_n K v_n \leq a^T_0 A a_0 + v^T_0 K v_0
\]

• Recursion bounds \( a_n \) and \( v_n \) when \( K \geq 0 \ \ \ A > 0 \)
\[
A = M + \frac{\Delta t}{2} C - \frac{\Delta t^2}{4} K
\]
\[
\Delta t \leq \frac{2}{\omega_c} \quad \text{where} \quad \omega_c^2 = \sup_u u^T K u / u^T M u
\]
Multipliers on background mesh: 2D Lagrange result

conforming

foreground

background
Multipliers on background mesh: 2D result

![Graph showing multipliers on background mesh]

- **Background disp**: slope = 1.97
- **Background energy**: slope = 1.15
- **Foreground disp**:
- **Foreground energy**:

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC.
- Use central difference explicit 2 step ALE approach
Use central difference explicit 2 step ALE approach

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

$V_e$
ALE implementation: with foreground Lagrange Mesh

- Use central difference explicit 2 step ALE approach

Load step
- Lagrange step
- Advection remap step (yields volume flux)
- Advance time step \( t_n \rightarrow t_{n+1} \)

\[
V_e + \Delta V_e^R
\]

\[
\Delta V_e^L = 0 \quad \Delta V_e^R
\]
Use central difference explicit 2 step ALE approach

- Load step
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- Advance time step $t_n \rightarrow t_{n+1}$
Verification/Validation: Conforming vs Immersed

Shock Tube

Buried Mine

Shell Pipe
Impacting Plates: contact
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
Nimble Vessel Analysis (Lam)
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
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 \iff FEM using nodal integration

\[ m_i a_i + (B^f \lambda)_i = \sum_{j=1}^{N} m_i m_j \left( \frac{\sigma_i}{\rho_i^2} + \frac{\sigma_j}{\rho_j^2} \right) \cdot \nabla W_{ij} \]

Consider EOM’s

\[
\begin{align*}
M^b a^b + B^{bT} \lambda &= F^b \\
M^f a^f + B^{fT} \lambda &= F^f \\
B^b v^b + B^f v^f - \bar{C}^{-1} \lambda &= 0
\end{align*}
\]

Background interface force

\[
B^{bT} \lambda \Rightarrow \int_{\Gamma} \phi^b_A(x) \lambda(x) \, d\Gamma = \sum_{e} \lambda_e \int_{\Gamma_e} \phi^b_A(x) \, d\Gamma
\]

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 $\Leftrightarrow$ FEM using nodal integration

$$m_i a_i + (B^f \lambda)_i = \sum_{j=1}^{N} m_i m_j \left( \frac{\sigma_i}{\rho_i^2} + \frac{\sigma_j}{\rho_j^2} \right) \cdot \nabla W_{ij}$$

Consider EOM’s

$$M^b a^b + B^{bT} \lambda = F^b$$
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$$B^{bT} \lambda \Rightarrow \int_{\Gamma} \phi^b_A(x) \lambda(x) \, d\Gamma = \sum_e \lambda_e \int_{\Gamma_e} \phi^b_A(x) \, d\Gamma$$

Foreground interface force

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

$$\tilde{W}_i(x) = \frac{W_i(x)}{\sum_j W_j(x)}$$
Embedded SPH vs Embedded FE
Validation: penetrators (Spangler)

- **0.5 cal bullet**
- **Embedded SPH**

Tates Formula: depth $= L\sqrt{\rho_{pen}/\rho_{target}} = 1.73$ cm
Embedded SPH: depth $= 1.65$ cm

(a) $V_i = 911$ m/s
Validation: AerMet steel cylinder & hubcap exp. (Tsuji)

Cylinder test geometry

Hemispherical shell test geometry ("hubcap")
Validation: Damage evolution with Embedded SPH

0 µs  10 µs  20 µs  30 µs  40 µs
High speed camera image of the cylinder is compared to FEusion/SPH

High speed images at t = 21 µs

Density at 21 µs
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
Validation: AerMet steel cylinder & hubcap experiments

Probe locations for cylinder and hubcap

Cylinder: Embedded SPH vs Experiment

Hubcap: Embedded SPH vs Experiment

velocity (cm/μs)

time (μs)

velocity (cm/μs)

time (μs)
Current Work: Unilateral contact and friction

Friction important for bar pull out, penetration $\mu = 0.4, 0.2, 0.01$
Contact Problems

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

  - **node to surface (n-s)**
    - single pass (inaccurate)
  - **surface to surface (s-s)**
    - double pass (locks)
    - 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
Many engineering problems are contact dominated

Different forms of constraint enforcement:

- **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
Surface to Surface options:

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

![Diagram of mortar and non-mortar sides]

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

![Diagram of piecewise linear field based on segments]

- Two pass mortar approach not biased also not stable

![Diagram of piecewise linear field based on nodes]
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**

  \[
  a(u_h, v_h) + b(\lambda_h, v_h) = \langle f, v_h \rangle \\
  b(\mu_h, u_h) = 0
  \]

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

  constraints 
  \( b_h(\mu_h, u_h) = \int_{\Gamma} \mu_A^{1/2} (u^1_h - u^2_h) \cdot d\Gamma \) 
  \( \mu_A^{1/2} \int_{\Gamma} \varphi_A^{1/2} (u^1_h - u^2_h) \cdot d\Gamma \)

  contact force 
  \( b_h(\lambda_h, v_h) = \int_{\Gamma} \lambda^1_h (v^1_h - v^2_h) \cdot d\Gamma \) 
  \( v_B^1 \cdot \int_{\Gamma} \lambda^1_h \varphi_B^1 d\Gamma - v_C^2 \cdot \int_{\Gamma} \lambda^1_h \varphi_C^1 d\Gamma \)
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- **Constraints**
  \[ b_h(\mu_h, u_h) = \int_{\Gamma} \mu^1_h (u^1_h - u^2_h) \, d\Gamma \Rightarrow g_A = n_A \cdot \int_{\Gamma} \varphi_A^1 (u^1_h - u^2_h) \, d\Gamma \geq 0 \]

- **Contact force**
  \[ b_h(\lambda_h, v_h) = \int_{\Gamma} \lambda^1_h (v^1_h - v^2_h) \, d\Gamma \Rightarrow v_B^1 \cdot \int_{\Gamma} \lambda^1_h \varphi^1_B \, d\Gamma - v_C^2 \cdot \int_{\Gamma} \lambda^1_h \varphi^2_C \, d\Gamma \]
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  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

  \[ a(u_h, v_h) + b(\lambda_h, v_h) = (f, v_h) \]
  
  \[ b(\mu_h, u_h) = 0 \]

  **strain energy**
  \[ a(u_h, v_h) = \int_{\Omega} \varepsilon(v_h) C \varepsilon(u_h) \, d\Omega \]
  
  \[ \varepsilon(u_h) = 1/2(\nabla u_h + \nabla^T u_h) \]

  **constraints**
  \[ b_h(\mu_h, u_h) = \int_{\Gamma} \mu_h^1 (u_h^1 - u_h^2) \cdot d\Gamma \Rightarrow g_A = n_A \cdot \int_{\Gamma} \varphi_A^1 (u_h^1 - u_h^2) \, d\Gamma \geq 0 \]

  **contact force**
  \[ b_h(\lambda_h, v_h) = \int_{\Gamma} \lambda_h^1 (v_h^1 - v_h^2) \cdot d\Gamma \Rightarrow f_B^1 = \int_{\Gamma} \lambda_h^1 \varphi_B^1 \, d\Gamma \quad f_C^2 = -\int_{\Gamma} \lambda_h^1 \varphi_C^2 \, d\Gamma \]
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- **Contact force**
  \[ b_h(\lambda_h, v_h) = \int_{\Gamma} \lambda_h^1 (v_h^1 - v_h^2) \cdot d\Gamma \Rightarrow f^c_B = \int_{\Gamma} \lambda_h^1 \varphi_B d\Gamma \quad f^c_C = -\int_{\Gamma} \lambda_h^1 \varphi_C^2 d\Gamma \]

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

no “modes” with standard mortar using \( \lambda = \lambda^1 \)
Stabilized two pass mortar approach

\[
a(u_h, v_h) + b(\lambda_h, v_h) = (f, v)
b(\mu_h, u_h) - j(\mu_h, \lambda_h) = 0
\]

\[
b(\lambda_h, v_h) = \frac{1}{2} \int_{\Gamma_c} (\lambda_h^1 - \lambda_h^2) \cdot (v_h^1 - v_h^2) \, d\Gamma
\]

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

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

\[ b(\lambda_h, u_h) = \frac{1}{2} \sum_{p=1}^{\text{#of pairs}} \left( \int_{\Gamma_{p,ab}} \lambda_h^{p,a} \cdot (u_h^{p,a} - u_h^{p,b}) \, d\Gamma + \int_{\Gamma_{p,ba}} \lambda_h^{p,b} \cdot (u_h^{p,b} - u_h^{p,a}) \, d\Gamma \right) \]
\[ j(\mu_h, \lambda_h) = \frac{h}{2} \sum_{p=1}^{\text{#of pairs}} \gamma^p \left( \int_{\Gamma_{p,ab}} \mu_h^{p,a} \cdot (\lambda_h^{p,a} + \lambda_h^{p,b}) \, d\Gamma + \int_{\Gamma_{p,ba}} \mu_h^{p,b} \cdot (\lambda_h^{p,b} + \lambda_h^{p,a}) \, d\Gamma \right) \]

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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?

\[ a(u_h, v_h) + b(\lambda_h, v_h) = \langle f, v \rangle \]
\[ b(\mu_h, u_h) - j(\mu_h, \lambda_h) = 0 \]
\[ b(\lambda_h, v_h) = \frac{1}{2} \int_{\Gamma_c} (\lambda^1_h - \lambda^2_h) \cdot (v^1_h - v^2_h) \, d\Gamma \]
\[ j(\mu_h, \lambda_h) = \frac{\gamma h}{2} \int_{\Gamma_c} (\mu^1_h + \mu^2_h) \cdot (\lambda^1_h + \lambda^2_h) \, d\Gamma \]

Stability: weak form $B$ must satisfy inf-sup (BNB) conditions:

\[ B((u_h, \lambda_h), (v_h, \mu_h)) = a(u_h, v_h) + b(\lambda_h, v_h) + b(\mu_h, u_h) - j(\mu_h, \lambda_h) \]

\[ \inf_{(u_h, \lambda_h)} \sup_{(v_h, \mu_h)} \frac{B((u_h, \lambda_h), (v_h, \mu_h))}{\|u_h, \lambda_h\| \cdot \|v_h, \mu_h\|} \geq c \]

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

\[ B((u_h, \lambda_h), (v_h, \mu_h)) \leq M \|u_h, \lambda_h\| \cdot \|v_h, \mu_h\| \]

\[ \|u_h, \lambda_h\|^2 = \sum_{i=1}^{2} (\|u^i_h\|^2 + \|\lambda^i_h\|^2_{-1/2,h} + \|\pi^i[u_h]|_{1/2,h}^2) \quad [u_h] = (u^1_h - u^2_h) \]

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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:

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

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

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

where we use the following mesh dependent norms

\[ \|\mu_h\|_{-1/2, h}^2 = h \int_{\Gamma} \mu_h \cdot \mu_h \, d\Gamma \]

\[ \|u_h\|_{1/2, h}^2 = \frac{1}{h} \int_{\Gamma} u_h \cdot u_h \, d\Gamma \]

and \( \pi^i \) is the \( L_2(\Gamma^i) \) projection

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

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

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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:

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

\[
b(\lambda_h, v_h) = \frac{1}{2} \int_{\Gamma^e} (\lambda_h^1 - \lambda_h^2) \cdot (v_h^1 - v_h^2) \, d\Gamma
\]

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

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

using the following test functions we can prove inf-sup

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

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

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Stabilized approach: test function ansatz

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

\[
\begin{align*}
    b(\lambda_h, v_h) &= \frac{1}{2} \int_{\Gamma_c} (\lambda_h^1 - \lambda_h^2) \cdot (v_h^1 - v_h^2) \, d\Gamma \\
    j(\mu_h, \lambda_h) &= \frac{\gamma h}{2} \int_{\Gamma_c} (\mu_h^1 + \mu_h^2) \cdot (\lambda_h^1 + \lambda_h^2) \, d\Gamma \\
    b(\mu_h, u_h) &= \frac{1}{2} \int_{\Gamma_c} (\mu_h^1 - \mu_h^2) \cdot (u_h^1 - u_h^2) \, d\Gamma = \frac{1}{2} \int_{\Gamma_c} (\mu_h^1 \cdot \pi^1[u_h] - \mu_h^2 \cdot \pi^2[u_h]) \, d\Gamma
\end{align*}
\]

using the following test functions we can prove inf-sup

\[
\begin{align*}
    v_h^1(x) &= u_h^1(x) + \beta h \lambda_h^1(x) & x \in \Omega_h^1, & \mu_h^1(x) = +\frac{\alpha}{h} \pi^1[u_h](x) - \lambda_h^1(x) & x \in \Gamma_h^1 \\
    v_h^2(x) &= u_h^2(x) + \beta h \lambda_h^2(x) & x \in \Omega_h^2, & \mu_h^2(x) = -\frac{\alpha}{h} \pi^2[u_h](x) - \lambda_h^2(x) & x \in \Gamma_h^2
\end{align*}
\]

Stabilized approach: test function ansatz

\[ B((u_h, \lambda_h), (v_h, \mu_h)) = a(u_h, v_h) + b(\lambda_h, v_h) + b(\mu_h, u_h) - j(\mu_h, \lambda_h) \]

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

using the following test functions we can prove inf-sup

\[ v_h^1(x) = u_h^1(x) + \beta h \lambda_h^1(x) \quad x \in \Omega_h^1, \quad \mu_h^1(x) = +\frac{\alpha}{h} \pi^1[u_h](x) - \lambda_h^1(x) \quad x \in \Gamma_h^1 \]
\[ v_h^2(x) = u_h^2(x) + \beta h \lambda_h^2(x) \quad x \in \Omega_h^2, \quad \mu_h^2(x) = -\frac{\alpha}{h} \pi^2[u_h](x) - \lambda_h^2(x) \quad x \in \Gamma_h^2 \]

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Stabilized approach: test function ansatz

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

\[
\begin{align*}
    b(\lambda_h, v_h) &= \frac{1}{2} \int_{\Gamma_c} (\lambda_h^1 - \lambda_h^2) \cdot (v_h^1 - v_h^2) \, d\Gamma \\
    j(\mu_h, \lambda_h) &= \frac{\gamma_h}{2} \int_{\Gamma_c} (\mu_h^1 + \mu_h^2) \cdot (\lambda_h^1 + \lambda_h^2) \, d\Gamma \\
    b(\mu_h, u_h) &= \frac{1}{2} \int_{\Gamma_c} (\mu_h^1 - \mu_h^2) \cdot (u_h^1 - u_h^2) \, d\Gamma = \frac{1}{2} \int_{\Gamma_c} (\mu_h^1 \cdot \pi^1[u_h] - \mu_h^2 \cdot \pi^2[u_h]) \, d\Gamma
\end{align*}
\]

using the following test functions we can prove inf-sup

\[
\begin{align*}
    v_h^1(x) &= u_h^1(x) + \beta h \lambda_h^1(x) & x \in \Omega_h^1, \\
    \mu_h^1(x) &= \frac{\alpha}{h} \pi^1[u_h](x) - \lambda_h^1(x) & x \in \Gamma_h^1 \\
    v_h^2(x) &= u_h^2(x) + \beta h \lambda_h^2(x) & x \in \Omega_h^2, \\
    \mu_h^2(x) &= -\frac{\alpha}{h} \pi^2[u_h](x) - \lambda_h^2(x) & x \in \Gamma_h^2
\end{align*}
\]

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Stabilized approach: test function ansatz

\[ B((u_h, \lambda_h), (v_h, \mu_h)) = a(u_h, v_h) + b(\lambda_h, v_h) + b(\mu_h, u_h) - j(\mu_h, \lambda_h) \]

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

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

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

using the following test functions we can prove inf-sup

\[ v_h^1(x) = u_h^1(x) + \beta h \lambda_h^1(x) \quad x \in \Omega_h^1 \]

\[ \mu_h^1(x) = -\frac{\alpha}{h} \pi^1[u_h](x) - \lambda_h^1(x) \quad x \in \Gamma_h^1 \]

\[ v_h^2(x) = u_h^2(x) + \beta h \lambda_h^2(x) \quad x \in \Omega_h^2 \]

\[ \mu_h^2(x) = -\frac{\alpha}{h} \pi^2[u_h](x) - \lambda_h^2(x) \quad x \in \Gamma_h^2 \]

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**a-priori error estimate**

Consider exact solution \((u, \lambda)\) and approximate FE solution \((u_h, \lambda_h)\), compute error

\[
\|u - u_h, \lambda - \lambda_h\| \leq \|u - v_h, \lambda - \mu_h\| + \|u_h - v_h, \lambda_h - \mu_h\| \quad \text{Triangle inequality}
\]

\[
\leq \|u - v_h, \lambda - \mu_h\| + \frac{1}{C} \sup_{(w_h, \rho_h)} B((u_h - v_h, \lambda - \mu_h), (w_h, \rho_h)) \quad \text{Using Galerkin orthogonality}
\]

Using the mesh dependent estimates

\[
\min\limits_{v_h \in V_h} \|u - v_h\| \leq C h^2 \|u\|_2 \quad \min\limits_{v_h \in V_h} \|u - v_h\|_1 \leq C h \|u\|_2
\]

\[
\min\limits_{v_h \in V_h} \|u - v_h\|_{1/2,h} \leq C h \|u\|_2 \quad \min\limits_{\lambda_h \in M_h} \|\lambda - \lambda_h\|_{1/2,h} \leq C h \|\lambda\|_{-1/2}
\]

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

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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 \(\gamma\)

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

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 \emph{is} in canonical form \emph{and} equivalent to above

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

\[
g(u, \mu) \geq 0 \quad \lambda \geq 0 \quad \lambda g(u, \mu) = 0
\]

\[
\begin{bmatrix}
A & 0 & -B^T \\
0 & J & -J \\
-B & -J & 0
\end{bmatrix}
\begin{bmatrix}
u \\
\mu \\
\lambda
\end{bmatrix}
= \begin{bmatrix}
F \\
0 \\
0
\end{bmatrix}
\]
Results:

two pass mortar: no locking

curved interface beam

two pass mortar

slope = 1

slope = 2

effective stress

contact pressure

dual

exact contact pressure

dual

two pass mortar $\alpha = 0.01$

two pass mortar $\alpha = 1.0$

two pass mortar $\alpha = 100$

energy error
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
Structure preserving time integration w/ contact

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

\[
\text{equations of motion: } M_{AB}(v^n_B - v^n_B)/\Delta t + f^{(int)n+1/2}_A - f^{(c)n+1/2}_A = 0
\]

\[
\text{midstep time integrator: } (x^{n+1}_A - x^n_A) = \frac{1}{2}(v^{n+1}_A + v^n_A)\Delta t
\]

\[
\frac{1}{2}v^{n+1}_A M_{AB}v^n_B - \frac{1}{2}v^n_A M_{AB}v^n_B + (x^{n+1}_A - x^n_A) \cdot f^{(int)n+1/2}_A = (x^{(n+1)}_A - x^n_A) \cdot f^{(c)n+1/2}_A
\]

\[
f^{(int)n+1/2}_A = \int_{\Omega} F_{n+1/2} S_{n+1/2} \nabla \varphi_A d\Omega \quad \text{e.g. } S_{n+1/2} = C \frac{1}{2}(E_{n+1} + E_n)
\]

\[
F \equiv \text{Deformation Gradient}, \quad E \equiv \text{Green Strain}
\]

Conservation: get classical results when \( f^c = 0 \)

- linear momentum: \( L_{n+1} - L_n = M_{AB}(v^{n+1}_B - v^n_B) = 0 \)
- angular momentum: \( J_{n+1} - J_n = x^{n+1}_A \times M_{AB}v^n_B - x^n_A \times M_{AB}v^n_B = 0 \)
- energy: \( \mathcal{E}_{n+1} - \mathcal{E}_n = (T_{n+1} + U_{n+1}) - (T_n + U_n) = 0 \)

\[
T_n = \frac{1}{2}v^n_A M_{AB}v^n_B \quad U_n = \frac{1}{2} \int_{\Omega} E_n CE_n d\Omega
\]

\[
\mathcal{E}(t) = \text{constant} \geq 0 \ \forall t \quad \text{bounds displacements and velocities } \Rightarrow \text{B stability}
\]
Structure preserving time integration w/ contact

- Stability and momentum conservation requirements for contact force

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

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

angular momentum: \[ \sum_A x_A \times f_A^c = x_A \times \sum_{A,B} G_{BA} \lambda_B = 0 \] result of choice of contact normal \( n_A \)

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

3 Step Process

Step 1: Solve for \( v_B^{n+1}, \lambda_B^{n+1/2} \) from EOM

\[
 M_{AB}(v_B^{n+1} - v_B^n)/\Delta t + f_A^{(int)n+1/2} - G_{BA}^{(c)n+1/2} \lambda_B^{n+1/2} = 0
\]

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

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

\[
 M_{AB}(\bar{v}_B^{n+1} - v_B^{n+1}) + G_{BA} \lambda_B^{n+1} = 0 \\
 G_{AB} \bar{v}_B^{n+1} = 0
\]

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

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

\[
 \frac{1}{2} v_A^{n+1} M_{AB} \bar{v}_B^{n+1} = \frac{1}{2} v_A^{n+1} M_{AB} v_B^{n+1} - \frac{1}{2} (v_A^{n+1} - v_A^{n+1}) M_{AB} (\bar{v}_B^{n+1} - v_B^{n+1}) \Rightarrow \varepsilon_{n+1} \leq \varepsilon_n \]
Structure preserving time integration w/ contact

- Can return dissipated energy upon contact release

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

\[
\text{plastic impact dissipation: } \bar{\kappa}_A
\]

\[
\frac{1}{2} \ddot{v}_A^{n+1} M_{AB} \ddot{v}_B^{n+1} - \frac{1}{2} \dot{v}_A^{n+1} M_{AB} \dot{v}_B^{n+1} = \frac{1}{2} (\ddot{v}_A^{n+1} - \dot{v}_A^{n+1}) M_{AB} (\ddot{v}_B^{n+1} - \dot{v}_B^{n+1}) = \sum_A -\bar{\kappa}_A \leq 0
\]

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

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

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

can show

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

Now using \( \ddot{v}_A^{n+1} \) energy is conserved i.e. \( \mathcal{E}_{n+1} = \mathcal{E}_n \) and set \( \ddot{v}_A^{n+1} = \ddot{v}_A^{n+1} \) for next time step.
Structure preserving time integration w/ contact

- Large rotation w/ contact
Structure preserving time integration w/ contact

- Large rotation w/ contact

\[ J_n = x_A^n \times M_{AB}v_B^n \]
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

  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)

optimize nylon layups (Weisgraber)

Q (in)  Q (out)
thermal expansion  vibration?
One-way coupling: energy not conserved!