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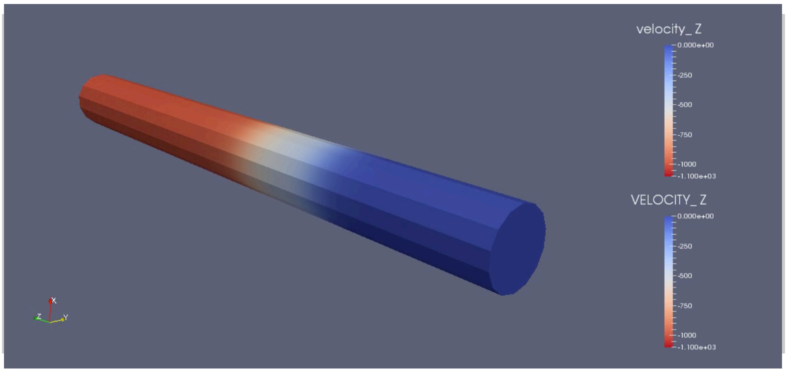

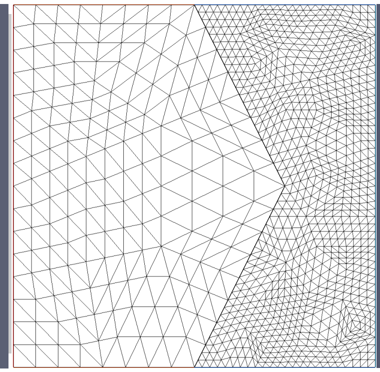

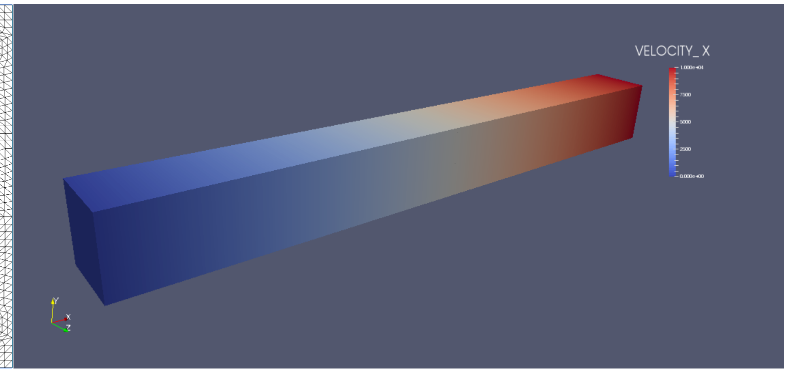

An explicit partitioned elastodynamics method based on Lagrange Multipliers

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LDRD

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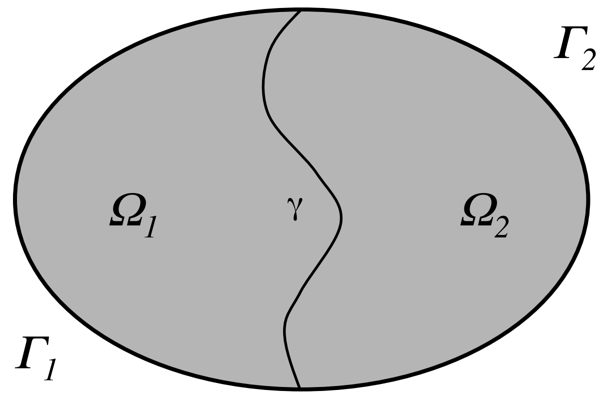
First in a series of two talks focusing on:

Problems with (physical or numerical) interfaces

$$
\begin{aligned}
\ddot{u} - \nabla \cdot \sigma(u) &= f && \text{in } \Omega \times T \\
u &= 0 && \text{on } \Gamma \times T \\
u(x,0) &= u_0(x) && \text{in } \Omega \times T \\
\dot{u}(x,0) &= \dot{u}_0(x) && \text{in } \Omega \times T
\end{aligned}
$$

$$\sigma(u) = \lambda(\nabla \cdot u)I + 2\mu\,\varepsilon(u)$$

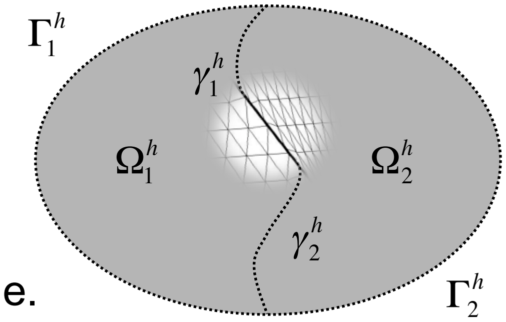


Solutions satisfy the continuity/transmission conditions

$$u\big|_{\gamma^-} = u\big|_{\gamma^+} \quad \textit{and} \quad \sigma(u^-) \cdot n_\gamma = \sigma(u^+) \cdot n_\gamma$$

Today we will talk about

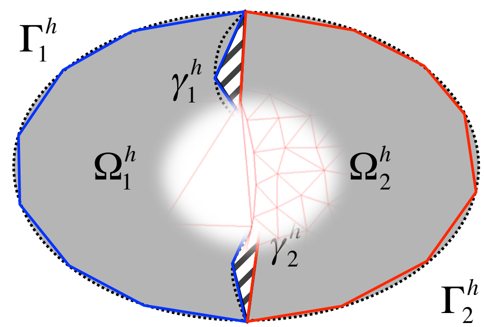
A partitioned algorithm under "practical constraints"



- Interface is physical, e.g., material property.
- Mesh is **interface-fitted** but not necessarily matching.
- Each subdomain problem is solved independently by a different code.
- Information exchange between codes is limited to nodal masses and forces.
- Motivated by the FORTE coupling of Sandia's Alegra and Sierra/SM codes.

Thursday: An optimization-based, mesh-tying algorithm (P. Kuberry, 9:00am)

- Interface is physical or numerical, e.g., due to meshing
- **Separate meshing** creates 2 distinct, **non-coincident** versions of the same interface.
- Data transfer between non-coincident interfaces remains a tough challenge.
- Existing approaches typically involve complex mesh manipulations.



Original "welded" interface coupling in Forte:

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"Welded" interface coupling

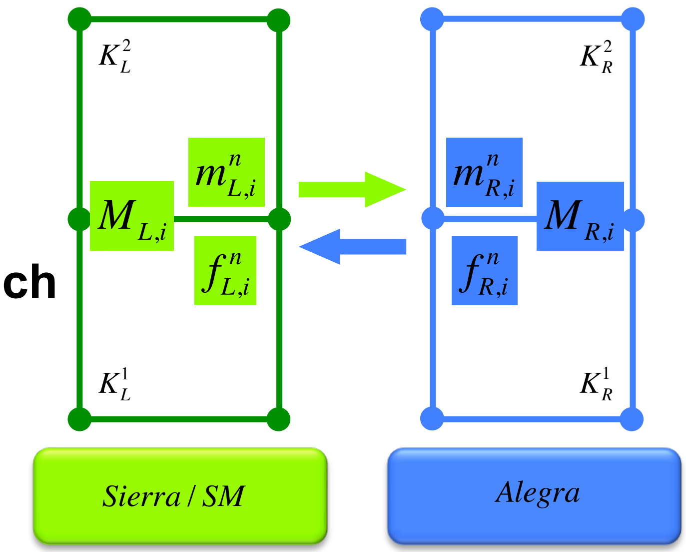
- Mass and forces **swapped** at nodes
- **Minimally intrusive** (black-box) coupling, but…
- Requires matching interface nodes
- One code may require **finer mesh**:

  ⇒ Forces **excessive mesh refinement**!

Discrete subdomain equations

$$M_L u_L^{n+1} = \vec{m}_L^n + \vec{f}_L^n \qquad M_R u_R^{n+1} = \vec{m}_R^n + \vec{f}_R^n$$

Mass-force exchange



Goal: develop a new partitioned algorithm, which

- Defaults to "welded" interface on **matching** grids.
- Handles interfaces with **non-matching** grids.
- Has **linear** consistency
- Is **second-order** accurate

Completed equation @ interface node:

$$(M_L + M_R) u_{L/R}^{n+1} = (\vec{m}_L^n + \vec{m}_R^n) + (\vec{f}_L^n + \vec{f}_R^n)$$

What does this swap mean mathematically?

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Let's reverse-engineer the "welded" interface coupling

$$(M_L + M_R)u_L^{n+1} = (\vec{m}_L^n + \vec{m}_R^n) + (\vec{f}_L^n + \vec{f}_R^n)$$
$$(M_L + M_R)u_R^{n+1} = (\vec{m}_L^n + \vec{m}_R^n) + (\vec{f}_L^n + \vec{f}_R^n)$$
$$u_L^{n+1} = u_R^{n+1}$$

This is a pair of identical "completed" equations at an interface node

Because they are the same, they imply continuity of the nodal displacement!

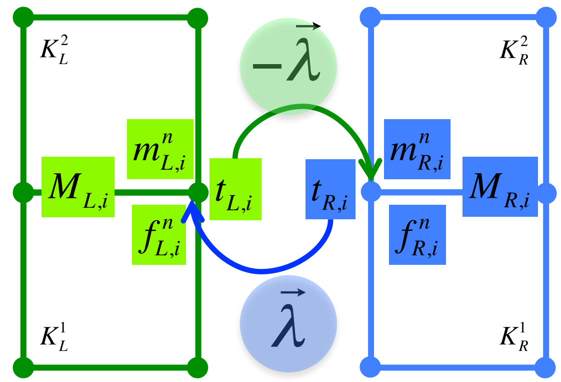
$$M_L u_L^{n+1} = (\vec{m}_L^n + \vec{f}_L^n) + (\vec{m}_R^n + \vec{f}_R^n - M_R u_L^{n+1})$$
$$M_R u_R^{n+1} = (\vec{m}_L^n + \vec{f}_R^n) + (\vec{m}_R^n + \vec{f}_L^n - M_L u_R^{n+1})$$
$$u_L^{n+1} = u_R^{n+1}$$

Let's group all terms from the "other" side

This is the contact force at the node!

It's beginning to look a lot like….

$$M_L u_L^{n+1} = (\vec{m}_L^n + \vec{f}_L^n) + \vec{\lambda}$$
$$M_R u_R^{n+1} = (\vec{m}_L^n + \vec{f}_R^n) - \vec{\lambda}$$
$$u_L^{n+1} = u_R^{n+1}$$



A mixed Lagrange multiplier formulation!

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Let's start from a monolithic formulation

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- Write the problem as a system of two subdomain equations with mixed boundary conditions.
- The Neumann boundary condition involves an unknown contact force λ.
- Close the system by adding the displacement continuity condition:

Monolithic formulation → **Semi-discrete version**

$$
\begin{aligned}
\ddot{u}_1 - \nabla\cdot\sigma(u_1) &= f_1 && \text{in } \Omega_1\times T\\
u_1 &= 0 && \text{on } \Gamma_1\times T\\
\sigma(u_1)\cdot n &= \lambda && \text{on } \gamma\times T
\end{aligned}
$$

$$
\begin{aligned}
\ddot{u}_2 - \nabla\cdot\sigma(u_2) &= f_2 && \text{in } \Omega_2\times T\\
u_2 &= 0 && \text{on } \Gamma_2\times T\\
-\sigma(u_2)\cdot n &= \lambda && \text{on } \gamma\times T
\end{aligned}
$$

$$u_1 - u_2 = 0 \quad \text{on } \gamma\times T$$

→

$$u_1 \in V_1^h \subset H^1_{\Gamma_1}(\Omega_1)$$

$$u_2 \in V_2^h \subset H^2_{\Gamma_2}(\Omega_2)$$

$$\lambda \in S^h \subset H^{-1/2}(\gamma)$$

→

$$M_1\ddot{u}_1 + G_1^T\lambda = F_1(u_1)$$

$$M_2\ddot{u}_2 - G_2^T\lambda = F_2(u_2)$$

$$G_1u_1 - G_2u_2 = 0$$

Mixed, KKT-like system

- System of 3 equations for 3 unknowns: subdomain displacements and contact force.
- **Contact force continuity** $\sigma(u_1)\cdot n_1 + \sigma(u_2)\cdot n_2 = 0$ on $\gamma\times T$ subsumed in the equations.
- **Displacement continuity** $u_1 - u_2 = 0$ on $\gamma\times T$ enforced explicitly
- For problems with an energy principle *t* can be identified with a Lagrange multiplier.

There's one problem though…

Lagrange multipliers are not the most natural setting for partitioned schemes

- Result in Index-2 DAE that are more difficult to solve
- Not compatible with explicit time integration

$$M_1\ddot{u}_1 + G_1^T\lambda = F_1(u_1)$$
$$M_2\ddot{u}_2 - G_2^T\lambda = F_2(u_2)$$
$$G_1 u_1 - G_2 u_2 = 0$$

Partial solution, *Carpenter et al, IJNME, 1991*

- References the multiplier one time increment ahead (forward increment LM method).
- Resulting method still not purely explicit

A (simple) solution: switch constraints from displacement to acceleration

$u_1 = u_2\big|_\gamma$ **index 2 DAE**

$\ddot{u}_1 = \ddot{u}_2\big|_\gamma$ **index 1 DAE**

implies the original constraint under suitable assumptions

$$\begin{bmatrix} M_{1,\sigma} & 0 & G_1^T & 0 & 0 \\ 0 & M_{2,\sigma} & -G_2^T & 0 & 0 \\ G_1 & -G_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & M_{1,0} & 0 \\ 0 & 0 & 0 & 0 & M_{2,0} \end{bmatrix} \begin{bmatrix} \ddot{\boldsymbol{u}}_{1,\sigma} \\ \ddot{\boldsymbol{u}}_{2,\sigma} \\ \lambda \\ \ddot{\boldsymbol{u}}_{1,0} \\ \ddot{\boldsymbol{u}}_{2,0} \end{bmatrix} = \begin{bmatrix} f_{1,\sigma} \\ f_{2,\sigma} \\ 0 \\ f_{1,0} \\ f_{2,0} \end{bmatrix}$$

- Caution: works for transmission problems but may not work for contact problems!

The master formulation on matching grids

The master monolithic (mixed) problem

$$\begin{bmatrix} M_{1,\sigma} & 0 & G_1^T & 0 & 0 \\ 0 & M_{2,\sigma} & -G_2^T & 0 & 0 \\ G_1 & -G_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & M_{1,0} & 0 \\ 0 & 0 & 0 & 0 & M_{2,0} \end{bmatrix} \begin{bmatrix} \ddot{\boldsymbol{u}}_{1,\sigma} \\ \ddot{\boldsymbol{u}}_{2,\sigma} \\ \lambda \\ \ddot{\boldsymbol{u}}_{1,0} \\ \ddot{\boldsymbol{u}}_{2,0} \end{bmatrix} = \begin{bmatrix} f_{1,\sigma} \\ f_{2,\sigma} \\ 0 \\ f_{1,0} \\ f_{2,0} \end{bmatrix}$$

$$\begin{bmatrix} M_{1,\sigma} & 0 & \tilde{M}_{1,\sigma} & 0 & 0 \\ 0 & M_{2,\sigma} & -\tilde{M}_{2,\sigma} & 0 & 0 \\ \tilde{M}_{1,\sigma} & -\tilde{M}_{2,\sigma} & 0 & 0 & 0 \\ 0 & 0 & 0 & M_{1,0} & 0 \\ 0 & 0 & 0 & 0 & M_{2,0} \end{bmatrix} \begin{bmatrix} \ddot{\boldsymbol{u}}_{1,\sigma} \\ \ddot{\boldsymbol{u}}_{2,\sigma} \\ \lambda \\ \ddot{\boldsymbol{u}}_{1,0} \\ \ddot{\boldsymbol{u}}_{2,0} \end{bmatrix} = \begin{bmatrix} f_{1,\sigma} \\ f_{2,\sigma} \\ 0 \\ f_{1,0} \\ f_{2,0} \end{bmatrix}$$

matching nodes specialization

Option A:(1,1) Schur

eliminate interface DOF

$$\begin{bmatrix} M_{1,\sigma} & 0 & \tilde{M}_{1,\sigma} \\ 0 & M_{2,\sigma} & -\tilde{M}_{2,\sigma} \\ \tilde{M}_{1,\sigma} & -\tilde{M}_{2,\sigma} & 0 \end{bmatrix} \begin{bmatrix} \ddot{\boldsymbol{u}}_{1,\sigma} \\ \ddot{\boldsymbol{u}}_{2,\sigma} \\ \lambda \end{bmatrix} = \begin{bmatrix} f_{1,\sigma} \\ f_{2,\sigma} \\ 0 \end{bmatrix}$$

Option B: (2,2) Schur

eliminate internal DOF

$$\begin{bmatrix} M_{1,\sigma} & 0 & \tilde{M}_{1,\sigma} \\ 0 & M_{2,\sigma} & -\tilde{M}_{2,\sigma} \\ \tilde{M}_{1,\sigma} & -\tilde{M}_{2,\sigma} & 0 \end{bmatrix} \begin{bmatrix} \ddot{\boldsymbol{u}}_{1,\sigma} \\ \ddot{\boldsymbol{u}}_{2,\sigma} \\ \lambda \end{bmatrix} = \begin{bmatrix} f_{1,\sigma} \\ f_{2,\sigma} \\ 0 \end{bmatrix}$$

$$\tilde{M}_{*,\sigma}(M_{1,\sigma}^{-1} + M_{2,\sigma}^{-1})\tilde{M}_{*,\sigma}\lambda = \tilde{M}_{*,\sigma}(M_{2,\sigma}^{-1}f_{2,\sigma} - M_{1,\sigma}^{-1}f_{1,\sigma})$$

VFR

MFR

$$\begin{aligned} (M_{1,\sigma}^i + M_{2,\sigma}^i)\ddot{\boldsymbol{u}}_{1,\sigma}^i &= f_{1,\sigma}^i + f_{2,\sigma}^i \\ (M_{1,\sigma}^i + M_{2,\sigma}^i)\ddot{\boldsymbol{u}}_{2,\sigma}^i &= f_{1,\sigma}^i + f_{2,\sigma}^i \end{aligned}$$

Identical Partitioned systems for matching nodes!

The master formulation on non-matching grids

$$\left[\begin{array}{ccc:cc} M_{1,\sigma} & 0 & G_1^T & 0 & 0 \\ 0 & M_{2,\sigma} & -G_2^T & 0 & 0 \\ G_1 & -G_2 & 0 & 0 & 0 \\ \hdashline 0 & 0 & 0 & M_{1,0} & 0 \\ 0 & 0 & 0 & 0 & M_{2,0} \end{array}\right] \left[\begin{array}{c} \ddot{\boldsymbol{u}}_{1,\sigma} \\ \ddot{\boldsymbol{u}}_{2,\sigma} \\ \lambda \\ \hdashline \ddot{\boldsymbol{u}}_{1,0} \\ \ddot{\boldsymbol{u}}_{2,0} \end{array}\right] = \left[\begin{array}{c} f_{1,\sigma} \\ f_{2,\sigma} \\ 0 \\ \hdashline f_{1,0} \\ f_{2,0} \end{array}\right]$$

Option A (VFR)

$$\left[\begin{array}{c:cc} M_{1,\sigma} & 0 & G_1^T \\ \hdashline 0 & M_{2,\sigma} & -\tilde{M}_{2,\sigma} \\ G_1 & -\tilde{M}_{2,\sigma} & 0 \end{array}\right] \left[\begin{array}{c} \ddot{\boldsymbol{u}}_{1,\sigma} \\ \hdashline \ddot{\boldsymbol{u}}_{2,\sigma} \\ \lambda \end{array}\right] = \left[\begin{array}{c} f_{1,\sigma} \\ \hdashline f_{2,\sigma} \\ 0 \end{array}\right]$$

$$\left[\begin{array}{c:cc} M_{2,\sigma} & 0 & -G_2^T \\ \hdashline 0 & M_{1,\sigma} & \tilde{M}_{1,\sigma} \\ G_2 & -\tilde{M}_{1,\sigma} & 0 \end{array}\right] \left[\begin{array}{c} \ddot{\boldsymbol{u}}_{2,\sigma} \\ \hdashline \ddot{\boldsymbol{u}}_{1,\sigma} \\ \lambda \end{array}\right] = \left[\begin{array}{c} f_{2,\sigma} \\ \hdashline f_{1,\sigma} \\ 0 \end{array}\right]$$

Option B (MFR)

$$\left[\begin{array}{cc:c} M_{1,\sigma} & 0 & G_1^T \\ 0 & M_{2,\sigma} & -G_2^T \\ \hdashline G_1 & -G_2 & 0 \end{array}\right] \left[\begin{array}{c} \ddot{\boldsymbol{u}}_{1,\sigma} \\ \ddot{\boldsymbol{u}}_{2,\sigma} \\ \hdashline \lambda \end{array}\right] = \left[\begin{array}{c} f_{1,\sigma} \\ f_{2,\sigma} \\ \hdashline 0 \end{array}\right]$$

$$(G_1 M_{1,\sigma}^{-1} G_1^T + G_2 M_{2,\sigma}^{-1} G_2^T)\lambda = G_2 M_{2,\sigma}^{-1} f_{2,\sigma} - G_1 M_{1,\sigma}^{-1} f_{1,\sigma}$$

- Requires 2 separate master systems for each side
- LM collocated with displacement on the opposite side
- LM spaces simple to construct
- Results in a generalized "mass-force exchange" between the subdomains

- Leads to a system for interface DOFs
- Requires preconditioning
- Index 1 enables explicit treatment of the LM
- Requires common mesh refinement for LM
- Potentially more accurate…
- Related to **Dual Schur Complement** systems in DD, FETI, hybrid methods,…

The two options in a nutshell

Options A and B are simply two different ways of expressing the contact force:

(A): **Indirect** representation: Generate

$$M + \Delta M = f + \Delta f$$

This is a **primal Schur** complement approach in which we express the contact force indirectly in terms of mass/force updates to the interface eqs.

(B) **Direct** representation: Generate

$$M = f + \Delta f$$

This is a **dual Schur** complement approach in which we solve an equation for the LM to obtain the contact force on the interface

Most approaches to partitioned algorithms are direct

Option A gives the desired generalization of FORTE

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Consider the system for subdomain 1 (LM collocated with interface on subdomain 2)

$$\begin{bmatrix} M_{1,\sigma} & 0 & \tilde{M}_{1,\sigma}\overleftarrow{\Pi} & 0 & 0 \\ 0 & M_{2,\sigma} & -\tilde{M}_2 & 0 & 0 \\ \tilde{M}_{2,\sigma}\overrightarrow{\Pi} & -\tilde{M}_{2,\sigma} & 0 & 0 & 0 \\ 0 & 0 & 0 & M_{1,0} & 0 \\ 0 & 0 & 0 & 0 & M_{2,0} \end{bmatrix} \begin{bmatrix} \ddot{\boldsymbol{u}}_{1,\sigma} \\ \ddot{\boldsymbol{u}}_{2,\sigma} \\ \lambda \\ \ddot{\boldsymbol{u}}_{1,0} \\ \ddot{\boldsymbol{u}}_{2,0} \end{bmatrix} = \begin{bmatrix} f_{1,\sigma} \\ f_{2,\sigma} \\ 0 \\ f_{1,0} \\ f_{2,0} \end{bmatrix}$$

Taking the (1,1) Schur complement gives a system for u_1

$$(M_{1,\sigma} + \tilde{M}_{1,\sigma}\overleftarrow{P}\tilde{M}_{2,\sigma}^{-1}M_{2,\sigma}\overrightarrow{P})\ddot{\boldsymbol{u}}_{1,\sigma} = f_{1,\sigma} + \tilde{M}_{1,\sigma}\overleftarrow{P}\tilde{M}_{2,\sigma}^{-1}f_{2,\sigma}$$

and analogously (using a second mixed problem) for u_2

$$(M_{2,\sigma} + \tilde{M}_{2,\sigma}\overrightarrow{P}\tilde{M}_{1,\sigma}^{-1}M_{1,\sigma}\overleftarrow{P})\ddot{\boldsymbol{u}}_{2,\sigma} = f_{2,\sigma} + \tilde{M}_{2,\sigma}\overrightarrow{P}\tilde{M}_{1,\sigma}^{-1}f_{1,\sigma}$$

generalization of Forte's mass-force exchange

mass $\Leftarrow$ exchange $\Rightarrow$ force

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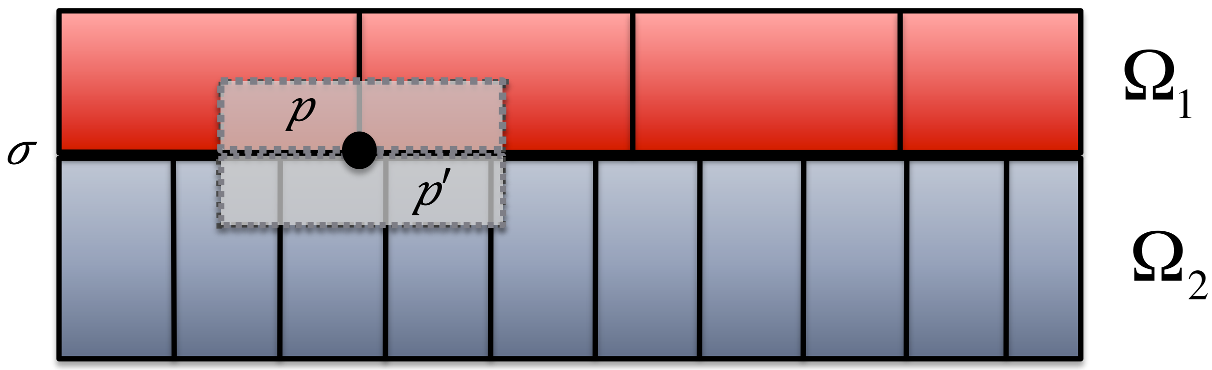
Comparison with a Slide Lines method

- We examine connections between Option A, i.e., generalized Forte coupling and slide lines for tied contact applications, Kuchařík et al. , *Comp. & Fluids*, 83 2013.



$$
\begin{aligned}
m^{p'} &= \alpha_i m_i^{p'} + \alpha_{i+1} m_{i+1}^{p'} \\
f^{p'} &= \alpha_i f_i^{p'} + \alpha_{i+1} f_{i+1}^{p'} \\
a^{p'} &= \alpha_i a_i^{p'} + \alpha_{i+1} a_{i+1}^{p'}
\end{aligned}
$$

- The slide line method is derived by considering virtual cells straddling the interface and then writing out contact conditions at *p=p'*:
  - Continuity of accelerations & continuity of the contact force
  - This leads to the following auxiliary system:

$$
\begin{aligned}
m^p \ddot{\boldsymbol{u}}^p &= f^p \\
m^{p'} \frac{a^p}{a^{p'}} \ddot{\boldsymbol{u}}^{p'} &= f^{p'} \frac{a^p}{a^{p'}}
\end{aligned}
\quad \longrightarrow \quad
(m^p + m^{p'} \frac{a^p}{a^{p'}}) \ddot{\boldsymbol{u}}^p = f^p + f^{p'} \frac{a^p}{a^{p'}}
$$

The slide line equation at interface node

Comparison with a Slide Lines method

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Slide lines (Kuchařík et al.)

$$\left(m^p + \frac{(\alpha_i m_i^{p'} + \alpha_{i+1} m_{i+1}^{p'}) a^p}{\alpha_i a_i^{p'} + \alpha_{i+1} a_{i+1}^{p'}}\right) \ddot{\boldsymbol{u}}^p = f^p + \frac{(\alpha_i f_i^{p'} + \alpha_{i+1} f_{i+1}^{p'}) a^p}{\alpha_i a_i^{p'} + \alpha_{i+1} a_{i+1}^{p'}}$$

Interpolate then scale vs. scale then interpolate

$$\left(m^p + \left(\alpha_i \frac{m_i^{p'}}{a_i^{p'}} + \alpha_{i+1} \frac{m_{i+1}^{p'}}{a_{i+1}^{p'}}\right) a^p\right) \ddot{\boldsymbol{u}}^p = f^p + \left(\alpha_i \frac{f_i^{p'}}{a_i^{p'}} + \alpha_{i+1} \frac{f_{i+1}^{p'}}{a_{i+1}^{p'}}\right) a^p$$

Generalized Forte

Thanks to M. Shashkov (LANL) for pointing out Slide Lines reference

Properties

Equivalence to a monolithic explicit solution for matching grid interfaces

For interfaces with matching nodes there holds $M_{1\sigma} = M_{2\sigma}$ and $\overleftarrow{P} = \vec{P} = I$

$$\left(M_1 + M_{1\sigma}\overleftarrow{P}M_{2\sigma}^{-1}M_2\vec{P}\right)\ddot{u}_1 = F_1 + M_{1\sigma}\overleftarrow{P}M_{2\sigma}^{-1}F_2 \quad\longrightarrow\quad \left(M_1 + M_2\right)\ddot{u}_1 = F_1 + F_2$$

$$\left(M_2 + M_{2\sigma}\vec{P}M_{1\sigma}^{-1}M_1\overleftarrow{P}\right)\ddot{u}_2 = F_2 + M_{2\sigma}\vec{P}M_{1\sigma}^{-1}F_1 \quad\longrightarrow\quad \left(M_2 + M_1\right)\ddot{u}_2 = F_2 + F_1$$

Interface	Vertical	Slanted
Mesh Ω_1	24x20	24x20
Mesh Ω_2	24x20	24x20
L_2 error Ω_1	3.38E-17	9.43E-17
L_2 error Ω_2	1.07E-15	1.05E-15
L_2 error Ω_1	2.49E-15	7.74E-15
L_2 error Ω_2	9.92E-14	1.23E-13

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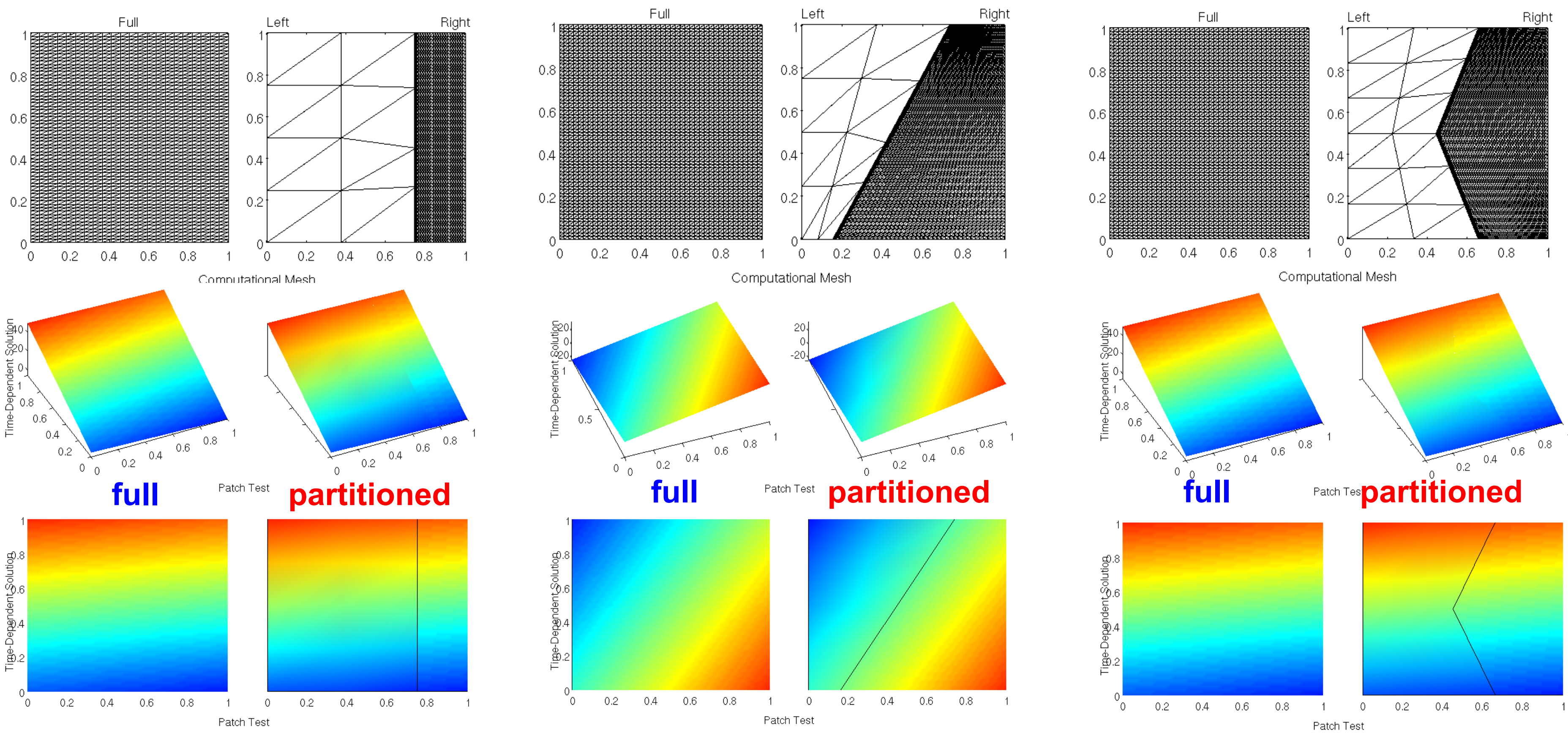
Properties

Recovery of linear displacements (patch test)

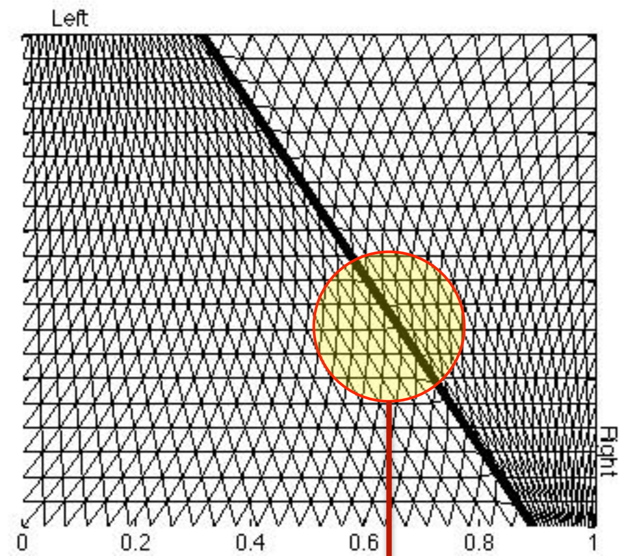


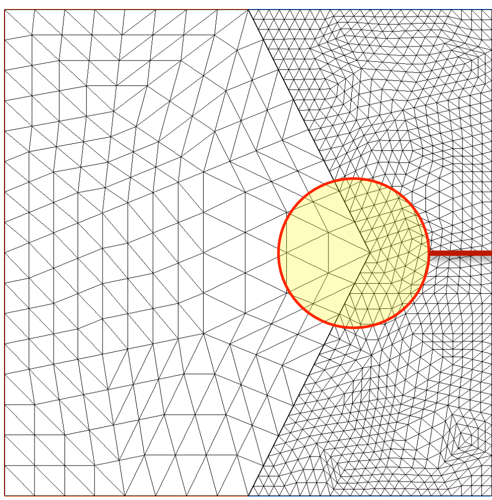
VFR approach recovers linear solution to machine precision on interfaces with non-matching grids.

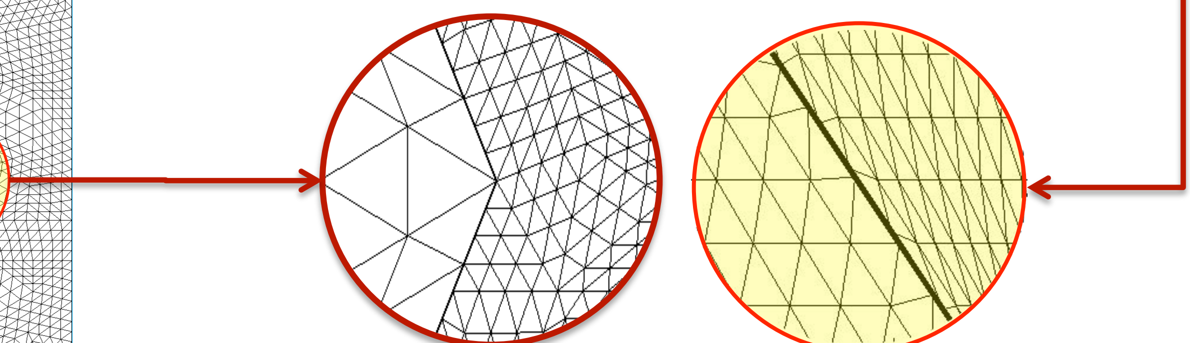
Properties

2^{nd} order accuracy on non-matching interfaces

	Error		Rate
Mesh Ω_1	28x40	56x80	
Mesh Ω_2	52x40	104x80	
L_2 error Ω_1	2.07E-03	5.15E-04	2.01
L_2 error Ω_2	3.79E-03	9.58E-04	1.99
H^1 error Ω_1	2.78E-01	1.39E-01	1.00
H^1 error Ω_2	8.22E-01	4.12E-01	1.00





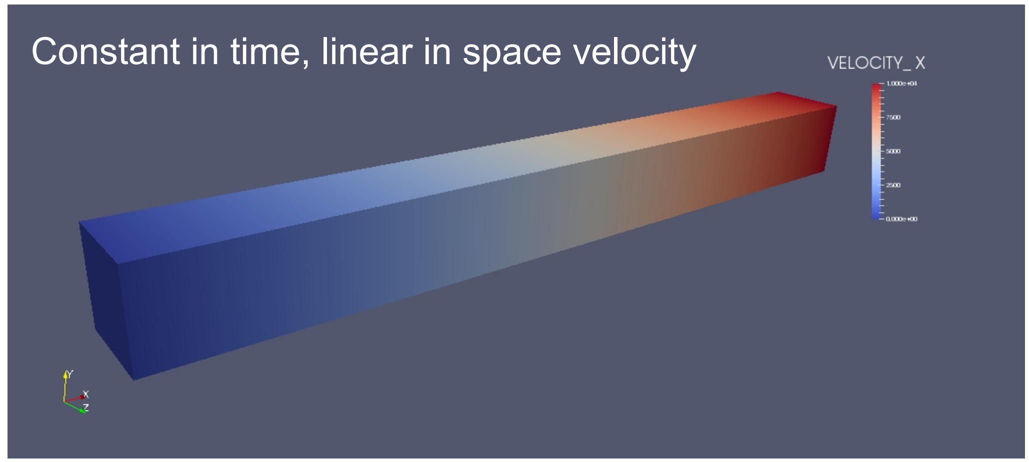


Implementation in production codes

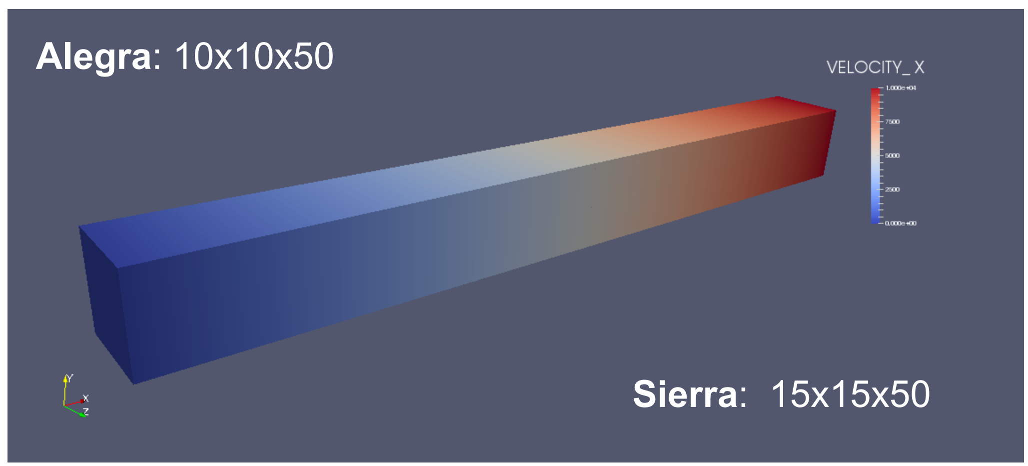
VFR coupling has been deployed in Sandia's Forte software.

Consistency test

Exact →



Forte+VFR →



Verification of Forte+VFR

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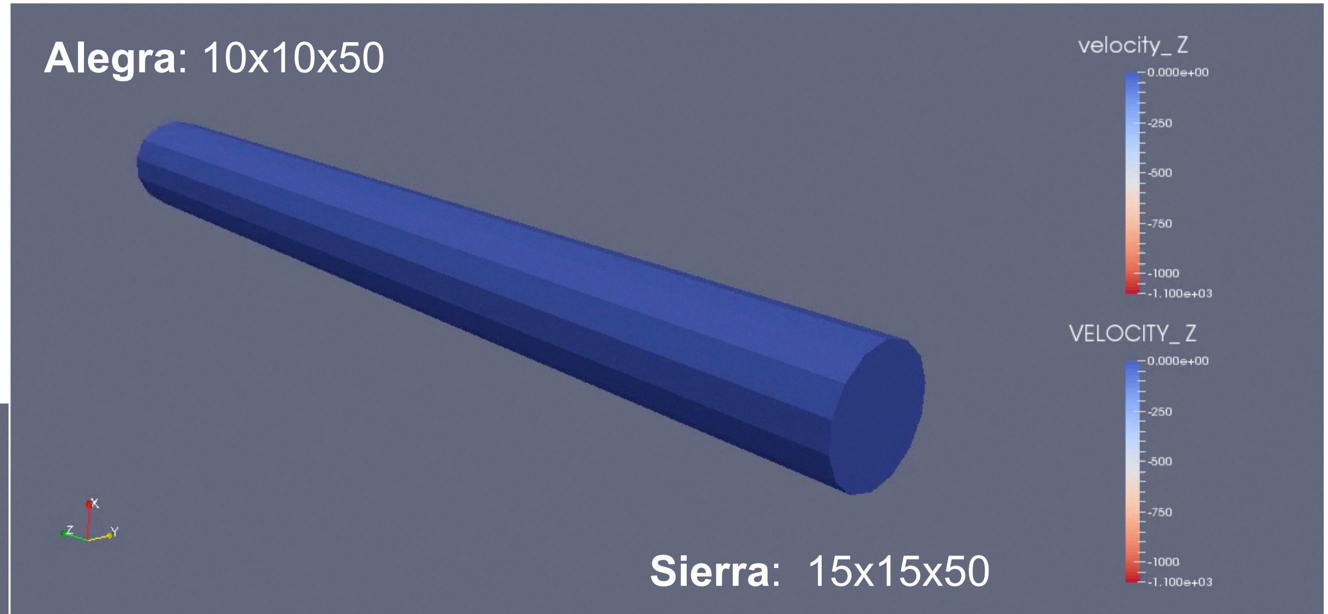
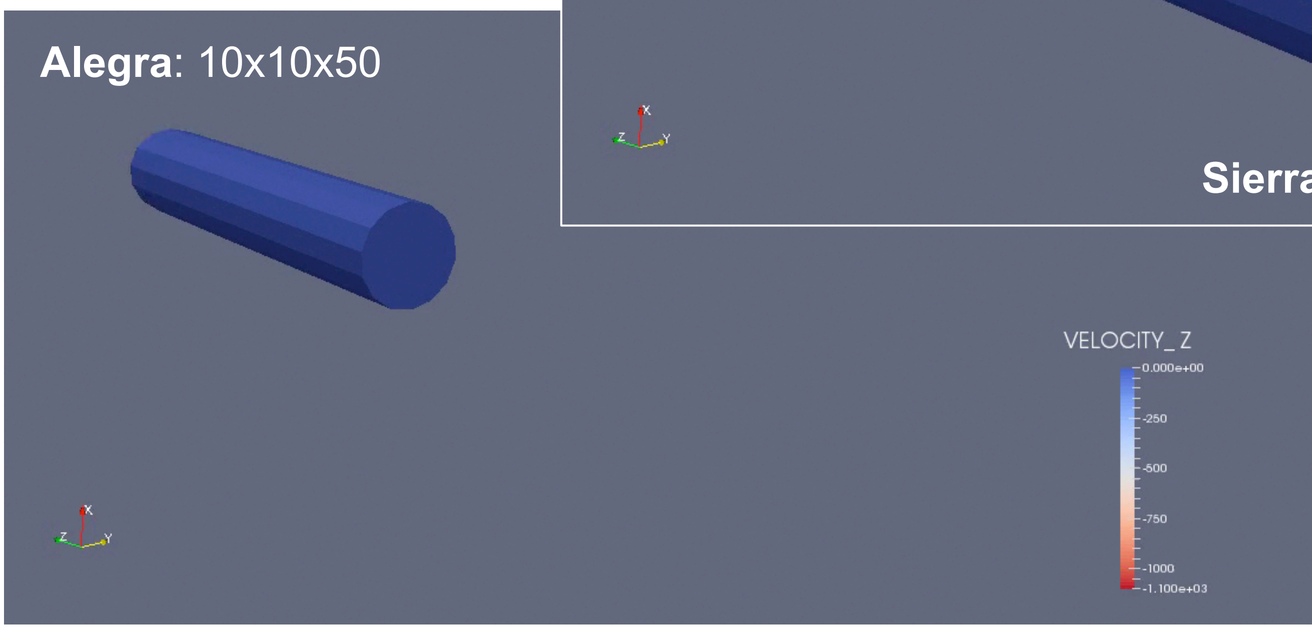
Axial pulse bar test





Conclusions

- **Developed a general framework** that reduces a DAE 2 to a DAE 1 and is based on Lagrange multipliers.
- **Framework provides** a way to generate partitioned approaches that can be traced back to a well-posed system including both direct and indirect contact force representation methods.
- **Operator simplification** allows for a diagonal mass update to the indirect approach, avoiding complicated linear solves in an explicit approach.
- **Equivalence to a monolithic solution (proved)** in the case of matching nodes, **passing a patch test (proved)**, and **second order convergence** rates observed in numerical experiments.

SAND2017-XXXX