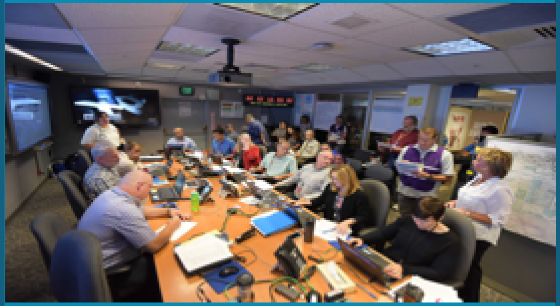
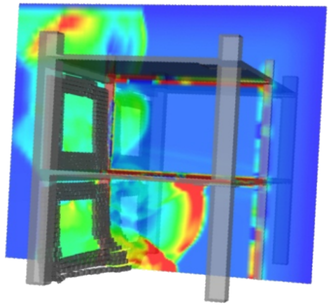
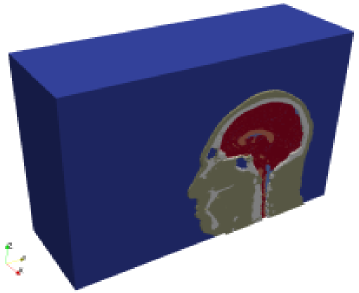
SAND2024-09275C

Modified Immersed Finite Element Method (mIFEM) For Explicit Eulerian to Explicit Lagrangian Coupling







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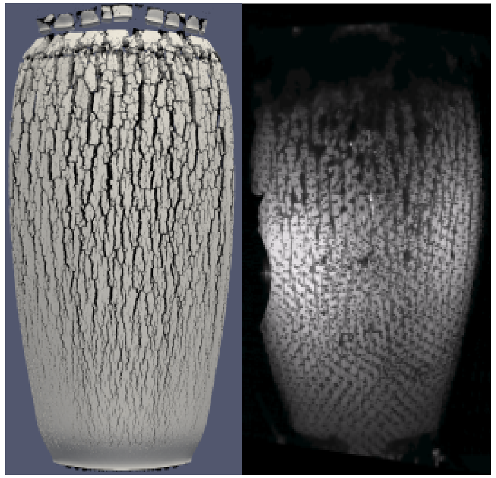
Many mechanical systems are naturally described by a combined Eulerian & Lagrangian description.

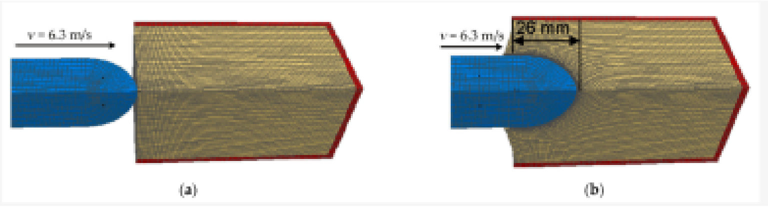
- Lagrangian for solids with low to moderate strain rates
- Eulerian description for materials that flow: fluids, solids at high strain rate

- Blast-on-structure is a common environment in the defense industry
  - Structural integrity
  - Lethality
  - System assessments
- Computational simulations are challenging
  - Fluid-structure interactions (FSI)
  - Particle velocity discrepancies introduce complexity
  - Differing numerical methods for the physics domains

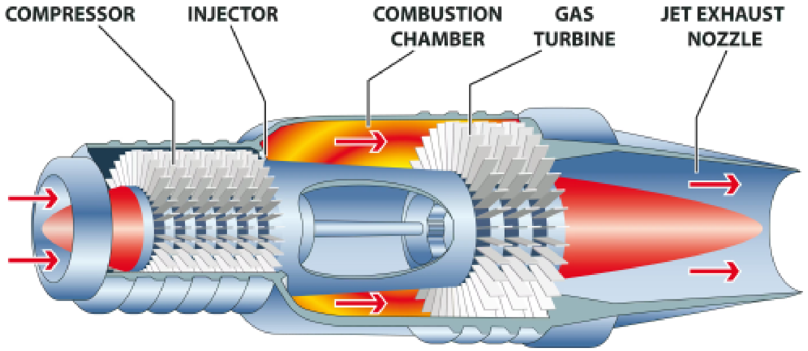


(a) Simulation (b) Experiment

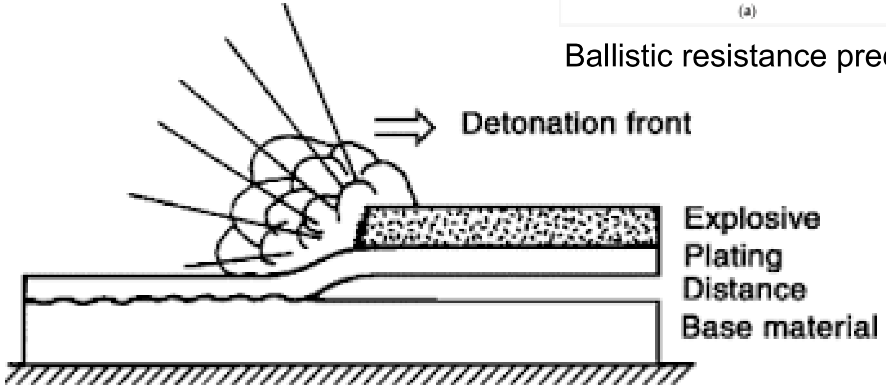
Fragmentation of bomb case (R. Teeter)



Ballistic resistance prediction (Zochowski et al., 2021)



Turbomachinery applications



Explosive welding

Our goal is to develop a robust and accurate coupling of existing finite element codes.

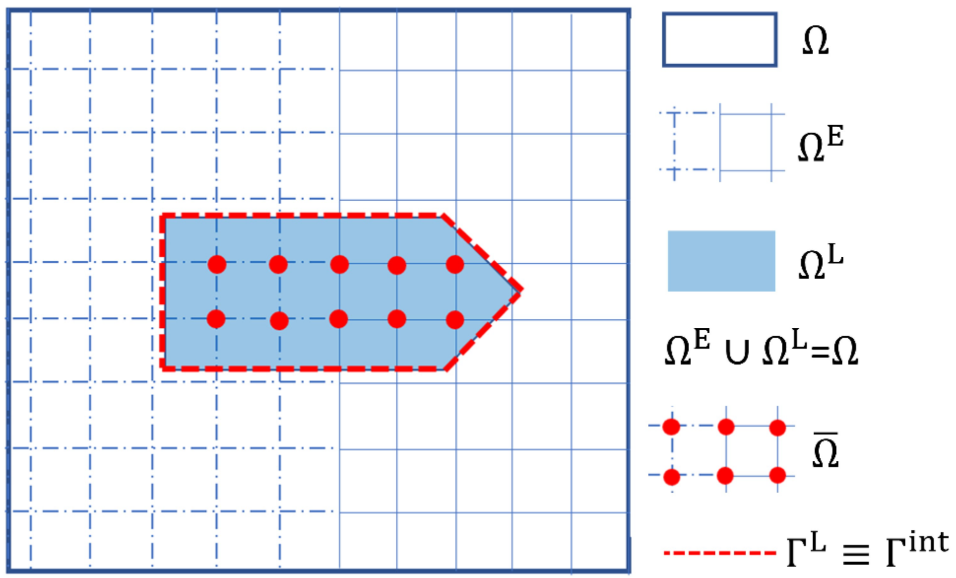
SABLE

- SABLE: Shock Adaptive BLock Eulerian
- Shock physics
  - Shock wave formation and propagation
  - Multi- and mixed-phase materials
  - Elastic, viscous, plastic solids with fracture/failures
  - High explosive detonations
  - Structured mesh with Adaptive Mesh Refinement (AMR)
  - Hex8 linear finite elements
  - Solves mass, momentum, energy equations
    - Equations of state
    - Constitutive models
  - Satisfies balance laws, including angular momentum
  - Lagrangian solution step followed by remap
  - Explicit time stepping – central difference

COMPSIM
SOLID MECHANICS

- Sierra Solid Mechanics (Sierra/SM)
- Large deformation, non-linear material behavior with fracture and failure
  - Linear and quadratic elements
  - Explicit and implicit solution procedures
  - Massively parallel implementation
  - Contact mechanics
  - Extensive material model library
  - Equation of state models
  - Explicit time stepping – central difference

Immersed methods are a natural choice for SABLE-to-Sierra Solid Mechanics coupling.



Schematic representation of the computational domain [Christon et al., SAND2022-12772]

- Structured background mesh
- Single (nodal) velocity field in SABLE
- No need to resolve "boundary layer" phenomena
  - Precise pointwise field values on the interface are not of primary importance
  - Prefer accuracy of integrated quantities (e.g. total force) over an appropriate collection of Lagrangian faces.

$$\mathbf{F}^{\mathrm{L}} = \sum_{f=1}^{N_{\mathrm{faces}}} \int_f \sigma^{\mathrm{E}}[\mathbf{n}]\,\mathrm{dS}$$

- Modified Immersed FEM (mIFEM, cf. Wang & Zhang, CMAME, 2013) is an approach that allows for separate Lagrangian and Eulerian solvers.

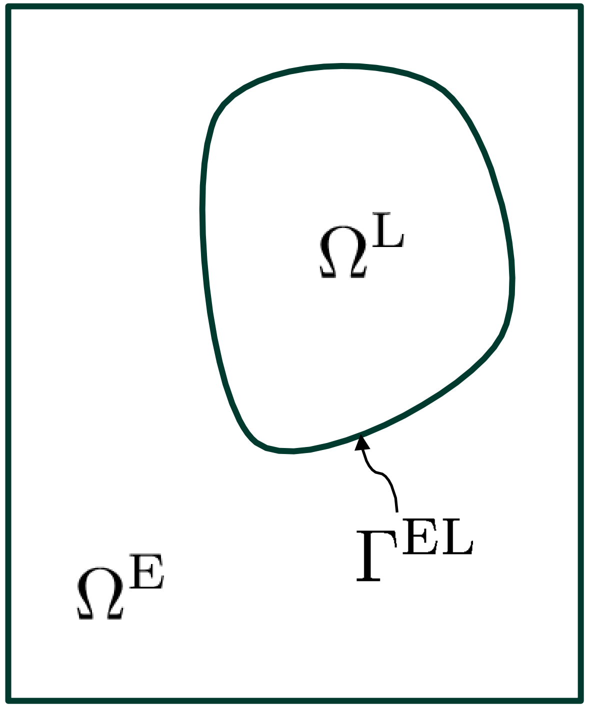
Domains are coupled via linear momentum balance.

$$\rho^{\mathrm{E}} \frac{\partial \mathbf{v}^{\mathrm{E}}}{\partial t} - \nabla \cdot \sigma^{\mathrm{E}} = \mathbf{0} \quad \text{in } \Omega^{\mathrm{E}}$$

$$\rho^{\mathrm{L}} \frac{\partial \mathbf{v}^{\mathrm{L}}}{\partial t} - \nabla \cdot \sigma^{\mathrm{L}} = \mathbf{0} \quad \text{in } \Omega^{\mathrm{L}}$$

$$\sigma^{\mathrm{L}}[\mathbf{n}^{\mathrm{L}}] + \sigma^{\mathrm{E}}[\mathbf{n}^{\mathrm{E}}] = \mathbf{0} \quad \text{on } \Gamma^{\mathrm{EL}} \qquad \text{(dynamic)}$$

$$G(\mathbf{v}^{\mathrm{E}}, \mathbf{v}^{\mathrm{L}}) = \mathbf{0} \quad \text{on } \Gamma^{\mathrm{EL}} \qquad \text{(kinematic)}$$

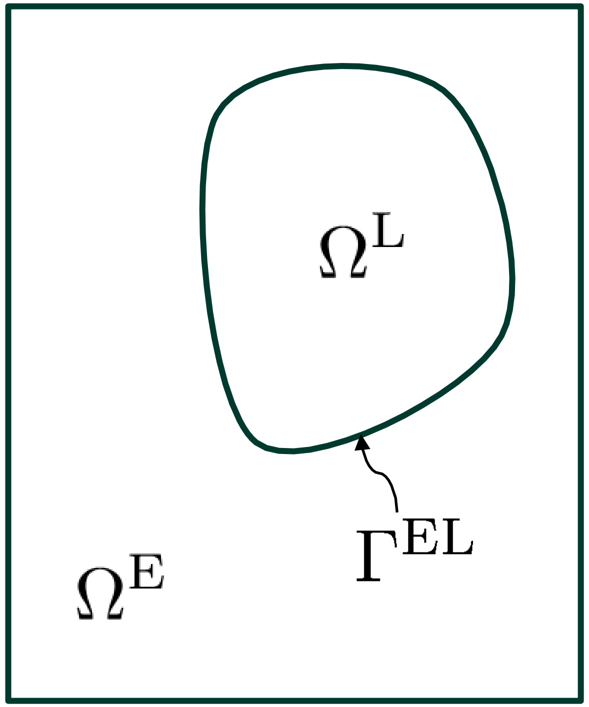


- Eulerian domain is doing a Lagrange step!
- Kinematic interface condition can be no-slip, slip, dynamic friction…
- *Body forces, initial & boundary conditions omitted for brevity

Virtual work statement is obtained via the immersed approach.

Problem 1 (Principle of virtual work)
Choose $\hat{\mathbf{v}} \in (H_0^1(\Omega))^d$. *Then,*

$$\int_{\Omega^{\mathrm{L}}} \left\{ \rho^{\mathrm{L}} \hat{\mathbf{v}} \cdot \frac{\partial \mathbf{v}^{\mathrm{L}}}{\partial t} + \nabla \hat{\mathbf{v}} \cdot \sigma^{\mathrm{L}} \right\} \mathrm{dV} + \int_{\Omega^{\mathrm{E}}} \left\{ \rho^{\mathrm{E}} \hat{\mathbf{v}} \cdot \frac{\partial \mathbf{v}^{\mathrm{E}}}{\partial t} + \nabla \hat{\mathbf{v}} \cdot \sigma^{\mathrm{E}} \right\} \mathrm{dV} = \mathbf{0}$$



- Immersed approach: single velocity field represents both Lagrangian and Eulerian materials.
- Multiply by **v**, integrate over each domain, integrate by parts, strongly enforce dynamic interface condition (force balance)
- Single velocity field has implications for E-L (inter-material) slip

Problem 2 (Weak form)
Find $\mathbf{v}^{\mathrm{E}} \in (H^1(\Omega^{\mathrm{E}}))^d$ *and* $\mathbf{v}^{\mathrm{L}} \in (H^1(\Omega^{\mathrm{L}}))^d$ *such that*

$$\int_{\Omega^{\mathrm{L}}} \left\{ \rho^{\mathrm{L}} \mathbf{v}^{\mathrm{L}} \cdot \frac{\partial \mathbf{v}^{\mathrm{L}}}{\partial t} + \nabla \hat{\mathbf{v}} \cdot \sigma^{\mathrm{L}} \right\} \mathrm{dV} + \int_{\Omega^{\mathrm{E}}} \left\{ \rho^{\mathrm{E}} \mathbf{v}^{\mathrm{E}} \cdot \frac{\partial \mathbf{v}^{\mathrm{E}}}{\partial t} + \nabla \hat{\mathbf{v}} \cdot \sigma^{\mathrm{E}} \right\} \mathrm{dV} = 0 \quad \forall\, \hat{\mathbf{v}} \in (H_0^1(\Omega))^d.$$

mIFEM introduces an artificial material to mimic the Lagrangian response.

- "Artificial" domain is the image of the Lagrangian domain immersed in the background
- Kinematics (velocity) on the artificial domain should mimic the Lagrangian kinematics
- Benefit: use existing solid models & Lagrangian codes
- Extend the Eulerian velocity and stress into the artificial domain:

$$\rho = \begin{cases} \rho^{\mathrm{A}} \text{ in } \Omega^{\mathrm{A}} \\ \rho^{\mathrm{E}} \text{ in } \Omega^{\mathrm{E}} \end{cases} \qquad \sigma = \begin{cases} \sigma^{\mathrm{A}} \text{ in } \Omega^{\mathrm{A}} \\ \sigma^{\mathrm{E}} \text{ in } \Omega^{\mathrm{E}} \end{cases}$$

$$\Omega = \Omega^{\mathrm{E}} \cup \Omega^{\mathrm{L}}$$

$$\Omega^{\mathrm{L}} \approx \Omega^{\mathrm{A}}$$

$$\rho^{\mathrm{A}} = \rho^{\mathrm{L}}, \ \sigma^{\mathrm{A}} = \sigma^{\mathrm{E}}$$

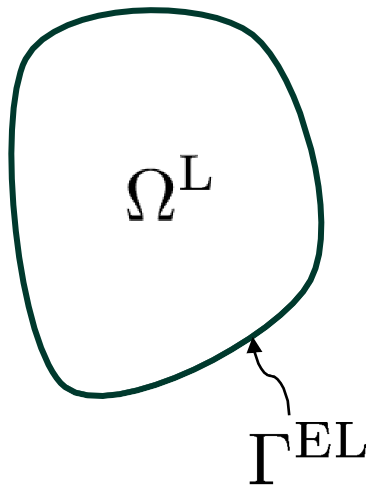
- In practice, desire:

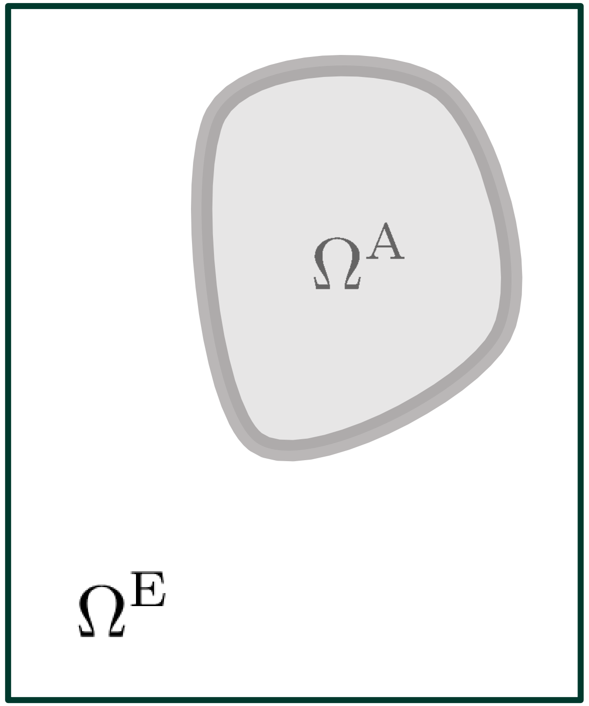
Problem 3 (Modified weak form)
Find $\mathbf{v} \in (H^1(\Omega))^d$ *such that*

$$\int_{\Omega} \left\{ \rho \hat{\mathbf{v}} \cdot \frac{\partial \mathbf{v}}{\partial t} + \nabla \hat{\mathbf{v}} \cdot \sigma \right\} \mathrm{dV} =$$

$$\int_{\Omega^{\mathrm{A}}} \left\{ \hat{\mathbf{v}} \cdot \left(\rho^{\mathrm{A}} \frac{\partial \mathbf{v}}{\partial t} - \rho^{\mathrm{L}} \frac{\partial \mathbf{v}^{\mathrm{L}}}{\partial t} \right) + \nabla \hat{\mathbf{v}} \cdot \left(\sigma^{\mathrm{A}} - \sigma^{\mathrm{L}} \right) \right\} \mathrm{dV}$$

$$\forall \hat{\mathbf{v}} \in (H_0^1(\Omega))^d.$$





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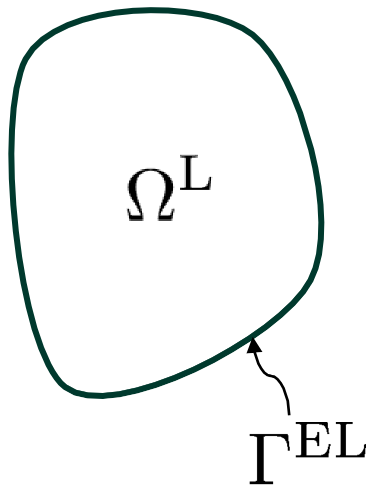
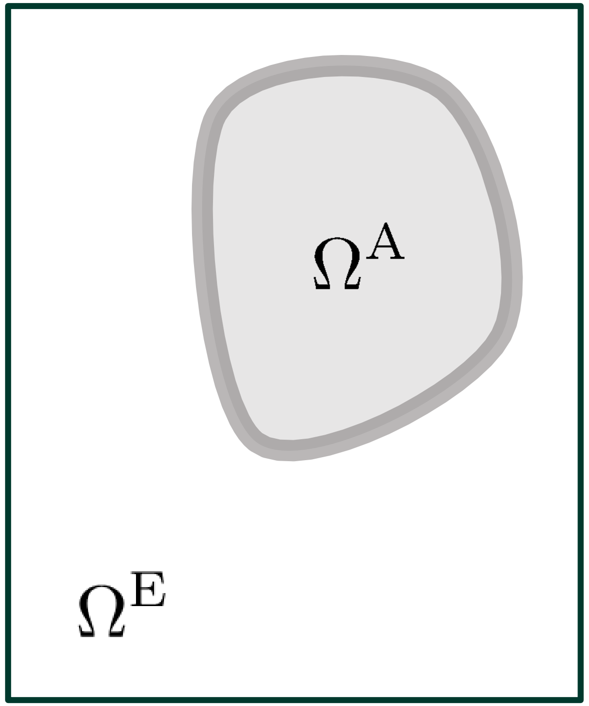




Problem 3 (Modified weak form)
Find $\mathbf{v} \in (H^1(\Omega))^d$ *such that*

$$\int_{\Omega} \left\{ \rho \hat{\mathbf{v}} \cdot \frac{\partial \mathbf{v}}{\partial t} + \nabla \hat{\mathbf{v}} \cdot \sigma \right\} \mathrm{dV} = \int_{\Omega^{\mathrm{A}}} \hat{\mathbf{v}} \cdot \mathbf{F}^{\mathrm{ELI}} \quad \forall \hat{\mathbf{v}} \in (H_0^1(\Omega))^d.$$

where

$$\int_{\Omega^{\mathrm{A}}} \hat{\mathbf{v}} \cdot \mathbf{F}^{\mathrm{ELI}} = \int_{\Omega^{\mathrm{A}}} \left\{ \hat{\mathbf{v}} \cdot \left(\rho^{\mathrm{A}} \frac{\partial \mathbf{v}}{\partial t} - \rho^{\mathrm{L}} \frac{\partial \mathbf{v}^{\mathrm{L}}}{\partial t} \right) + \nabla \hat{\mathbf{v}} \cdot \left(\sigma^{\mathrm{A}} - \sigma^{\mathrm{L}} \right) \right\} \mathrm{dV}$$

mIFEM solution algorithm advances Lagrangian and Eulerian domains sequentially without iterations.

For each time step:

1. Interpolate traction on Lagrangian boundary from background material: $\mathbf{t}^{\mathrm{L}} = \sigma^{\mathrm{E}}[\mathbf{n}^{\mathrm{L}}]$
2. Solve Lagrangian solid dynamics

Problem 4 (Lagrangian weak form)
Find $\mathbf{v}^{\mathrm{L}} \in (H^1(\Omega^{\mathrm{L}}))^d$ *such that*

$$\int_{\Omega^{\mathrm{L}}} \left\{ \rho^{\mathrm{L}} \hat{\mathbf{v}}^{\mathrm{L}} \cdot \frac{\partial \mathbf{v}^{\mathrm{L}}}{\partial t} + \nabla \hat{\mathbf{v}}^{\mathrm{L}} \cdot \sigma^{\mathrm{L}} \right\} \mathrm{dV} - \int_{\Gamma^{\mathrm{EL}}} \hat{\mathbf{v}}^{\mathrm{L}} \cdot \sigma^{\mathrm{E}}[\mathbf{n}^{\mathrm{L}}] \, \mathrm{dS} = \mathbf{0}$$

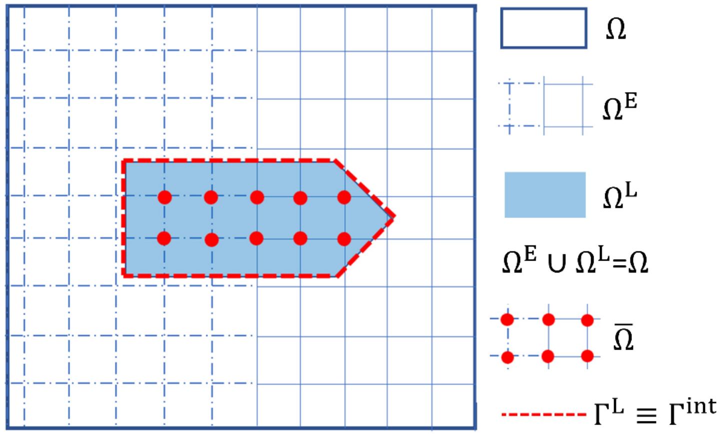
$$\forall \hat{\mathbf{v}}^{\mathrm{L}} \in (H^1_0(\Omega^{\mathrm{L}}))^d.$$

$$\mathbf{a}^{\mathrm{L}}_n = \mathbf{M}^{-1} \left[\mathbf{F}^{\mathrm{ext}}(\mathbf{u}^{\mathrm{L}}_n) - \mathbf{F}^{\mathrm{int}}(\mathbf{u}^{\mathrm{L}}_n) \right]$$

$$\mathbf{v}^{\mathrm{L}}_{n+1/2} = \mathbf{v}^{\mathrm{L}}_{n-1/2} + \frac{1}{2} \left(\Delta t_{n-1/2} + \Delta t_{n+1/2} \right) \mathbf{a}^{\mathrm{L}}_n$$

$$\mathbf{u}^{\mathrm{L}}_{n+1} = \mathbf{u}^{\mathrm{L}}_n + \Delta t_{n+1/2} \mathbf{v}^{\mathrm{L}}_{n+1/2}$$

3. Identify artificial domain Ω^{A} as the image of the foreground Lagrangian domain in the background mesh (via an 'indicator function')



Schematic representation of the computational domain [Christon et al., SAND2022-12772]

mIFEM solution algorithm advances Lagrangian and Eulerian domains sequentially without iterations.

For each time step:

4. Evaluate the coupling force

$$\hat{\mathbf{v}} \cdot \mathbf{F}^{\mathrm{ELI}} = \hat{\mathbf{v}} \cdot \left(\rho^{\mathrm{A}} \frac{\partial \mathbf{v}}{\partial t} - \rho^{\mathrm{L}} \frac{\partial \mathbf{v}^{\mathrm{L}}}{\partial t} \right) + \nabla \hat{\mathbf{v}} \cdot \left(\sigma^{\mathrm{A}} - \sigma^{\mathrm{L}} \right)$$

5. Solve the Eulerian (background) domain

Problem 3 (Modified weak form)
Find $\mathbf{v} \in (H^1(\Omega))^d$ *such that*

$$\int_{\Omega} \left\{ \rho \hat{\mathbf{v}} \cdot \frac{\partial \mathbf{v}}{\partial t} + \nabla \hat{\mathbf{v}} \cdot \sigma \right\} \mathrm{dV} = \int_{\Omega^{\mathrm{A}}} \hat{\mathbf{v}} \cdot \mathbf{F}^{\mathrm{ELI}} \quad \forall \hat{\mathbf{v}} \in (H_0^1(\Omega))^d.$$

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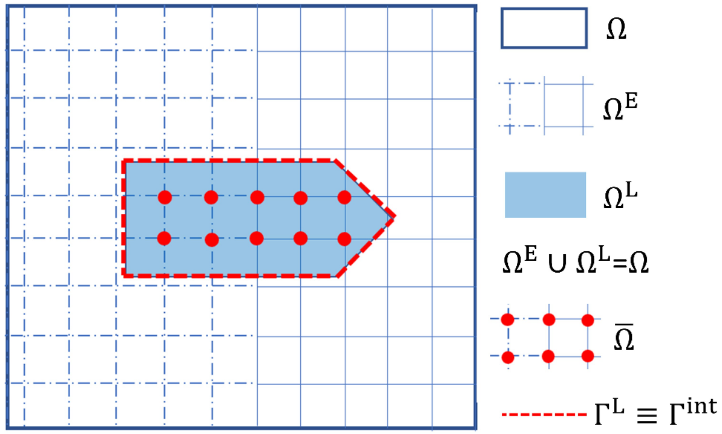
- Mass conservation and internal energy are also solved
- Calculate fluxes and remap deformed state to initial grid

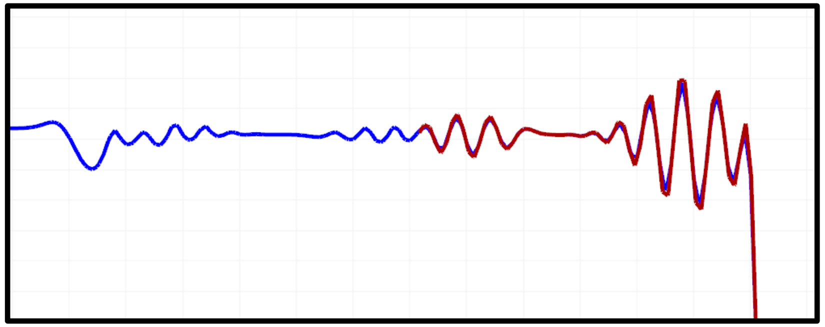


Schematic representation of the computational domain [Christon et al., SAND2022-12772]

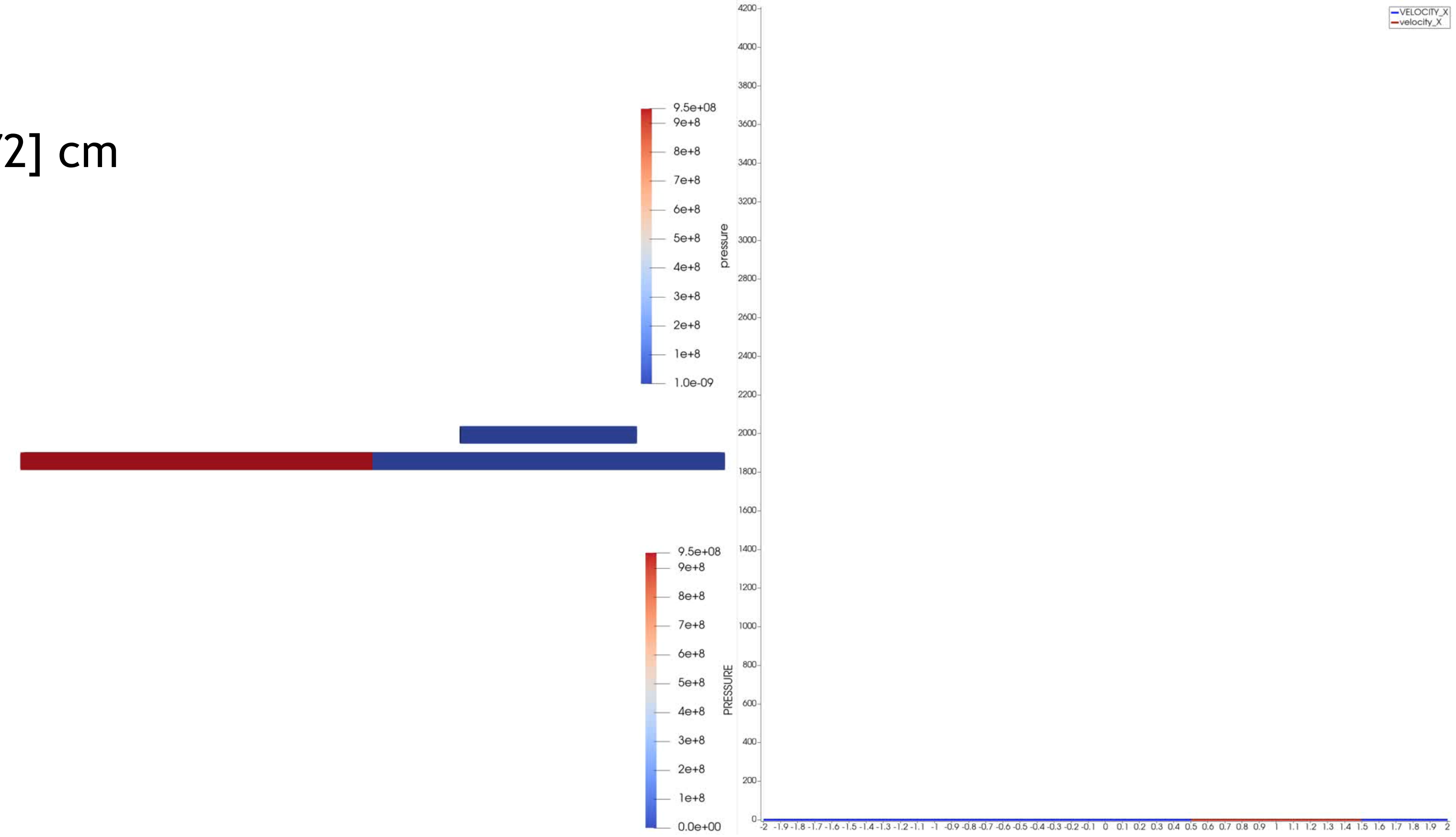
Example: impedance matched shock wave propagation

Eulerian domain:
- Dimensions: [-2,2]x[-0.05,]x[-0.72,0.72] cm
- Elements: 400x10x10
- Material: Mie-Gruneisen (linearized)
- Pressure differential = 1e8 Pa
- Density differential = 0.05 g/cm^3

Lagrangian domain:
- Dimensions: [0.5,1.5]x[-0.05,]x[-0.72,0.72] cm
- Material: elastic, impedance matched



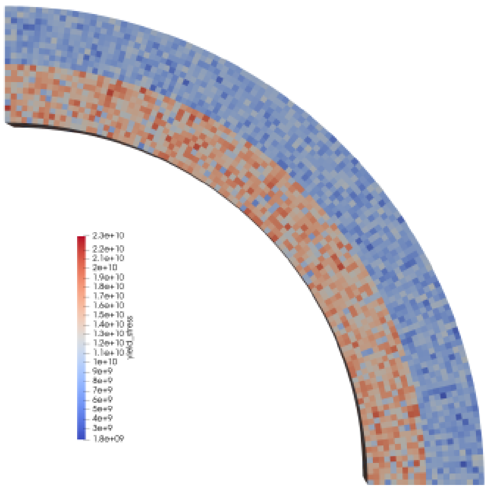
Eulerian and Lagrangian velocities agree in overlap region.



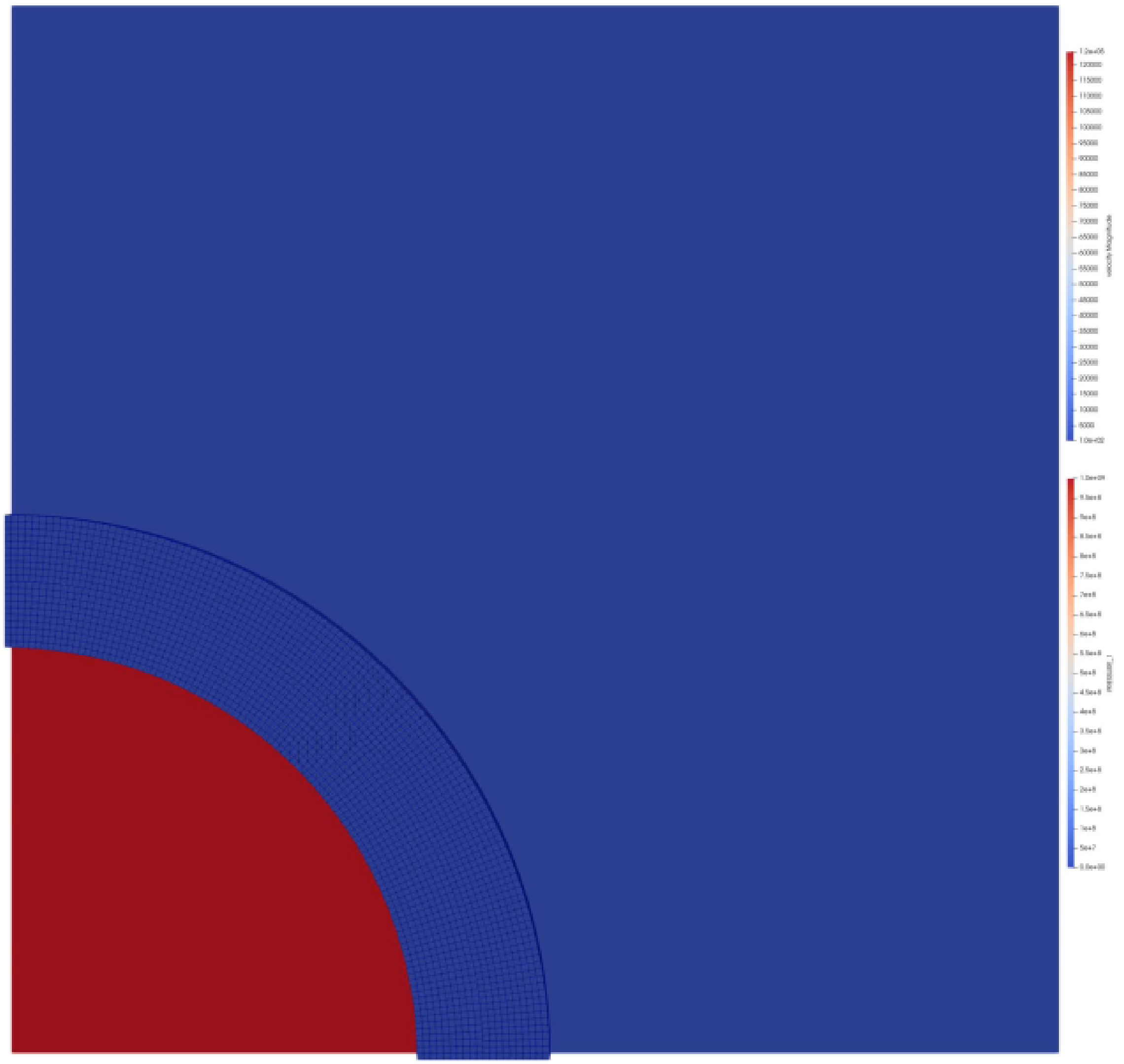
Example: Fragmentation of concentric rings

Eulerian domain:
- Dimensions: [0,28.8]x[0,28.8]x[-0.72,0.72] cm
- Elements: 80x80x2 = 12,800 total
- Material: Air (tabulated equation of state)
- Initial inner pressure = 1e10 Pa
- Initial outer pressure = 0.82e6 Pa

Lagrangian domain:
- Inner radius = 11.2 cm
- Ring thickness = 1.8 cm
- Materials: Tungsten - inner, 8400 elements
  Steel – outer, 9680 elements



Weibull distribution of yield stress adds stochasticity



Take-away messages

1. Two-way immersed coupling of Sierra Solid Mechanics (FEM) and SABLE (shock physics) for explicit transient dynamics simulations will be an enabling technology for next-generation blast-on-structure analysis.
2. Immersed FEM approach is needed for block structured shock physics code
3. Modified IFEM coupling methodology offers features needed for our coupling strategy: theoretical basis, partitioned solvers, additional flexibility
4. Initial investigations show promising results for high strain rate scenarios
5. Research and development work is in progress
    1. Stability and convergence results – theory &
    2. Z-scheme (e.g. CSS) temporal offsets for robustness and accuracy
    3. Strong scaling and running ‘at scale’ needs to be demonstrated