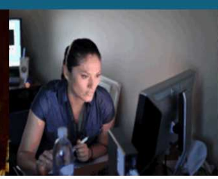
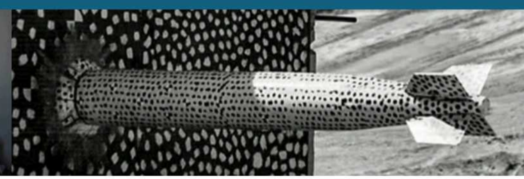
SAND2019-10456C

Multi-material dynamic domain topology changes in the Lagrangian Grid Reconnection (LGR) code





MULTIMAT 2019

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SAND 2019-XXXX

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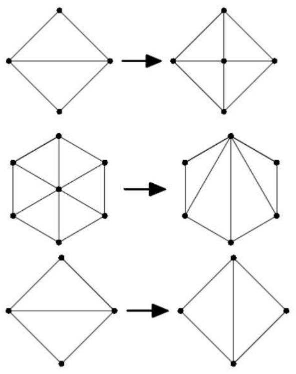
LGR (formerly Alexa)

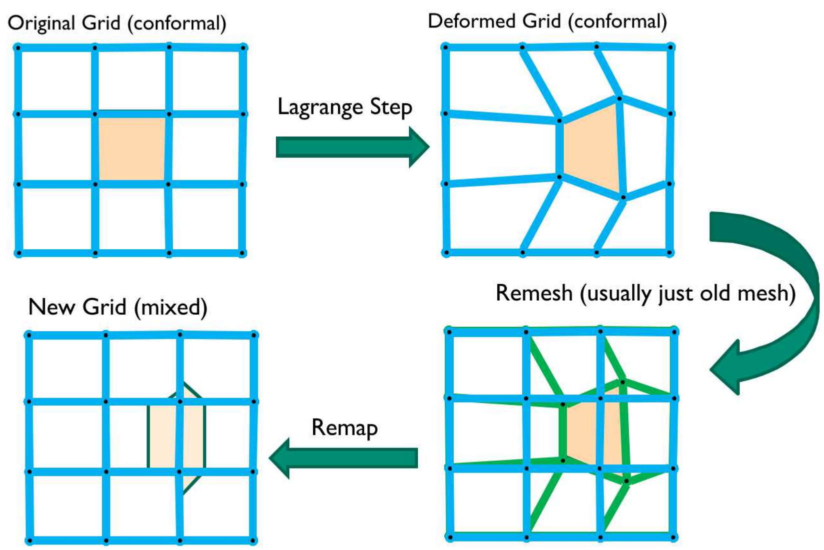
- The LGR research code for GPU-performant shock hydrodynamics
- Adaptive Lagrangian: Like ALE (Arbitrary Lagrangian-Eulerian) except no Eulerian component, does adaptation (remeshing) by local modification, maintains single-material elements
- Local topology changes ("flooding") for fracture and penetration
- Completed Open-Source (to GitHub), renamed to Lagrangian Grid Reconnection Tool Kit (github.com/SNLComputation/lgrtk)
- Extended to 1D and 2D, including better V&V

Adaptive Tet Meshes: A New Approach to ALE

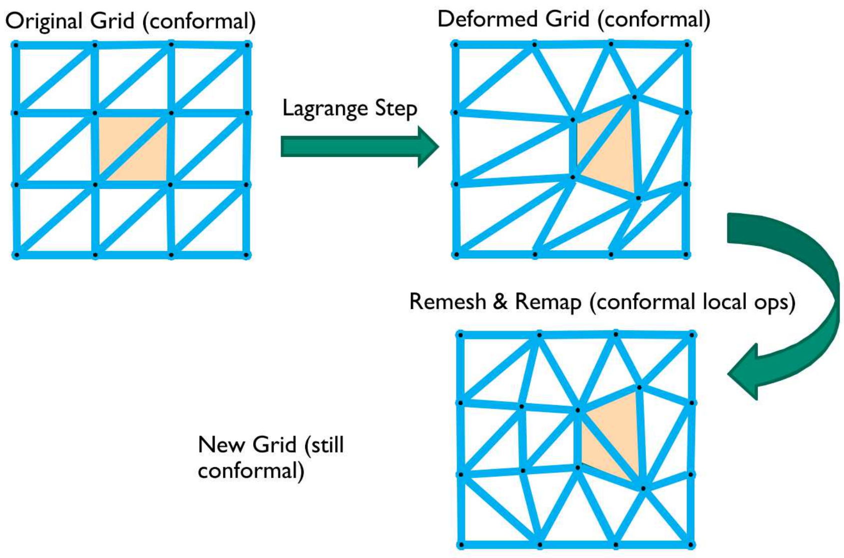
- Adopt ideas from aerospace mesh generation and adaptation: triangle/tetrahedral grids can adapt (reconnect) on the fly
- Always single-material elements: no volume fraction issues
- Easier body-fitted mesh generation, better geometric fidelity in shock simulations



ALE



LGR



Lagrangian continuum equations

- Conservation of linear momentum:

$$\langle \delta\boldsymbol{\varphi}, \rho\dot{\mathbf{v}} \rangle \; + \; \langle \mathrm{grad}[\delta\boldsymbol{\varphi}], \boldsymbol{\sigma} \rangle = 0 \quad \forall \boldsymbol{\varphi}$$

- Balance of internal energy:

$$\langle \delta\theta, \rho\dot{\varepsilon} \rangle - \langle \delta\theta, \mathrm{grad}[\mathbf{v}] \bullet \boldsymbol{\sigma} \rangle = 0 \quad \forall \delta\theta$$

- Kinematics:

$$\dot{\mathbf{x}} - \mathbf{v} = \mathbf{0}$$

$$\mathbb{F} := \mathrm{GRAD}[\mathbf{x}] \qquad J := \det(\mathbf{F})$$

- Conservation of mass:

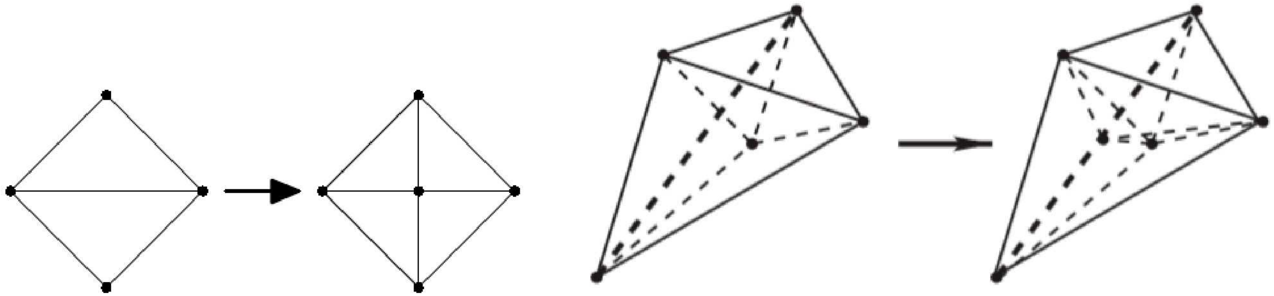
$$\rho = J^{-1}\rho_0$$

- Constitutive model:

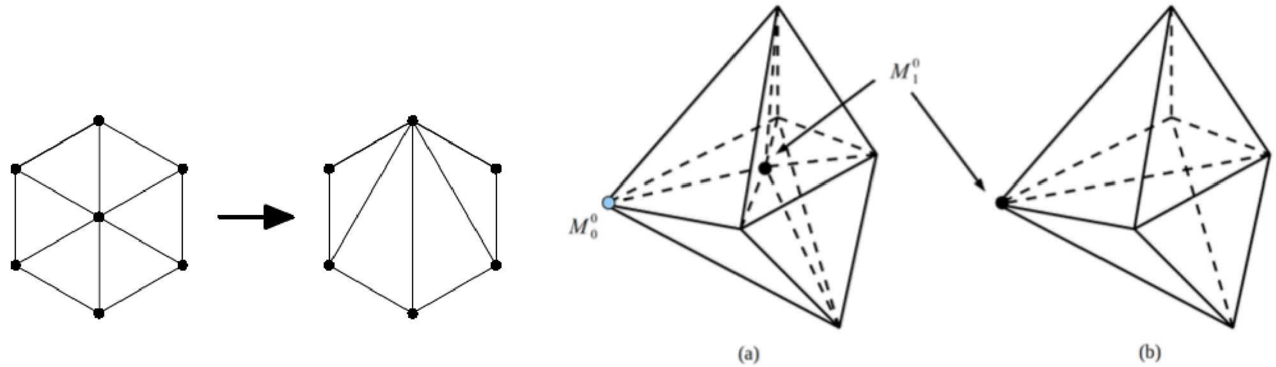
$$\boldsymbol{\sigma} := -\hat{p}(\rho, \epsilon)\mathbf{I} + \boldsymbol{\sigma}_{\mathrm{dev}} + \boldsymbol{\sigma}_{\mathrm{art}}$$

Adaptivity: Local Cavity Modifications

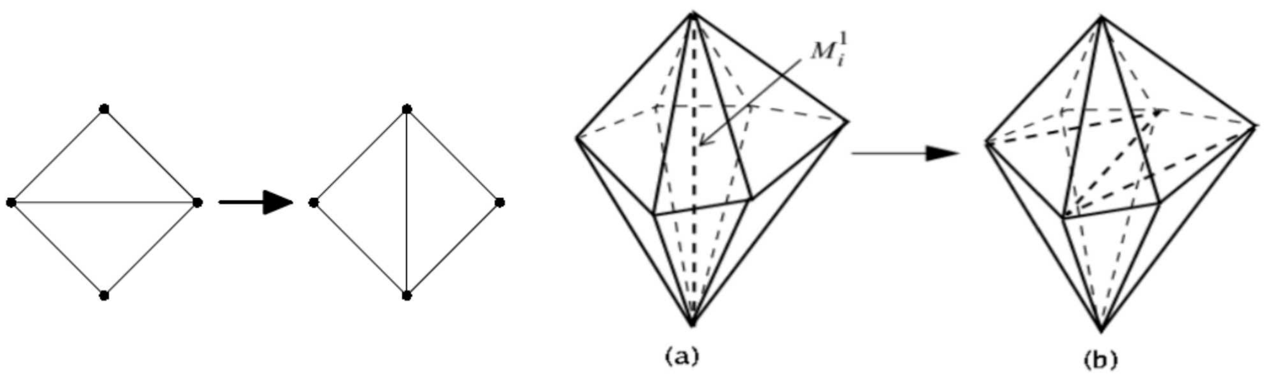
Split



Collapse



Swap



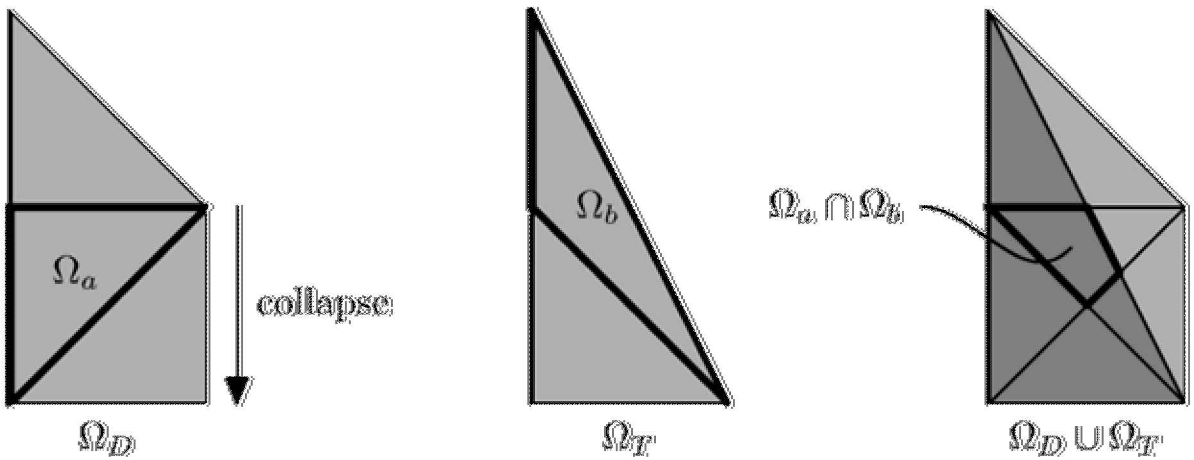
Adaptivity: Conserved cell-average quantities

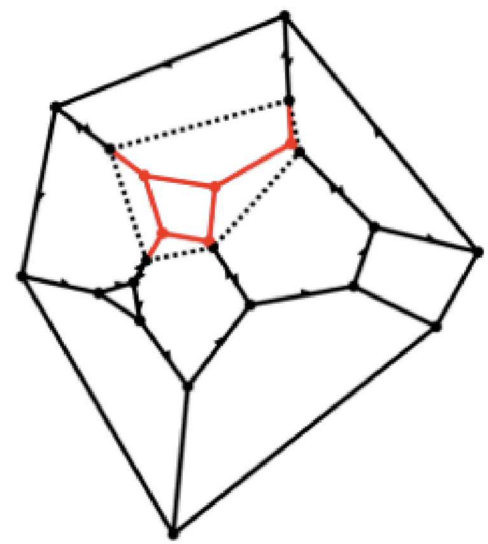
For refinement, simply divide by two, assign to child cells

Use R3D-based intersection remap on interior cavities

- Conservative and bounds-preserving

For curved boundary collapses, keep same density, record conservation error in "error field"





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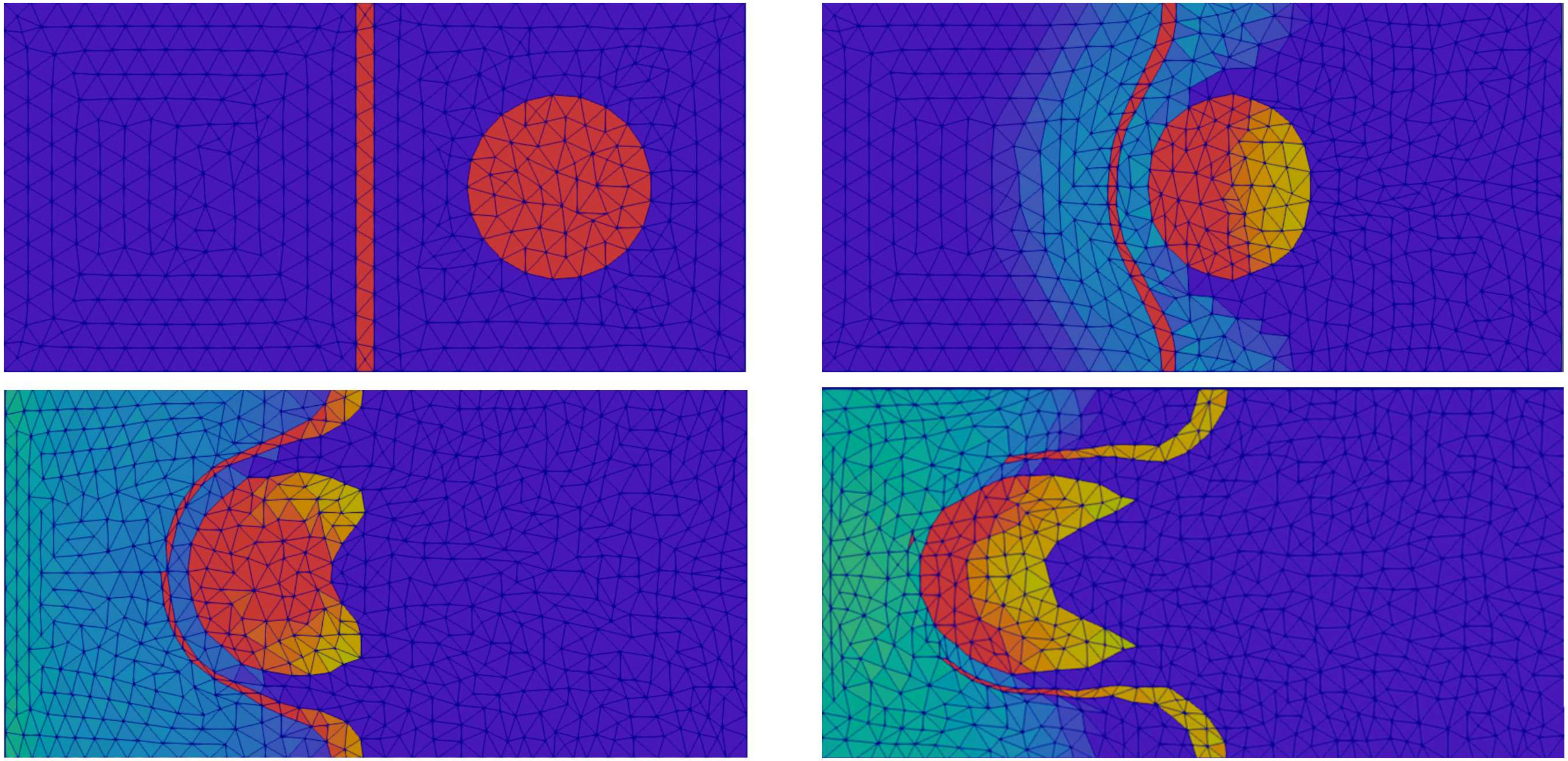
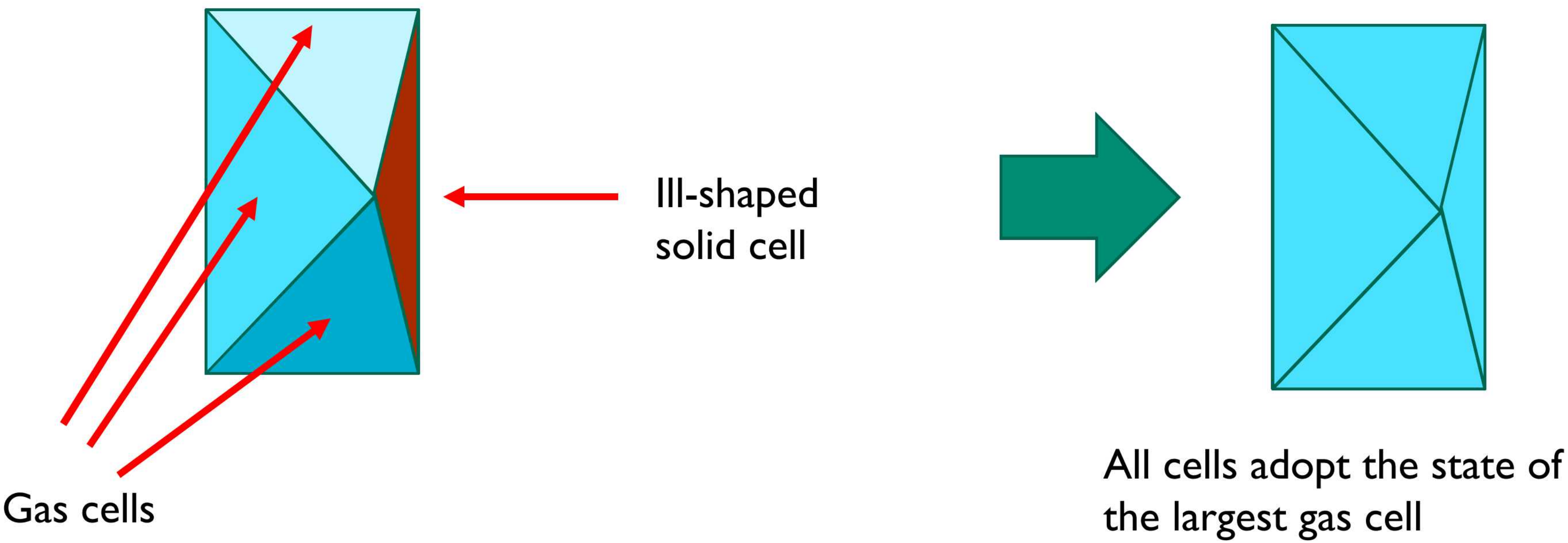
Recent development: Topology Change

- Always-conformal adaption is great, but…
- How to deal with fracture & collision?
- Elements compressed below very small size will be replaced with “background”



Topology Change: "Flooding"

- Our topology change algorithm is inspired by the paper:
  - Bernard, Étienne, et al. "Lagrangian method enhanced with edge swapping for the free fall and contact problem." *ESAIM: Proceedings*. Vol. 24. EDP Sciences, 2008.
- Étienne et al's algorithm is mass-conservative, ours is density-preserving but not mass-conservative
- Still follows the "cavity" idea: each node is considered a focal point for flooding

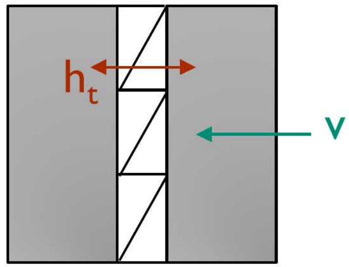


Topology Change: “Flooding”

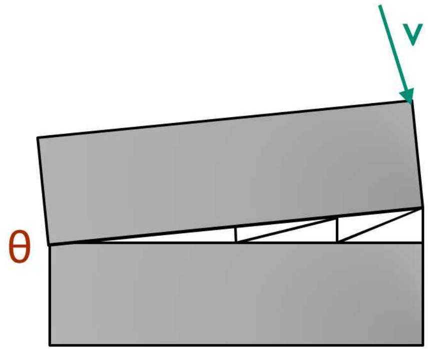
Adaptivity alone cannot always guarantee good element quality.

Examples:

- Elements of one material squeezed such that thinner than target h

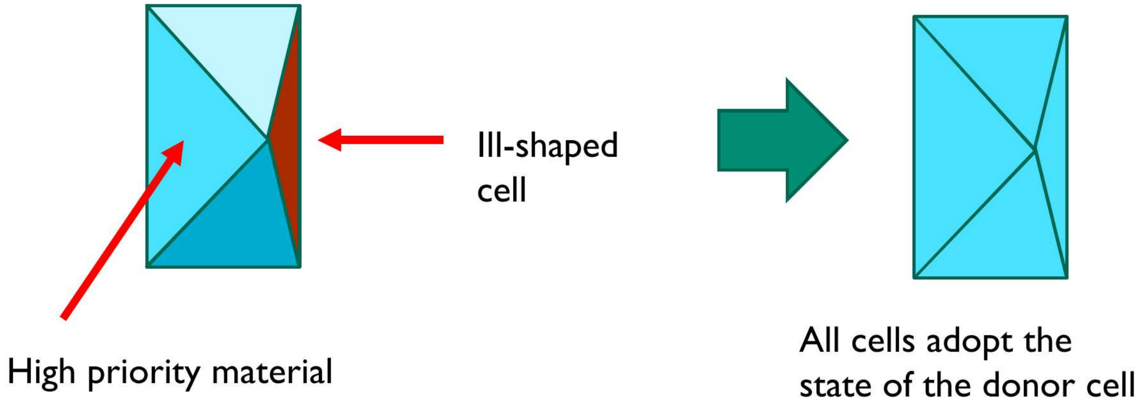


- Cavity collapsing drives angle to zero



Flooding algorithm

1. Take a Lagrangian time step (update positions, thermodynamic state, etc.)
2. Evaluate element quality metric $\eta_k = \left(\frac{V_k}{\gamma_k l_{k,RMS}^3}\right)^{2/3}$
3. For poor quality elements, adapt using split, collapse, swap
4. Remap cell centered and node centered quantities
5. If elements are still low quality
   i. Each node of the bad element defines a "cavity" that contains all elements connected to that node
   ii. Find the cavity with the highest priority "donor" material, use largest volume in case of ties
   iii. Replace bad element with donor element material & thermodynamic state

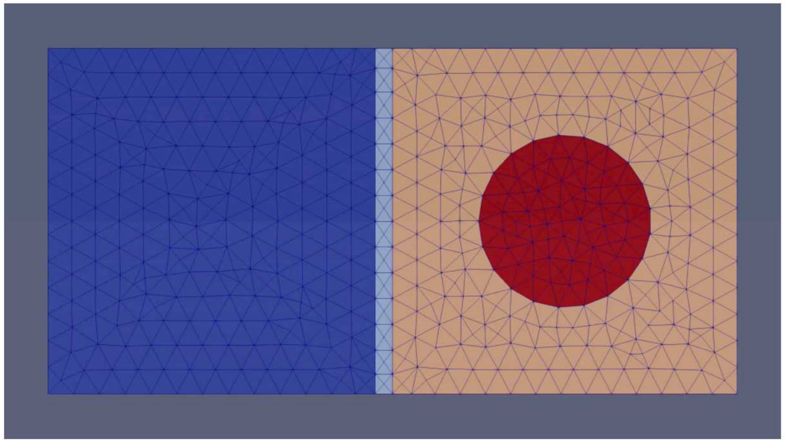


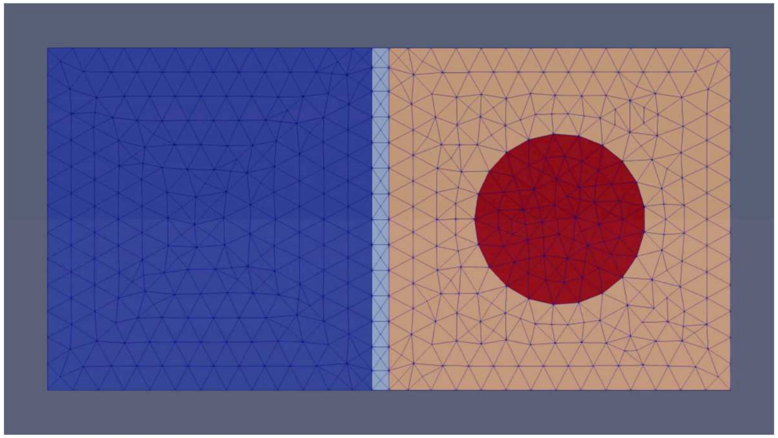
Why don't we conserve mass?

Because we don't conserve volume

- There is, in general, no upper bound on the density of new elements after flooding if mass is to be conserved
- Large increase in density leads to increase in pressure, spurious behavior
- Favor stable thermodynamic state over conservation

Flooding in action



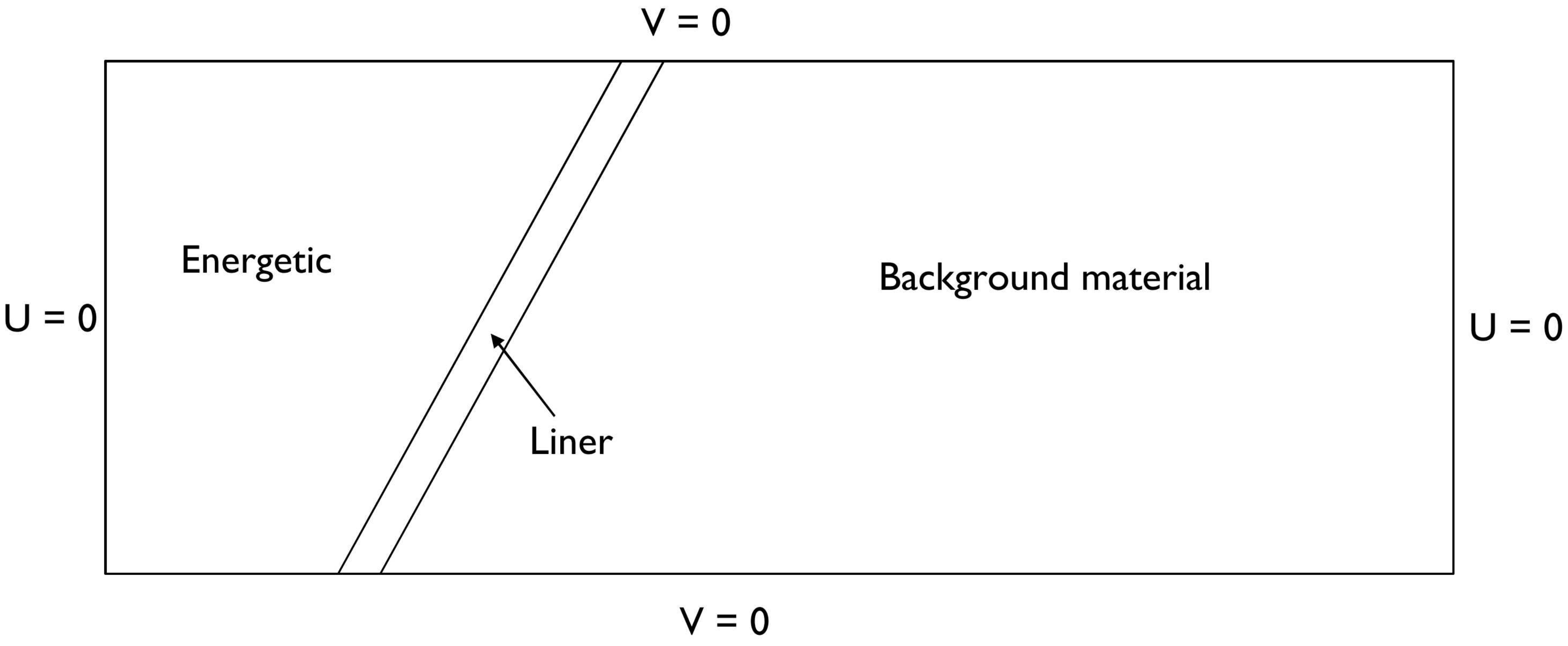


Linear Shape Charge Jet

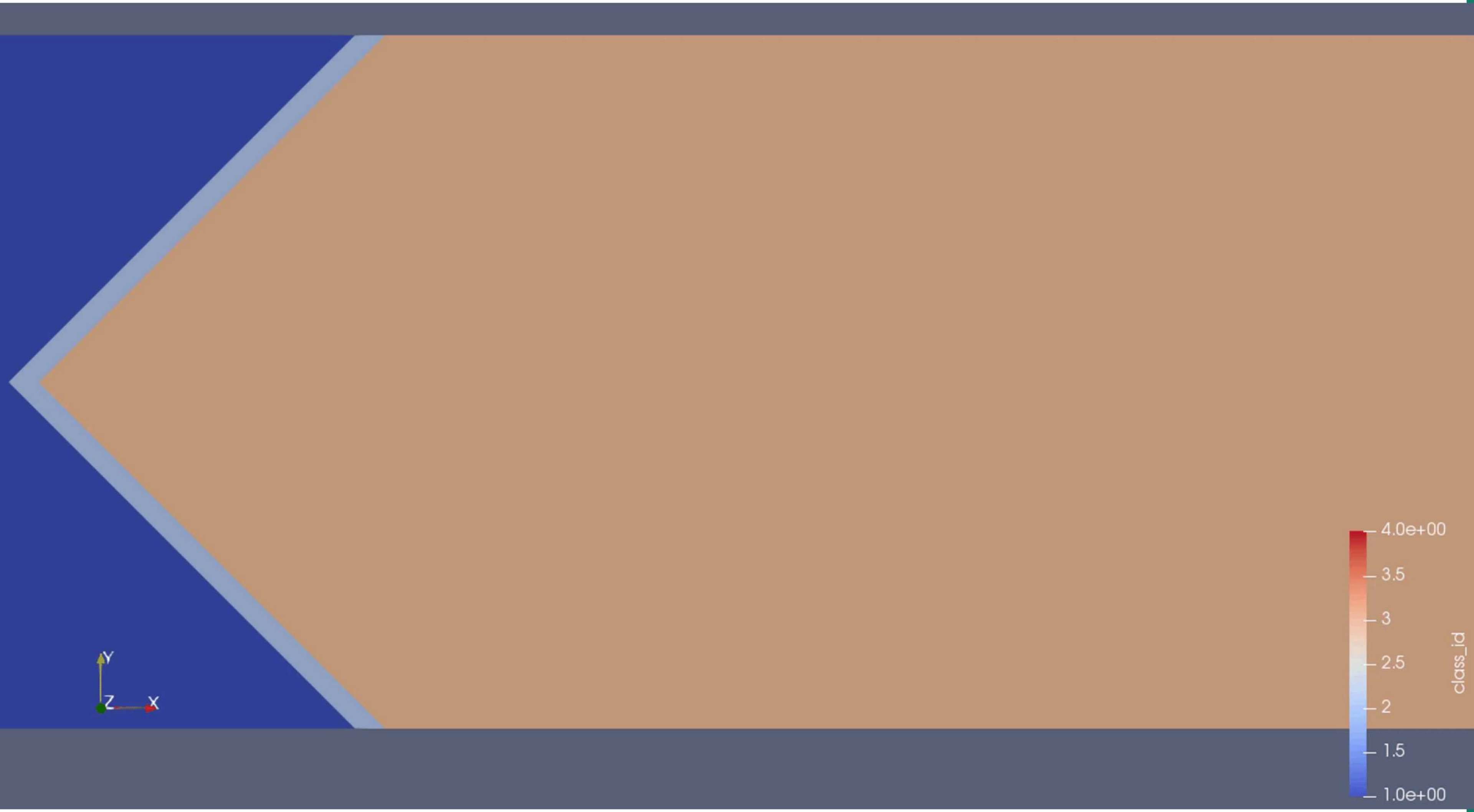
Energetic: Ideal gas with energy deposition

Liner: Copper, Mie-Gruneisen EOS, no strength (yet!)

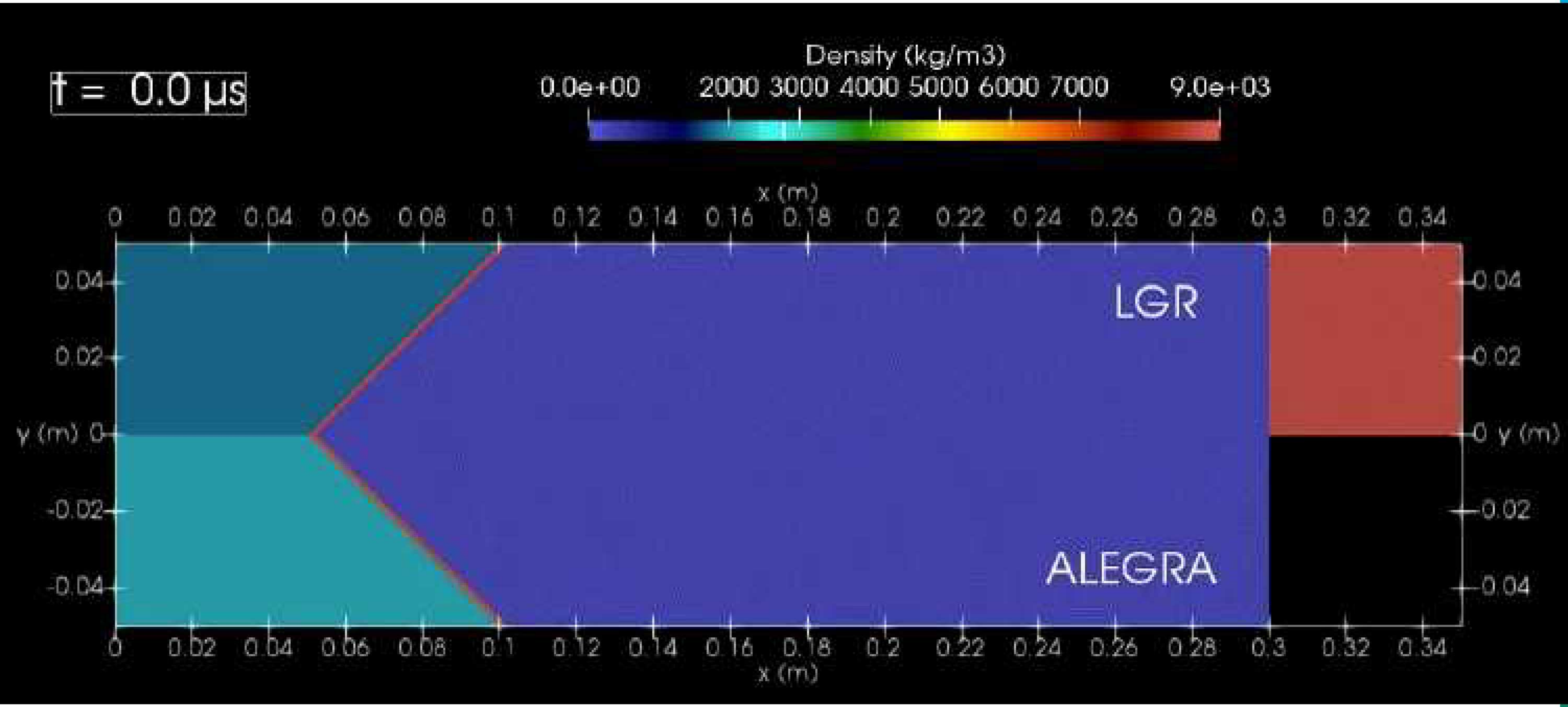
Background material: Air, ideal gas



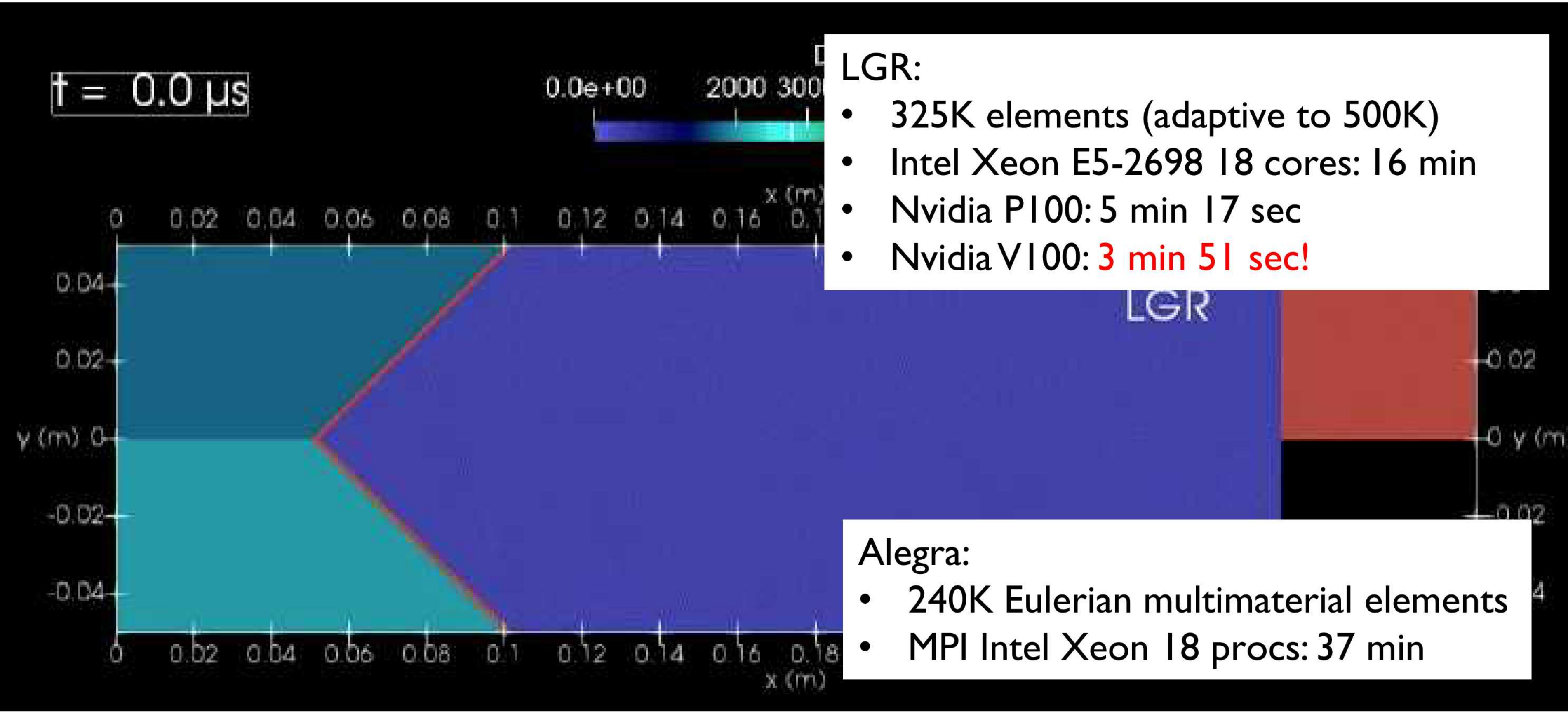
Jet Formation



Shaped Charge: Alegra vs LGR



Shaped Charge: Alegra vs LGR



LGR:

- 325K elements (adaptive to 500K)
- Intel Xeon E5-2698 18 cores: 16 min
- Nvidia P100: 5 min 17 sec
- Nvidia V100: 3 min 51 sec!

Alegra:

- 240K Eulerian multimaterial elements
- MPI Intel Xeon 18 procs: 37 min

Future work

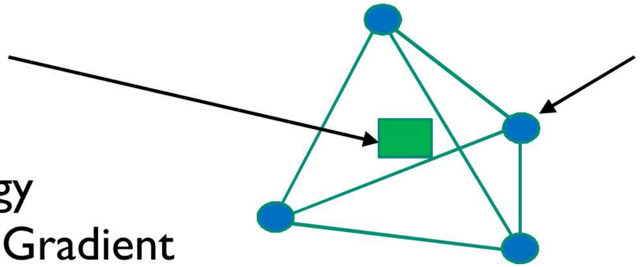
Thank you!

Extra Slides

Implementational details

Use *VMS four-node tetrahedral* elements (for now).

Cell-Centered:
- Density
- Internal Energy
- Deformation Gradient
- Pressure



Nodal:
- Displacement
- Velocity
- Pressure

Use *second order explicit predictor-corrector* time integration.

Tensor shock-capturing artificial viscosity.

Current material models:
- Ideal gas
- Mie-Gruneisen
- Neo-hookean thermo-elastic
- Mechanical multiplicative J-2 plasticity

VMS Formulation

- Conservation of linear momentum:

$$\langle \delta\boldsymbol{\varphi}^h, \rho\dot{\mathbf{v}}^h \rangle \; + \; \langle \text{grad}[\delta\boldsymbol{\varphi}^h], -p^h \rangle + \langle \text{grad}\delta\boldsymbol{\varphi}^h, \text{dev}\boldsymbol{\sigma} \rangle + \langle \text{grad}\delta\boldsymbol{\varphi}^h, -p' \rangle = 0 \quad \forall\boldsymbol{\varphi}^h$$

- Balance of internal energy:

$$\langle \delta\theta^h, \rho\dot{\varepsilon} \rangle - \langle \delta\theta^h, \text{grad}[\mathbf{v}] \bullet (-p^h\mathbf{I} + \text{dev}\boldsymbol{\sigma} - p'\mathbf{I}) \rangle = 0 \quad \forall\delta\theta^h$$

- Pressure projection:

$$\langle \eta^h, p^h \rangle - \langle n^h, p \rangle + \langle \text{grad}\eta^h, -\mathbf{u}' \rangle = 0 \quad \forall\eta^h$$

Multi-scale fields:

$$p' = -\tau(\dot{p}^h + \rho c^2 \text{div } \mathbf{v}^h)$$

$$\mathbf{v}' = -\frac{\tau}{\rho}\left(\rho\dot{\mathbf{v}}^h + \text{grad}p^h - \text{div}(\text{dev}\boldsymbol{\sigma})\right) \qquad \mathbf{u}' = \int_0^{\text{t}} \rho c^2 \mathbf{v}'(\text{t})\text{dt}$$

- The pressure-prime term is designed to stabilize zero-energy volume modes for materials without deviatoric response.

- The displacement-prime term is designed to stabilize the inf-sup condition for continuous nodal pressure element formulations.

- The goal is for this element to be applicable for both compressible gas dynamics (no zero-energy modes) and nearly incompressible elasticity simulations (no locking).

- Yes, that is a lot to ask of a single element formulation! Maybe too much…

$$\text{for}(\text{int } i = 0; i < 2; {+}{+}i)\{$$

Define $\boldsymbol{\sigma} := -p^h \mathbf{I} - p' + \boldsymbol{\sigma}_{\text{dev}}$

1. Update nodal velocity:

$$\left\langle \delta\boldsymbol{\varphi}^h, \rho(\mathbf{v}_{n+1}^{(i+1)} - \mathbf{v}_n) \right\rangle + \Delta\text{t} \left\langle \text{grad}[\delta\boldsymbol{\varphi}^h], \boldsymbol{\sigma}_{n+\frac{1}{2}}^{(i)} \right\rangle = 0$$

2. Update element-centered internal energy:

$$\left\langle \delta\theta^h, \rho(\varepsilon_{n+1}^{(i+1)} - \varepsilon_n) \right\rangle - \Delta\text{t} \left\langle \delta\theta^h, \text{grad}[\mathbf{v}_{n+\frac{1}{2}}^{(i+1)}] \bullet \boldsymbol{\sigma}_{n+\frac{1}{2}}^{(i)} \right\rangle = 0$$

3. Update nodal coordinates:

$$\mathbf{x}_{n+1}^{(i+1)} - \mathbf{x}_n - \Delta\text{t} \cdot \mathbf{v}_{n+\frac{1}{2}}^{(i+1)} = \mathbf{0}$$

4. Update deformation gradient, volume element, and spatial density.
5. Update element-centered material models.

Time Integration (continued)

6. Update nodal pressure field:

$$\left\langle \eta^h, p_{n+1}^{h(i+1)} \right\rangle - \langle \eta^h, p_{n+1}^{i+1} \rangle + \left\langle \text{grad}\eta^h, -\mathbf{u}'^{(i+1)}_{n+\frac{1}{2}} \right\rangle = 0$$

7. Update element-centered fine scale fields:

$$\mathbf{v}' := -\frac{\tau}{\rho^{(i+1)}_{n+\frac{1}{2}}} \left[\rho^{(i+1)}_{n+\frac{1}{2}} \left(\mathbf{v}^{(i+1)}_{n+1} - \mathbf{v}_n \right) \Delta \mathrm{t}^{-1} + \text{grad } p^{h(i+1)}_{n+\frac{1}{2}} \right]$$

$$\mathbf{u}'^{(i+1)}_{n+1} = \mathbf{u}'_n + \left[\rho^{(i+1)}_{n+\frac{1}{2}} c^{(i+1)^2}_{n+\frac{1}{2}} \right] (\mathbf{v}' \Delta \mathrm{t})$$

}

The sequence of steps here is explicitly designed to discretely conserve total energy.

$$V := \int \mathrm{d}^3\mathrm{x}$$

$$\mathbf{b}_A := \int \nabla N_A \, \mathrm{d}^3\mathrm{x}$$

$$h := \frac{1}{\sqrt{2}} \frac{V}{\sum_{A=0}^{3} (\mathbf{b}_A \bullet \mathbf{b}_A)}$$

$$h_{\mathrm{art}} := \max_{e=0,5} \|\mathbf{x}_{e_1} - \mathbf{x}_{e_0}\|$$

$$\mathbf{d} := \mathrm{symm}\,[\nabla \mathbf{v}]$$

$$c := \frac{\mathrm{d}p}{\mathrm{d}\rho}(\rho, \eta)$$

$$c_1 := \mathcal{O}(0.15) \qquad c_2 := \mathcal{O}(1.2)$$

$$\xi := \frac{h_{\mathrm{art}}}{h} \left[c_1 + c_2 \frac{h_{\mathrm{art}}}{c} |\mathrm{trace}(\mathbf{d})| \right]$$

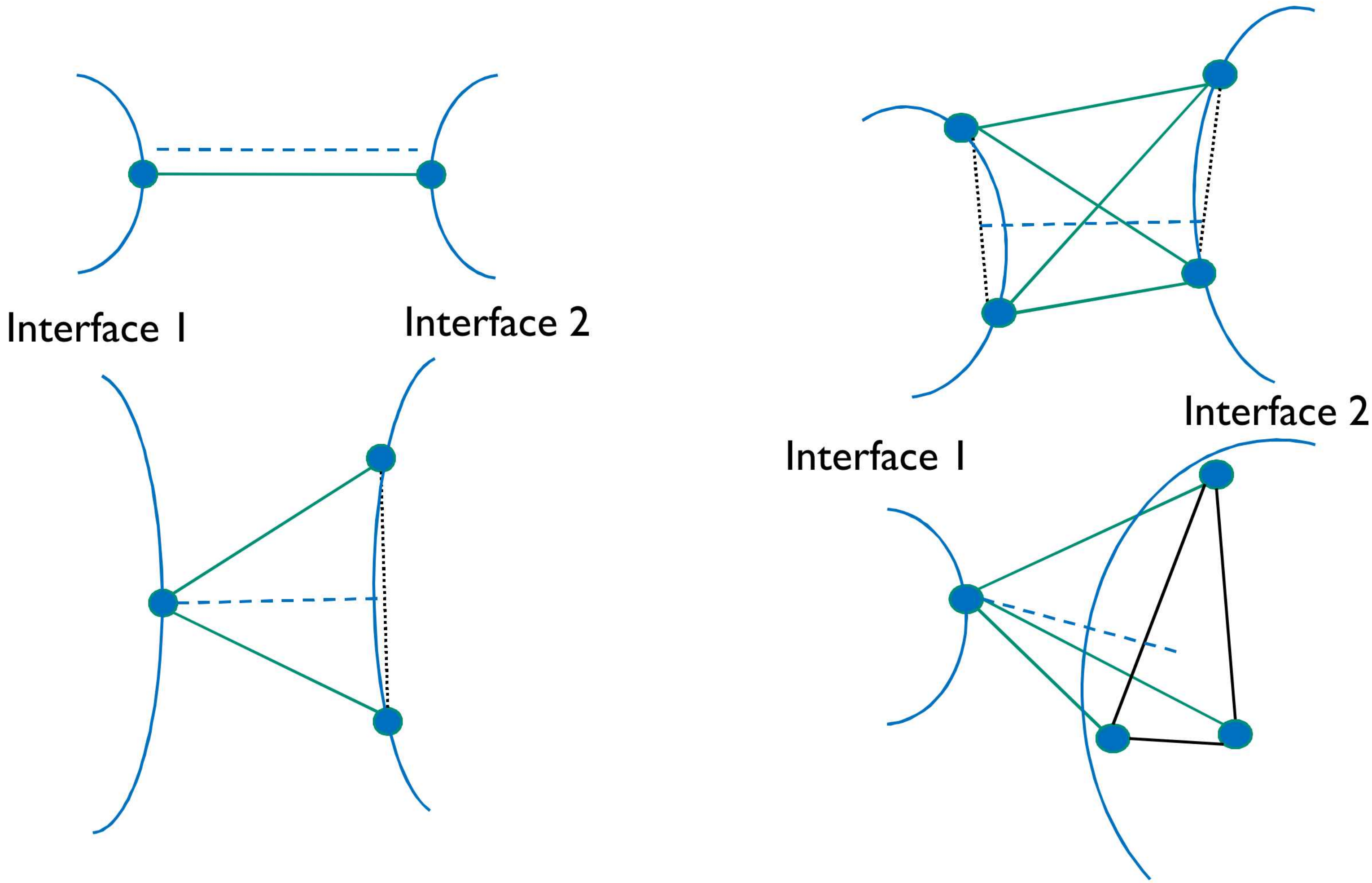
$$\Omega := \frac{2}{\sqrt{1 + \xi^2} + \xi}$$

$$\boxed{\boldsymbol{\sigma}_{\mathrm{art}} := \rho h_{\mathrm{art}} \left[c_1 c + h_{\mathrm{art}} c_2 \mathrm{trace}(\mathbf{d}) \right] \mathbf{d}}$$

$$\boxed{\Delta \mathrm{t} \leq \left(\frac{\Omega}{2} \right) \left(\frac{h}{c} \right)}$$

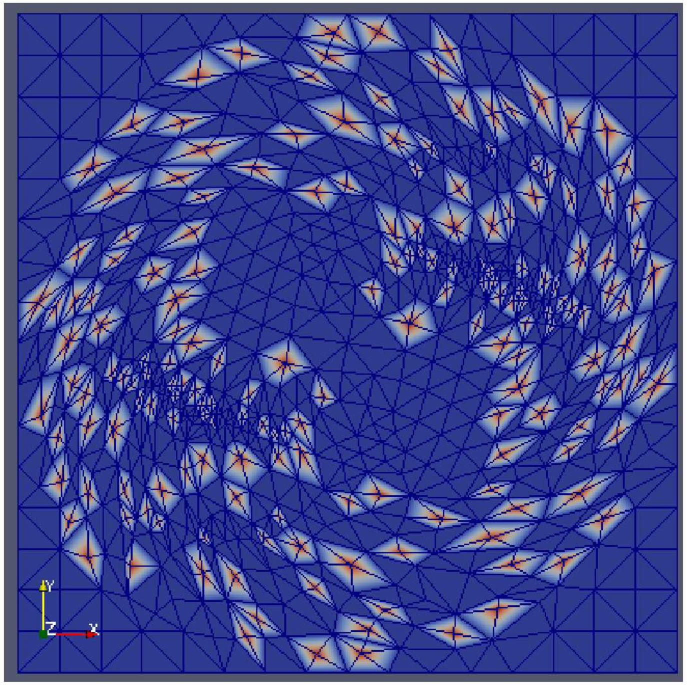
Two-Interface Proximity Detection

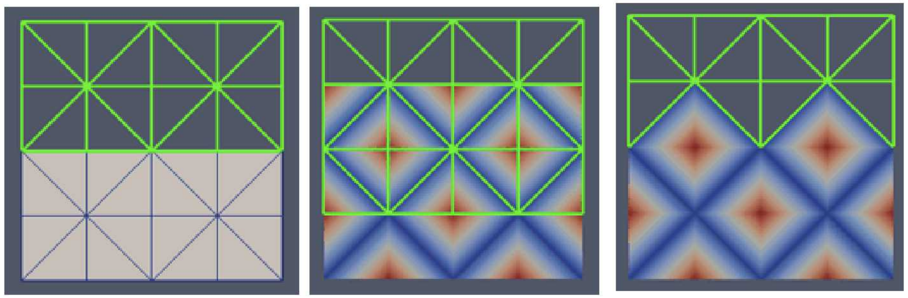
Measure shortest distance across single elements



One Round of Changes

- All of the same kind
- Non-overlapping (independent set)
- Runs in parallel with minimal and scalable communication
- Construct new mesh from old mesh
- Selection and modification are fully determinisitic
- Serial-parallel consistent!





Metric Tensor Field

- Symmetric Positive Definite tensor

$$\mathcal{M} = R^T \Lambda R,\ R^T R = I,\ \Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_d),\ \forall i \in [1, d] : \lambda_i > 0$$

- Exist linear transform(s) from real space to “metric space”

$$Q = \Lambda^{\frac{1}{2}} R,\ \Lambda^{\frac{1}{2}} = \mathrm{diag}(\sqrt{\lambda_1}, \ldots, \sqrt{\lambda_d})$$

- Defines an inner product, transform-then-dot

$$\mathbf{u}^T \mathcal{M} \mathbf{v} = \mathbf{u}^T R^T \Lambda R \mathbf{v} = \mathbf{u}^T R^T \Lambda^{\frac{1}{2}} \Lambda^{\frac{1}{2}} R \mathbf{v} = \mathbf{u}^T Q^T Q \mathbf{v} = (Q\mathbf{u})^T (Q\mathbf{v}) = \tilde{\mathbf{u}}^T \tilde{\mathbf{v}}$$

- Defines an ellipsoid of desired resolution in each direction

F. Alauzet and P. Frey
Estimateur d’erreur géométrique et métriques anisotropes pour l’adaptation de maillage.
Partie I : aspects théoriques