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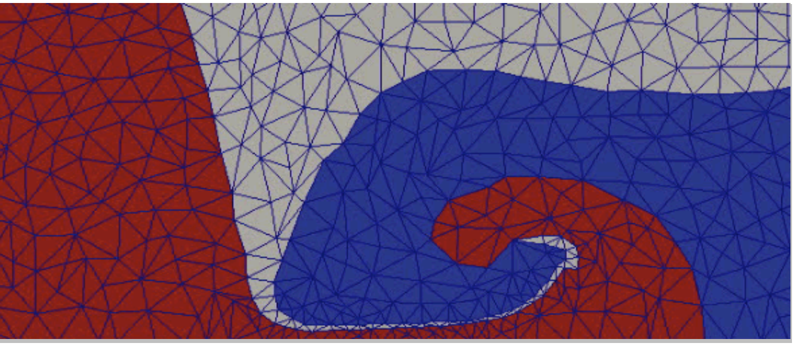
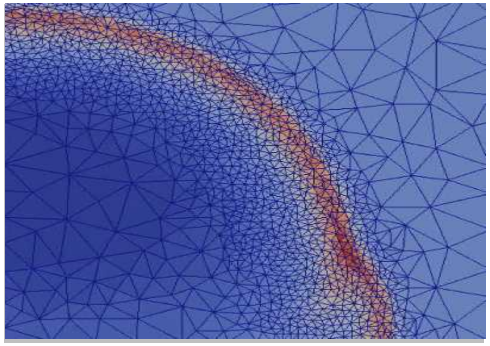
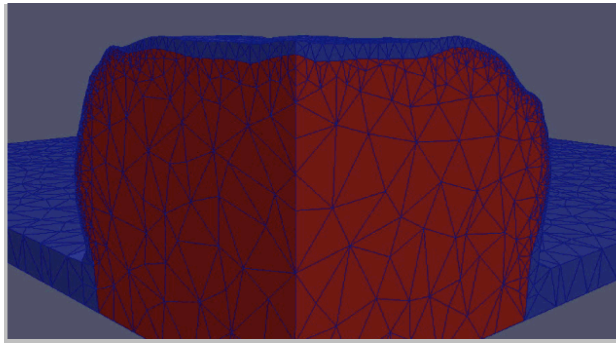

Alexa: MPI+X Shock Hydrodynamics on Dynamically Adaptive Tetrahedral Meshes

G. Hansen, D. Ibanez, E. Love, J. Overfelt,
N. Roberts and T. Voth MULTIMAT 2017

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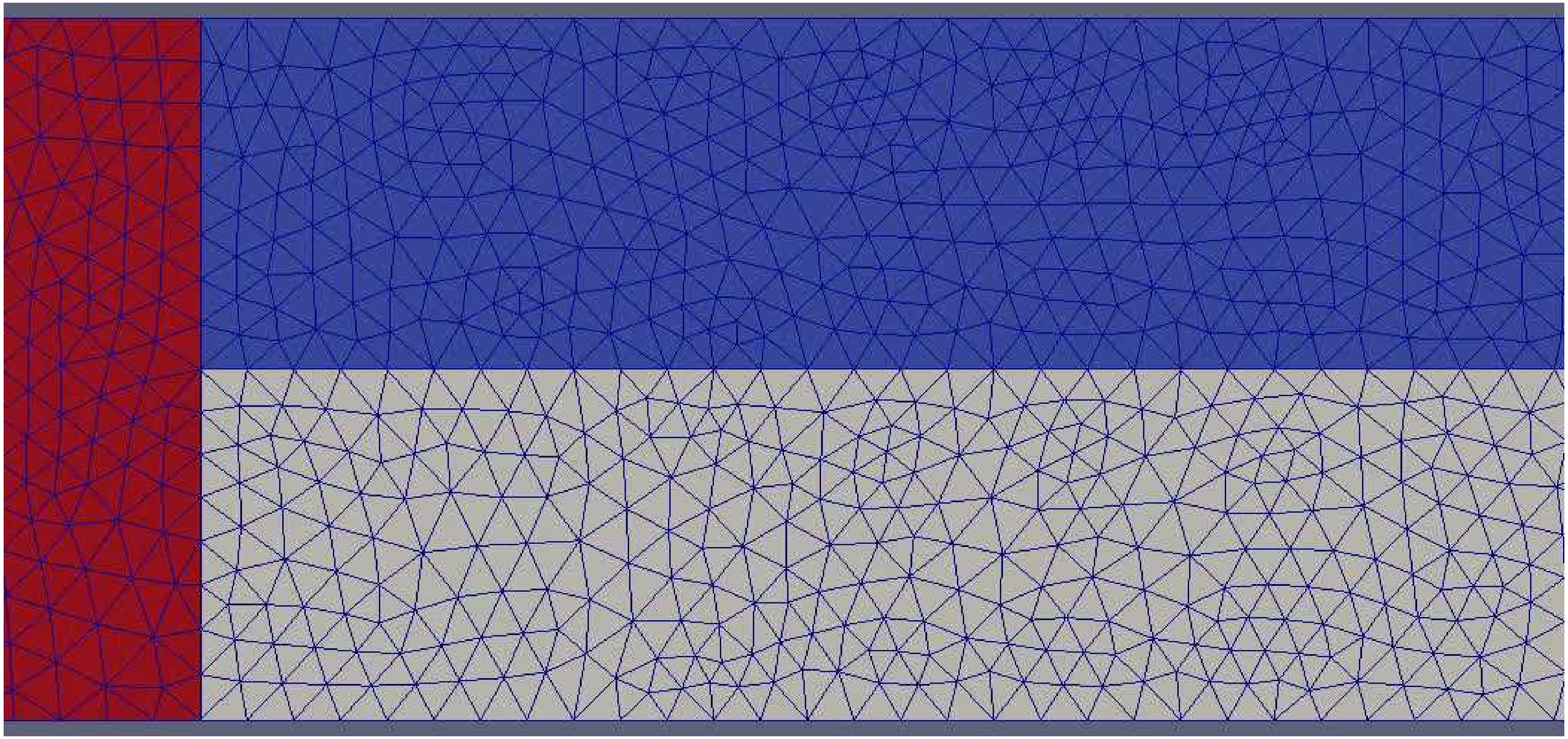
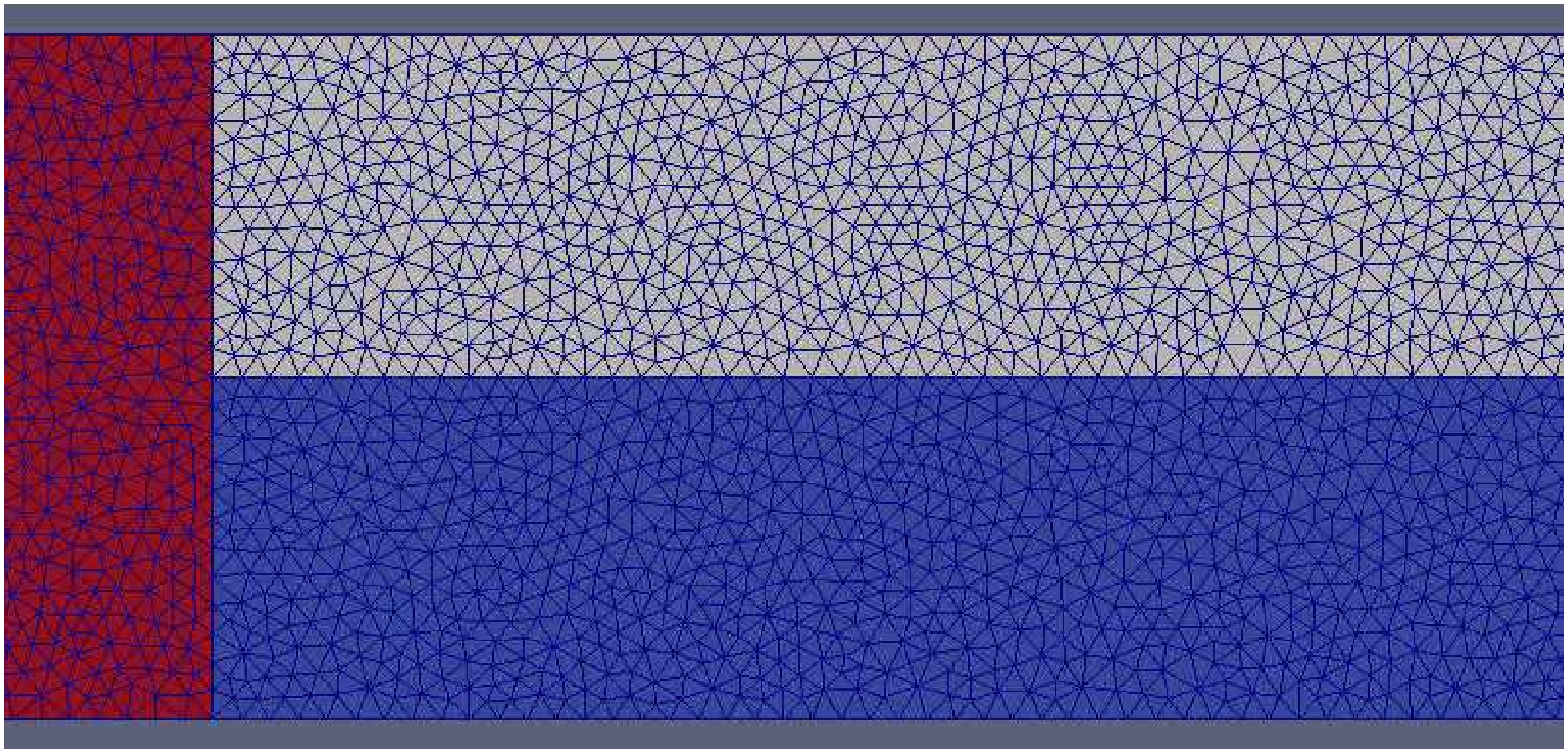
Alexa

- Portably Performant: runs efficiently on most modern hardware, especially NVIDIA GPUs
- Adaptive Lagrangian: Like ALE (Arbitrary Lagrangian-Eulerian) except no Eulerian component, does adaptation (remeshing) by local modification, maintains single-material elements
- Shock Hydrodynamics: Compressible gases, elastic and plastic solids, and more material models combined to form true multi-material simulations
- All in 3D!

Pure Lagrangian Triple-Point



Adaptive Lagrangian Triple-Point



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:

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

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

- Conservation of mass:

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

- Constitutive model:

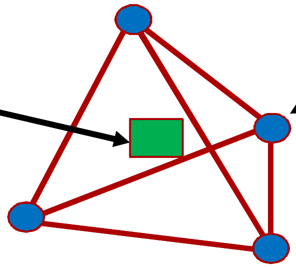
$$\boldsymbol{\sigma} := -\hat{p}(\rho, \epsilon)\mathbf{I} + \boldsymbol{\sigma}_{\mathrm{dev}} + \boldsymbol{\sigma}_{\mathrm{art}}$$

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*.
- Limited number of 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:

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

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

VMS Formulation

- 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…

Time integration

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

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:

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

7. Update element-centered fine scale fields:

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

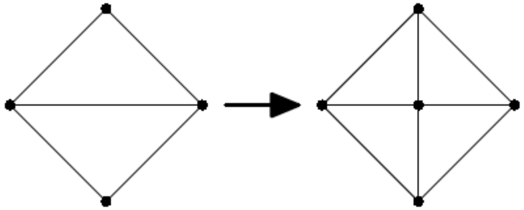
$$\mathbf{u}'^{(i+1)}_{n+1} = \mathbf{u}'_n + \left[\rho_{n+\frac{1}{2}}^{(i+1)} {c_{n+\frac{1}{2}}^{(i+1)}}^2 \right] (\mathbf{v}' \Delta \mathrm{t})$$

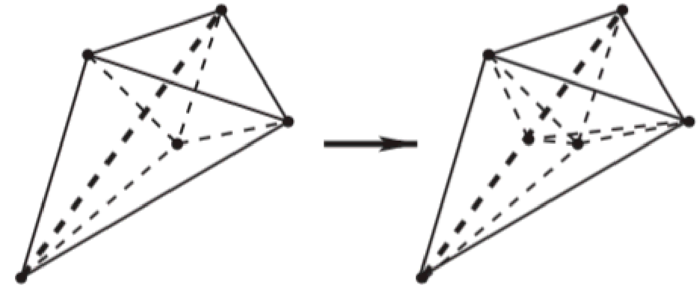
}

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

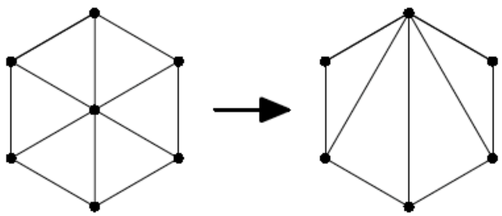
Local Cavity Modifications

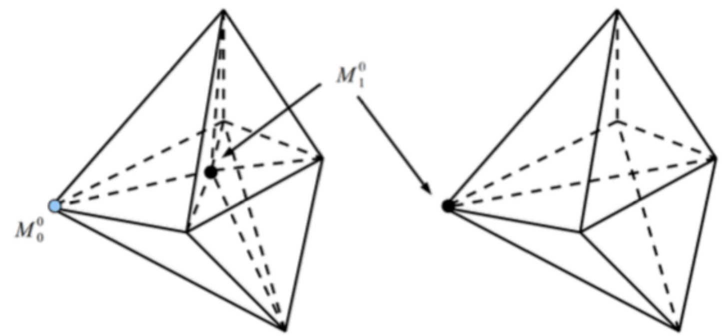
- Split





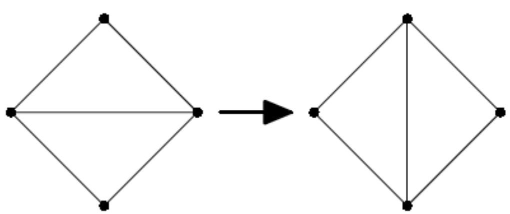
- Collapse

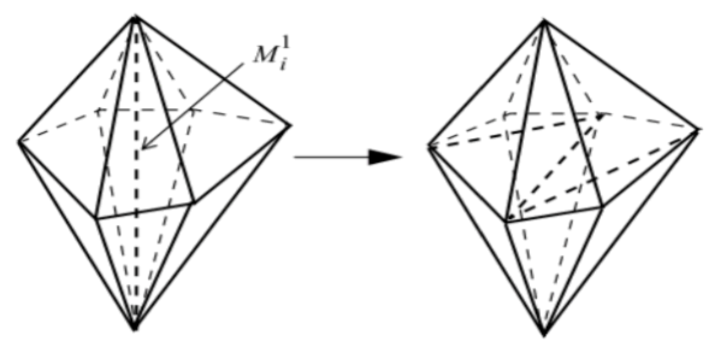




(a) (b)

- Swap





(a) (b)

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"

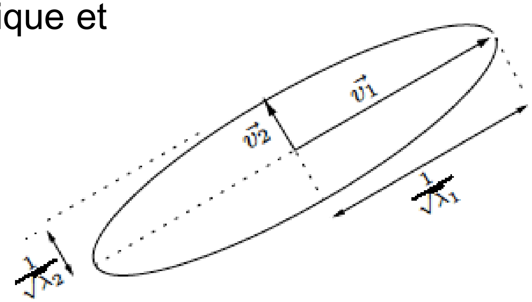
$$Q = \Lambda^{\frac{1}{2}} R,\ \Lambda^{\frac{1}{2}} = \mathrm{diag}(\sqrt{\lambda_1}, \ldots, \sqrt{\lambda_d})$$

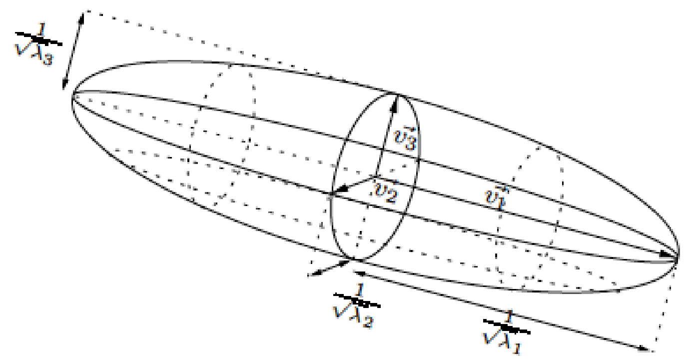
- Defines an inner product, transform-then-dot

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

- Defines an ellipsoid of <u>desired resolution in each direction</u>

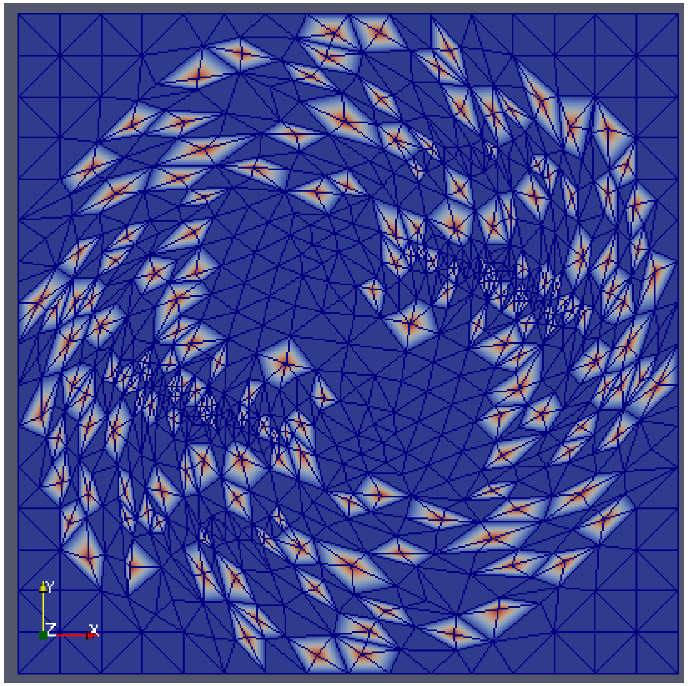
F. Alauzet and P. Frey
Estimateur d'erreur géométrique et métriques anisotropes pour l'adaptation de maillage.
Partie I : aspects théoriques

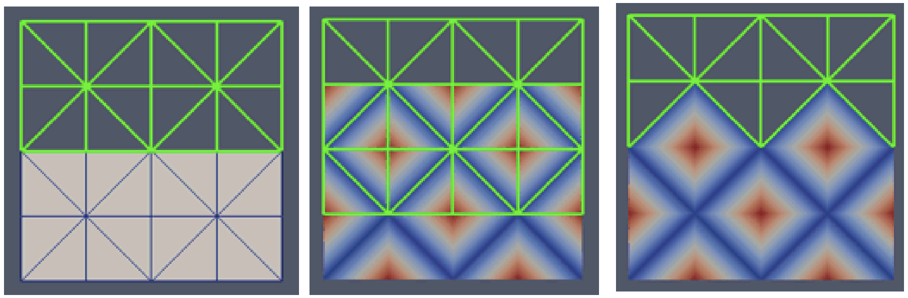




One Round of Changes

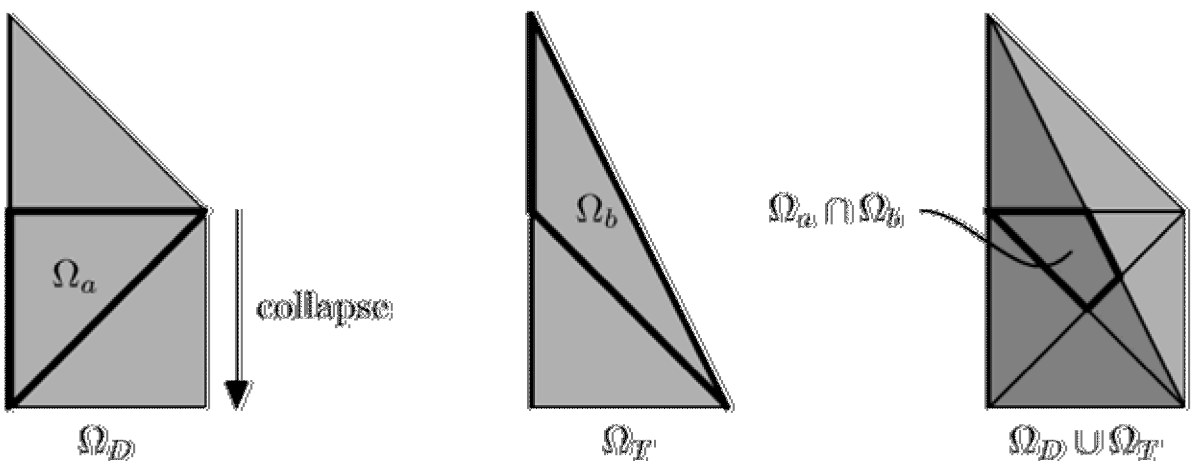
- All of the same kind
- Non-overlapping (independent set)
- Runs in parallel with minimal and scalable communication
- Construct new mesh from old mesh
- Selection and modification are fully determinisitic
- Serial-parallel consistent!

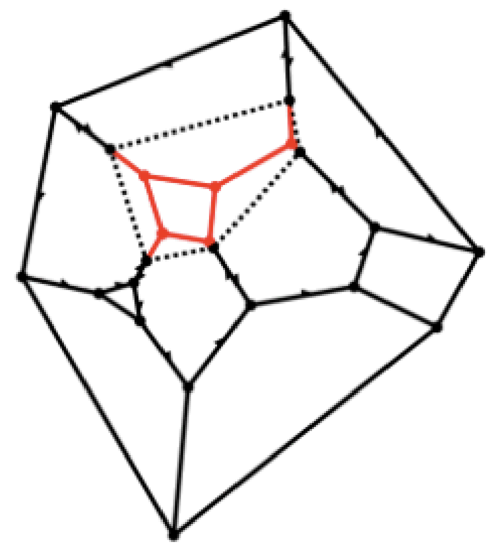




Conserved cell-average quantities

- For refinement, simply divide by two, assign to child cells
- Use R3D-based intersection remap on interior cavities
  - Conservative and bounds-perserving
- For curved boundary collapses, keep same density, record conservation error in “error field”





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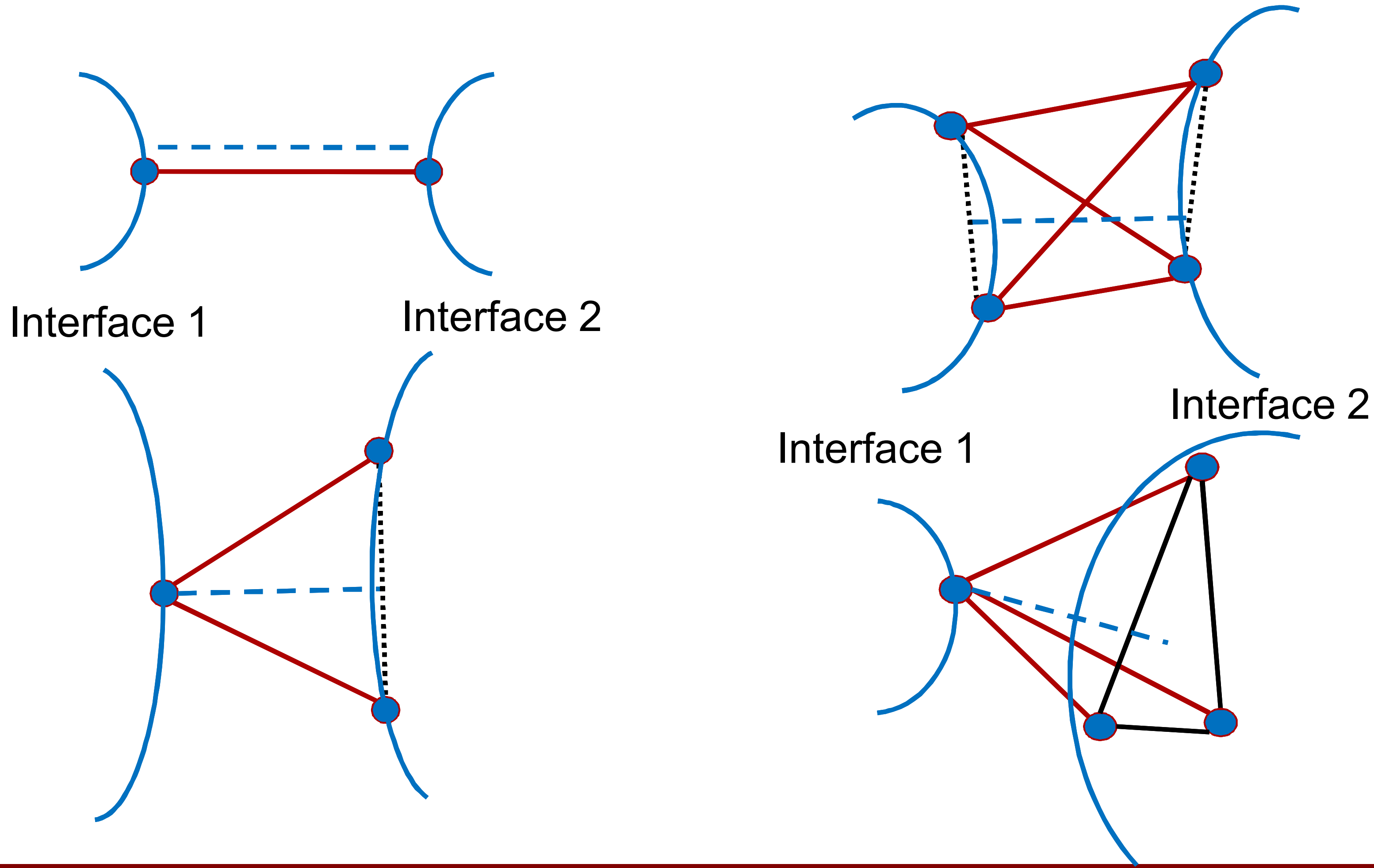
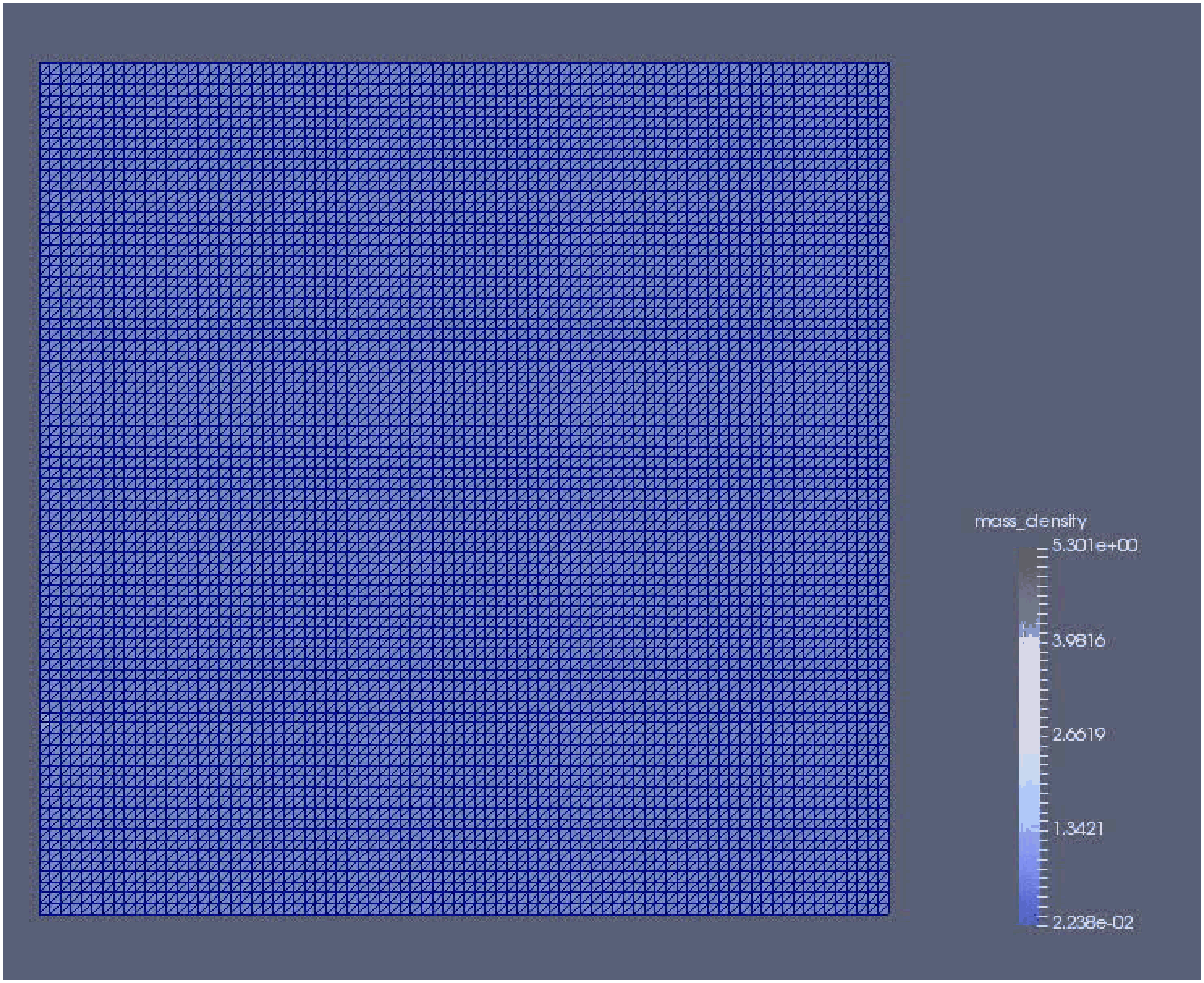
Two-Interface Proximity Detection

- Measure shortest distance across single elements

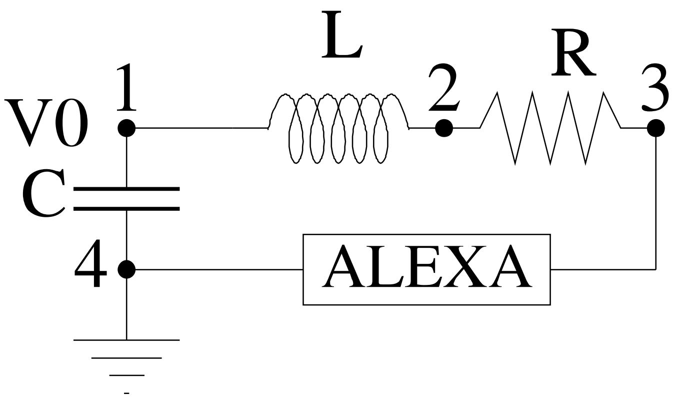


Airblast



Low-Rm MHD (Joule Heating)

- We model a circuit with Joule heating connected to our mesh.
- We allow an RLC circuit, and a scalar conductivity σ.



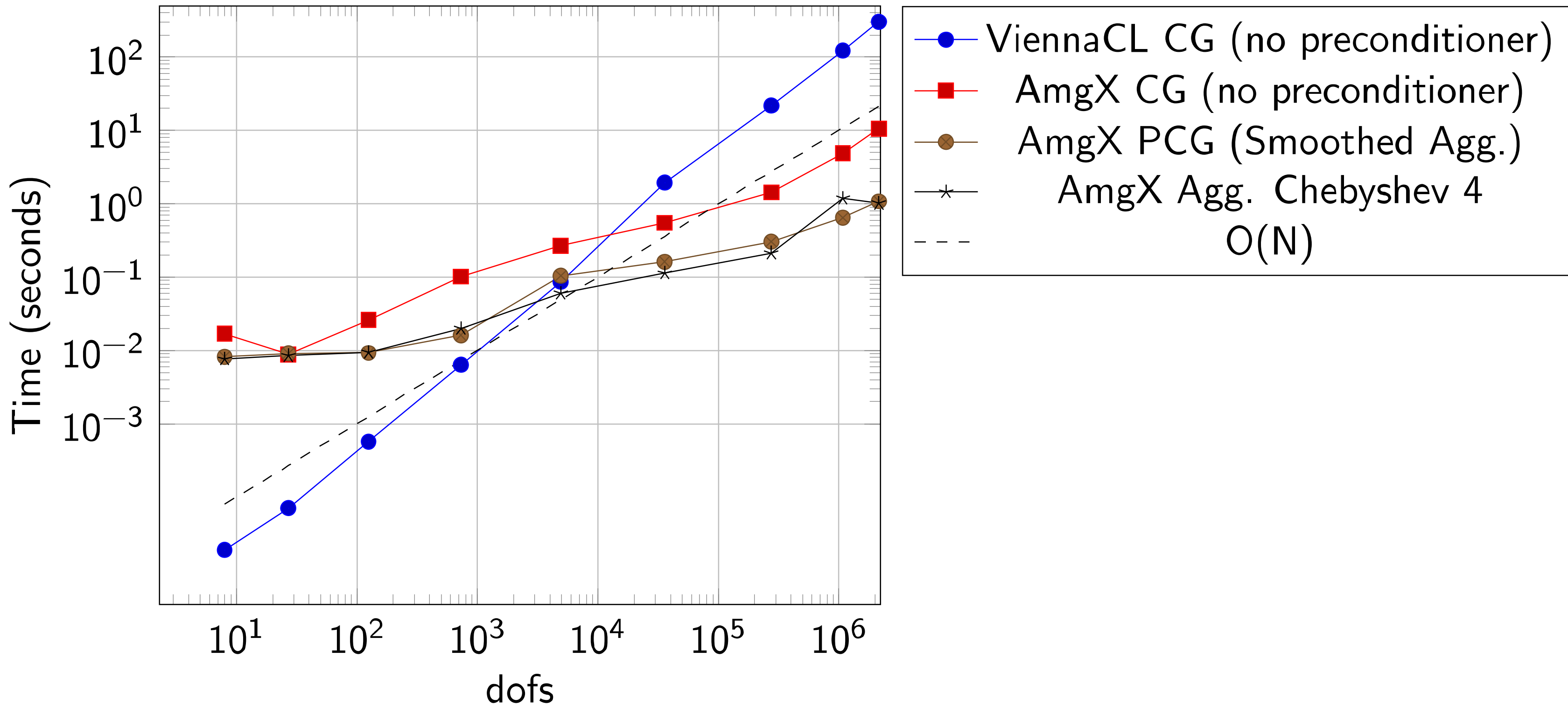
- Computationally intensive part of this is the Poisson solve:

$$(\nabla\phi, \sigma\nabla v)_\Omega = (f, v)_\Omega \quad \forall v$$

To gauge performance on a problem that approximates the physics of interest, we use a high-contrast $\sigma = (10^6 - 1)x^2 + 1$ and solve on $\Omega = [0, 1]^3$. We use GPU-accelerated solvers a single NVIDIA P100.

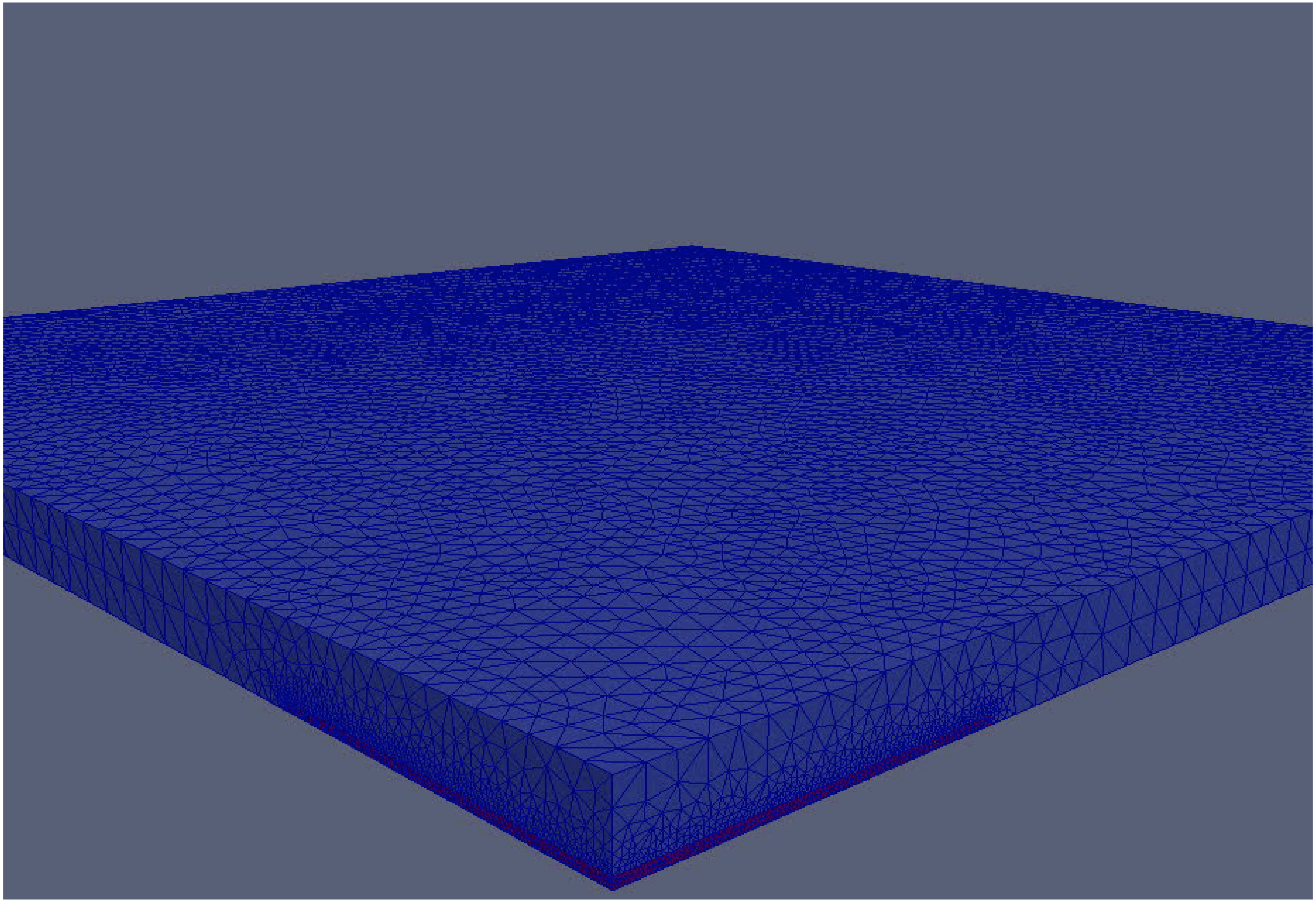
Higher-Contrast Poisson: Timings

White P100 3D FEM (higher-contrast Poisson), performance comparison



Convergence criterion: reduce residual by factor of 10^{-10}.

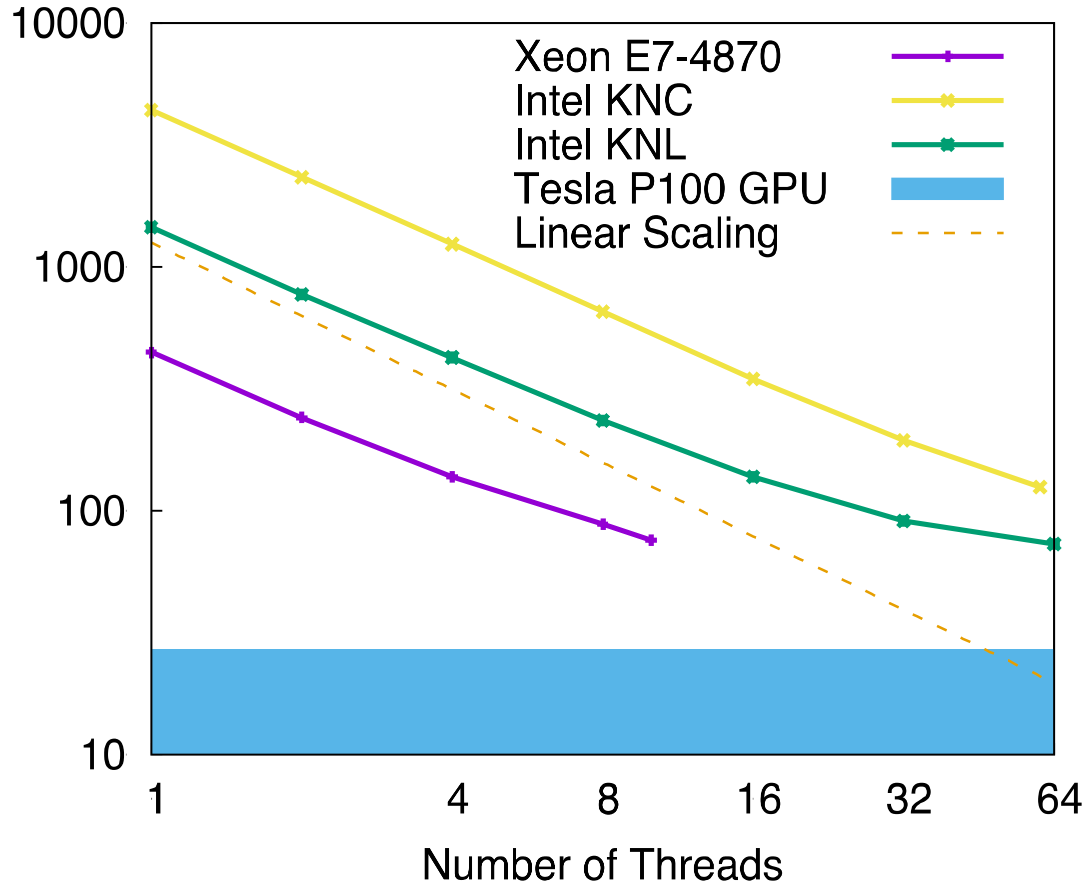
Electrified Foil



Performance Portability

- Kokkos is used for on-node parallelism
- Good performance across Intel Xeon Phi and NVIDIA cards

Time (seconds)
to run electrified foil
problem using 1M tets



Thank You

... Questions ?

Glen Hansen

Dan Ibanez

Ed Love

James Overfelt,

Nate Roberts

Tom Voth