Parallel ReALE Calculations of Large-Scale Multimaterial Problems

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Overview

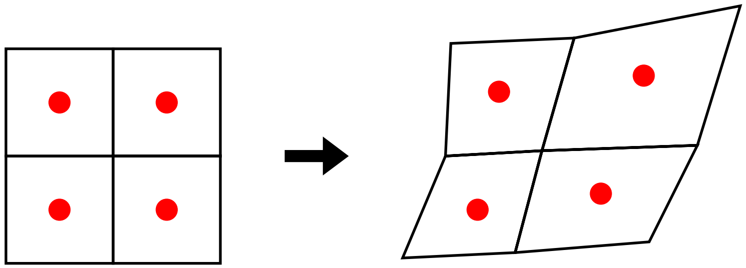
- ReALE Background
  - Code decisions and integration
- Reconnection
  - Mesh optimization
  - Generator motion
- Numerical Findings
  - Reconnection in Sedov and Triple Point Problems
- Code Capabilities and Results
- Future Work

ReALE is a 3-stage remap procedure

Lagrangian Stage

- Update state with your favorite hydro scheme
- Generators move with local Lagrangian velocity

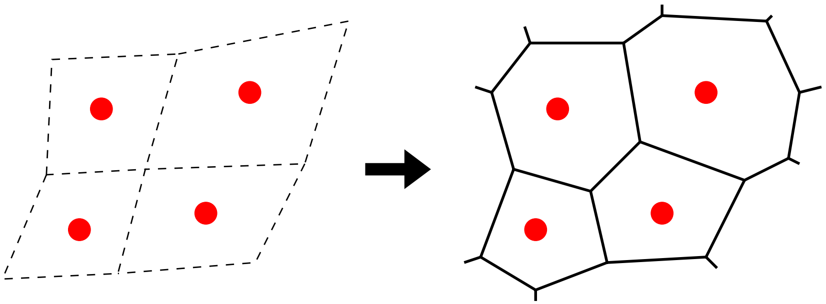
Requirement: Hydro scheme on arbitrary polygons



Rezone Stage

- Generators create new mesh elements
- Mesh topology changes

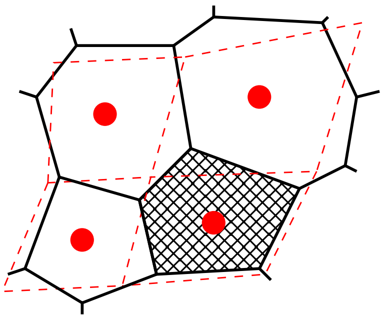
Requirement: Tool for generating Voronoi mesh data



Remap Stage

- Geometric overlay from post-Lagrange mesh to Voronoi mesh
- Volume-based, polygon-polygon intersections

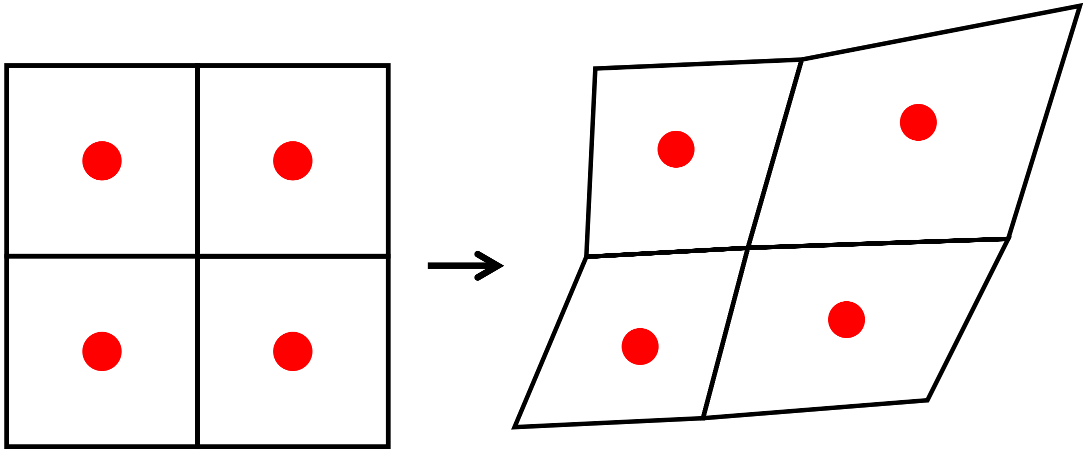
Requirement: Geometric overlay tool



Code Decisions: Lagrangian Stage

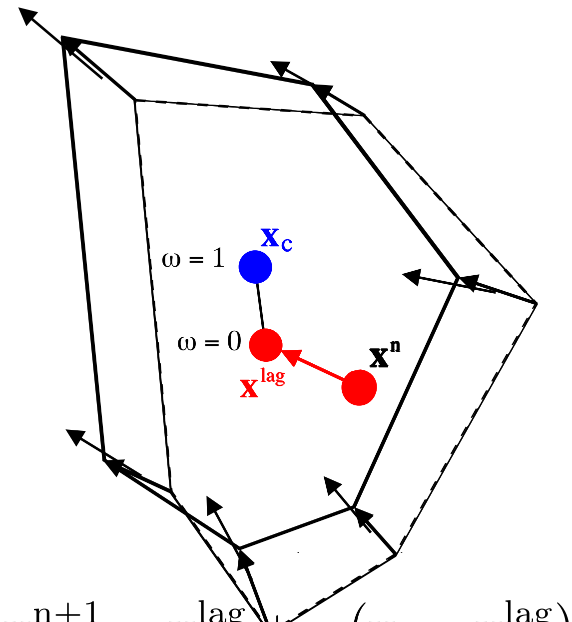
KULL Code

- LLNL ASC Code [Rathkopf et al, 2000]
- Production multi-physics code for ICF
- Compatible staggered Lagrange hydro formulation [Caramana et al, 1998]
- Caramana-Shashkov-Whalen edge-centered Q [Caramana et al, 1998]
- Energy conservative



Generator Motion

- Zone generator given time-centered Lagrangian velocity
- Average of nodal velocities around each zone
- Centroidal component applied generator motion to smooth



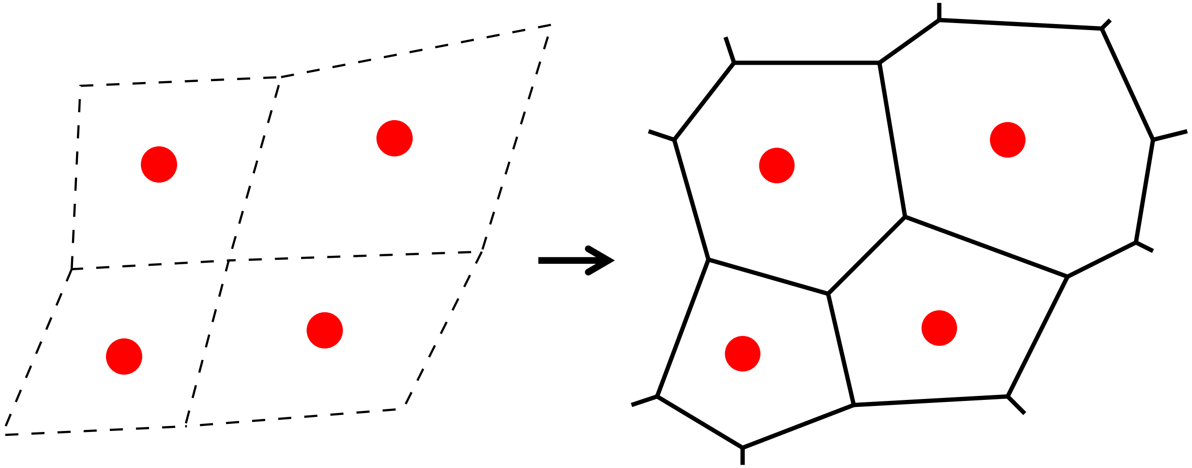
$$\mathbf{x}^{n+1} = \mathbf{x}^{lag} + \omega\left(\mathbf{x}_c - \mathbf{x}^{lag}\right)$$

NOTE: ω chosen to preserve Galilean invariance [Loubere et al, 2010]

Code Decisions: Rezone Stage

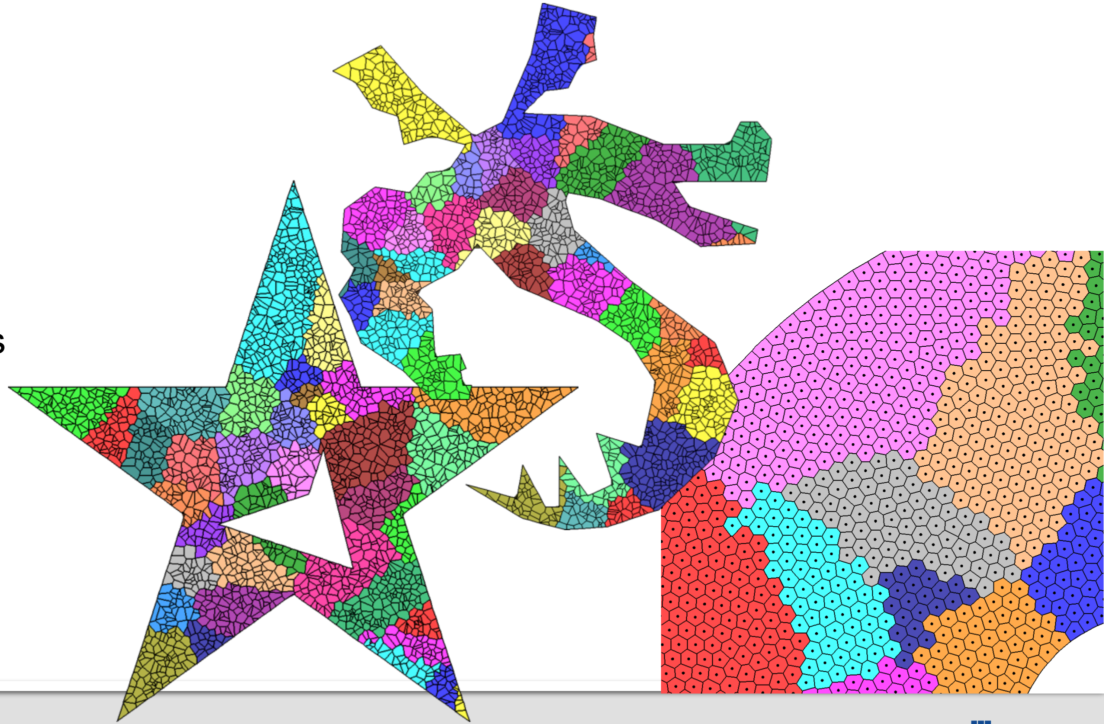
Polytope

- Open-source meshing software
  [Starinshak, Owen, Johnson, 2013]
- Generates unstructured meshes from Delaunay/Voronoi graphs
- See poster for more info



Parallelism

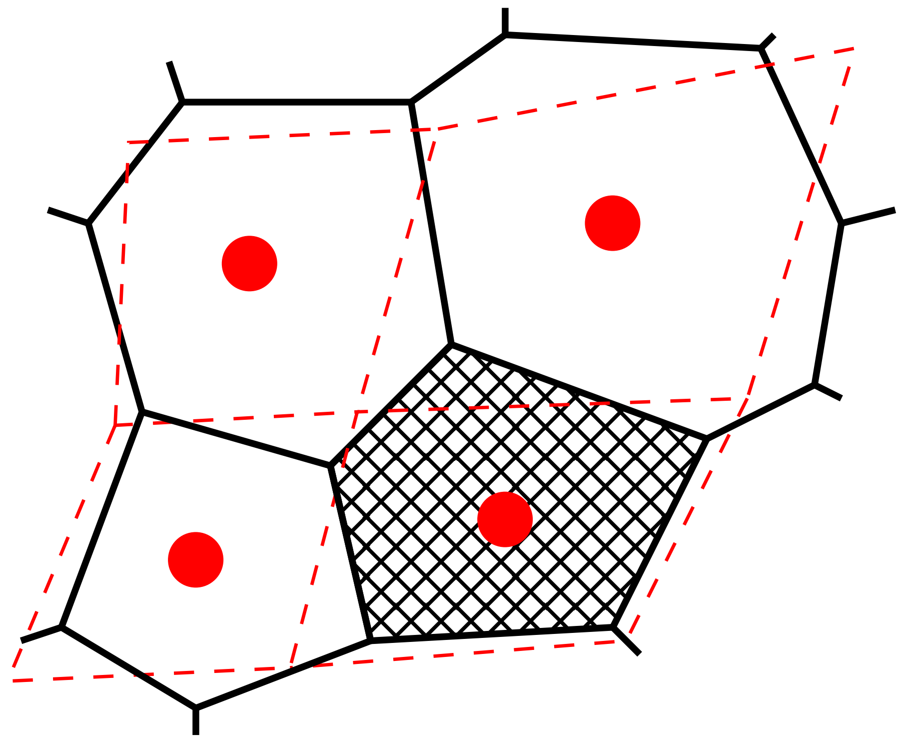
- The high bar for parallel ReALE
- Generators distributed across processors
- Mesh construction performed in parallel
- Communication data structures recomputed for each ReALE cycle



Code Decisions: Remap Stage

Overlink

- Second-order geometric overlay on polygonal/polyhedral grids [Grandy, 1999]
- Slope-limited linear reconstruction preserves monotonicity
- Supports zone- and node-centered quantities
- Multimaterial: supports mixed zones through material volume fractions



Parallelism

- Massively parallel (100,000+ cores)
- Uses communication structures of the donor and target meshes

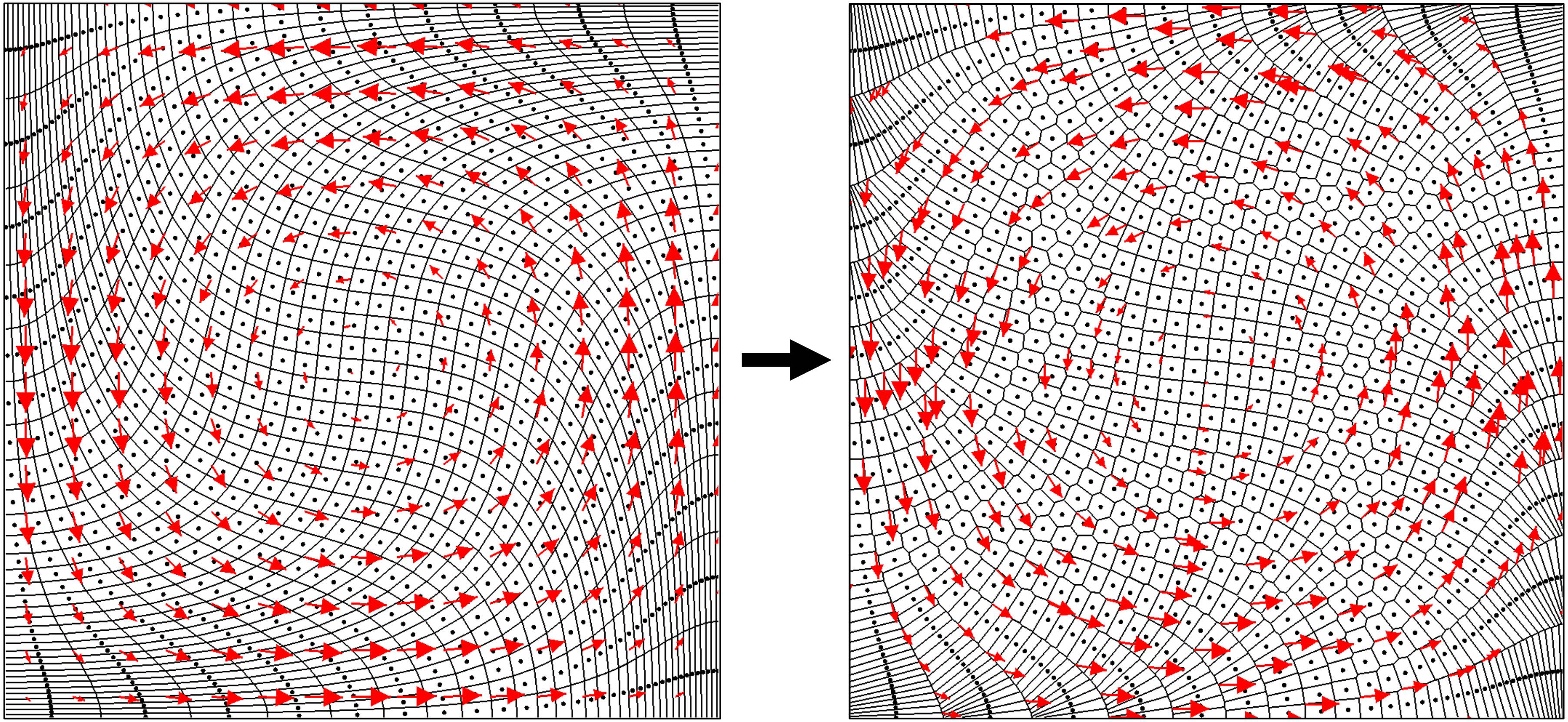
Momentum currently not conserved

- Compatible staggered hydro defines nodal mass using subzonal densities
- Subzonal quantities lack an (efficient) remap in Overlink
- We have a novel solution ready for testing (stay tuned…)

Rezoning Offers Many Attractive Properties

Mesh topology is not fixed

- Robust to tangling and locking
- Avoids mesh stiffness



Rezoning Offers Many Attractive Properties

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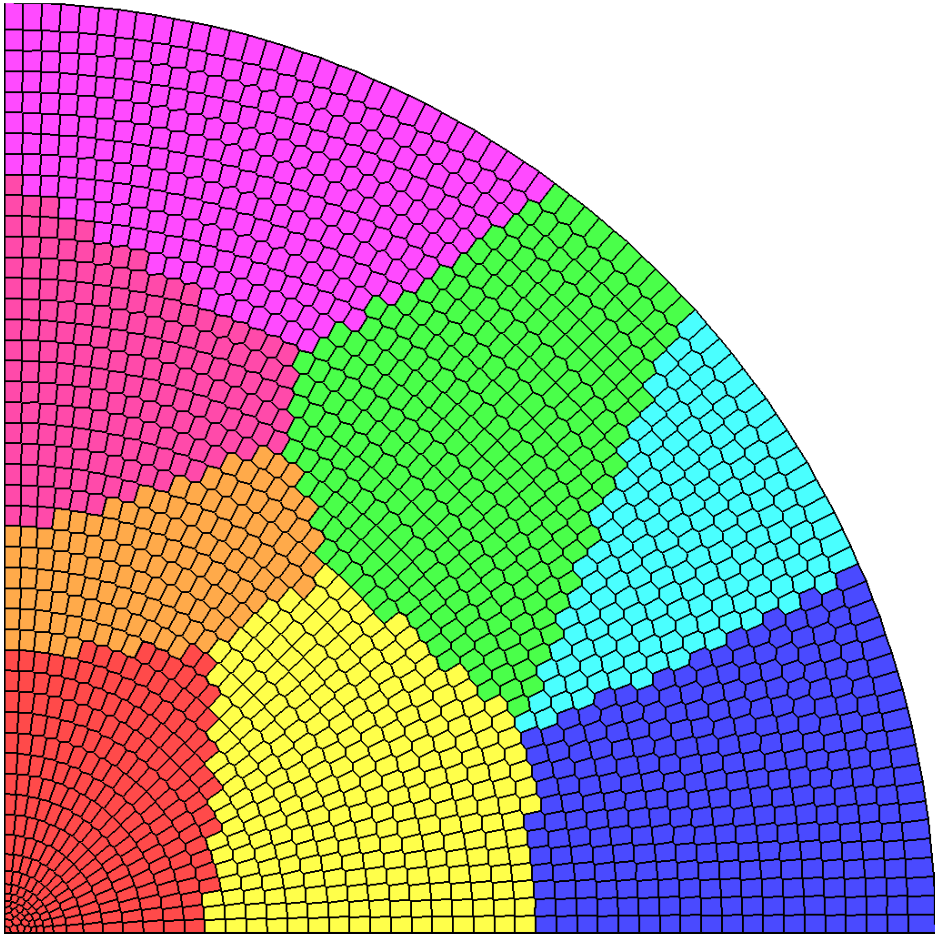
Automatic mesh generation

- Mesh topology based on Voronoi is well-defined
- Convex polygonal zones (if domain is also convex)



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Automatic mesh generation

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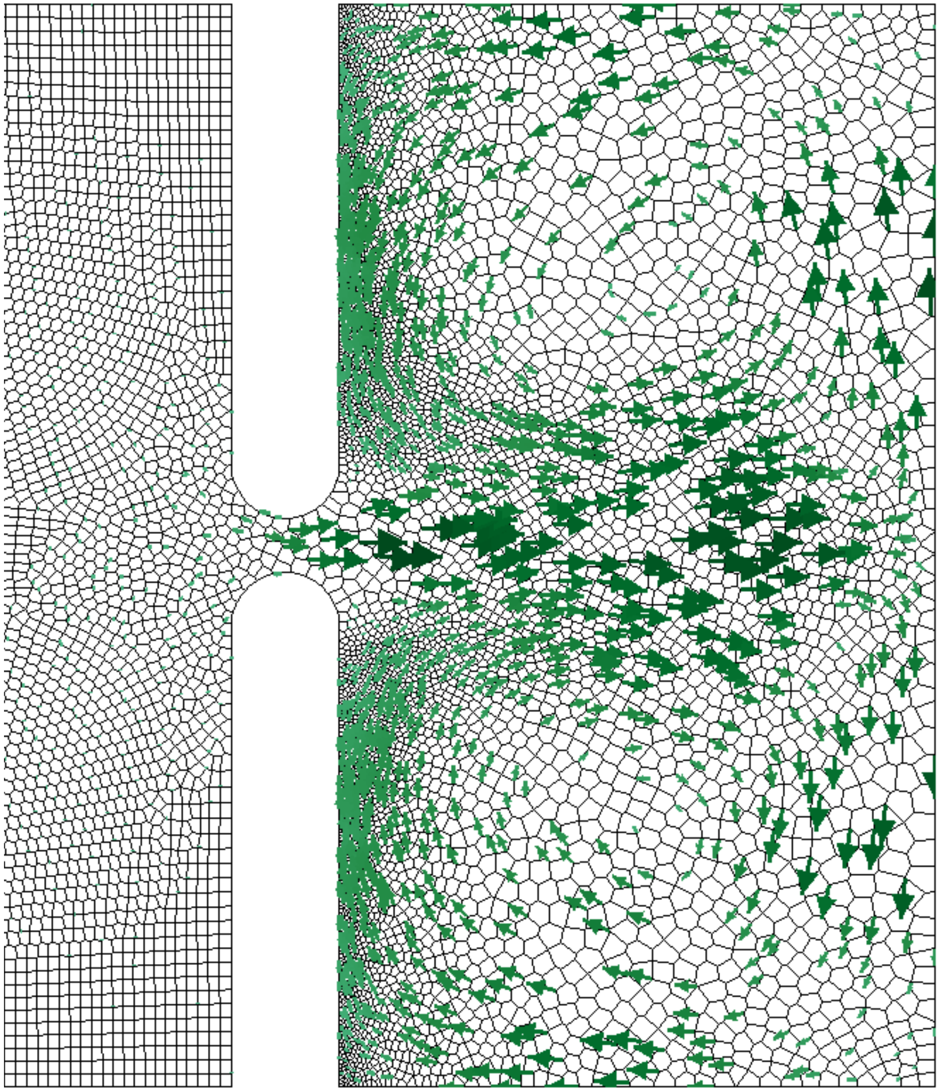
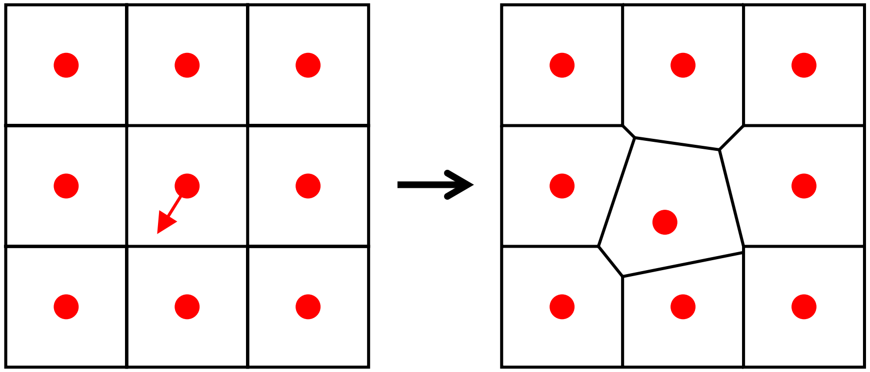
Generators are Lagrangian objects

- Tracks Lagrangian-frame physics



The Voronoi Doesn't Solve All of Your Problems



Mesh Topology Not Easily Controlled

- Displacing a generator influences neighbor cells
- Can lose grid regularity
- Small edges and zone angles can result
- Generators do not coincide with zone centers

Standard ReALE Strategies

Mesh Cleaning: Delete small edges in the Voronoi mesh

Smoothing: Iteratively move generators to zone centroids to regularize mesh (Lloyd's algorithm)

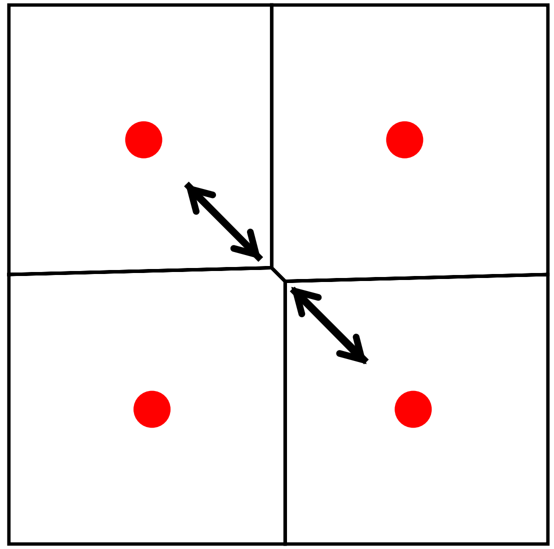
Concerns Looking Forward:

- Zone faces can lose alignment with flow features after Voronoi rezoning
  - Can we constrain generator motion to better track fronts and material interfaces?
- Rezoning and remapping need not occur everywhere
  - Can ReALE be limited to a subset of the domain? Implementation?
- How does generator motion and mesh cleaning impact numerical accuracy?

Eliminating Small Edges Due to Voronoi Rezoning

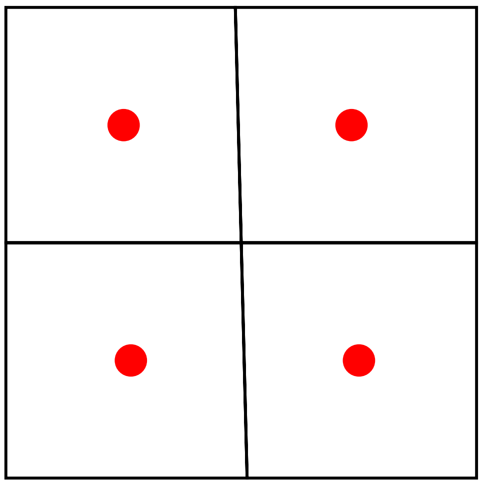
Mesh Cleaning

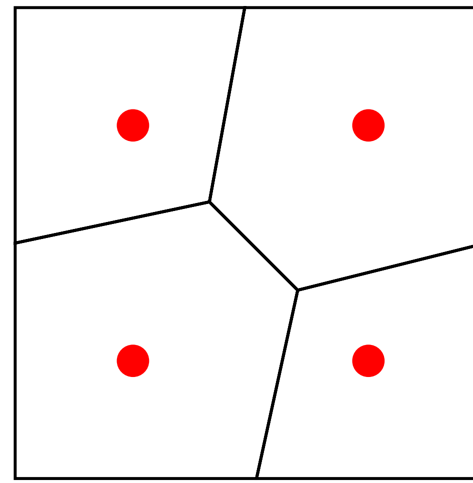
- Delete small edges based on relative/absolute tolerance
- Force mesh back into degenerate configuration



Mesh Relaxation

- Accept rezoned mesh topology
- Optimize resulting zones based on local geometric considerations





Mesh is not topologically Voronoi

- Can break symmetry
- Can introduce new communication in parallel
- Can invalidate mesh topology (if not careful)

Mesh is not geometrically Voronoi

- Generators not consistent with location of mesh nodes/edges/faces
- Relaxers may be problem-specific and subject to prior knowledge

Considerations for Generator Motion

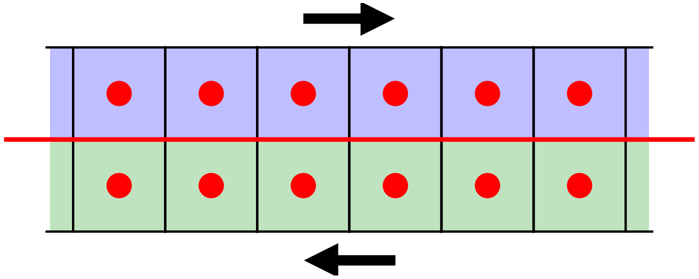
Important Properties:

Galilean Invariance – maintain Lagrangian motion when flow corresponds to translation or rotation

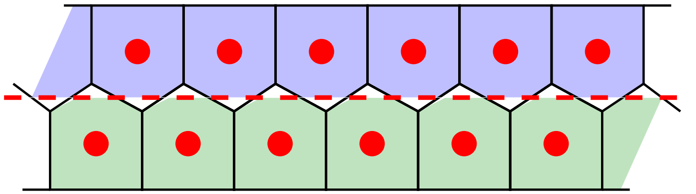
Numerical consistency – generator motion obeys boundary conditions

Numerical stability – generator motion should inform timestepping

Additional Concerns

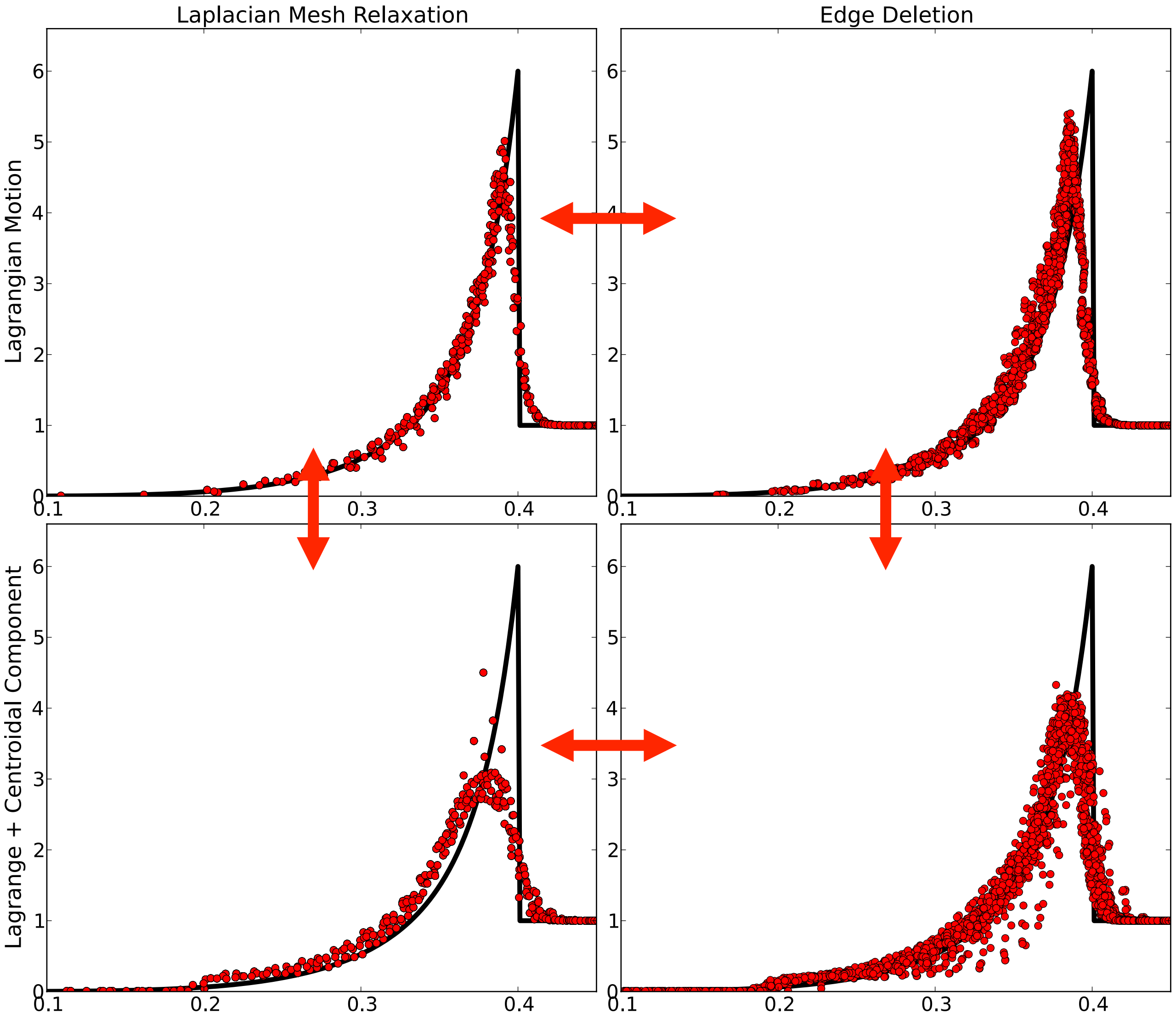


- Averaging nodal velocities can trigger spurious generator motion
  - Consistency error – generator can displace before signal has reached it
- Interpolated sub-zonal velocities can pick up high-mode fluctuations
  - Signals below the resolution of the grid



- Centroidal smoothing deviations from Lagrangian dynamics
  - Generators no longer track Lagrangian-frame feature
  - Zone density can coarsen as generators approach CVT
  - Smoothing is nonlocal – centroidal displacements can propagate ahead of flow

Sedov: Sensitivities due to generator motion and small edge mitigation.



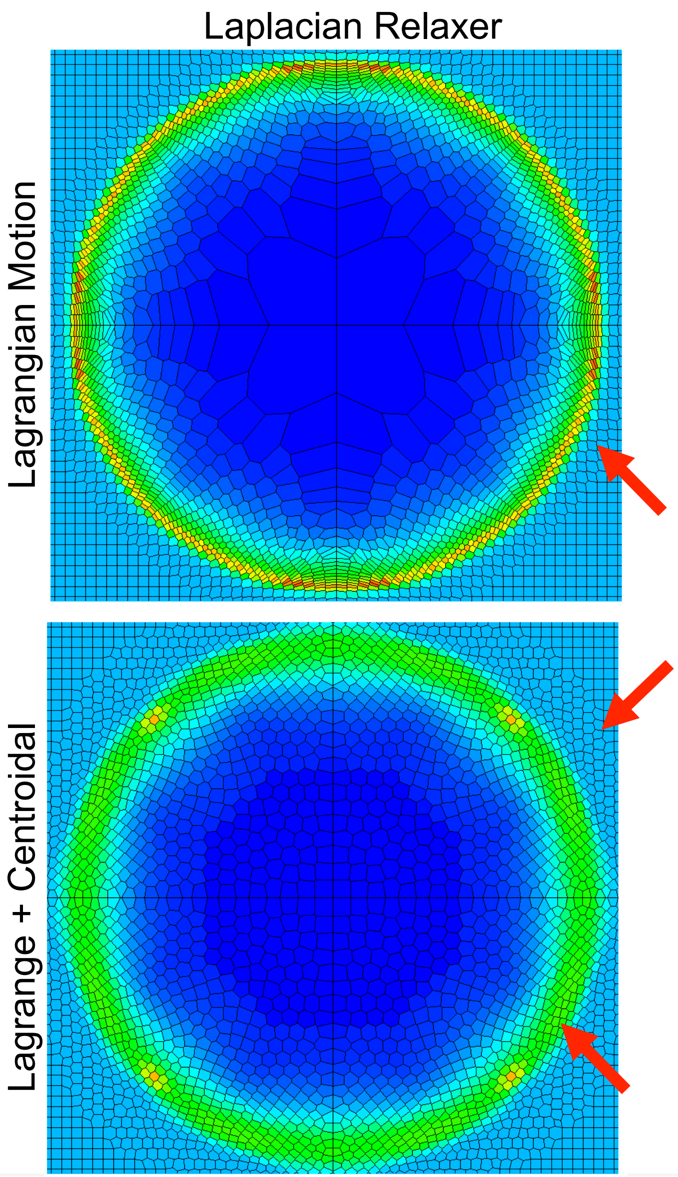
Symmetry breaking

- Deleting small edges does not preserve symmetry
- Greater radial scatter

Numerical Diffusion

- Centroidal smoothing regularizes mesh
- Grid coarsening at and behind shock front
- Comparable to running Eulerian

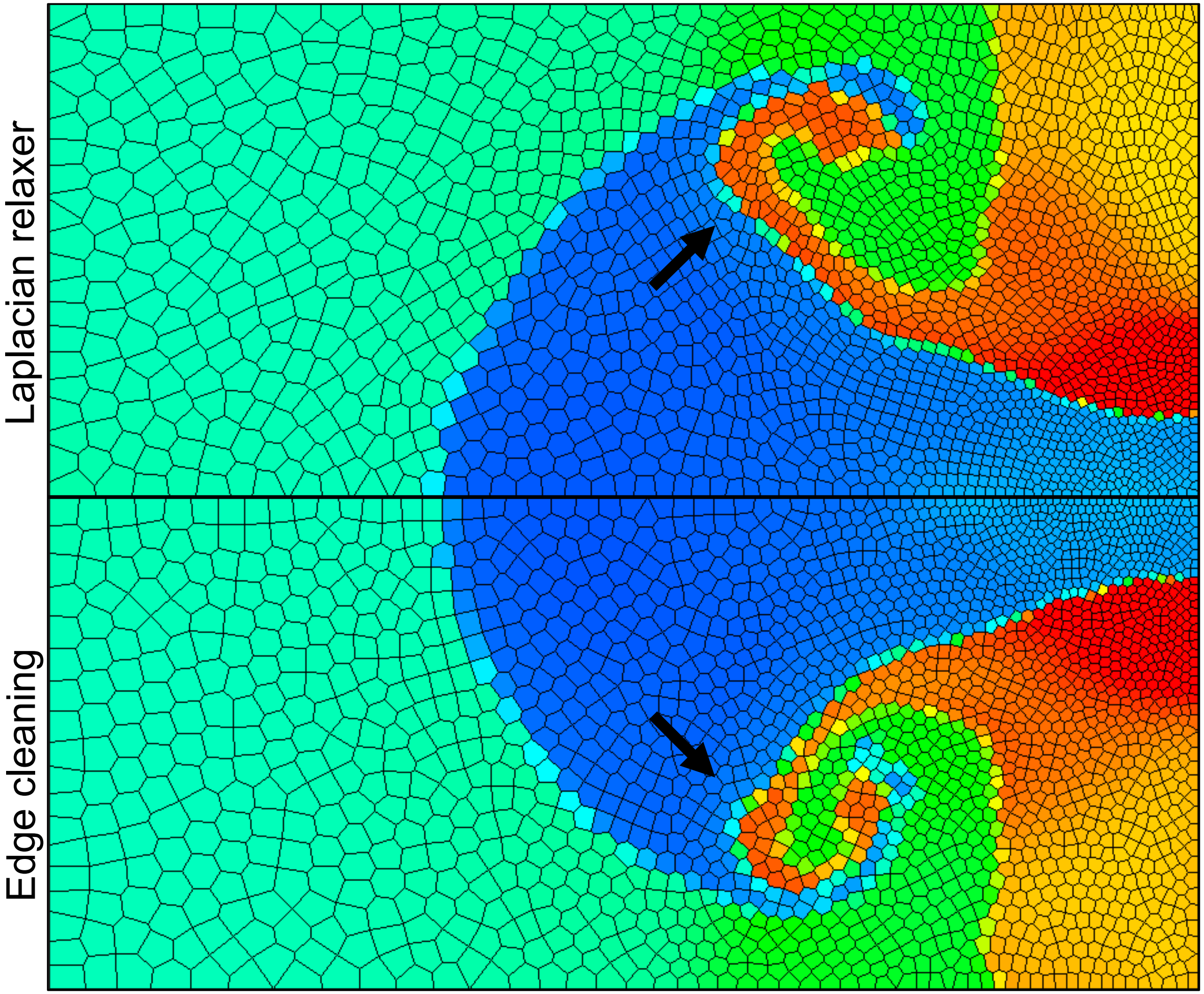
Sedov: Sensitivities due to generator motion and small edge mitigation.



Winslow-Crowley Laplacian relaxer preserves symmetry

Centroidal smoothing coarsens mesh everywhere

Triple Point Problem: Mesh Cleaning Versus Relaxing



W-C Laplacian appears to stiffen mesh during vortical roll-up

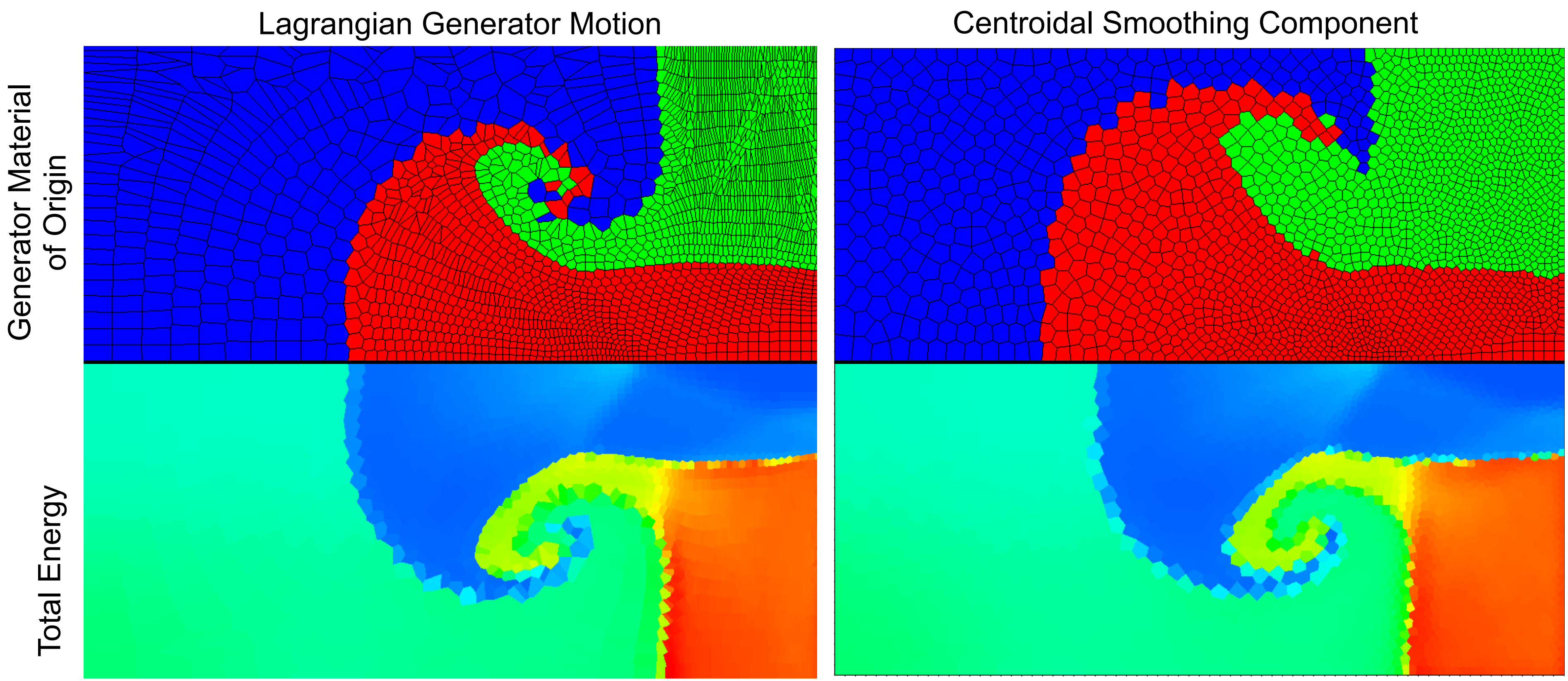
Strategies for mesh relaxation are problem-dependent

Improvements Needed

- **Better limiting on where and how much relaxers work**
- **Implement new relaxers such as the Reference Jacobian Method** [Knupp et at, 2001]

Triple Point Problem: Centroidal Smoothing Effects

Smoothed generators do not correctly track Lagrangian features such as interfaces

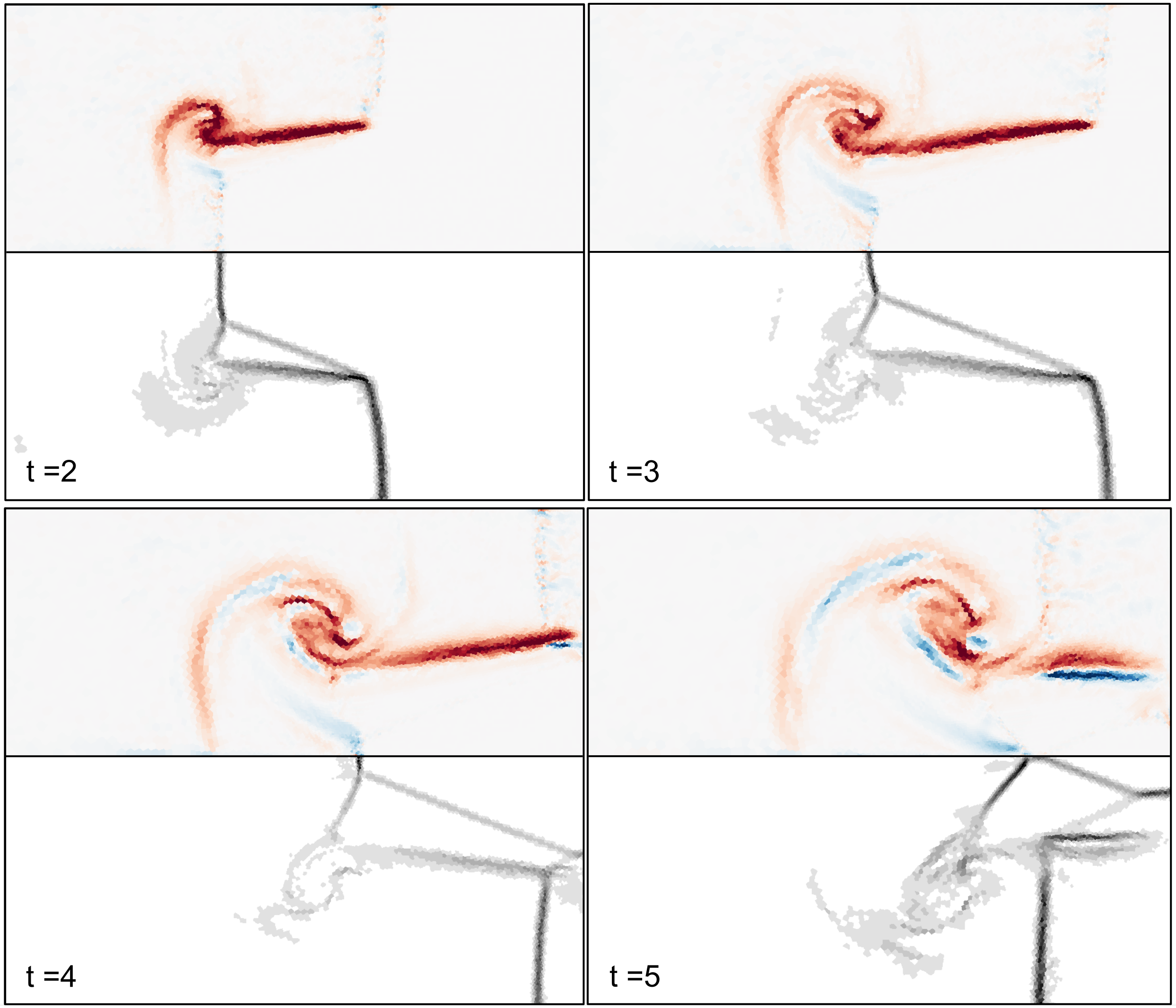


Centroidal smoothing

- Turns on at shock fronts and along roll-up
- Some portion of displacement due to Lagrangian velcoity is lost

Triple Point Problem: Centroidal Smoothing Over Time

Centroidally-smoothed generator update: $$\mathbf{x}^{n+1} = \mathbf{x}^{\mathrm{lag}} + \omega\left(\mathbf{x}_c - \mathbf{x}^{\mathrm{lag}}\right)$$



Vorticity

Red: negative (CW)

Blue: positive (CCW)

Galilean-Invariant Smoothing Parameter ω

White: Purely Lagrangian $(\omega = 0)$

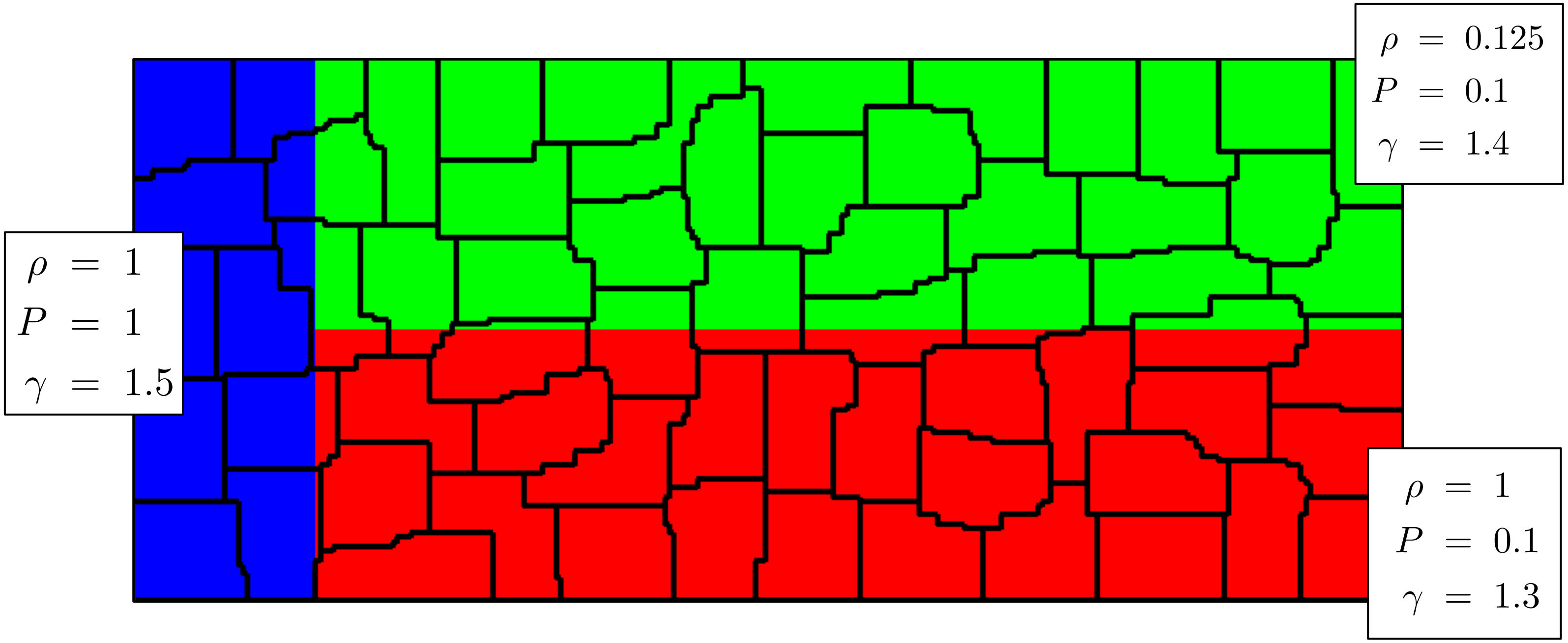
Black: Purely Centroidal $(\omega = 1)$

Gray: Some amount of Lagrangian motion goes into smoothing

NOTE:

- **Smoothing should turn off if zone translates or rotates**
- **Generators in roll-up region smoothed at every cycle**
- **Smoothing can coarsen zone density and increase numerical diffusion during remap**

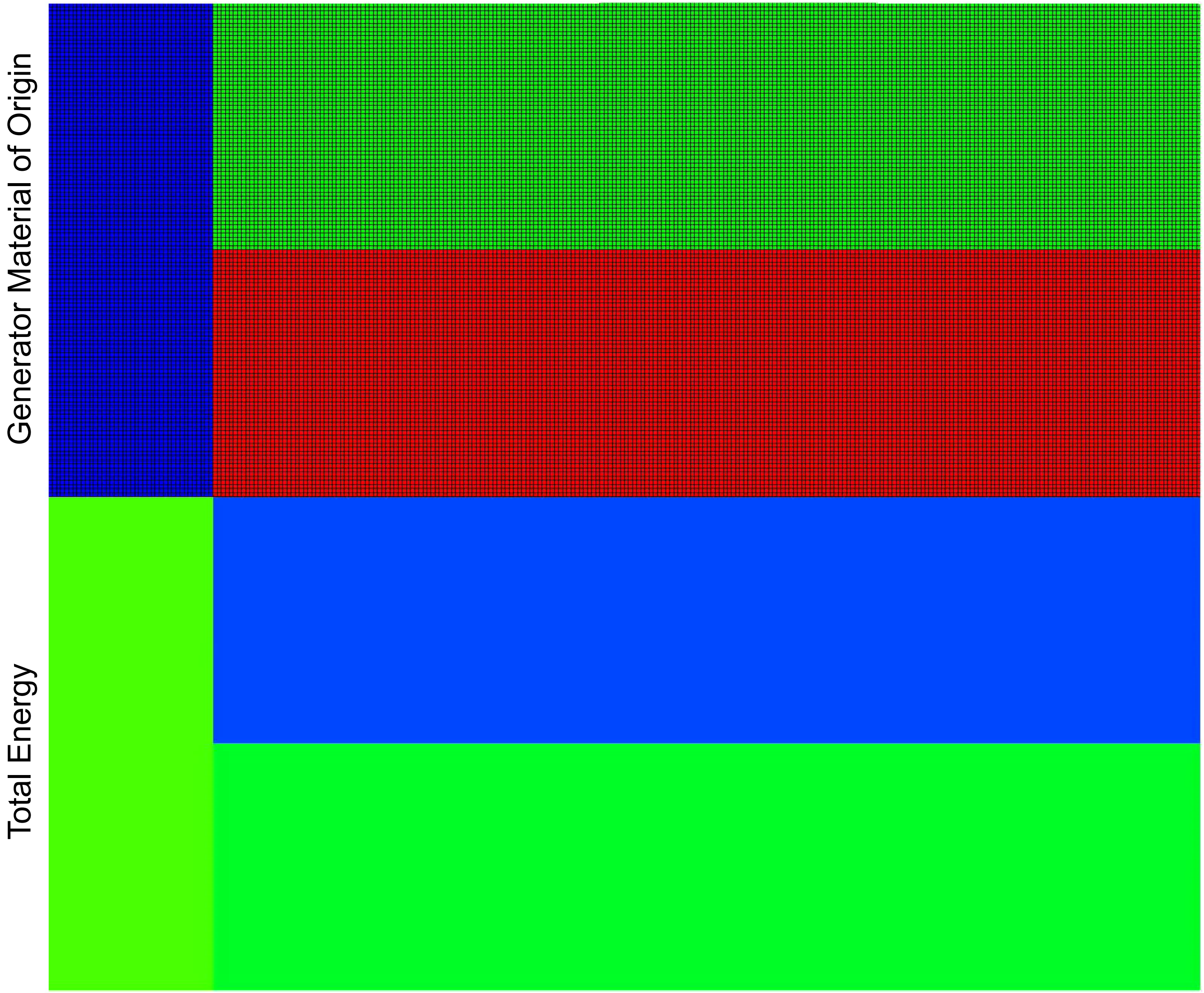
Triple Point Problem in Parallel – Initialization



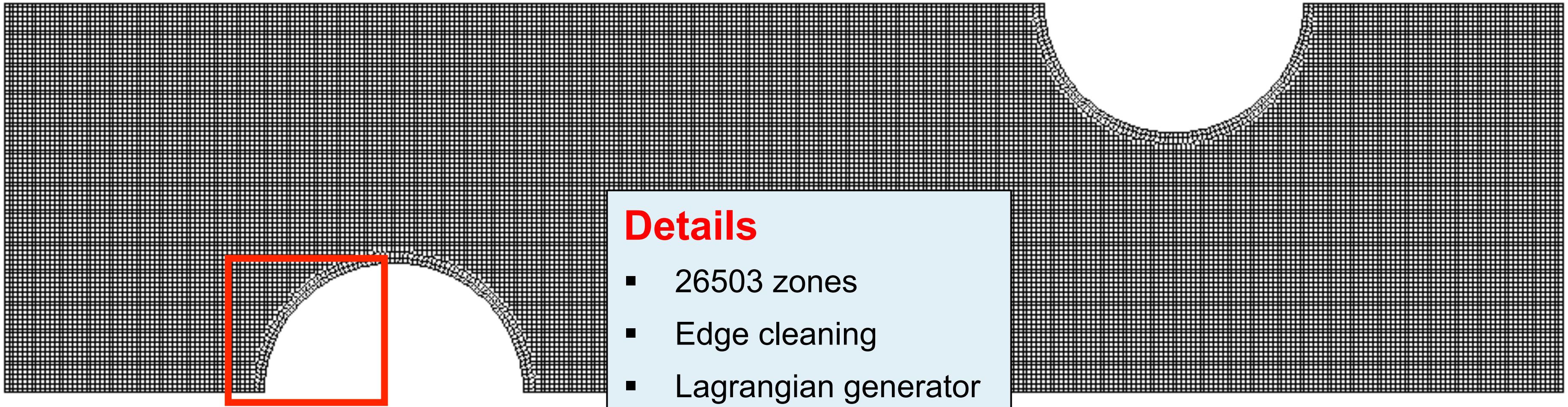
Details

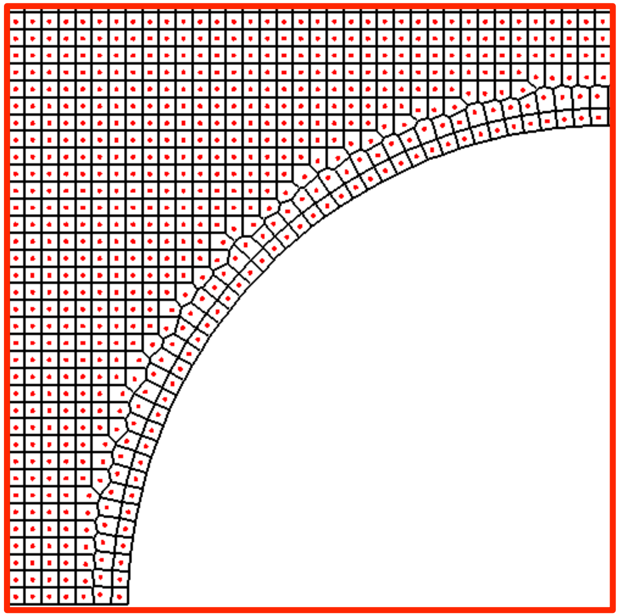
- 280 x 120 square mesh initially (degenerate Voronoi config.)
- 64 processors
- Laplacian mesh relaxer
- Lagrangian generator motion with centroidal smoothing

Triple Point Problem in Parallel – Results



Interacting Strong Shocks – Initialization



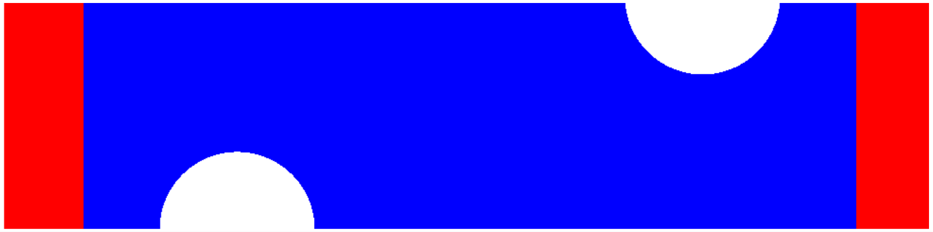


Details

- 26503 zones
- Edge cleaning
- Lagrangian generator motion with centroidal smoothing

Double shock tube initial condition

Hot gas state	Cold gas state
$\rho = 1$	$\rho = 10^{-2}$
$P = 2/3$	$P = 10^{-7}$
$\gamma = 5/3$	$\gamma = 5/3$



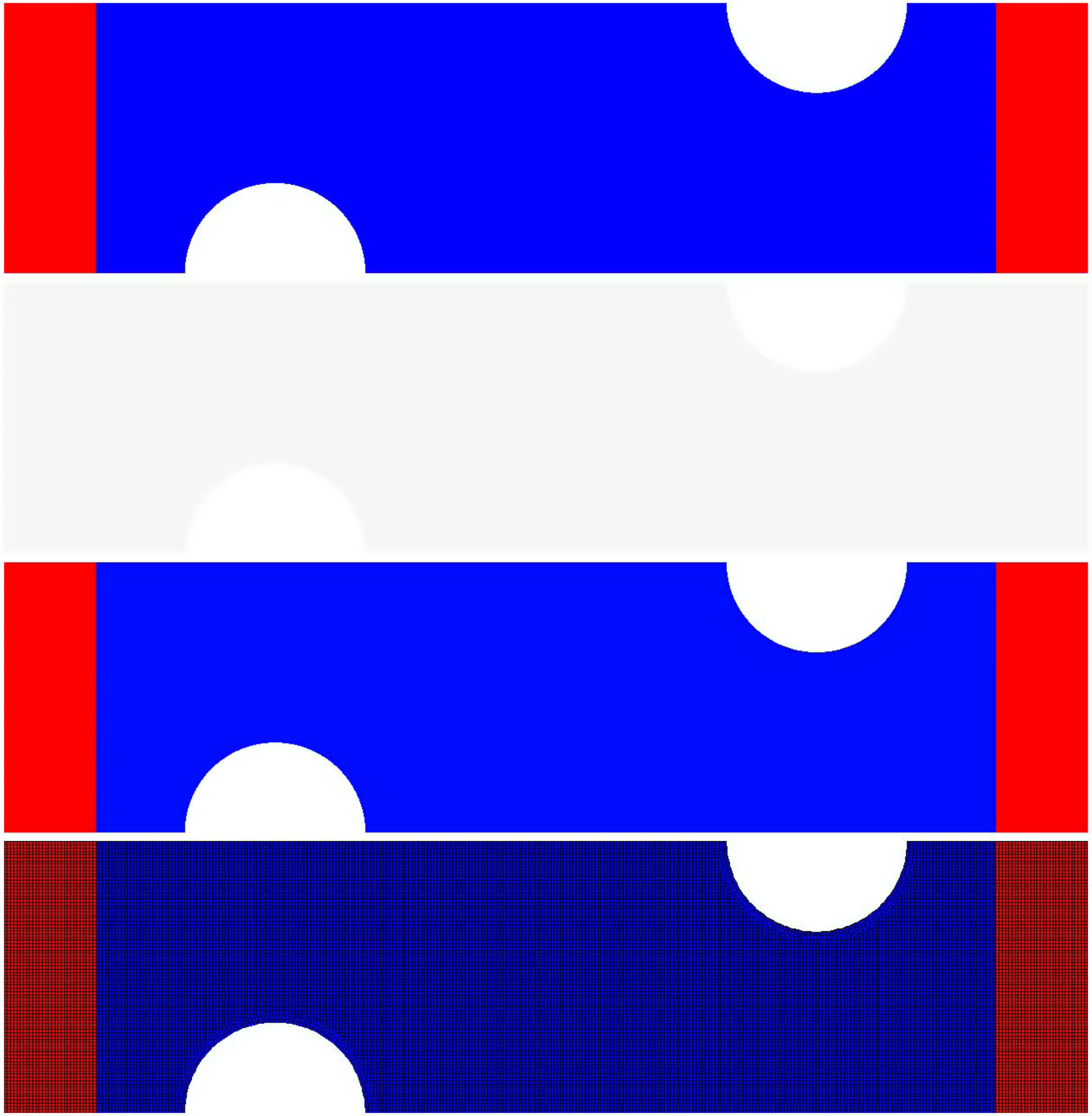
Interacting Strong Shocks – Results

Volume Fraction

Vorticity

Density

Generator Material of Origin



Constricted Shock Tube – Initialization and Results

Shock tube initial condition through 2D "nozzle"

Hot gas state

$\rho = 1$

$P = 2/3$

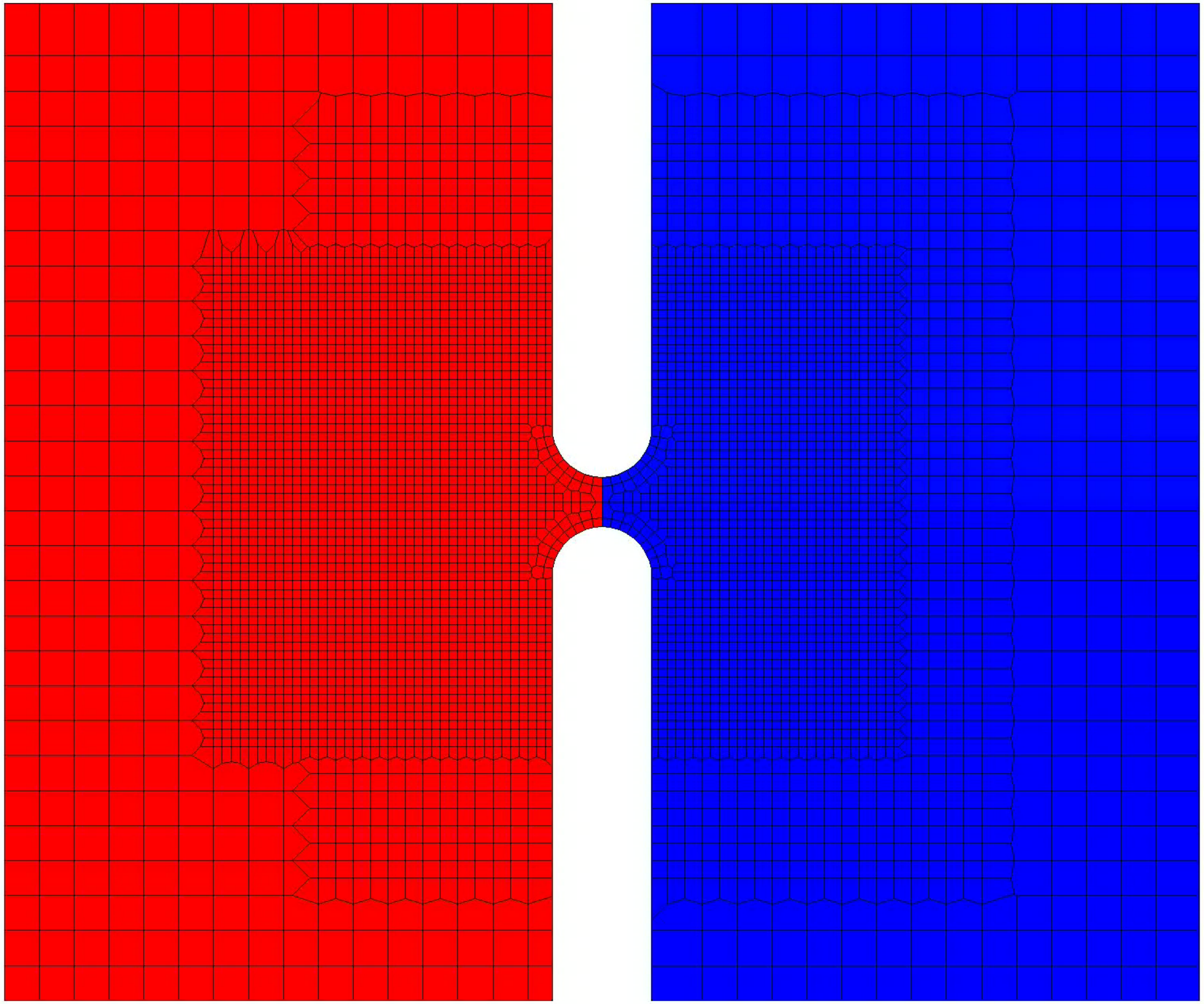
$\gamma = 5/3$

Cold gas state

$\rho = 10^{-2}$

$P = 10^{-7}$

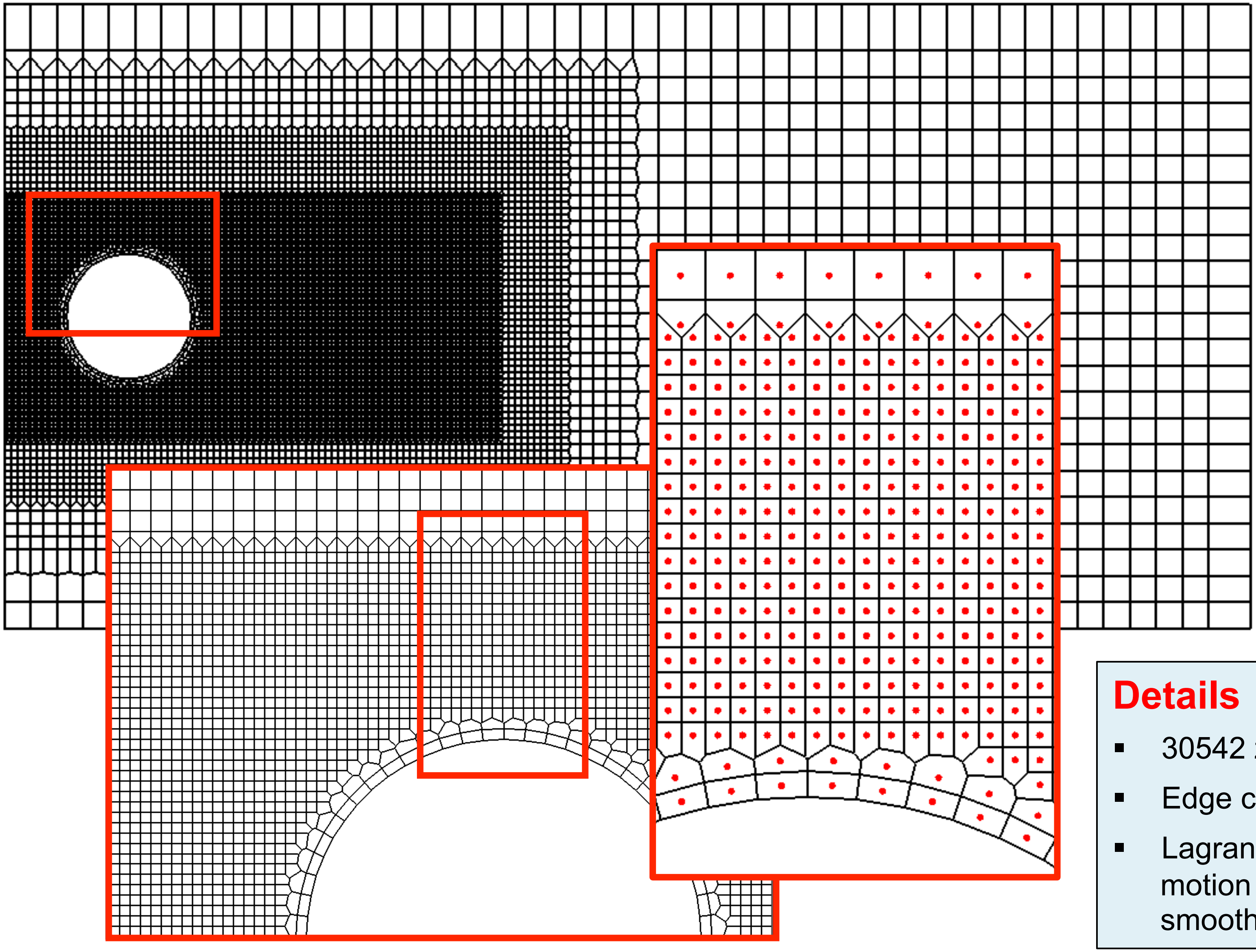
$\gamma = 5/3$



Density

Generator Material of Origin

Shock Over a Cylindrical Barrier – Initialization



Hot gas state

$\rho = 1$

$P = 2/3$

$\gamma = 5/3$

Cold gas state

$\rho = 10^{-2}$

$P = 10^{-7}$

$\gamma = 5/3$

Details

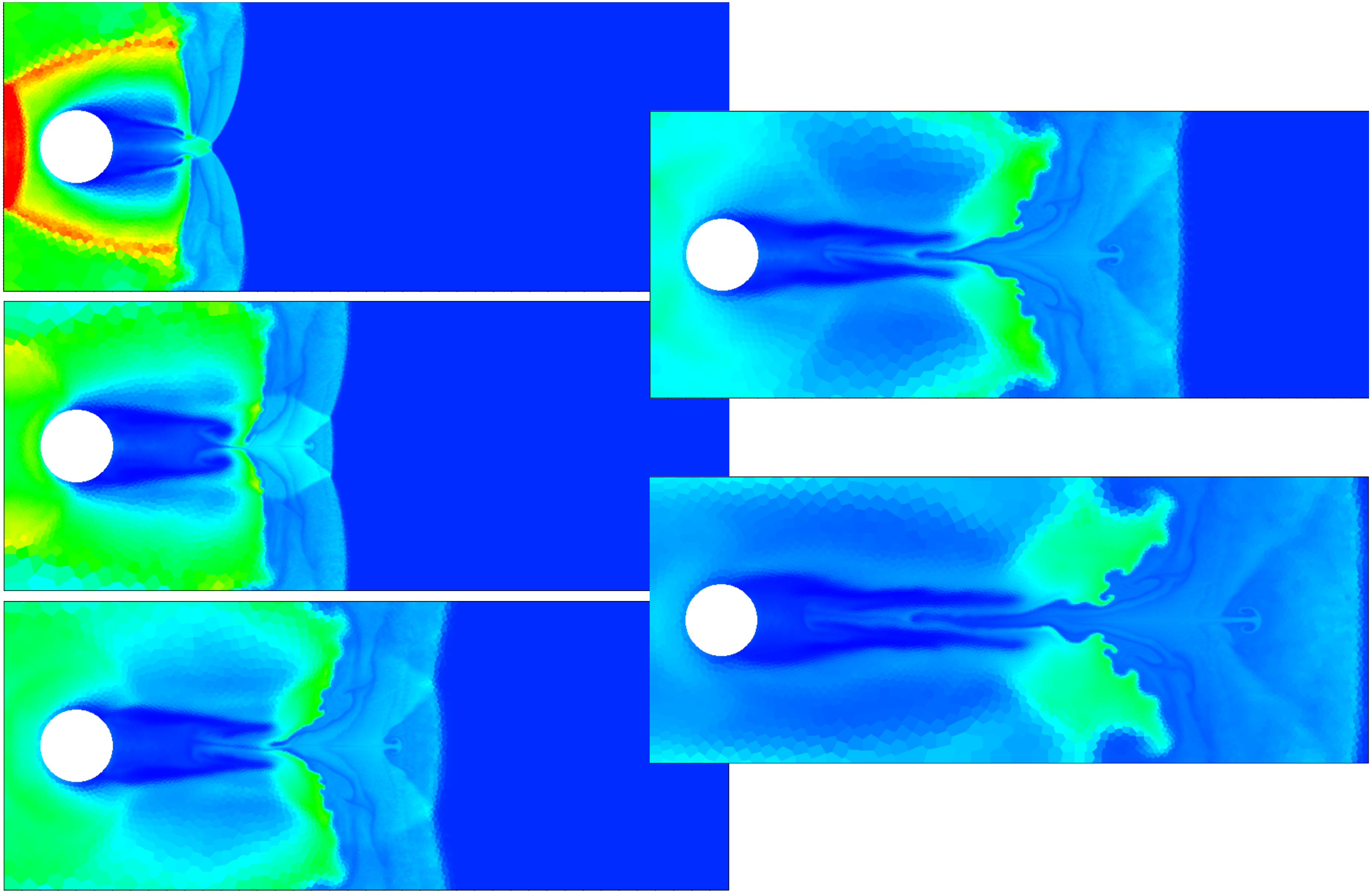
- 30542 zones
- Edge cleaning
- Lagrangian generator motion with centroidal smoothing

Shock Over a Cylindrical Barrier – Results

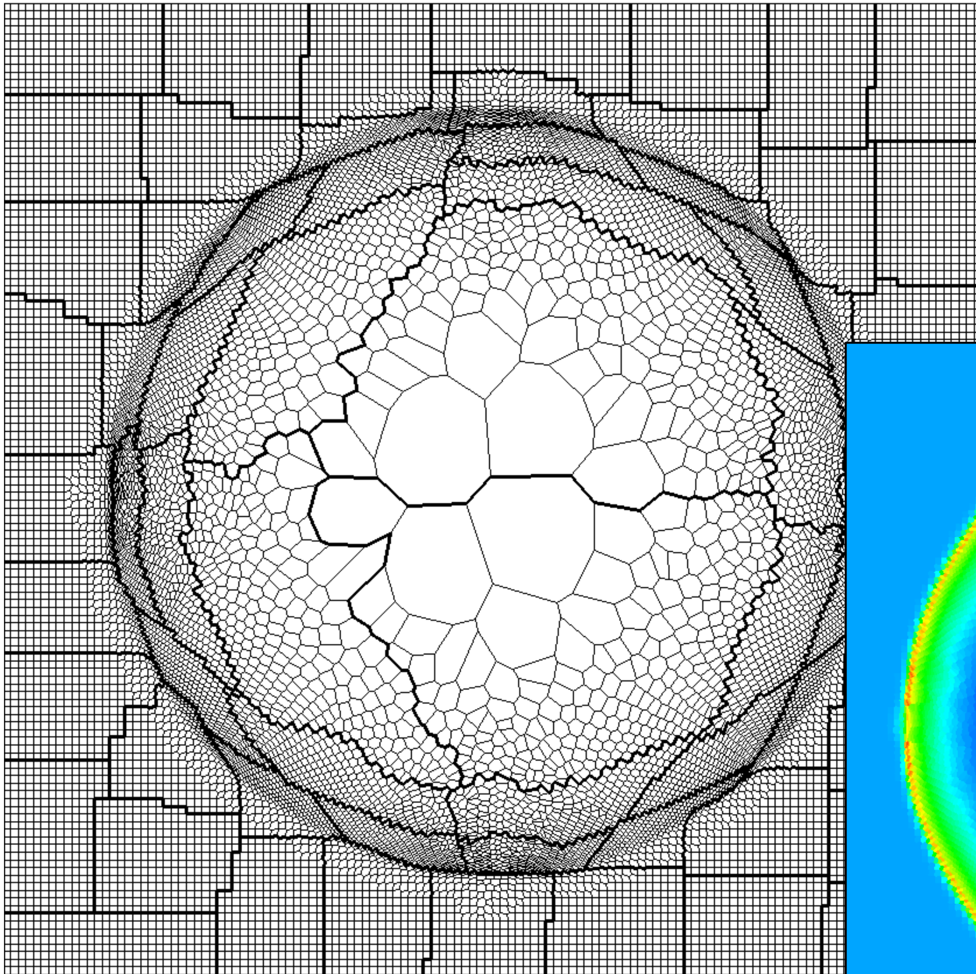
Density

Vorticity

Shock Over a Cylindrical Barrier – Results (Refinement)

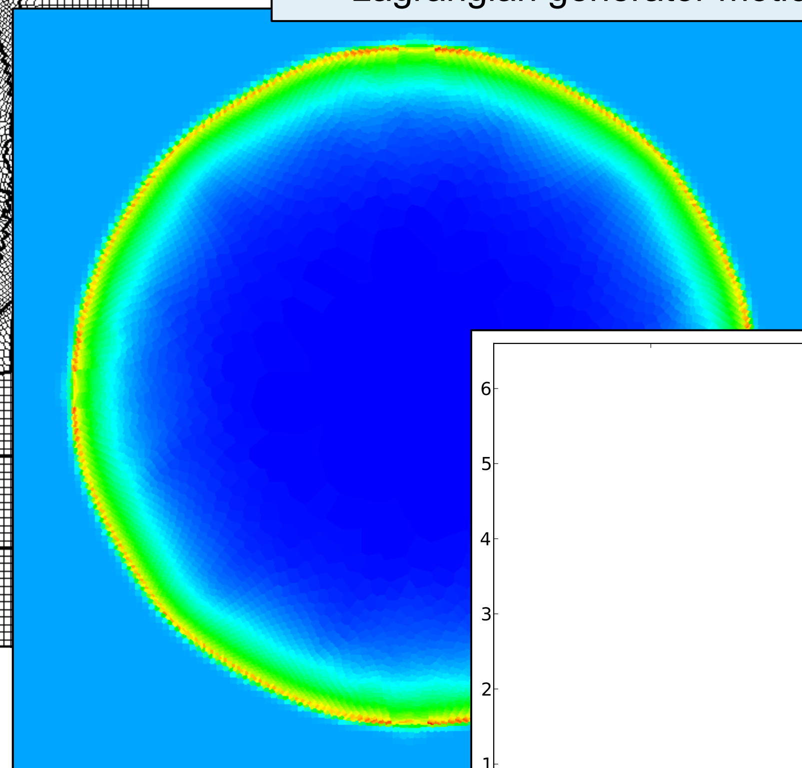


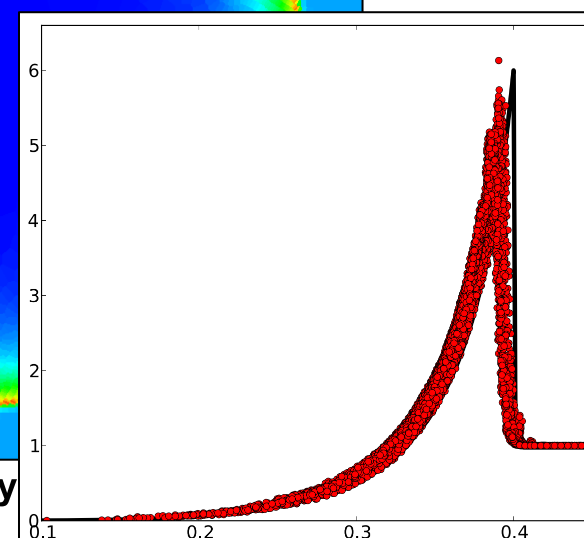
Domain Imprinting Visible in Parallel Sedov Test



Details

- 128 x 128 square mesh initially
- 64 processors
- Laplacian mesh relaxer
- Lagrangian generator motion





density

NOTE: Overlink remaps nodal values on processor boundaries differently than on interior nodes.

Future Directions

Pure Hydro

- Investment in mesh optimizers
  - Reference Jacobian mesh relaxer
- More experimentation in generator motion
  - Quantitative impact on accuracy
- Address Overlink's domain imprinting error in parallel
- Implement momentum-conservative overlay treatment
  - Have devised variation-diminishing technique for staggered hydro
- ReALE on subsets of the mesh

Multiphysics

- Demonstrate first rad-hydro ReALE calculations
- Model problem: reconnection of an ablating surface flow

Acknowledgements

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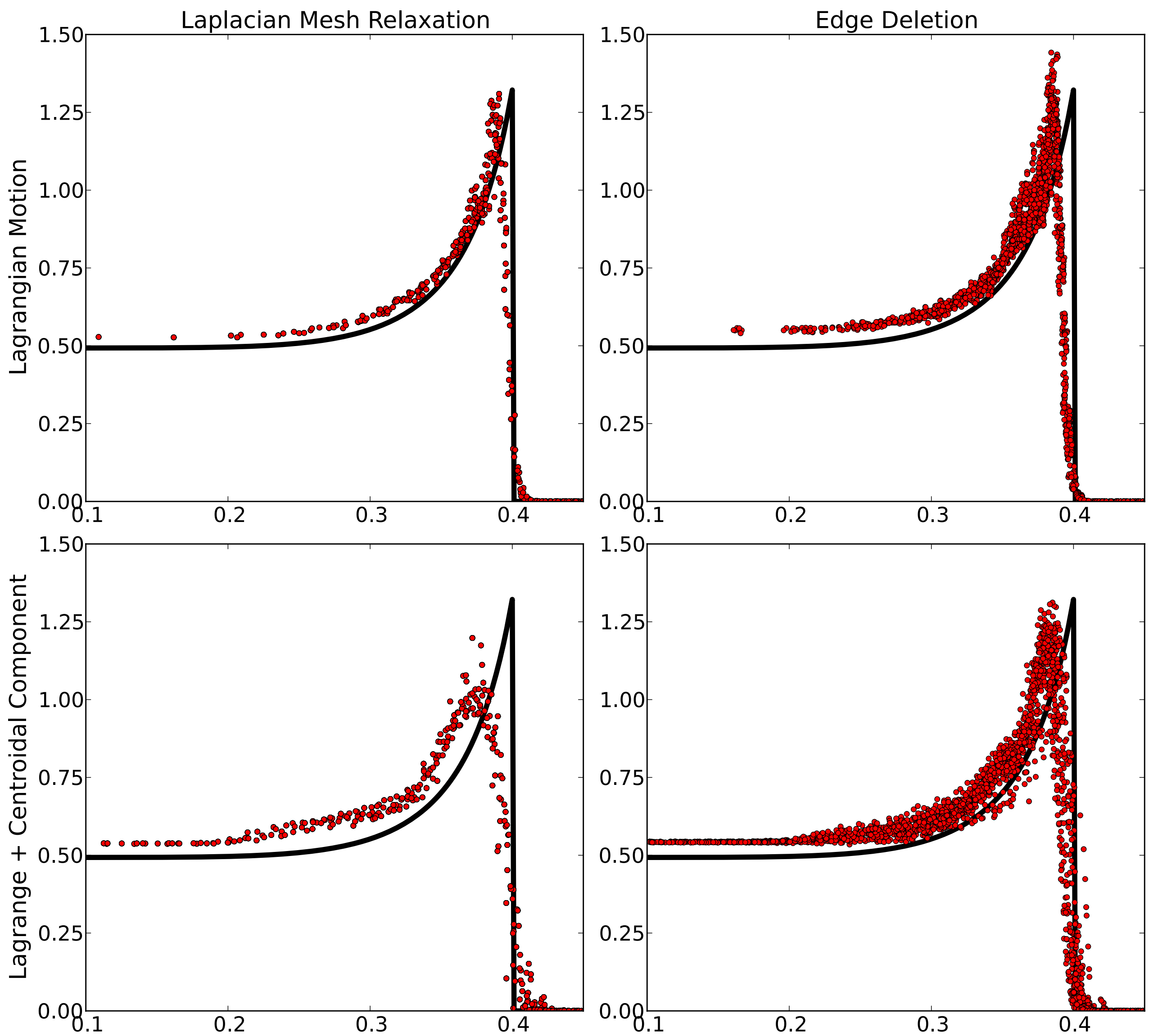
Sedov: shock moves at incorrect velocity due to remap



Linear momentum currently not conserved in overlay remap

Constricted Shock Tube – Initialization and Results

Shock tube initial condition through 2D "nozzle"

Hot gas state	Cold gas state
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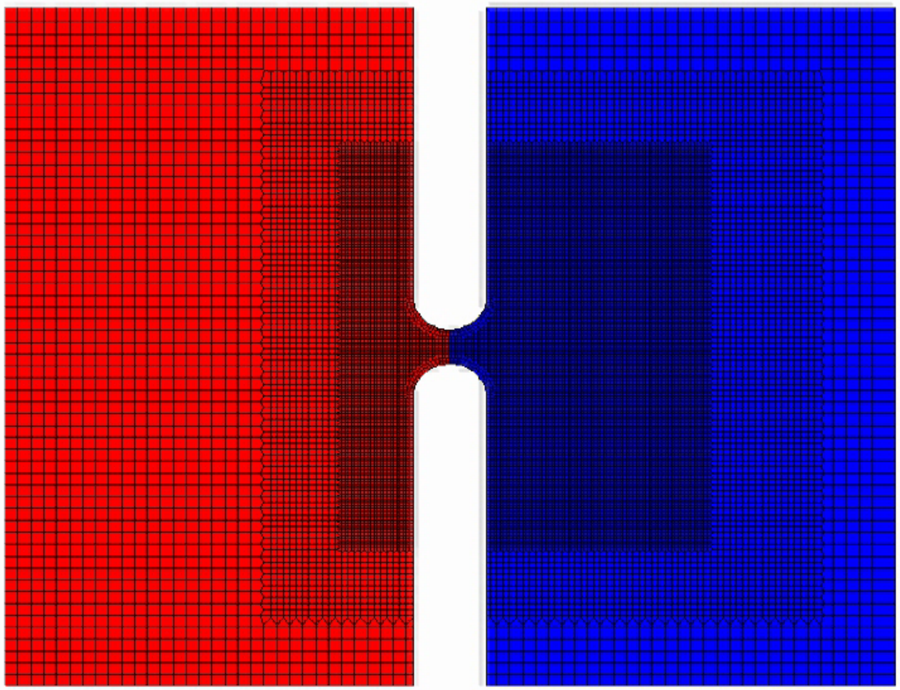
Generator Material of Origin



Density