Adaptation of Curved Meshes in ALE Hydrodynamics

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CASC
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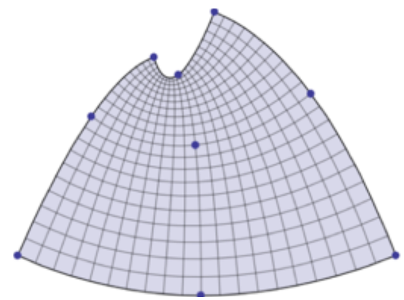
Overview and motivation

- General framework for mesh optimization.
  - Meshes are modified by node movement.
  - Extension of TMOP to curved meshes and adaptivity.
  - User targets (ideal geometry), mesh quality metrics, nonlinear optimization.
  - Algebraic routines - no geometrical operations in physical space.

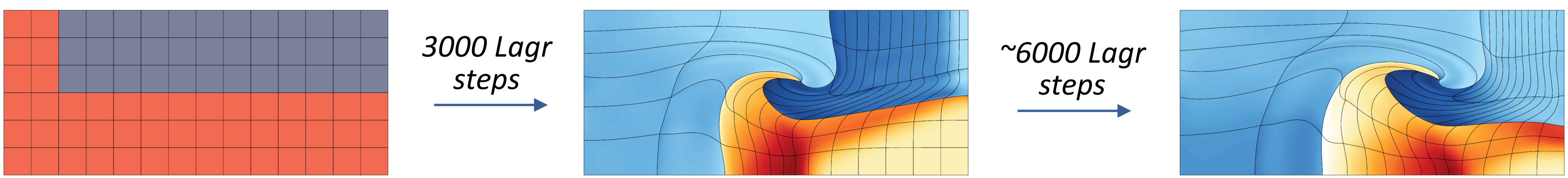
- Application to multi-material ALE hydro.
  - Demonstration code - BLAST (high-order FE on curved grids).
  - Adaptivity to discrete features (interfaces, materials, shocks, etc).
  - Adaptive ALE triggers.

Discretization and ALE framework in BLAST

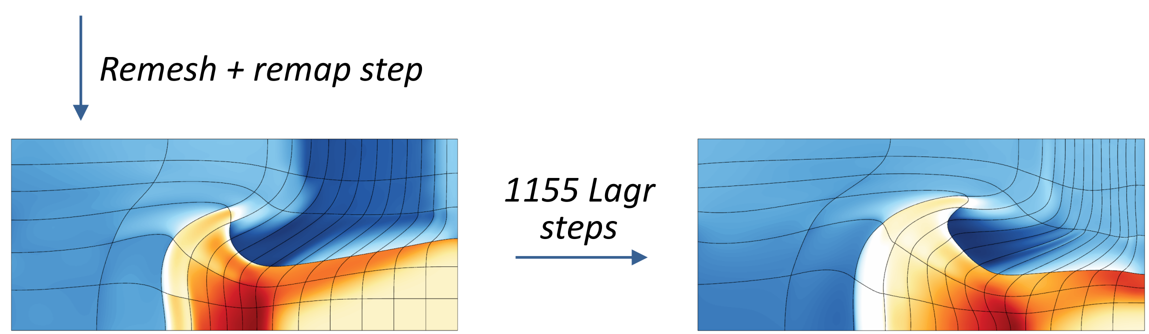
- Lagrange + remap, high-order finite elements.
- Curved meshes: $\boldsymbol{x} = (\boldsymbol{x}_1 \ldots \boldsymbol{x}_N)^T, \quad x_q(\bar{x}_q) = \sum_{i=1}^{N} \boldsymbol{x}_i \bar{w}_i(\bar{x}_q)$
- Any number of Lagrangian steps between two ALE steps.



Example of a Q_2 element



Triple point, Q3Q2, 84 elements

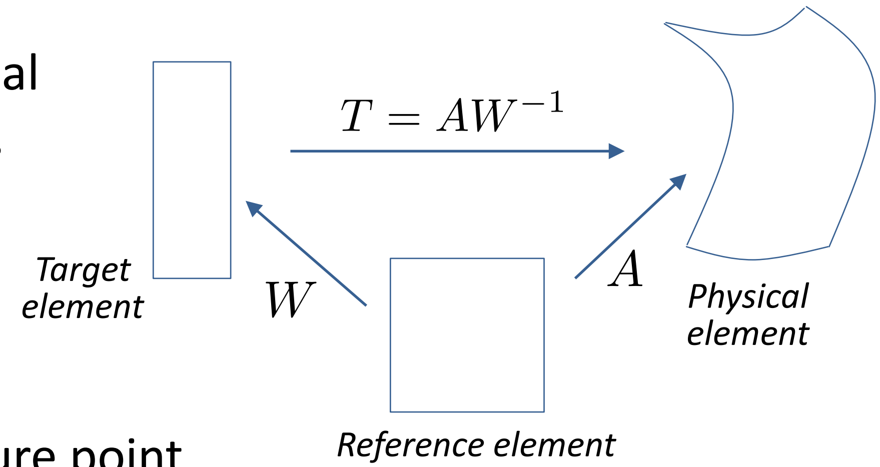


Towards what to optimize the mesh?

How often to perform ALE steps?

Target - Matrix Optimization Paradigm (TMOP)

- Target construction: the user defines ideal elements by specifying the Jacobians W.



- Minimize $\displaystyle\sum_{E \in \mathcal{M}} \int_{E_t} \mu(T(x_t))$

  Mesh quality metric

- $T, \mu(T)$ are computed at every quadrature point.

- Default option: Newton's method (+ line search) to solve $\partial F(x) \,/\, \partial \boldsymbol{x} = 0$.
  - Efficient parallel implementation in contrast to derivative-free methods.

- Requires calculation of $\partial\mu(T) \,/\, \partial T$ and $\partial^2\mu(T) \,/\, \partial T^2$ for the metric.

Dobrev, Knupp, Kolev, Mittal, Tomov "The Target-Matrix Optimization Paradigm for High-Order Meshes", SIAM J. Sci. Comp, 2019.

TMOP mesh quality metrics

We have explored more than 60 metrics divided into 7 metric types

- Jacobian decomposition: $W =$ [volume] [orientation] [skew] [aspect ratio].
- Shape metrics – control over skew and aspect ratio. Minimized when A is a scaled rotation of W.

$$\mu_2(T) = 0.5\frac{|T|^2}{\det(T)} - 1$$

- Size metrics – control over volume. Minimized when $\det(A) = \det(W)$.

$$\mu_{77}(T) = 0.5\left(\det(T) - \frac{1}{\det(T)}\right)^2$$

- Alignment metrics – control over orientation and skew. Minimized when $A = \mathrm{W} * \mathrm{Diag}$.

$$\mu_{30}(A,W) = |\boldsymbol{a}_1||\boldsymbol{w}_1| - (\boldsymbol{a}_1 \cdot \boldsymbol{w}_1) + |\boldsymbol{a}_2||\boldsymbol{w}_2| - (\boldsymbol{a}_2 \cdot \boldsymbol{w}_2)$$

- Implicit combinations. SH+SZ, SH+AL, SZ+AL, SH+SZ+AL.

$$\mu_7(T) = |T - T^{-t}|^2 \qquad \mu_{14}(T) = |T - I|^2$$

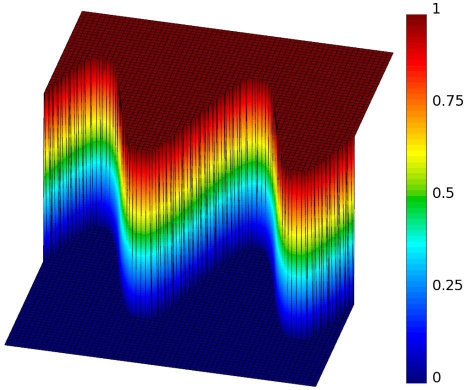
- Explicit combinations.

$$\mu(T) = \alpha\mu_i(T) + (1-\alpha)\mu_j(T)$$

P. Knupp, "Algebraic mesh quality metrics", SIAM J. Sci. Comp., 23(1):193-218, 2001.

Main steps in the adaptivity procedure

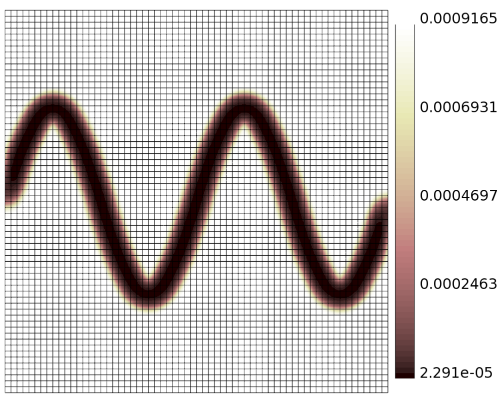
Example of adapting size and aspect ratio to a material interface



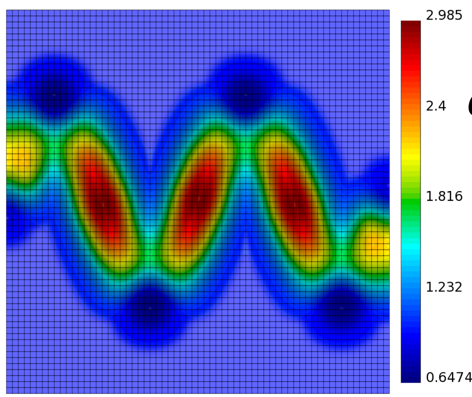
1. Start with simulation data (material interface η here)

2. Choose adaptation goal
- *volume = ζ*
- *orientation angle = θ*
- *skew angle = ϕ*
- *aspect ratio = ρ*

3. Transform into geometric data on the initial mesh



Size function $S(x) \approx |\nabla \eta|$



Aspect ratio $A(x) \approx |\eta_x / \eta_y|$

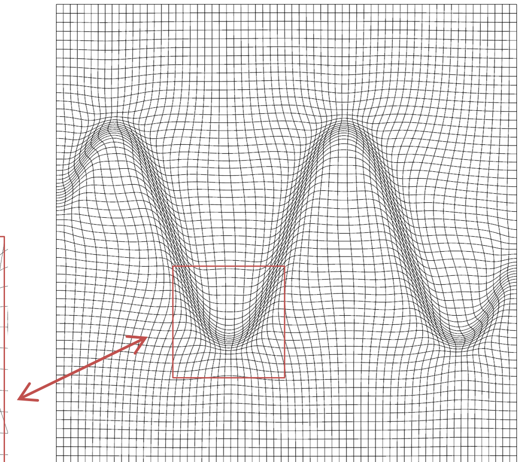
Construct target Jacobians

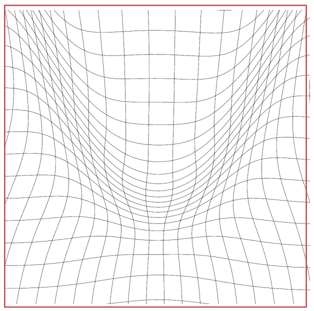
$$W(x) = \left(\frac{S(x)}{A(x)}\right)^{\frac{1}{2}} \begin{bmatrix} 1 & 0 \\ 0 & A(x) \end{bmatrix}$$

General formula in 2D:

$$X = \sqrt{\zeta} \begin{pmatrix} \frac{1}{\sqrt{\rho}} \cos\theta & \sqrt{\rho}\cos(\theta + \phi) \\ \frac{1}{\sqrt{\rho}} \sin\theta & \sqrt{\rho}\sin(\theta + \phi) \end{pmatrix}$$

Choose quality metric and optimize the nonlinear functional





Adaptivity field values on intermediate meshes

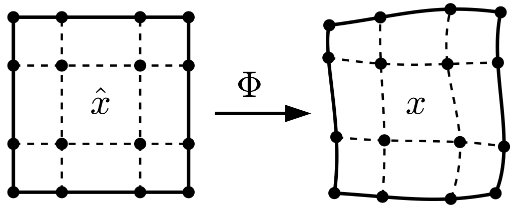
The values of $\eta_0(x_0)$ are transferred on different meshes

- Iterative solvers use a series of intermediate meshes to reach convergence.

- Method 1: physical -> logical space interpolation.
  - Iterate over a set of candidate elements.
  - Invert the reference -> physical map for each.

$$\bar{x_0}^{n+1} = \bar{x_0}^{n} + A^{-1}(\bar{x_0}^{n})\left[x - \Phi_{E_0}(\bar{x_0}^{n})\right]$$

  - Challenging parallel implementation.



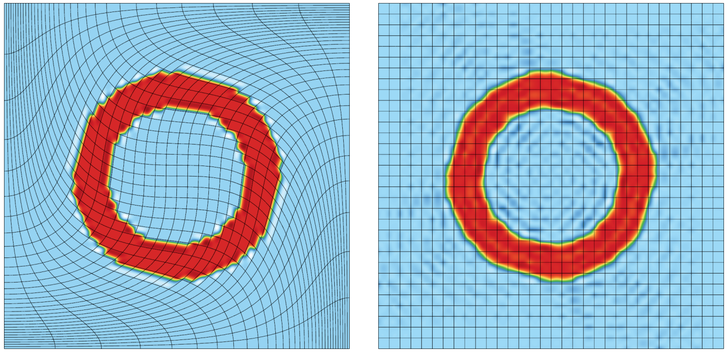
3rd order transformation

- Method 2: advection remap.
  - Define pseudo-time τ and mesh velocity u.

$$\tau \in [0,1], \quad u = x - x_0$$

$$\frac{d\eta}{d\tau} = u \cdot \nabla \eta, \quad \eta(x_0, 0) = \eta_0(x_0)$$

  - CG advection, no monotonicity treatment.



CG remap of a 3rd order field on 3rd order mesh

Differentiation of adaptive target matrices

Major difference compared to geometry-based optimization

- As W depends on η, derivative-based solvers need its derivatives in $\boldsymbol{x}$.

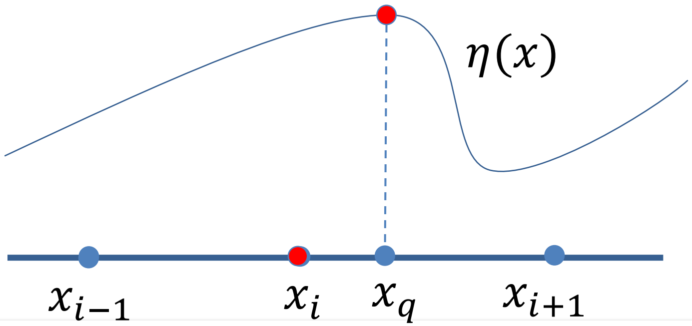
$$F(x) := \sum_{E \in \mathcal{M}} \int_{E_t} \mu(T(x_t)) dx_t = \sum_{E \in \mathcal{M}} \sum_{x_q \in E_t} w_q \det(W(\bar{x}_q)) \, \mu(T(x_q))$$

$$\frac{\partial \mu(T)}{\partial x_{ij}} = \left(\nabla \bar{w}_i W^{-1}(\eta(x)) - A(x) W^{-1} \frac{\partial W}{\partial \eta} \left(\nabla \eta \cdot \frac{\partial x}{\partial x_{ij}} \right) W^{-1} \right) : \frac{\partial \mu(T)}{\partial T}$$

New term due to r-adaptivity

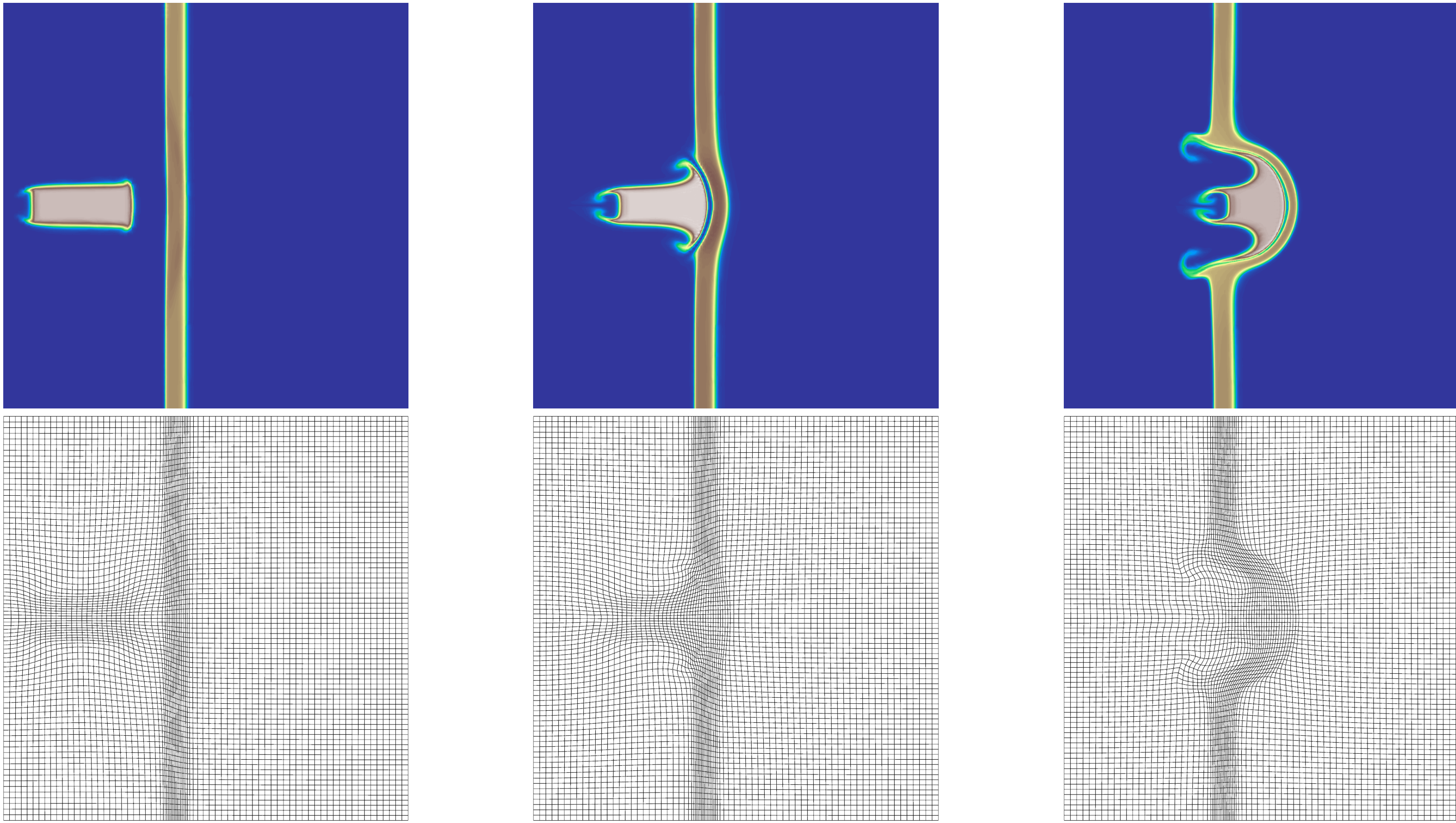
$$A(\boldsymbol{x}) = \sum_i \boldsymbol{x}_i \nabla \bar{w}_i(\bar{x}) \,, \quad x = \sum_i \boldsymbol{x}_i \bar{w}_i(\bar{x}) \,, \quad \eta(\boldsymbol{x}) = \sum_i \eta_i w_i(\boldsymbol{x}) \,, \quad \left[\frac{\partial \mu}{\partial T} \right]_{kl} = \frac{\partial \mu}{\partial T_{kl}}$$

- The above derivative is still an approximation. It doesn't consider transfer errors.



Example of r-adaptivity in an impact simulation

45000 Lagrange steps / 80 ALE steps / 690 pseudo advection steps

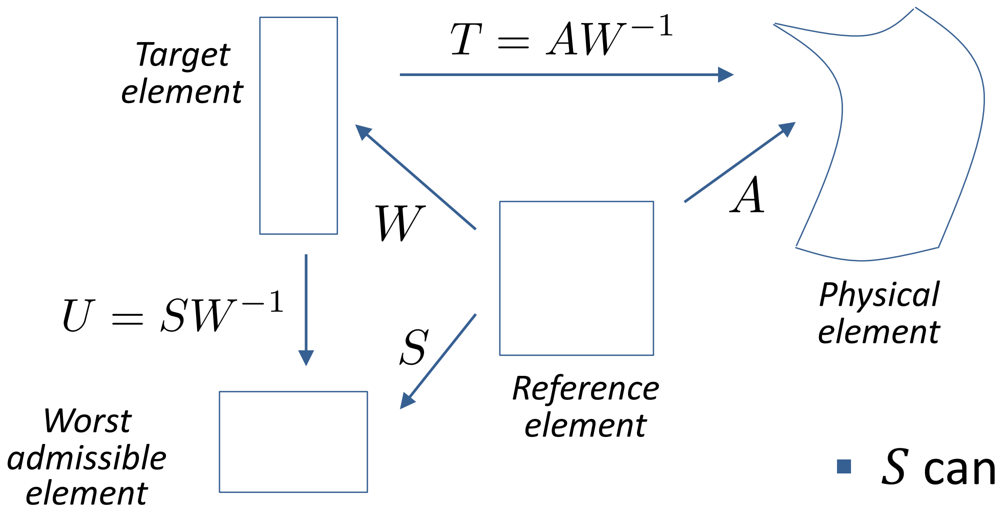


t = 0.5 *t = 2.0* *t = 4.0*

TMOP-based quality detection and ALE triggers

User-defined admissible local quality can trigger the ALE step

- Too few ALE steps - deterioration of mesh quality can cause simulation failure.
- Too frequent - affects accuracy (remap is artificial transport).
- ALE frequency must be based on mesh quality.
  - Lagrangian steps don't always deteriorate mesh quality!
- The user defines admissible local quality.
  Jacobian S of the reference -> *worst admissible* element transformation.



- ALE step is triggered whenever

$$\mu(T) > \mu(U)$$

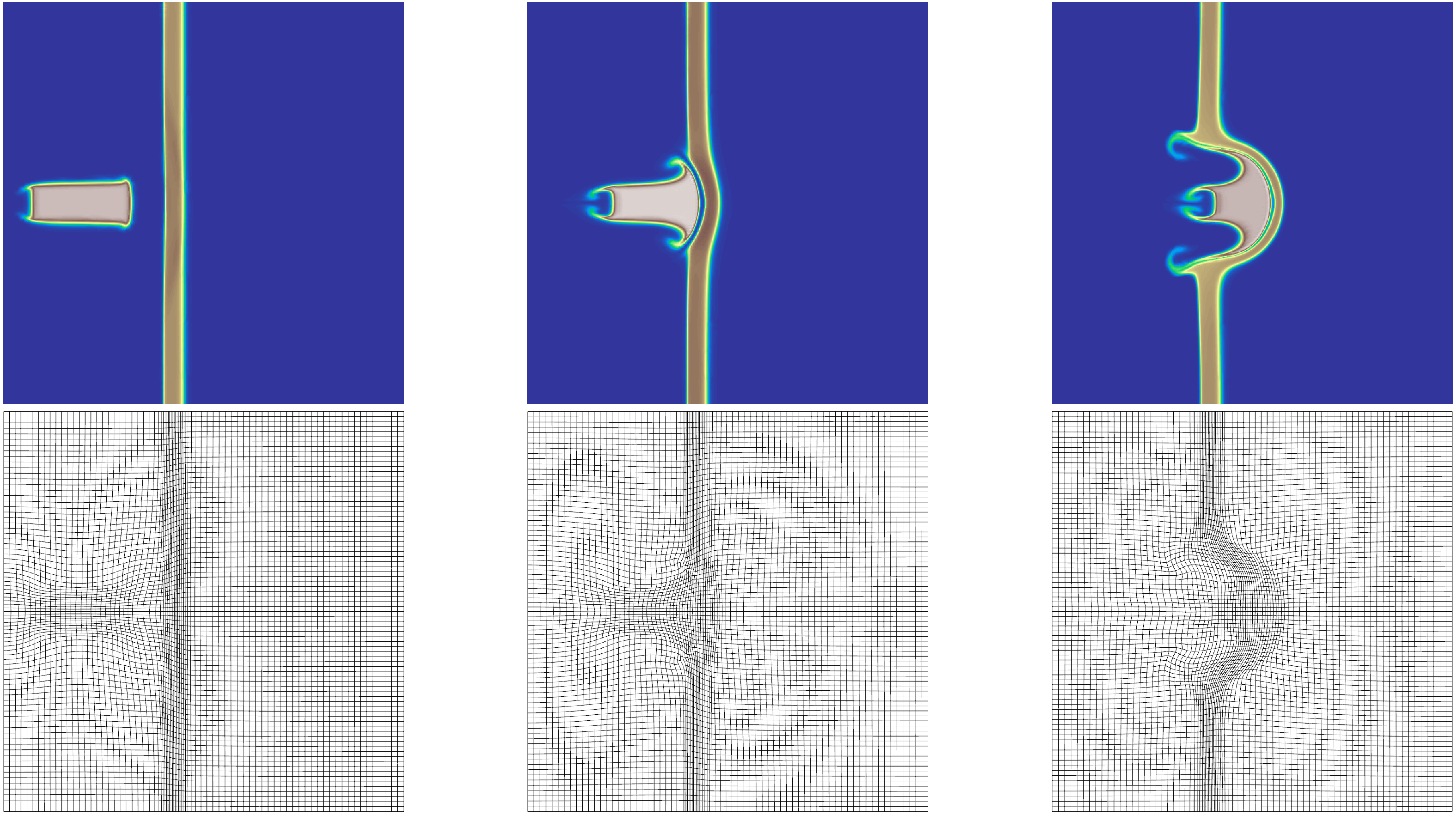
- S and W must be in sync!
  - Might get stuck otherwise.

- S can be adapted through η.

S = [volume] [orientation] [skew] [aspect ratio].

Example of r-adaptivity in an impact simulation

45000 Lagrange steps / 80 ALE steps / 690 pseudo advection steps



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Example of r-adaptivity in an impact simulation

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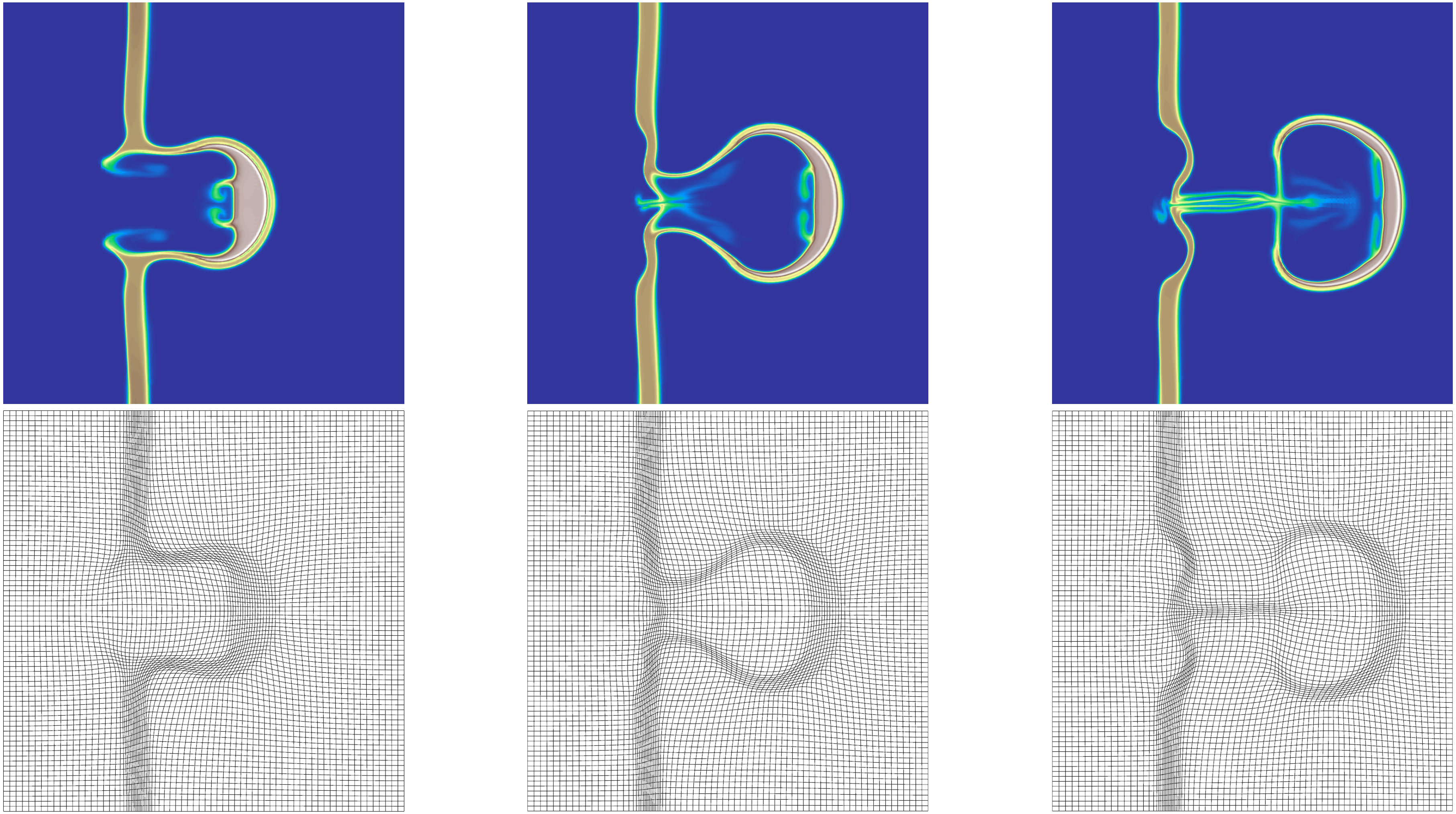
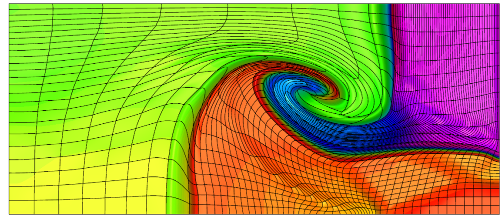


t = 6.0 *t* = 8.0 *t* = 10.0

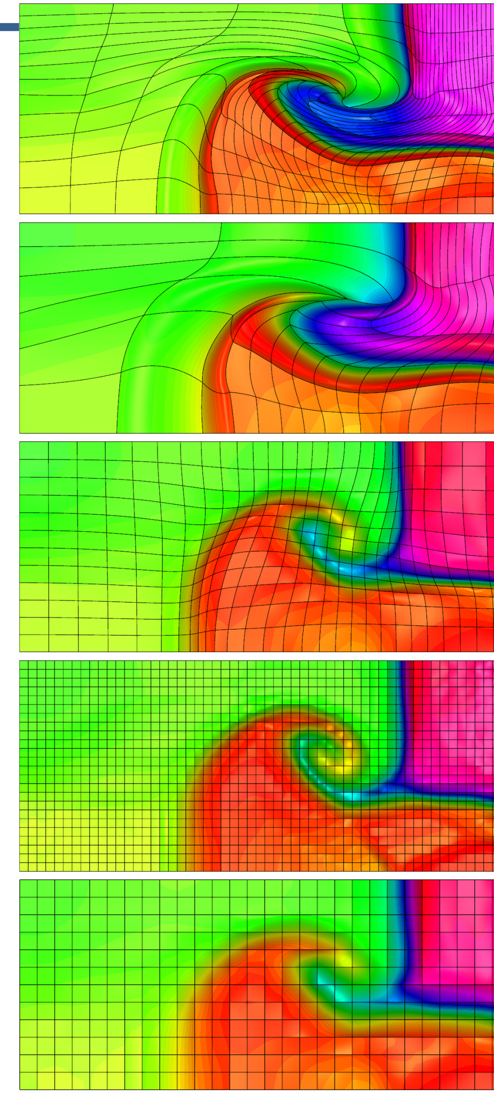
A more quantitative example

Solutions on different meshes are compared through interpolation

- Triple point to time 5, Q2Q1. Skew angle trigger at $\pi/4$.



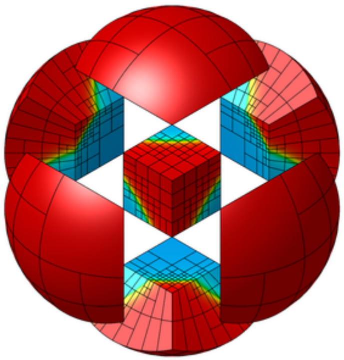
Method	Refs	L Cycles	Runtime	# ALE	Error
Lagrangian	2	93 833	-	0	0
Lagrangian	1	18 482	266	0	0.069
Lagrangian	0	3 034	11.2	0	0.138
Adapted to interfaces	1	1 577	54.4	19	0.099
Eulerian	2	1 508	134	21	0.098
Eulerian	1	802	18.5	11	0.143



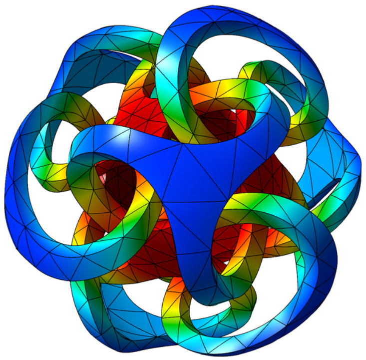
MFEM open source implementation

- All presented methods are (or will be) available in MFEM.

- MFEM contains **12** 2D metrics, **7** 3D metrics, all metric derivatives, **6** target construction methods.



mfem.org



glvis.org

- User interface provided by the ***mesh_optimizer*** and ***pmesh_optimizer*** miniapps.
  - Choice of target construction / quality metric / adaptivity fields / parameters.
  - Visualization through GLVis.

V. Dobrev, P. Knupp, Tz. Kolev, K. Mittal, V. Tomov, "The target-matrix optimization paradigm for high-order meshes", SISC, 2018.
V. Dobrev, P. Knupp, Tz. Kolev, V. Tomov, "Towards simulation-driven optimization of high-order meshes by the target-matrix optimization paradigm", IMR 2018 Proceedings.

Summary and future work

- The TMOP framework can be beneficial in ALE hydro.
  - Flexible adaptivity options.
  - Simulation-based ALE triggers.

- General framework for improving quality of high-order curved meshes.
  - Point-wise quality metrics + target constructions.
  - Sub-element control over shape / size / alignment.

- Extension to r-adaptivity based on discrete adaptivity fields.
  - Interpolation / advection to obtain values of η on intermediate meshes.
  - Additional derivative terms in the nonlinear solvers.

- Future work:
  - Approximate preservation of discrete surfaces.
  - Combination of TMOP and AMR adaptivity (hr-adaptivity).
  - Improved nonlinear solvers, physical interpolation, general TMOP components.

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Combinations of metrics and limiting terms

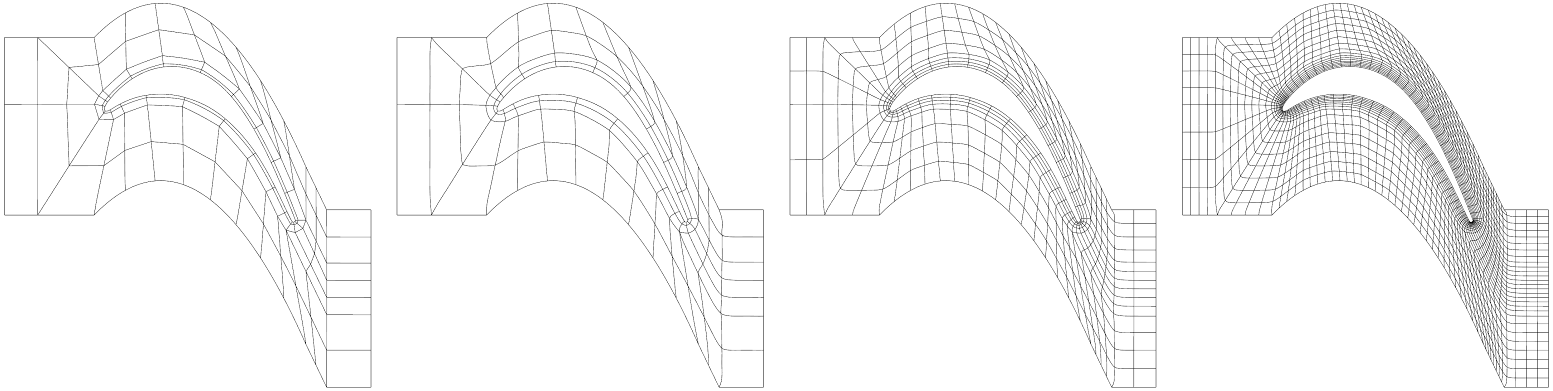
All terms are normalized relative to the unit value

- Users expect similar displacement under mesh refinement / change of units.
- Users expect reasonable, O(1) adjustable constants for each problem.

$$F(x) = \alpha \frac{1}{n} \frac{\sum_{E(x)} \int_{E_t} \mu_{i_1}(T)}{\sum_{E(x_0)} \int_{E_t} \mu_{i_1}(T_0)} + \dots \beta \frac{1}{n} \frac{\sum_{E(x)} \int_{E_t} \mu_{i_n}(T)}{\sum_{E(x_0)} \int_{E_t} \mu_{i_n}(T_0)} + \varepsilon \frac{\sum_E \int_{E_t} \frac{(x-x_0)^2}{d^2}}{\sum_E \int_{E_t} 1}$$

Behavior under refinement for fixed d 4th order mesh, Shape optimization

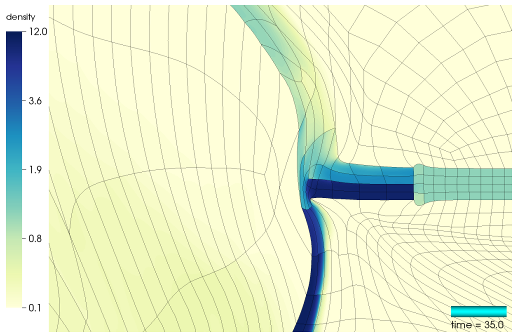
Refs	Final F	μ part	Limiting part	Max displacement
0	0.7548	0.6915	0.0632	0.0216
1	0.7542	0.6913	0.0629	0.0217
2	0.7541	0.6912	0.0628	0.0217



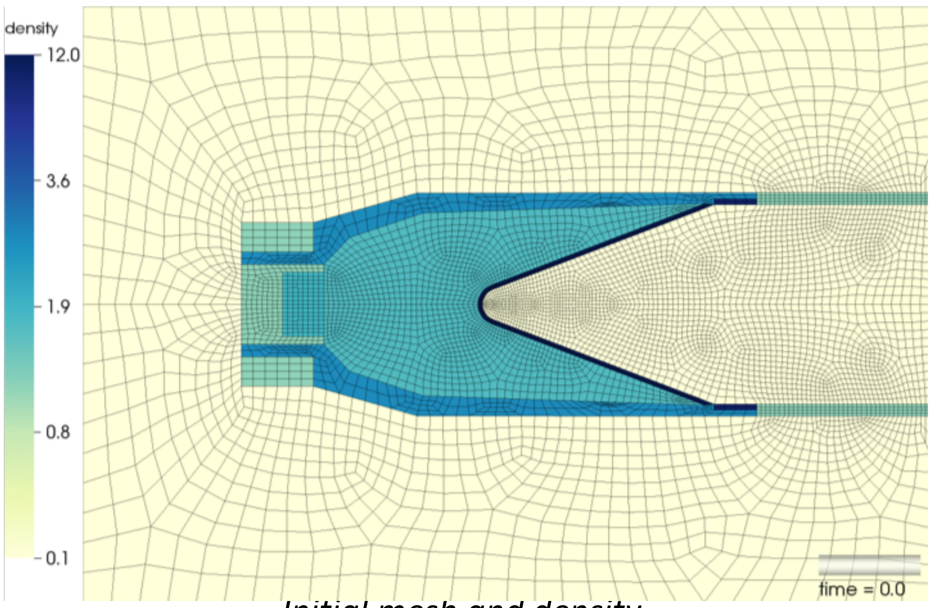
Feature preservation and local optimization

- Local optimization by using space-dependent d. No mesh motion for $d \to 0$.
- Applicable when the starting mesh has certain desirable features.

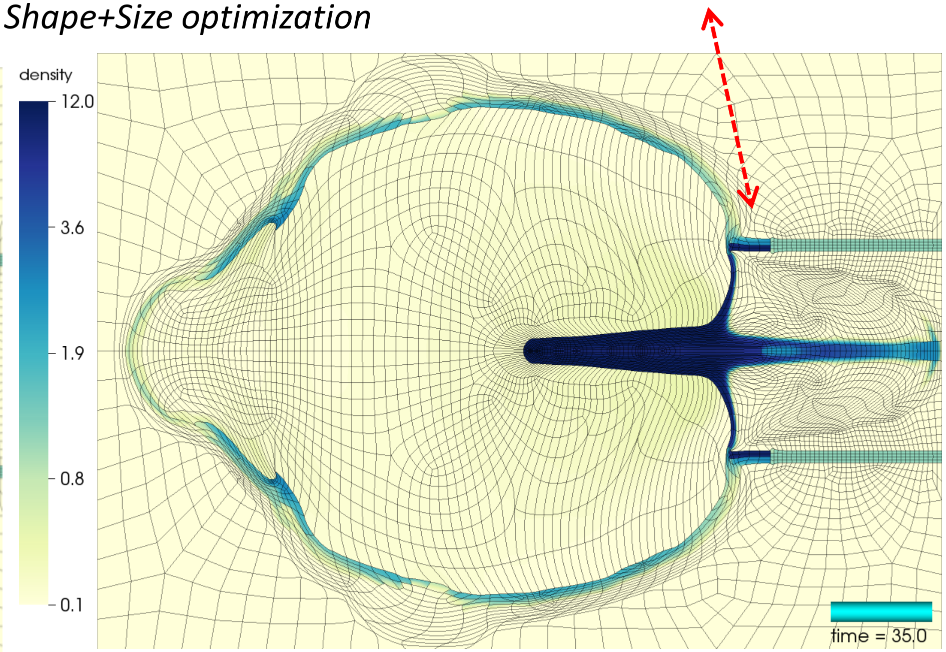
$$\sum_E \int_{E_t} \frac{(x - x_0)^2}{d^2}$$



Shaped charge simulation on an unstructured NURBS mesh, Shape+Size optimization



Initial mesh and density



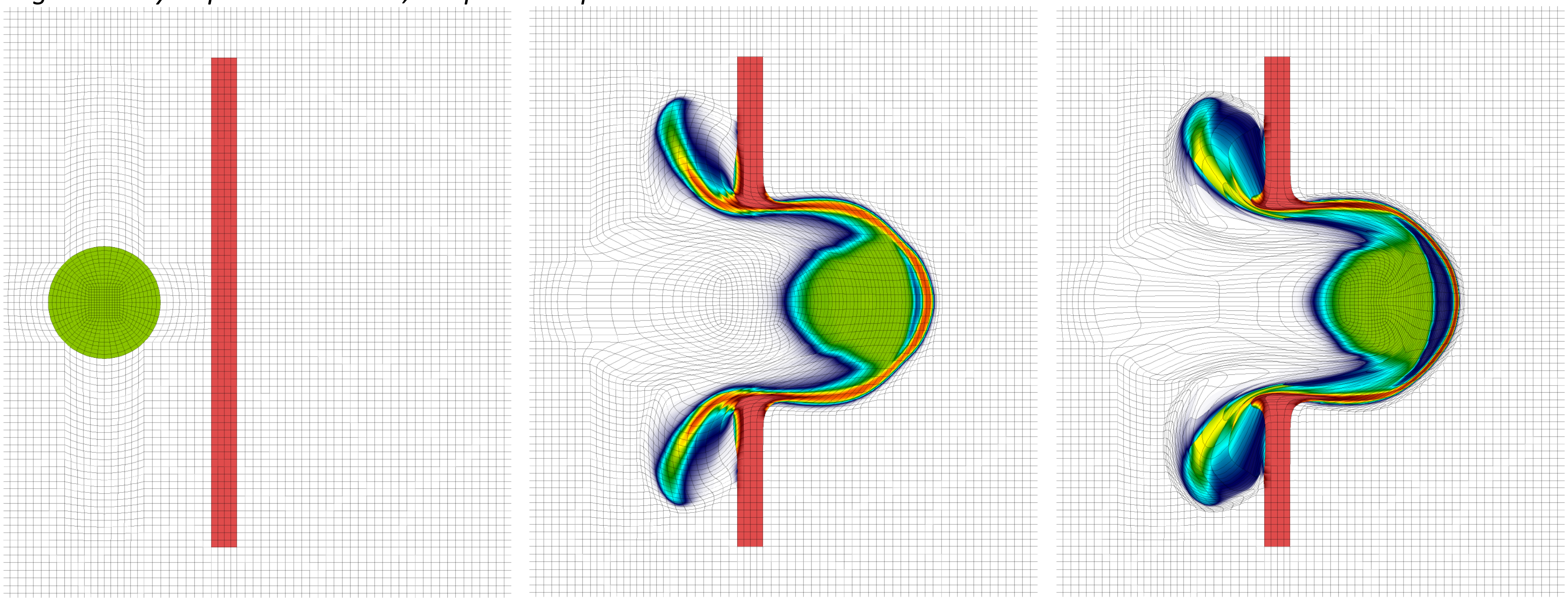
Mesh and density at final time

Feature preservation in moving mesh applications

- Optimization can be adapted to the problem dynamics. Example: $d \sim \alpha$[mesh displacement] in ALE simulations.
- Allows tradeoffs between mesh quality feature preservation.

$$\sum_{E} \int_{E_t} \frac{(x - x_0)^2}{d^2}$$

High-velocity impact simulation, Shape+Size optimization



Initial condition | *Higher d – better mesh / more diffusion* | *Lower d – worse mesh / less diffusion*