Recent advances in high-order mesh adaptivity using the target-matrix optimization paradigm

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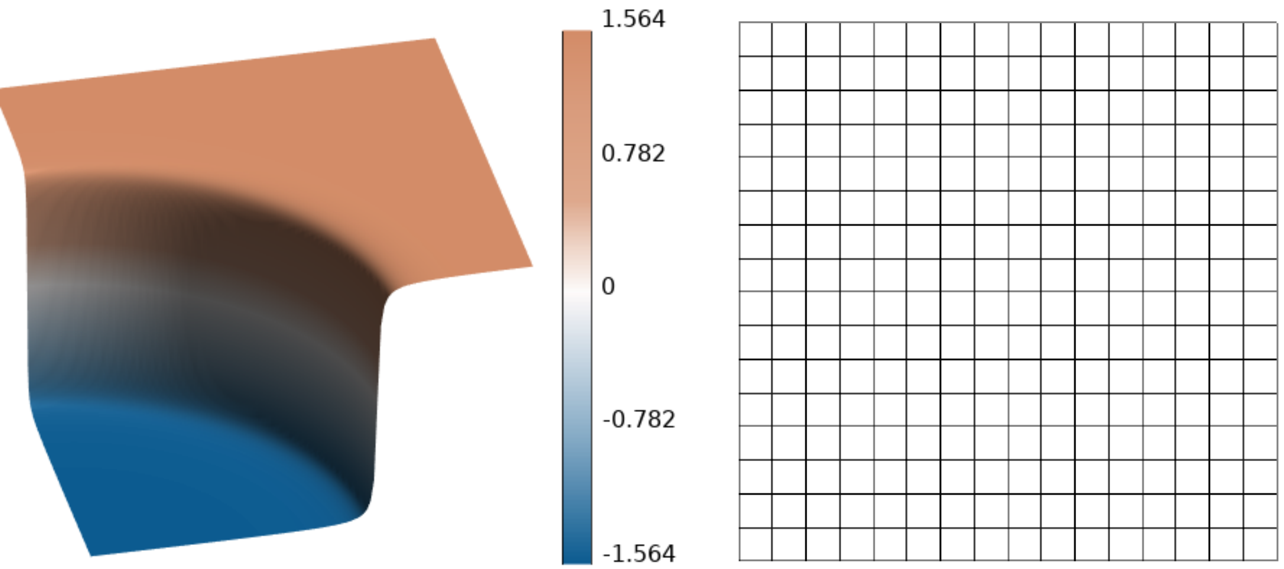
Overview

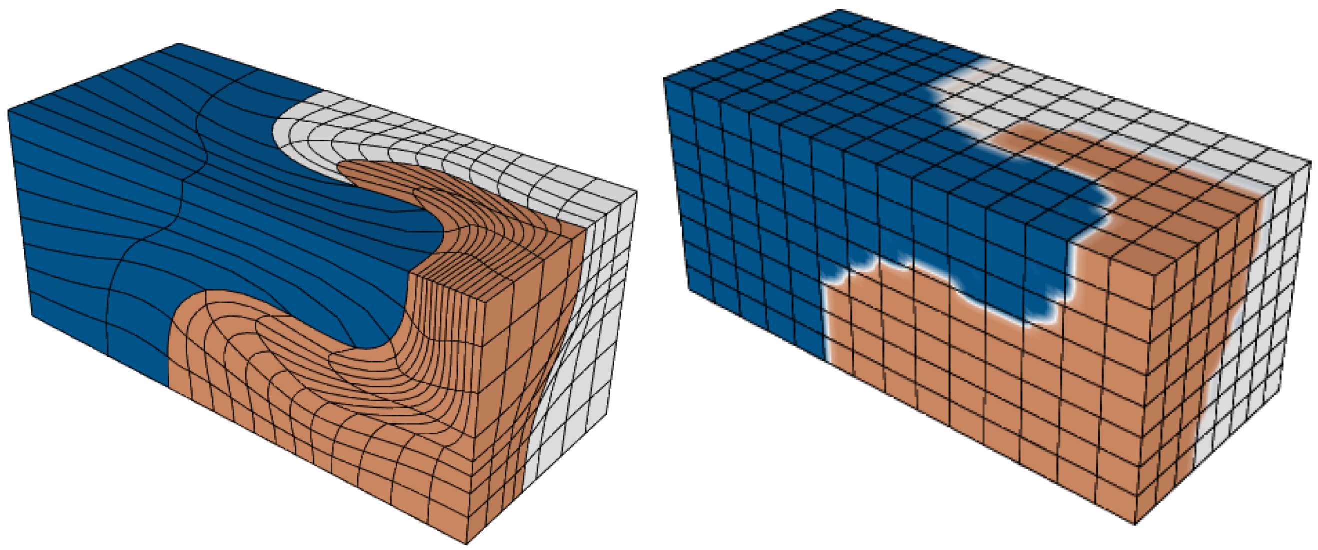
- Introduction
- Overview of Target Matrix Optimization Paradigm (TMOP) for r-adaptivity
- Recent advances
  - Target construction and mesh quality metrics
  - hr-adaptivity
  - Tangential relaxation and interface fitting
- Future work

Introduction

- Why mesh optimization?



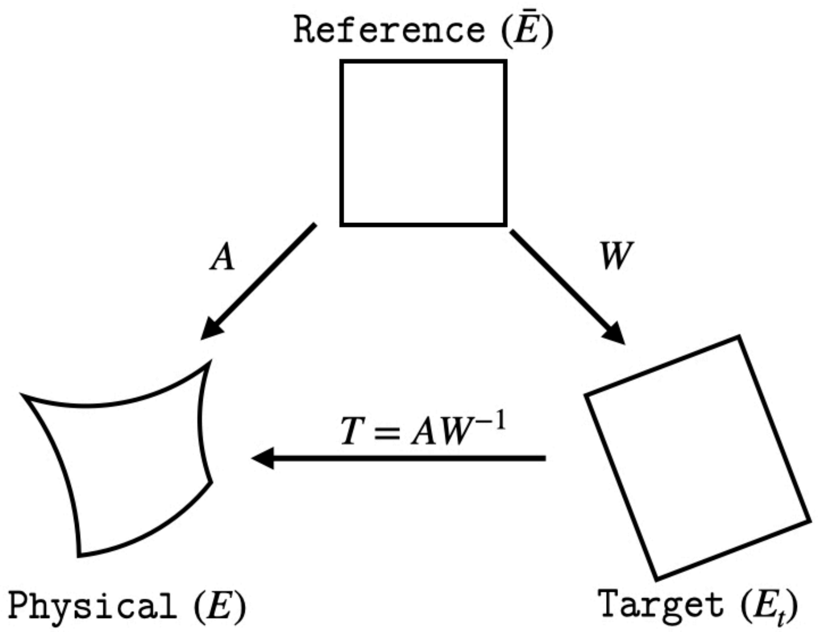
Outwards propagating shock wave



Multimaterial Lagrangian hydrodynamics

- Mesh optimization can help adapt the mesh to the solution and ultimately reduce error.
- Improve conditioning of the resulting system.

Target Matrix Optimization Paradigm (TMOP)



- Any Jacobian transformation can be represented using four geometric parameters:

$$W = \underbrace{\zeta}_{\text{[volume]}} \quad \underbrace{R}_{\text{[rotation]}} \quad \underbrace{Q}_{\text{[skewness]}} \quad \underbrace{D}_{\text{[aspect-ratio]}}$$

- The transformation T from the active to target element can be defined using the Jacobian transformation A and W.

TMOP Mesh Quality Metrics

- Quality metric $\mu(T)$ is a measure of the deviation between the active and target Jacobian transformation.

- Different metrics depend on different geometric parameters.

  - $\mathtt{Shape}$ metric - depends on Skew (*Q*) and Aspect-ratio (*D*). $\mu_2(T) = 0.5\frac{|T|^2}{\det(T)} - 1$

  - $\mathtt{Size}$ metric - depends on ζ. $\mu_{77}(T) = 0.5\left(\det(T) - \frac{1}{\det(T)}\right)^2$

  - Other kinds include $\mathtt{Alignment}$, $\mathtt{Shape} + \mathtt{Size}$, $\mathtt{Shape} + \mathtt{Alignment}$, etc.

  - We typically deploy $\mathtt{Shape} + \mathtt{Size}$ metrics but seldom also use $\mathtt{Alignment}$ metrics.

Node Movement with TMOP

- Using the quality metric and the Jacobian transformation T, the TMOP objective function is defined as:

$$F(\mathbf{x}) = \sum_{E \in \mathcal{M}} F_E(\mathbf{x}_E) = \sum_{E(\mathbf{x}_E)} \int_{E_t} \omega(\mathbf{x}) \mu(T(\mathbf{x})) d\mathbf{x}_t$$

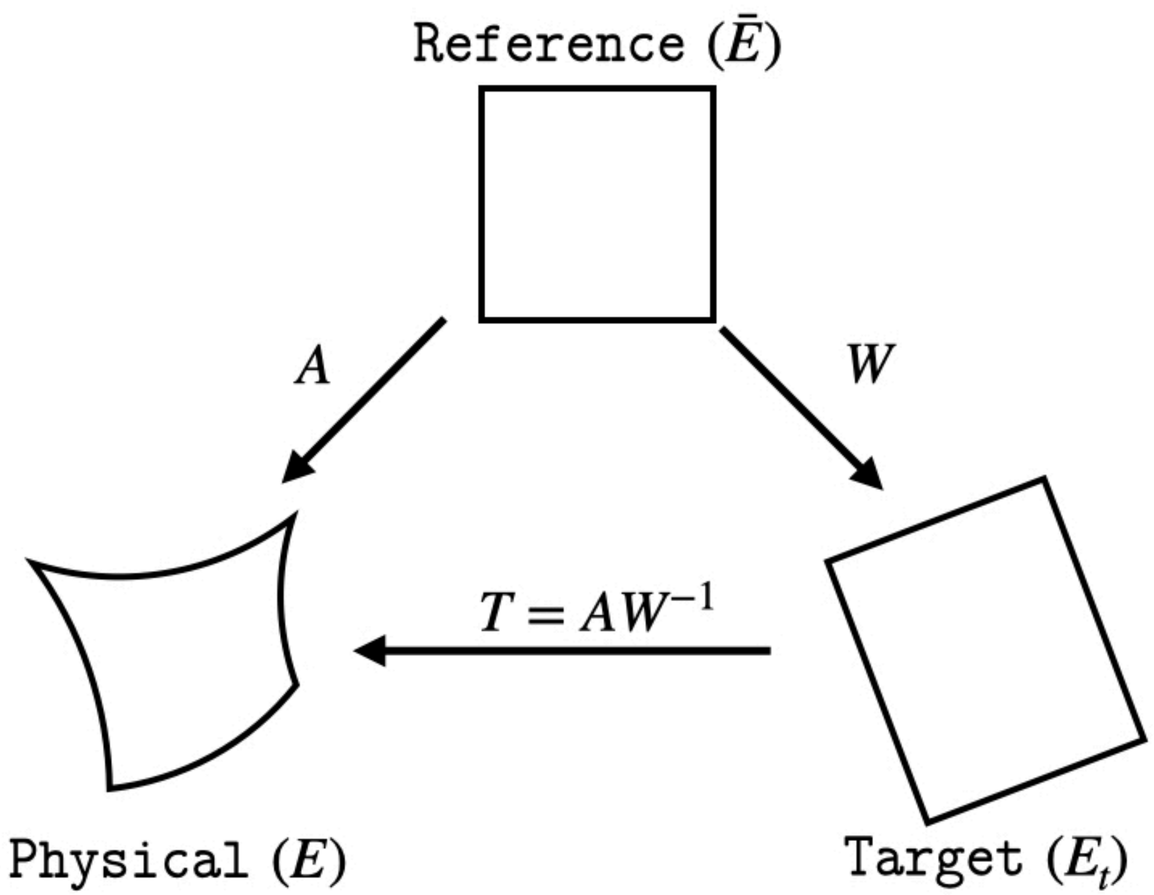
where $\mathbf{x}$ represents mesh coordinates, ω is a user-defined spatial weight. The element-by-element integral is computed as:

$$\sum_{E \in \mathcal{M}} \int_{E_t} \omega(\mathbf{x}_t) \mu(T(\mathbf{x}_t)) d\mathbf{x}_t = \frac{1}{N_E} \sum_{E \in \mathcal{M}} \sum_{\mathbf{x}_q \in E_t} w_q \det(W(\bar{\mathbf{x}}_q))\, \omega(\mathbf{x}_q) \mu(T(\mathbf{x}_q))$$

- In practice, we can use multiple metrics with different spatial weights.
- r-adaptivity - $F(\mathbf{x})$ is minimized using a technique such as the Newton's method to optimize the mesh [2].

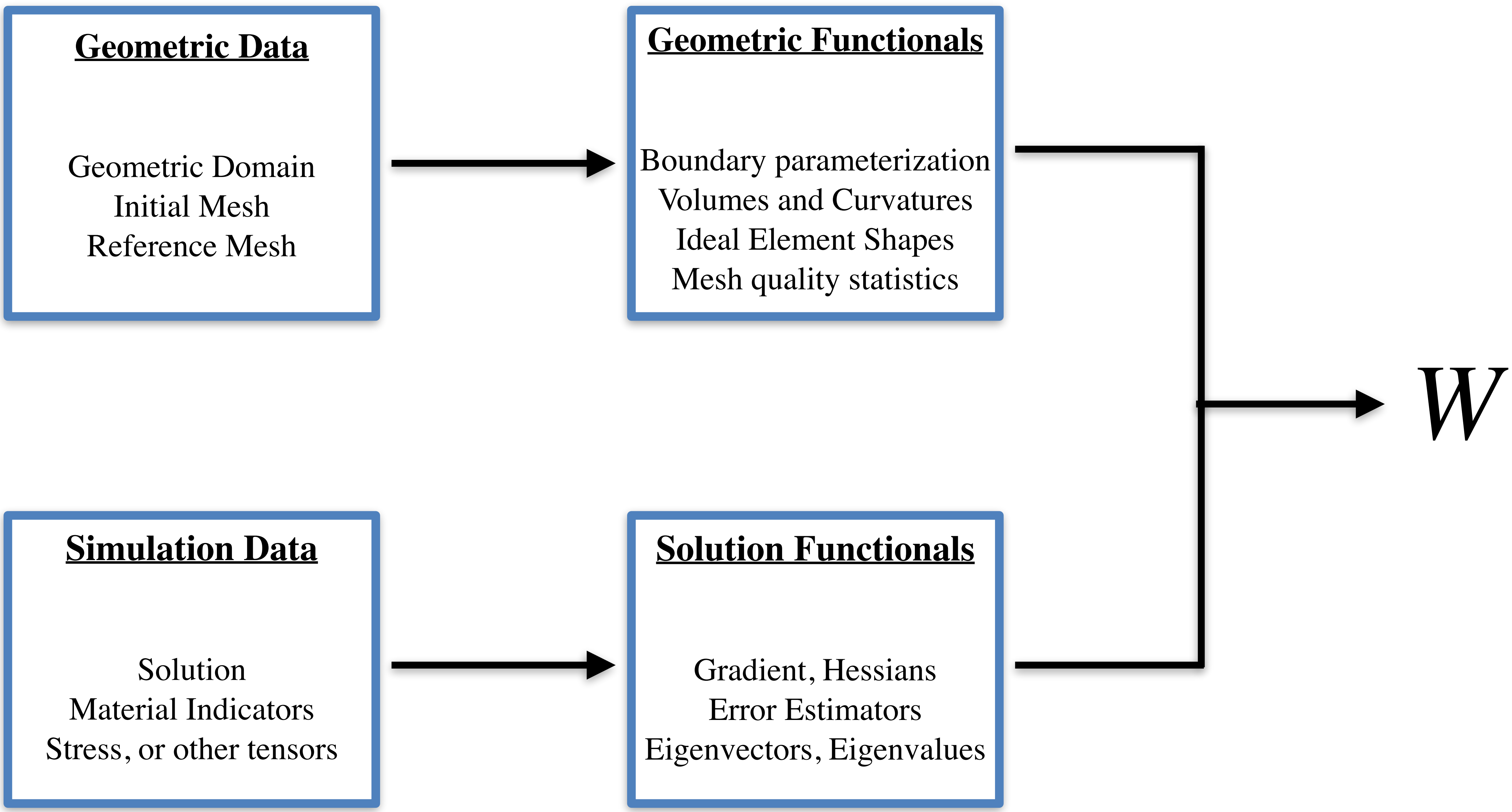
Target Construction & Mesh Quality Metric

- Use of TMOP relies on choice of W and a compatible quality metric satisfying certain convexity requirements.
- Recent developments have advanced the state-of-the-art on both fronts.



Target Construction

- Knupp describes various techniques with examples in “Target formulation and construction in mesh quality improvement”, LLNL-TR-795097.



Metric polyconvexity

- Existence of minimum can be established, in part, by showing that the metric is polyconvex [Garanzha].

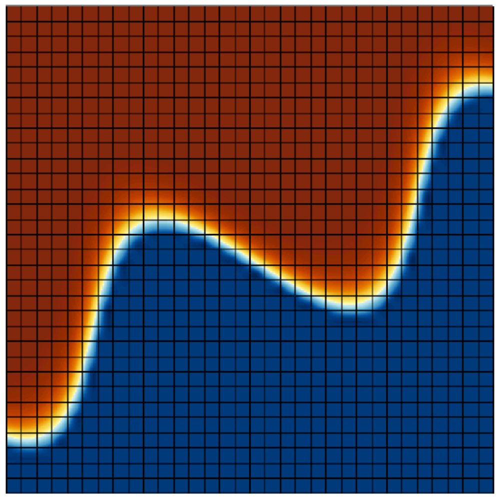
- Knupp has developed various metrics for TMOP in "*Metric type in the target-matrix mesh optimization paradigm*", LLNL-TR-817490.

  - Over 100 different metrics divided into 8 Types based on geometric properties.

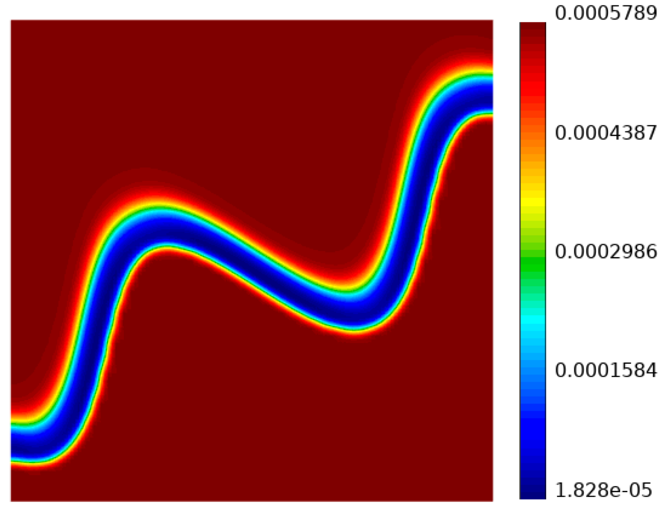
  - Analyzes polyconvexity of each metric.

  - Determined at-least one polyconvex metric for $\mathtt{Shape}$, $\mathtt{Shape} + \mathtt{Size}$, $\mathtt{Orientation} + \mathtt{Size}$, and $\mathtt{Shape} + \mathtt{Orientation} + \mathtt{Size}$.

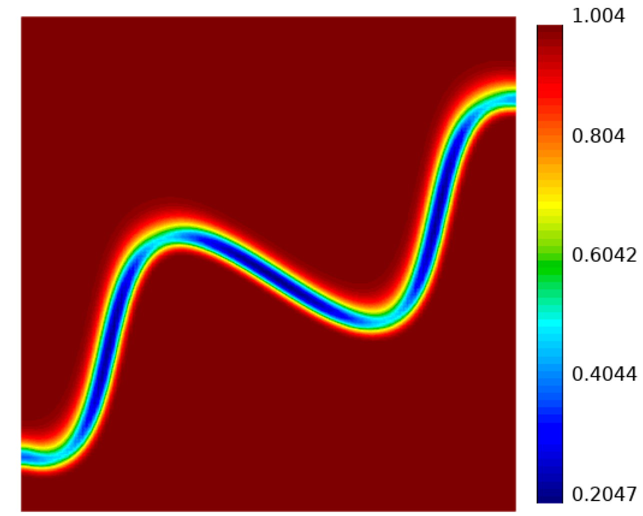
Simulation-driven Adaptivity



Simulation data material indicator (η)



Size - $\zeta \propto 1/|\nabla \eta|$



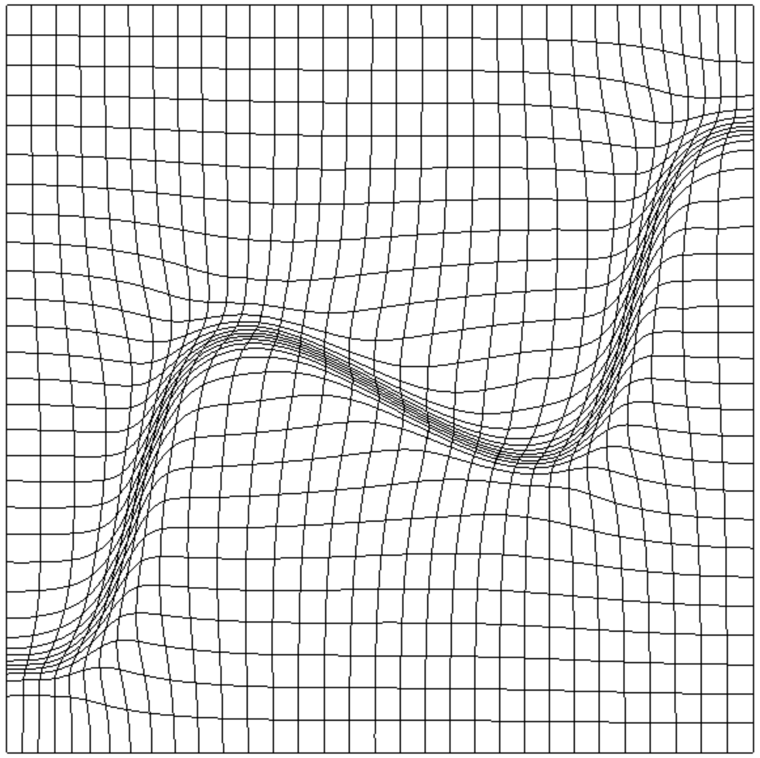
Aspect-Ratio - $\rho \propto |\eta_x/\eta_y|$

$$W = \sqrt{\zeta}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix}1 & \cos\phi\\ 0 & \sin\phi\end{bmatrix}\begin{bmatrix}\frac{1}{\sqrt{\rho}} & 0\\ 0 & \sqrt{\rho}\end{bmatrix},$$

- $\phi = \frac{\pi}{2}$ for an ideal square.
- Use a $\mathtt{Shape} + \mathtt{Size}$ polyconvex metric, $\mu_{80} = (1-\gamma)\mu_2 + \gamma\mu_{77}$.

$$\mu_2(T) = 0.5\frac{|T|^2}{\det(T)} - 1 \qquad \mu_{77}(T) = \frac{1}{2}(\tau - \frac{1}{\tau})^2$$

- Note: η must be remapped between and after Newton iterations.

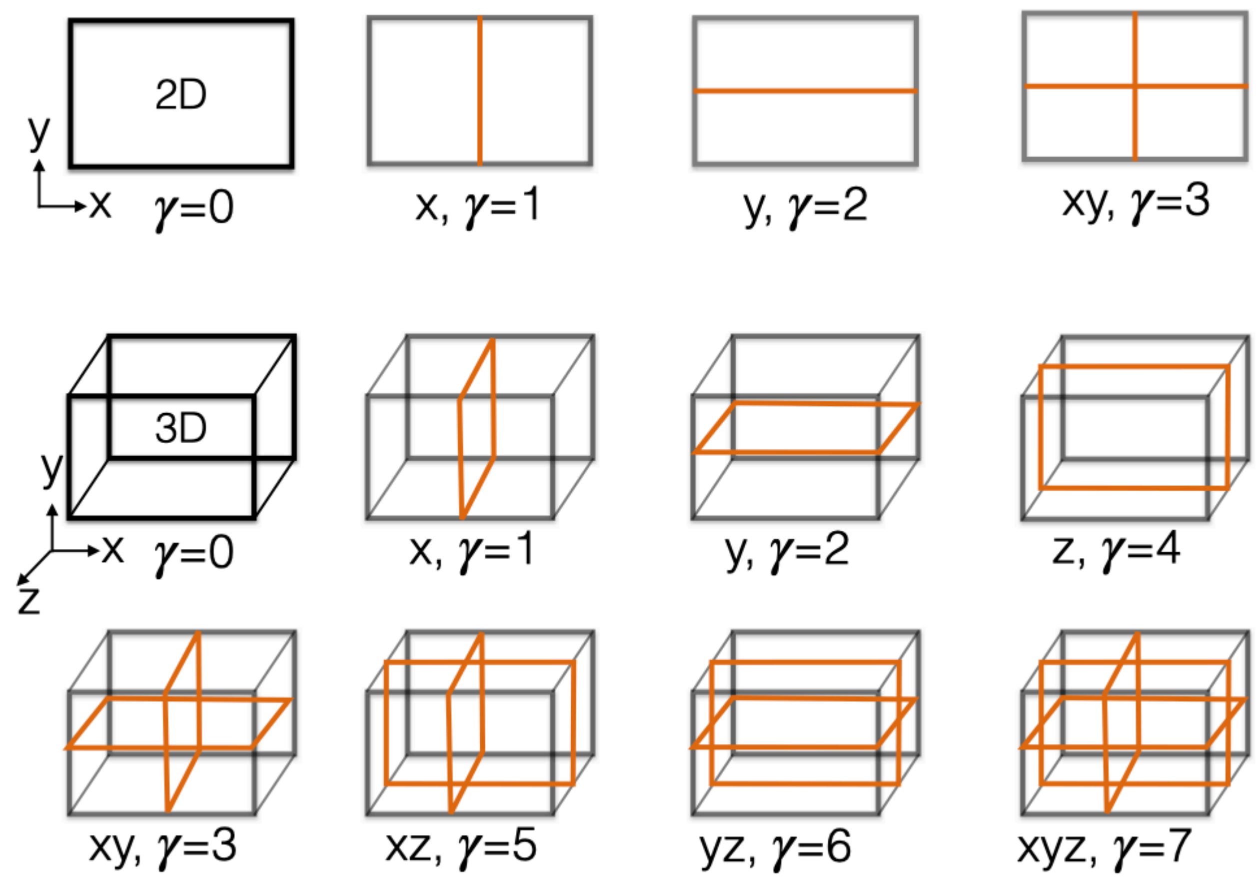


"*Simulation-driven optimization of high-order meshes in ALE hydrodynamics.*" Computers & Fluids 208 (2020): 104602.

hr-adaptivity

- Effectiveness of r-adaptivity can be limited due to the topology of the original mesh.
- h-adaptivity introduces addition degrees of freedom by splitting existing elements.
- Nonconforming high-order mesh refinement framework introduced by Cerveny et al. [6]
  - Supports **nonconforming isotropic** and **anisotropic** refinement/derefinement in 2D and 3D for **triangles/quads** and **tetrahedrons/cubes**.
  - Requires use of an error estimator for refinement/derefinement decisions during simulation.

AMR for Mesh Optimization



Different types of refinements for a quad and a cube

- Anisotropic refinements impact the shape and size of an element, and isotropic refinement impacts only the size of an element.
- Refinements also impact skew, but this impact cannot be directly controlled.

TMOP-based Refinement Error Estimator

- Based on μ, define Γ as the set of refinement types to be considered:
  - $\mathtt{Shape}$ metric - $\gamma = 1{,}2$ in 2D and 1-6 in 3D.
  - $\mathtt{Size}$ metric - $\gamma = 3$ in 2D and 7 in 3D.
  - $\mathtt{Shape} + \mathtt{Size}$ metric - $\gamma = 1 - 3$ in 2D and 1-7 in 3D.
- For a given element E and refinement type $\gamma \in \Gamma$:

Difference in energy for a given refinement. → $$\Delta F_E^{\gamma} = F_E^{\gamma=0} - \frac{F_E^{\gamma}}{N_c},$$

Sum of TMOP energy for children of a given element. → where $F_E^{\gamma} = \sum_{i=1}^{N_c} F_{E_c}$

TMOP energy for a given element. → $$F_E = \sum_{\mathbf{x}_q \in E_t} w_q \det(W(\bar{\mathbf{x}}_q))\, \omega(\mathbf{x}_q) \mu(T(\mathbf{x}_q))$$

- Refinement type is picked based on: $\max_{\gamma} \Delta F_E^{\gamma},\ \gamma \in \Gamma$

TMOP-based Derefinement Error Estimator

- Derefinement is important for time-dependent problems where regions that require resolution can change with time.
- Elements that are already refined, are considered for derefinement:
  - If E_p is an element that was refined to span N_c children at a previous iteration:

Difference in energy for a derefinement.

$$\Delta F_{E_p} = \sum_{i=1}^{N_c} \frac{F_{E_c}}{N_c} - F_{E_p}$$

- ΔF_E^γ for refinement and ΔF_{E_p} for derefinement are compliments of each other.
- Note: Determining ΔF_E^γ and ΔF_{E_p} requires the discrete functions to be mapped between children and parent elements.

hr-adaptivity

$\mathbf{x_0}$ - original mesh
μ - TMOP quality metric
ϵ - Newton convergence
N_h - h-adaptivity iterations per step.

Target construction

N_R - Number of elements refined at previous iteration
N_D - Number of elements derefined at previous iteration

r-adaptivity with Newton's method (ϵ)

N_h iterations of h-adaptivity

- Note: quality metric can be different for *r*- and *h*-adaptivity component.

Algorithm 1: $hr-$adaptivity

Input: $\mathbf{x}_0$, μ, ε, N_h.

Output: $\mathbf{x}_s$ (initialized to $\mathbf{x}_0$).

Construct W_i for each integration-point i using target-construction.

while $N_R \neq 0$ `or` $N_D \neq 0$ **do**

  $r-$adaptivity:

  $\mathbf{x}_s \rightarrow \arg\min_{\mathbf{x}} \sum_{E \in \mathscr{M}} \sum_{\mathbf{x}_q \in E_t} w_q \det(W(\bar{\mathbf{x}}_q))\, \omega(\mathbf{x}_q) \mu(T(\mathbf{x}_q))$.

  $h-$adaptivity:

  for $i \in 1 \ldots N_h$ **do**

    $\forall\ E_p \in \mathscr{M}$, determine ΔF_{E_p}.

    Derefine element E_p if $\Delta F_{E_p} > 0$.

    $\forall\ E \in \mathscr{M}$, determine $\Delta F_E^\gamma\ \forall\ \gamma \in \Gamma$.

    Refine element E based on $\max_\gamma \Delta F_E^\gamma$.

  end

end

[Derefinement estimator]

[Refinement estimator]

2D Benchmark Using Poisson Equation

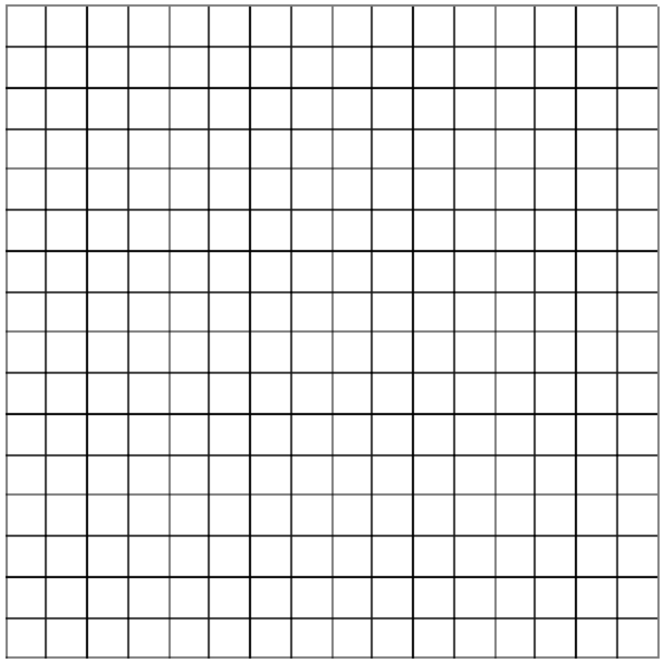
- Solve the Poisson problem:

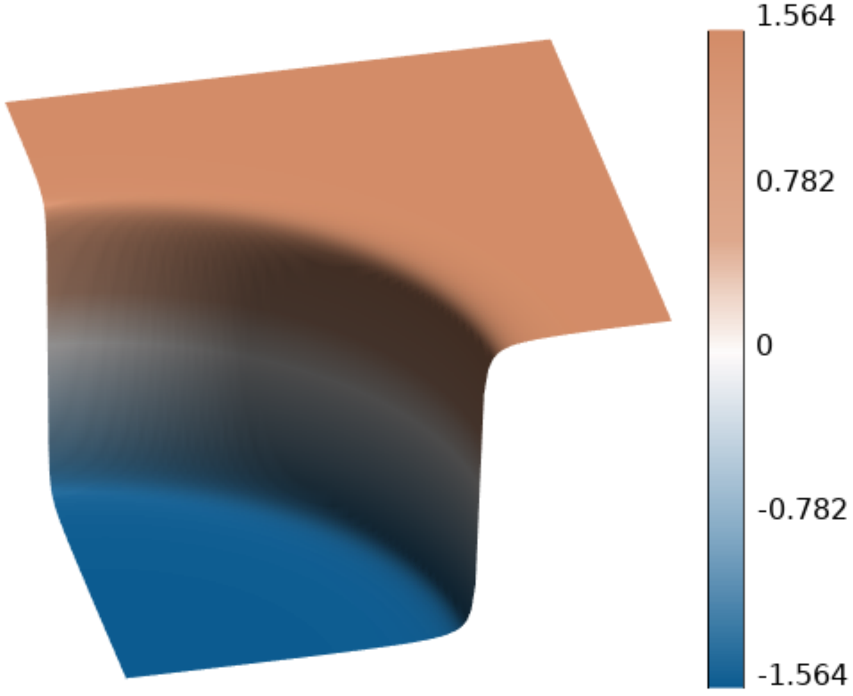
$$\nabla^2 u = f, \qquad \Omega = [0,1]^2$$

with a known exact solution to mimic a sharp circular wave front of radius r centered at (x_c, y_c)

$$u = \arctan\left[\alpha\left(\sqrt{(x-x_c)^2 + (y-y_c)^2} - r\right)\right]$$

- $\alpha = 200,\ (x_c, y_c) = (-0.05, -0.05),\ r = 0.7$



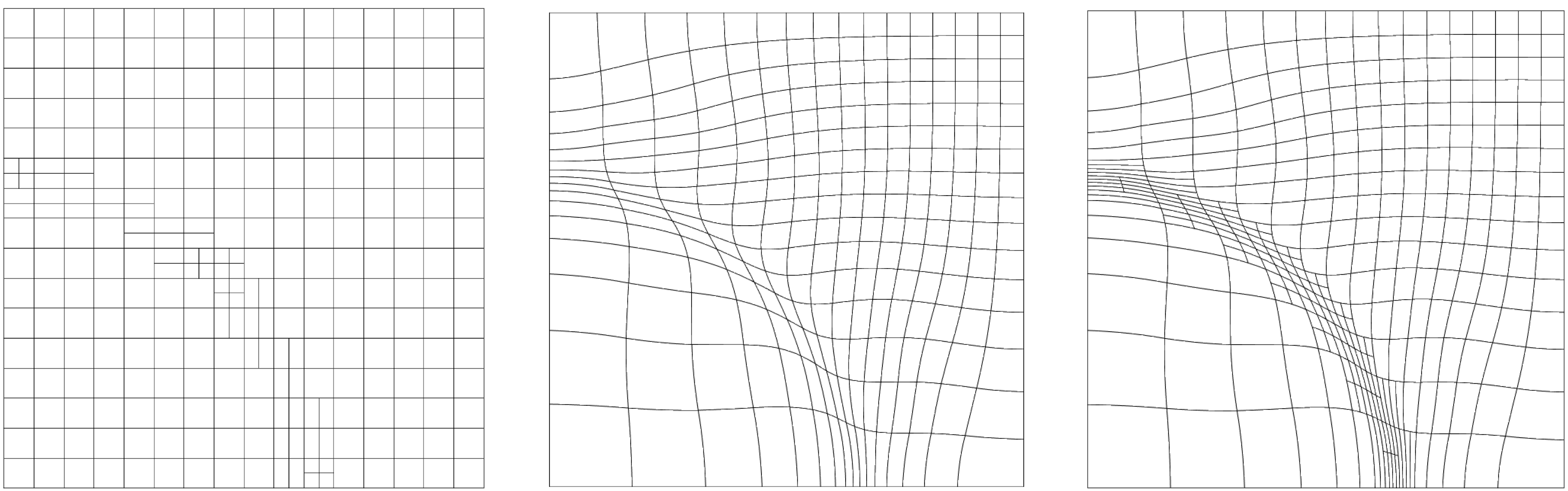


2D Benchmark Using Poisson Equation

- Target construction using gradient of the discrete function on the mesh, as earlier.

$$W = \sqrt{\zeta}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}\begin{bmatrix}1 & \cos\phi\\0 & \sin\phi\end{bmatrix}\begin{bmatrix}\frac{1}{\sqrt{\rho}} & 0\\0 & \sqrt{\rho}\end{bmatrix}$$

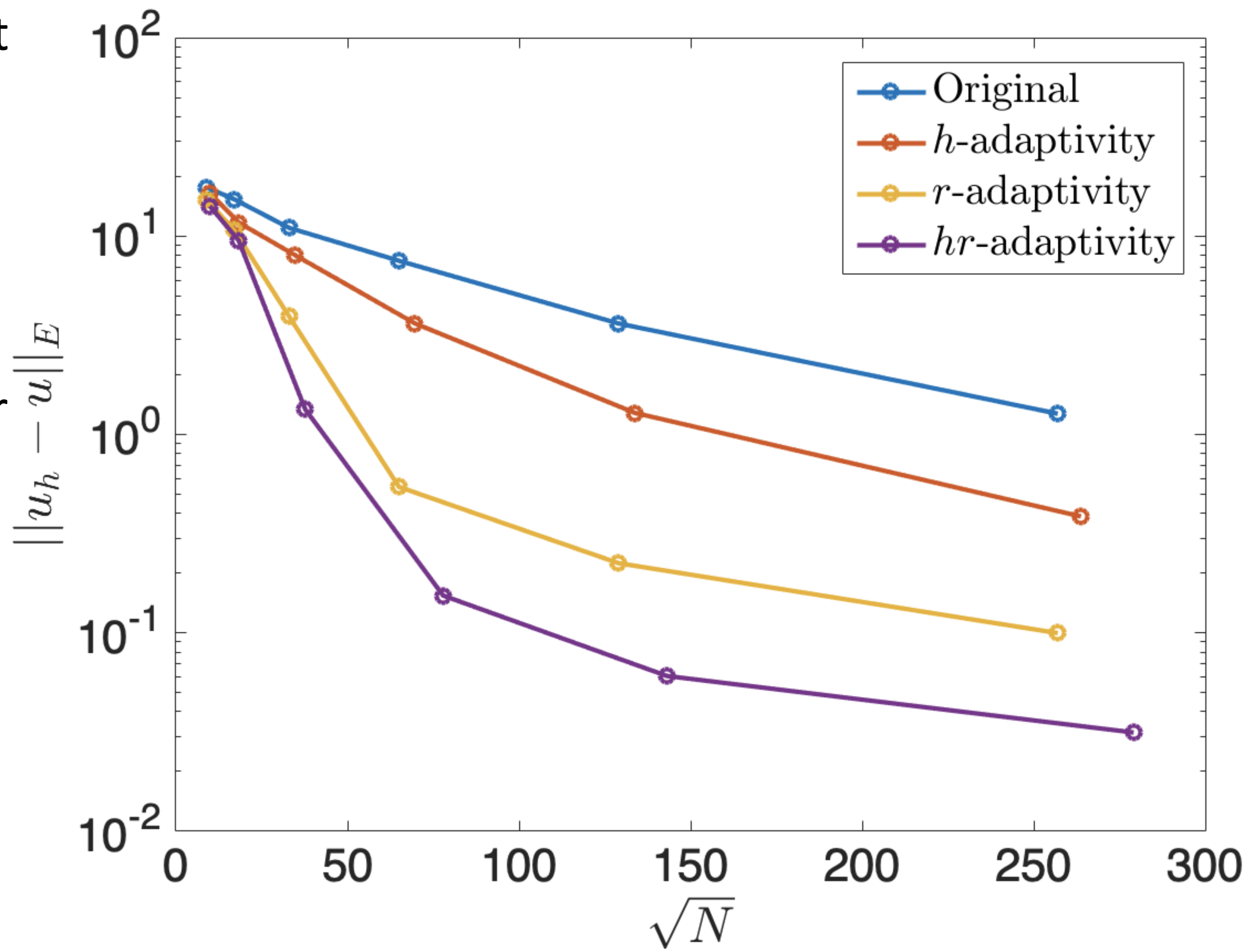
- To compare *h*-, *r*-, and *hr*-adaptivity, we start with a mesh and do 1 iteration of *h*- and/or *r*-adaptivity, using a $\texttt{Shape} + \texttt{Size}$ metric



h-adaptivity r-adaptivity hr-adaptivity

2D Benchmark Using Poisson Equation

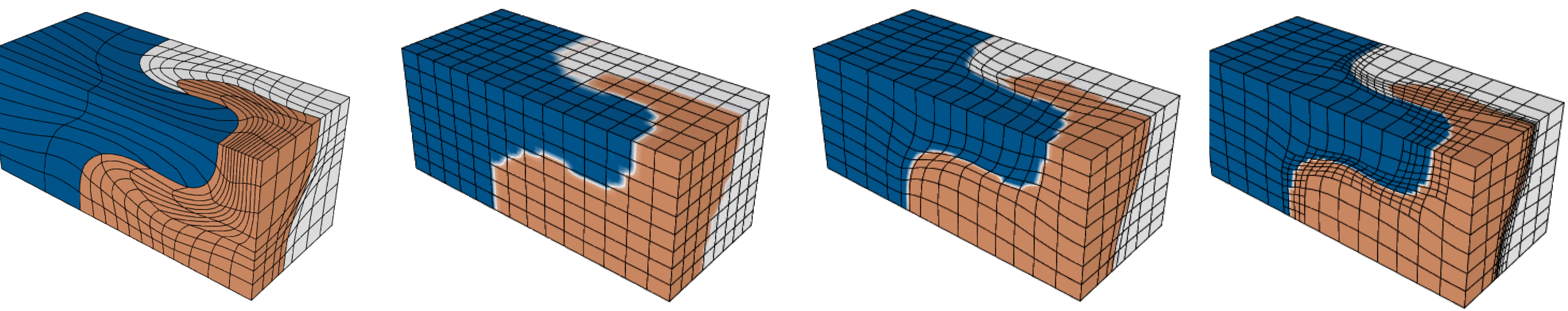
- Error comparison for different adaptivity techniques shows effectiveness of *hr*-adaptivity.
- *hr*-adaptivity requires 66% fewer degrees of freedoms in comparison to *r*-adaptivity for a given accuracy in the solution.



Application to ALE Hydrodynamics

- Triple point problem using Laghos in MFEM.
- Large mesh deformations lead to mesh tangling in Lagrangian framework.
- TMOP-based *r*- and *hr*-adaptivity improves mesh quality and provides resolution in regions with material interaction.

$$e = \int_\Omega \left(\eta_L(\mathbf{x}_L) - \eta(\mathbf{x}_s) \right)^2$$



(a) Lagrangian mesh $\eta_L(\mathbf{x}_L)$ (b) Original mesh $e = 1.71$ (c) *r*-adaptivity $e = 0.62$ (d) *hr*-adaptivity $e = 0.078$

"*hr-Adaptivity for nonconforming high-order meshes with the target matrix optimization paradigm.*" Engineering with Computers (2021): 1-17.

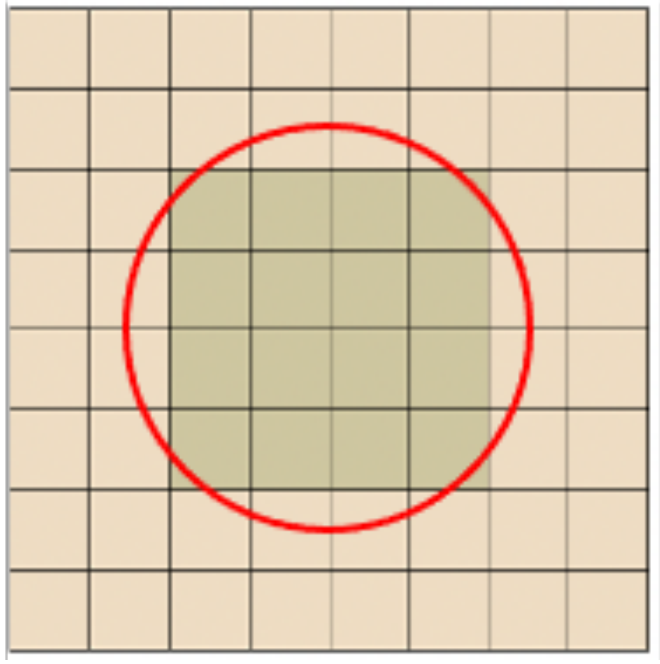
Adaptive Interface Fitting

- The surface of interest is given as a discrete level set (no analytic parametrization).

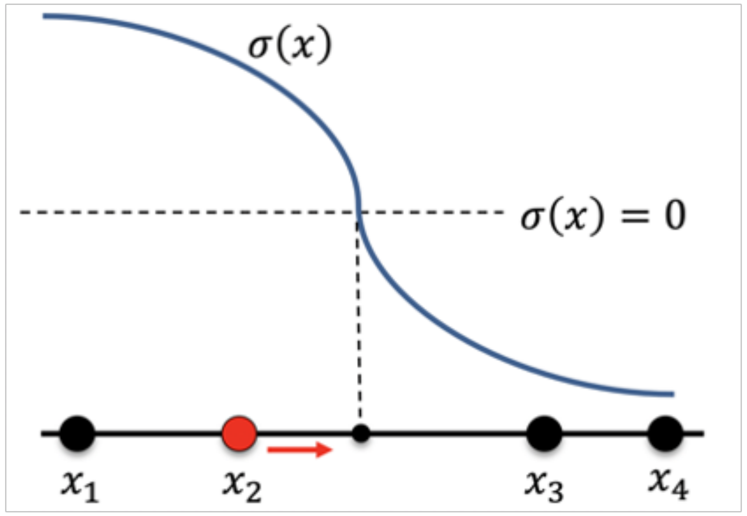
- Penalty formulation (quality / fitting tradeoff).
  - All mesh nodes move simultaneously.
  - One approach for fitting / tangential relaxation.

$$F(x) = F_\mu + w_\sigma \int_\Omega \bar{\sigma}(x)^2$$

- The restricted level set function $\bar{\sigma}$ penalizes the deviation from the zero level set.
  - Marking is not a trivial procedure.



Multimaterial mesh with target level set



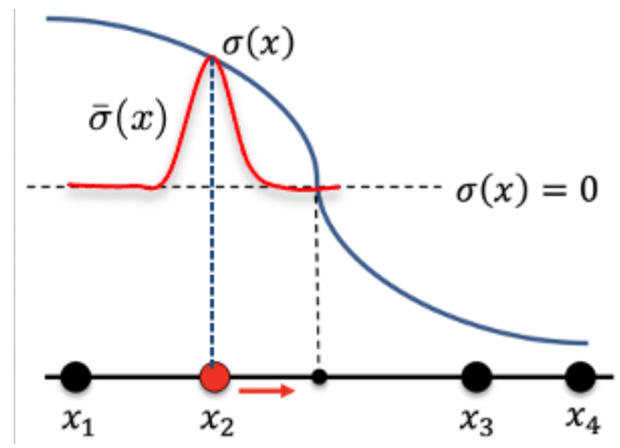
The extra term affects only the position of the red DOF

Adaptive Interface Fitting

- We restrict σ to the set of marked nodes:

$$\bar{\sigma}_i = \begin{cases} \sigma_i & \text{if } i \in \mathcal{S}, \\ 0 & \text{otherwise.} \end{cases}$$

- Goal: move the mesh so that $\sigma_i \equiv \sigma(\mathbf{x}_i) = 0$.
  - Interpolatory finite element basis functions.



- Requires derivative computation, $\frac{\partial \sigma}{\partial \mathbf{x}}$, and transfer of $\sigma(\mathbf{x}_0)$ as the mesh moves during optimization.

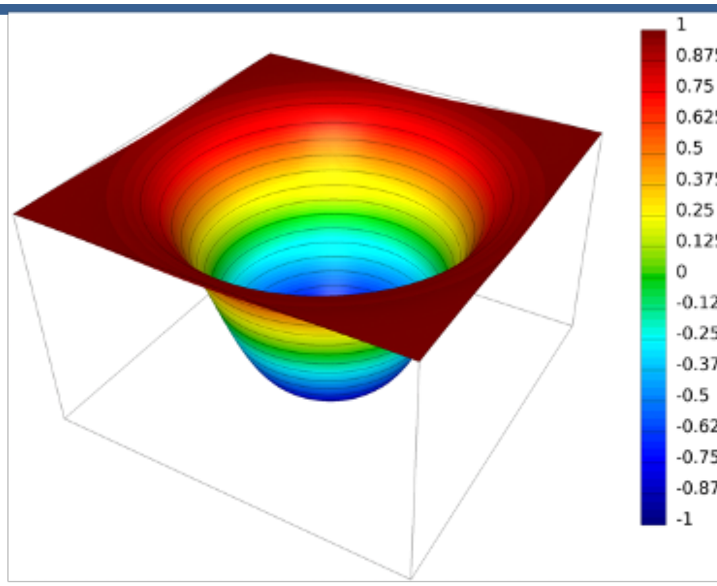
"Adaptive Surface Fitting and Tangential Relaxation for High-Order Mesh Optimization", International Meshing Roundtable, 2021.

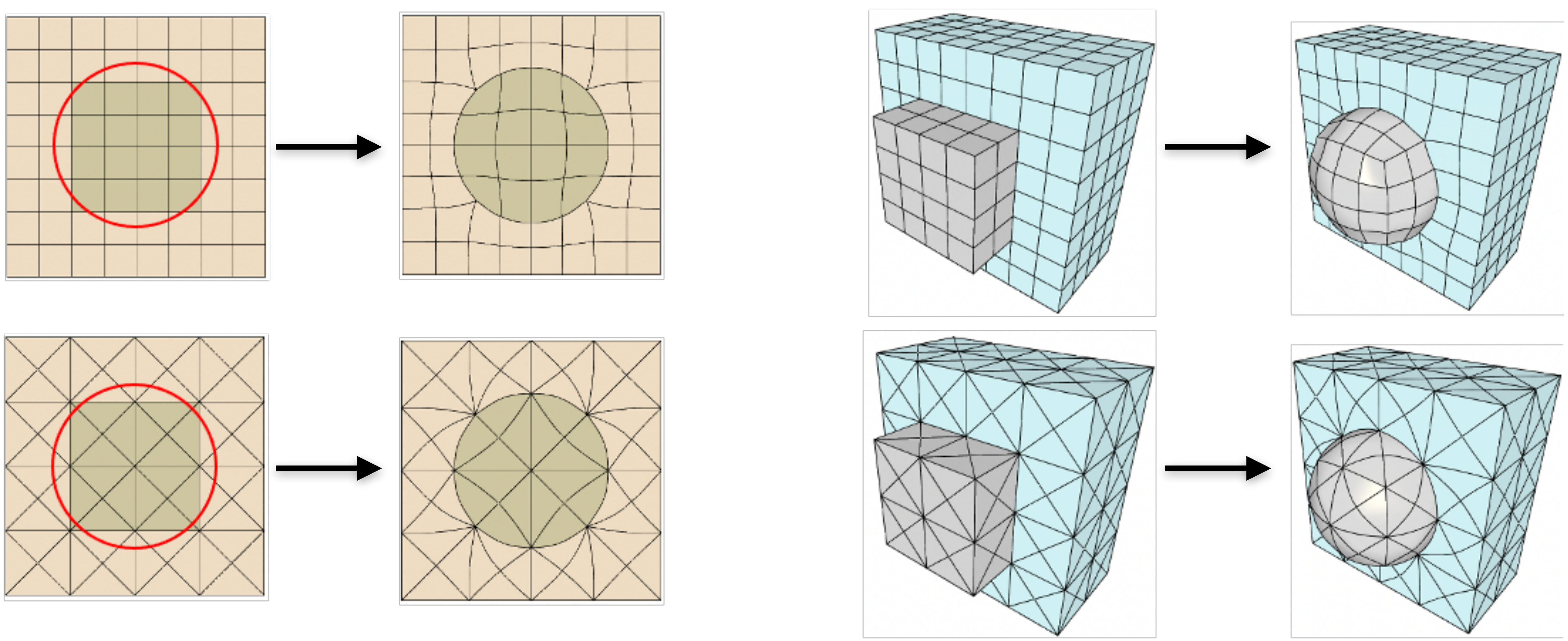
Adaptive Interface Fitting

- In all cases σ is a discrete FE function.
  - Ball at the center of the domain.

2D metric: $$\mu_{80} = (1-\gamma)\left(0.5\frac{|T|^2}{\tau} - 1\right) + \gamma\left(0.5\left(\tau - \frac{1}{\tau}\right)^2\right)$$

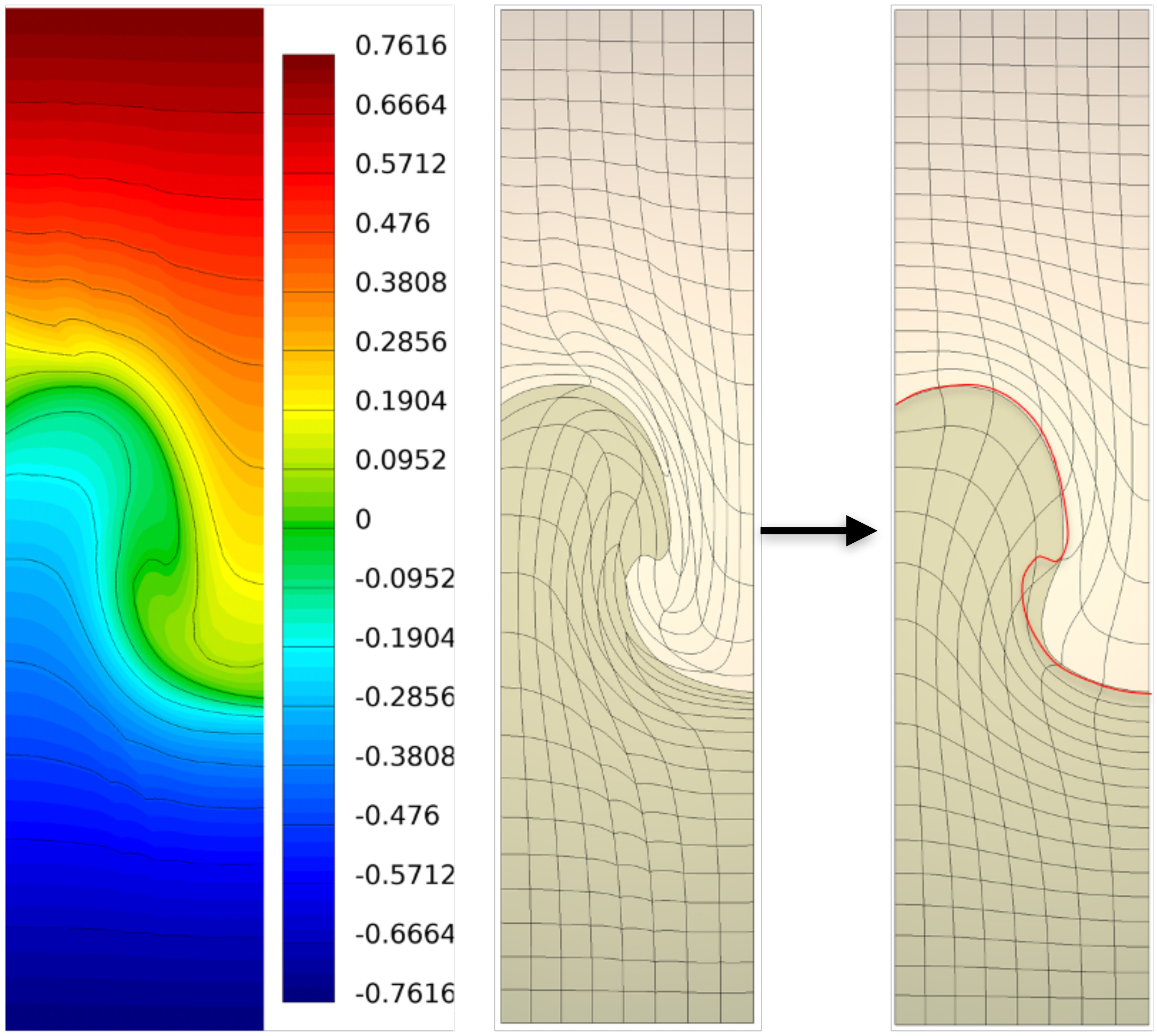
3D metric: $$\mu_{333} = (1-\gamma)\left(\frac{|T|^2|T^{-1}|^2}{9} - 1\right) + \gamma\left(0.5\left(\tau + \frac{1}{\tau}\right) - 1\right)$$

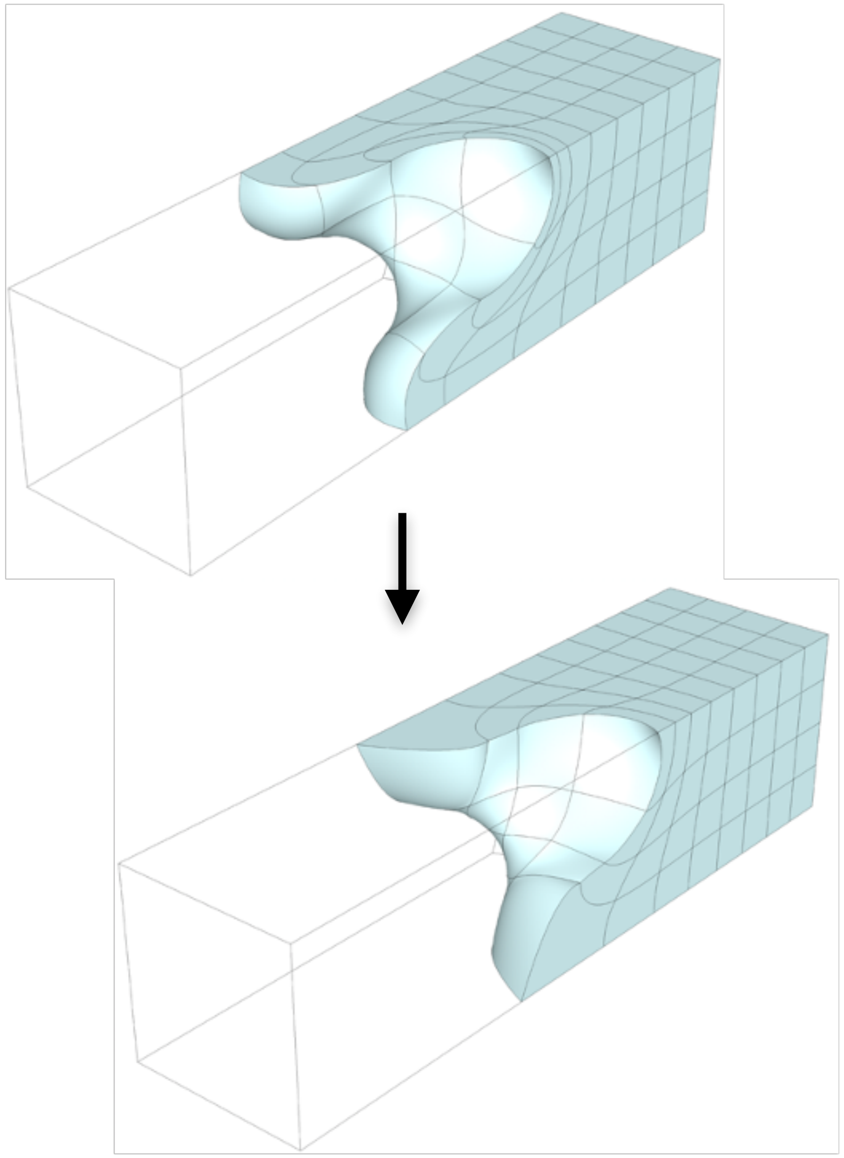




Adaptive Interface Fitting

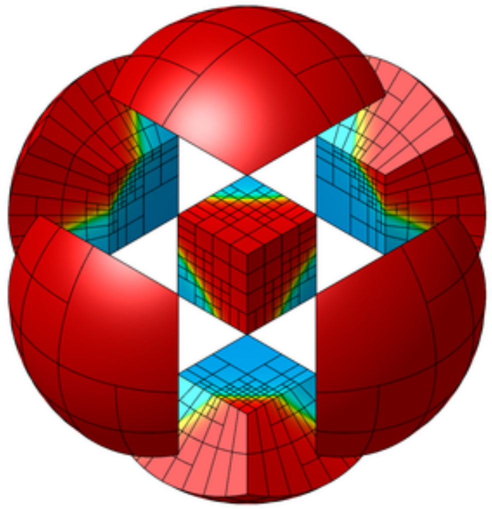
- For non-smooth practical cases, further research and methods are required.



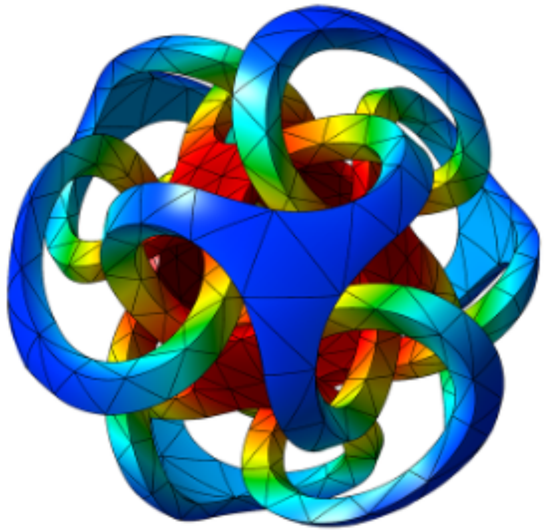


Summary

- Theoretical and practical advances in target construction and metric types for TMOP.
- TMOP-based *hr*-adaptivity for nonconforming high-order meshes helps improve mesh quality while reducing DOFs required for a given accuracy in solution.
  - Dobrev et al. "***hr*-adaptivity for nonconforming high-order meshes with the target matrix optimization paradigm**". Engineering With Computers, 2021.
- Surface fitting and tangential relaxation through an adaptive FE formulation.
  - Discrete representation of the surface; no analytic parametrization
  - Weak enforcement through a variational penalty term
- All presented methods are (or will be) available in MFEM.



mfem.org



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