Optimization, Adaptivity, and Surface Fitting of High-Order Meshes

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CASC
Center for Applied Scientific Computing

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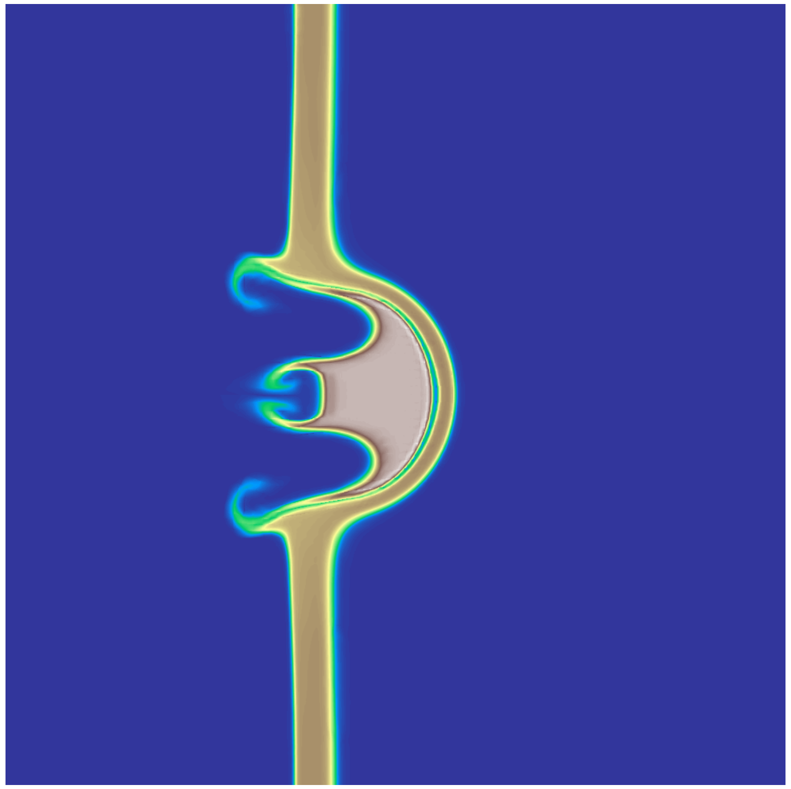
Motivation

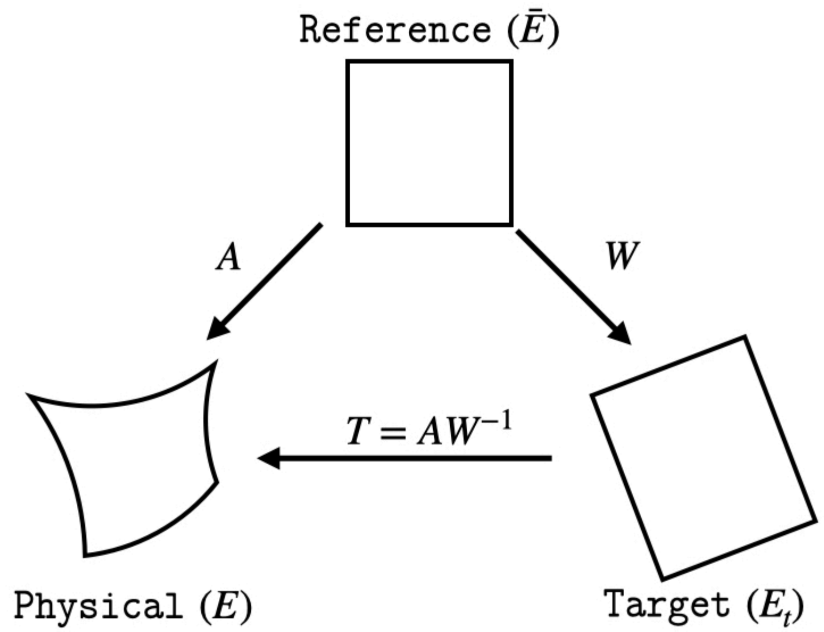
- Take easy to generate Cartesian meshes and optimize them for simulation needs.



Time dependent problem where we wish to ensure sufficient resolution with key features of the simulation.

Multi-material Fischer-Tropsch reactor domain to be meshed for shape optimization

Target Matrix Optimization Paradigm (TMOP)



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

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

- The transformation T from the physical to target element is defined using the Jacobian transformation A and W.

TMOP based Mesh Optimization

- Quality metric $\mu(T)$ is a measure of the difference between the active and target Jacobian transformation.
  - Shape metric ($\mu_{Sh}(T) = 0.5\frac{|T|^2}{det(T)} - 1$), Size metric ($\mu_{Sz}(T) = 0.5(det(T) - \frac{1}{det(T)})^2$)
- Using the quality metric and the Jacobian transformation T, the TMOP objective function is defined as:

$$F_\mu(\mathbf{x}) = \sum_{E(\mathbf{x}_E)} \int_{E_t} \mu(T(\mathbf{x}))d\mathbf{x}_t$$

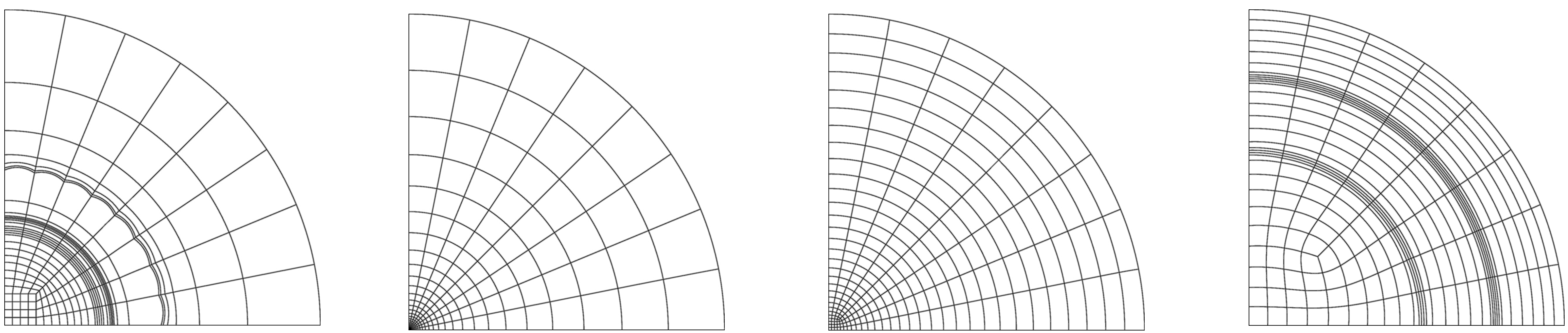
where $\mathbf{x}$ represents mesh coordinates, and E_t is the target element.

- r-adaptivity - $F(\mathbf{x})$ is minimized using a technique such as the Newton's method to optimize the mesh.

Geometric r-adaptivity

- TMOP for *r-adaptivity*:

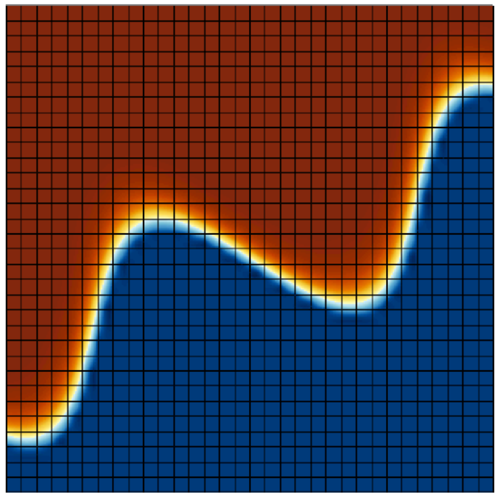
$$W = \sqrt{\zeta}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix}1 & \cos\phi\\ 0 & \sin\phi\end{bmatrix}\begin{bmatrix}\frac{1}{\sqrt{\rho}} & 0\\ 0 & \sqrt{\rho}\end{bmatrix}$$



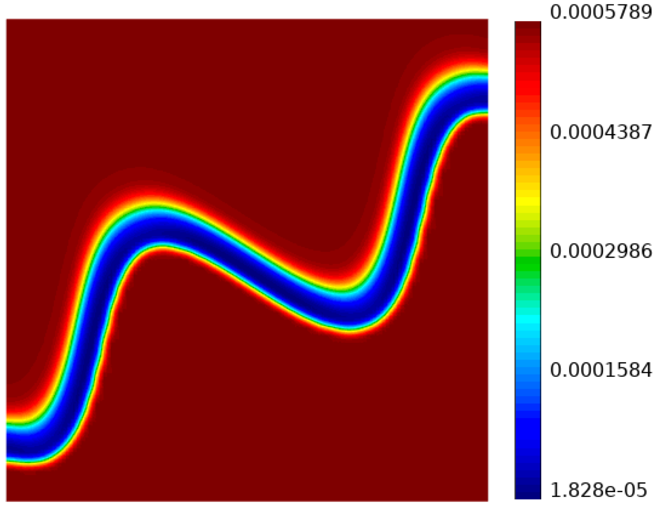
Original mesh | $\phi = \frac{\pi}{2}, \rho = 1, \mu_{Sh}(T)$ | $\zeta = \frac{\mathscr{V}}{N_E}, \phi = \frac{\pi}{2}, \rho = 1, \mu_{ShSz}(T)$ | $\zeta(\mathbf{x}), \phi = \frac{\pi}{2}, \rho = 1, \mu_{ShSz}(T)$

Geometric optimization for a high-order mesh

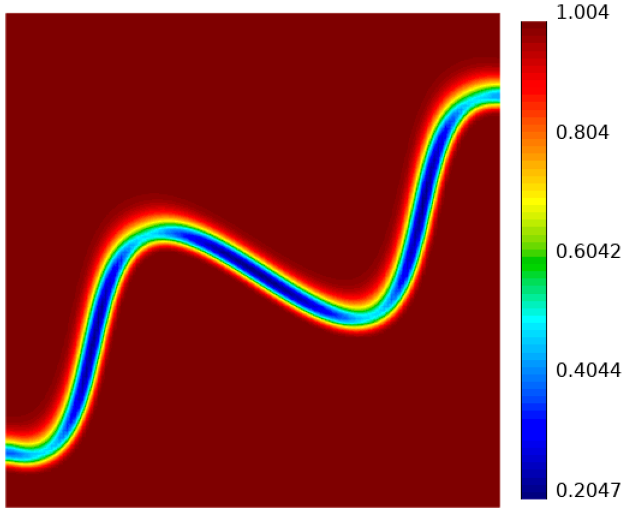
Simulation-driven r-adaptivity



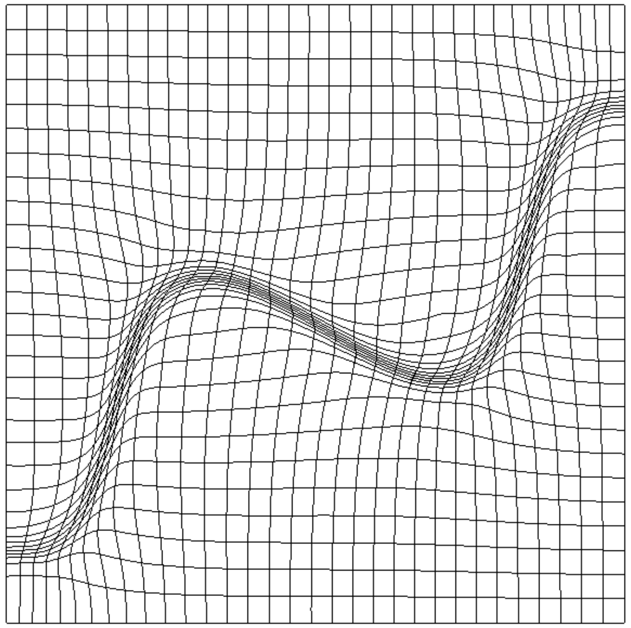
Sinusoidal material indicator (η)



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

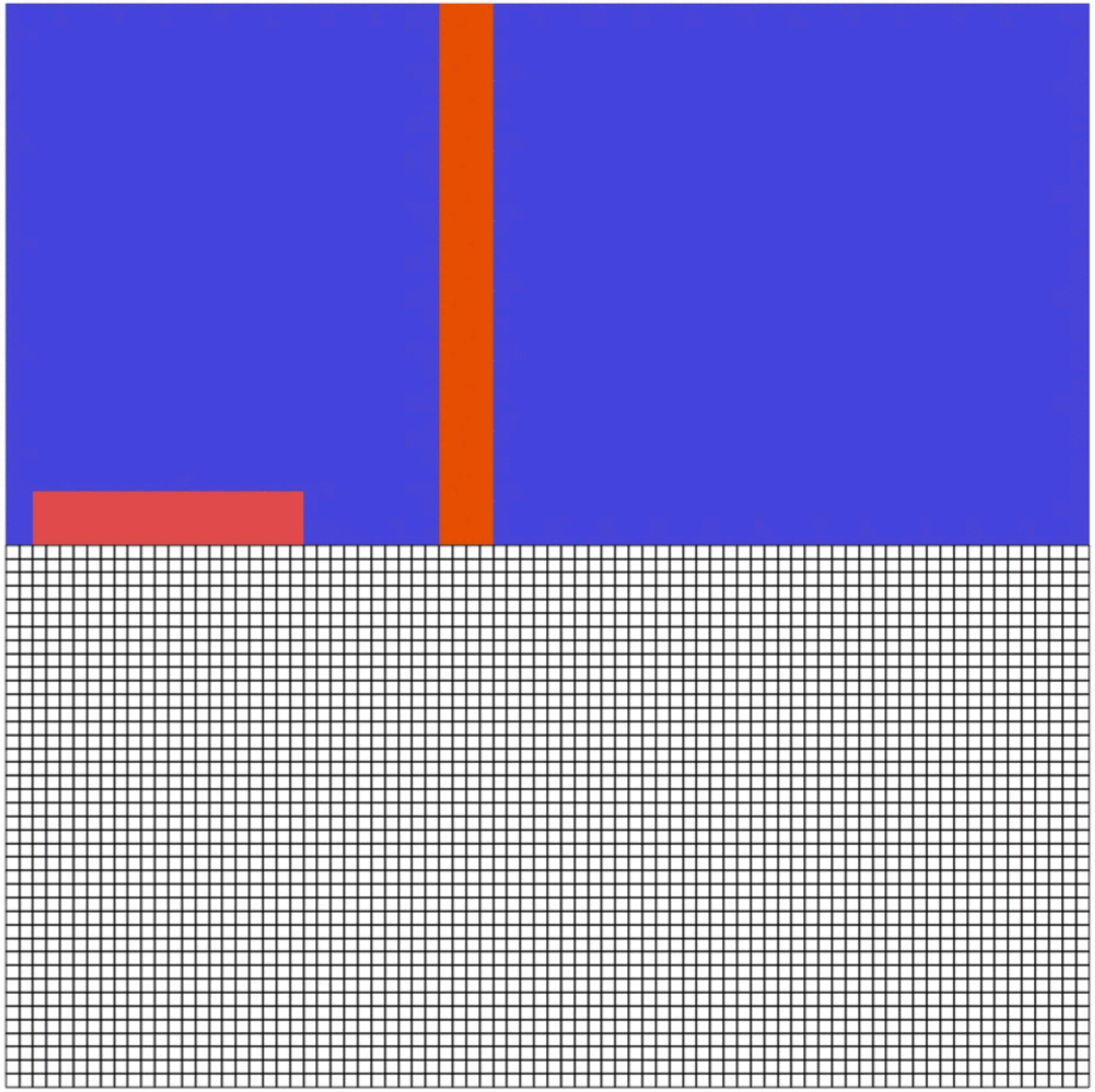


Aspect-Ratio - $\rho \propto |\eta_x/\eta_y|$



Optimized mesh

Simulation-driven r-adaptivity

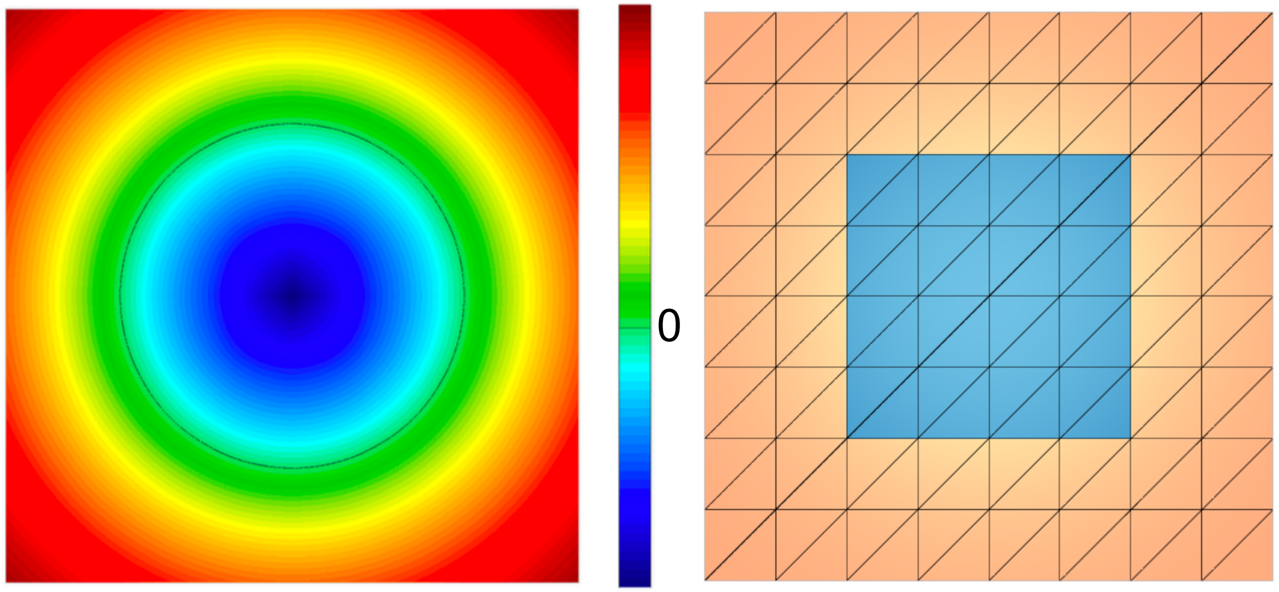


r-adaptivity for the gas impact test using TMOP

"Simulation-driven optimization of high-order meshes in ALE hydrodynamics." Computers & Fluids, 2020.

Boundary and Interface Fitting Method

- Our approach for boundary and interface fitting is to fit the mesh to surface of interest given as the zero level set of a discrete function ($\sigma(\mathbf{x})$), using a penalty-based formulation.



$\sigma(\mathbf{x})$ describing target interface and mesh to be optimized

$$F(\mathbf{x}) = \underbrace{\sum_{E(\mathbf{x}_E)} \int_{E_t} \mu(T(\mathbf{x})) d\mathbf{x}_t}_{F_\mu} + \underbrace{w_\sigma \int_{\mathcal{S}} \sigma^2(\mathbf{x})}_{F_\sigma}, \text{ where}$$

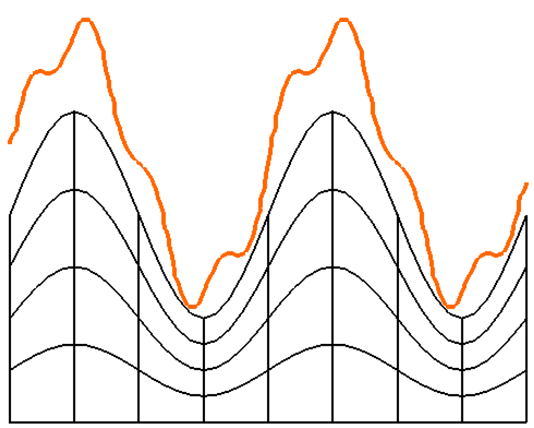
σ - Discrete function

$\mathcal{S}$ - Nodes marked for fitting

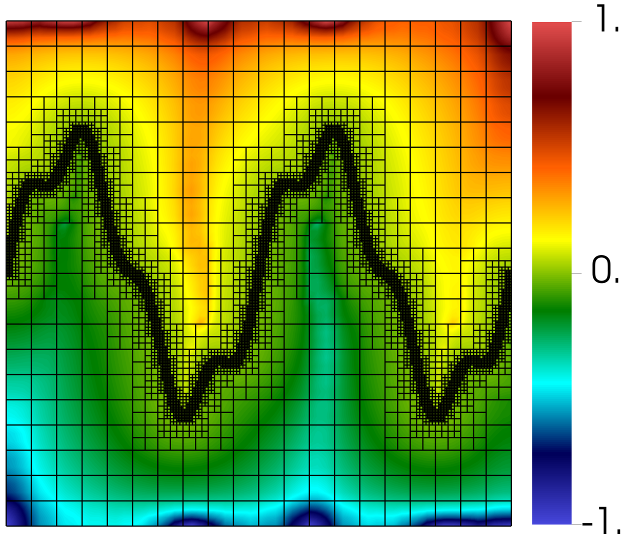
w_σ - Penalization weight

Level Set Function Representation

- Using the mesh being optimized for representing $\sigma(\mathbf{x})$ results in a sub-optimal fit if
  - The mesh does not have sufficient resolution around the zero level-set of $\sigma(\mathbf{x})$.
  - If the zero level-set of $\sigma(\mathbf{x})$ is outside the domain of the mesh.
- We use a background/source mesh with AMR to ensure accuracy in $\sigma(\mathbf{x}_B)$ and its gradient.



Current mesh and target level set



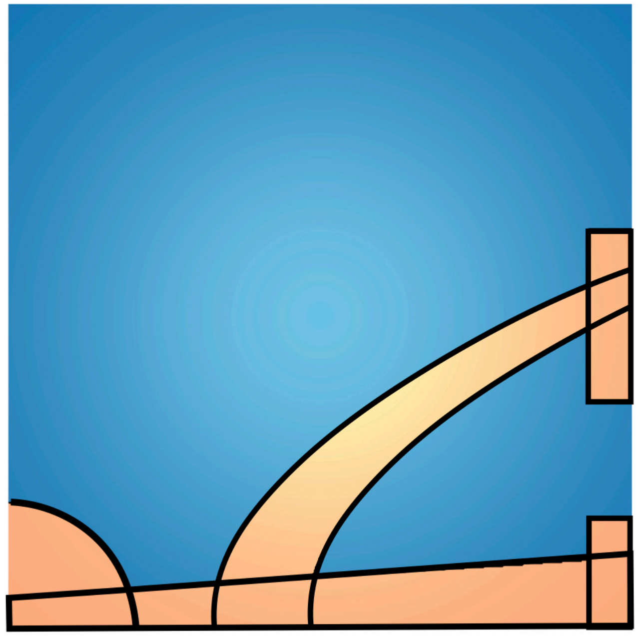
Level set on a background mesh

- We use FindPointsGSLIB in MFEM (a wrapper around the gslib high-order interpolation library) to transfer information from the background mesh to the current mesh.

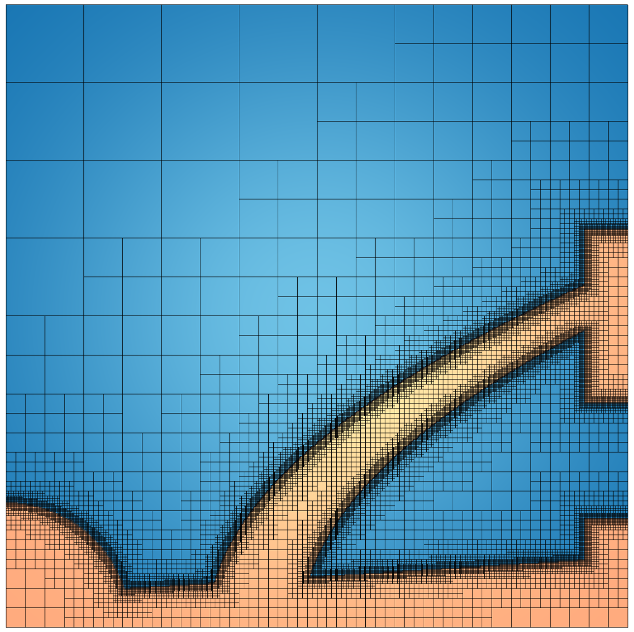
$$\sigma(\mathbf{x}) = I(\mathbf{x}, \mathbf{x}_B, \sigma(\mathbf{x}_B))$$

Level Set Function Representation for Complex Domains

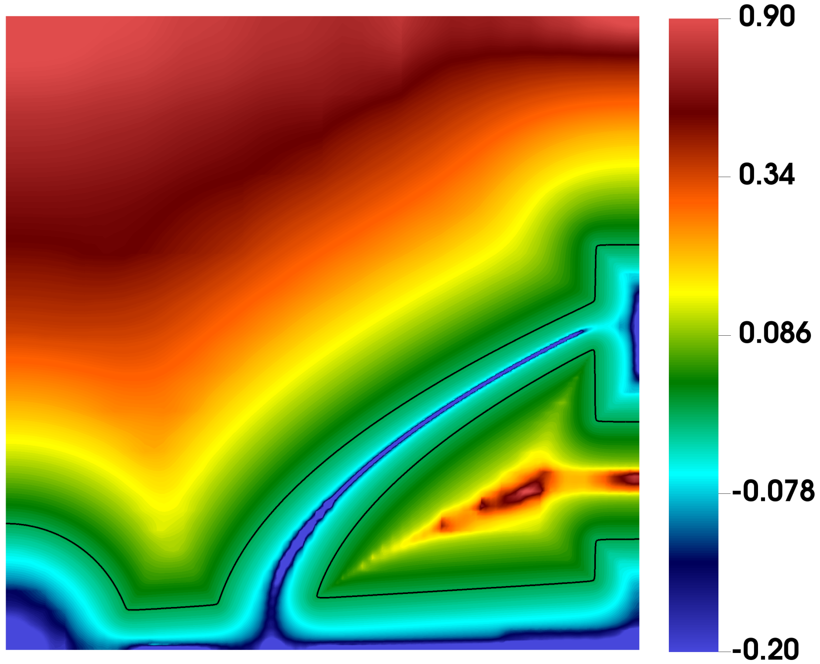
- To define non-trivial geometries with sufficient accuracy, we use geometric primitives along with a method for distance function.



Fischer-Tropsch reactor like domain using CSG



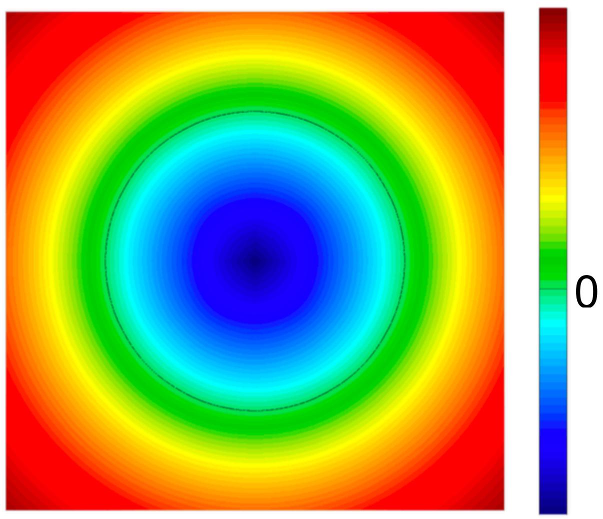
AMR around the 0 level set



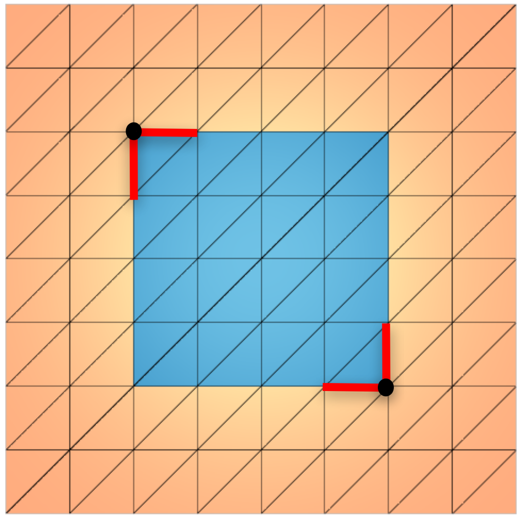
Distance function from the 0 level set

Marking for Interface Fitting

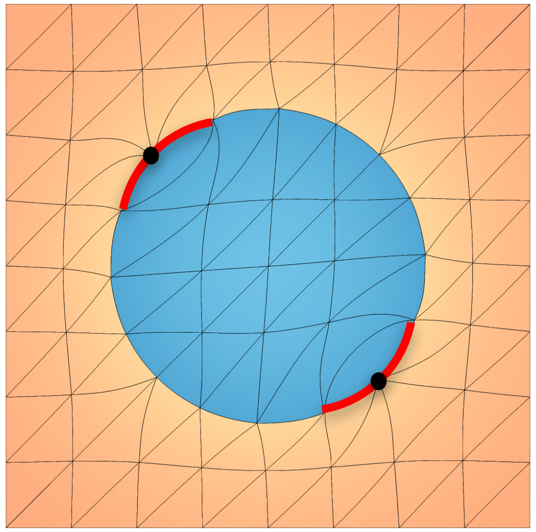
- Marking for interface fitting is not trivial and impacts the quality of the final mesh.



Level set function

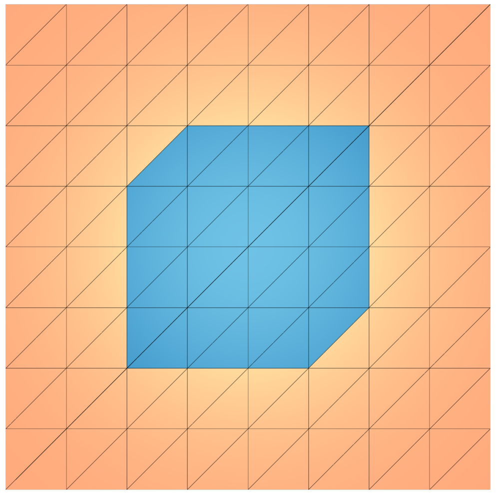


Initial mesh marked for fitting

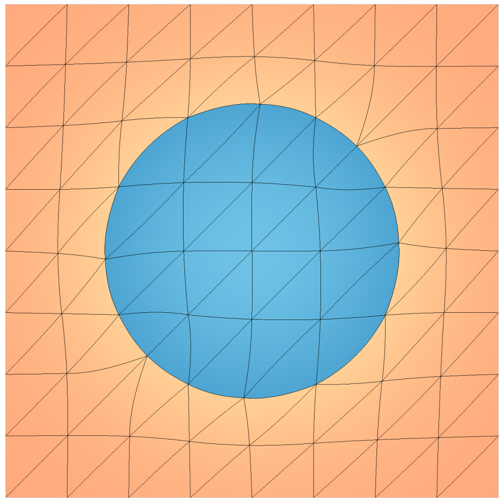


Optimized mesh

- The fit might be sub-optimal if multiple faces of an element are trying to align along a curve.



Adaptive marking

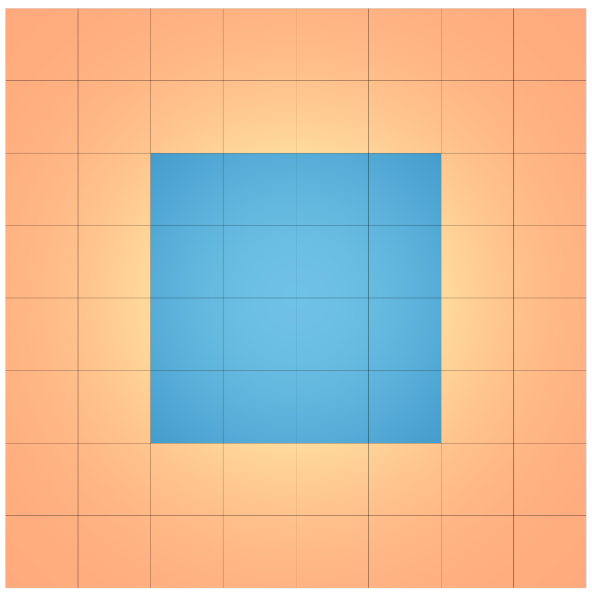


Optimized mesh

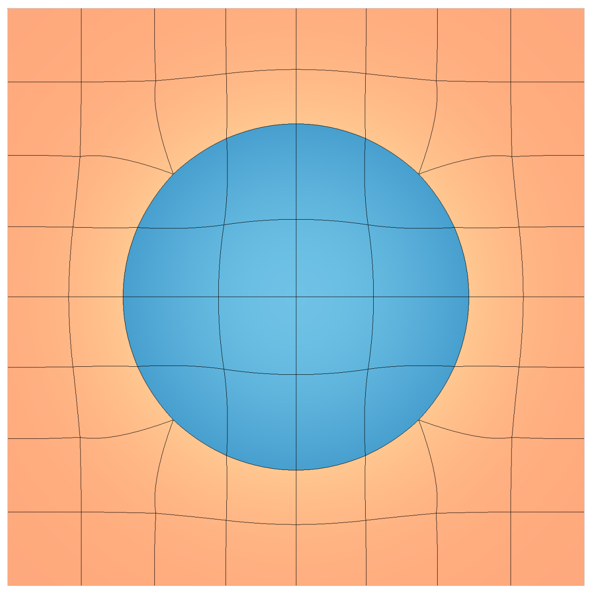
- Using an adaptive marking strategy can significantly improve the fit.

Marking for Interface Fitting

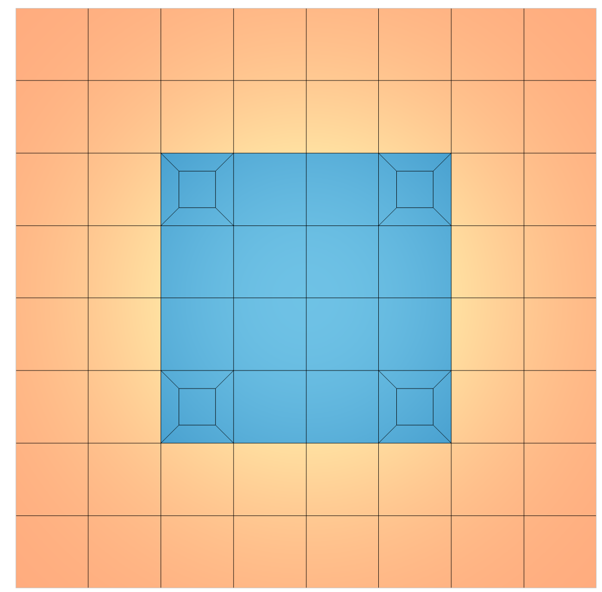
- With quadrilateral elements, we can do a *conforming* split to improve the fit.



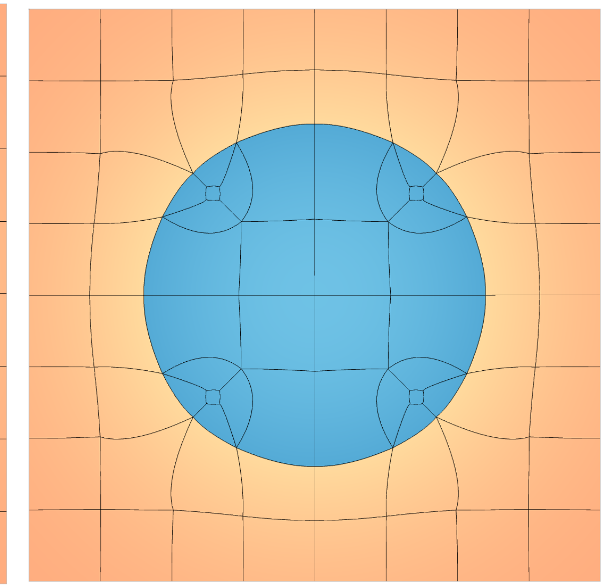
Initial mesh marked for fitting



Optimized mesh



Mesh with conformal splits

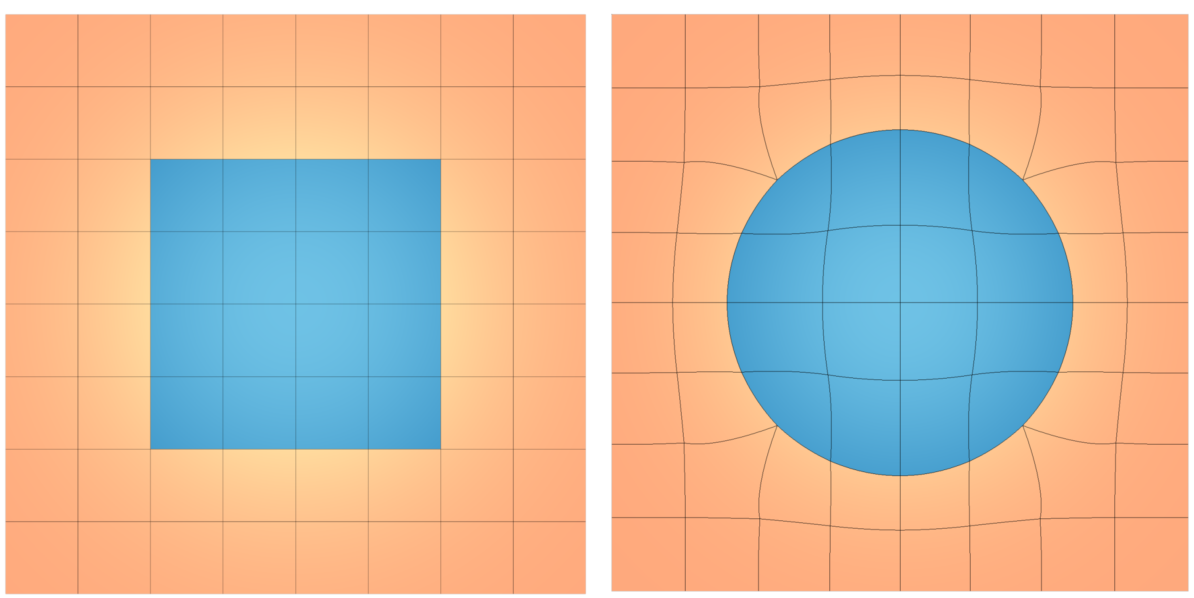


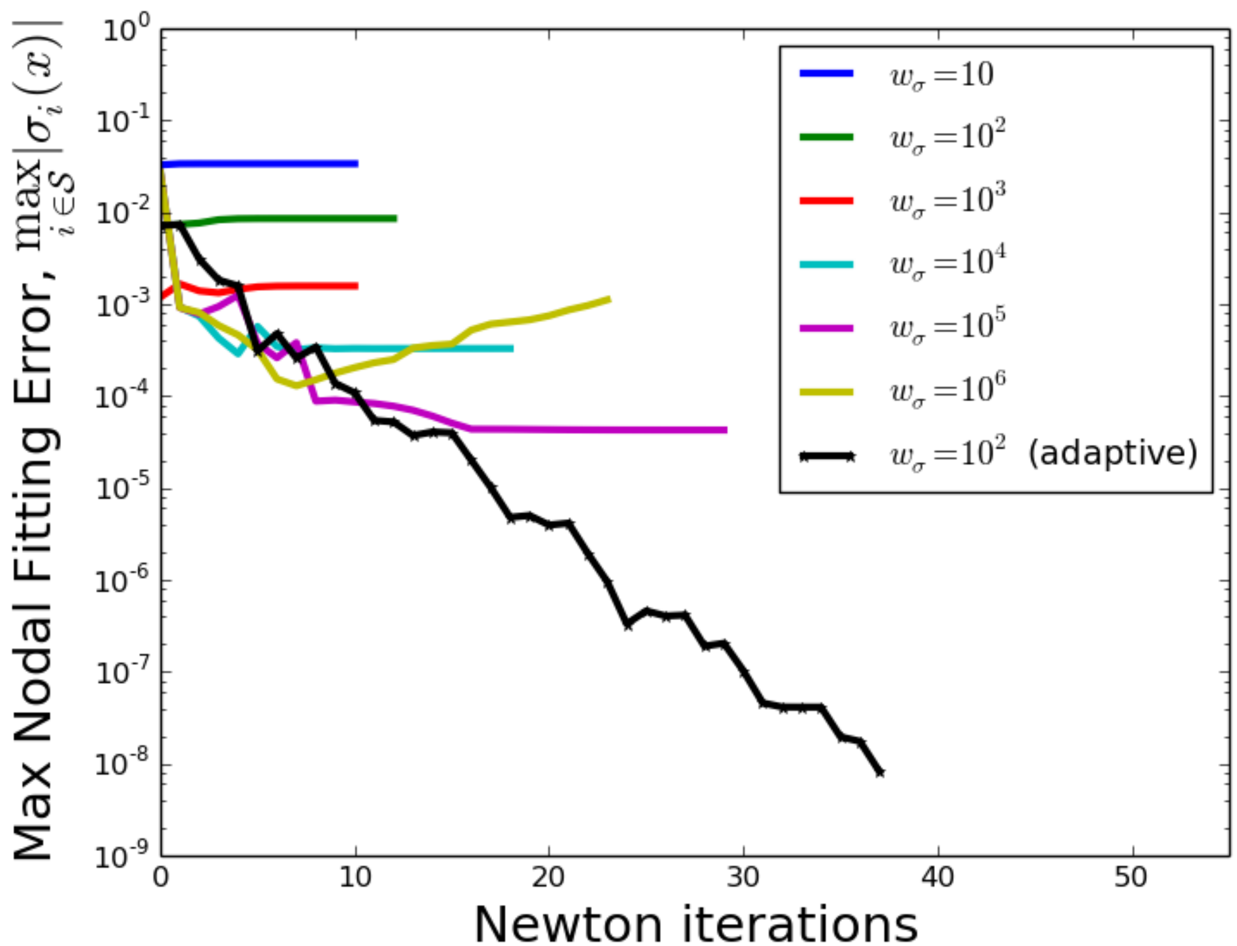
Optimized mesh

- Similar splitting strategy in hexahedral elements does not guarantee optimal fit and we are currently working on that problem.

Adaptive Penalization Weight

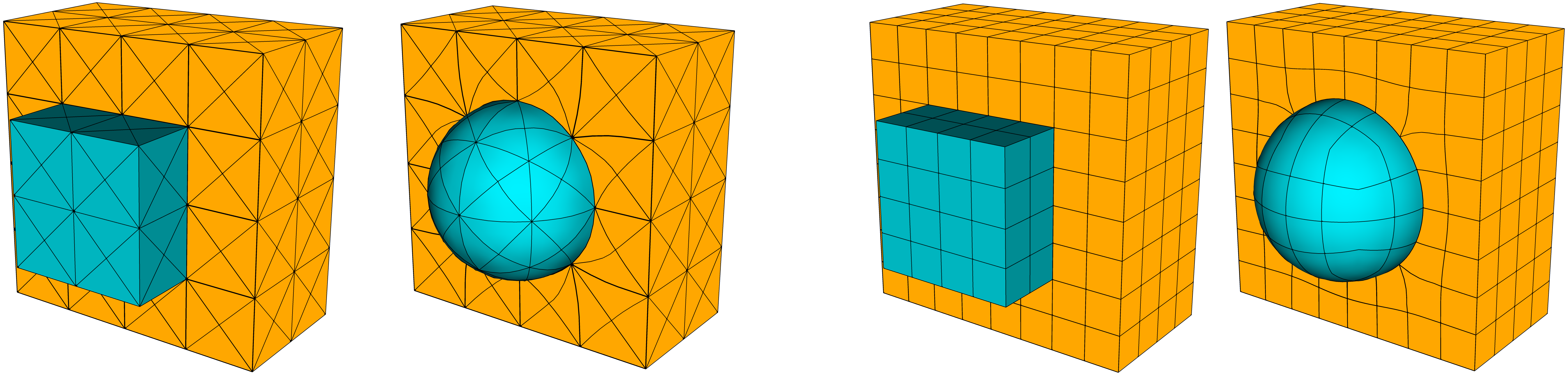
- Using a constant penalization weight w_σ requires tuning to get the best fit for a given mesh topology and level set function.
- We adapt w_σ by monitoring the maximum fitting error, $|\sigma|_{\mathcal{S},\infty} := \max_{i\in\mathcal{S}} |\sigma_i(\mathbf{x})|$, at the marked nodes, and increasing w_σ if $|\sigma|_{\mathcal{S},\infty}$ does not decrease sufficiently across subsequent Newton iterations.





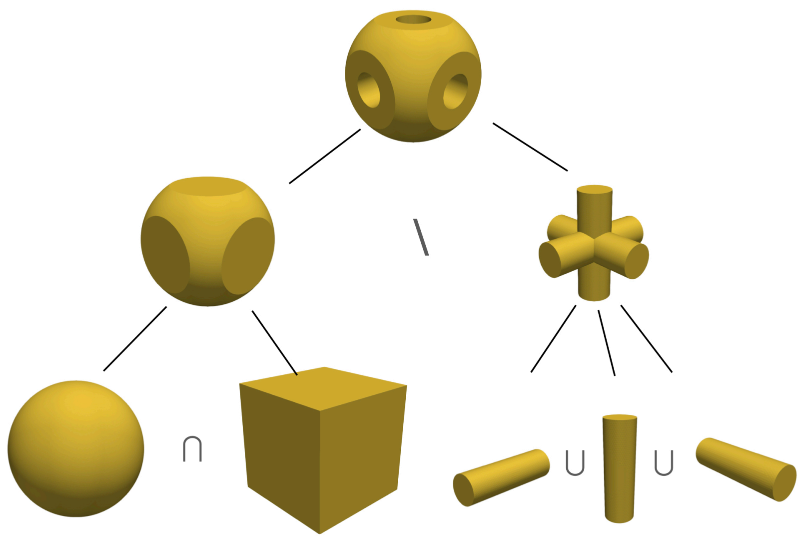
Applications - Interface Fitting to a Sphere

- $T = I, \;\; \mu_{Sh}(T) = \frac{|T|^2}{3det(T)^{\frac{2}{3}}} - 1$

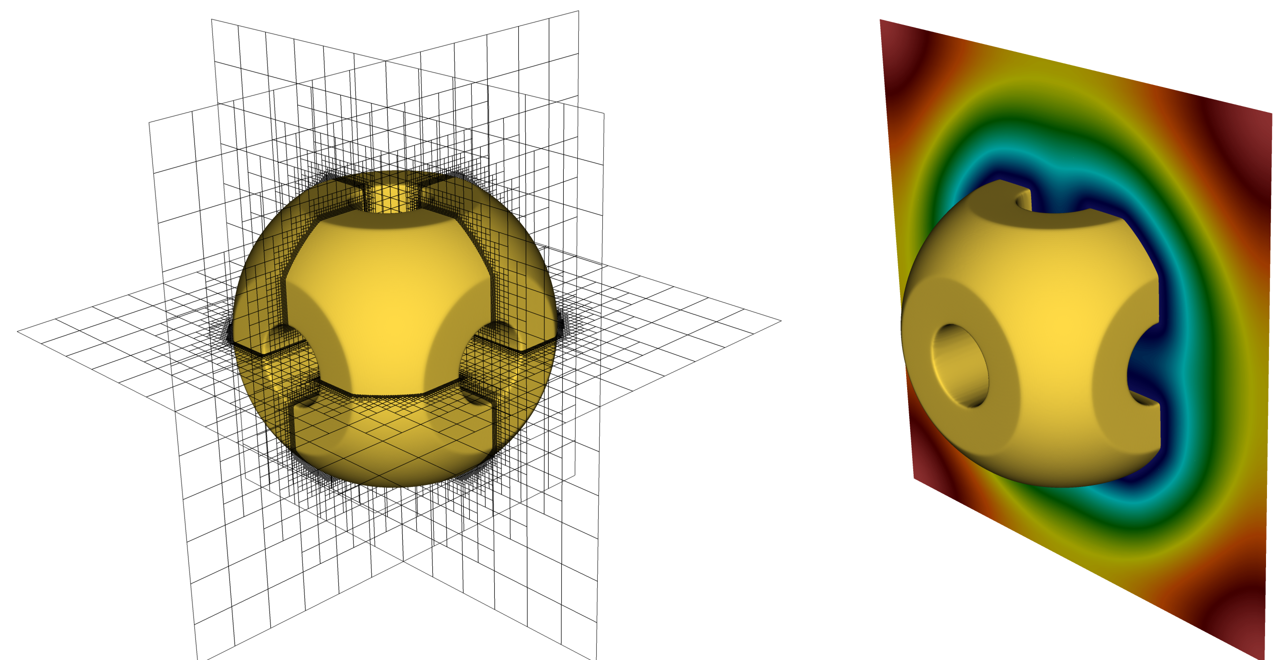


Multimaterial tet- and hex-meshes fitted to a sphere

Boundary Fitting for a Complex 3D Domain



CSG Tree for a curvilinear domain

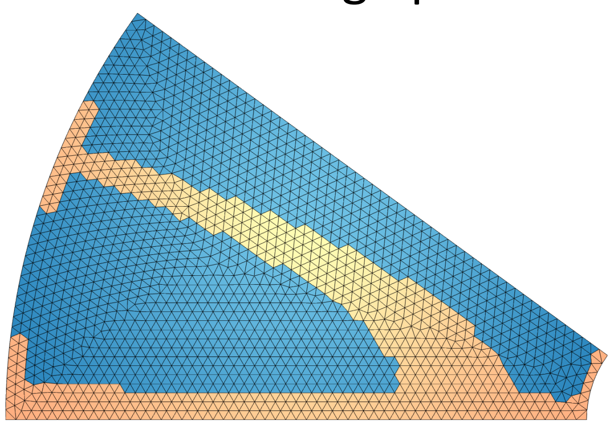


Background mesh and distance function

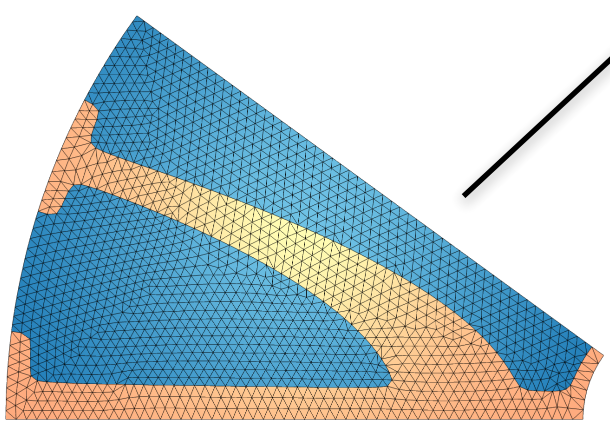
Uniform Cartesian (second-order) mesh trimmed and fit to the level-set function.

Interface Fitting for the Reactor Design Problem

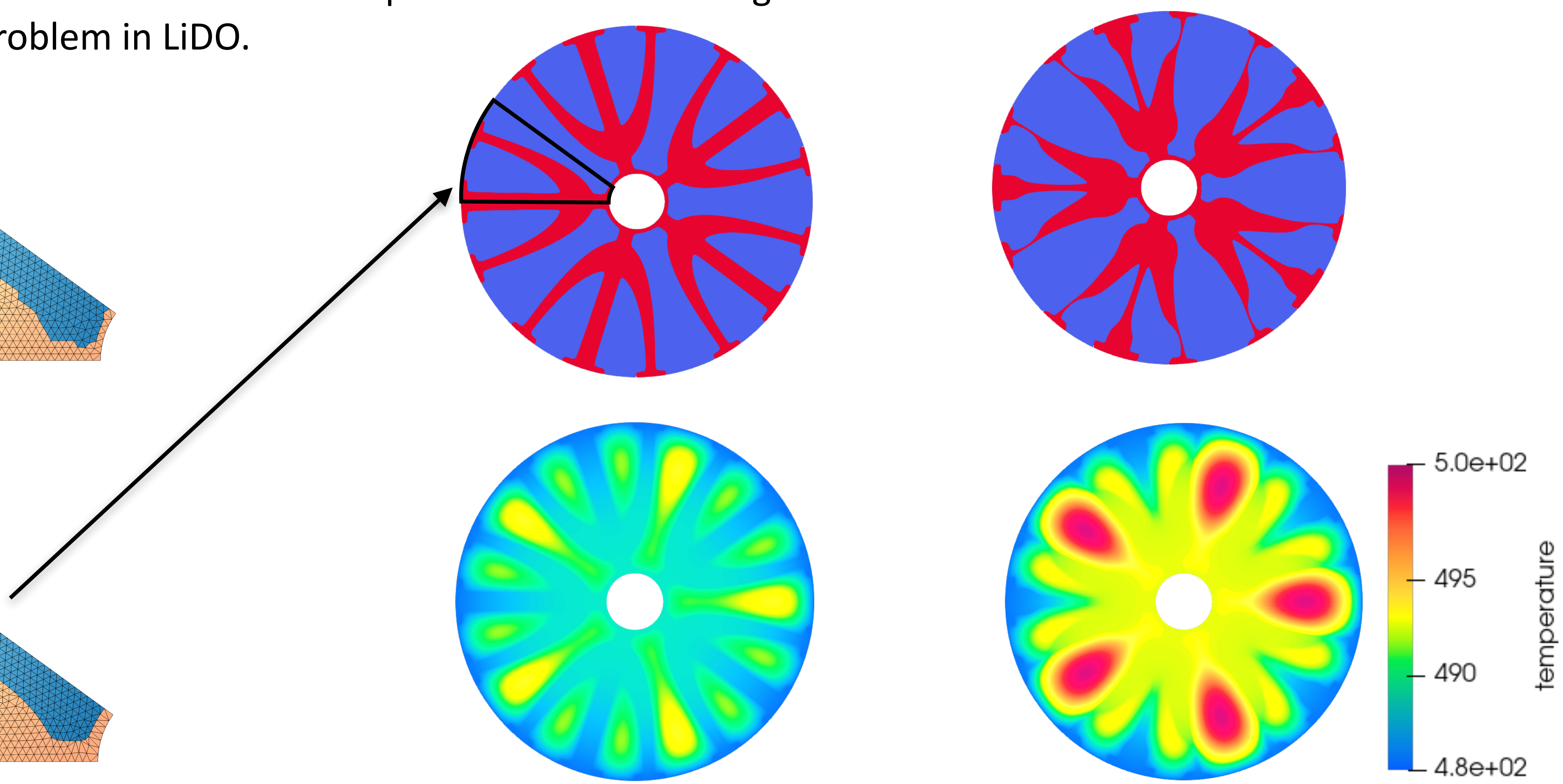
- Reactor design problem: Maximize the energy produced by the system while keeping the volume of the aluminum fins fixed (*red/orange* in plots below).
- We first generate a uniform mesh and optimize it in MFEM to get an initial mesh to be used for the reactor design problem in LiDO.



Initial mesh



Interface fitting mesh



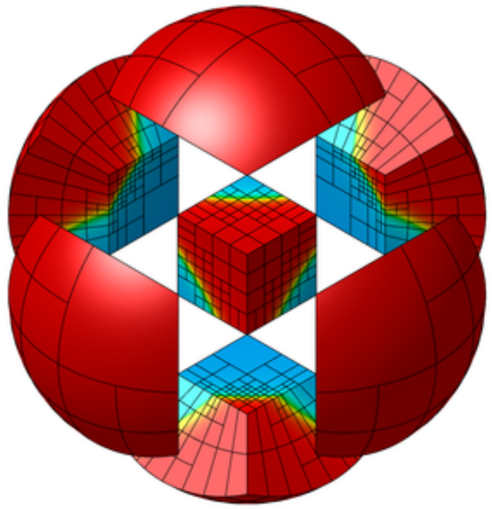
Initial fitted mesh

Fitted mesh optimized for energy production

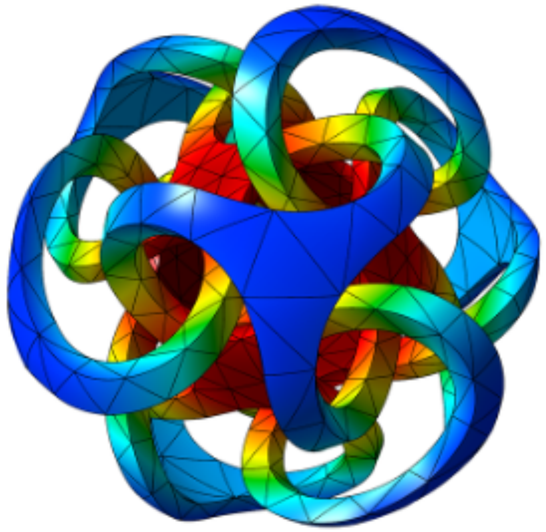
LLNL LDRD for Shape Optimization on Conformal Meshes, PI: Jorge-Luis Barrera

Summary

- Simulation-driven optimization of high-order meshes using TMOP.
- Boundary and interface fitting through a penalization-based formulation.
- All presented methods are (or will be) available in MFEM.



mfem.org



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