Shape and Topology Optimization Powered by MFEM

MFEM Workshop

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OxEon energy

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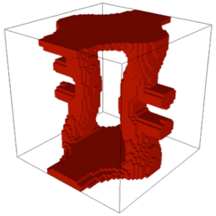
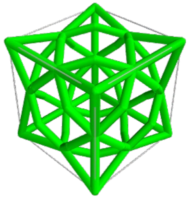
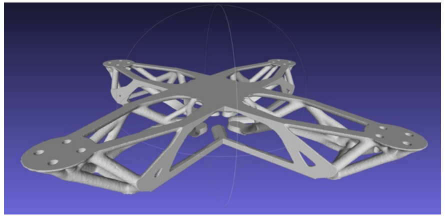
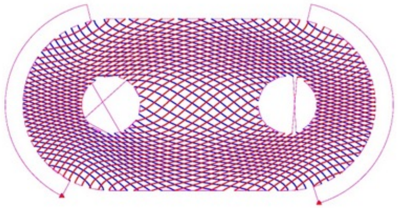
Systematic Design Optimization

Livermore **D**esign **O**ptimization (**LiDO**) code:

- Developing production-quality design optimization tools for Lab community and collaborators
- HPC-enabled design for coupled, transient, and nonlinear physics
- Developing and using optimization-aware machine learning models
- AM process optimization
- Manufacturing constraints
- Design under uncertainty

Serac


Bramwell


White


Mish

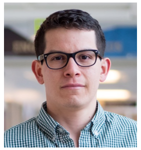

Dayton


Chapman


Andrej

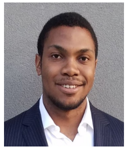

Chin

LiDO

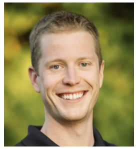

Barrera


Chapman


Epperly


Johnson


Schmidt

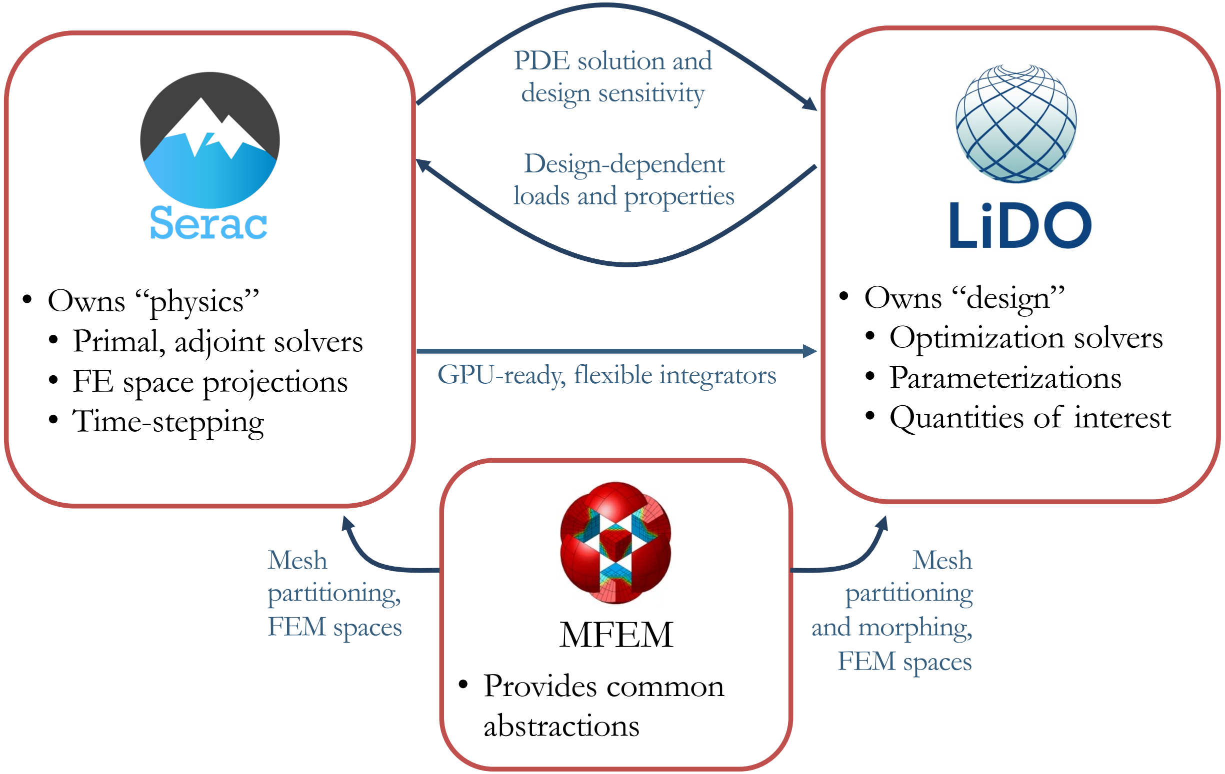

Swartz


Villanueva


Watts

Optimization Framework: Building Blocks

Smith and LiDO are being co-developed to improve utility, integration, and performance

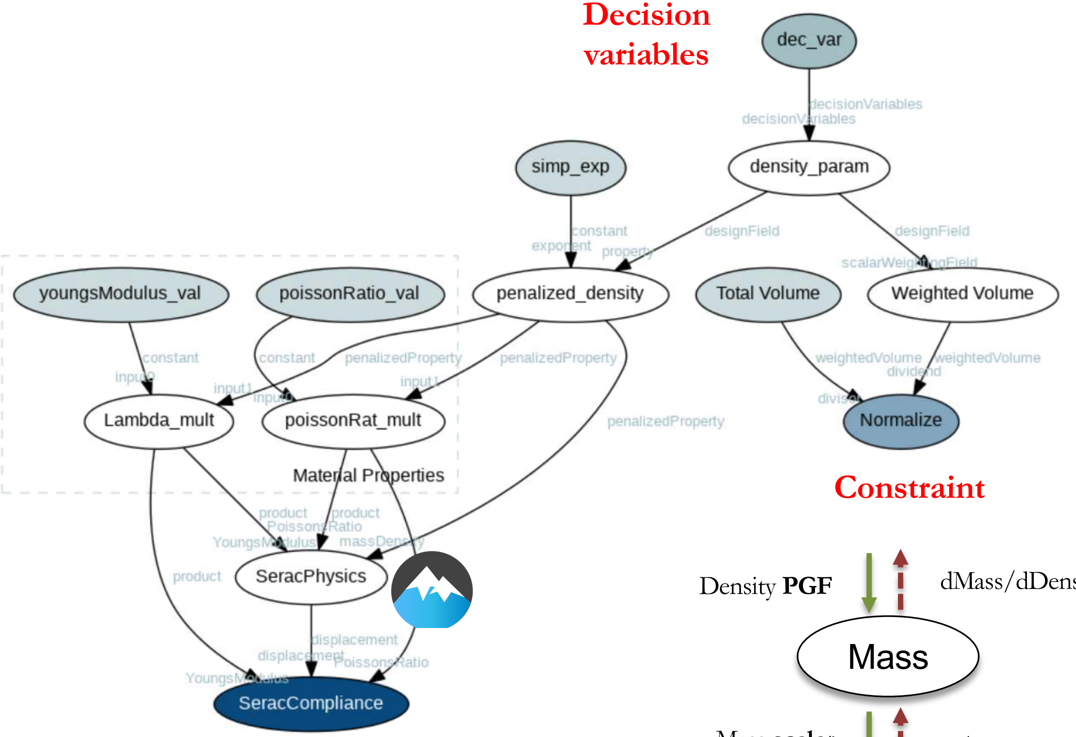


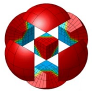
Example of LiDO Graph Data Flow

Derivatives w.r.t. decision variables

Forward physical analysis

Decision variables





Constraint

Backward sensitivity analysis

Density **PGF**

dMass/dDensity **PLF**

Mass **scalar**

d*/dMass **PLF**

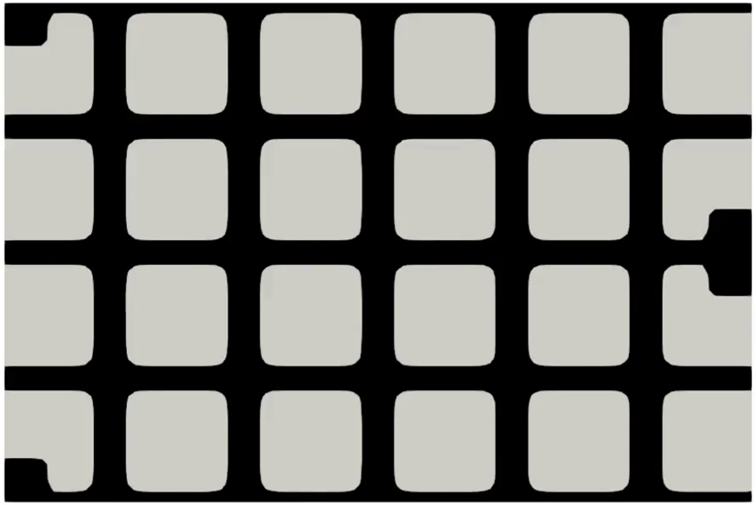
Performance metric (i.e., objective and constraints)

Objective

Note: data/computations of any vertex can come from user-defined module!

Gradient-based topology and shape optimization

Current alternatives for gradient-based optimization in LiDO:

Design evolves **automatically** via	**Topology optimization (TopOpt)**	**Shape optimization (ShapeOpt*)**
		
Parameterizes	Fields $\int_{\Omega} \nabla \boldsymbol{w} \cdot \mathbb{C}(\boldsymbol{d}) \, [\nabla \boldsymbol{u}] \, dv = 0$	Domain $\int_{\Omega(\boldsymbol{d})} \nabla \boldsymbol{w} \cdot \mathbb{C} \, [\nabla \boldsymbol{u}] \, dv = 0$

*Under active development

TopOpt: Multi-material design considering geometric measures

A mass mock part designed for additive manufacturing with two materials (red and clear) to match a given total mass, center of mass, and multiple moments of inertia.

$$\min_{p} \quad \theta(\boldsymbol{p}) = w_0 \int_{\Omega} p\,(1.0 - p)\,dV$$

$$\text{such that} \quad g_1(p) = w_1 \left(\mathcal{M}(p)/\bar{\mathcal{M}} - 1.0\right)^2 \leq 0$$

$$g_2(p) = w_2 \left(\mathcal{I}_{XX}(p)/\bar{\mathcal{I}}_{XX} - 1.0\right)^2 \leq 0$$

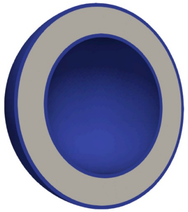
$$g_3(p) = w_3 \left(\mathcal{I}_{YY}(p)/\bar{\mathcal{I}}_{YY} - 1.0\right)^2 \leq 0$$

$$g_4(p) = w_4 \left(\mathcal{I}_{ZZ}(p)/\bar{\mathcal{I}}_{ZZ} - 1.0\right)^2 \leq 0$$

$$g_5(p) = w_5 \left(\mathcal{C}_X(p) - \bar{\mathcal{C}}_X\right)^2 \leq 0$$

$$g_6(p) = w_6 \left(\mathcal{C}_Y(p) - \bar{\mathcal{C}}_Y\right)^2 \leq 0$$

$$g_7(p) = w_7 \left(\mathcal{C}_Z(p) - \bar{\mathcal{C}}_Z\right)^2 \leq 0$$



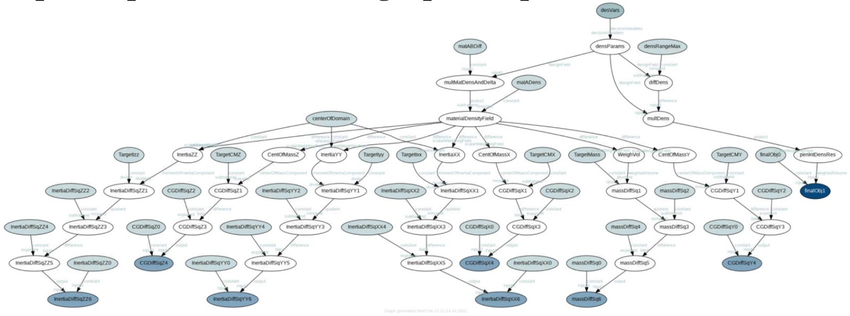
Skin thickness of 0.1 inches

w_i : weights to adjust sensitivity contributions

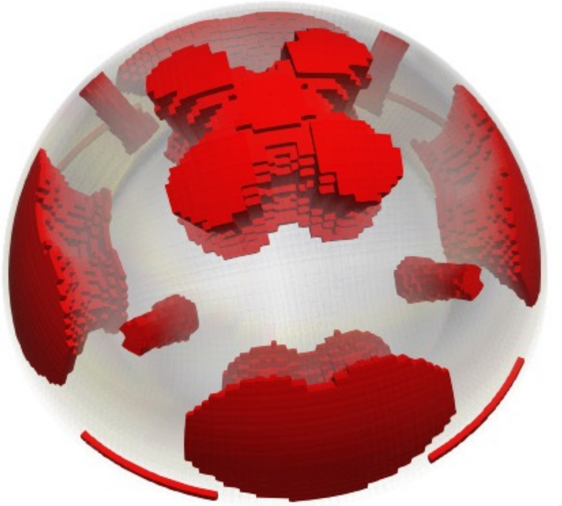
$$\mathcal{M}(p) = \int_{\Omega} \rho(p) dV$$

$$\rho = \rho_A + p\,(\rho_B - \rho_A)$$

Simple implementation of graph despite number of vertices.



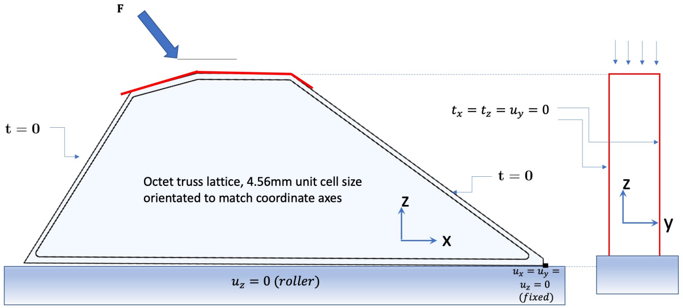
Optimal design

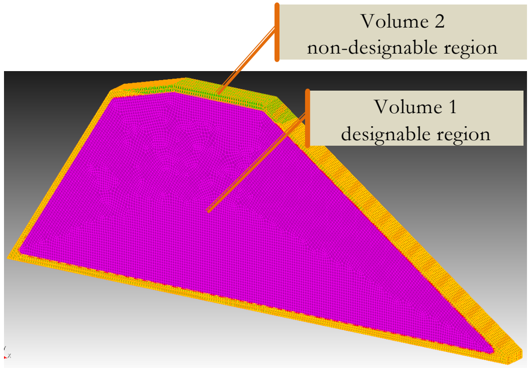


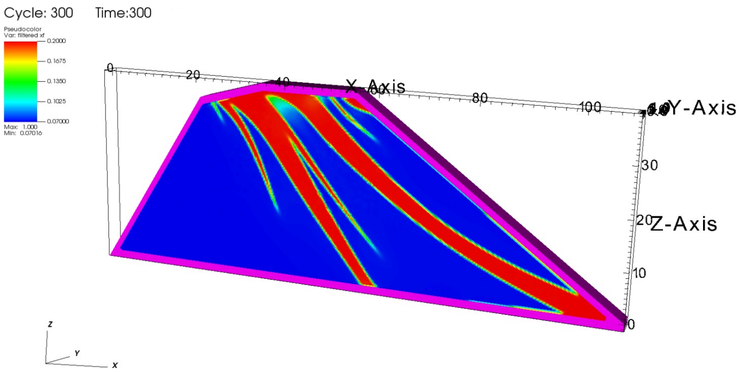
TopOpt: Field-based octet truss lattice structural design

Minimize compliance, subject to the mass fraction constraint:

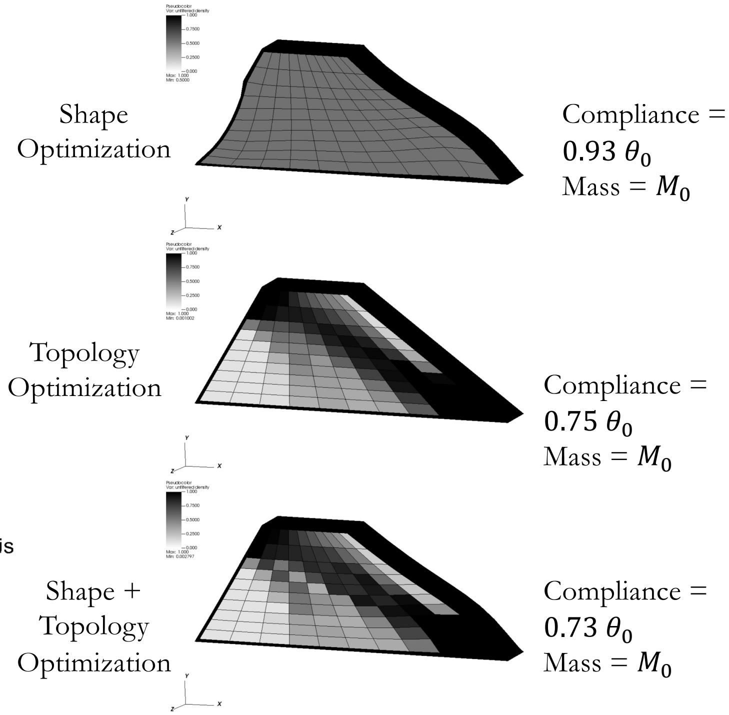
- mass fraction of designable region ≤ 10%, where the designable region is made up of an octet lattice.





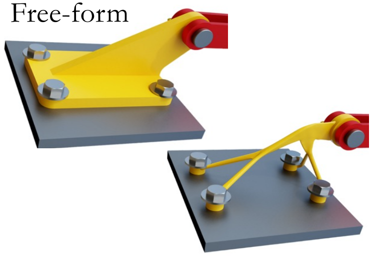


Combining design optimization approaches

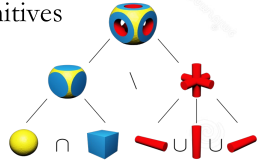


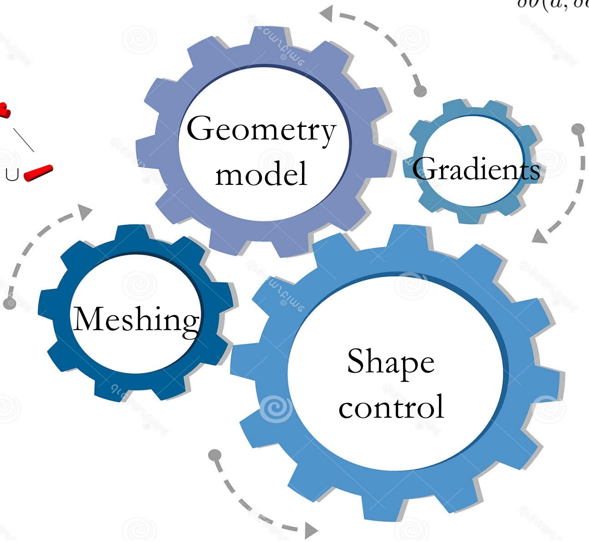
Shape Optimization 101

Free-form



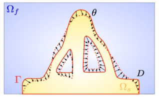
Combining geometric primitives



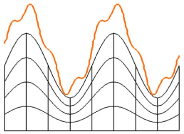


Shape sensitivity analysis

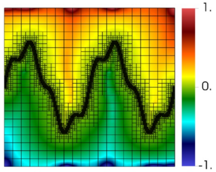
$$\delta\theta(d;\delta d) = \int_\Omega \left(-\frac{\partial g}{\partial \nabla \mathbf{u}} \cdot \nabla \mathbf{u}\, \nabla \mathbf{v}_d + g\, \mathrm{div}\, \mathbf{v}_d \right) dv - \int_\Omega \left(-\nabla \mathbf{w}\, \nabla \mathbf{v}_d \cdot \boldsymbol{\sigma} - \nabla \mathbf{w} \cdot \frac{\partial \boldsymbol{\sigma}}{\partial \nabla \mathbf{u}} [\nabla \mathbf{u}\, \nabla \mathbf{v}_d] - \mathbf{w} \cdot \overset{\star}{\mathbf{b}} + (\nabla \mathbf{w} \cdot \boldsymbol{\sigma} - \mathbf{w} \cdot \mathbf{b})\, \mathrm{div}\, \mathbf{v}_d \right) dv$$



Discretization

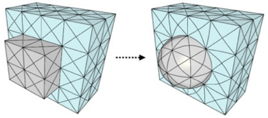


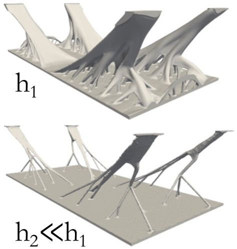
Current mesh and target level set



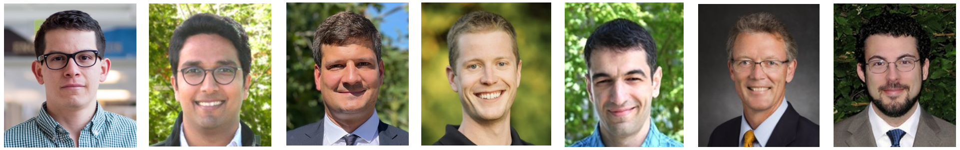
Level set on a background mesh

Accurate mesh morphing, feature size control, …





Shape Optimization Team

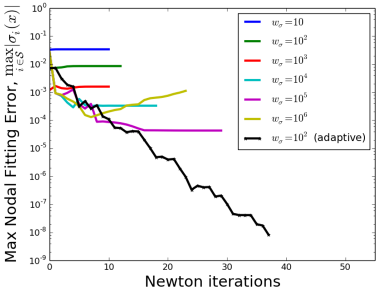


Barrera **Mittal** **Schmidt** **Swartz** **Tomov** **Tortorelli** **Watts**

ShapeOpt: Pre-processing Discretized Design Domain

- MFEM's TMOP adapt structured meshes to parameterized geometry (uses GSLib too)

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



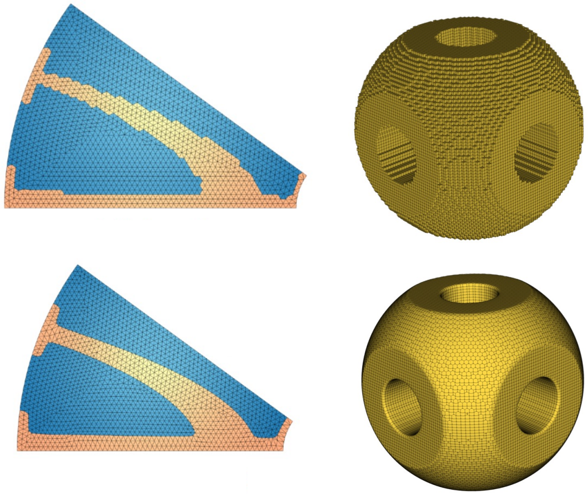
$$\frac{\partial F_\sigma(\mathbf{x})}{\partial x_{a,i}} = 2\omega_\sigma \sum_{s\in\mathcal{S}} \sigma(x_s) \frac{\partial \sigma(x_s)}{\partial x_a} \frac{\partial x_a(\bar{x}_s)}{\partial x_{a,i}} = 2\omega_\sigma \sum_{s\in\mathcal{S}} \sigma(x_s) \frac{\partial \sigma(x_s)}{\partial x_a} \bar{w}_i(\bar{x}_s),$$

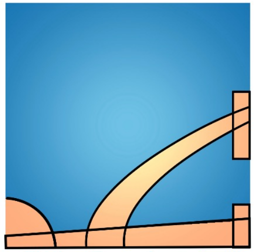
$$\frac{\partial^2 F_\sigma(\mathbf{x})}{\partial x_{b,j}\partial x_{a,i}} = 2\omega_\sigma \sum_{s\in\mathcal{S}} \left(\frac{\partial \sigma(x_s)}{\partial x_b} \frac{\partial \sigma(x_s)}{\partial x_a} + 2\omega_\sigma \frac{\partial^2 \sigma(x_s)}{\partial x_b \partial x_a} \right) \bar{w}_i(\bar{x}_s)\bar{w}_j(\bar{x}_s),$$

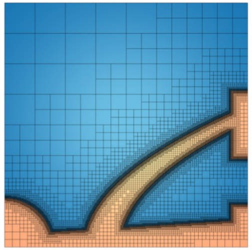
$$a, b = 1 \ldots d, \quad i, j = 1 \ldots N_x.$$

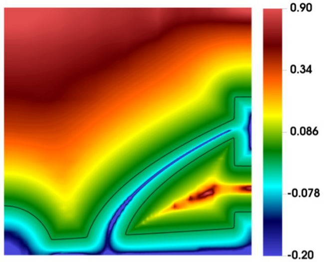
Initial mesh

Morphed mesh



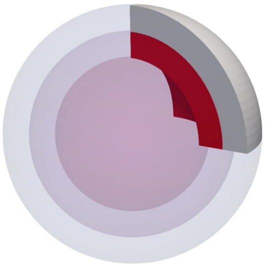

Fischer-Tropsch reactor like domain using CSG


AMR around the 0 level set

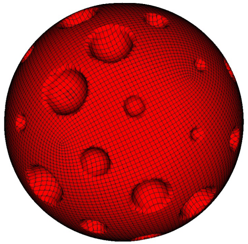


Distance function from the 0 level set

Initial mesh



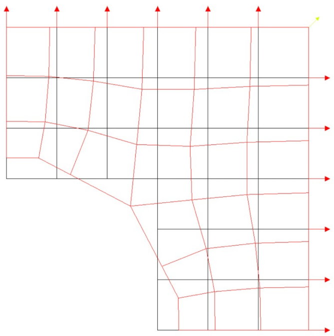
Flexible parameterization


Number of spheres = 40
Sphere radii range = 0.05-0.20

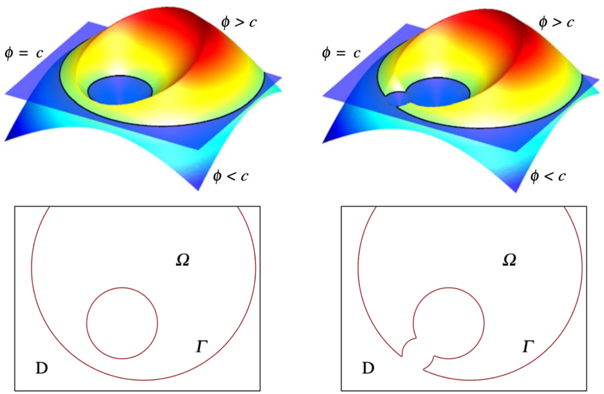

Number of spheres = 180
Sphere radius = 0.1

ShapeOpt: Alternatives Explored

Option 1: node coordinates as decision variables



Option 2: interface/boundary defined implicitly by isocontour of a level set function



Node aware shape optimization

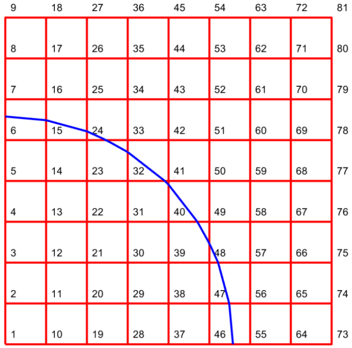
$$r_d(\tilde{\mathbf{u}}_d, \tilde{\mathbf{w}}, \mathbf{u}_d) = 0 \quad = \int_{\Omega_0} (\nabla \tilde{\mathbf{w}} \cdot \gamma \, \nabla \tilde{\mathbf{u}}_d + \tilde{\mathbf{w}} \cdot \tilde{\mathbf{u}}_d) \, dv - \int_{\Omega_0} \tilde{\mathbf{w}} \cdot \mathbf{u}_d \, dv$$

$$\min_{\tilde{\mathbf{u}}_d \in \mathcal{H}_c} \quad \theta_\gamma = \int_{\Omega_0} |\tilde{\mathbf{u}}_d - \mathbf{u}_d|^2 \, dv + \gamma \int_{\Omega_0} |\nabla \tilde{\mathbf{u}}_d|^2 \, dv$$

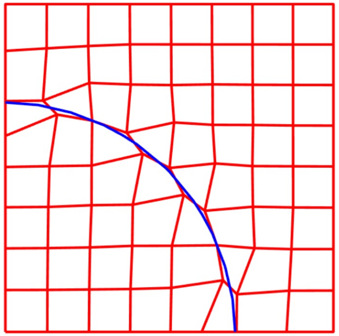
$$\delta\theta_i(\tilde{\mathbf{u}}_d; \delta\tilde{\mathbf{u}}_d) = \delta\theta_i^E(\mathbf{x}; \delta\mathbf{x}) - \delta r^E(\mathbf{u}, \mathbf{w}, \mathbf{x}; \delta\mathbf{x})$$

Level set shape optimization

Design (fixed) mesh

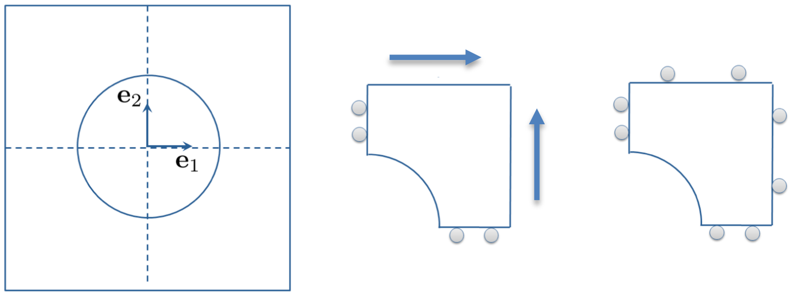


Analysis (morphing) mesh



ShapeOpt: Structural design of benchmark stress problem

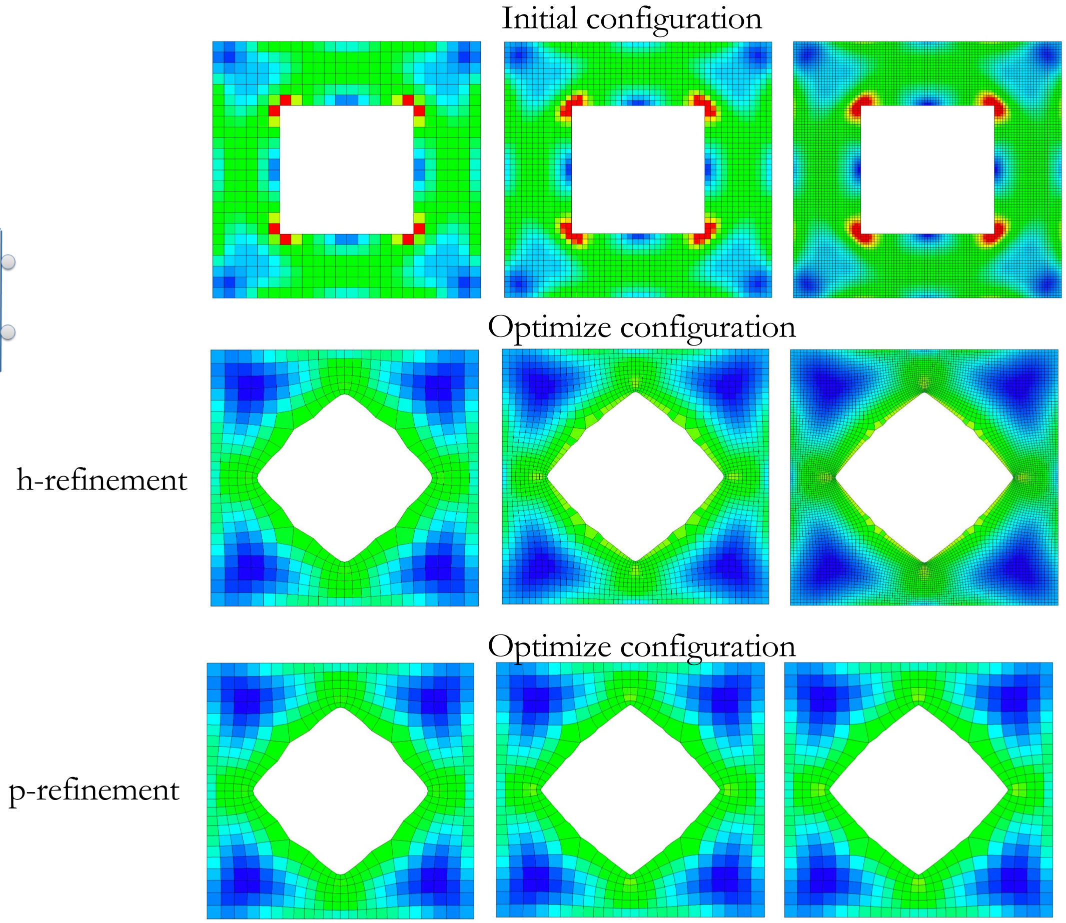
Plate with Hole:



$$\min_{\mathbf{u}_d \in \mathcal{H}_H} \quad \theta_0 = \left(\int_\Omega \sigma_{VM}^p \, dv \right)^{\frac{1}{p}}$$

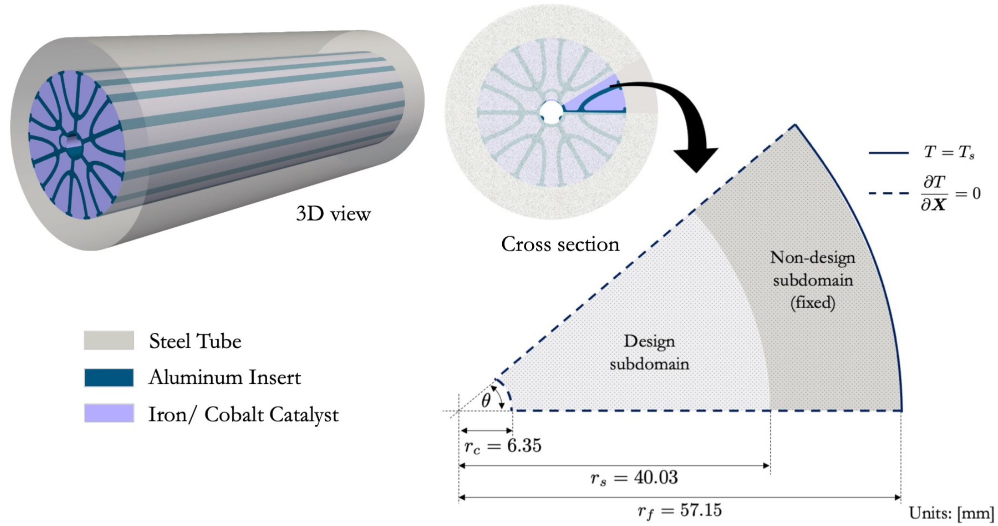
$$\text{such that} \quad \theta_1 = \int_\Omega dv - \overline{V} = 0$$

$$\underline{u}_d \leq \mathbf{u}_d \cdot \mathbf{e}_i \leq \overline{u}_d \text{ for } i = 1, 2$$

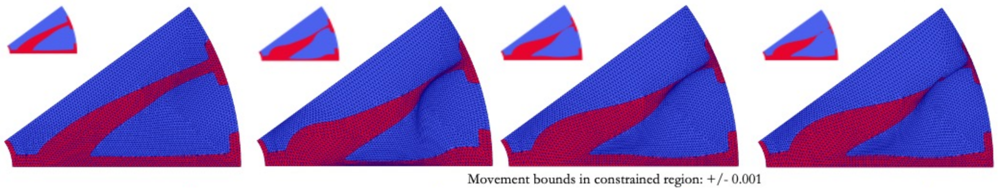


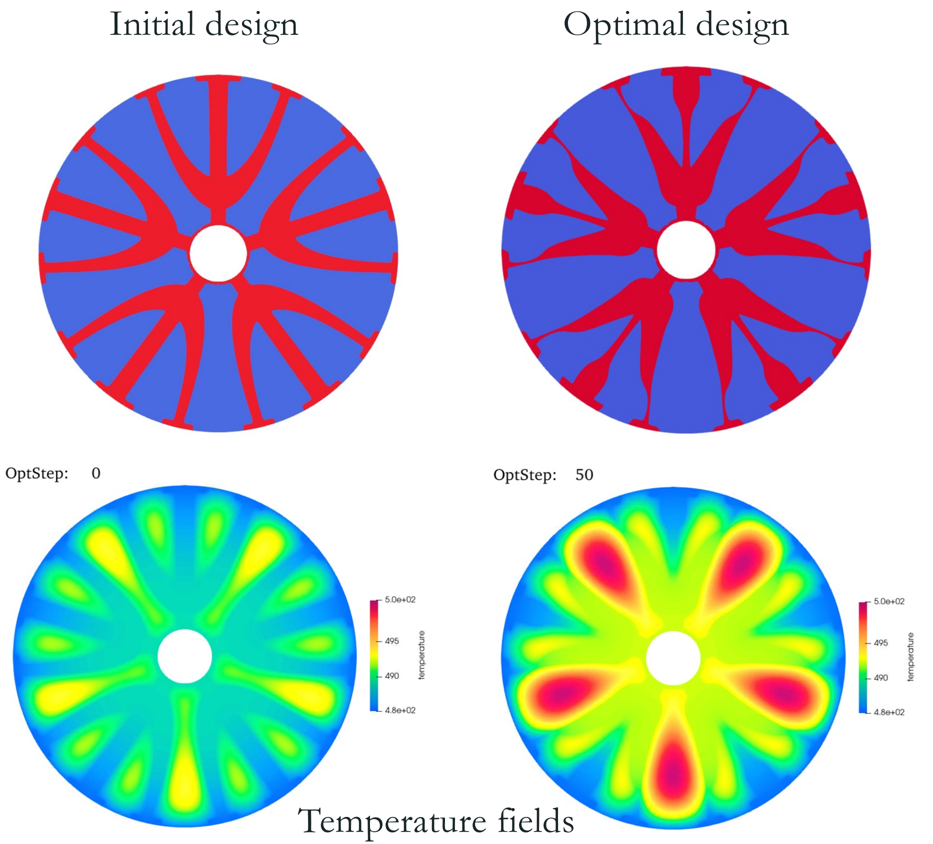
ShapeOpt: Reactor Design for Thermal Management

Design optimization of integrated cooling inserts in modular Fischer-Tropsch reactors



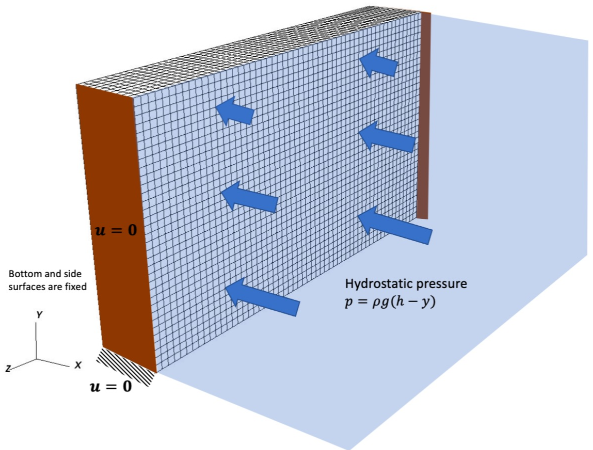
Controlling minimum feature size in topology preserving designs





ShapeOpt: Dam Structural Design

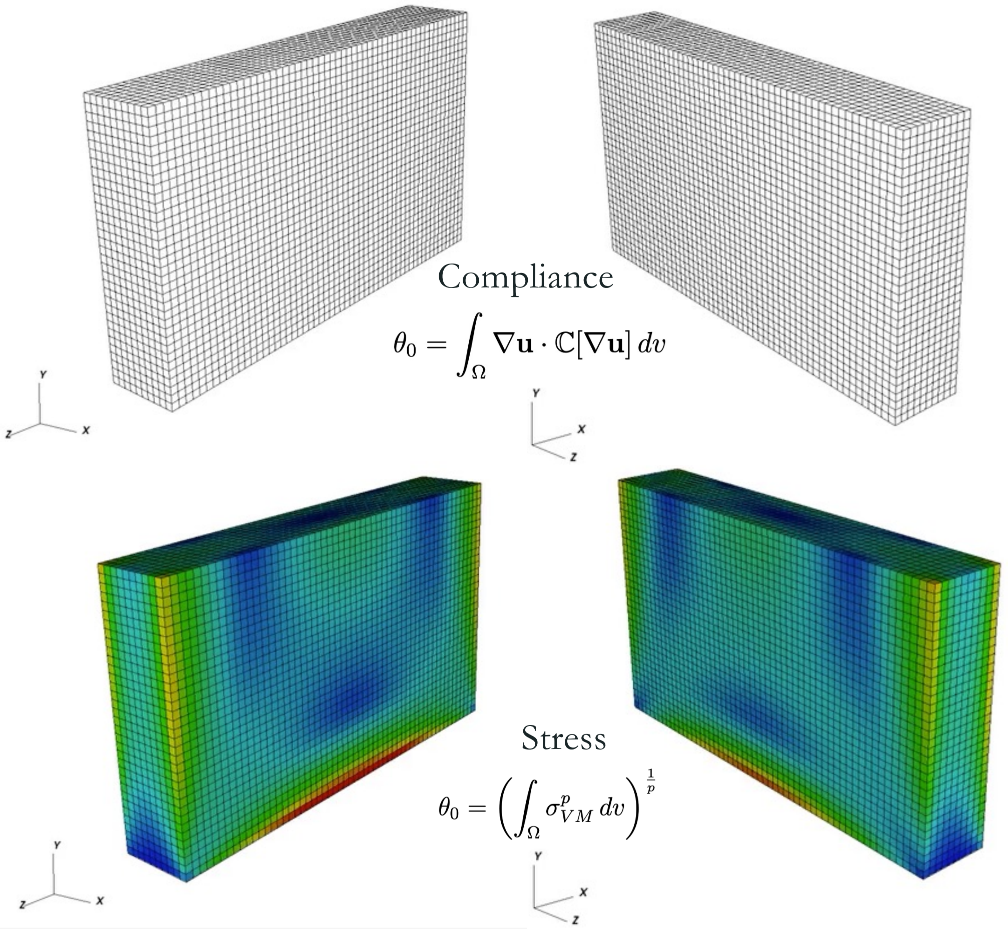
Shape optimization of a concrete dam. Enforcing an anisotropic stress constraint yields a familiar compression arch shape.



$$\min_{\mathbf{u}_d \in \mathcal{H}_H} \quad \theta_0$$

$$\text{such that} \quad \theta_1 = \int_\Omega dv - \overline{V} = 0$$

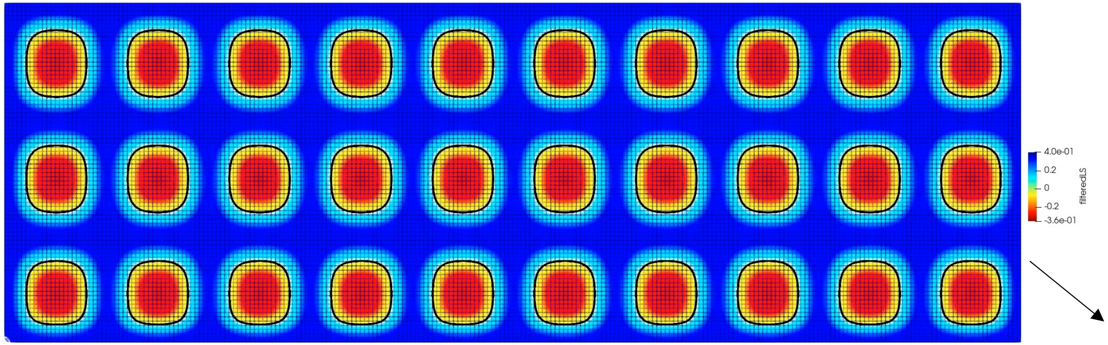
$$\underline{u}_d \le \mathbf{u}_d \cdot \mathbf{e}_i \le \overline{u}_d \text{ for } i = 1, 2$$



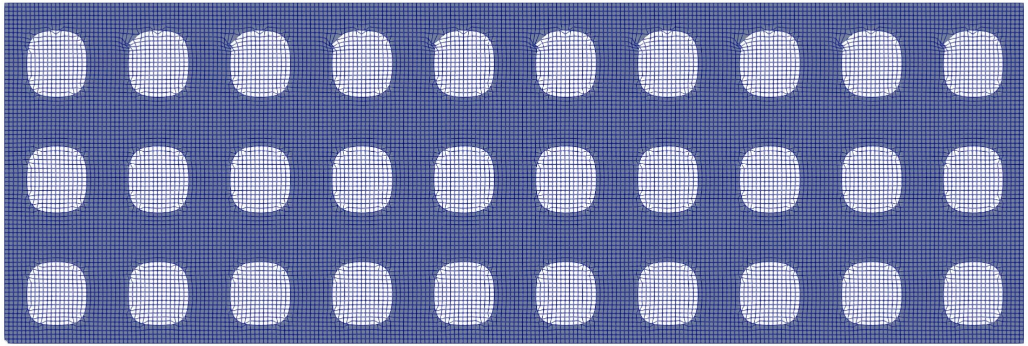
ShapeOpt: Parameter-free via Level Sets

- Two meshes: one fixed for design and another that morphs for analysis.
- Leverages graph, TMOP, and (in the near future) Serac's shape sensitivities.
- Current approach allows for topological changes and circumvents remeshing by redefining the element attributes of the mesh to be morphed.

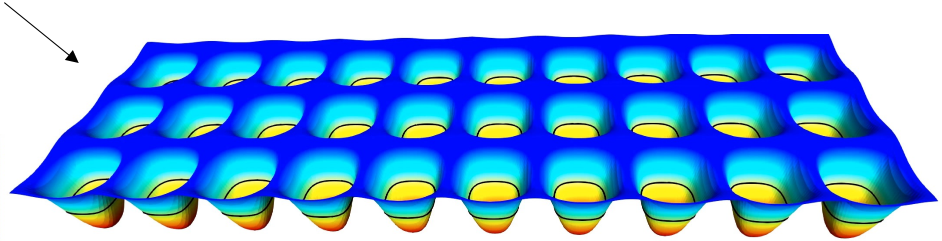
MBB Beam compliance minimization with mass constraint



Opt Iter: 1

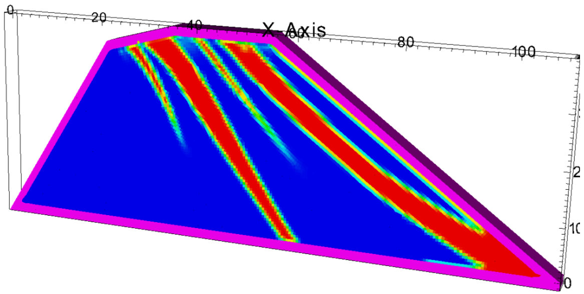


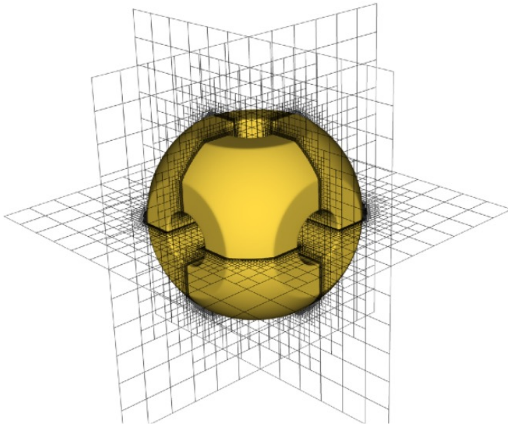
LS regularization via Heat Method using MFEM's Miniapp to compute a signed distance function.

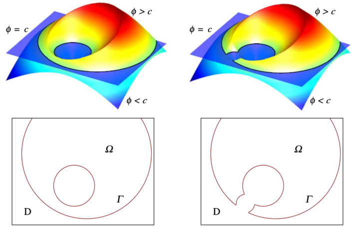


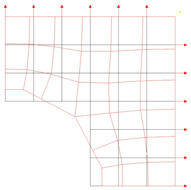
Summary

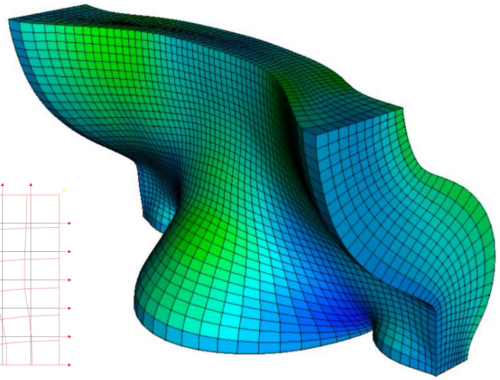
- LiDO->Serac-> MFEM
- Graph paradigm aids in modularization.
- Flexibility to exchange building blocks based on applications.
- Robust topology optimization (fictitious density/volume fraction fields) for various physics in 2D and 3D.
- Level set shape optimization using TMOP for mesh morphing.
- Potential application of shape optimization approaches to large scale problems since they are purely based on MFEM abstractions.

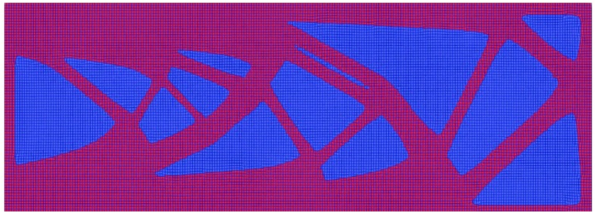












Thank you!

Any questions?

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