Topology Optimization using the Level Set and Extended Finite Element Methods

Theory and Applications

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Overview

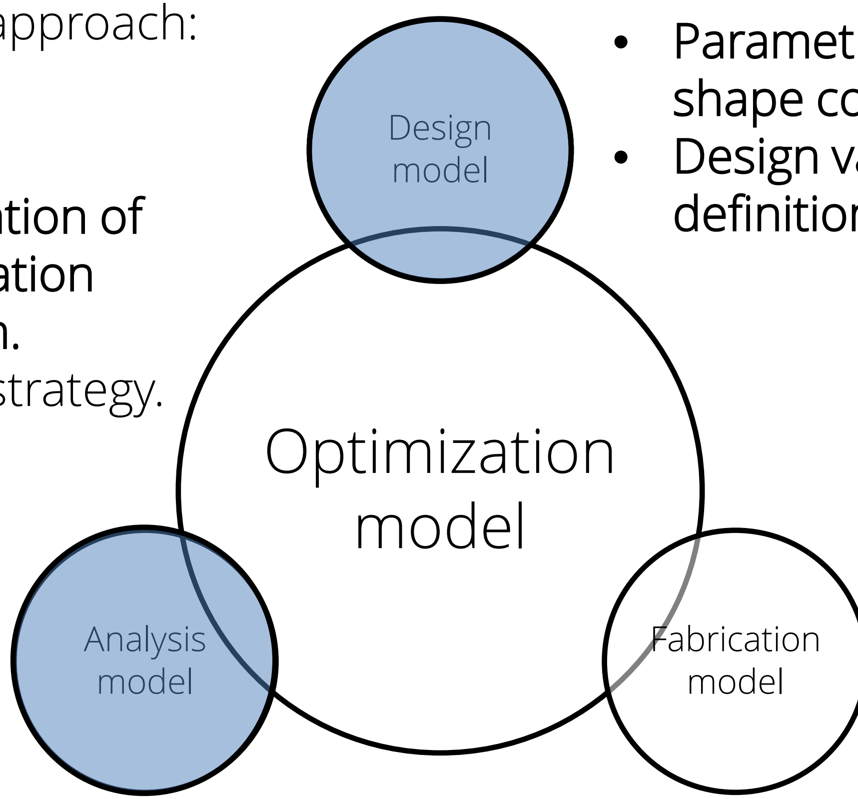
- Introduction.
- Goals and objectives.
- Case studies.
  - Structural linear elasticity.
  - Incompressible Navier-Stokes flow with scalar transport.
  - Curvature.
  - Incompressible Navier-Stokes with multiple scalar fields.
- Conclusions.

Goals and motivation

INTRODUCTION

Topology optimization

- Topology optimization is an inverse problem.
- Find a realizable distribution and geometry of materials and components with desired functionality.
  - i.e. Minimize a target value via configuring the material layout in some design domain.
- Computational approach:



- **Parametrization and shape control.**
- **Design variables definition.**

- **Formulation of optimization problem.**
- Search strategy.

- **Multiscale and multiphysics analysis.**

- Fabrication constraints and costs.

Structural topology optimization

- Minimize $\mathcal{F}_{\mathrm{SE}} = \int \frac{1}{2} \boldsymbol{\sigma}(\mathbf{x}) : \boldsymbol{\varepsilon}(\mathbf{x})\, \mathrm{d}\Omega$
- Satisfy equations:

$$-\nabla \cdot \boldsymbol{\sigma} = \mathbf{b} \quad \text{in } \Omega$$
$$\mathbf{u} = \bar{\mathbf{u}} \quad \text{on } \Gamma_D$$
$$\boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{f} \quad \text{on } \Gamma_N$$

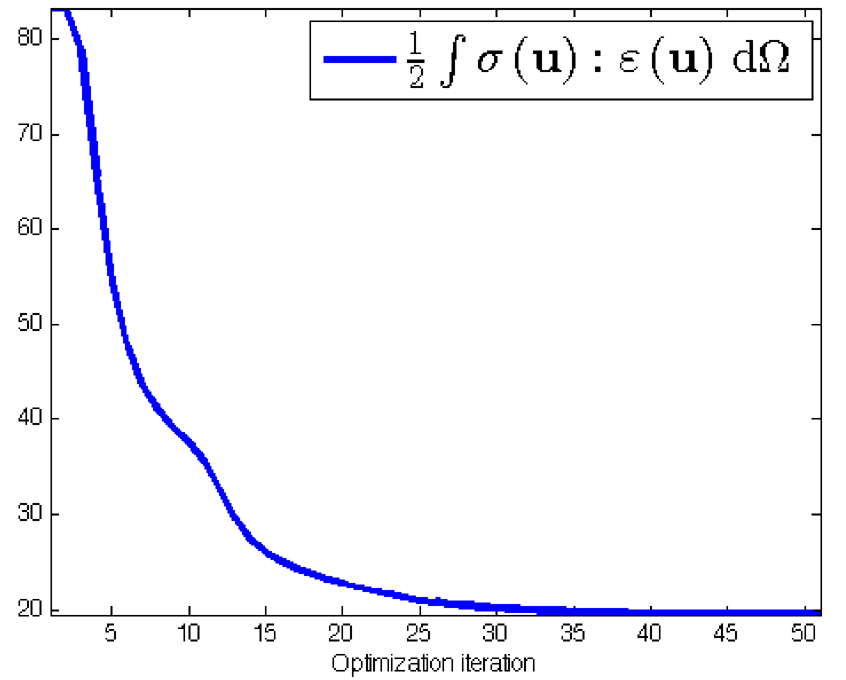
- Subject to $\mathcal{G}_s = \frac{\int \rho \mathrm{d}\Omega}{0.5 \int \mathrm{d}\Omega} < 1$
- Optimization solved by nonlinear mathematical programming algorithm (GCMMA).
- Design variables are the artificial densities of the finite elements.

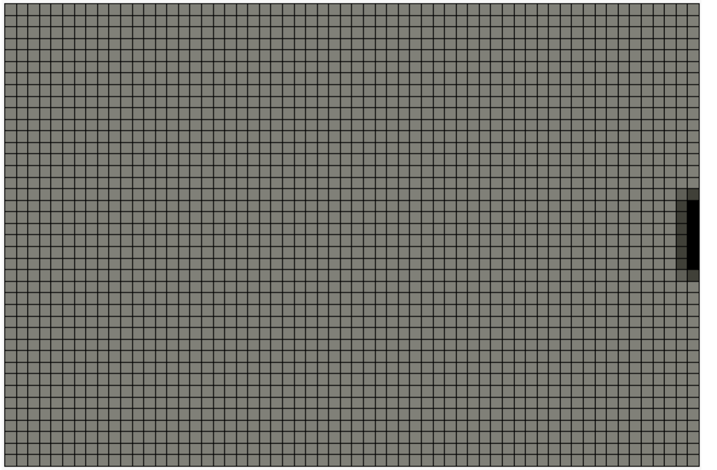
  $\rho(\mathbf{x}) = 1.0 \rightarrow$ solid.

  $\rho(\mathbf{x}) = 0.0 \rightarrow$ void.
- Design to physical model:

  $\boldsymbol{\sigma} = \mathbb{C}(\rho) : \boldsymbol{\varepsilon}$
- Relax by allowing a continuum between the materials.

  Intermediate material.





Optimized geometry

Incompressible Navier-Stokes flow topology optimization

- Minimize pressure difference:

$$F_{\mathrm{PD}} = \frac{\int_{\Gamma_{\mathrm{in}}}\left(p+\frac{\rho|\mathbf{u}|^2}{2}\right)d\Gamma}{\int_{\Gamma_{\mathrm{in}}} d\Gamma} - \frac{\int_{\Gamma_{\mathrm{out}}}\left(p+\frac{\rho|\mathbf{u}|^2}{2}\right)d\Gamma}{\int_{\Gamma_{\mathrm{out}}} d\Gamma}$$

- Satisfy equations:

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla p + \mu\nabla^2\mathbf{u} - \alpha\mathbf{u}$$

- Subject to $\mathcal{G}_s = \frac{\int \gamma \mathrm{d}\Omega}{0.25\int \mathrm{d}\Omega} < 1$

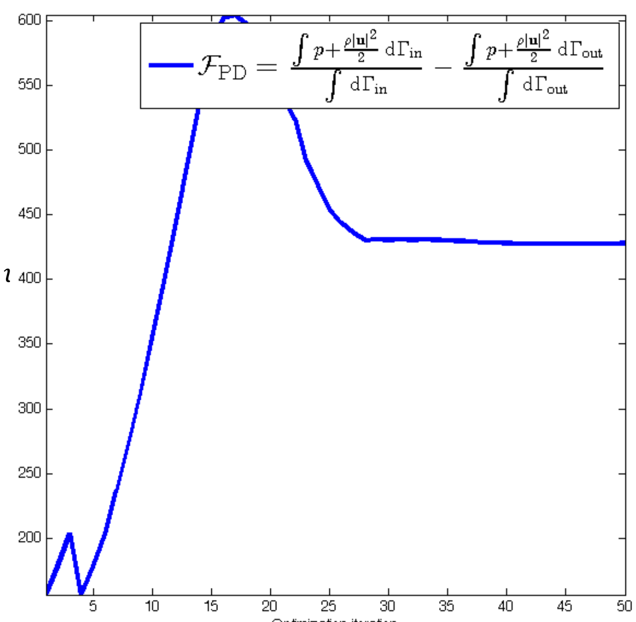
- Design variables are the porosity of the finite elements.

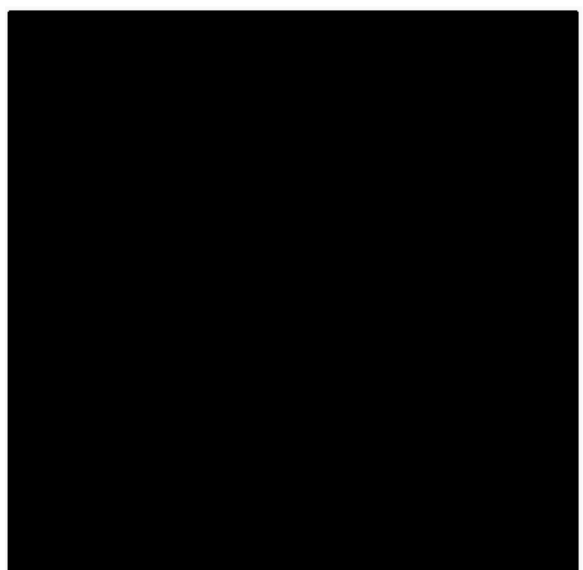
$\gamma(\mathbf{x}) = 1.0 \rightarrow$ fluid.

$\gamma(\mathbf{x}) = 0.0 \rightarrow$ solid.

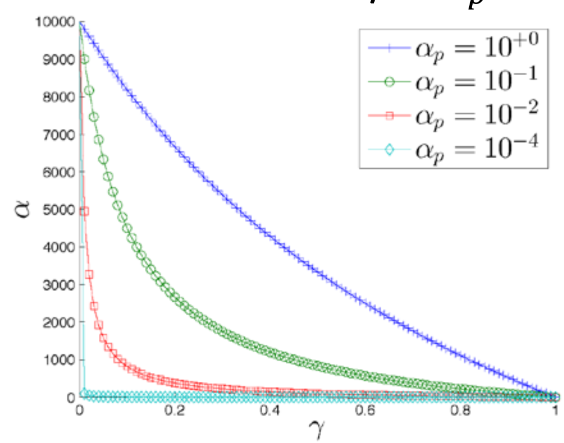
- Brinkman coefficient uses interpolation to avoid large gradients in flow.

$$\alpha(\gamma) = \alpha_{max} + \gamma\cdot(\alpha_{min} - \alpha_{max})\frac{1+\alpha_p}{\gamma+\alpha_p}$$





Optimized geometry.

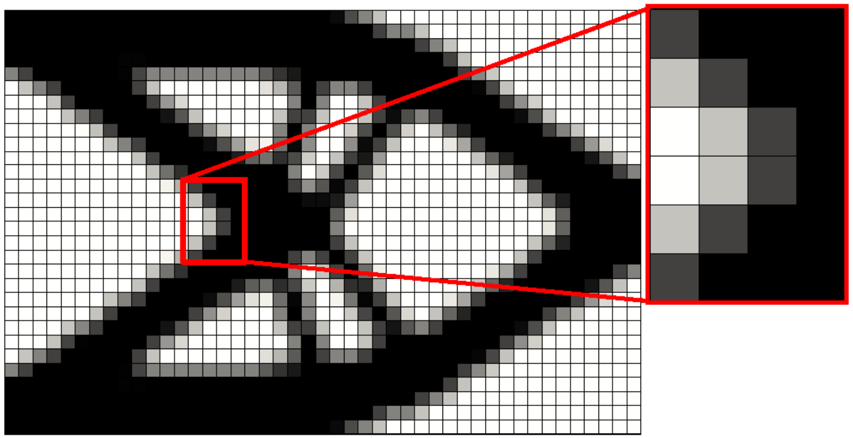


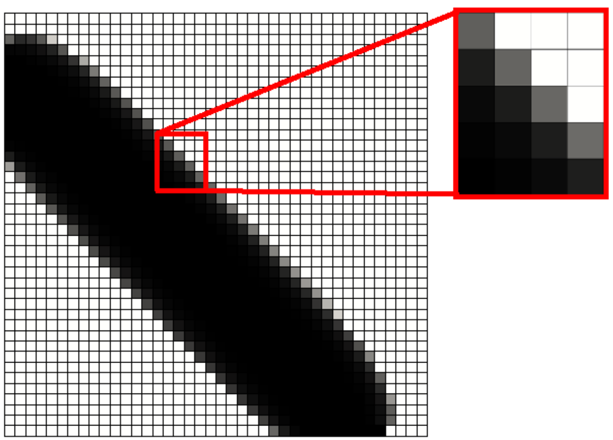
$$\alpha_{max} = \left(1 + \frac{1}{Re}\right)\cdot 10^4$$

$$\alpha_{min} = 0$$

$$\alpha_p = 0.01$$

Density optimization methods





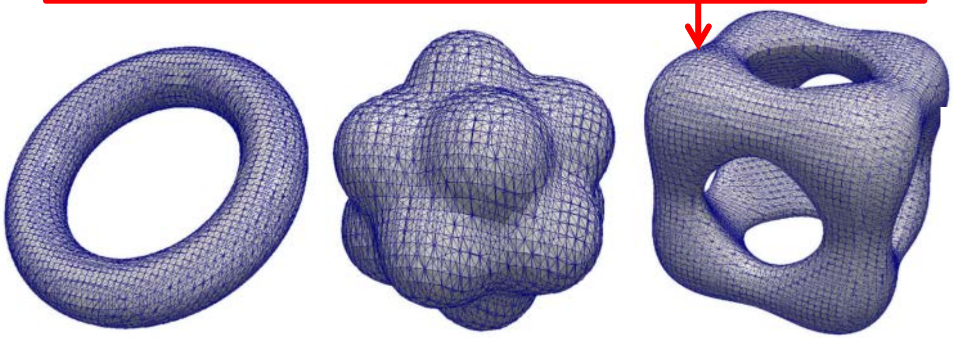
- Interface between different material domains represented by using intermediate ("grey") densities → jagged boundaries.
- Enforcement of boundary conditions at the interface is hindered.

- Jagged boundaries cause:
  - Premature yielding in structural mechanics due to stress singularities (Maute et al., 1998).
  - Fluid flow penetrating solid material in low Reynolds number flow (Kreissl and Maute, 2011) .
  - Scalar fields diffusing through solid material at low Péclet number flow (Makhija et al., 2012).
  - Especially in **nonlinear problems**.
- These problems can be overcome by **adaptive remeshing**.
  - Expensive for three dimensional problems.
- Density methods implemented in most comme

Level set method

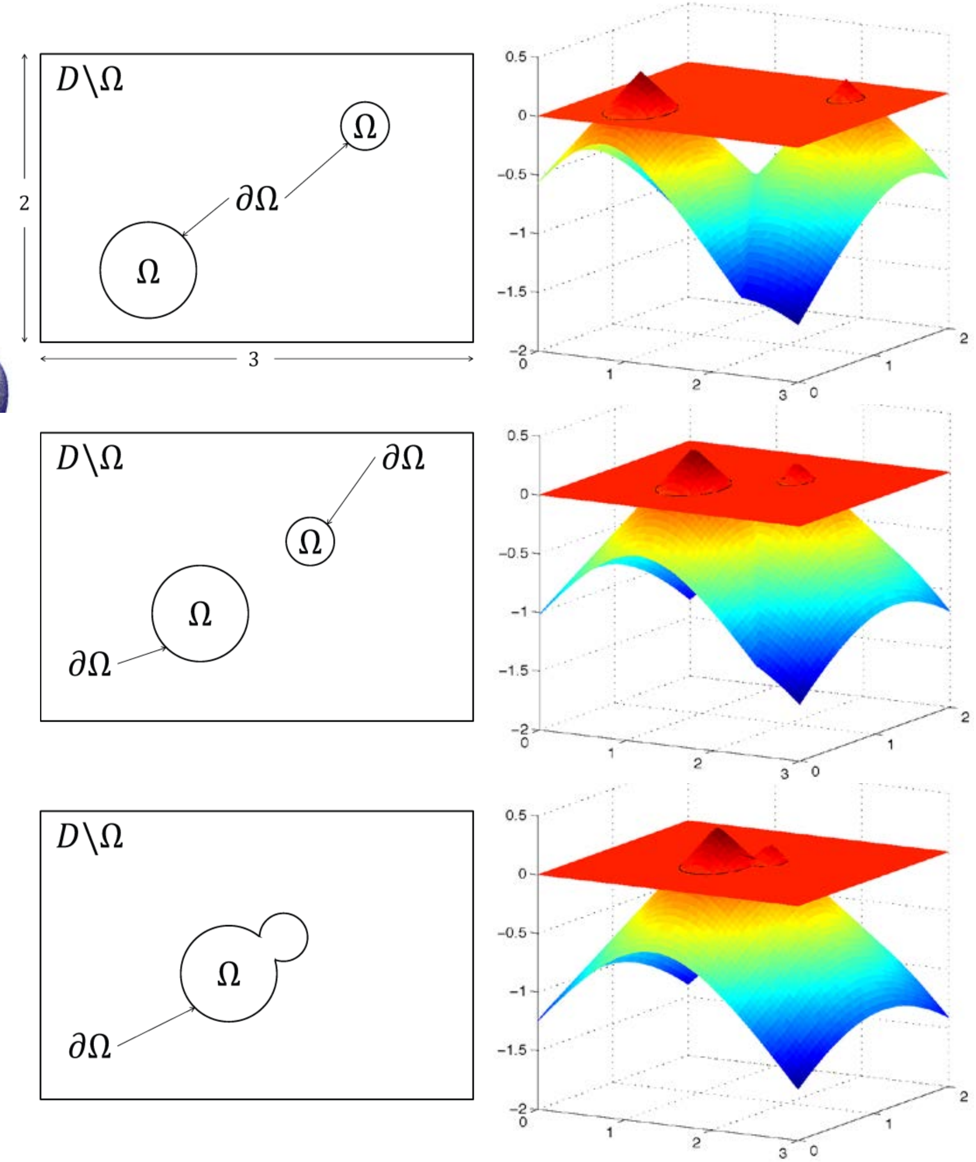
- Alternative to geometry description of density methods.
- Shape boundary $\partial\Omega$ is a curve or surface expressed as the zero level set of a higher dimensional implicit function.

$$\boxed{\begin{aligned}\phi(\mathbf{x}) = (x^2+y^2-4)^2+(z^2-1)^2+(y^2+z^2-4)^2 \\ -(x^2-1)^2+(z^2+y^2-4)^2+(y^2-1)^2-15\end{aligned}}$$



- Smooth changes in $\phi(\mathbf{x})$ leads to changes in topology:
  - Form holes.
  - Split into multiple pieces.
  - Merge with other level set functions.

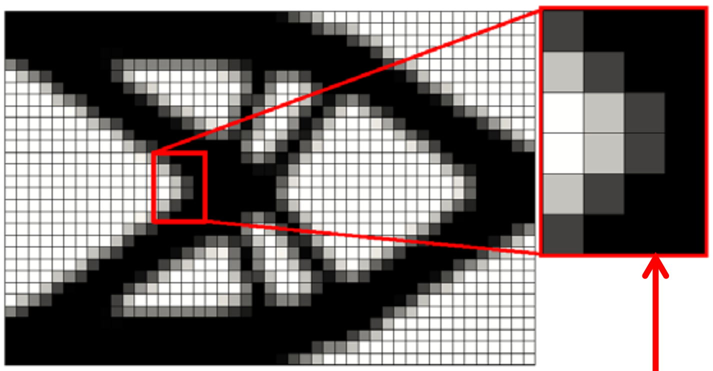
$\phi(\mathbf{x}) > 0$	$\forall\mathbf{x} \in \Omega\backslash\partial\Omega$	inside the region
$\phi(\mathbf{x}) = 0$	$\forall\mathbf{x} \in \partial\Omega$	on the boundary
$\phi(\mathbf{x}) < 0$	$\forall\mathbf{x} \in D\backslash\Omega$	outside the region



Geometry representation comparison: density and level set

Design variables, $\mathbf{s}(\mathbf{x})$, are associated with nodes in these examples.

Density method

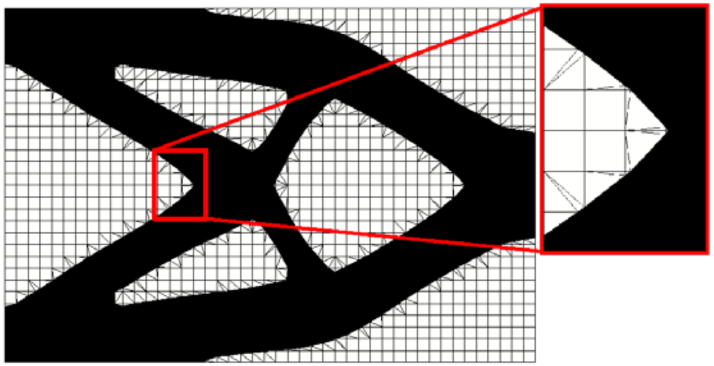


$$\tilde{\rho}(\mathbf{s}) = \frac{\sum_{i=1}^{E} w_i s_i}{\sum_{i=1}^{E} w_i}$$

$$w_i = \max\left(0, r_\rho - \|\mathbf{x}_i - \mathbf{x}\|\right)$$

- Prevents formation of features smaller than r_ρ.
- At cost of intermediate ("grey") densities.

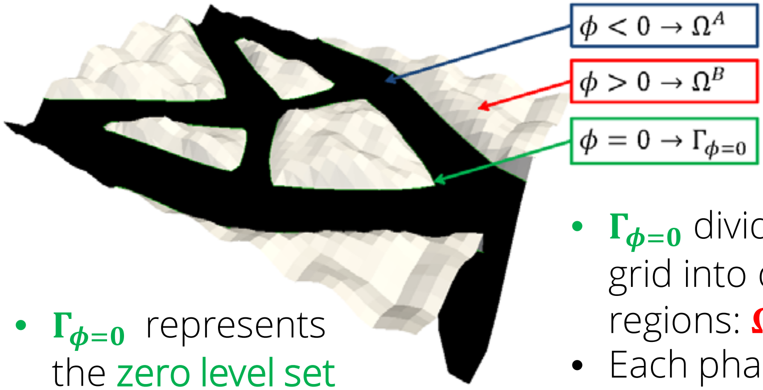
Level set method



$$\phi(\mathbf{s}) = \frac{\sum_{i=1}^{N} w_i s_i}{\sum_{i=1}^{N} w_i}$$

$$w_i = \max\begin{pmatrix} 0, \\ r_\phi - \|\mathbf{x}_i - \mathbf{x}\| \end{pmatrix}$$

- Does not provide a minimum feature size control.

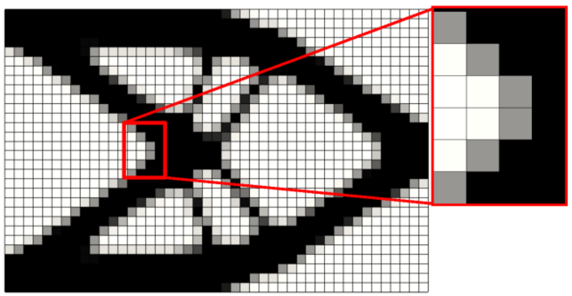


- $\boldsymbol{\Gamma}_{\boldsymbol{\phi}=0}$ represents the zero level set isolevel of the level set function $\phi(\mathbf{x})$.

- $\boldsymbol{\Gamma}_{\boldsymbol{\phi}=0}$ divides the fixed mesh grid into different phase regions: $\boldsymbol{\Omega}^{\boldsymbol{A}}$ and $\boldsymbol{\Omega}^{\boldsymbol{B}}$.
- Each phase represents a different material, i.e. solid and void.

Material representation comparison: SIMP, Ersatz material, remeshing

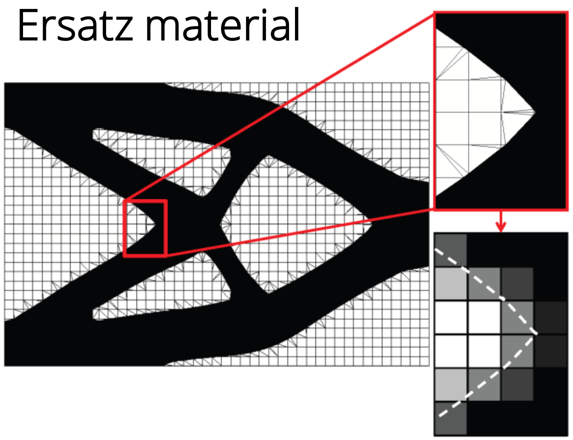
Solid Isotropic Material with Penalization



$E(\mathbf{x})$ plot

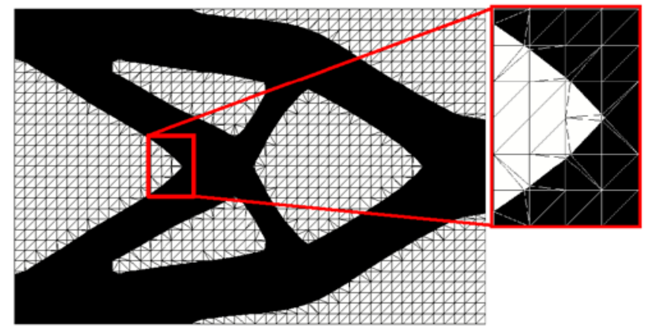
- SIMP models relation between density and stiffness.
  $E(\mathbf{x}) = \tilde{\rho}^p \boldsymbol{E_A} + (1 - \tilde{\rho}^p)\boldsymbol{E_B}$
- $p \geq 3$ recovers binary distribution.
- $\boldsymbol{E_B} = \mathbf{0}$ for void material.

Ersatz material

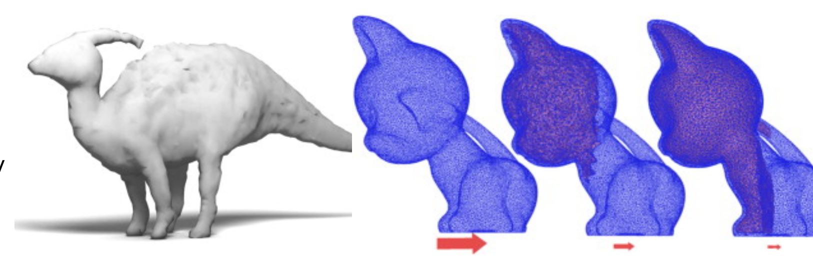


- The material properties of each finite element are interpolated proportional to the volumes of the solid and void phases.
- Similar issues as density methods.

Remeshing



- Circumvent Ersatz material.
- New meshes align with geometry of $\boldsymbol{\Gamma_{\phi=0}}$.
- Suffers from robustness and efficiency.
- Affects the convergence of the optimization process (Schleupen et al., 2000 and Wilke et al. 2006).
- There have been recent developments, but still tricky:

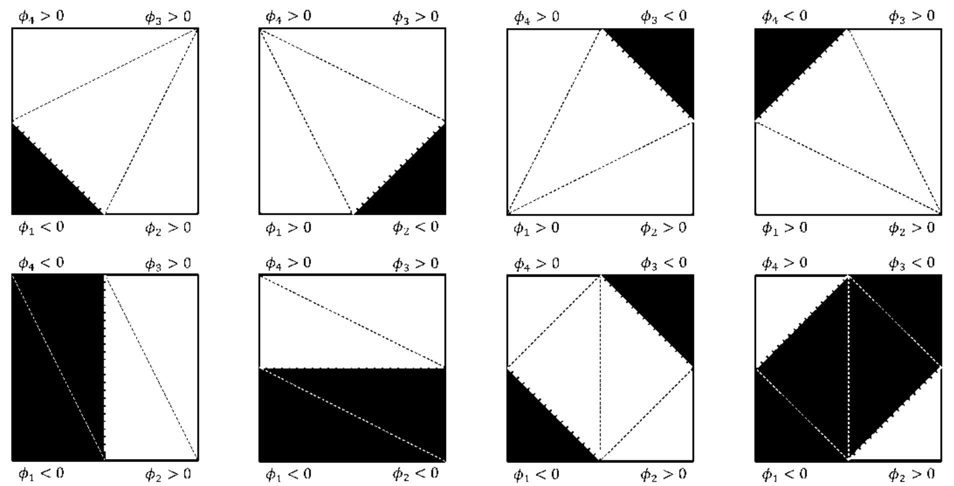


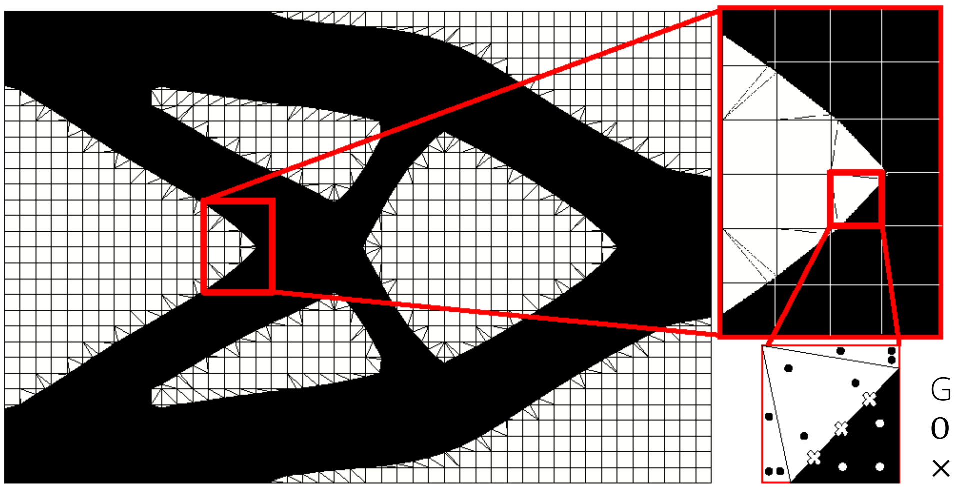
Toy models optimized with remeshing to improve balance while maintaining the initial shape.

Material representation: eXtended Finite Element Method

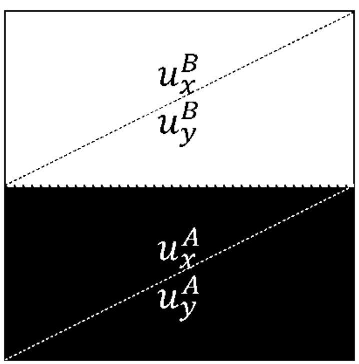
- Immersed boundary technique.
- Decomposes finite elements into subdomains and interfaces for integration.
- Enriches solution space, allowing for discontinuities.

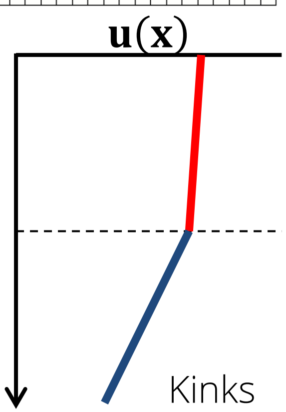
Decomposition examples for 2D finite elements.

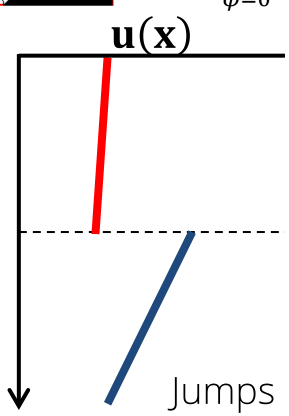




Gaussian quadrature points.
$0 \rightarrow \Omega_{\text{tri}}$
$\times \rightarrow \Gamma_{\phi=0}$





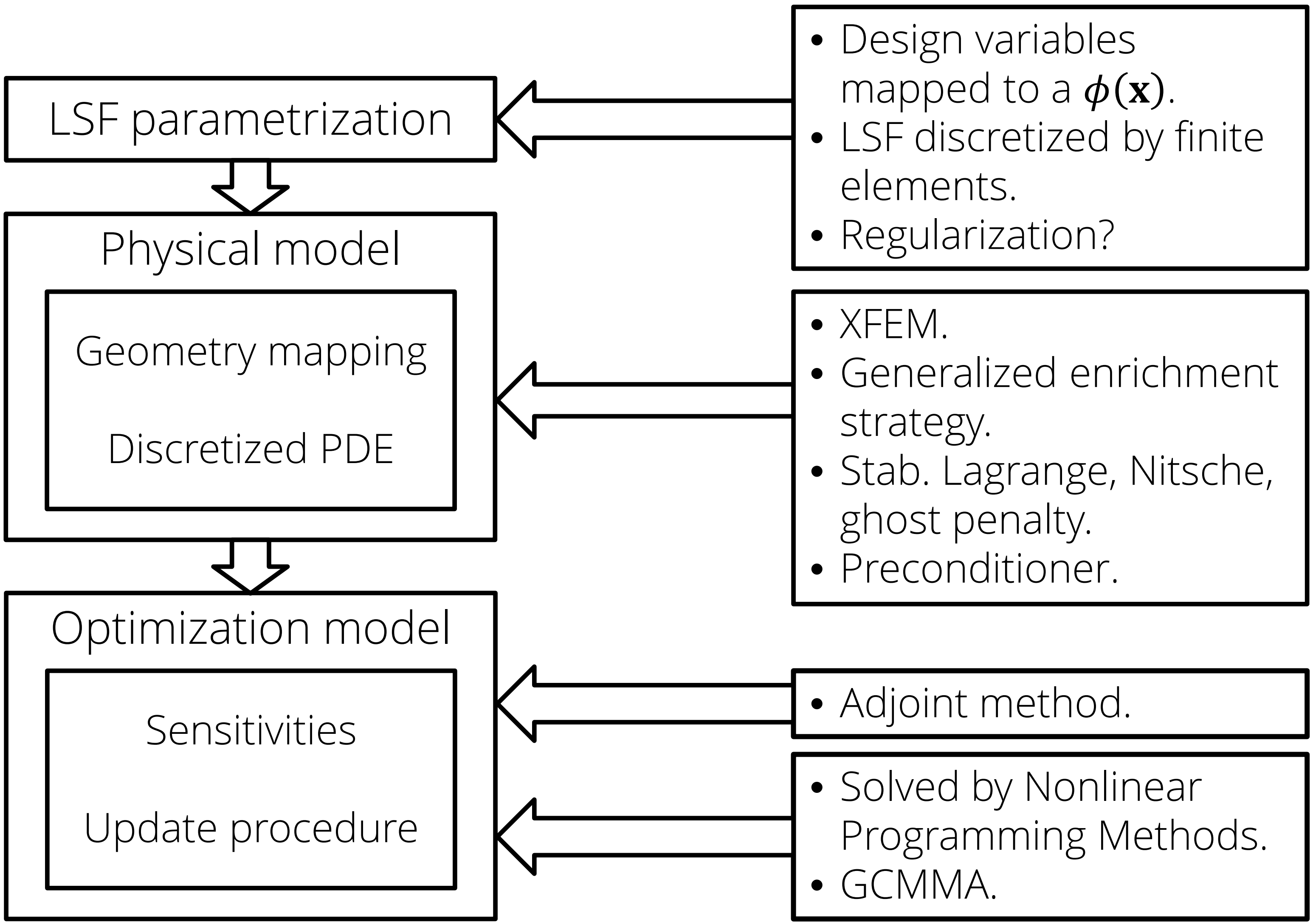


- Solution approximation by **standard enrichment.**

$$\mathbf{u}(\mathbf{x}) = H(-\phi)\sum_{i=1}^{n} \mathbf{N}_i \mathbf{u}_i^A + H(\phi)\sum_{i=1}^{n} \mathbf{N}_i \mathbf{u}_i^B$$

$$H(z) = \begin{cases} 1, & z < 0 \\ 0, & z \geq 0 \end{cases}$$

The LSM-XFEM framework



GOALS AND HYPOTHESES

Goals and objectives

- Generate a generic, robust, and efficient LSM-XFEM topology optimization framework.
- **Generic**:
  - Develop a **generic** optimization approach.
  - LSM-XFEM can be used for different physics.
  - In contrast with density methods.
    - Requires a **different interpolation scheme** for each physics.
    - Structural linear elasticity: $E(\mathbf{x}) = \tilde{\rho}^p \boldsymbol{E_A} + (1 - \tilde{\rho}^p)\boldsymbol{E_B}$
    - Incompressible Navier-Stokes: $\alpha(\gamma) = \alpha_{max} + \gamma \cdot (\alpha_{min} - \alpha_{max}) \frac{1+\alpha_p}{\gamma+\alpha_p}$
  - LSM-XFEM can be used for 2D and 3D problems.
  - LSM-XFEM can be used for multi-material problems.
- **Robust**:
  - Material interpolation in SIMP is robust for linear problems.
    - Not as accurate in nonlinear problems.
  - Apply to linear and nonlinear problems.
  - Study shape control capabilities.
  - Study boundary condition enforcement at phase interface.
- **Efficiency**:
  - Study computational cost.
  - Mesh size requirements.

Goals and objectives

- Compare the LSM-XFEM optimization scheme with traditional density methods.
  - Study the advantages and disadvantages.
- Explore characteristics of framework through case studies:
  - Structural linear elasticity,
  - Incompressible Navier-Stokes flow.
  - Scalar transport.
  - Real-world incompressible Navier-Stokes with multiple scalar fields transport problem.
  - Each one of them requires special treatment in density method.

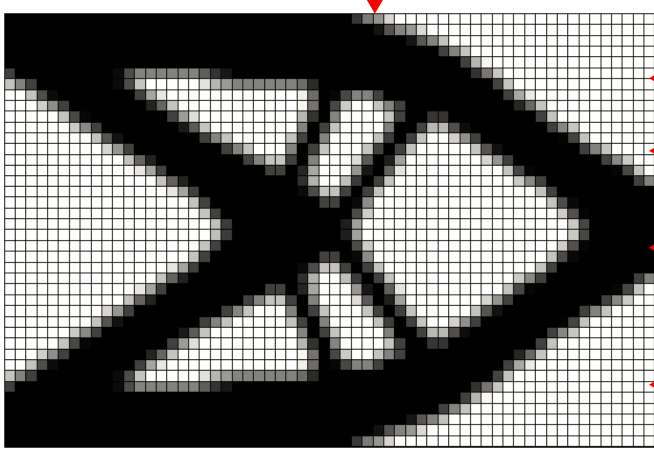
  - Two “material–void” and “material–material” problems.
  - Three dimensional.
  - Help understand the characteristics and capabilities of the framework.

Structural topology optimization

CASE STUDY I

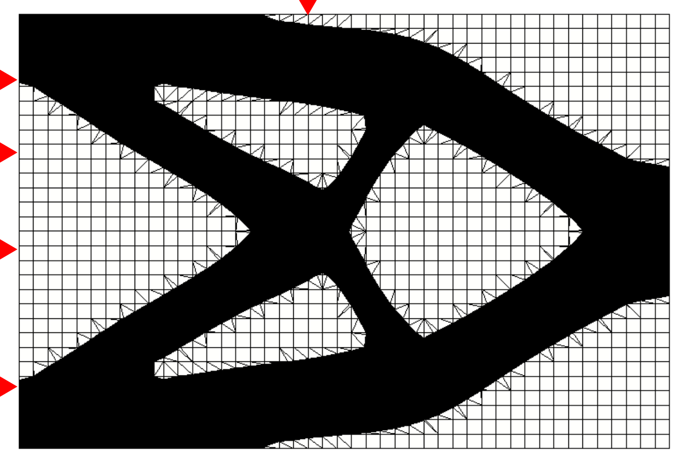
Goals and objectives

- **Objective:**
  - Implement algorithms for LSM-XFEM framework in 3D.
  - Compare LSM-XFEM framework against density methods, such as SIMP, with a structural linear elastic problem.
- **Hypotheses**:
  - Requires **coarser meshes** which may lead to **faster computations**.
  - Provides ability to extract surface meshes from level set function to **manufacture** design.
- **Open issues**:



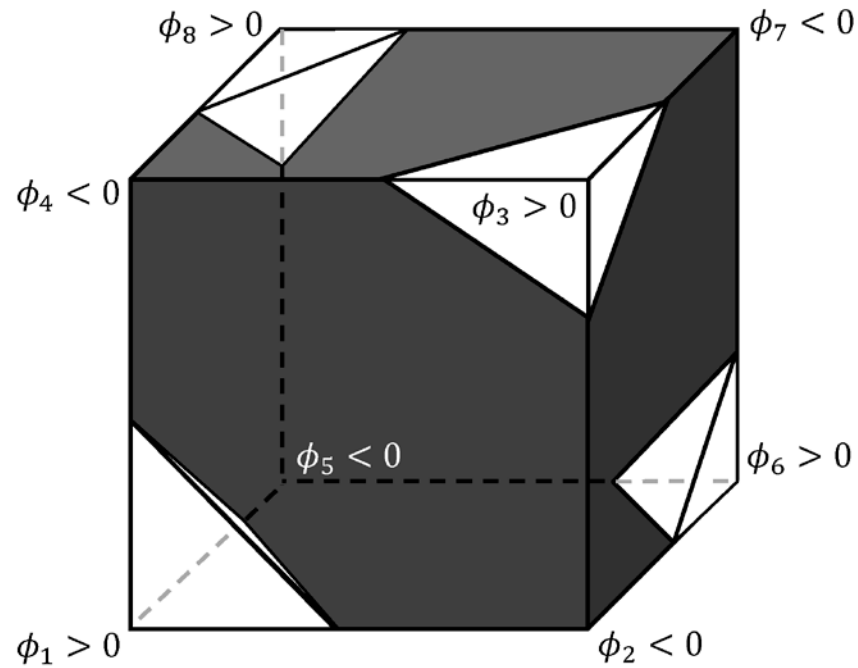
Comparison against density methods*.
Convergence rates?*
Shape control?*
Postprocessing for manufacturing?*
Influence of initial design?*

*for selected case studies.



Issue: XFEM implementation in three dimensions

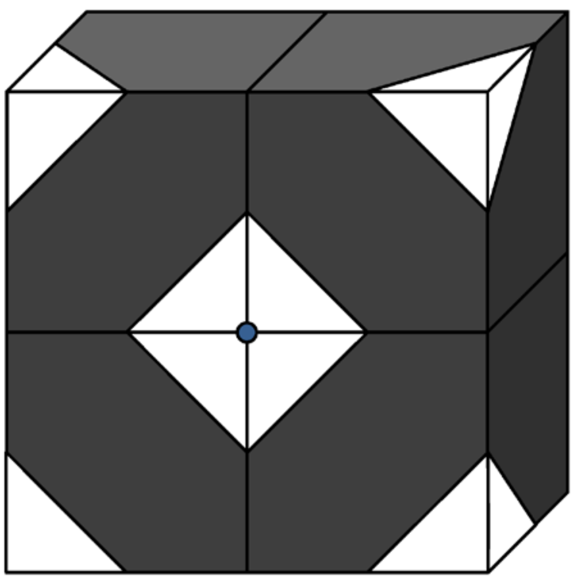
- **Objective**:
  - Expand the **triangulation**, **enrichment**, and **preconditioner** formulations to 3D.
- **Open issues**:
  - What is the algorithmic complexity?
  - Use **computer vision algorithms** to "see" disconnected phase regions?
  - How expensive is it computationally?



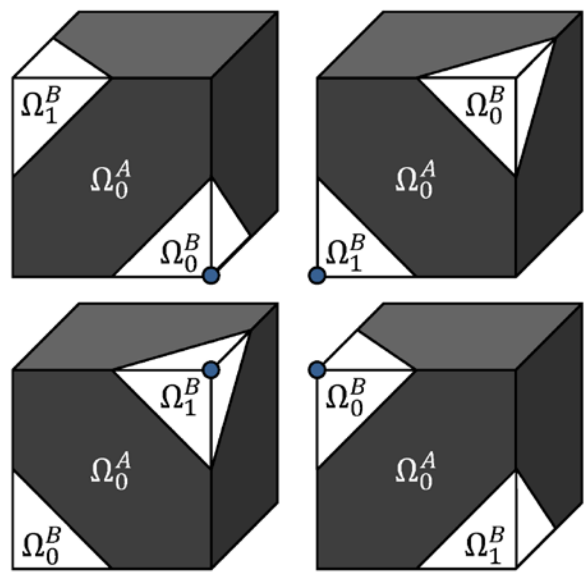
Intersection pattern can be numerous and complex in three dimensions.

Approach: generalized enrichment strategy for 3D XFEM

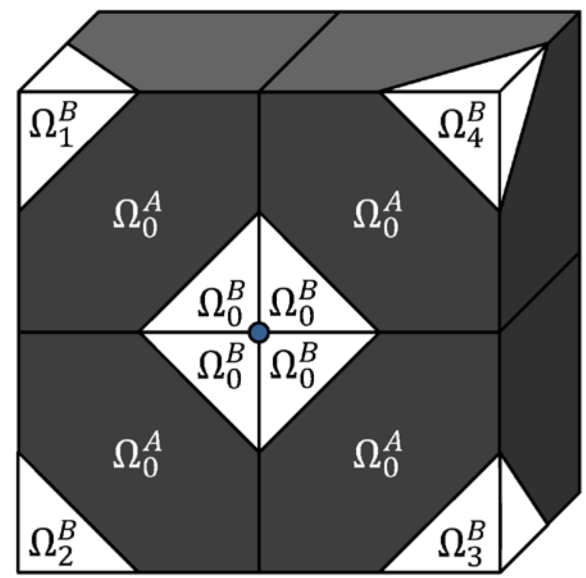
- Grounded on **flood fill** computer vision algorithm.
- Several implementation algorithms attempted.
  - Latest version reduced computation time from ~10 minutes on average to milliseconds.



Intersection configuration



Local elemental enrichment



Nodal cluster enrichment

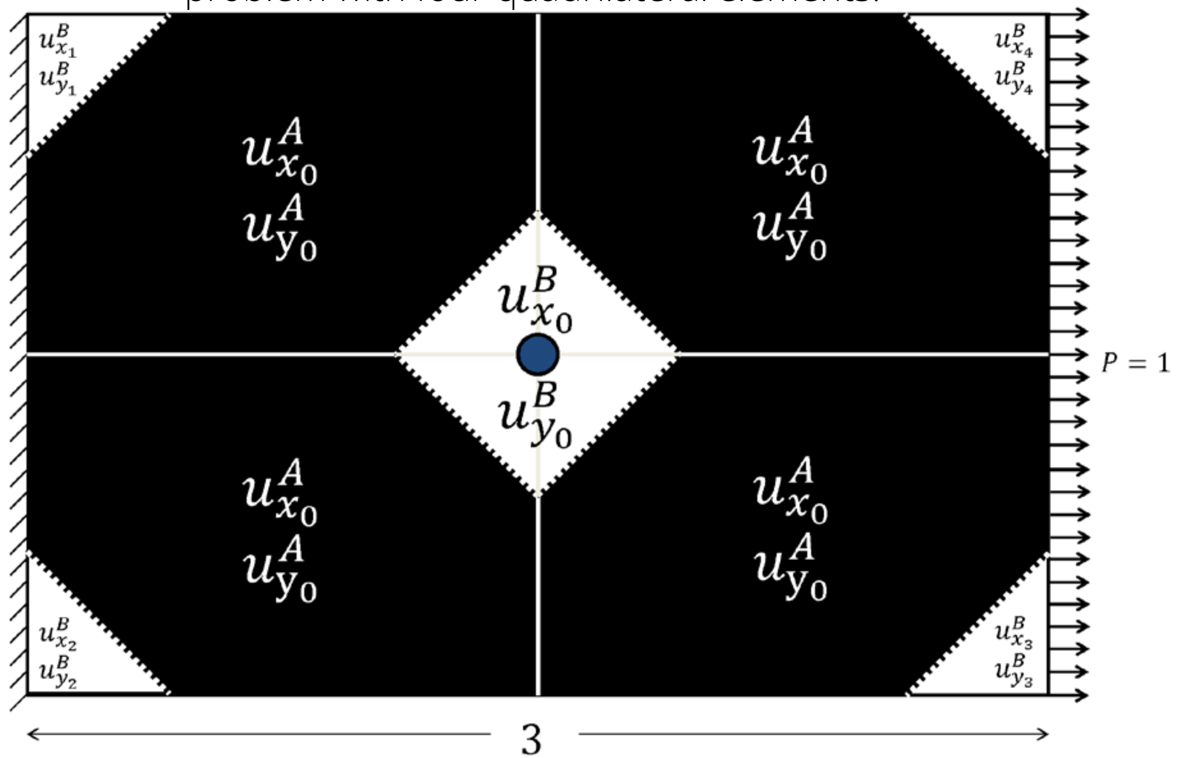
Issue: generalized description of discontinuities

- Multiple disconnected regions of the same phase may appear during optimization.
- **Approach**:
  - Augments the standard function space with additional "enriched" degrees-of-freedom.
  - Heaviside enrichment formulation of Hansbo and Hansbo (2004).

$$\mathbf{u}(\mathbf{x}) = \sum_{m=1}^{M} \left(H(-\phi) \sum_{i=1}^{n} \mathbf{N}_i \mathbf{u}_{i,m}^{A} + H(\phi) \sum_{i=1}^{n} \mathbf{N}_i \mathbf{u}_{i,m}^{B} \right)$$

m	:	Enrichment level.
M	:	Maximum number of enrichment levels for each phase.
$\mathbf{u}_{i,m}^{l}$	:	Vector of degrees-of-freedom.
$l = [A, B]$	:	Phase region.

Two dimensional structural linear elastic problem with four quadrilateral elements.



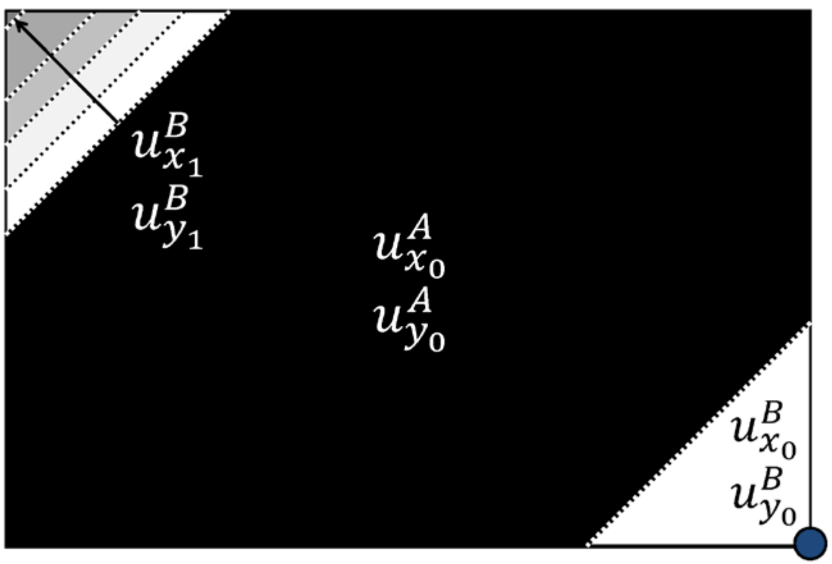
Phase "A"		Phase "B"	
$u_{x_0}^A$	$u_{x_0}^A$	$u_{x_0}^B$	$u_{x_0}^B$
$u_{x_1}^A$	$u_{x_1}^A$	$u_{x_1}^B$	$u_{x_1}^B$
$u_{x_2}^A$	$u_{x_2}^A$	$u_{x_2}^B$	$u_{x_2}^B$
$u_{x_3}^A$	$u_{x_3}^A$	$u_{x_3}^B$	$u_{x_3}^B$
$u_{x_4}^A$	$u_{x_4}^A$	$u_{x_4}^B$	$u_{x_4}^B$

- Center node uses different dofs to describe disconnected phase regions.
- Subscripts denote the m enrichment level.
- Maximum number of enrichment levels for each phase $M = 5$.

■ Active for phase "A".
■ Active for phase "B".
■ Inactive.

Issue: Ill-conditioned analysis problems

- Changes in topology may cause vanishing zone of influence for certain degrees-of-freedom. 💣
- Ill-conditioning is **more pronounced in 3D** (more intersection patterns).



Example of vanishing zone of influence for $u^B_{x_1}$ and $u^B_{x_1}$.

- The condition number of the stiffness matrix increases. 💣

Approach:

- Balance the influence of all degrees of freedom in the system (Lang et a., 2013).

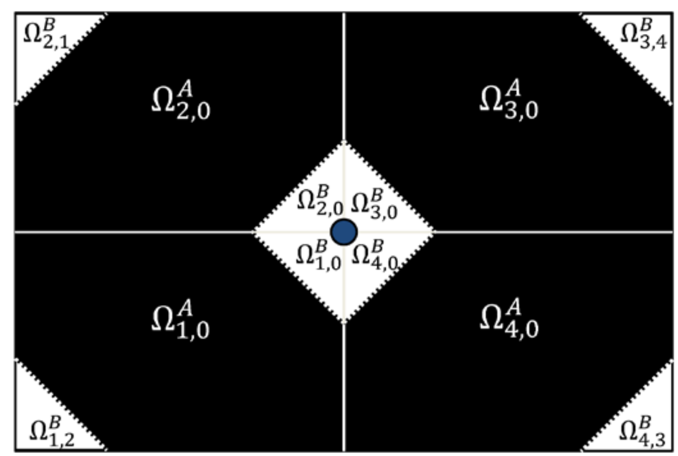
$$\mathbf{T}^l_{i,m} = \left(\max_{e \in E_i} \frac{\int_{\Omega^l_{e,m}} \nabla \mathbf{N}_i(\mathbf{x}) \cdot \nabla \mathbf{N}_i(\mathbf{x}) \mathrm{d}\mathbf{x}}{\int_{\Omega_e} \nabla \mathbf{N}_i(\mathbf{x}) \cdot \nabla \mathbf{N}_i(\mathbf{x}) \mathrm{d}\mathbf{x}} \right)^{-1/2}$$

E_i : Set of elements connected to node $\boldsymbol{i}$.

$\Omega^l_{e,m}$: Element domain of phase l.

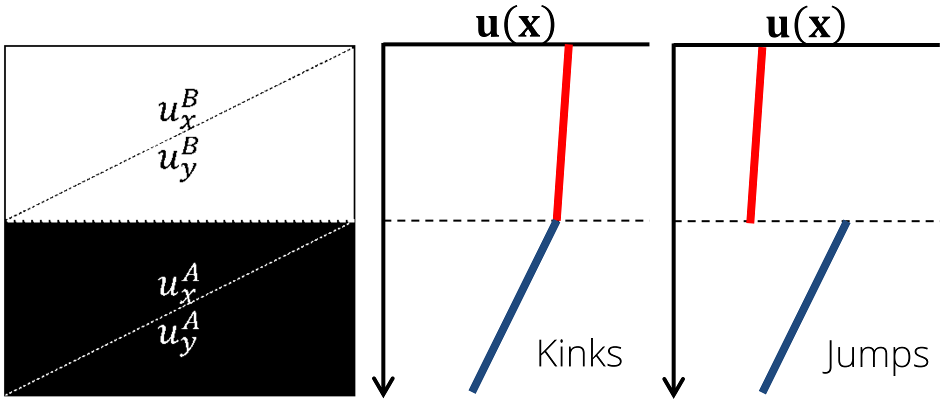
- Constraint degrees-of-freedom

$$\mathbf{T}^l_{i,m} > \mathbf{T}_{tol}$$



- Preconditioner expanded to 3D and built upon enrichment information.

Issue: Ensure continuity of solution at phase boundary $\Gamma_{\phi=0}$



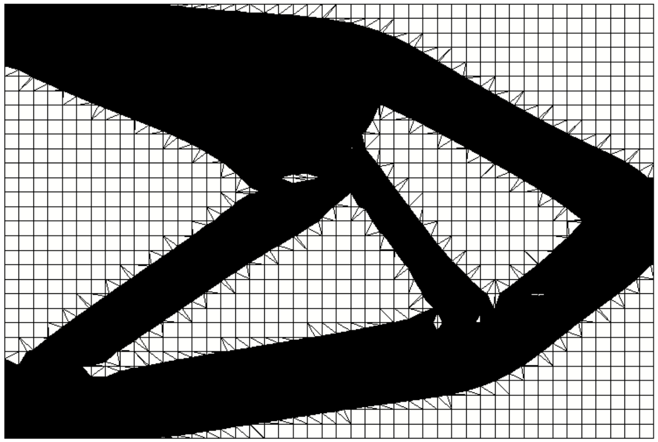
- The Heaviside function allows for discontinuities of the states $\mathbf{u}$ along the phase boundaries.

- **Hypothesis**:
  - Can we accurately **enforce boundary conditions** on the phase interface without extensive **mesh refinement**?
  - Can we ensure continuity of solution? $\mathbf{u}^A = \mathbf{u}^B \text{ on } \Gamma_{\phi=0}$ for "material-material" problems.
- **Approach**:
  - Stabilized Lagrange multipliers.

$$\int_{\phi=0} \delta\boldsymbol{\lambda} \cdot \left(\boldsymbol{\lambda} - \left(\frac{1}{2}(\boldsymbol{\sigma}^A + \boldsymbol{\sigma}^B)\right) \cdot \mathbf{n}_{\Gamma_{\phi=0}}\right) \mathrm{d}\Gamma - \int_{\phi=0} \delta\boldsymbol{\lambda} \cdot (\mathbf{u}^A - \mathbf{u}^B) \mathrm{d}\Gamma - \int_{\phi=0} \delta(\mathbf{u}^A - \mathbf{u}^B) \cdot \boldsymbol{\lambda} \mathrm{d}\Gamma$$

  - Nitsche method (penalty enforcement).
  - Proper treatment of interface conditions is key to obtaining accurate solution gradient along interface. 💣

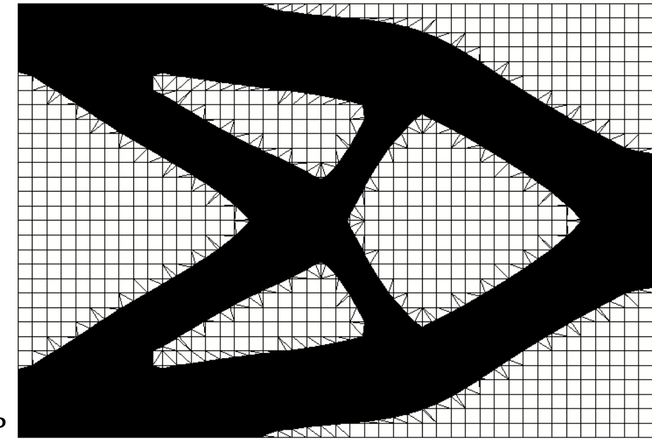
Issue: Controlling the shape of the level set function



Minimize $\mathcal{F}_{\mathrm{SE}}$

Motivation:
- Emergence of numerical artifacts in optimization problem.
- Convergence to local minima.

Minimize $\mathcal{F}_{\mathrm{SE}} + \mathcal{F}_{\mathrm{P}}$



Hypothesis:
- We can control the shape of the design through regularization techniques.

Objective:
- Use regularization technique to:
  - Avoid local minima with poor performance.
  - **Control geometrical properties.**

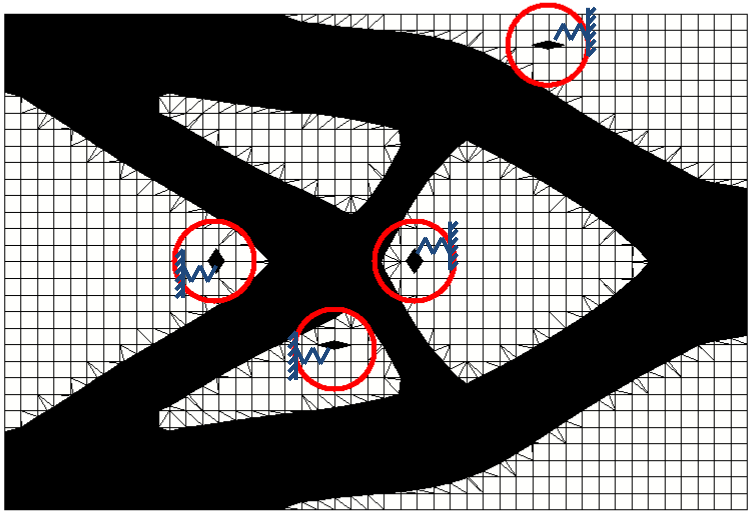
$$\mathcal{F}_{\mathrm{P}} = \int_{\phi=0} \mathrm{d}\Gamma \qquad \text{Perimeter}$$

$$\mathcal{F}_{\mathbf{n}} = \int_{\phi=0} \nabla \cdot \mathbf{n}\, \mathrm{d}\Gamma \qquad \text{Curvature}$$

Open issues:
- What are the effects of applying a **perimeter constraint** in 3D?
- Does it provide **local shape control**? e.g. minimum feature size?

Issue: Emergence of numerical geometrical artifacts

- For "solid-void" problems, designs with free floating pieces of material may be generated in the course of the optimization process.
- Causes ill-conditioning of the system.

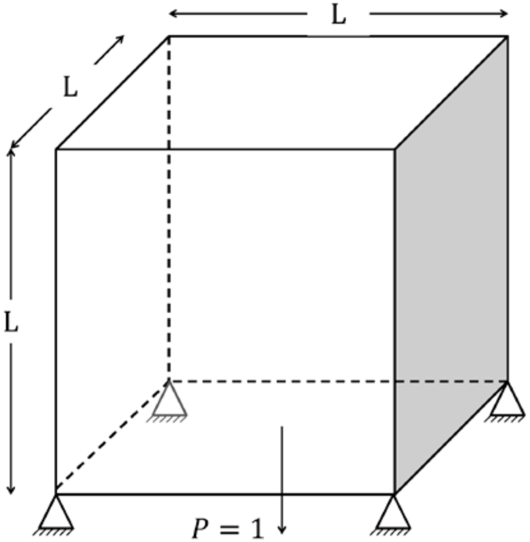


- **Approach**:
  - Adding soft springs between every material point and a fictitious support.

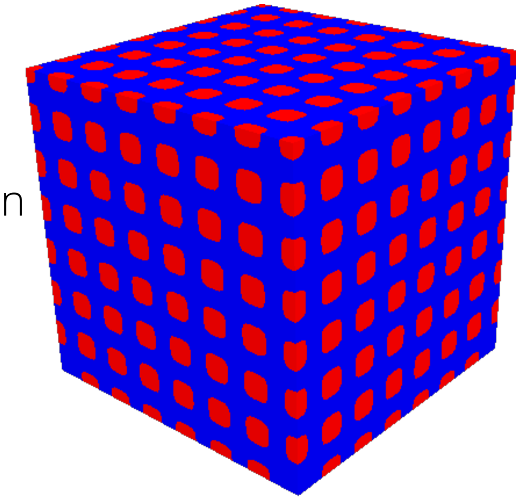
$$\int k_A \mathbf{N} \cdot \mathbf{u} \mathrm{d}\Omega^A$$

  - k_A denotes the stiffness of the distributed system of springs, $\mathbf{10^{-6}}$, for all examples.
  - Minimize perimeter of $\Gamma_{\phi=0}$ with $\mathcal{F}_{\mathrm{P}}$.

Convergence rate / feature size control

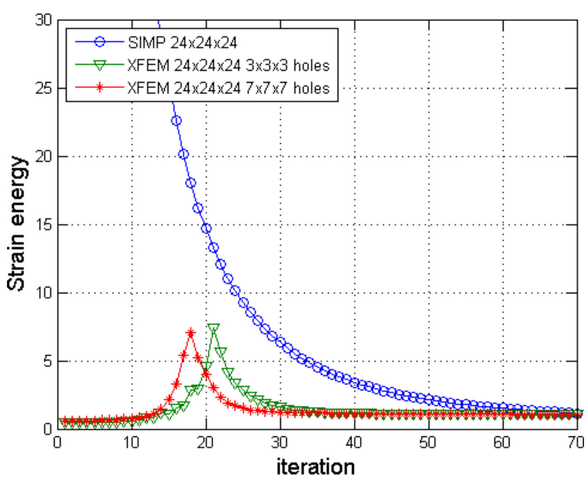


- Minimize $\mathcal{F}_{\mathrm{SE}}(+\mathcal{F}_{\mathrm{P}})$
- Maximum stiffness for given mass 10%
- $r_\rho = r_\phi = 1.6 \cdot h$
- $65 \times 65 \times 65$



Issue:
- Design sensitivities differ from zero near the interface.
- No new domains of solid can emerge, only possible to merge existing.

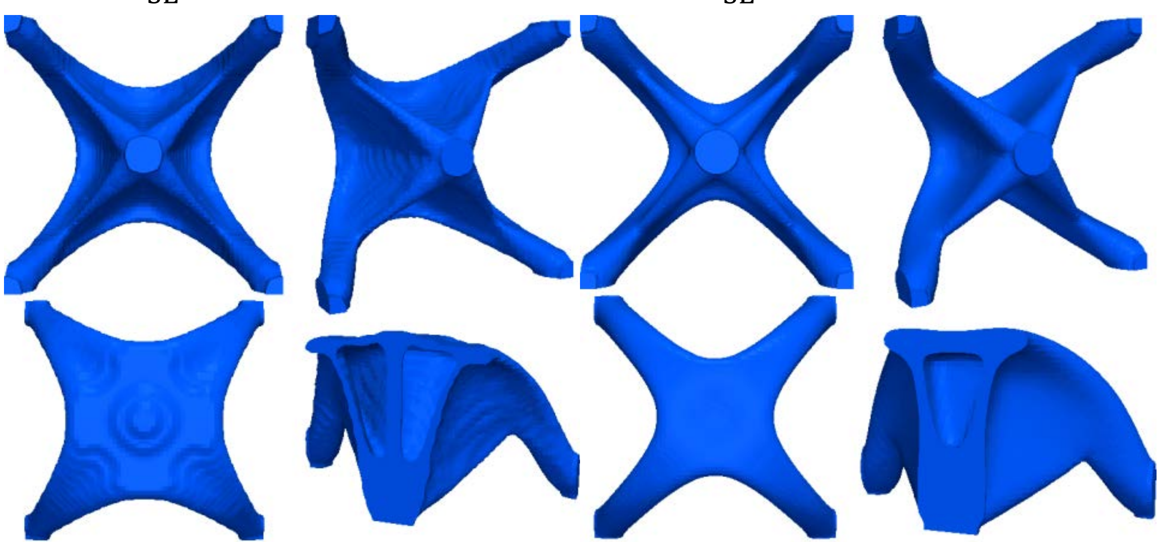
Approach:
- Seeding the initial design with several void areas.



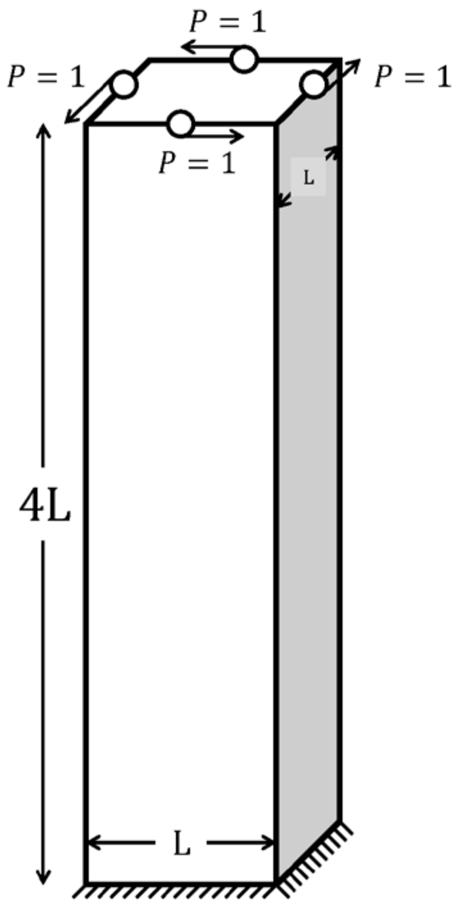
- No issues with minimum feature size.
- Strain energies are similar.
- Convergence is faster.

SIMP $\mathcal{F}_{\mathrm{SE}} = 3.5519 \times 10^{-2}$

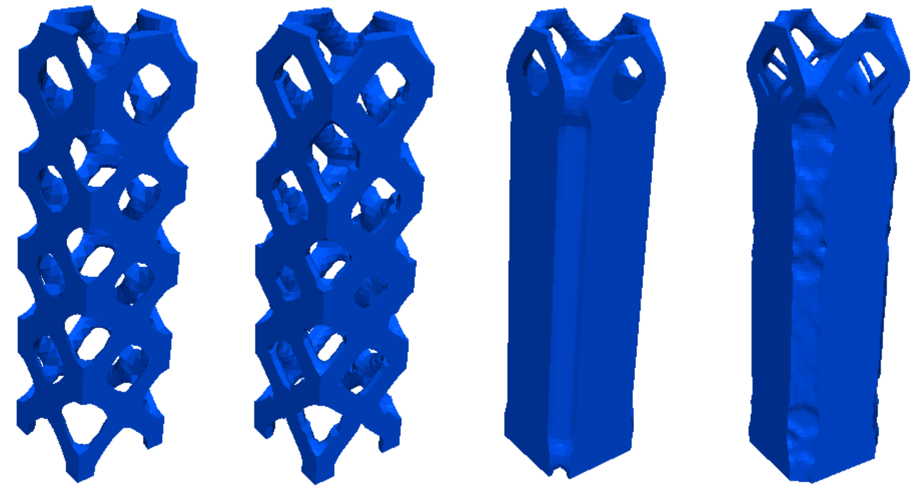
LSM-XFEM $\mathcal{F}_{\mathrm{SE}} = 3.5244 \times 10^{-2}$



SIMP and XFEM comparison: Mesh convergence



SIMP

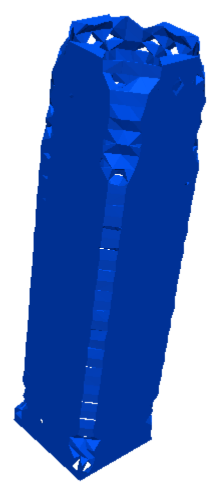


$\mathcal{F}_{\mathrm{SE}} = 2.6555 \times 10^3$

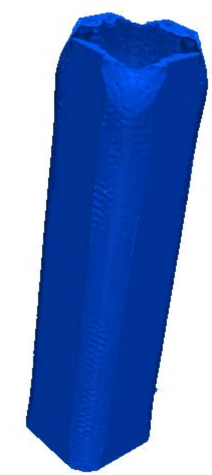
$40 \times 10 \times 10$ $\quad 60 \times 15 \times 15$ $\quad 80 \times 20 \times 20$ $\quad 120 \times 30 \times 30$

$\mathcal{F}_{\mathrm{SE}} = 9.8262 \times 10^2$

LSM-XFEM



- SIMP design changes with mesh refinement because of r_ρ.
- In XFEM, only local details are improved.

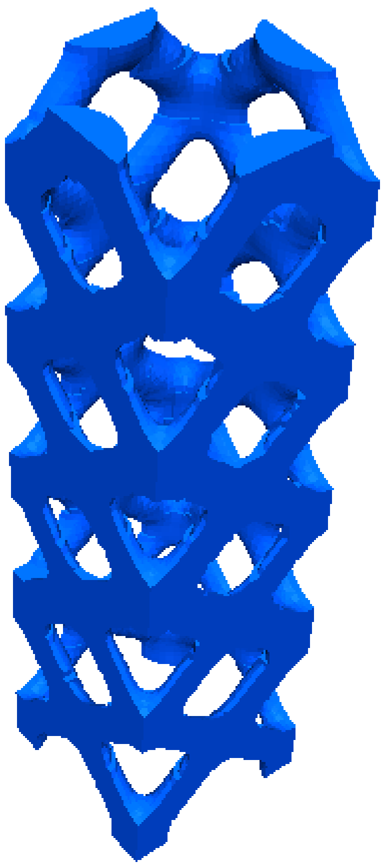


- Minimize $\mathcal{F}_{\mathrm{SE}}(+\mathcal{F}_{\mathrm{P}})$
- Maximum stiffness for given mass 10%
- $r_\rho = r_\phi = 1.6 \cdot h$

Smoothing filter / feature size control

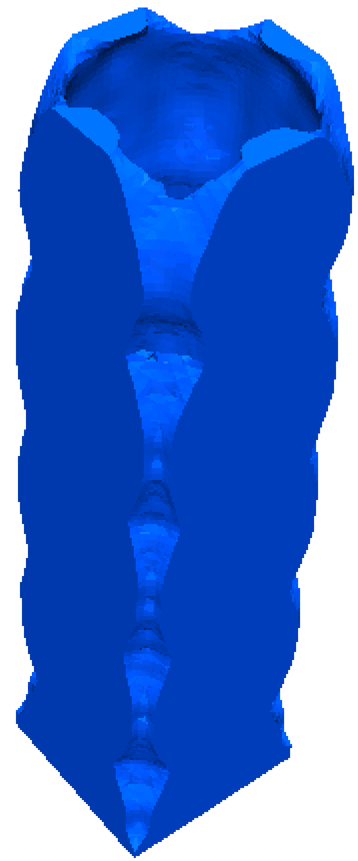
$120 \times 30 \times 30$

SIMP



$r_\rho = 0.16$

- SIMP approach leads to the same layout for a mesh independent filter.
- Increasing r_ϕ results in a less smooth design.
- r_ϕ does not control shape.



$r_\phi = 0.16$

LSM-XFEM

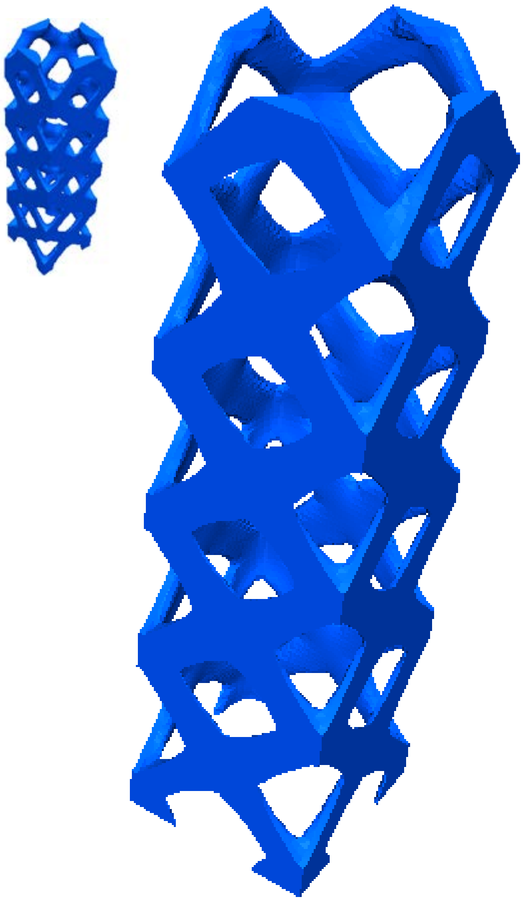
Initial design / feature size control

$$120 \times 30 \times 30$$

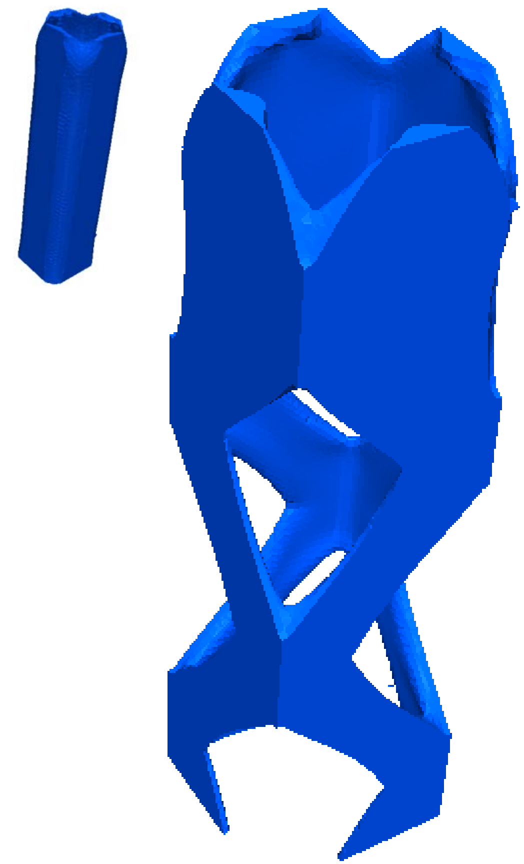
- Constrain the perimeter $\mathcal{G}_{\mathbf{P}}$ using perimeter from SIMP.

- **Open issues**:
  - Neither perimeter constraint nor smoothing control the local feature size.
  - Effect of a perimeter constraint is non-intuitive.

- **Approach**:
  - A minimum feature size control approach is outside the scope of this work.



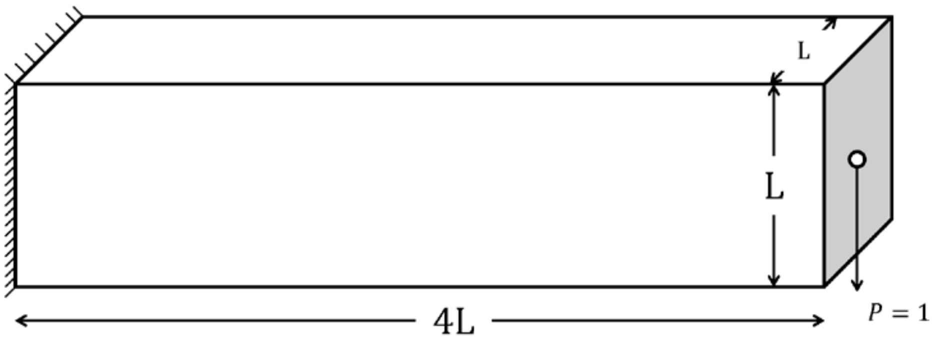
LSM-XFEM restarted from SIMP design.



LSM-XFEM restarted from XFEM design.

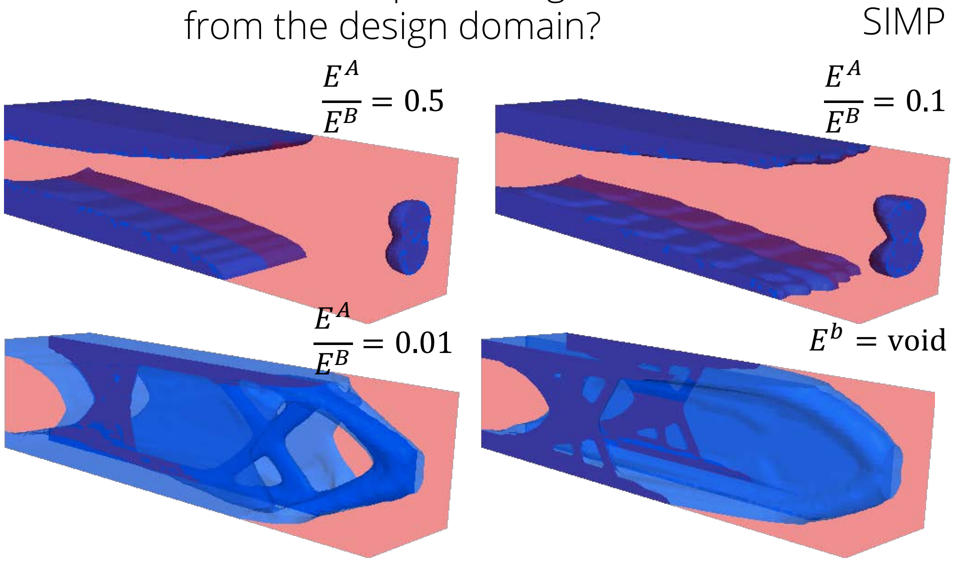
Two-phase problem / manufacturing

Manufacturing example of a two-phase "solid-solid" problem using 3D printing.

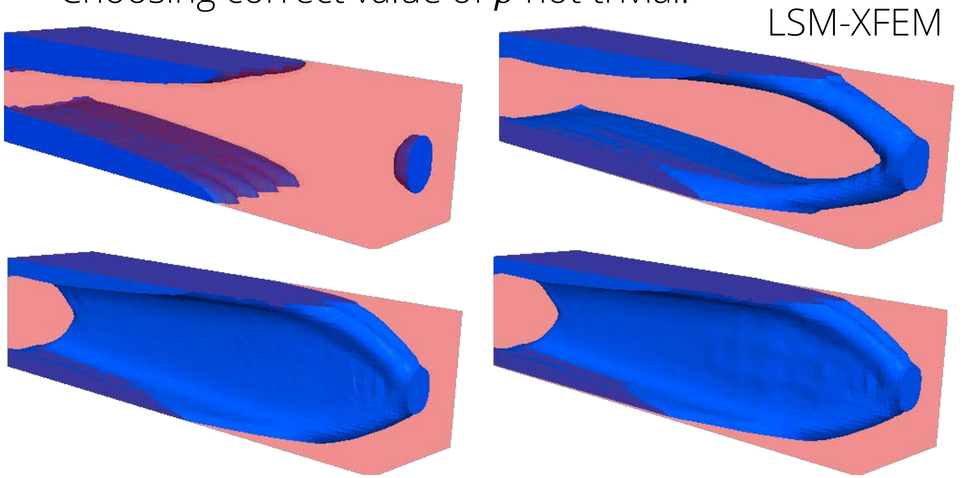


- Minimize $\mathcal{F}_{\mathrm{SE}}(+\mathcal{F}_{\mathrm{P}})$
- Maximum stiffness for given mass 30%
- $r_\rho = r_\phi = 1.6 \cdot h$
- $120 \times 30 \times 30$

How do we extract optimized geometries from the design domain?



- Extract surface through isolevels of ρ.
- Choosing correct value of ρ not trivial.



- Extract threshold of subdomains for specific region.

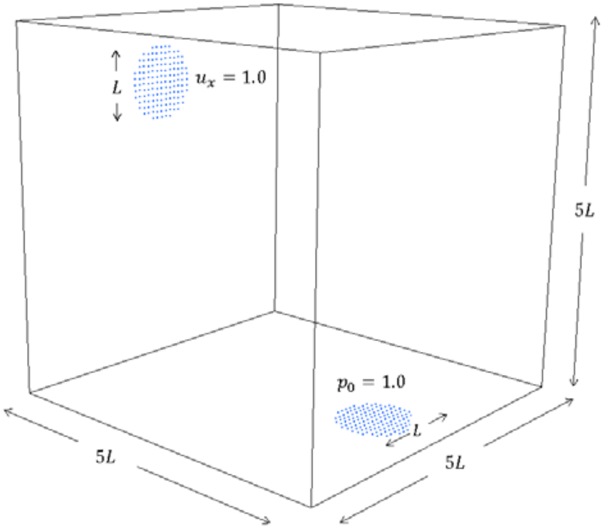
Incompressible Navier-Stokes and scalar transport

CASE STUDY II

Goals and objectives

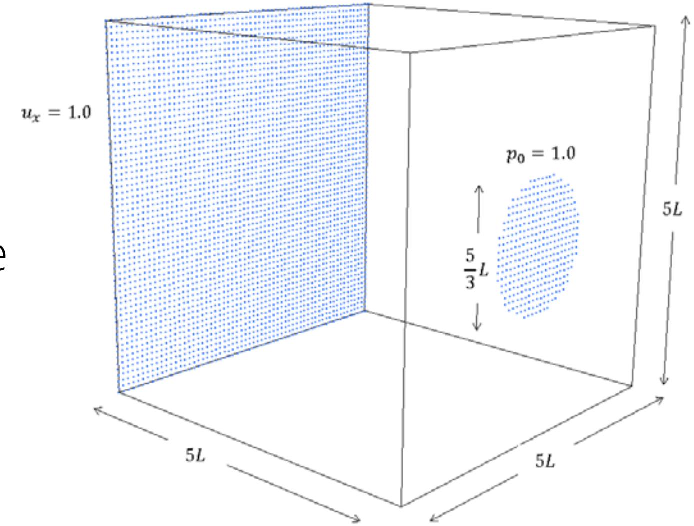
- Study the characteristics of the LSM-XFEM framework for three dimensional incompressible Navier-Stokes flow and scalar transport problems.
  - Enforcement of boundary conditions at the phase interface for high Reynolds number flow.
- Motivation:
  - Density methods in fluids, such as the Brinkman penalization cause spurious pressure diffusion through solid material.
- Approach:
  - LSM-XFEM framework.
  - Stabilized Lagrange multipliers.

Pipebend and diffuser



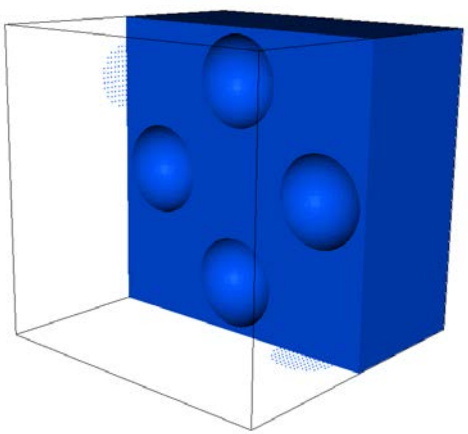
Pipebend

- "Fluid-solid" problem.
- Minimize $\mathcal{F}_{\mathbf{PD}}$.
- Maximum volume fraction of fluid phase 25% and 50%.
- $Re = 1.0$
- $r_\phi = 2.4 \cdot h$

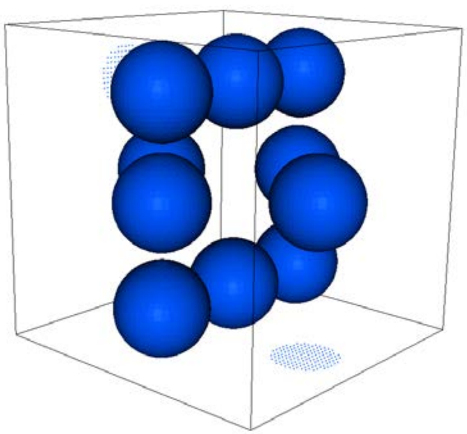


Diffuser

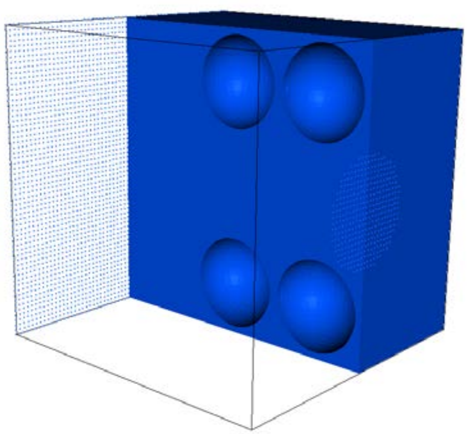
Initial designs.



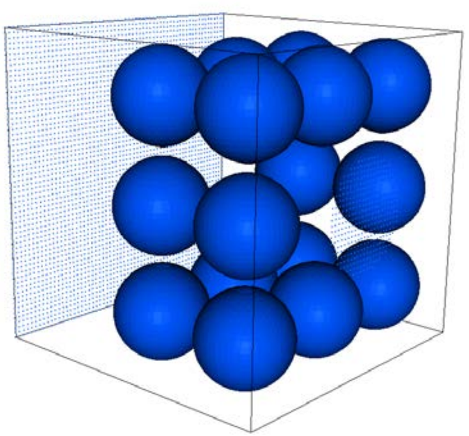
Fluid



Solid

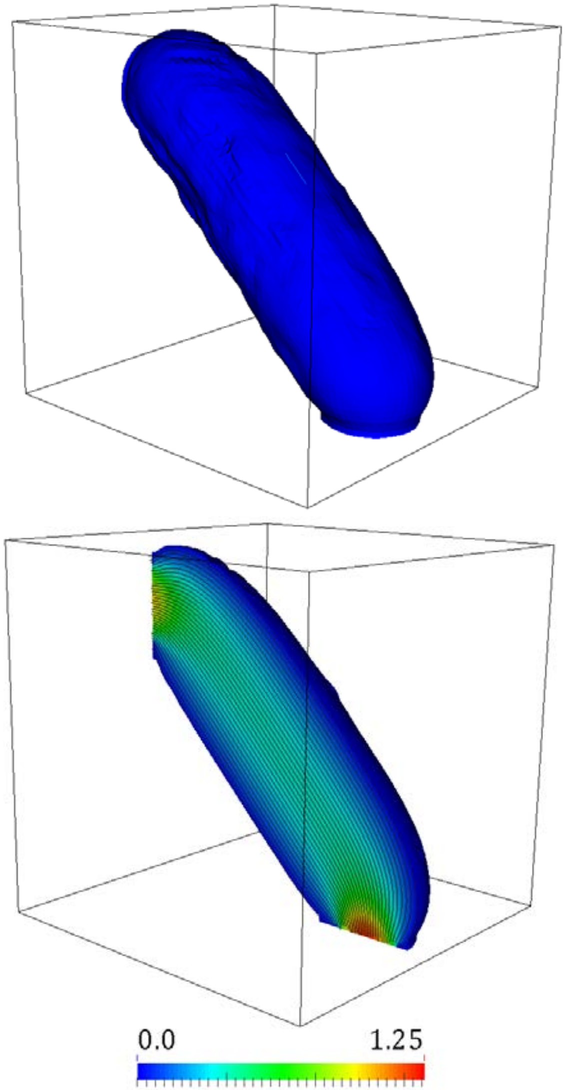


Fluid

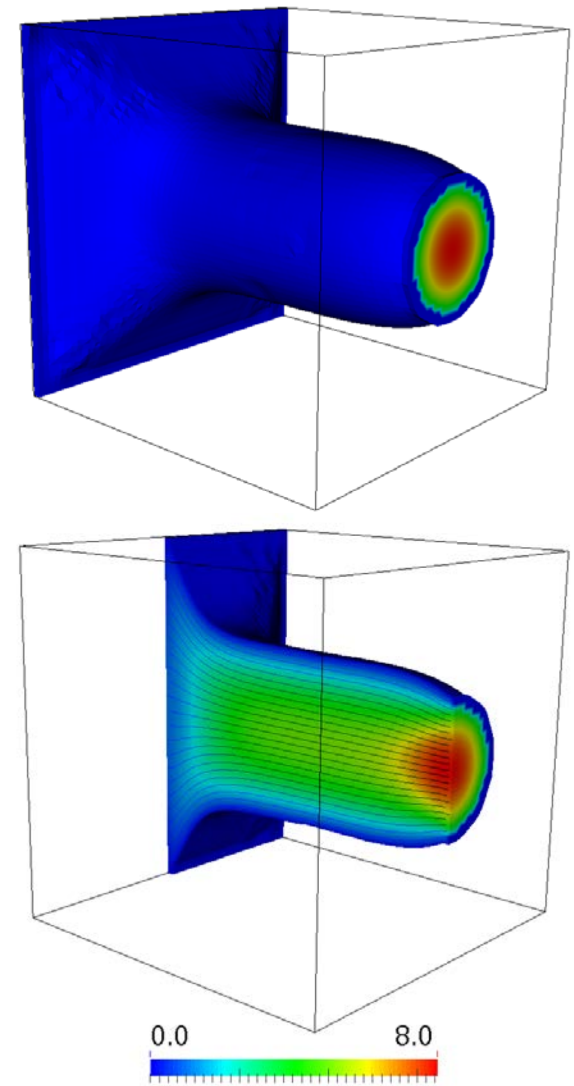


Solid

Pipebend and diffuser



- Identical results for Stokes and Navier-Stokes formulation with $Re = 1.0$.
- Open issues:
  - Higher Re flow does not converge for certain topologies.
  - Oscillations occur near interface.
- Approach:
  - Explore **Nitsche** method for enforcing continuity at interface.
  - Use **face-oriented ghost penalty** to increase stability.



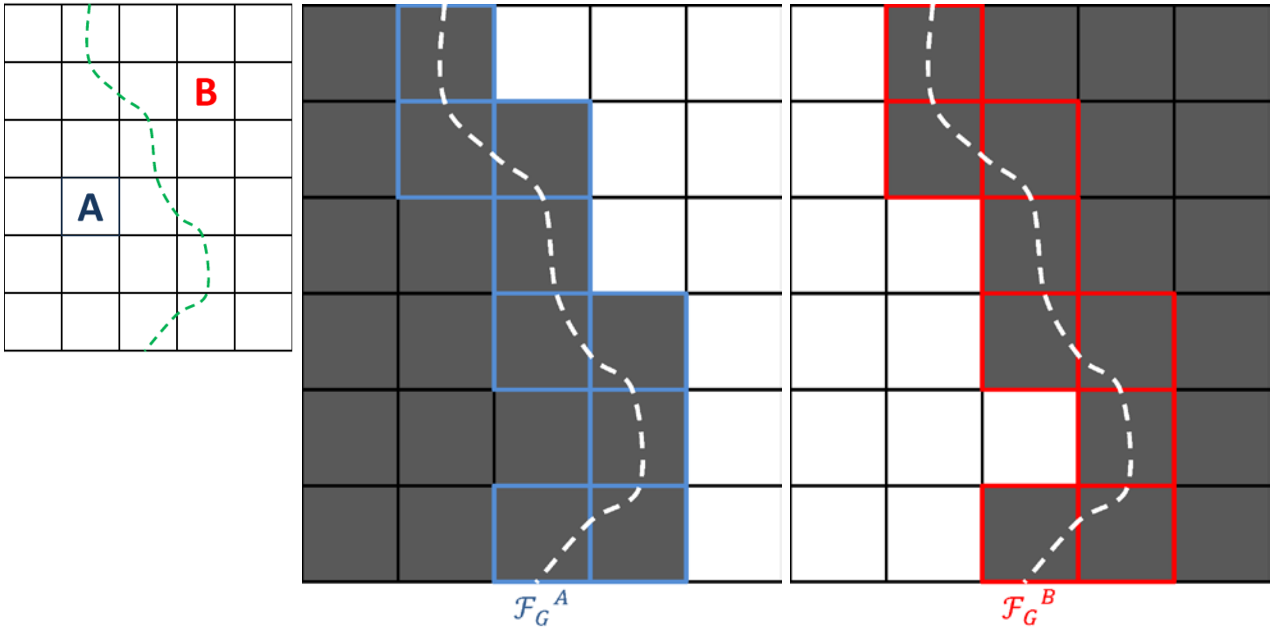
Approach: Face-oriented ghost-penalty

- Objective:
  - Overcome stability issues on cut elements for viscous flows.
  - Control higher-order derivatives on a cut element.
  - Method used for single enrichment diffusion and incompressible Navier –Stokes flow (Burman and Hansbo, 2012; Schott et al., 2014).
- Hypothesis:
  - Smoothing the gradient of the solution across the element facets reduces condition number.
- Open issues:
  - Expand methodology to 3D.
  - Apply method in topology optimization.
  - With multiple enrichment functions.

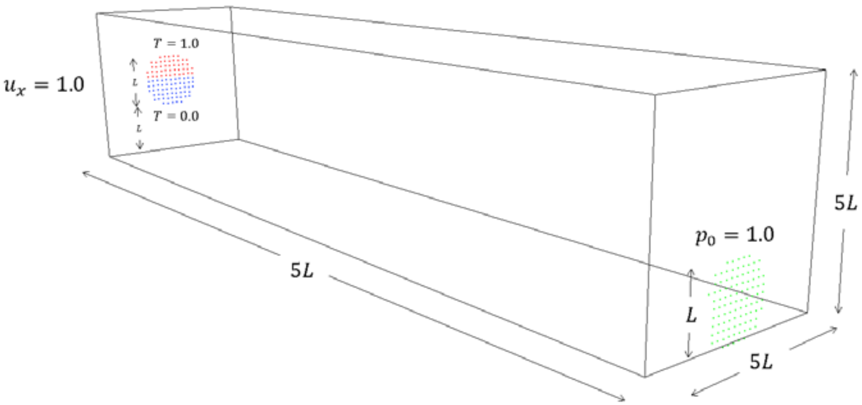
For incompressible Navier-Stokes:

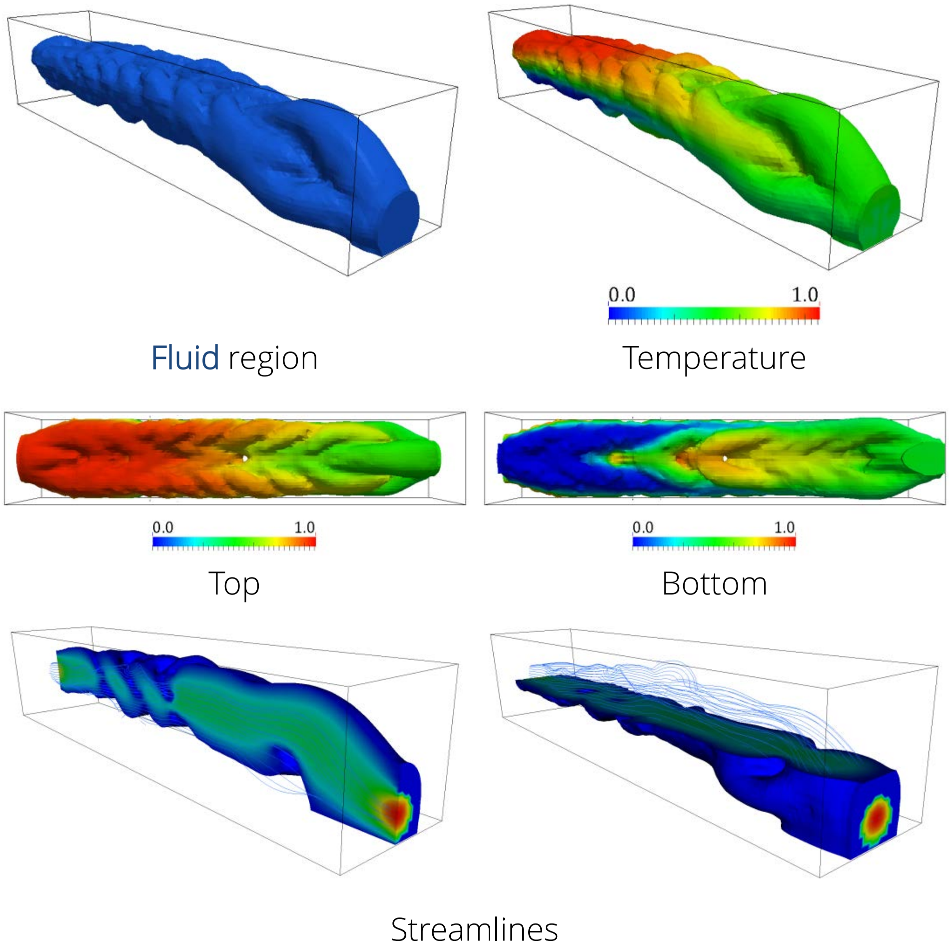
$$\sum_{l\in\{A,B\}}\sum_{m=1}^{M}\sum_{F\in\mathcal{F}_{G_m}^{k}}\sum_{i=1}^{D}\int_F \alpha_{\mathrm{GP},\mu}\mu^l h_F^{2(i-1)+1}\left[\frac{\partial^i \mathbf{N}}{\partial \mathbf{x}^i}\right]\cdot\mathbf{n}_F : \left[\frac{\partial^i \mathbf{u}_m^l}{\partial \mathbf{x}^i}\right]\cdot\mathbf{n}_F\,\mathrm{d}s$$

$$+\sum_{l\in\{A,B\}}\sum_{m=1}^{M}\sum_{F\in\mathcal{F}_{G_m}^{k}}\sum_{i=1}^{D}\int_F \alpha_{\mathrm{GP},\mu}{\mu^l}^{-1} h_F^{2i+1}\left[\frac{\partial^i \mathbf{N}}{\partial \mathbf{x}^i}\right]\cdot\mathbf{n}_F : \left[\frac{\partial^i p_m^l}{\partial \mathbf{x}^i}\right]\cdot\mathbf{n}_F\,\mathrm{d}s$$



Micromixer





- Minimize:

$$\mathcal{F}_{\text{TSV}} = \frac{1}{\beta} \ln \left(\int_{\Gamma} e^{\beta (T - T_{ref})^2} d\Gamma \right)$$

- Maximum volume fraction of fluid phase 50%.
- $Re = 1.0$
- $r_\phi = 2.4 \cdot h$

- Open issues:
    - Same as issues as pipebend and diffuser problems for higher Re. 💣

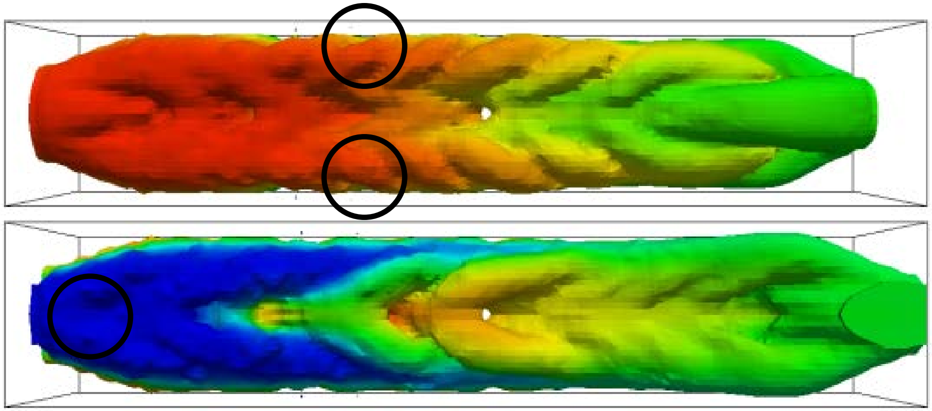
Identical results for Stokes and Navier-Stokes formulation with $Re = 1.0$.

Curvature regularization

CASE STUDY III

Goals and objectives

- **Issues**:
  - Can we get rid of **floating particles** and **rough surfaces** without a perimeter penalty/constraint?
  - To avoid losing wavy pattern.



- **Objective**:
  - Control the smoothness of the level set interface without creating flat designs.
  - Smooth surface meshes are important for manufacturing.

- **Approach**:
  - Include smoothness measure in optimization problem.
  - To control optimization parameters.

How do we measure smoothness?

- Curvature measures how much the normal unit vector changes as we move along a curve.

$$\kappa = \left\| \frac{\mathrm{d}\mathbf{n}}{\mathrm{d}s} \right\|$$

- Image recognition community minimizes **squared curvature to smooth images**.
- Measuring curvature along $\Gamma_{\phi=0}$.

$$\mathcal{F}_\kappa = \int_{\phi=0} (\nabla \cdot \mathbf{n})^2 \,\mathrm{d}\Gamma = \int_{\phi=0} \left\| \frac{\mathrm{d}\mathbf{n}}{\mathrm{d}s} \right\|^2 \mathrm{d}\Gamma$$

How do we measure $\mathbf{n}$?

$\mathbf{n}_\phi$

- Enforced in the strong form with $\mathbf{N}$.

$$\mathbf{n}_\phi = \frac{\nabla\phi}{\|\nabla\phi\|}$$

$\mathbf{n}_u$

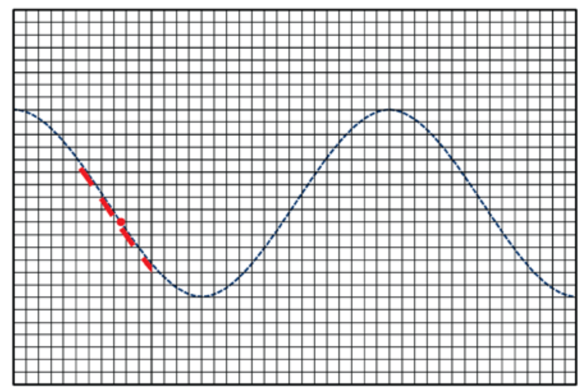
- Enforced in the weak form.

$$\int_\Omega \delta\mathbf{n}_u(\mathbf{n}_u\|\nabla\phi\| - \nabla\phi)\,\mathrm{d}\Omega = 0$$

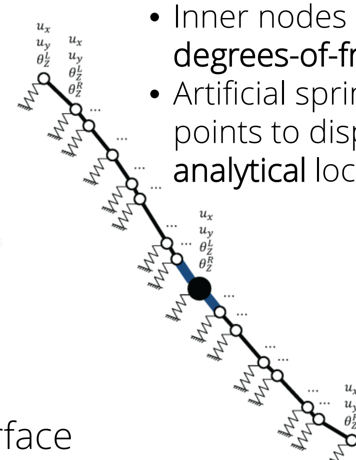
$\mathbf{n}_g$

- Model interface as structural linear beam elements.

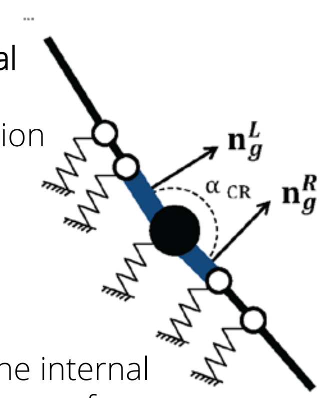
$$\mathcal{F}_\kappa = \int_{\phi=0}\left\|\frac{\mathrm{d}\mathbf{n}}{\mathrm{d}s}\right\|^2 \mathrm{d}\Gamma = \frac{1}{2}\int_{\phi=0}\sigma : \varepsilon\,\mathrm{d}\Gamma$$



- Sinusoidal wave with an amplitude of 0.50.
- Mesh discretization is 45×30 elements.
- --- All cut elements within a radius $r_\kappa = 0.4$.



- Inner nodes have **two rotational degrees-of-freedom**.
- Artificial springs allow intersection points to displace to their **analytical** location.



- Continuity in the internal rotational degrees-of-freedom with Lagrange multipliers. $\theta_z^L - \theta_z^R = \alpha_{CR}$

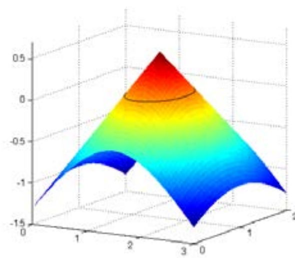
$\mathbf{n}_\psi$

- Project ϕ with hyperbolic tangent function.

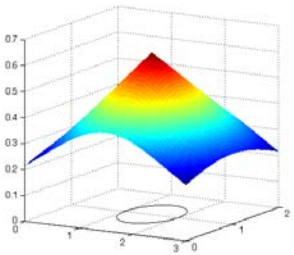
$$\psi(\phi) = \frac{1}{2}\left(\tanh\left(\frac{\phi}{2\epsilon}\right) + 1\right)$$

- Enforce in the weak form.

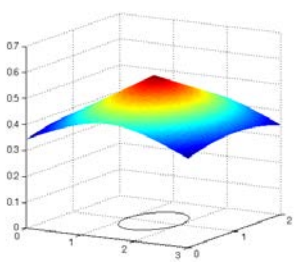
$$\int_\Omega \delta\mathbf{n}_\psi(\mathbf{n}_\psi\|\nabla\psi\| - \nabla\psi)\,\mathrm{d}\Omega = 0$$



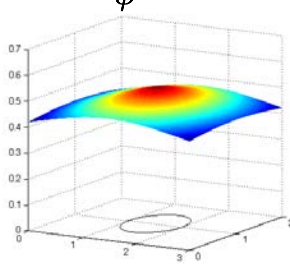
ϕ



$\epsilon = 1.0$



$\epsilon = 2.0$

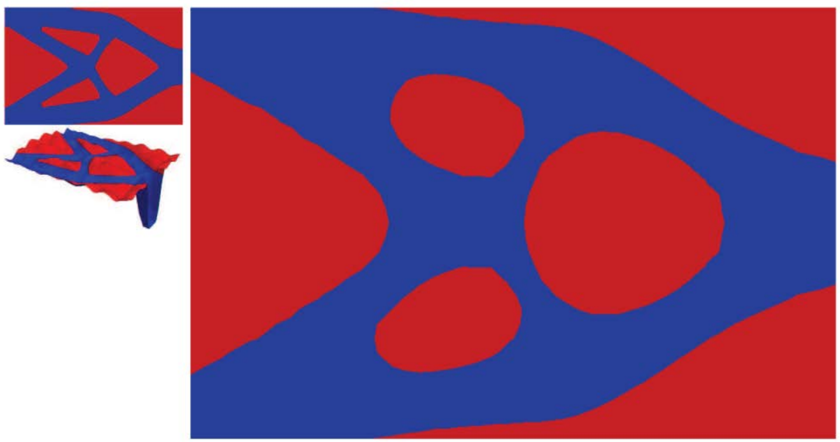


$\epsilon = 4.0$

- Open issues:
  - What is the influence of computing $\mathbf{n}$ from the interface vs. geometrically on the smoothness measure?

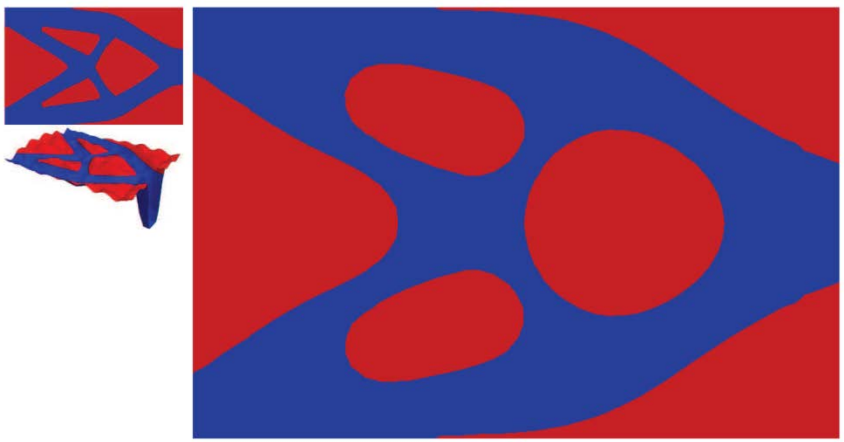
Preliminary results

Minimize $\mathcal{F}_{\mathrm{SE}} + \mathcal{F}_{\kappa}$ using $\mathbf{n}_u$



- $\mathcal{F}_{\kappa}$ using $\mathbf{n}_u$ yields a smooth design yet with a few kinks.

Minimize $\mathcal{F}_{\mathrm{SE}} + \mathcal{F}_{\kappa}$ using $\mathbf{n}_g$



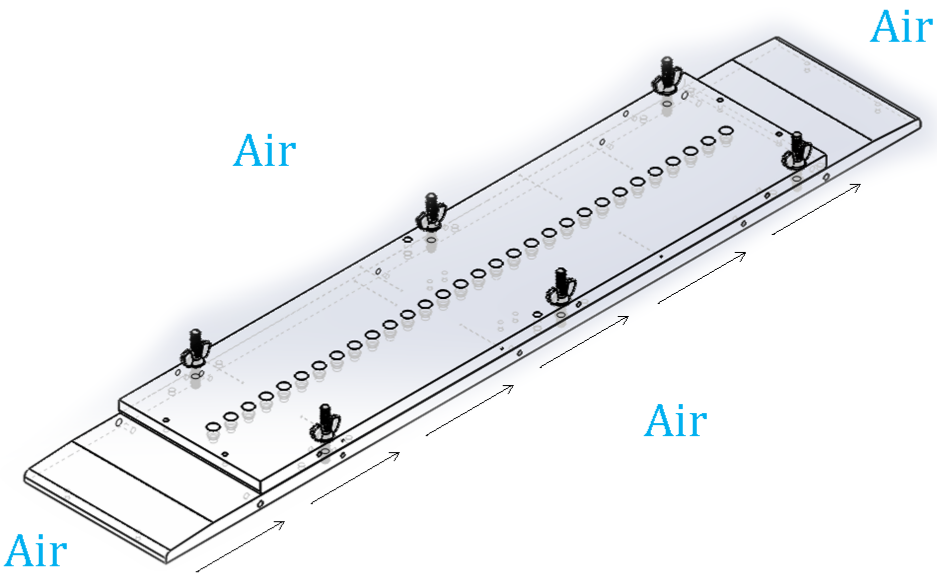
- $\mathcal{F}_{\kappa}$ using $\mathbf{n}_g$ is computed directly at the intersection points.
  - Smoother results.
- Open issues:
  - Too smooth? 💣
  - Penalize only sharp corners?

Incompressible Navier-Stokes flow with multiple scalar fields

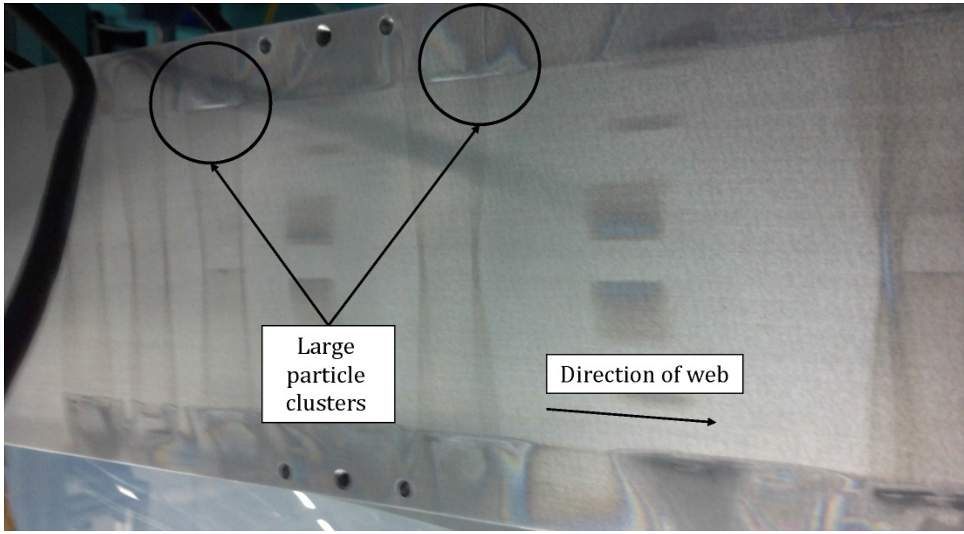
CASE STUDY IV

Atomic Layer Deposition

- ALD is a thin film deposition technique in which two or more chemicals react with the surface of a material.



- Holes at the top are inlets through which the chemical reactants enter.
- Conveyor belt moves a web on which the chemicals are deposited.



Issues:
- Machine has open boundaries which may cause reactions with air.
- Lead to imperfections in the deposition.

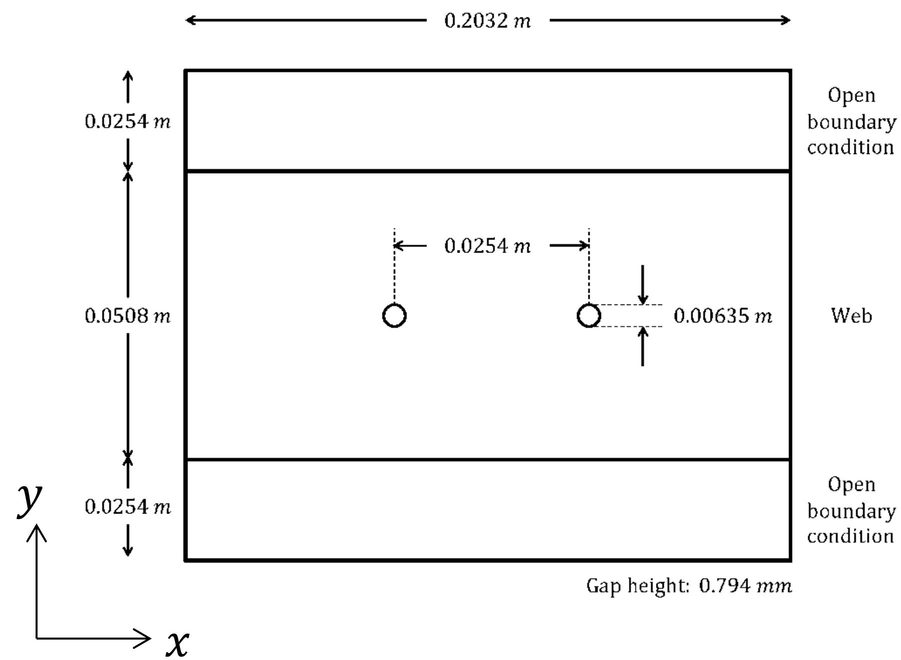
Approach:
- Model an incompressible Navier-Stokes flow problem with multiple scalar transport fields.
- Model interaction of multiple reactants with outside sources.

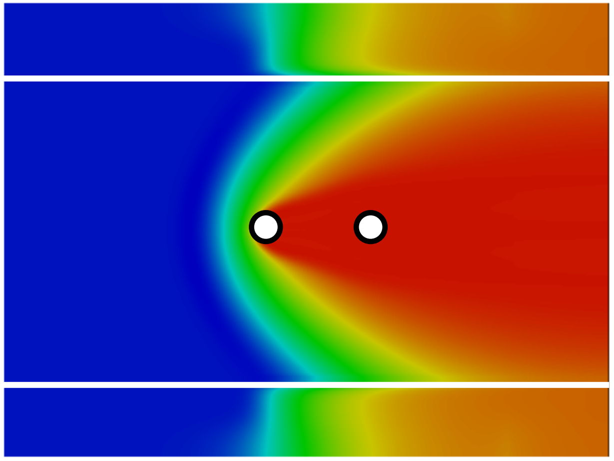
Atomic Layer Deposition

- Scalar transport equation:
  $$\frac{\partial c}{\partial t} - \mathbf{u} \cdot \nabla c - d\nabla^2 c - q = 0$$
  where c is the species concentration and d is the diffusivity.
- The inflow velocity of the inlets is:
  $$u_{inlet_z} = 1.0 * 0.53 \frac{m}{s}$$
- Material properties:
  $$\nu_{\mathrm{N2}} = 1.52 \cdot 10^{-5} \frac{m^2}{s}$$
  $$\rho_{\mathrm{N2}} = 1.16 \frac{kg}{m^3}$$
  $$d_{\mathrm{N2,H2O}} = 2 \cdot 10^{-5} \frac{m^2}{s}$$

Objective:

- Expand our scalar transport model to simulate multiple scalar transport fields.
  $$\frac{\partial \mathbf{c}}{\partial t} - \mathbf{u} \cdot \nabla \mathbf{c} - d\nabla^2 \mathbf{c} - q = 0$$
- Research the interaction of the reactant with the outside sources, such as air.
- Optimize the layout of the gas source heads.
- Minimize mixing.
  $$\mathcal{F}_{\mathrm{MX}} = \int_t \int_\Gamma \sqrt[n]{\left((c - c_1)(-c + c_2)\right)^n}\, \mathrm{d}\Gamma \mathrm{d}t$$
  where c_1 and c_2 are the concentration of the inlets.





Diffusion of gases

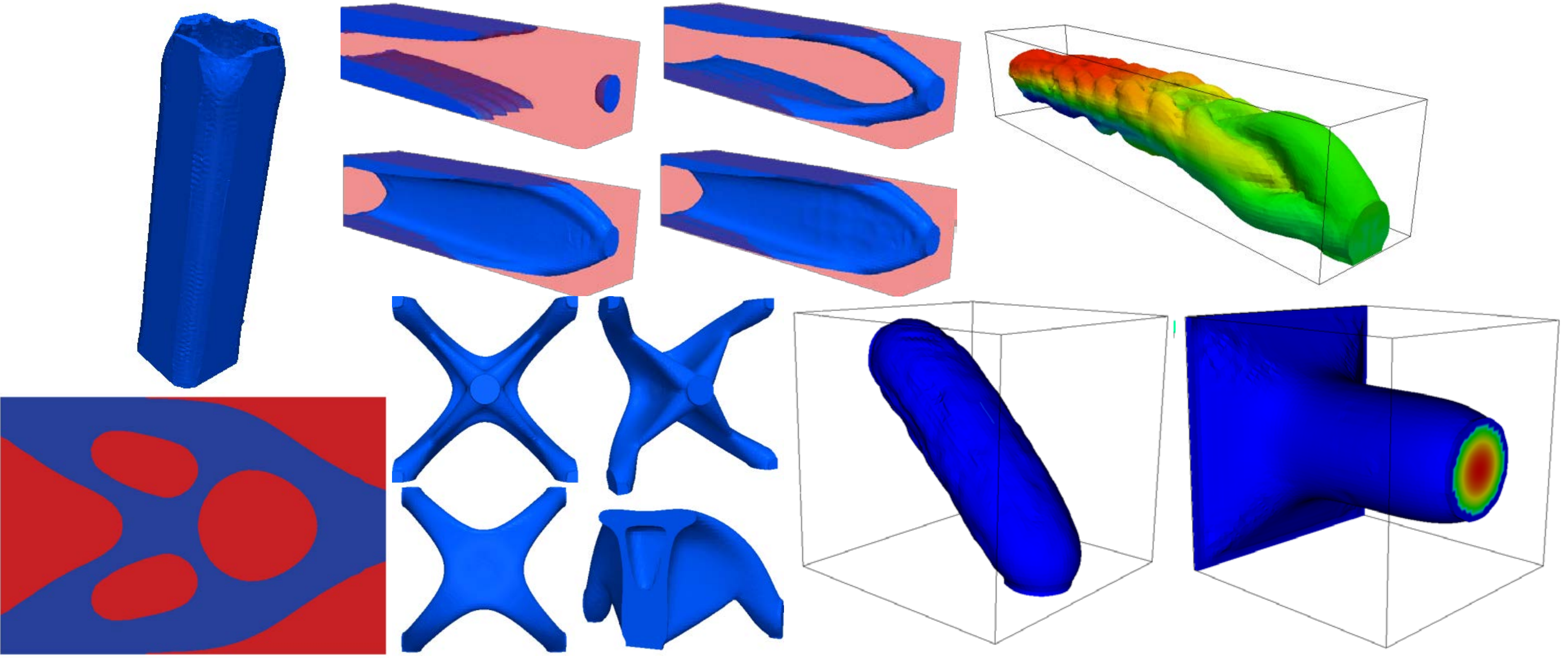
CONCLUSIONS

Conclusions

- The LSM can describe the geometry and the XFEM can predict the structural response.
- Built upon generalized enrichment and preconditioning schemes.
- Applied method to:
  - Two “material–void” and “material–material” problems in 3D.
  - Structural linear elasticity.
  - Incompressible Navier-Stokes flow.
  - Scalar transport.

Is it generic?

- Used the same optimization approach for:
  - Multiphysics problems.
  - Two-phase "material–void" and "material–material" problems.
  - 2D and 3D problems.
- LSM can describe complex geometries.
- XFEM can model discontinuities with generalized enrichment strategy.



Is it efficient?

- Method is significantly more complex in regards of implementation.
- Similar assembly time for “material–void ” problems.
- More time for “material–material” due to larger linear system.
    - Faster optimization convergence rate.
- Ability to represent thin-walled structures on coarse meshes.
- Enforce boundary conditions on coarse meshes.
- Alternative to density methods for problems where a high mesh resolution is not tolerable.

Is it robust?

- Perimeter and curvature provide global shape control.
- Capability to mitigate numerical artifacts.
- Method can be used in linear and nonlinear problems.

- Open issues:
  - Smoothing filter and perimeter constraint do not control local feature size.
    - Outside the scope of this work.
  - Interface conditions need to be enforced accurately for higher Re flow.
  - Using $\mathbf{n}_g$ may yield too smooth designs.

- Hypothesis:
  - Boundary conditions are not enforced accurately.
  - Small intersection regions cause ill-conditioning.
  - Stabilized Lagrange multipliers (to solve for $\boldsymbol{\sigma}$ at $\Gamma_{\phi=0}$) fail due to ill-conditioning.

Is it robust?

Remaining work:

- Structural linear elasticity:
  - Study stress constrains with **face-oriented ghost penalty** in structural linear elasticity.
- Incompressible Navier-Stokes with scalar transport:
  - Explore **Nitsche** method for enforcing continuity at interface in higher Re flow
  - Explore **face-oriented ghost penalty** to increase stability in higher Re flow.
- Curvature regularization:
  - Study influence of $\mathbf{n}$ in the smoothness measure.
  - Penalize intermediate curvatures to better control the shape.
- Atomic layer deposition:
  - Expand our scalar transport model to simulate multiple scalar transport fields.
  - Research the interaction of the reactant with the outside sources, such as air.

Timeline

- Need to complete this slide.

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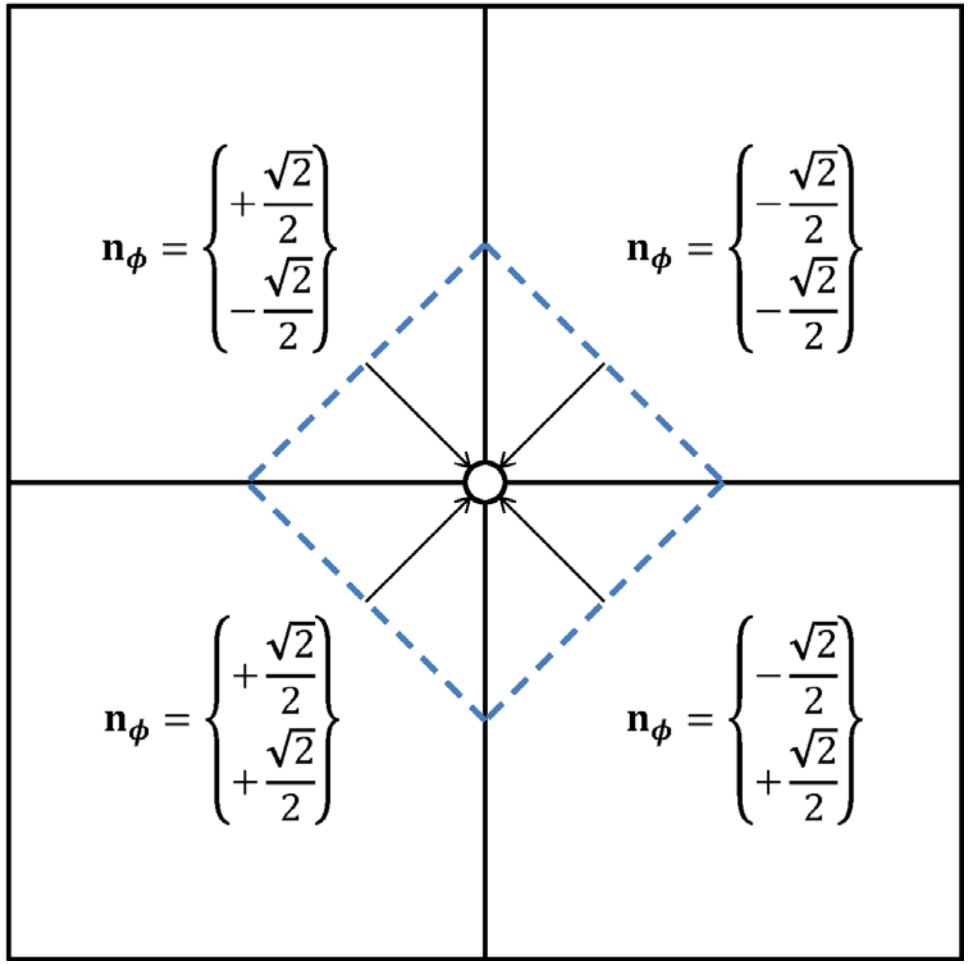

$\mathbf{n}_\phi = \begin{Bmatrix} +\frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} \end{Bmatrix}$
$\mathbf{n}_\phi = \begin{Bmatrix} -\frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} \end{Bmatrix}$
$\mathbf{n}_\phi = \begin{Bmatrix} +\frac{\sqrt{2}}{2} \\ +\frac{\sqrt{2}}{2} \end{Bmatrix}$
$\mathbf{n}_\phi = \begin{Bmatrix} -\frac{\sqrt{2}}{2} \\ +\frac{\sqrt{2}}{2} \end{Bmatrix}$