Shape derivative method and application to optimal design problems

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Introduction

Let $\Omega \subset \mathbb{R}^d$ be open and bounded set.
Two phases each with different isotropic conductivity: α, β $(0 < \alpha < \beta)$.
q_α is the prescribed volume of the first phase α $(0 < q_\alpha < |\Omega|)$.
$\chi \in \mathrm{L}^\infty(\Omega)$ such that

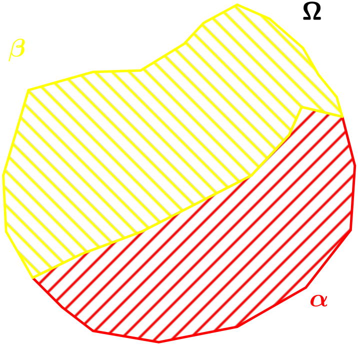
$$\begin{cases} \chi = 1, & \text{phase } \alpha \\ \chi = 0, & \text{phase } \beta \end{cases}.$$

Conductivity can be expressed as

$$\mathbf{A}(\chi) := \chi\alpha\,\mathbf{I} + (1-\chi)\beta\,\mathbf{I},$$

where

$$\int_\Omega \chi(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = q_\alpha.$$



Introduction

State functions $u_i \in \mathrm{H}_0^1(\Omega),\ i = 1, 2, ..., m$ are given as a solution of the following boundary value problems:

$$(\mathrm{S}) \qquad \begin{cases} -\mathrm{div}(\mathbf{A}\,\nabla u_i) = f_i & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega, \end{cases} \qquad i = 1, 2, ..., m,$$

with $\mathbf{A} = \chi\alpha\,\mathbf{I} + (1-\chi)\beta\,\mathbf{I}$. Denote $\boldsymbol{u} = (u_1, ..., u_m)$.
Energy functional:

$$J(\chi) := \sum_{i=1}^{m} \mu_i \int_{\Omega} f_i(\boldsymbol{x}) u_i(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x},$$

where $\mu_i > 0,\ i = 1, 2, ..., m.$

Statement of the problem

Optimal design problem:

$$
\text{(P)} \qquad \begin{cases} J(\chi) = \sum_{i=1}^{m} \mu_i \int_\Omega f_i u_i \, \mathrm{d}\boldsymbol{x} \to \max \\ \text{s.t.} \quad \chi \in L^\infty(\Omega, \{0,1\}), \quad \int_\Omega \chi \, \mathrm{d}\boldsymbol{x} = q_\alpha, \\ \boldsymbol{u} \text{ solves (S) with } \mathbf{A} = \chi\alpha\,\mathbf{I} + (1-\chi)\beta\,\mathbf{I}. \end{cases}
$$

If solution χ exists for (P) we call it *classical solution.*

Important: For general optimal design problems the classical solutions usually do not exist.

Assumptions:

- $\Omega \subset \mathbb{R}^d$ is ball or annulus,
- right hand sides f_i are radial functions.

With this assumptions one can construct classical solutions.

Relaxed design

For characteristic functions relaxation consists of:

$$\chi \in \mathrm{L}^\infty(\Omega, \{0,1\}) \quad \rightsquigarrow \quad \theta \in \mathrm{L}^\infty(\Omega, [0,1]), \tag{1}$$

with

$$\int_\Omega \theta \, \mathrm{d}\boldsymbol{x} := q_\alpha .$$

Notion of H-convergence is introduced for conductivity $\mathbf{A}$.

Effective conductivities:

$$\mathcal{K}(\theta) \subset M_d(\mathbb{R}) \text{ with local fraction } \theta \in [0,1].$$

Precisely, $A \in \mathcal{K}(\theta)$ iff there exists sequence of characteristic functions

$$\begin{cases} \chi_n \xrightarrow{L^\infty *} \theta \\ \mathbf{A}^n = \chi_n \alpha \mathbf{I} + (1-\chi_n)\beta \mathbf{I} \xrightarrow{H} A. \end{cases}$$

Effective conductivities - set $\mathcal{K}(\theta)$

$\mathcal{K}(\theta)$ is given in terms of eigenvalues

$$\lambda_\theta^- \leq \lambda_j \leq \lambda_\theta^+ \quad j = 1, \ldots, d$$

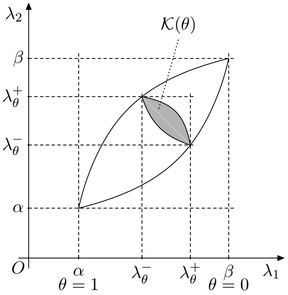
$$\sum_{j=1}^{d} \frac{1}{\lambda_j - \alpha} \leq \frac{1}{\lambda_\theta^- - \alpha} + \frac{d-1}{\lambda_\theta^+ - \alpha}$$

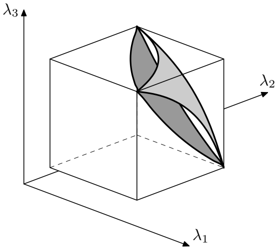
$$\sum_{j=1}^{d} \frac{1}{\beta - \lambda_j} \leq \frac{1}{\beta - \lambda_\theta^-} + \frac{d-1}{\beta - \lambda_\theta^+},$$

where

$$\lambda_\theta^+ = \theta\alpha + (1-\theta)\beta$$

$$\frac{1}{\lambda_\theta^-} = \frac{\theta}{\alpha} + \frac{1-\theta}{\beta}.$$





Generalized (convex) problem

Relaxed design:

$$\mathcal{A} = \left\{ (\theta, \mathbf{A}) \in L^\infty(\Omega, [0,1] \times \mathrm{Sym}_d) \;\middle|\; \begin{array}{c} \int_\Omega \theta \, \mathrm{d}\boldsymbol{x} = q_\alpha, \\ \mathbf{A}(\boldsymbol{x}) \in \mathcal{K}(\theta(\boldsymbol{x})), \text{ a.e. } \boldsymbol{x} \end{array} \right\}$$

Relaxed problem can be written as:

$$\text{(A)} \qquad \max_{(\theta,\mathbf{A})\in\mathcal{A}} J(\theta, \mathbf{A}) = \max_{(\theta,\mathbf{A})\in\mathcal{A}} \sum_{i=1}^{m} \mu_i \int_\Omega f_i u_i \, \mathrm{d}\boldsymbol{x}$$

Unfortunately, $\mathcal{A}$ is not a convex set. To achieve convexity, an enlarged set is introduced:

$$\mathcal{B} = \left\{ (\theta, \mathbf{A}) \in L^\infty(\Omega, [0,1] \times \mathrm{Sym}_d) \;\middle|\; \begin{array}{c} \int_\Omega \theta \, \mathrm{d}\boldsymbol{x} = q_\alpha, \\ \lambda^-_{\theta(\boldsymbol{x})} \mathbf{I} \le \mathbf{A}(\boldsymbol{x}) \le \lambda^+_{\theta(\boldsymbol{x})} \mathbf{I}, \text{ a.e. } \boldsymbol{x} \end{array} \right\}$$

and with it

$$\text{(B)} \qquad \max_{(\theta,\mathbf{A})\in\mathcal{B}} J(\theta, \mathbf{A}) = \max_{(\theta,\mathbf{A})\in\mathcal{B}} \sum_{i=1}^{m} \mu_i \int_\Omega f_i u_i \, \mathrm{d}\boldsymbol{x}$$

Rewrite B as a max-min problem

Define $\mathcal{S} := \left\{ \boldsymbol{\sigma} = (\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, ..., \boldsymbol{\sigma}_m) \;\middle|\; \boldsymbol{\sigma}_i \in \mathrm{L}^2(\Omega, \mathbb{R}^d),\ -\mathrm{div}(\boldsymbol{\sigma}_i) = f_i \right\}$

One can rewrite functional J in terms of fluxes:

$$J(\theta, \mathbf{A}) = \min_{\boldsymbol{\sigma} \in \mathcal{S}} \sum_{i=1}^{m} \mu_i \int_\Omega \mathbf{A}^{-1} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_i$$

With notation $\mathcal{C} = \left\{ (\theta, \mathbf{A}) \,|\, (\theta, \mathbf{A}^{-1}) \in \mathcal{B} \right\}$

$$\begin{aligned} \max_{(\theta,\mathbf{A}) \in \mathcal{B}} J(\theta, \mathbf{A}) &= \max_{(\theta,\mathbf{A}) \in \mathcal{B}} \min_{\boldsymbol{\sigma} \in \mathcal{S}} \sum_{i=1}^{m} \mu_i \int_\Omega \mathbf{A}^{-1} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_i \\ &= \max_{(\theta,\mathbf{B}) \in \mathcal{C}} \min_{\boldsymbol{\sigma} \in \mathcal{S}} \sum_{i=1}^{m} \mu_i \int_\Omega \mathbf{B} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_i \end{aligned}$$

Observe that

$$L(\boldsymbol{\sigma}, (\theta, \mathbf{B})) = \sum_{i=1}^{m} \mu_i \int_\Omega \mathbf{B}\, \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_i$$

$$\boldsymbol{\sigma} \mapsto L(\boldsymbol{\sigma}, (\theta, \mathbf{B}))$$

- quadratic (strictly convex)
- continuous in $L^2(\Omega)$ (l.s.c.)
- $(\exists(\theta, \mathbf{B})) \quad \boldsymbol{\sigma} \mapsto L(\boldsymbol{\sigma}, (\theta, \mathbf{B}))$ $\lim_{\|\boldsymbol{\sigma}\| \to +\infty} L(\boldsymbol{\sigma}, (\theta, \mathbf{B}))) = +\infty$

$$(\theta, \mathbf{B}) \mapsto L(\boldsymbol{\sigma}, (\theta, \mathbf{B}))$$

- linear (concave)
- continuous in $L^\infty *$ (u.s.c.)
- set $\mathcal{C}$ is compact (in $L^\infty *$).

Min-max theory

Previous conclusions for the Lagrange functional L implies:

- set of saddle points $\mathcal{S}_0 \times \mathcal{C}_0 \subset \mathcal{S} \times \mathcal{C}$ is not empty
- min and max are interchangeable
- $\boldsymbol{\sigma} \mapsto L(\boldsymbol{\sigma}, (\theta, \mathbf{B}))$ is strictly convex $\quad \Rightarrow \quad \mathcal{S}_0 = \{\boldsymbol{\sigma}^*\}$.

This means that there exists **unique** $\boldsymbol{\sigma}^*$ such that this holds

$$\begin{aligned}
\max_{(\theta,\mathbf{A})\in\mathcal{B}} J(\theta, \mathbf{A}) &= \max_{(\theta,\mathbf{B})\in\mathcal{C}} \min_{\boldsymbol{\sigma}\in\mathcal{S}} L(\boldsymbol{\sigma}, (\theta, \mathbf{B})) \\
&= \max_{(\theta,\mathbf{B})\in\mathcal{C}} L(\boldsymbol{\sigma}^*, (\theta, \mathbf{B})) \\
&= \max_{(\theta,\mathbf{B})\in\mathcal{C}} \sum_{i=1}^{m} \mu_i \int_\Omega \mathbf{B}\, \boldsymbol{\sigma}_i^* \cdot \boldsymbol{\sigma}_i^*
\end{aligned}$$

Conclusions

Instead of solving convex problem B, one can solve the following optimization problem:

$$
\text{(I)} \qquad \begin{cases} I(\theta) = \sum_{i=1}^{m} \mu_i \int_\Omega f_i u_i \, \mathrm{d}\boldsymbol{x} \to \max \\ s.t. \quad \theta \in L^\infty(\Omega, [0,1]), \ \int_\Omega \theta = q_\alpha, \ \text{where } u_i \text{ satisfies} \\ -\operatorname{div}(\lambda_\theta^- \nabla u_i) = f_i, \quad u_i \in \mathrm{H}_0^1(\Omega), \ i = 1, 2, ..., m \end{cases}
$$

For spherically symmetric problem such that:

- $\Omega = R(\Omega)$ for any rotation R
- f_i are radial functions

it can be proved that there exists radial solution θ_R^* of (I).

In particular, it can be shown that

$$
\max_{(\theta, \mathbf{A}) \in \mathcal{A}} J(\theta, \mathbf{A}) = I(\theta_R^*).
$$

Conclusions

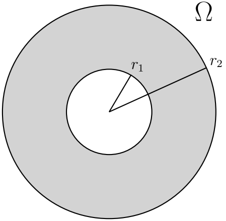
Define

$$\Psi := \sum_{i=1}^{m} \mu_i |\boldsymbol{\sigma}_i{}^*|^2 .$$

Lemma

The necessary and sufficient condition of optimality for solution θ^* of optimal design problem (I) *simplifies to the existence of a Lagrange multiplier $c \geq 0$ such that*

$$\begin{aligned} \Psi > c \quad &\Rightarrow \quad \theta^* = 1\,, \\ \Psi < c \quad &\Rightarrow \quad \theta^* = 0\,. \end{aligned} \tag{2}$$



Single state equation:

$$(3) \qquad \begin{cases} -\operatorname{div}(\lambda_\theta^-(x)\nabla u) = 1 & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

where $\lambda_\theta^-(x) = \left(\frac{\theta(x)}{\alpha} + \frac{1-\theta(x)}{\beta}\right)^{-1}$.

Optimization problem:

$$(4) \qquad \begin{cases} I(\theta) = \displaystyle\int_\Omega u \, \mathrm{d}\boldsymbol{x} \to \max \\ s.t. \quad \theta \in \mathrm{L}^\infty(\Omega, [0,1]), \ \displaystyle\int_\Omega \theta = q_\alpha, \ \text{where } u \text{ satisfies (3)} \end{cases}$$

Single state optimal design problem

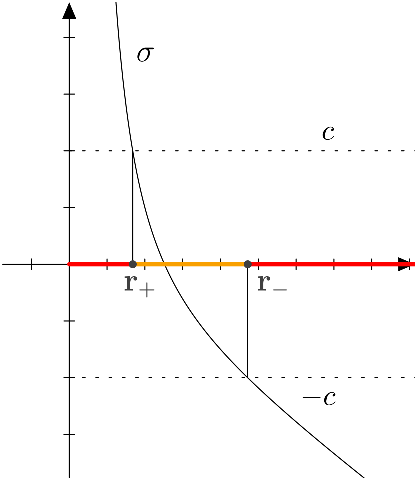
One can rewrite (3) in polar coordinates :

$$-\frac{1}{r^{d-1}}(r^{d-1}\underbrace{\lambda_\theta^- u'(r)}_{\sigma})' = 1 \text{ in } \langle r_1, r_2\rangle\,, \quad u(r_1) = u(r_2) = 0.$$

Observe that σ satisfies

$$\sigma = -\frac{r}{d} + \frac{\gamma}{r^{d-1}}, \quad \gamma > 0$$

$\sigma(r) : \langle 0, \infty\rangle \to \mathbb{R}$ is a strictly decreasing function.



The necessary and sufficient condition of optimality for θ^* states

$$
\begin{aligned}
|\sigma^*| > c \quad &\Rightarrow \quad \theta^* = 1\,, \\
|\sigma^*| < c \quad &\Rightarrow \quad \theta^* = 0\,.
\end{aligned}
$$

There are only three possible candidates for optimal design:

1) $\theta^*(r) = \begin{cases} 1, & r \in [r_1, r_+\rangle \\ 0, & r \in [r_+, r_-\rangle \\ 1, & r \in [r_-, r_2] \end{cases}$

2) $\theta^*(r) = \begin{cases} 1, & r \in [r_1, r_+\rangle \\ 0, & r \in [r_+, r_2\rangle \end{cases}$

3) $\theta^*(r) = \begin{cases} 0, & r \in [r_1, r_-\rangle \\ 1, & r \in [r_-, r_2\rangle \end{cases}$

Simplification to a non-linear system

From condition of optimality a non-linear system (with unknowns γ, c, r_+, r_-) is created:

$$
\text{(NS)} \qquad \begin{cases} S_d \displaystyle\int_{r_1}^{r_2} \theta(\rho)\rho^{d-1}\,\mathrm{d}\rho = q_\alpha \\ u(r_2) = 0 \iff \gamma \displaystyle\int_{r_1}^{r_2} \left(\frac{1}{a(\rho)\rho^{d-1}}\right) \mathrm{d}\rho = \int_{r_1}^{r_2} \frac{\rho}{a(\rho)}\,\mathrm{d}\rho \\ \sigma(r_+) = c, \quad \sigma(r_-) = -c, \qquad \text{where } c > 0 \end{cases}
$$

where

$$
\sigma(r) = \frac{\gamma}{r^{d-1}} - \frac{r}{d}, \quad \& \quad a(r) = \left(\frac{\theta(r)}{\alpha} + \frac{1-\theta(r)}{\beta}\right)^{-1}.
$$

Important: For solving (NS) optimal design is assumed.

(Optimal design for annulus $d = 2, 3,\ f = 1$)

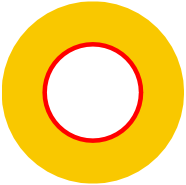
With previous assumptions problem (I) admits optimal solution with two possible designs:

1) $$\theta^*(r) = \begin{cases} 1, & r \in [r_1, r_+\rangle \\ 0, & r \in [r_+, r_-\rangle \\ 1, & r \in [r_-, r_2] \end{cases}$$ **alpha-beta-alpha**

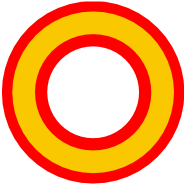
2) $$\theta^*(r) = \begin{cases} 1, & r \in [r_1, r_+\rangle \\ 0, & r \in [r_+, r_2\rangle \end{cases}$$ **alpha-beta**

If q_α is small design 2) is optimal.

alpha-beta
($q_\alpha <$ critical value)



alpha-beta-alpha
($q_\alpha >$ critical value)

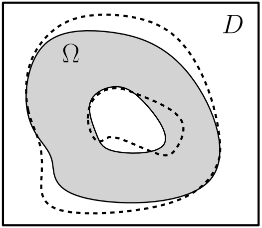


Shape derivative

Perturbation of the set Ω is given with

$$\Omega_t = (\mathrm{Id} + t\psi)\Omega$$

where $\psi \in W^{k,\infty}(\mathbb{R}^d, \mathbb{R}^d)$.



Definition (Shape derivative)

Let $J = J(\Omega)$ be a shape functional. J is said to be shape differentiable at Ω in direction ψ if

$$J'(\Omega, \psi) := \lim_{t \searrow 0} \frac{J(\Omega_t) - J(\Omega)}{t}$$

exists and the mapping $\psi \mapsto J'(\Omega, \psi)$ is linear and continuous. $J'(\Omega, \psi)$ is called the **shape derivative**.

Single state problem

For single state optimal design problem (with transmission condition):

$$
(5)\qquad \begin{cases} J(\chi) = \int_\Omega f u \, \mathrm{d}\boldsymbol{x} \to \max \\ \text{s.t.} \quad \chi \in L^\infty(\Omega, \{0,1\}), \quad \int_\Omega \chi \, \mathrm{d}\boldsymbol{x} = q_\alpha, \\ u \text{ solves (S) with } \mathbf{A} = \chi\alpha\,\mathbf{I} + (1-\chi)\beta\,\mathbf{I} \end{cases}
$$

shape derivative is given with:

$$
\begin{aligned} J'(\Omega, \psi) &= \int_\Omega \mathbf{A}(-\operatorname{div}(\psi) + \nabla\psi + \nabla\psi^\tau)\nabla u_0 \cdot \nabla u_0 \, \mathrm{d}\boldsymbol{x} \\ &+ \int_\Omega 2(\operatorname{div}(\psi) f + \nabla f \cdot \psi) u_0 \, \mathrm{d}\boldsymbol{x} \end{aligned}
$$

where u_0 is solution of BVP (S) on domain Ω with $\mathbf{A} = \chi\alpha\,\mathbf{I} + (1-\chi)\beta\,\mathbf{I}$.

Gradient method, Lagrange approach

Heuristics: do several iterations of the method, check results and adapt parameters.

Algorithm 1: iteration of the method

1 Input : mesh $\mathcal{T}_k$ - boundary is discretized (it is desirable to make a new triangulation)

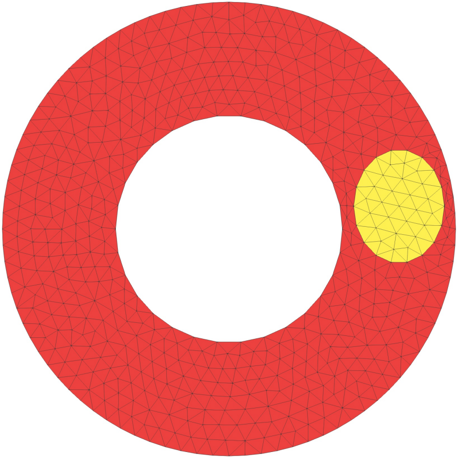
2 Create function space `Vh` na $\mathcal{T}_k$ (P1,P2,...)

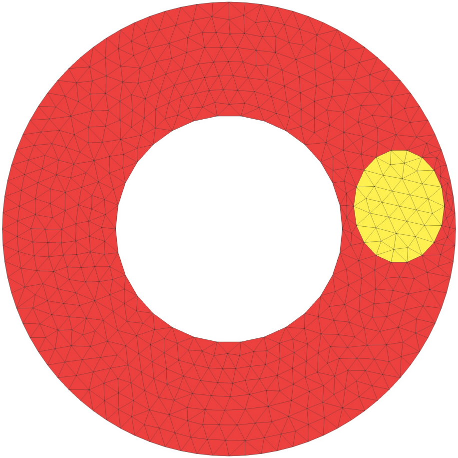
3 Determine ascent vector $\psi \in$ `Vh` from shape derivative

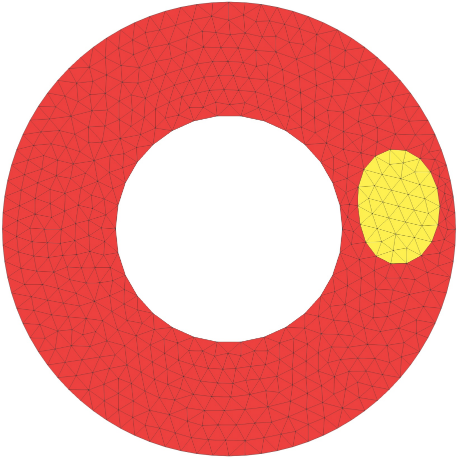
4 Calculate size of the step $t_0 > 0$ $\mathcal{T}_k$ (in order to avoid creating elements with negative volume)

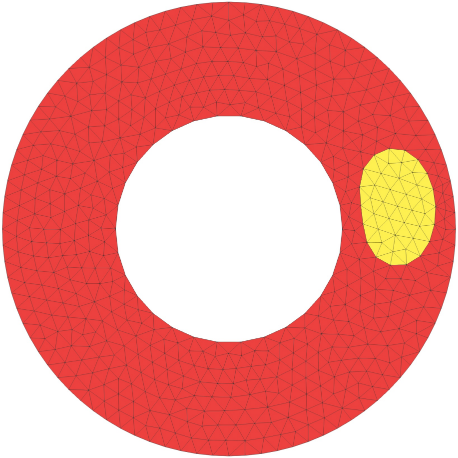
5 Update mesh $\mathcal{T}_{k+1} = (\mathrm{Id} + t_0\psi)\mathcal{T}_k$

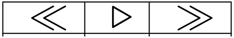
The main drawback of implementation is the need for frequent triangulation of the domain.
Regardless, the above-implemented method is fairly stable and quickly approximates the optimal shape with minimal user intervention.

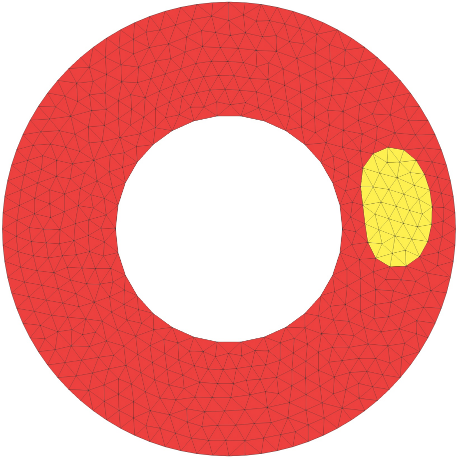


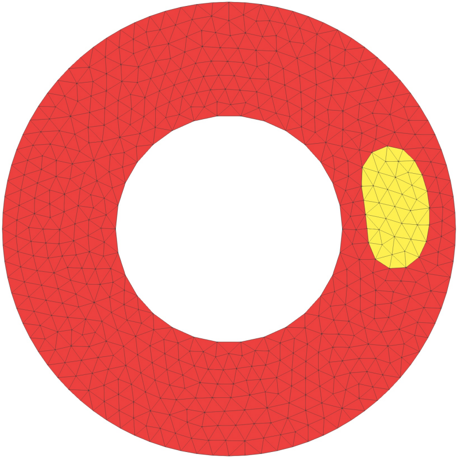


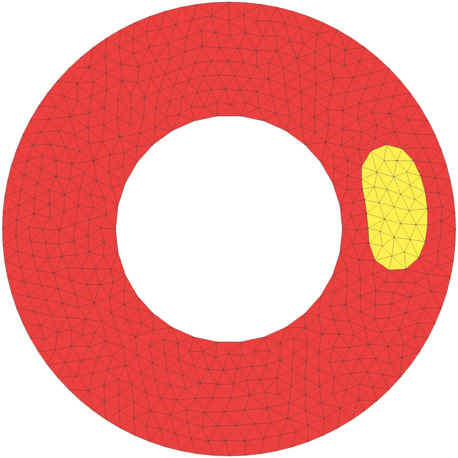


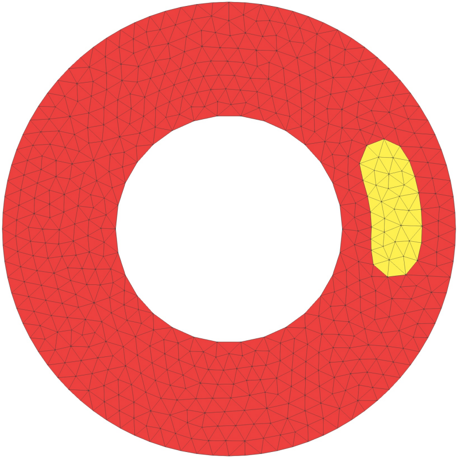


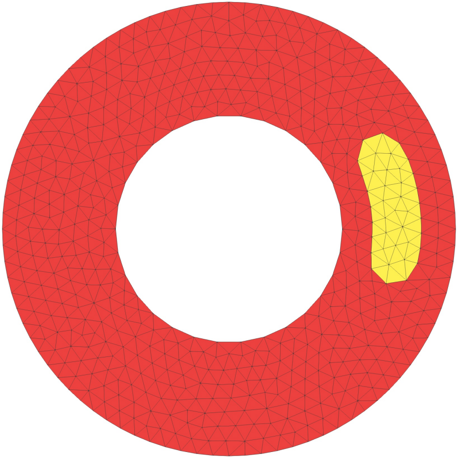


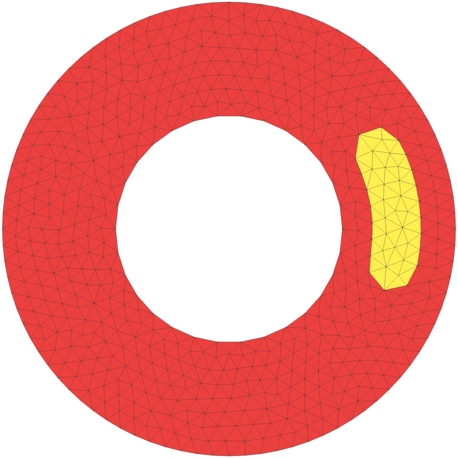


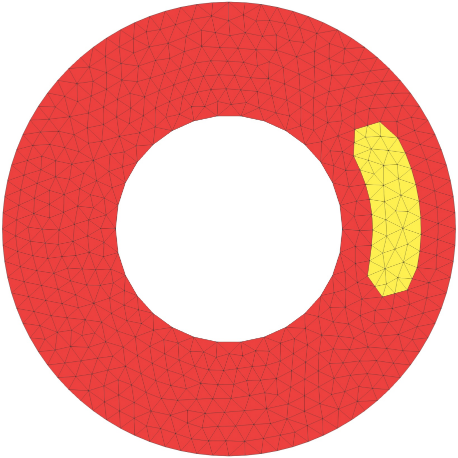


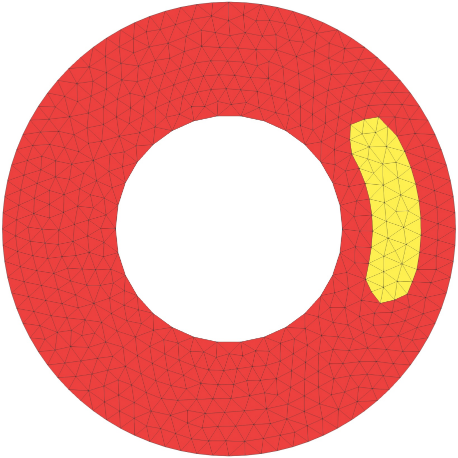


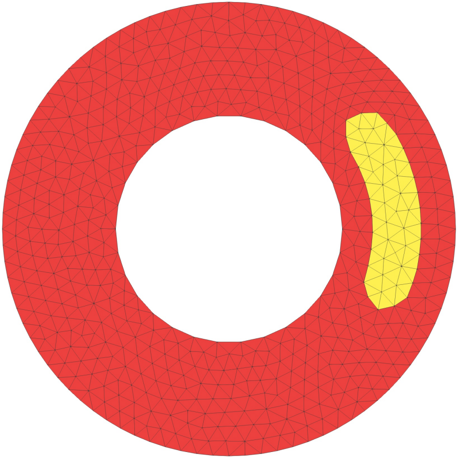


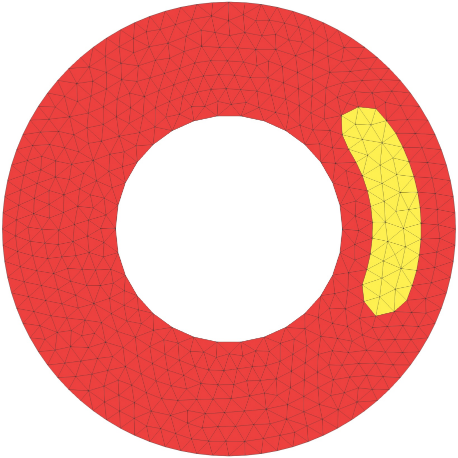


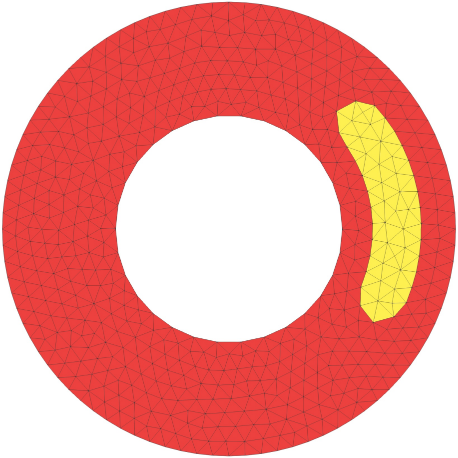


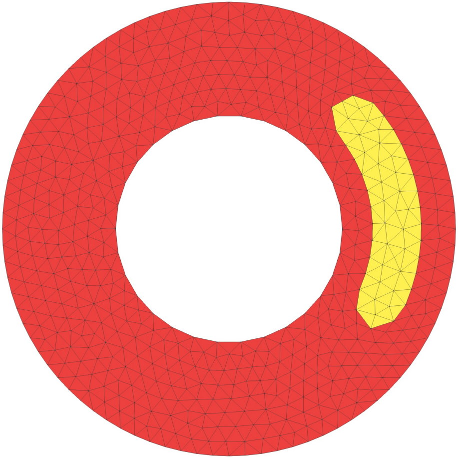


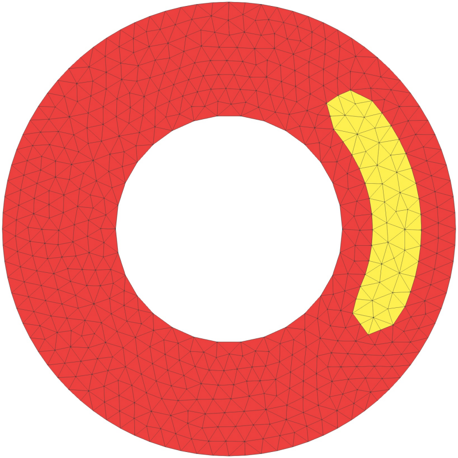


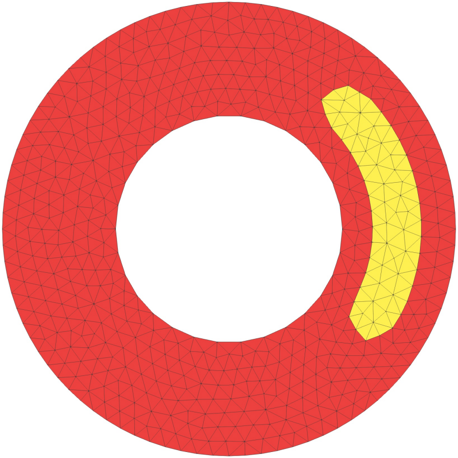


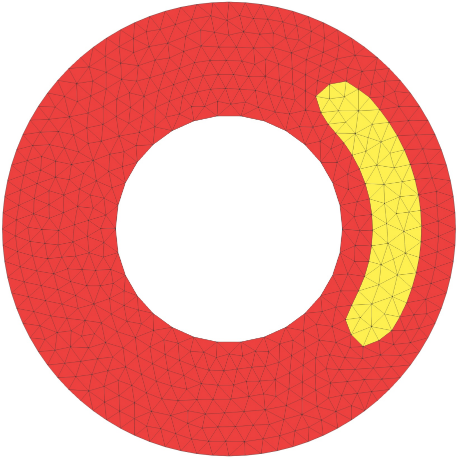


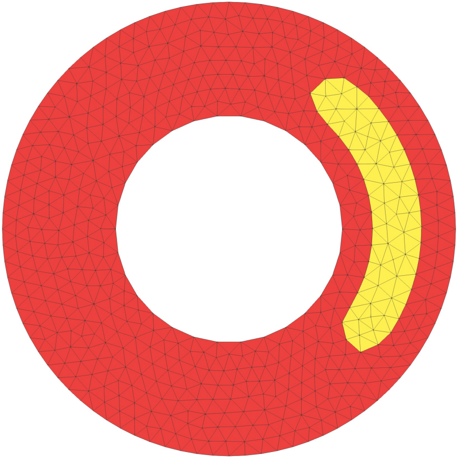


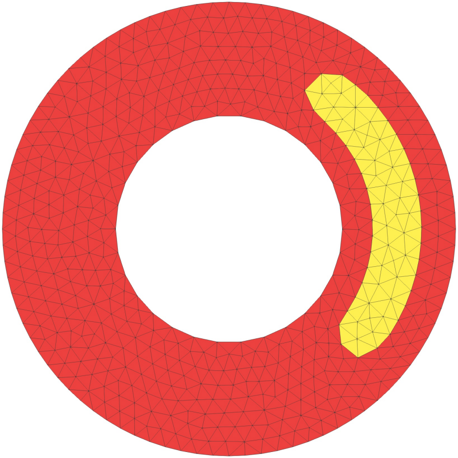


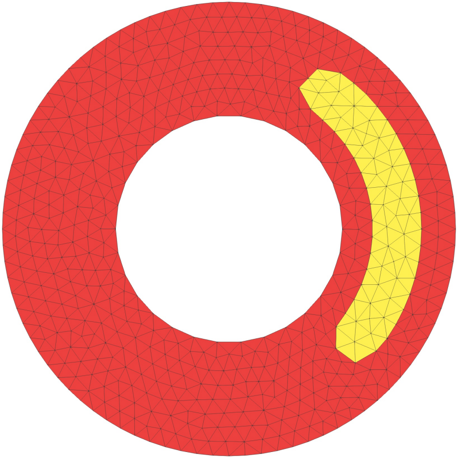


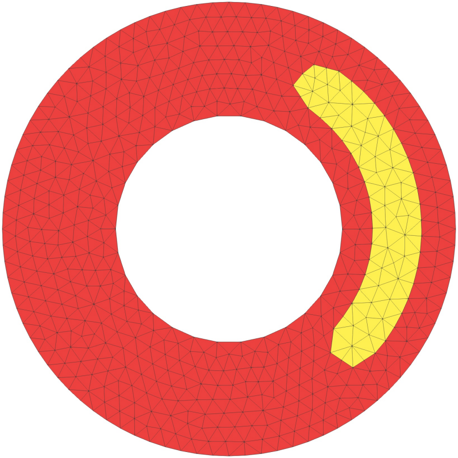


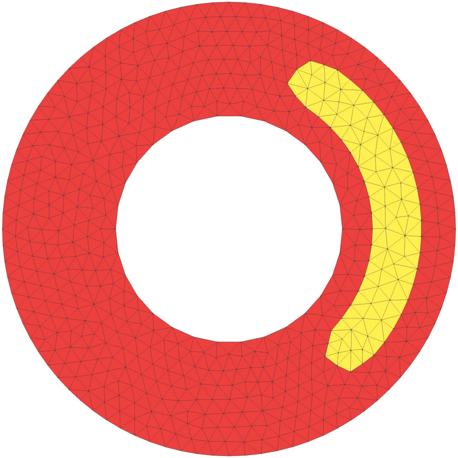


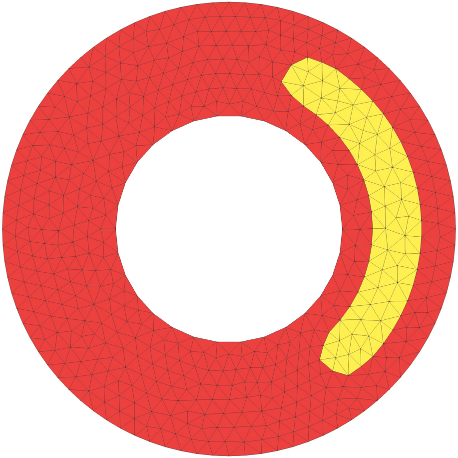


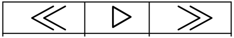


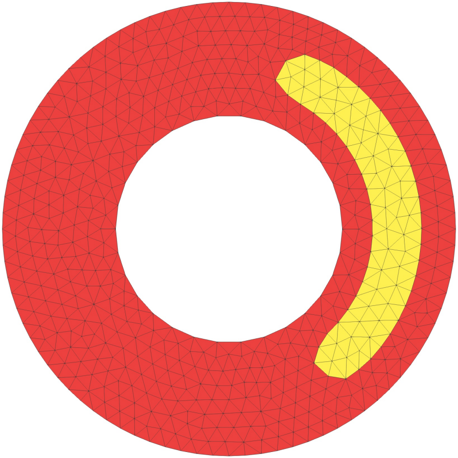


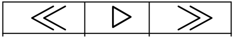


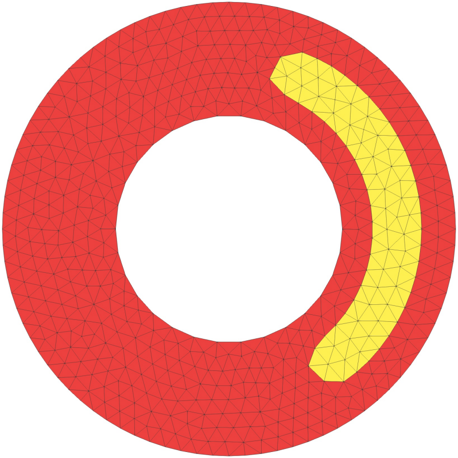


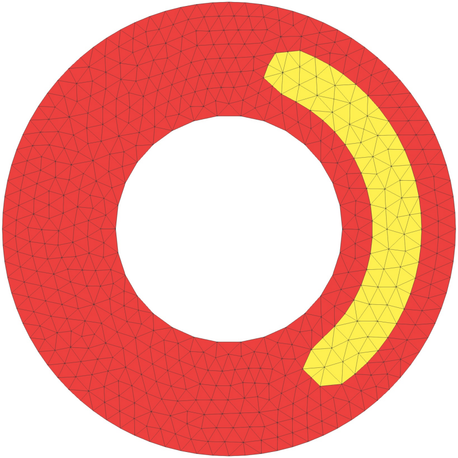


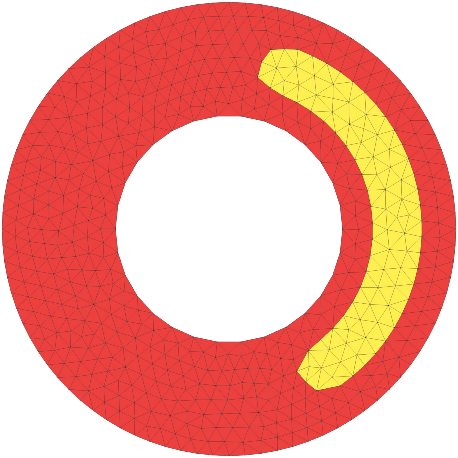


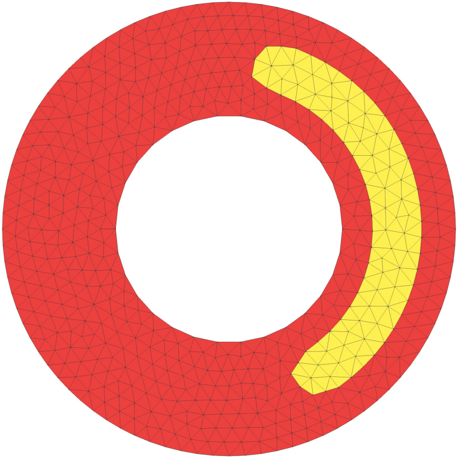


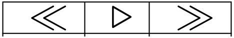


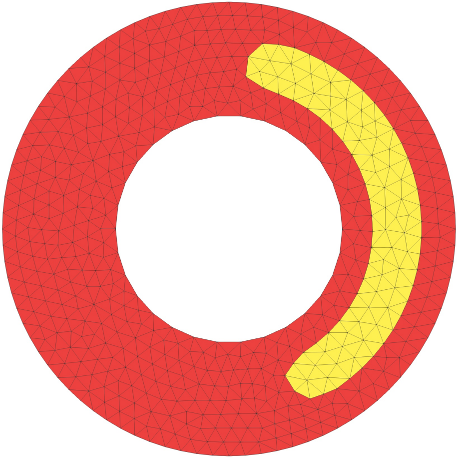


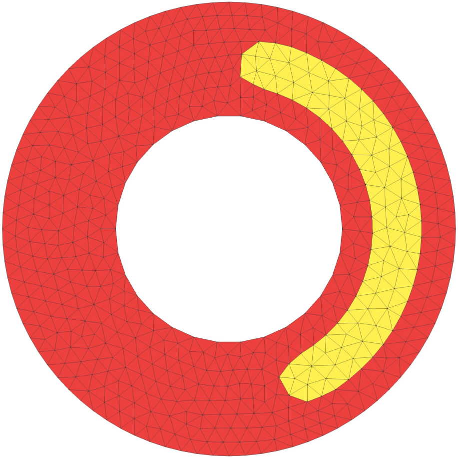


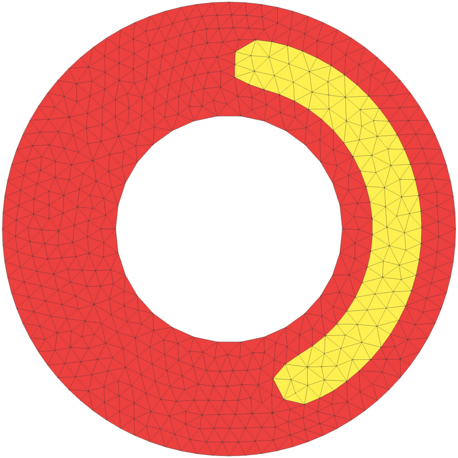


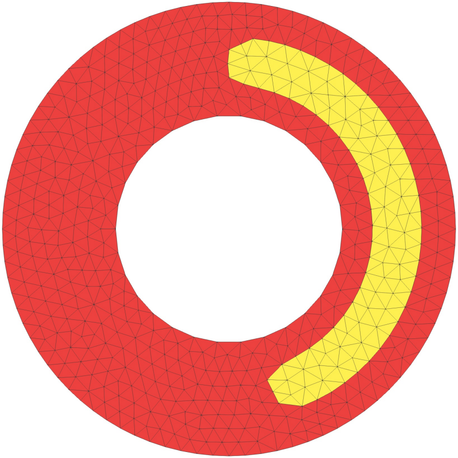


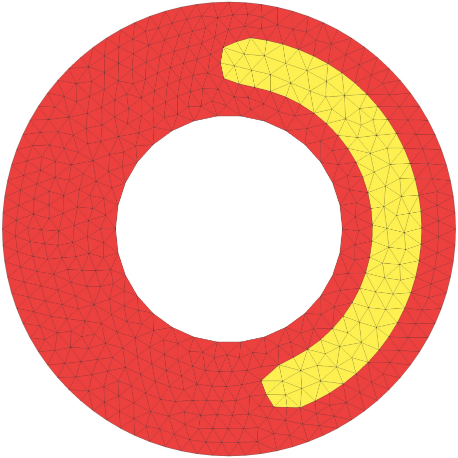


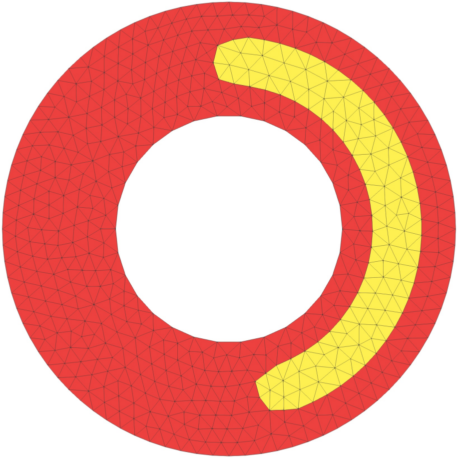


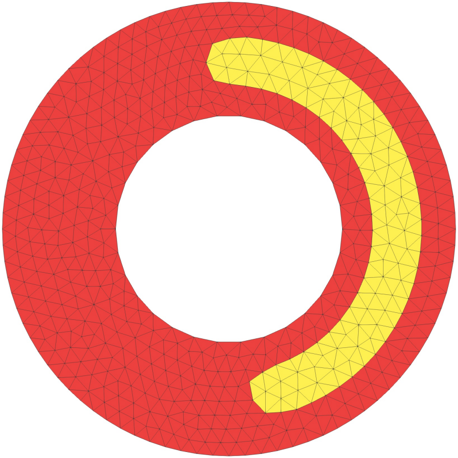


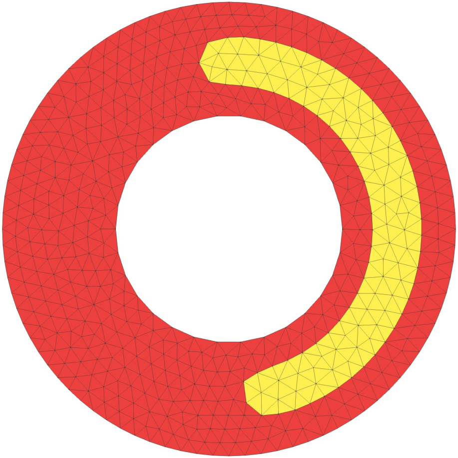


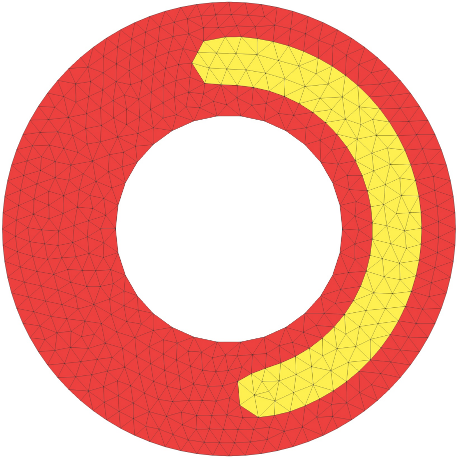


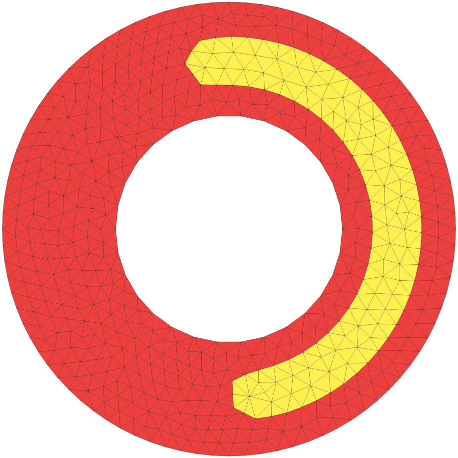


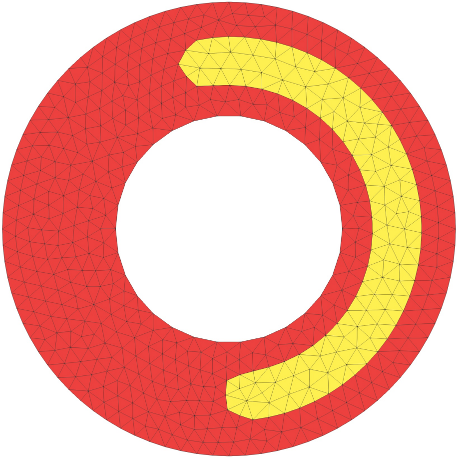


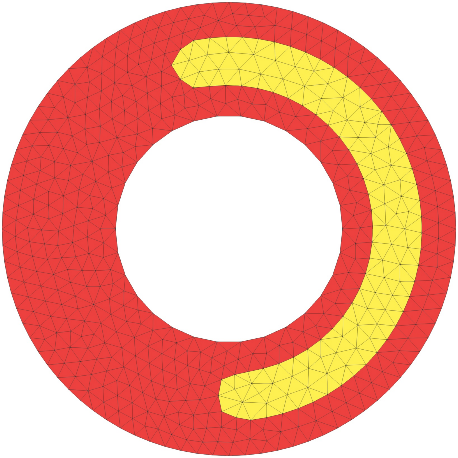


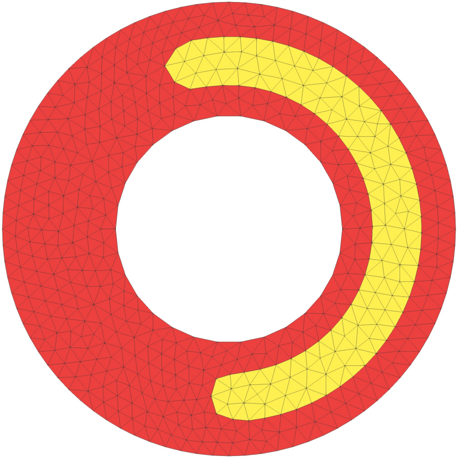


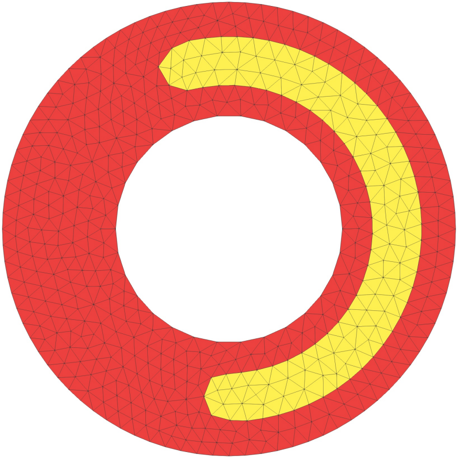


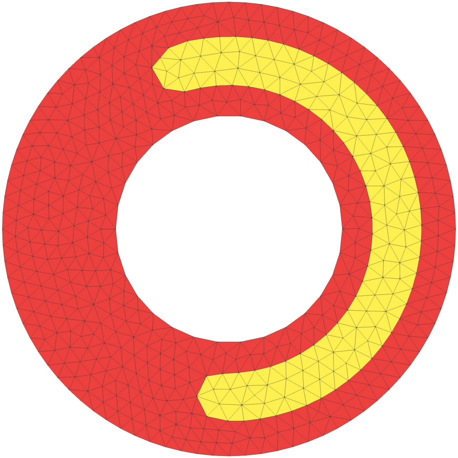


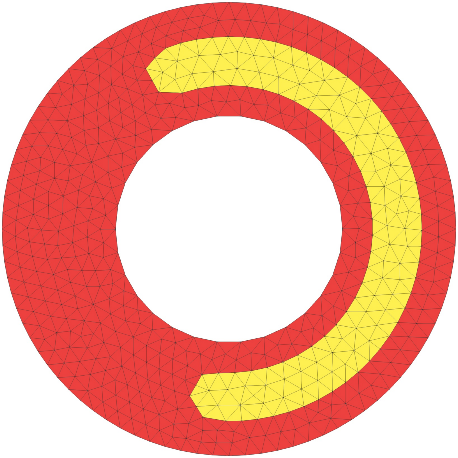


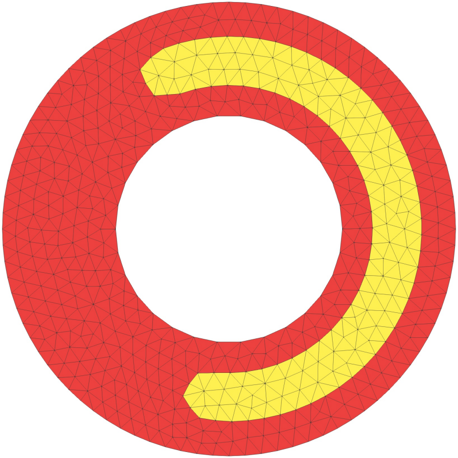


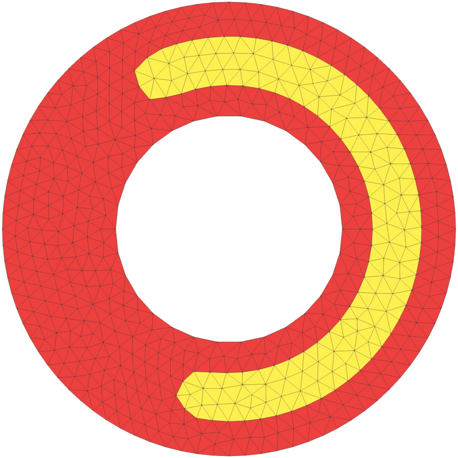


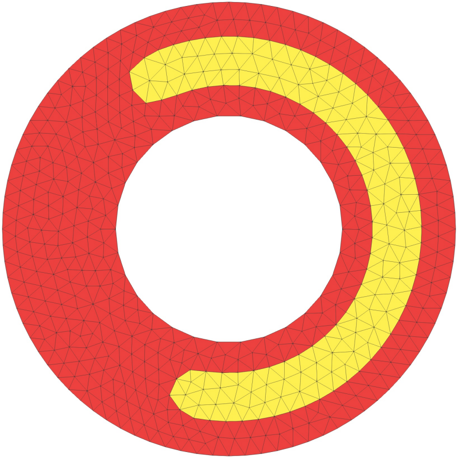


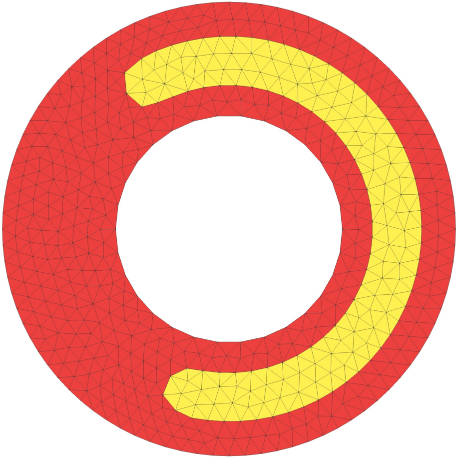


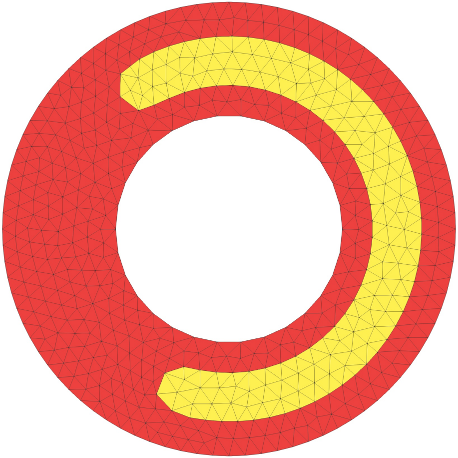


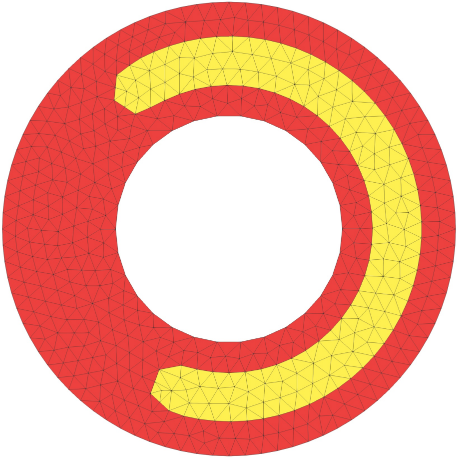


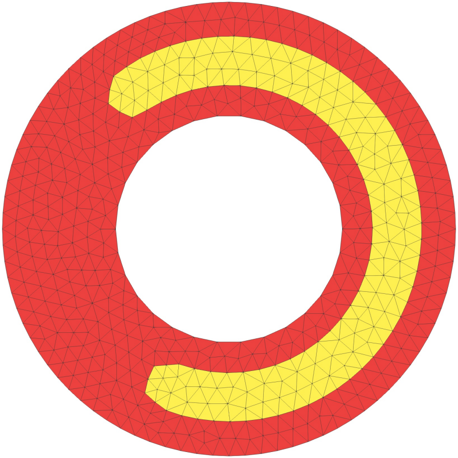


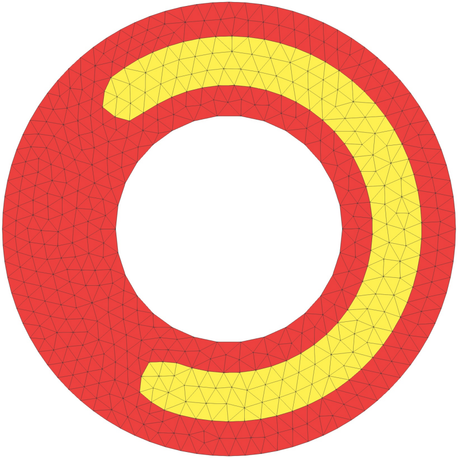


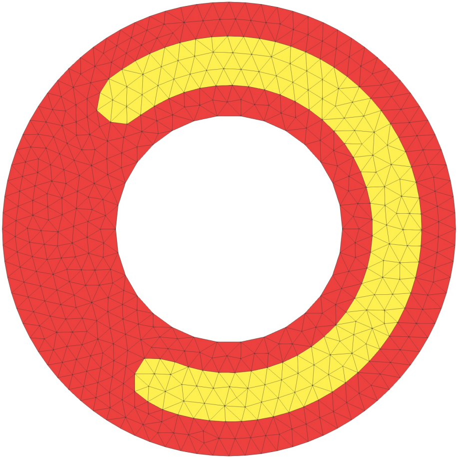


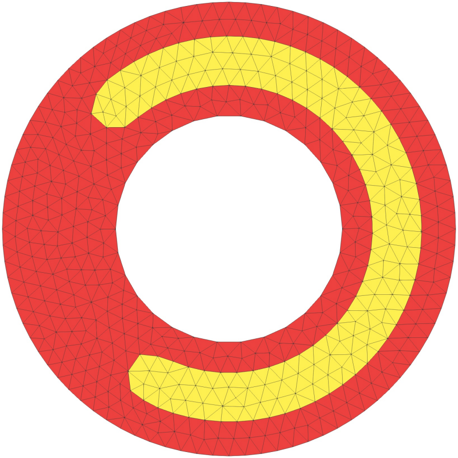


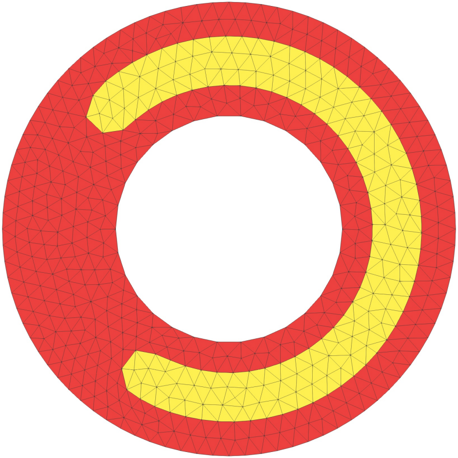


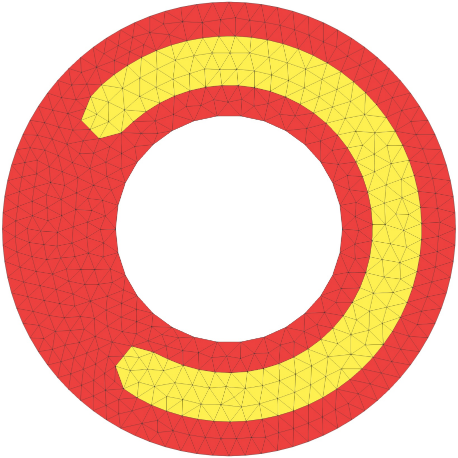


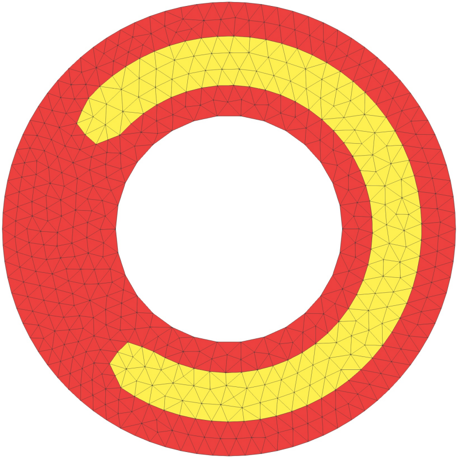


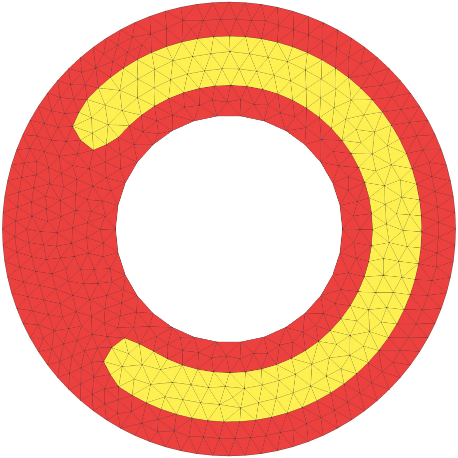


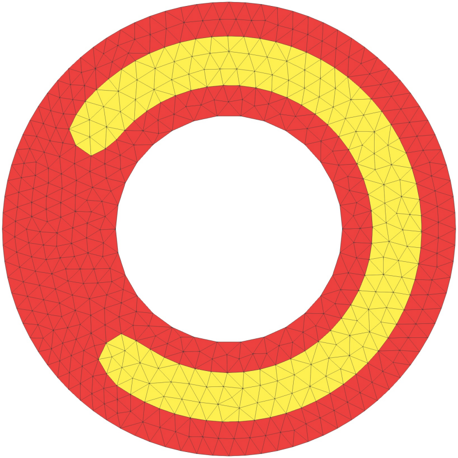


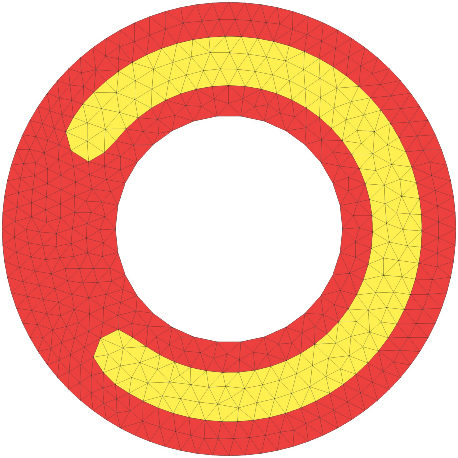


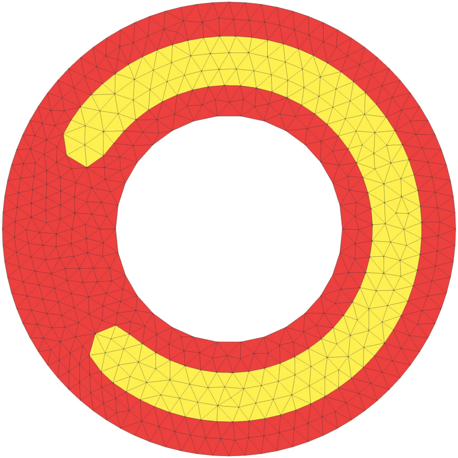


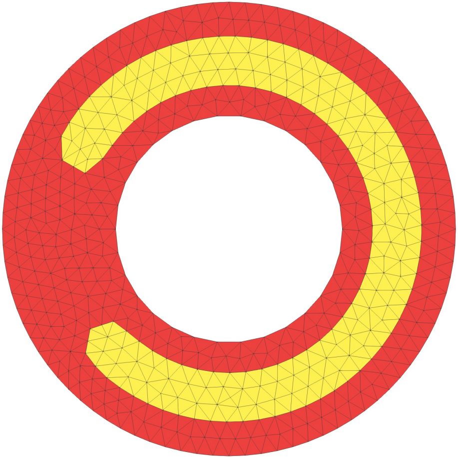


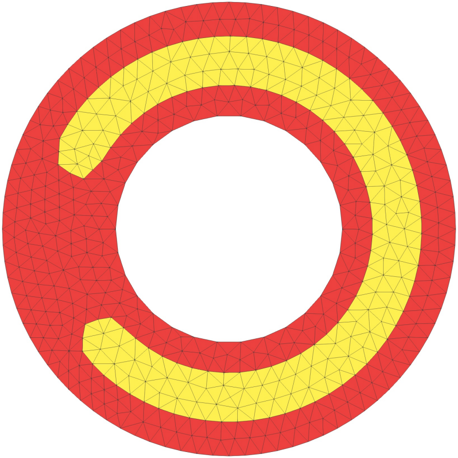


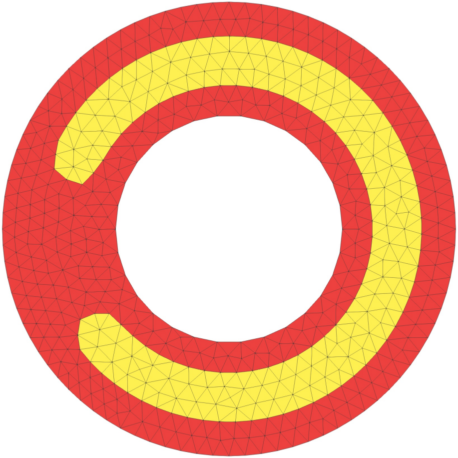


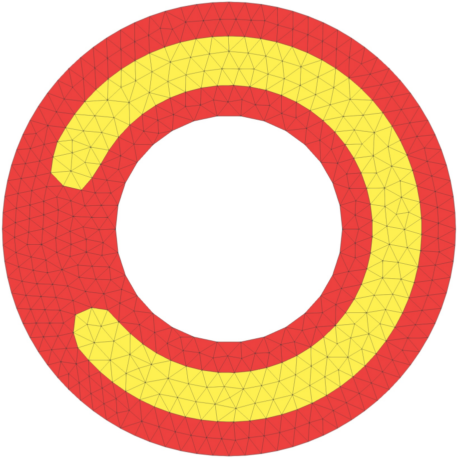


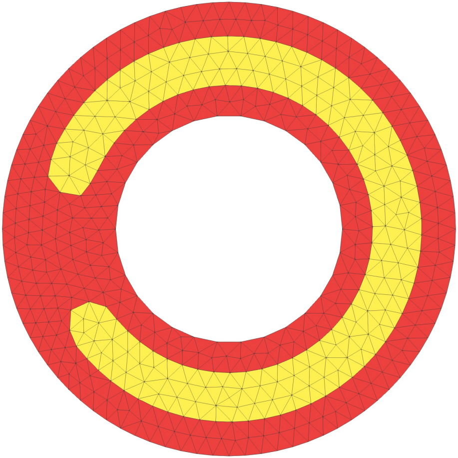


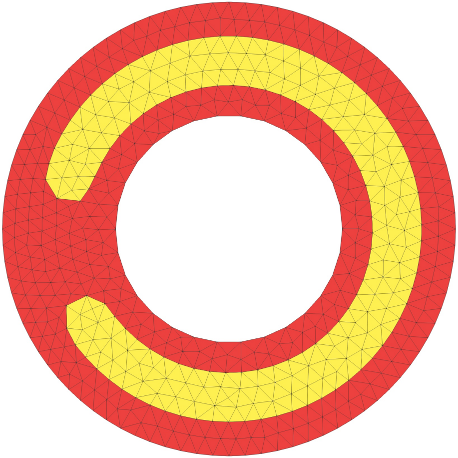


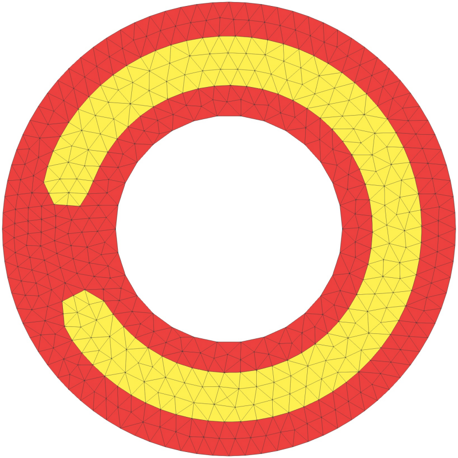


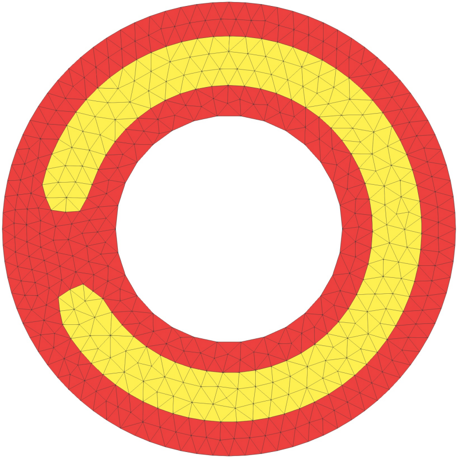


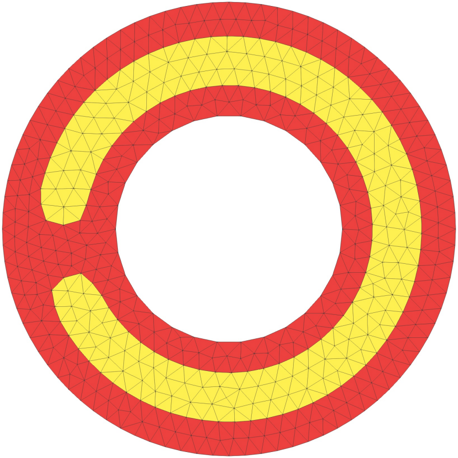


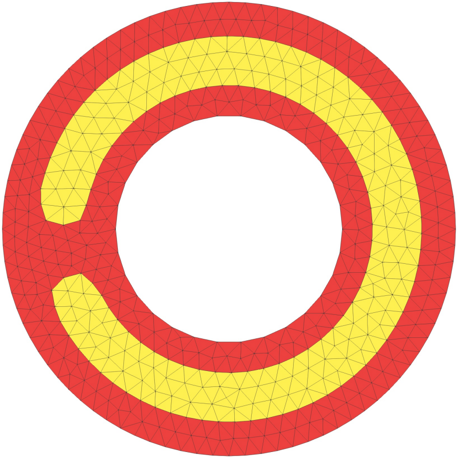


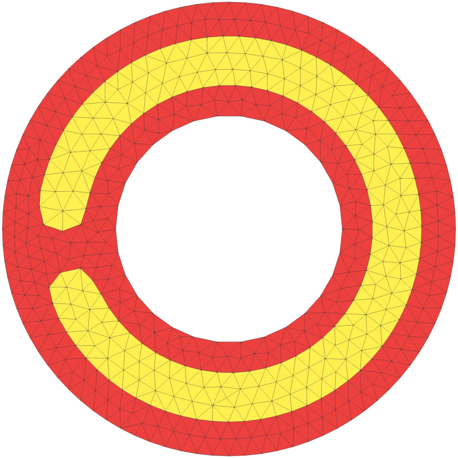


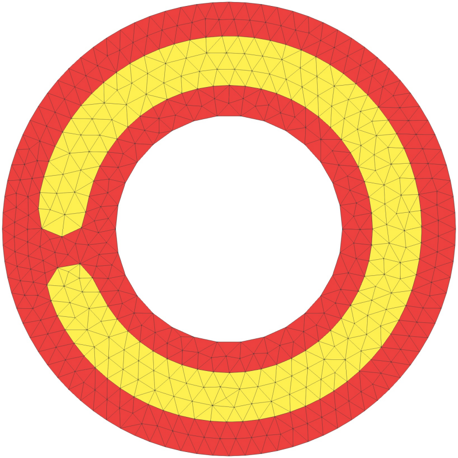


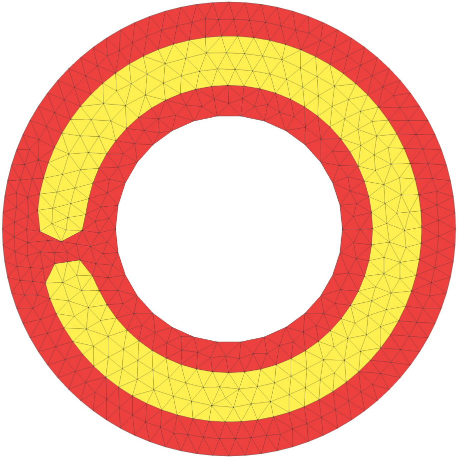


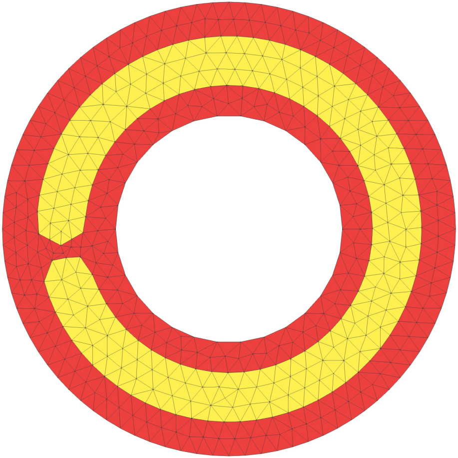


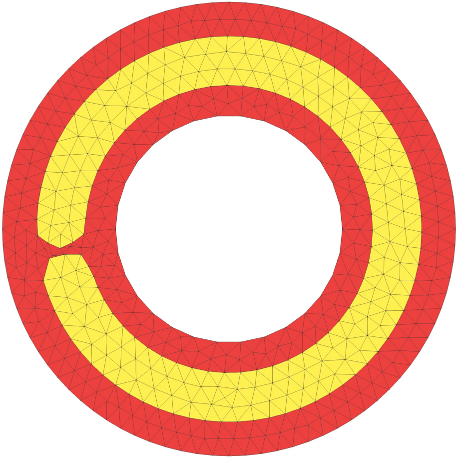


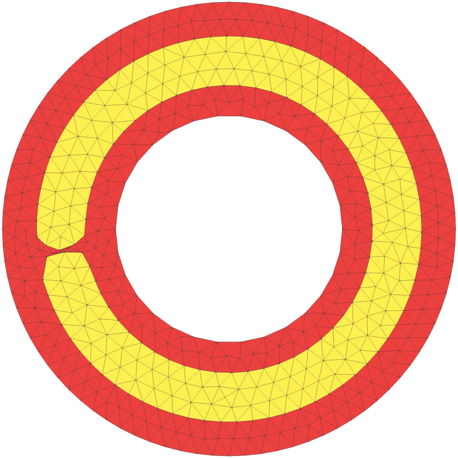


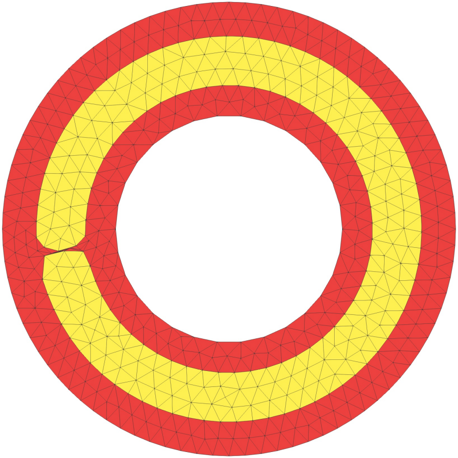


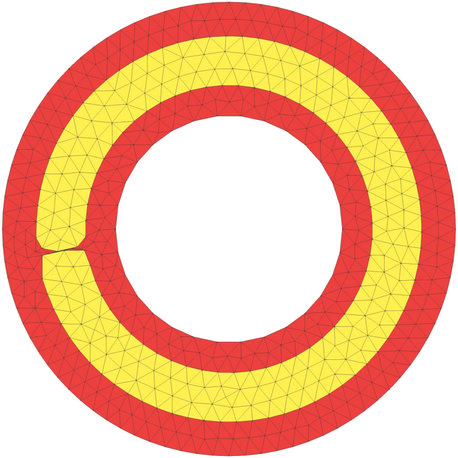


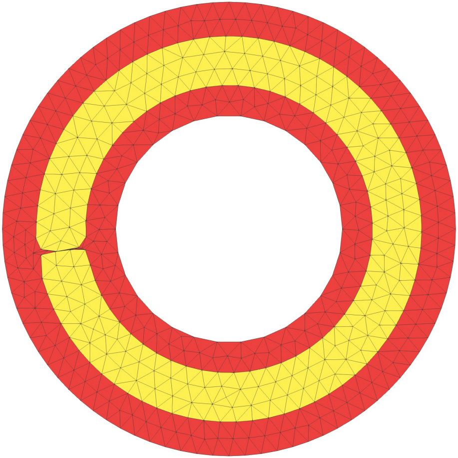


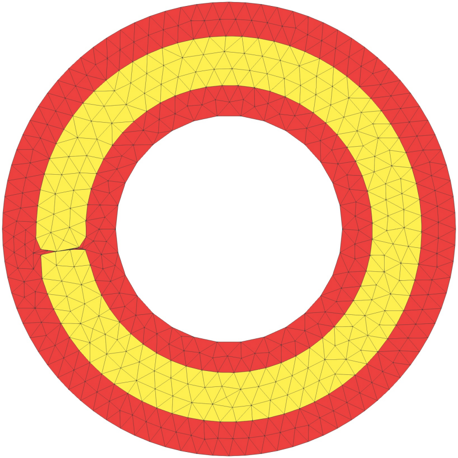


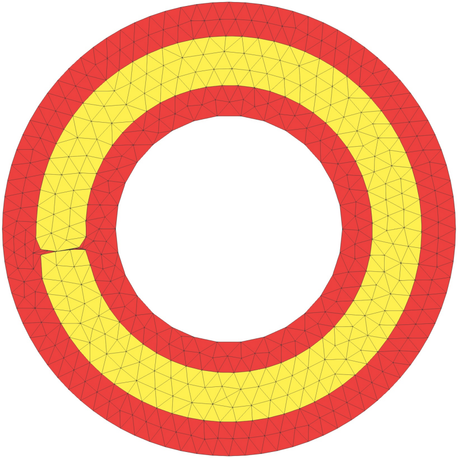


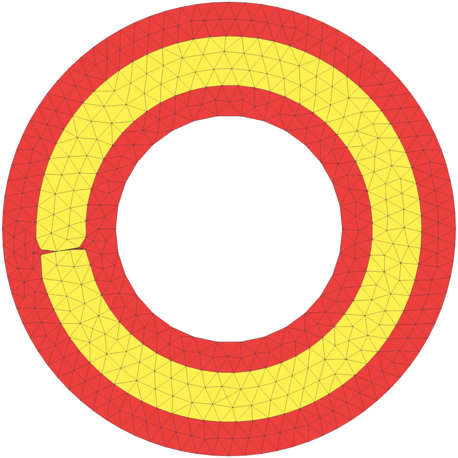


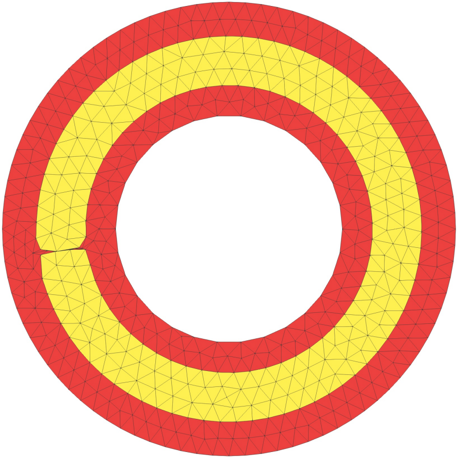


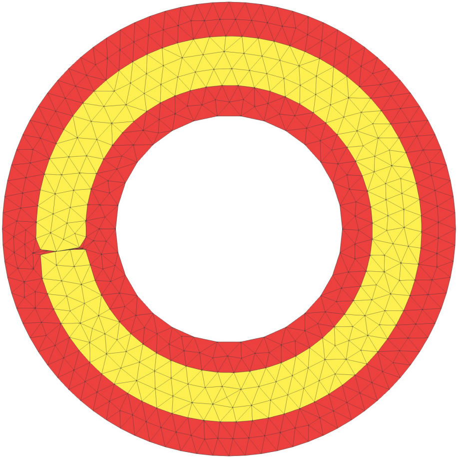


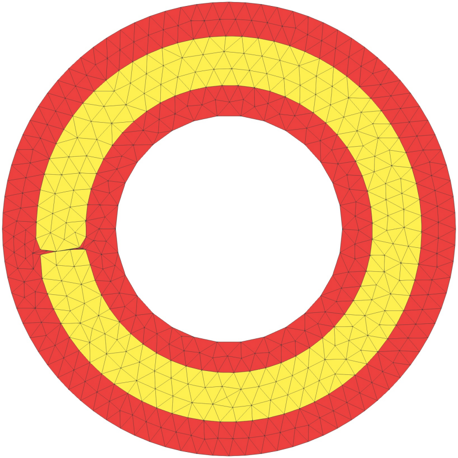


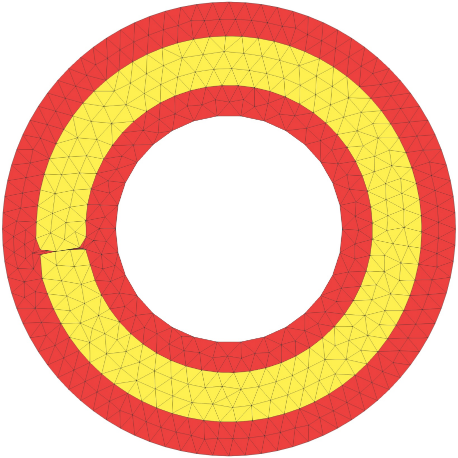


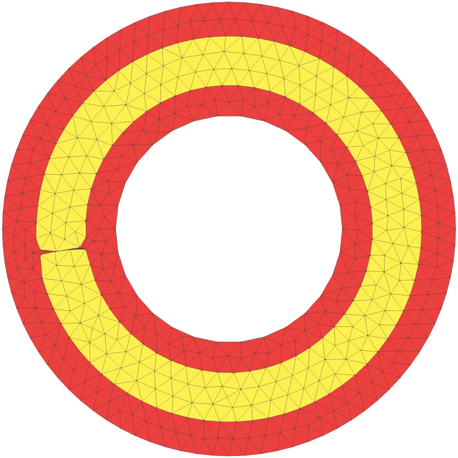


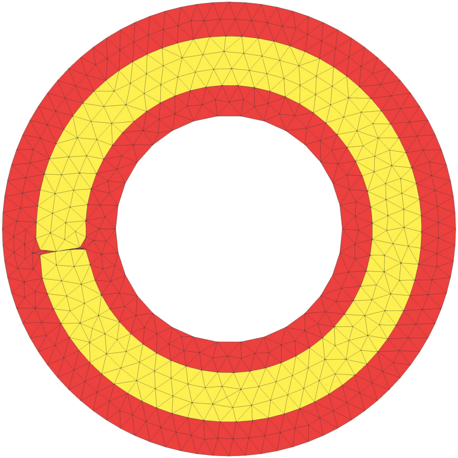


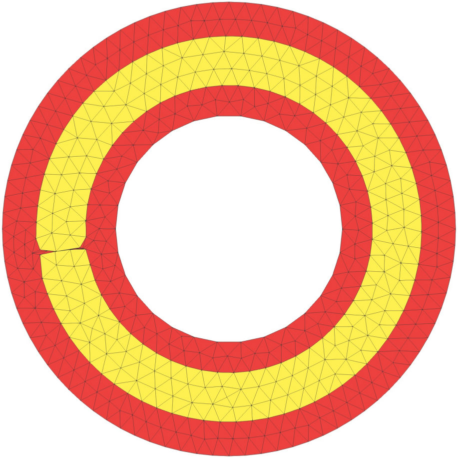


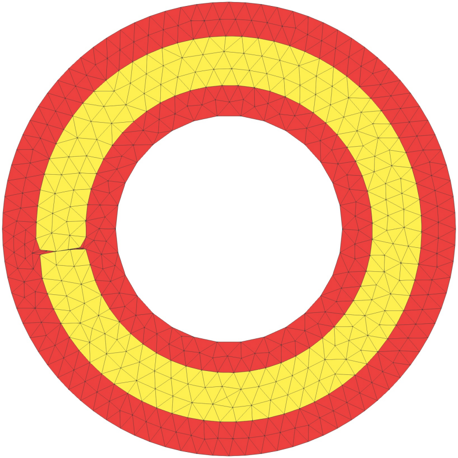


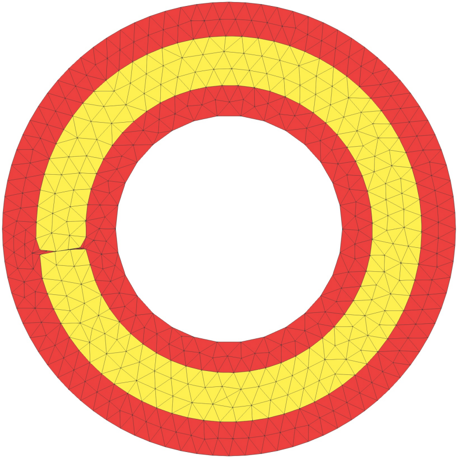


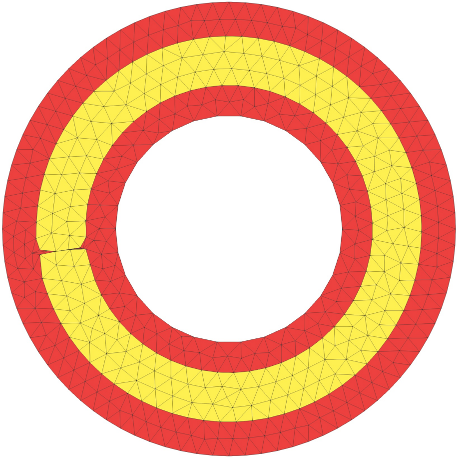


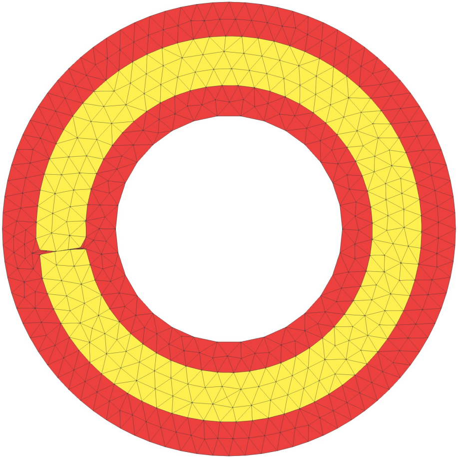


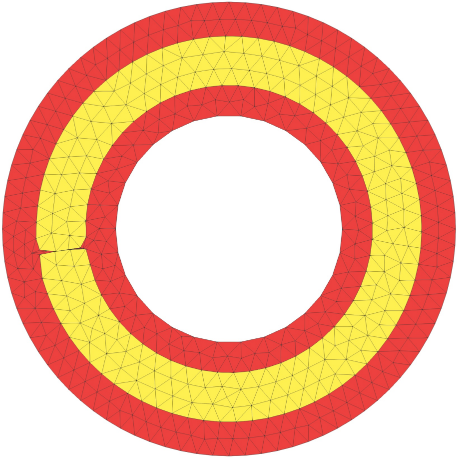


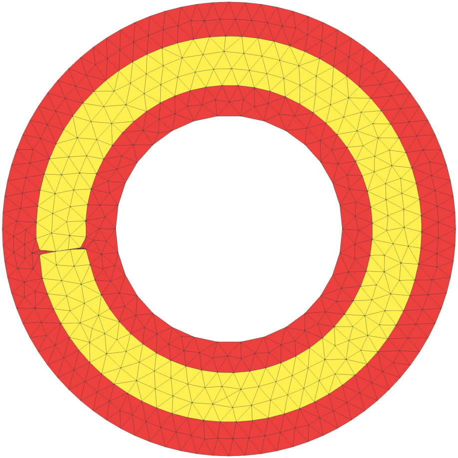




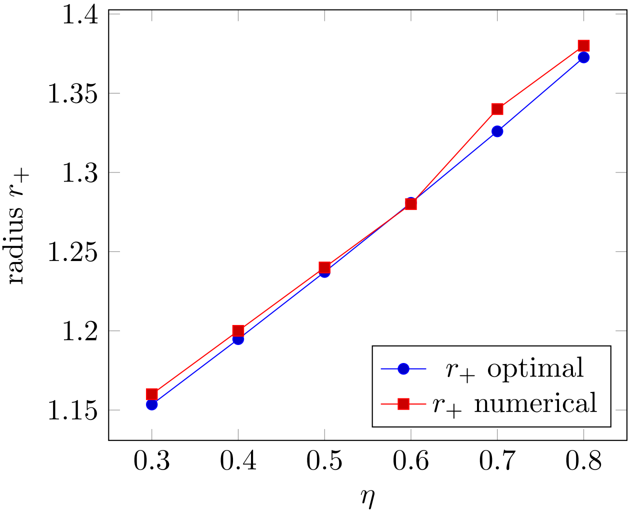




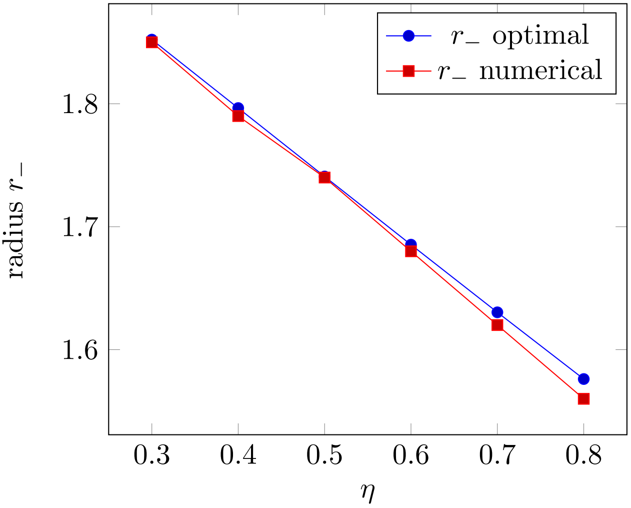


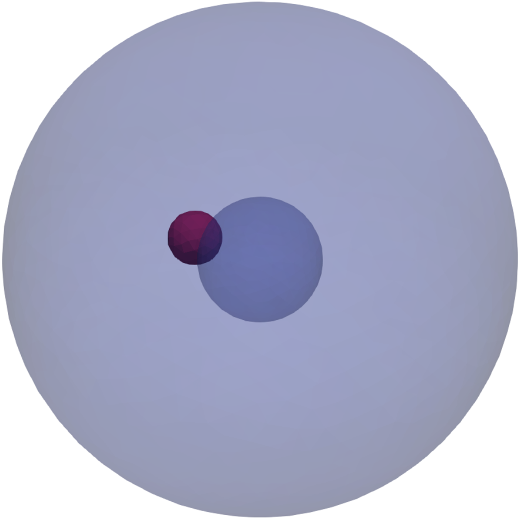


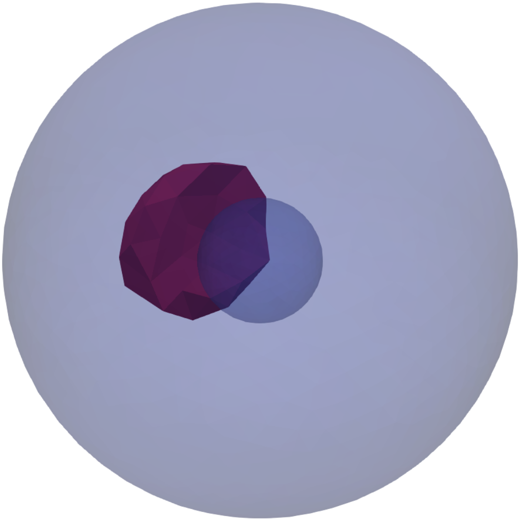
Numerical results

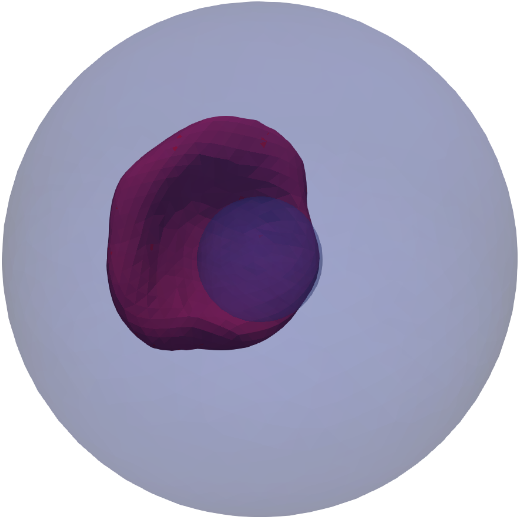


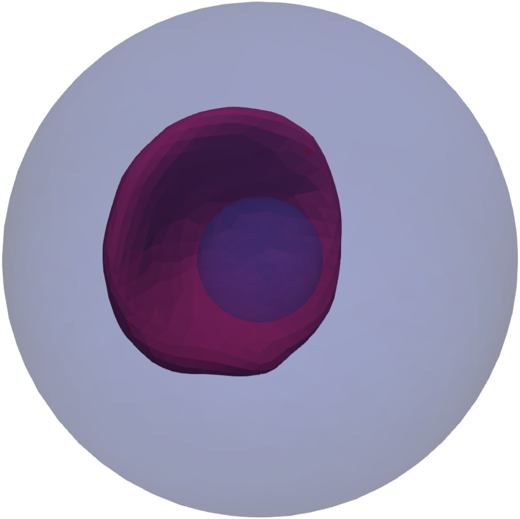
Numerical results

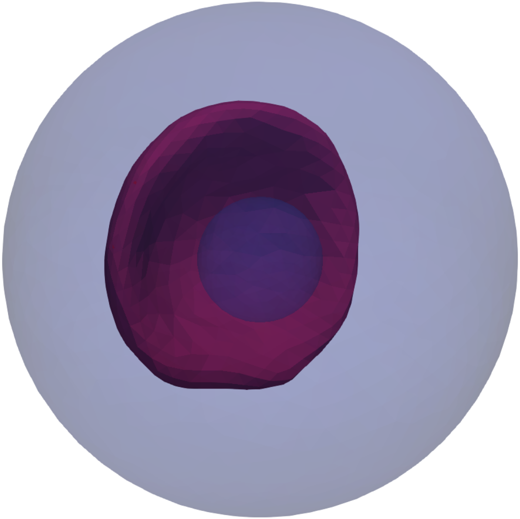


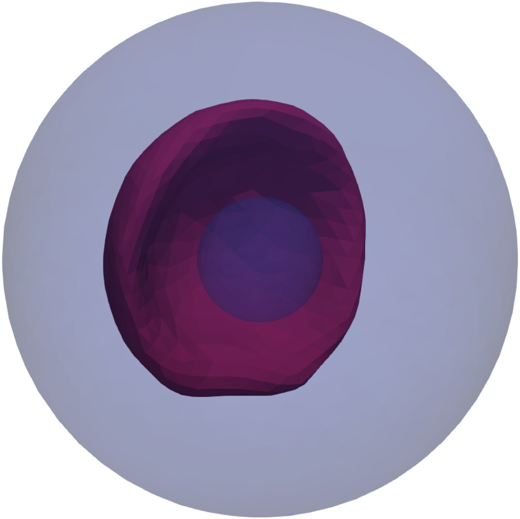


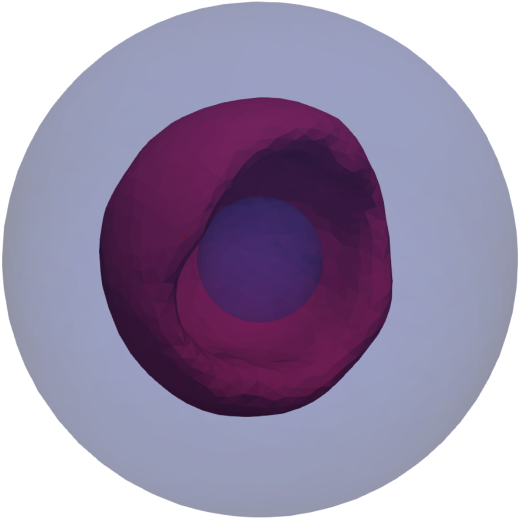


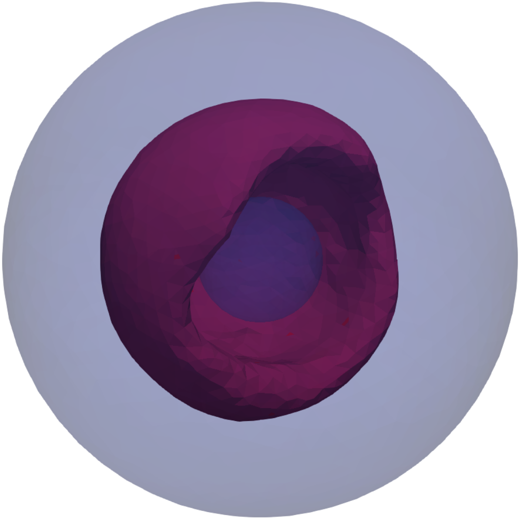


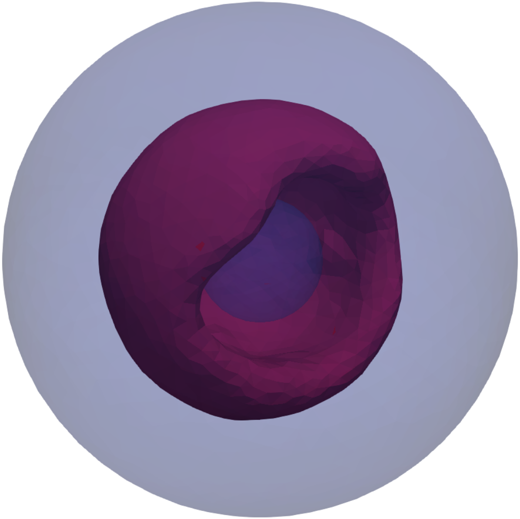


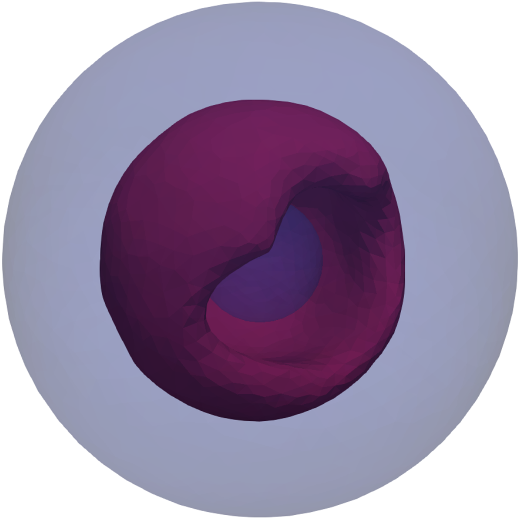


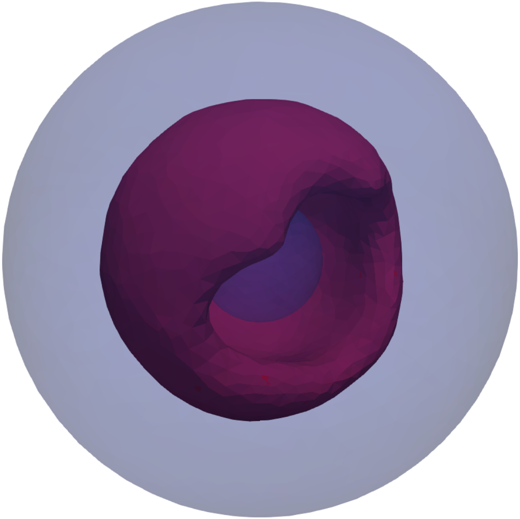


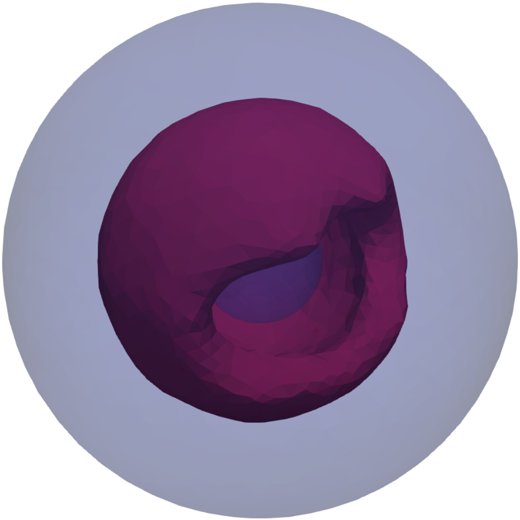












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