

# Methods based on shape derivative for the optimal design on annulus

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VIII Partial differential equations, optimal design and numerics

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# Part I: Construction of classical solutions for optimal design problems

# Introduction

Let  $\Omega \subset \mathbb{R}^d$  be open and bounded set.

Two phases each with different isotropic conductivity:  $\alpha, \beta$  ( $0 < \alpha < \beta$ ).

$q_\alpha$  is the prescribed volume of the first phase  $\alpha$  ( $0 < q_\alpha < |\Omega|$ ).  
 $\chi \in L^\infty(\Omega)$  such that

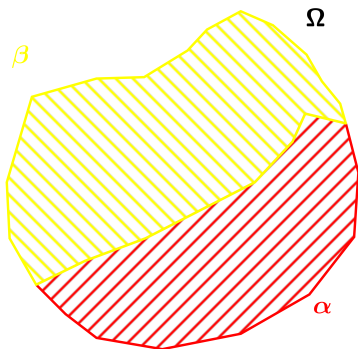
$$\begin{cases} \chi = 1, & \text{phase } \alpha \\ \chi = 0, & \text{phase } \beta \end{cases} .$$

Conductivity can be expressed as

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

where

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



# Introduction

State functions  $u_i \in H_0^1(\Omega)$ ,  $i = 1, 2, \dots, m$  are given as a solution of the following boundary value problems:

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

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

Energy functional:

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

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

# Statement of the problem

Optimal design problem:

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

If solution  $\chi$  exists for (P) we call it *classical solution*.

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

## Results from general theory

$$(I) \quad \begin{cases} I(\theta) = \sum_{i=1}^m \mu_i \int_{\Omega} f_i u_i \, d\mathbf{x} \rightarrow \max \\ s.t. \quad \theta \in L^{\infty}(\Omega, [0, 1]), \quad \int_{\Omega} \theta = q_{\alpha}, \quad \text{where } u_i \text{ satisfies} \\ \quad -\operatorname{div}(\lambda_{\theta}^{-} \nabla u_i) = f_i, \quad u_i \in H_0^1(\Omega), \quad i = 1, 2, \dots, m \end{cases}$$

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

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  $\theta_R^*$  of (I).

In particular, it can be shown that if  $\theta_R^*$  is classical it is also a solution of problem (P). Also, state functions  $u_i$  and fluxes  $\sigma_i = \mathbf{a} \nabla u_i$  are radial functions and  $\sigma_i$  are unique.

Define

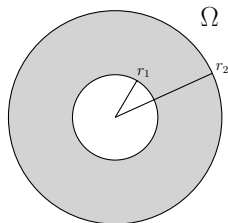
$$\Psi := \sum_{i=1}^m \mu_i |\sigma_i^*|^2.$$

### Lemma

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

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

# Single state optimal design problem



**Single state equation:**

$$(2) \quad \begin{cases} -\operatorname{div}(\lambda_{\theta}^{-}(x)\nabla u) = 1 & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

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

**Optimization problem:**

$$(3) \quad \begin{cases} I(\theta) = \int_{\Omega} u \, d\mathbf{x} \rightarrow \max \\ \text{s.t. } \theta \in L^{\infty}(\Omega, [0, 1]), \int_{\Omega} \theta = q_{\alpha}, \text{ where } u \text{ satisfies (2)} \end{cases}$$



# Single state optimal design problem

One can rewrite (2) 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  $\sigma$  satisfies

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

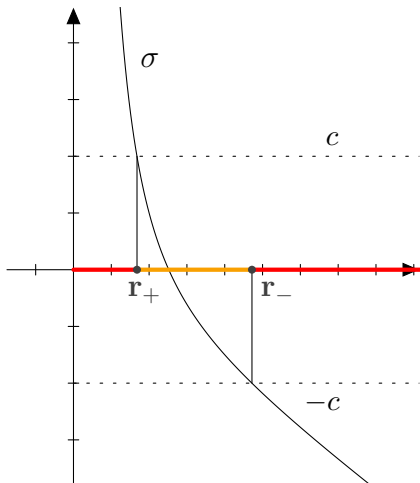
$\sigma(r) : \langle 0, \infty \rangle \rightarrow \mathbb{R}$  is a strictly decreasing function.

The necessary and sufficient condition of optimality for  $\theta^*$  states

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

There are only three possible candidates for optimal design:

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



## Simplification to a non-linear system

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

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

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 $d = 2, 3, f = 1$ )

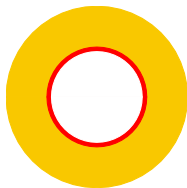
With previous assumptions problem (I) admits optimal solution with two possible designs:

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

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

If  $q_\alpha$  is small design 2) is optimal.

**alpha-beta**  
( $q_\alpha < \text{critical value}$ )



**alpha-beta-alpha**  
( $q_\alpha > \text{critical value}$ )



# Part II: Numerical methods based on shape derivative

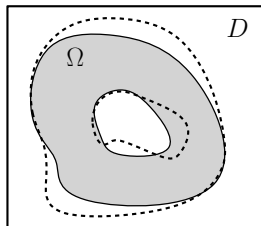
description of methods, numerical solutions in 2D & 3D.

# Shape derivative

Perturbation of the set  $\Omega$  is given with

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

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  $\Omega$  in direction  $\psi$  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):

$$(4) \quad \begin{cases} J(\chi) = \int_{\Omega} f u \, d\mathbf{x} \rightarrow \max \\ \text{s.t. } \chi \in L^{\infty}(\Omega, \{0, 1\}), \quad \int_{\Omega} \chi \, d\mathbf{x} = q_{\alpha}, \\ u \text{ solves (S) with } \mathbf{A} = \chi\alpha\mathbf{I} + (1 - \chi)\beta\mathbf{I} \end{cases}$$

shape derivative is given with:

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

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

# Gradient method based on shape derivative

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

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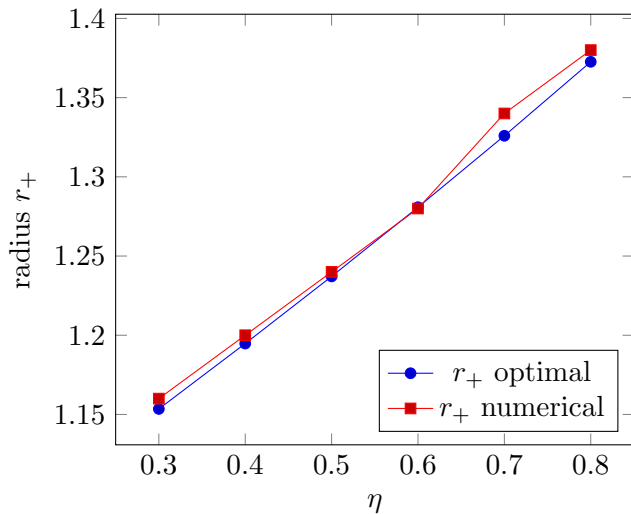
**Algorithm 1:** iteration of the method

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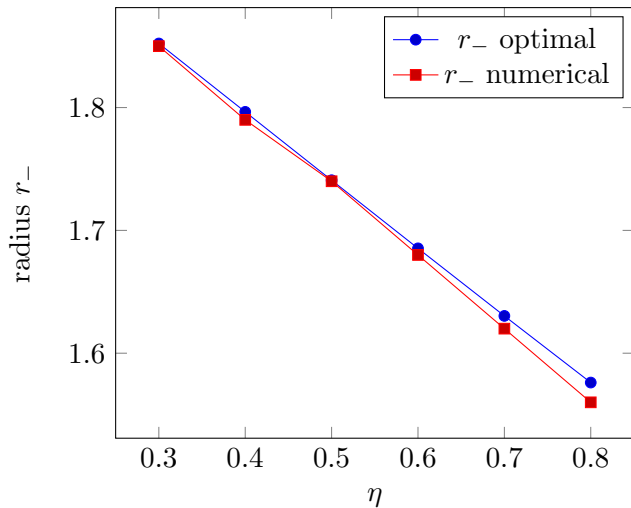
- 1 Input : interface is given implicitly (LSF) or explicitly as discretized set of points - triangulation mesh  $\mathcal{T}_k$
  - 2 Create function space  $\mathbf{V}_h$  on  $\mathcal{T}_k$  (P1,P2,...)
  - 3 Determine ascent vector  $\psi \in \mathbf{V}_h$  from shape derivative (consists of solving several PDEs)
  - 4 Output: update interface (depends highly on considered representation of interface)
- 
- above implemented methods are fairly stable with minimal user intervention
  - in 2D it quickly approximates the optimal shape and script is under 100 lines of code

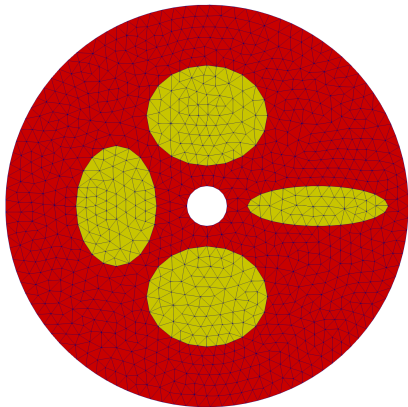


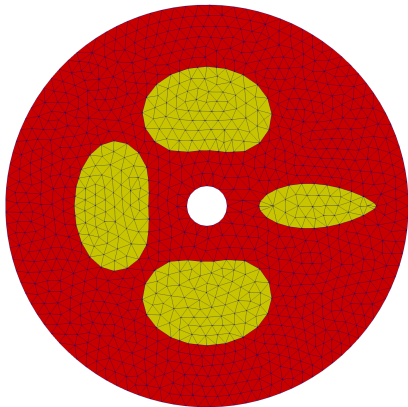
# Numerical results

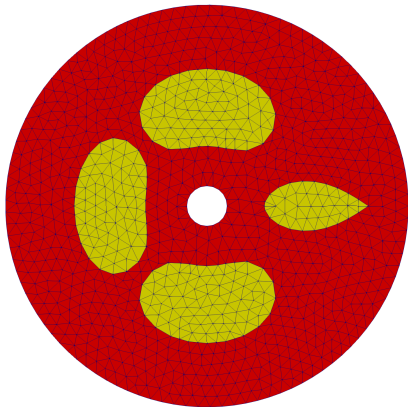


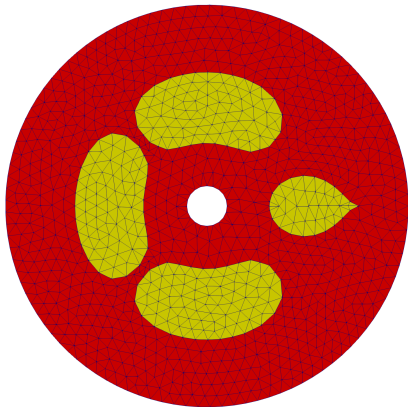
# Numerical results

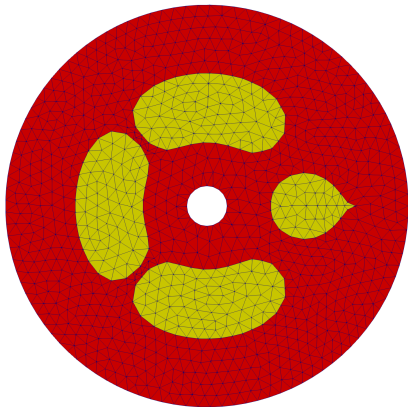


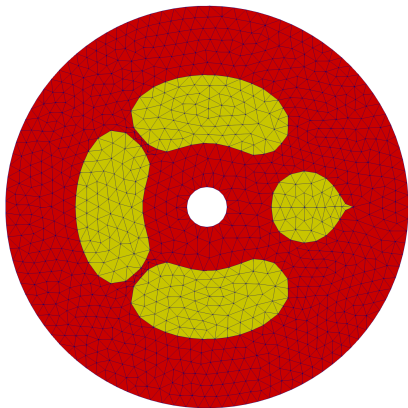




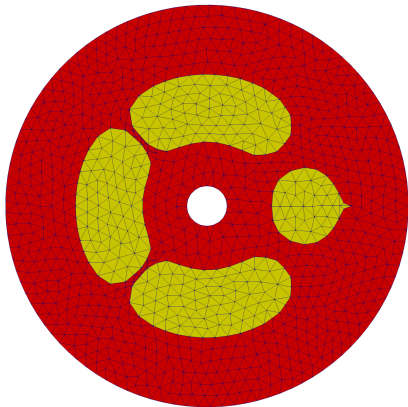


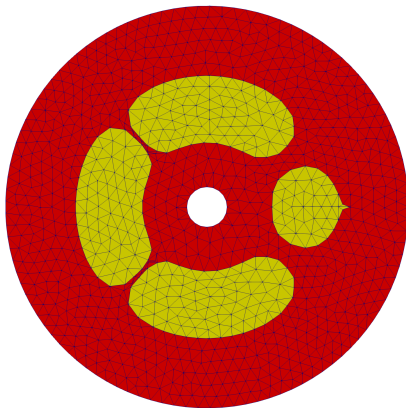


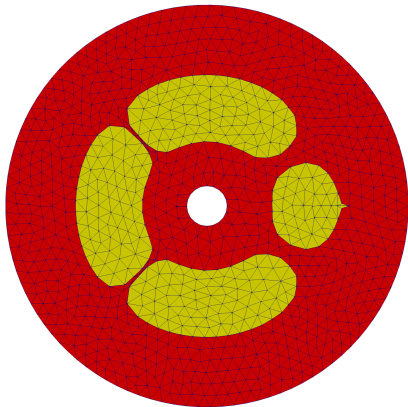


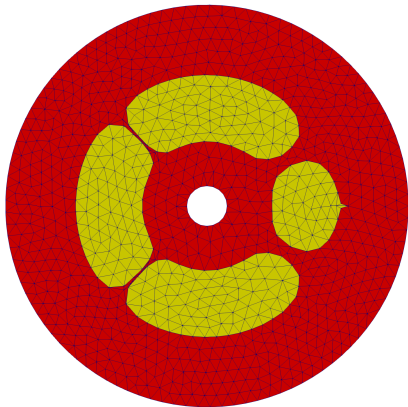


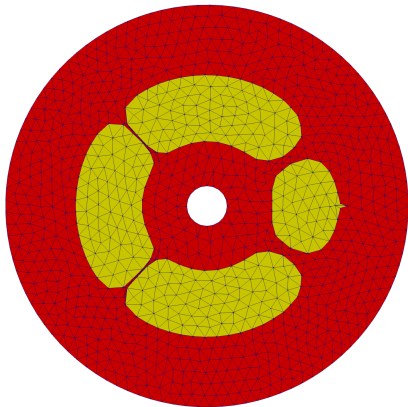


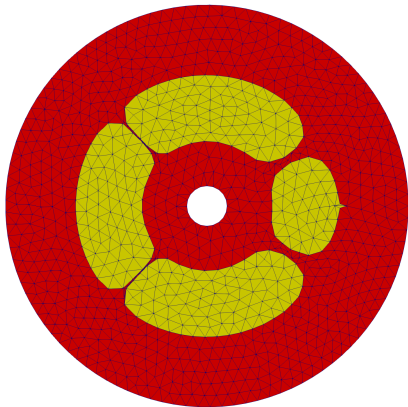


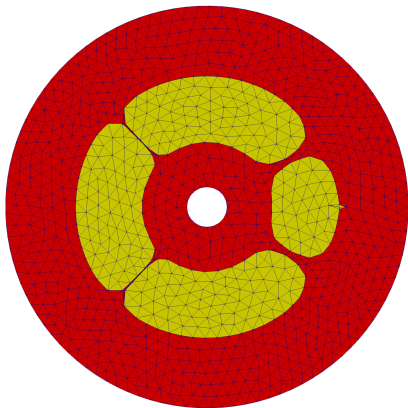


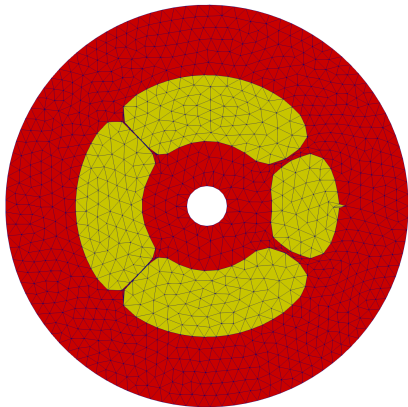




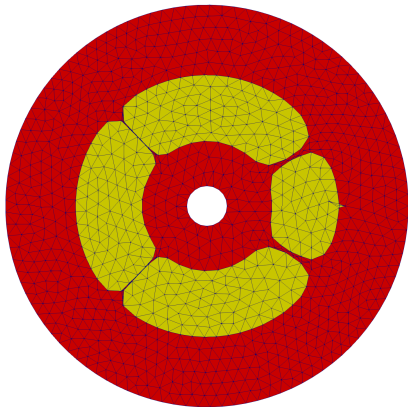


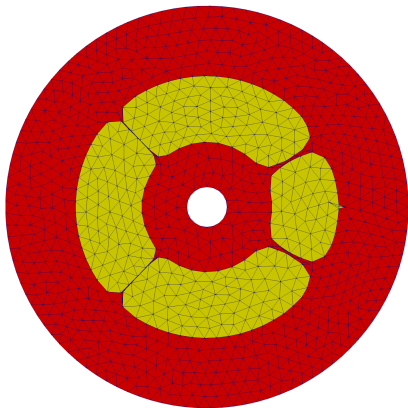


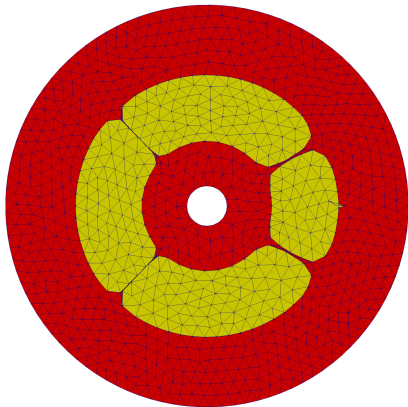


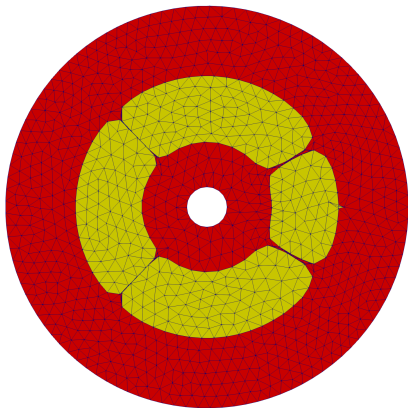


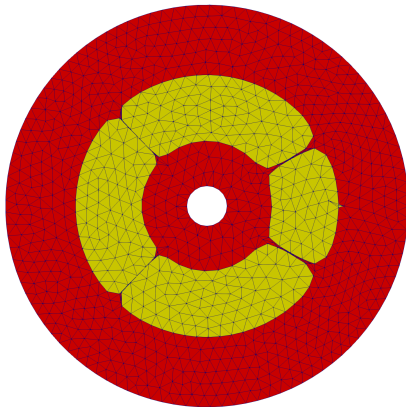


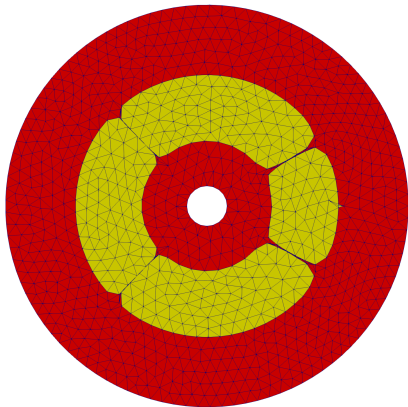


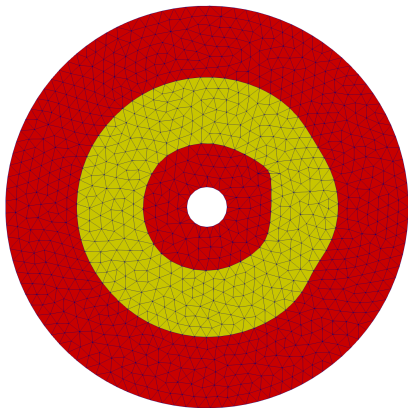


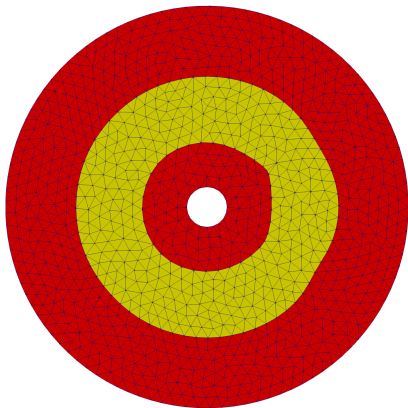




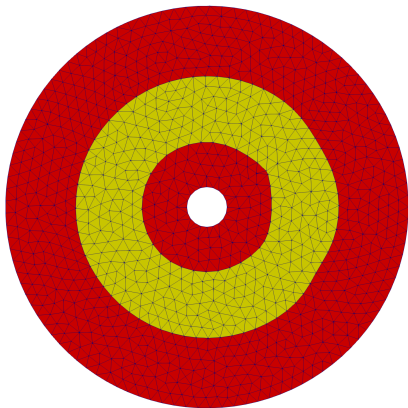


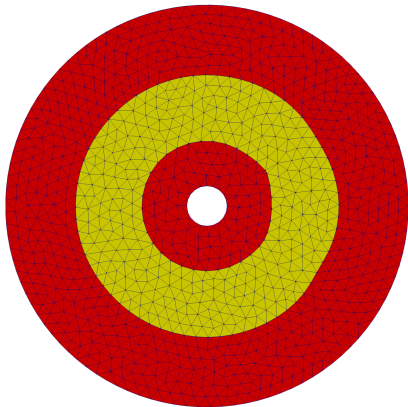


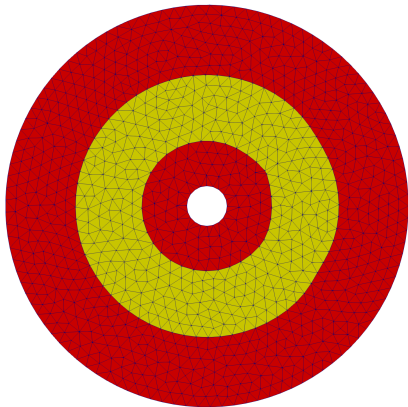


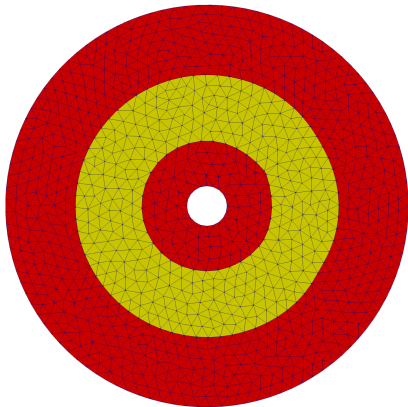


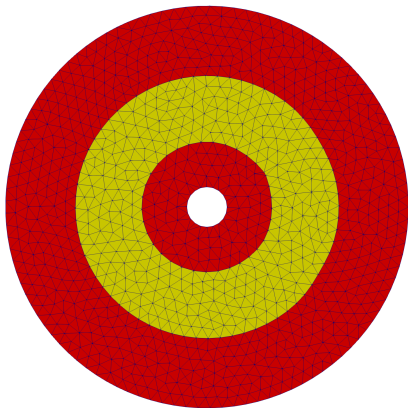


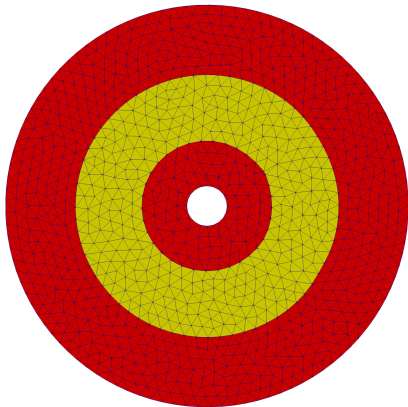


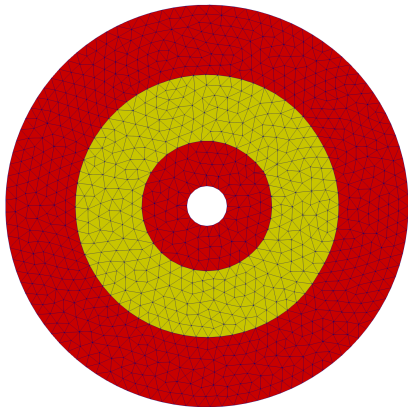


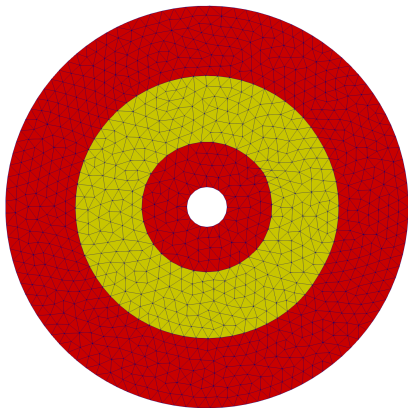




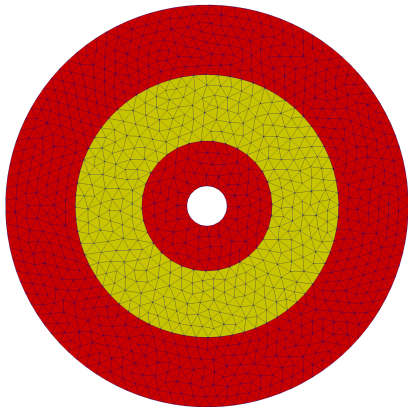






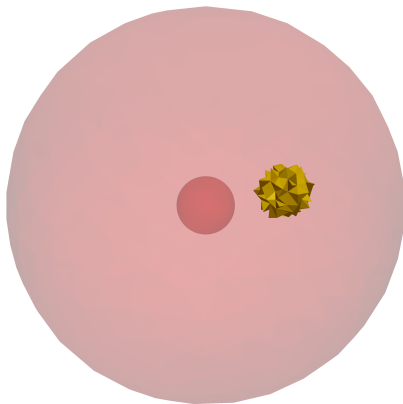




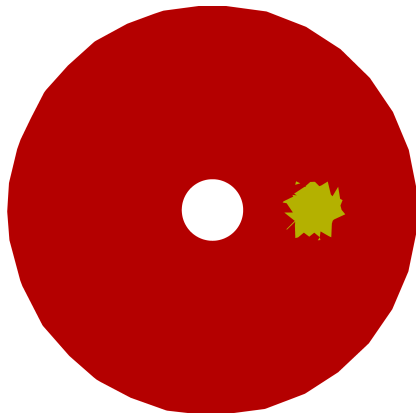




(a) 3D representation of material  $\beta$   
(yellow)

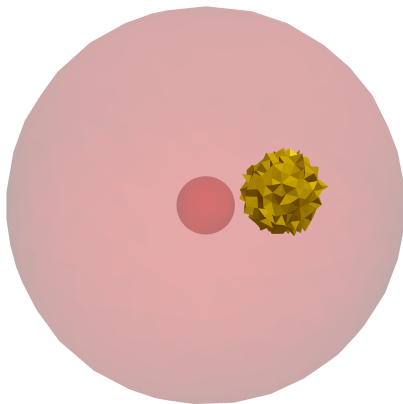


(b) slice of volume representation  
at  $z = 0$

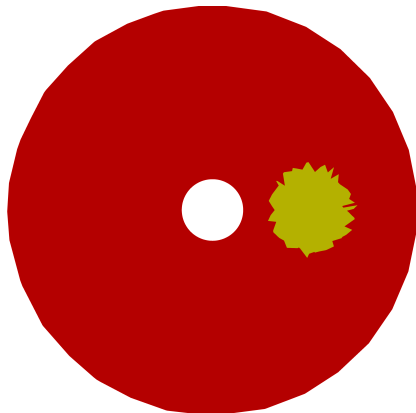




(a) 3D representation of material  $\beta$   
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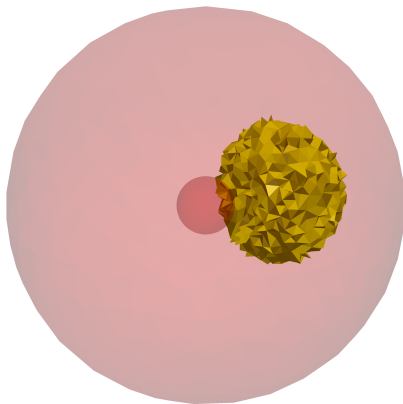


(b) slice of volume representation  
at  $z = 0$

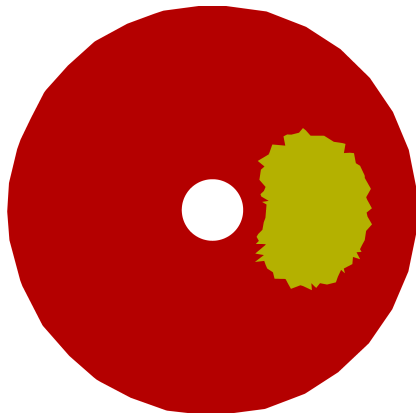




(a) 3D representation of material  $\beta$   
(yellow)

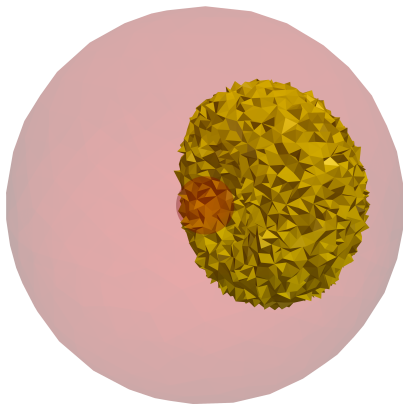


(b) slice of volume representation  
at  $z = 0$





(a) 3D representation of material  $\beta$   
(yellow)

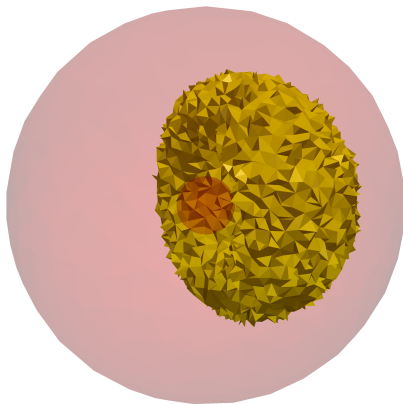


(b) slice of volume representation  
at  $z = 0$





(a) 3D representation of material  $\beta$   
(yellow)

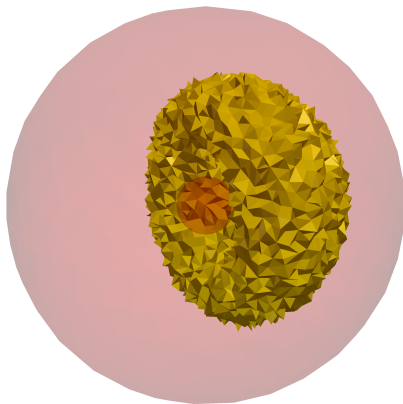


(b) slice of volume representation  
at  $z = 0$

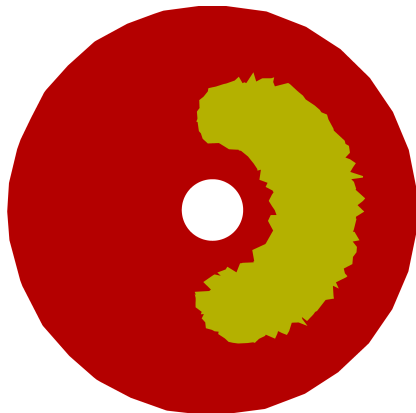




(a) 3D representation of material  $\beta$   
(yellow)

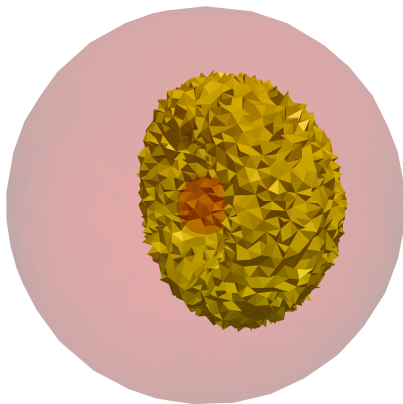


(b) slice of volume representation  
at  $z = 0$





(a) 3D representation of material  $\beta$   
(yellow)



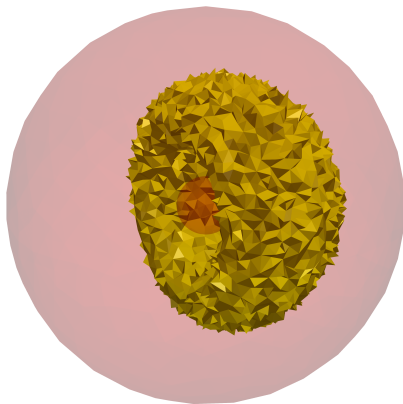
(b) slice of volume representation  
at  $z = 0$







(a) 3D representation of material  $\beta$   
(yellow)

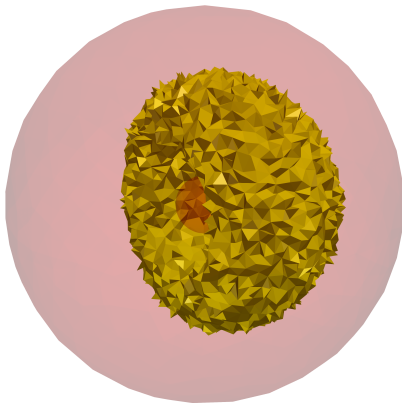


(b) slice of volume representation  
at  $z = 0$





(a) 3D representation of material  $\beta$   
(yellow)

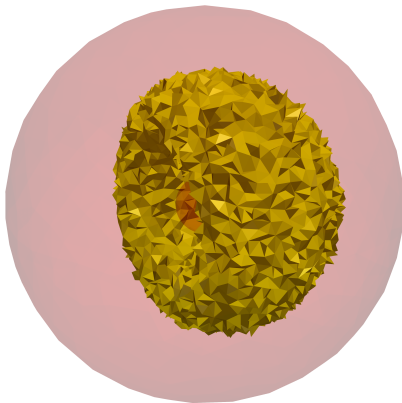


(b) slice of volume representation  
at  $z = 0$





(a) 3D representation of material  $\beta$   
(yellow)

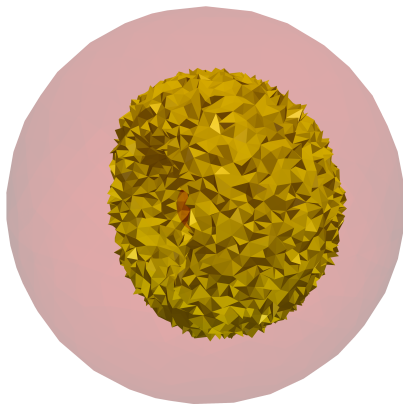


(b) slice of volume representation  
at  $z = 0$





(a) 3D representation of material  $\beta$   
(yellow)

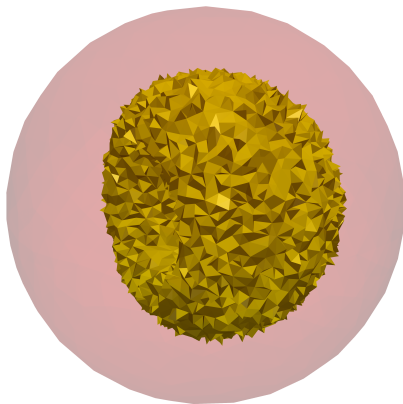


(b) slice of volume representation  
at  $z = 0$





(a) 3D representation of material  $\beta$   
(yellow)

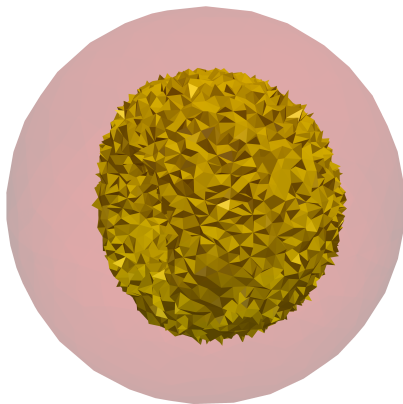


(b) slice of volume representation  
at  $z = 0$





(a) 3D representation of material  $\beta$   
(yellow)

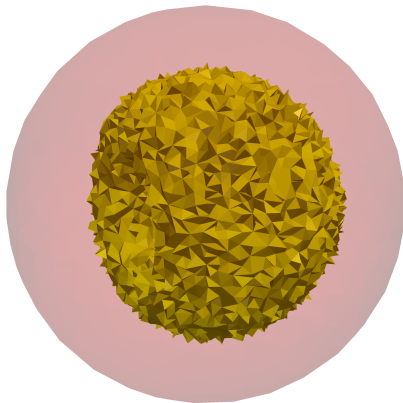


(b) slice of volume representation  
at  $z = 0$





(a) 3D representation of material  $\beta$   
(yellow)

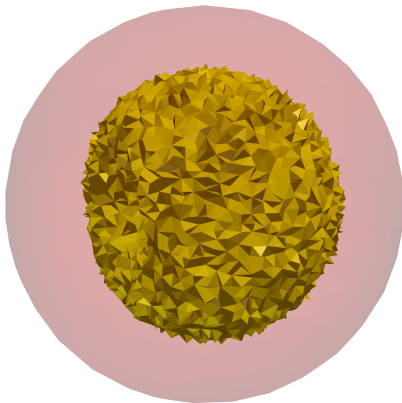


(b) slice of volume representation  
at  $z = 0$





(a) 3D representation of material  $\beta$   
(yellow)



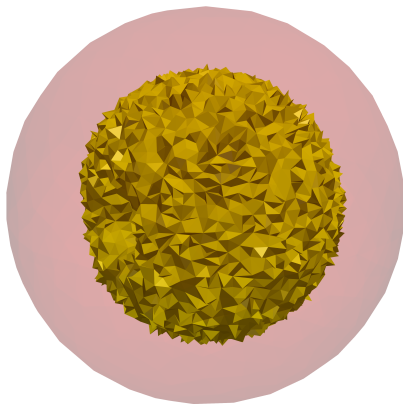
(b) slice of volume representation  
at  $z = 0$







(a) 3D representation of material  $\beta$   
(yellow)

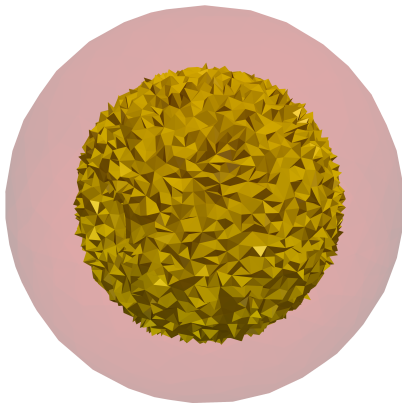


(b) slice of volume representation  
at  $z = 0$





(a) 3D representation of material  $\beta$   
(yellow)

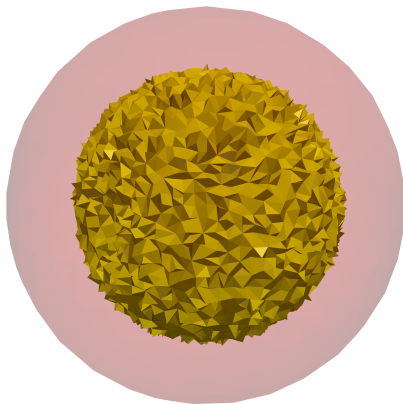


(b) slice of volume representation  
at  $z = 0$





(a) 3D representation of material  $\beta$   
(yellow)

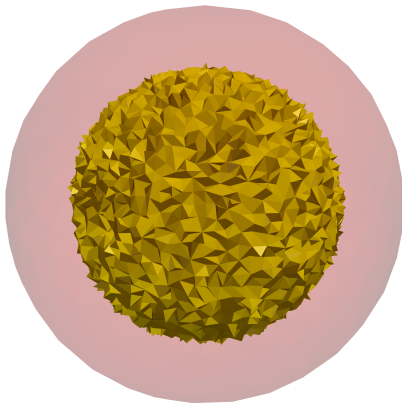


(b) slice of volume representation  
at  $z = 0$





(a) 3D representation of material  $\beta$   
(yellow)

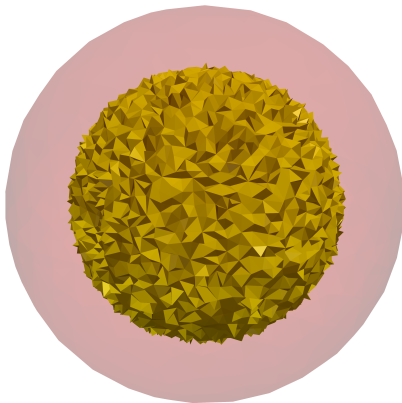


(b) slice of volume representation  
at  $z = 0$

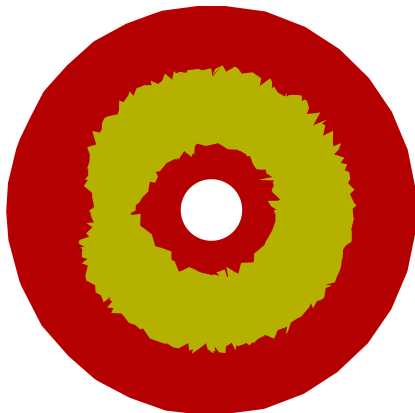




(a) 3D representation of material  $\beta$   
(yellow)

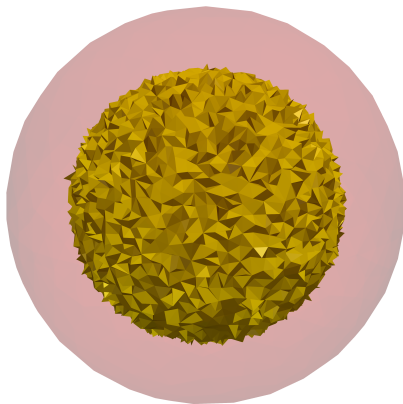


(b) slice of volume representation  
at  $z = 0$

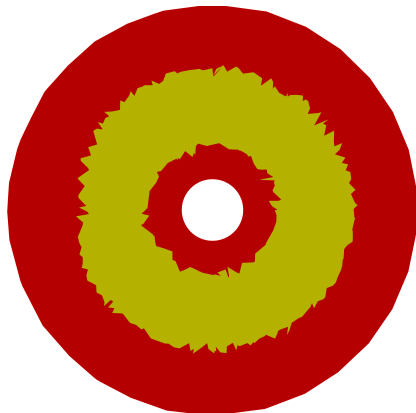




(a) 3D representation of material  $\beta$   
(yellow)

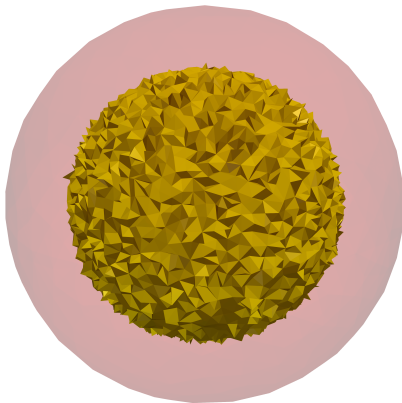


(b) slice of volume representation  
at  $z = 0$

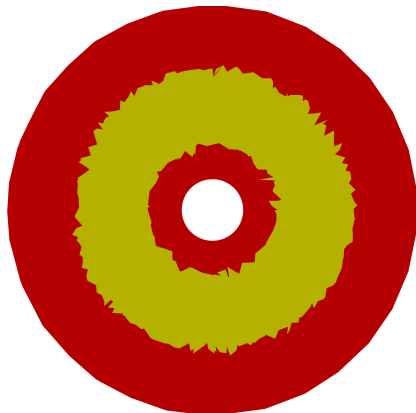




(a) 3D representation of material  $\beta$   
(yellow)

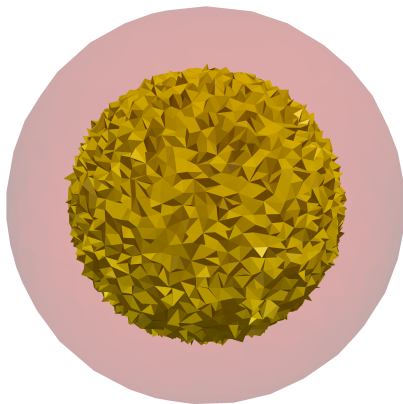


(b) slice of volume representation  
at  $z = 0$

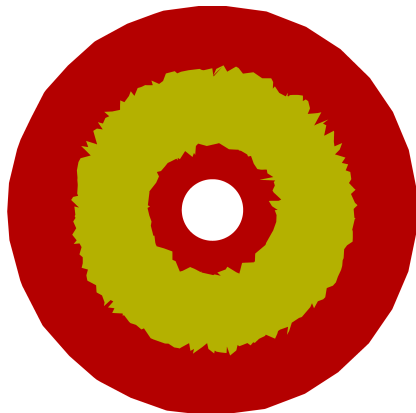




(a) 3D representation of material  $\beta$   
(yellow)



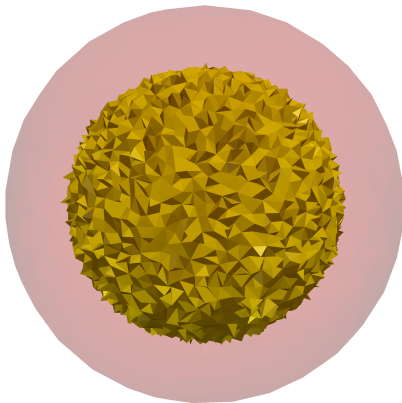
(b) slice of volume representation  
at  $z = 0$



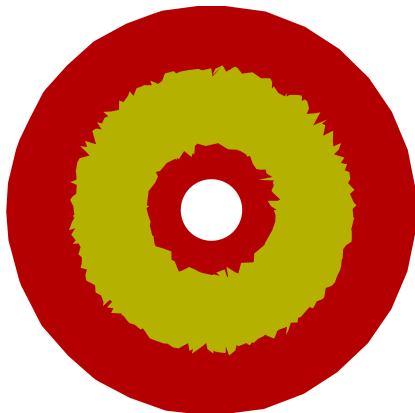




(a) 3D representation of material  $\beta$   
(yellow)

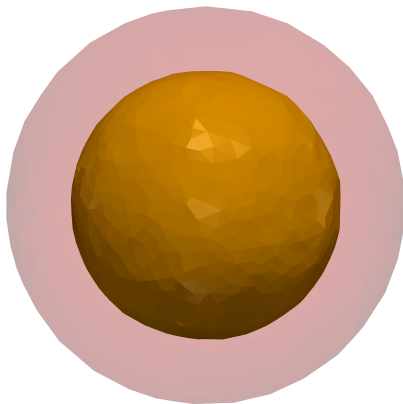


(b) slice of volume representation  
at  $z = 0$

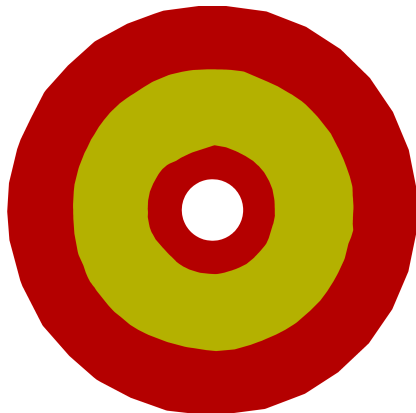




(a) 3D representation of material  $\beta$   
(yellow)

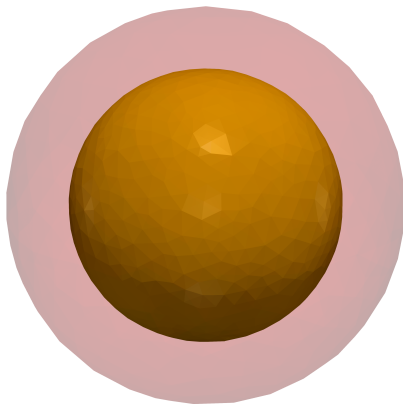


(b) slice of volume representation  
at  $z = 0$

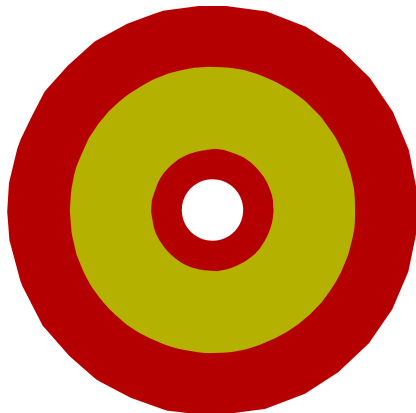




(a) 3D representation of material  $\beta$   
(yellow)

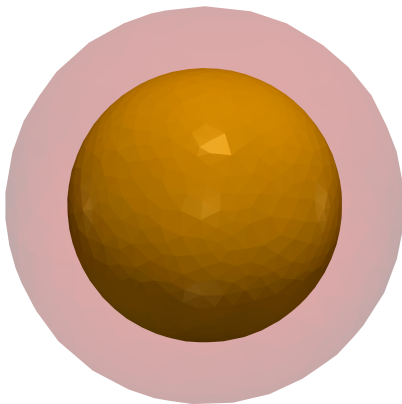


(b) slice of volume representation  
at  $z = 0$

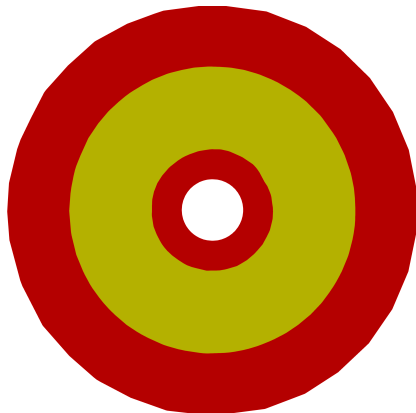




(a) 3D representation of material  $\beta$   
(yellow)

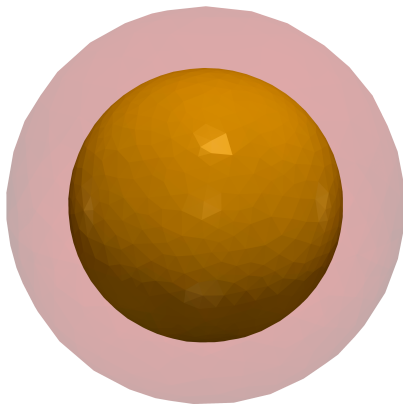


(b) slice of volume representation  
at  $z = 0$

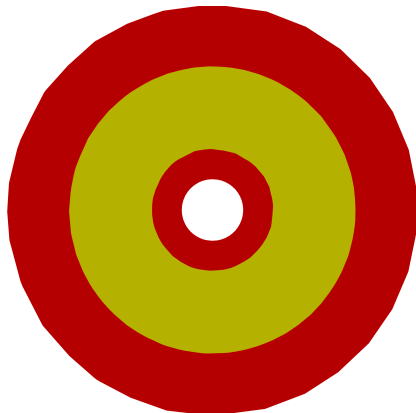




(a) 3D representation of material  $\beta$   
(yellow)



(b) slice of volume representation  
at  $z = 0$



# Part III: Second order shape derivative

Work in progress

We are interested in the second order expansions of  $J$ :

$$J((\text{Id} + \psi)\Omega) = J(\Omega) + J'(\Omega; \psi) + \frac{1}{2}J''(\Omega; \psi, \psi) + o(\|\psi\|_k^2)$$

**Important:** This is not a variations of first order shape derivative

$$J''(\Omega; \psi_1, \psi_2) \neq (J'(\Omega; \psi_1))'(\Omega; \psi_2) = \lim_{t \rightarrow 0} \frac{1}{t} (J'(\text{Id} + t\psi_2)\Omega; \psi_1) - J'(\Omega; \psi_1).$$

but the following identity holds

$$J''(\Omega; \psi_1, \psi_2) = (J'(\Omega; \psi_1))'(\Omega; \psi_2) - J'(\Omega; \nabla\psi_1\psi_2).$$

By standard method of using local derivative  $u'(\psi)$ :

$$\begin{aligned}
J''(\Omega; \psi_1, \psi_2) = & \\
& \alpha \int_{\Gamma} (\psi_1 \cdot \mathbf{n}_\alpha)(\psi_2 \cdot \mathbf{n}_\alpha) \left\{ \mathbf{H} \left[ 2 \left| \frac{\partial u_\alpha}{\partial \mathbf{n}_\alpha} \right|^2 - |\nabla u_\alpha|^2 \right] + \frac{\partial}{\partial \mathbf{n}_\alpha} \left[ 2 \left| \frac{\partial u_\alpha}{\partial \mathbf{n}_\alpha} \right|^2 - |\nabla u_\alpha|^2 \right] \right\} dS \\
& - \beta \int_{\Gamma} (\psi_1 \cdot \mathbf{n}_\alpha)(\psi_2 \cdot \mathbf{n}_\alpha) \left\{ \mathbf{H} \left[ 2 \left| \frac{\partial u_\beta}{\partial \mathbf{n}_\alpha} \right|^2 - |\nabla u_\beta|^2 \right] + \frac{\partial}{\partial \mathbf{n}_\alpha} \left[ 2 \left| \frac{\partial u_\beta}{\partial \mathbf{n}_\alpha} \right|^2 - |\nabla u_\beta|^2 \right] \right\} dS \\
& - \frac{2(\beta + \alpha)\alpha}{\beta - \alpha} \int_{\Omega_\alpha} \nabla u'_\alpha(\psi_1) \cdot \nabla u'_\alpha(\psi_2) dx + \frac{2(\beta + \alpha)\beta}{\beta - \alpha} \int_{\Omega_\beta} \nabla u'_\beta(\psi_1) \cdot \nabla u'_\beta(\psi_2) dx \\
& + \frac{2\alpha\beta}{\beta - \alpha} \int_{\Gamma} u'_\beta(\psi_1) \frac{\partial u'_\alpha(\psi_2)}{\partial \mathbf{n}_\alpha} + u'_\alpha(\psi_2) \frac{\partial u'_\beta(\psi_1)}{\partial \mathbf{n}_\alpha} + u'_\alpha(\psi_1) \frac{\partial u'_\beta(\psi_2)}{\partial \mathbf{n}_\alpha} + u'_\beta(\psi_2) \frac{\partial u'_\alpha(\psi_1)}{\partial \mathbf{n}_\alpha} dS \\
& + \alpha \int_{\Gamma} Z(\psi_1, \psi_2) \left[ 2 \left| \frac{\partial u_\alpha}{\partial \mathbf{n}_\alpha} \right|^2 - |\nabla u_\alpha|^2 \right] dS - \beta \int_{\Gamma} Z(\psi_1, \psi_2) \left[ 2 \left| \frac{\partial u_\beta}{\partial \mathbf{n}_\alpha} \right|^2 - |\nabla u_\beta|^2 \right] dS
\end{aligned}$$



where

$$Z(\psi_1, \psi_2) = \nabla \mathbf{n}_\alpha^T (\psi_1)_\Gamma \cdot (\psi_2)_\Gamma - \nabla_\Gamma (\psi_1 \cdot \mathbf{n}_\alpha) \cdot (\psi_2)_\Gamma - \nabla_\Gamma (\psi_2 \cdot \mathbf{n}_\alpha) \cdot (\psi_1)_\Gamma$$

and  $u$  is a solution of (S). Local derivative  $u'(\psi) \in H^1(\Omega_\alpha \cup \Omega_\beta)$  is a solution of the following transmission problem with discontinuous jumps on the interface:

$$(5) \quad \left\{ \begin{array}{ll} \Delta u'(\psi) = 0 & \text{in } \Omega_\alpha \cup \Omega_\beta, \\ u'_\alpha(\psi) - u'_\beta(\psi) = \frac{\alpha - \beta}{\beta} (\nabla u_\alpha \cdot \mathbf{n}_\alpha)(\psi \cdot \mathbf{n}_\alpha) & \text{on } \Gamma, \\ \alpha \nabla u'_\alpha(\psi) \cdot \mathbf{n}_\alpha - \beta \nabla u'_\beta(\psi) \cdot \mathbf{n}_\alpha = (\alpha - \beta) \operatorname{div}_\Gamma (\nabla_\Gamma u(\psi \cdot \mathbf{n}_\alpha)) & \text{on } \Gamma, \\ u'(\psi) = 0 & \text{on } \partial\Omega. \end{array} \right.$$

Volume representation:








(6)

$$\begin{aligned}
 J''(\Omega; \psi_1, \psi_2) &= \int_{\Omega} \mathbf{a} \left[ -\operatorname{div} \psi_1 \operatorname{div} \psi_2 \mathbf{I} + \nabla \psi_1 : \nabla \psi_2^T \mathbf{I} - \nabla \psi_1 \nabla \psi_2^T - \nabla \psi_2 \nabla \psi_1^T \right] \nabla u \cdot \nabla u \, dx \\
 &+ \int_{\Omega} \mathbf{a} \left[ -\nabla \psi_1 \nabla \psi_2 - \nabla \psi_2 \nabla \psi_1 - \nabla \psi_1^T \nabla \psi_2^T - \nabla \psi_2^T \nabla \psi_1^T \right] \nabla u \cdot \nabla u \, dx \\
 &+ \int_{\Omega} \mathbf{a} \left[ \operatorname{div} \psi_1 (\nabla \psi_2 + \nabla \psi_2^T) + \operatorname{div} \psi_2 (\nabla \psi_1 + \nabla \psi_1^T) \right] \nabla u \cdot \nabla u \, dx \\
 &+ 2 \int_{\Omega} [f \operatorname{div} \psi_1 \operatorname{div} \psi_2 + \psi_1 \cdot \nabla f \operatorname{div} \psi_2 + \psi_2 \cdot \nabla f \operatorname{div} \psi_1 + H f \psi_2 \cdot \psi_1] u \, dx \\
 &- 2 \int_{\Omega} \nabla \psi_1 : \nabla \psi_2^T f u \, dx + \frac{1}{2} \int_{\Omega} \mathbf{a} \nabla v(\psi_1) \cdot \nabla v(\psi_2) \, dx
 \end{aligned}$$

where  $u$  is a solution of (S) and  $v(\psi) \in H_0^1(\Omega)$  satisfies following equality for any  $\varphi \in H_0^1(\Omega)$ :

$$(7) \quad \int_{\Omega} \mathbf{a} \nabla v(\psi) \cdot \nabla \varphi \, dx = 2 \int_{\Omega} \operatorname{div}(f\psi) \varphi \, dx + 2 \int_{\Omega} \mathbf{a} \left[ -\operatorname{div}(\psi) \mathbf{I} + \nabla \psi + \nabla \psi^T \right] \nabla u \cdot \nabla \varphi \, dx.$$

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