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Boundary Element Methods for Shape Optimisation in Homogenisation

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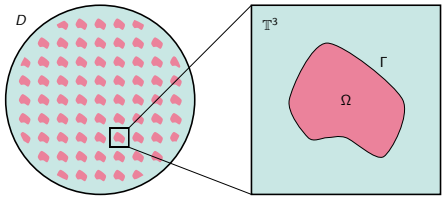
Motivation

- Shape Optimisation has many applications in the industry.
- A bone implant should have the same material properties as a real bone.
- We can think of a bone as a periodic scaffold structure.
- How shall we choose the shapes of the holes?



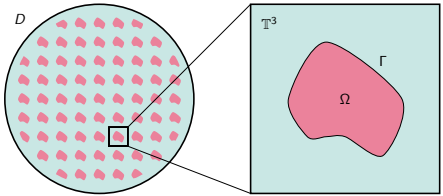
Outline

1. Motivation
2. Homogenisation
3. Shape Optimisation
4. Boundary Elements
5. Implementation
6. Numerical Examples

Homogenisation

- Define $\mathbb{T}^3 = \mathbb{R}^3 / \left[-\frac{1}{2}, \frac{1}{2}\right]^3$.
- Let $\mathbf{A} : \mathbb{T}^3 \to \mathbb{R}^{3\times 3}$, $\varepsilon > 0$ and $\mathbf{A}^\varepsilon(\boldsymbol{x}) = \mathbf{A}\left(\frac{\boldsymbol{x}}{\varepsilon}\right)$.
- For a domain $D \subseteq \mathbb{R}^3$, we are interested in the solution u^ε of the partial differential equation

$$\begin{cases} -\operatorname{div}\left(\mathbf{A}^\varepsilon \nabla u^\varepsilon\right) = f & \text{in } D, \\ u^\varepsilon = 0 & \text{on } \partial D. \end{cases}$$

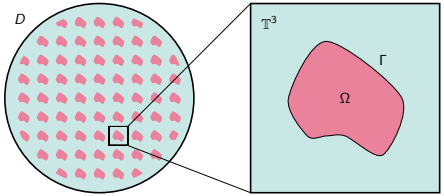


Homogenisation

- Homogenisation treats the behaviour of u^ε in the limit case $\varepsilon \to 0$.
- There exists a homogenised problem

$$\begin{cases} -\operatorname{div}\left(\mathbf{A}_0 \nabla u_0\right) = f & \text{in } D, \\ u_0 = 0 & \text{on } \partial D. \end{cases}$$

with a homogenised solution u_0 such that $u^\varepsilon \rightharpoonup u_0$ weakly in $H^1(D)$.



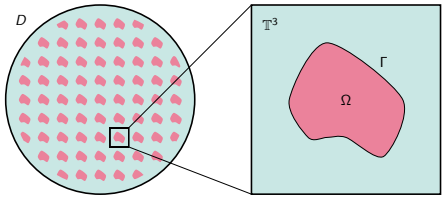
Homogenisation

The effective material tensor $\mathbf{A}_0 = \left[a_{i,j}\right]_{i,j=1}^{3}$, is given by the entries

$$a_{i,j} = \int_{\mathbb{T}^3} \left\langle \mathbf{A}(\boldsymbol{e}_i + \nabla w_i),\ \boldsymbol{e}_j + \nabla w_j \right\rangle \mathrm{d}V,$$

where for $i = 1, 2, 3$, w_i is the solution of the cell problem

find $w_i \in H^1_{per}(\mathbb{T}^3)$ s.t. $\operatorname{div}\left(\mathbf{A}(\boldsymbol{e}_i + \nabla w_i)\right) = 0.$



Homogenisation

- For a scaffold structure, we define $\mathbf{A} = \mathbb{1}_{\mathbb{T}^3 \setminus \overline{\Omega}} \mathbf{I}$.
- Then, the cell problem is equivalent to the exterior Neumann problem

$$\begin{cases} \Delta w_i = 0 & \text{in } \mathbb{T}^3 \setminus \overline{\Omega}, \\ \partial_{\boldsymbol{n}} w_i = -n_i & \text{on } \Gamma = \partial\Omega. \end{cases}$$

- The compatibility condition is satisfied, as

$$\int_\Gamma -n_i \, \mathrm{d}A = -\int_\Gamma \langle \boldsymbol{e}_i, \boldsymbol{n} \rangle \, \mathrm{d}A = -\int_\Omega \operatorname{div}(\boldsymbol{e}_i) \, \mathrm{d}V = 0.$$

- The effective material tensor only depends on the size and the shape of Ω.

Shape Optimisation

For a desired material tensor $\mathbf{B}$, we define the shape functional

$$J(\Omega) = \frac{1}{2}\left\|\mathbf{A}_0(\Omega) - \mathbf{B}\right\|_F^2 = \frac{1}{2}\sum_{i,j=1}^{3}\left(a_{i,j}(\Omega) - b_{i,j}\right)^2.$$

Goal: Optimise the shape of Ω such that $J(\Omega)$ is minimal.

It is crucial to know the behaviour of $J(\Omega)$ when Ω is slightly deformed.

Shape Optimisation

- Let $\tilde{\boldsymbol{f}} : \left[-\frac{1}{2}, \frac{1}{2}\right]^3 \to \left[-\frac{1}{2}, \frac{1}{2}\right]^3$ be a sufficiently smooth vector field with compact support, and $\boldsymbol{f} : \mathbb{T}^3 \to \mathbb{T}^3$ be the periodic continuation of $\tilde{\boldsymbol{f}}$.
- We define the perturbation of the identity as

$$T_{t,\boldsymbol{f}}(\boldsymbol{x}) = \boldsymbol{x} + t\boldsymbol{f}(\boldsymbol{x}).$$

  For $t > 0$ small enough, $T_{t,\boldsymbol{f}}$ is a diffeomorphism that preserves each cell.
- We define the shape derivative of $a_{i,j}$ in the direction of $\boldsymbol{f}$ as

$$a'_{i,j}[\boldsymbol{f}](\Omega) = \left[\frac{\mathrm{d}}{\mathrm{d}t} a_{i,j}\big(T_{t,\boldsymbol{f}}(\Omega)\big)\right]_{t=0} = \lim_{t\to 0} \frac{a_{i,j}\big(T_{t,\boldsymbol{f}}(\Omega)\big) - a_{i,j}(\Omega)}{t}.$$

- Consequently,

$$J'[\boldsymbol{f}](\Omega) = \sum_{i,j=1}^{3} a'_{i,j}[\boldsymbol{f}](\Omega)\big(a_{i,j}(\Omega) - b_{i,j}\big).$$

Shape Optimisation

Remember the solutions of the cell problems w_i. By defining $\phi_i = x_i + w_i$, it holds:

Theorem (Dambrine and Harbrecht, 2020)

The coefficient $a_{i,j}(\Omega)$ and its shape derivative are given by

$$a_{i,j}(\Omega) = \int_{\mathbb{T}^3 \setminus \overline{\Omega}} \left\langle \nabla \phi_i,\ \nabla \phi_j \right\rangle \, \mathrm{d}V,$$

$$a'_{i,j}[\boldsymbol{f}](\Omega) = -\int_{\Gamma} \left\langle \nabla_\Gamma \phi_i,\ \nabla_\Gamma \phi_j \right\rangle \langle \boldsymbol{f}, \boldsymbol{n} \rangle \, \mathrm{d}A,$$

where ∇_Γ is the tangential gradient.

Boundary Elements

Remember that we have to solve the exterior Neumann problems

$$\begin{cases} \Delta w_i = 0 & \text{in } \mathbb{T}^3 \setminus \overline{\Omega}, \\ \partial_{\boldsymbol{n}} w_i = -n_i & \text{on } \Gamma = \partial\Omega. \end{cases}$$

- In every iteration step, the shape of the domain Ω changes.
- The values of w_i will be needed on the boundary $\Gamma = \partial\Omega$ only.
- The resulting shape might not be convex.

Solution: Use Boundary Elements.

Boundary Elements: Theoretical Background

Definition

Let $d \in \mathbb{N}$, $\Omega \subseteq \mathbb{R}^d$, and let $\mathcal{L}$ be an elliptic, second order differential operator. The **fundamental solution** or **Green's function** is a function that satisfies the distributional equation

$$\mathcal{L}_{\boldsymbol{y}} G(\boldsymbol{x}, \boldsymbol{y}) = \delta_{\mathbf{0}}(\boldsymbol{x} - \boldsymbol{y}).$$

Examples:

$$\mathcal{L} = -\Delta, \qquad G(\boldsymbol{x}, \boldsymbol{y}) = \begin{cases} -\frac{1}{2\pi} \log\left(\|\boldsymbol{x} - \boldsymbol{y}\|\right), & d = 2, \\ \frac{1}{4\pi\|\boldsymbol{x}-\boldsymbol{y}\|}, & d = 3. \end{cases}$$

$$\mathcal{L} = -\Delta - \kappa^2 \mathcal{I}, \qquad G(\boldsymbol{x}, \boldsymbol{y}) = \begin{cases} \frac{i}{4} H_0^{(1)}\left(\kappa\|\boldsymbol{x} - \boldsymbol{y}\|\right), & d = 2, \\ \frac{\exp\left(i\kappa\|\boldsymbol{x}-\boldsymbol{y}\|\right)}{4\pi\|\boldsymbol{x}-\boldsymbol{y}\|}, & d = 3. \end{cases}$$

Boundary Elements: Theoretical Background

Let $\Omega \subseteq \mathbb{R}^3$ with a Lipschitz boundary $\Gamma = \partial\Omega$. Consider the interior Laplace problem with Dirichlet boundary conditions

$$\begin{cases} \Delta u = 0 & \text{in } \Omega, \\ u = g & \text{on } \Gamma. \end{cases}$$

Green's representation formula gives us

$$\begin{aligned} u(\boldsymbol{x}) &= -\int_\Omega \big(\Delta_{\boldsymbol{y}} G\big)(\boldsymbol{x},\boldsymbol{y}) u(\boldsymbol{y}) \,\mathrm{d}V_{\boldsymbol{y}} \\ &= \int_\Gamma G(\boldsymbol{x},\boldsymbol{y}) \big(\partial_{\boldsymbol{n}} u\big)(\boldsymbol{y}) \,\mathrm{d}A_{\boldsymbol{y}} - \int_\Gamma \big(\partial_{\boldsymbol{n}_{\boldsymbol{y}}} G\big)(\boldsymbol{x},\boldsymbol{y}) u(\boldsymbol{y}) \,\mathrm{d}A_{\boldsymbol{y}}, \qquad \boldsymbol{x} \in \Omega. \end{aligned}$$

Boundary Elements: Theoretical Background

Using the trace properties, one obtains

$$\mathcal{V}\partial_{\boldsymbol{n}} u = \left(\mathcal{K} + \frac{1}{2}\mathcal{I}\right) u|_{\Gamma},$$

with

$$\mathcal{V}\varrho(\boldsymbol{x}) = \int_{\Gamma} G(\boldsymbol{x},\boldsymbol{y})\varrho(\boldsymbol{y})\ \mathrm{d}A_{\boldsymbol{y}}, \qquad \mathcal{K}\varrho(\boldsymbol{x}) = \int_{\Gamma} \partial_{\boldsymbol{n}_{\boldsymbol{y}}} G(\boldsymbol{x},\boldsymbol{y})\varrho(\boldsymbol{y})\ \mathrm{d}A_{\boldsymbol{y}}.$$

Having $\partial_{\boldsymbol{n}} u$, one can calculate $u(\boldsymbol{x})$ for every $\boldsymbol{x} \in \Omega$ according to Green's representation formula.

Boundary Elements: Theoretical Background

- On a Lipschitz domain in three dimensions, the operator $\mathcal{V} : H^{-1/2+s}(\Gamma) \to H^{1/2+s}(\Gamma)$ is continuous for $|s| \leq \frac{1}{2}$, and invertible for $s = 0$.
- On a Lipschitz domain in three dimensions, the operator $\mathcal{K} : H^{1/2+s}(\Gamma) \to H^{1/2+s}(\Gamma)$ is continuous for $|s| \leq \frac{1}{2}$, but $\ker\left(\mathcal{K} + \frac{1}{2}\mathcal{I}\right) = \operatorname{span}\{\mathbb{1}\}$.
- In a periodic setting, the fundamental solution satisfies $-\Delta_{\boldsymbol{y}} G(\boldsymbol{x}, \boldsymbol{y}) = \delta_{\boldsymbol{0}}(\boldsymbol{x} - \boldsymbol{y}) - 1$.
- In a periodic setting, the fundamental solution cannot be represented explicitly, but as the series

$$G(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{4\pi\|\boldsymbol{x} - \boldsymbol{y}\|} + \frac{\|\boldsymbol{x} - \boldsymbol{y}\|^2}{6} + \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \alpha_n^m \phi_n^m(\boldsymbol{x} - \boldsymbol{y}).$$

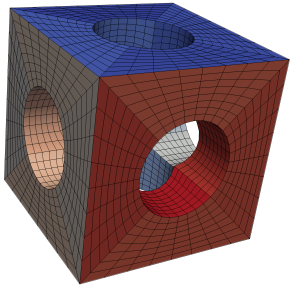
Here, $\alpha_n^m \in \mathbb{C}$ are scalar coefficients and ϕ_n^m denote the solid spherical harmonics.

Boundary Elements: Discretisation

Definition

For an admissible decomposition $\mathcal{T} = \{T_1, ..., T_N\}$ of Γ, with nodes $\{\boldsymbol{x}_1, ..., \boldsymbol{x}_M\}$, we define the **ansatz space** $\boldsymbol{S_h^1(\Gamma)} = \text{span}\{\psi_1, ..., \psi_M\}$, where

$$\psi_i(\boldsymbol{x}) = \begin{cases} 1, & \boldsymbol{x} = \boldsymbol{x}_i, \\ 0, & \boldsymbol{x} = \boldsymbol{x}_j,\ i \neq j, \\ \text{transformed bilinear}, & \text{else.} \end{cases}$$



Boundary Elements: Discretisation

Remember that we want to solve

$$\mathcal{V}t = \left(\mathcal{K} + \frac{1}{2}\mathcal{I}\right) g,$$

where $t = \partial_{\boldsymbol{n}} u$ and $g = u\big|_{\Gamma}$ are the given Dirichlet data.

Boundary Elements: Discretisation

Remember that we want to solve

$$\mathcal{V}t = \left(\mathcal{K} + \frac{1}{2}\mathcal{I}\right) g,$$

where $t = \partial_{\boldsymbol{n}} u$ and $g = u\big|_\Gamma$ are the given Dirichlet data.

We can pose the variational problem

find $t \in L^2(\Gamma)$, such that

$$\langle \mathcal{V}t,\ \psi\rangle_\Gamma = \left\langle \left(\mathcal{K} + \frac{1}{2}\mathcal{I}\right) g,\ \psi \right\rangle_\Gamma \qquad \text{for any } \psi \in L^2(\Gamma).$$

Boundary Elements: Discretisation

Remember that we want to solve

$$\mathcal{V}t = \left(\mathcal{K} + \frac{1}{2}\mathcal{I}\right) g,$$

where $t = \partial_{\boldsymbol{n}} u$ and $g = u\big|_{\Gamma}$ are the given Dirichlet data.

If $Q_h : L^2(\Gamma) \to S_h^1(\Gamma)$ denotes the $L^2(\Gamma)$-orthogonal projection, we solve the Galerkin problem

$$\text{find } t_h \in S_h^1(\Gamma), \text{ such that}$$
$$\langle \mathcal{V} t_h,\ \psi_i \rangle_{\Gamma} = \left\langle \left(\mathcal{K} + \frac{1}{2}\mathcal{I}\right) Q_h g,\ \psi_i \right\rangle_{\Gamma}, \qquad i = 1, ..., M.$$

Boundary Elements: Discretisation

Let us define

$$\mathbf{K}_h = \left[\left\langle \mathcal{K}\psi_j, \psi_i \right\rangle_\Gamma\right]_{i,j=1}^{M}, \qquad \mathbf{V}_h = \left[\left\langle \mathcal{V}\psi_j, \psi_i \right\rangle_\Gamma\right]_{i,j=1}^{M},$$
$$\mathbf{M}_h = \left[\left\langle \psi_j, \psi_i \right\rangle_\Gamma\right]_{i,j=1}^{M}, \qquad \boldsymbol{g}_h = \left[\left\langle g, \psi_i \right\rangle_\Gamma\right]_{i=1}^{M}.$$

Then, the Galerkin variational formulation is equivalent to

$$\mathbf{V}_h \boldsymbol{t}_h = \left(\mathbf{K}_h + \frac{1}{2}\mathbf{M}_h\right)\mathbf{M}_h^{-1}\boldsymbol{g}_h.$$

Boundary Elements: Neumann Problem

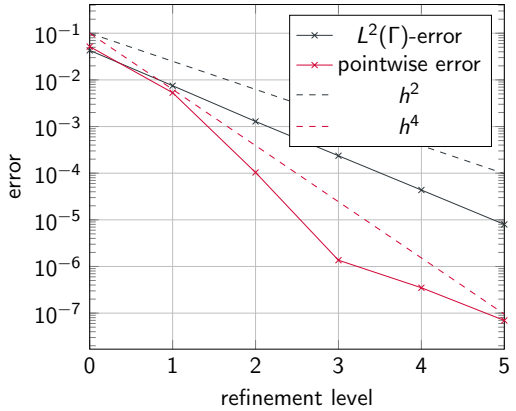
- For an exterior Neumann problem, the resulting equation is $\left(\mathcal{K} - \frac{1}{2}\mathcal{I}\right) u\big|_\Gamma = \mathcal{V}\partial_{\boldsymbol{n}} u$.
- The operator $\left(\mathcal{K} - \frac{1}{2}\mathcal{I}\right) : H^s(\Gamma) \to H^s(\Gamma)$ is continuously invertible for $s = 0, 1/2$.
- To make the solution of an interior Neumann problem unique, one can factor out the constant, i.e., set

$$\tilde{t}_h = t_h - \frac{\langle t_h,\ \mathbb{1}\rangle_\Gamma}{\|\mathbb{1}\|^2_{L^2(\Gamma)}}\mathbb{1}, \qquad \tilde{\boldsymbol{t}}_h = \boldsymbol{t}_h - \frac{\boldsymbol{t}_h^T \mathbf{M}_h \mathbf{1}_h}{\mathbf{1}_h^T \mathbf{M}_h \mathbf{1}_h}\mathbf{1}_h.$$

Boundary Elements: Convergence

Using the described procedure, one can show that

$$\left\|u - u_h\right\|_{L^2(\Gamma)} \leq Ch^2 \|u\|_{H^2(\Gamma)}, \qquad \left|u(\boldsymbol{x}) - u_h(\boldsymbol{x})\right| \leq Ch^4 \|u\|_{H^2(\Gamma)}, \quad \boldsymbol{x} \in \Omega.$$



Boundary Elements: Remarks

- The equation is solved on the boundary only.
- No volume mesh has to be generated, or updated, respectively.
- Singularities arising from the geometry are treated in a natural way.
- One dimension lower, but full matrices instead.
- There exist fast boundary element methods to overcome the full population.

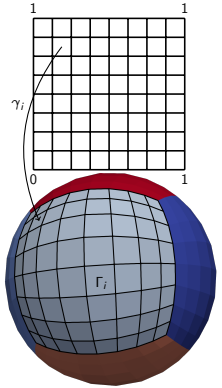
Implementation

We use the **B**oundary **E**lement **M**ethod **B**ased **E**ngineering **L**ibrary **BEMBEL**.

- Written in `C++`, compatible with `Eigen3`.
- Fast multipole method, combined with $\mathcal{H}^2$-matrices.
- Parametric surface representation.

Implementation: Shape Representation

- Decomposition into surface patches Γ_i with parametrisations γ_i.
- On each element, the parametrisation γ_i is approximated by a piecewise polynomial.
- In the case of a quintic polynomial, we achieve an $L^2\big([0,1]^2\big)$-accuracy of $\mathcal{O}(h^6)$.



Implementation: Shape Discretisation

- Take a correlation kernel $C(r)$, for example a Matérn kernel.
- Calculate the eigenfunctions of the corresponding Hilbert-Schmidt operator.
- This gives us a deformation basis, with some spacial relation to the geometry.
  - A Sphere delivers spherical harmonics.
  - Each geometry delivers another basis
- Calculate the deformation functions by a quintic interpolation.

Implementation: Shape Calculus

Lemma (Harbrecht, Multerer, and v. R., 2021)

It holds

$$a_{i,j}(\Omega) = \delta_{i,j}\big(1 - |\Omega|\big) - \int_\Gamma w_j \langle \boldsymbol{e}_i, \boldsymbol{n}\rangle \,\mathrm{d}A,$$

$$a'_{i,j}[\boldsymbol{f}](\Omega) = -\int_\Gamma \Big[\big\langle \boldsymbol{e}_i + \nabla_\Gamma w_i,\ \boldsymbol{e}_j + \nabla_\Gamma w_j\big\rangle - \langle \boldsymbol{e}_i, \boldsymbol{n}\rangle\langle \boldsymbol{n}, \boldsymbol{e}_j\rangle\Big]\langle \boldsymbol{f}, \boldsymbol{n}\rangle \,\mathrm{d}A.$$

- It holds
$$|\Omega| = \int_\Omega \operatorname{div}\left(\frac{\boldsymbol{x}}{3}\right) \,\mathrm{d}V = \frac{1}{3}\int_\Gamma \langle \boldsymbol{x}, \boldsymbol{n}\rangle \,\mathrm{d}A.$$
- For $\boldsymbol{b} \in \operatorname{span}\{\boldsymbol{n}\}^\perp$, and $\boldsymbol{c} \in \mathbb{R}^3$, we have $\langle \boldsymbol{b}, \boldsymbol{c}\rangle = \langle \boldsymbol{n} \times \boldsymbol{b},\ \boldsymbol{n} \times \boldsymbol{c}\rangle$. This allows us to use the surface curl instead of the tangential gradient.

Implementation: Shape Update

- Let us define

$$g(\boldsymbol{y}) = J\big((\mathbf{I} + y_1\boldsymbol{f}_1 + ... + y_N\boldsymbol{f}_N)(\Omega)\big).$$

  We use the direction of the steepest descent

$$\boldsymbol{d} = -\nabla g(\mathbf{0}) = -\big[J'[\boldsymbol{f}_1](\Omega), ..., J'[\boldsymbol{f}_N](\Omega)\big]^T.$$

- If $g(\boldsymbol{d}) < g(\mathbf{0})$, set

$$\Omega_{\text{new}} = \big(\mathbf{I} + d_1\boldsymbol{f}_1 + ... + d_N\boldsymbol{f}_N\big)(\Omega).$$

  If not, decrease the step size.

Implementation: Shape Update

- In practice, we calculate the quadratic polynomial $h(t)$, which interpolates $g(t\boldsymbol{d})$ at the points
$$\big(0,\ g(\mathbf{0})\big), \quad \big(0,\ g'(\mathbf{0})\big), \quad \big(1,\ g(\boldsymbol{d})\big).$$
Afterwards, we use its minimum $t^* \in (0,1)$ as the new step size.
- An evaluation of the shape functional is expensive, so we do not want to apply an Armijo line search.
- The BFGS method was also applied, but did not perform well.

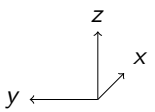
Numerical Examples

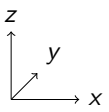
- The initial deformation basis is used throughout the whole process.
- In all of the subsequent examples, the optimisation was stopped if $J(\Omega) < 1\mathrm{e}{-5}$.
- The calculations were carried out on the fourth refinement level, resulting in

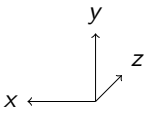
$$N \sim N_p\left(2^4 + 1\right)^2$$

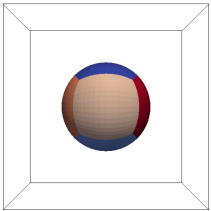
  unknowns.
- If not stated otherwise, $N = 16$ deformation functions were used.

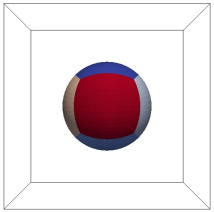
Numerical Examples: Sphere

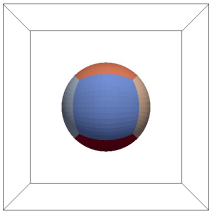






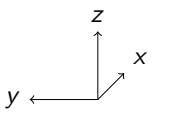


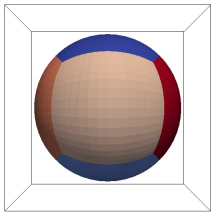


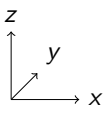


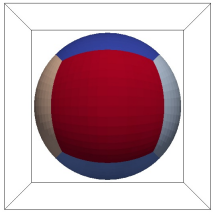
Desired Tensor $\mathbf{B} = 0.9\mathbf{I}$, Initial Guess $\mathcal{B}_{0.3}(0)$, Iterations: 3.

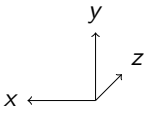
Numerical Examples: Sphere

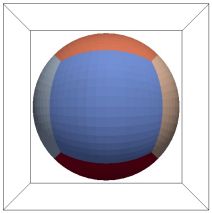






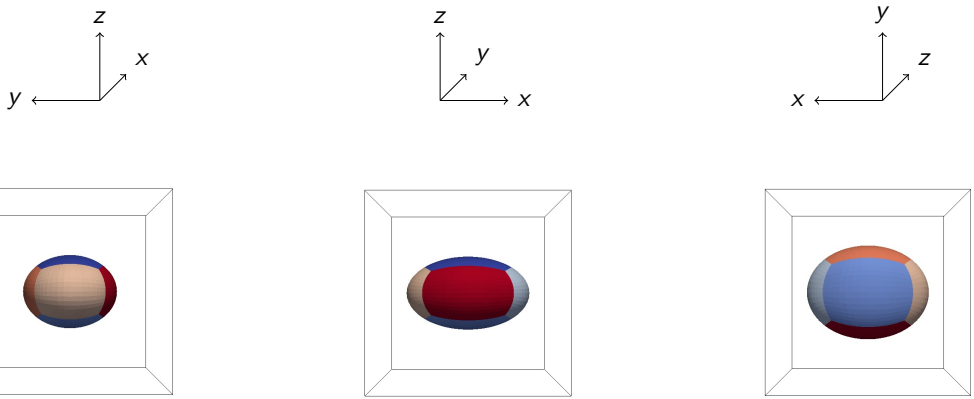






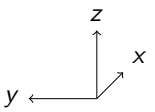
Desired Tensor $\mathbf{B} = 0.6\mathbf{I}$, Initial Guess $\mathcal{B}_{0.3}(0)$, Iterations: 6.

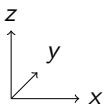
Numerical Examples: Sphere

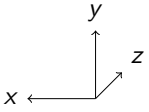


Desired Tensor $\mathbf{B} = \mathrm{diag}(0.9, 0.88, 0.86)$, Initial Guess $\mathcal{B}_{0.3}(0)$, Iterations: 17.

Numerical Examples: Sphere



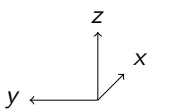


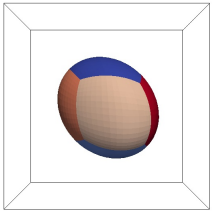


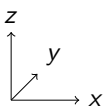
For the next example, we define the transformation matrix $\mathbf{T}$ as

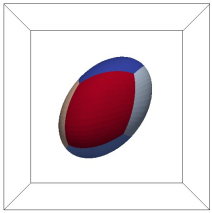
$$\mathbf{T} = \begin{bmatrix} \frac{1}{\sqrt{3}} & 0 & \frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} \end{bmatrix}.$$

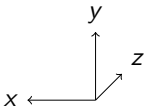
Numerical Examples: Sphere

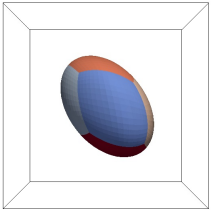






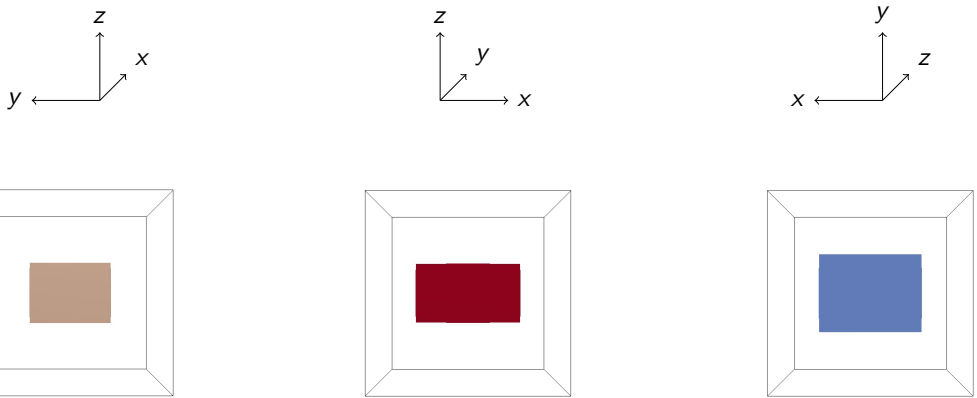






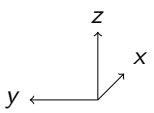
Desired Tensor $\mathbf{B} = \mathbf{T}\text{diag}(0.9, 0.88, 0.86)\mathbf{T}^T$, Initial Guess $\mathcal{B}_{0.3}(0)$, Iterations: 25.

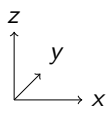
Numerical Examples: Cube

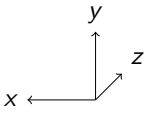


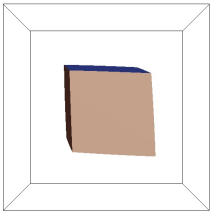
Desired Tensor $\mathbf{B} = \mathrm{diag}(0.9, 0.88, 0.86)$, Initial Guess $[-0.15, 0.15]^3$, Iterations: 13.

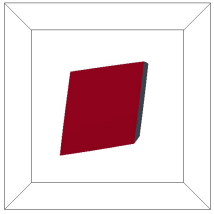
Numerical Examples: Cube

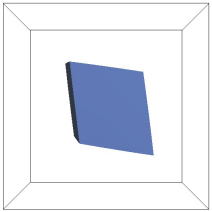






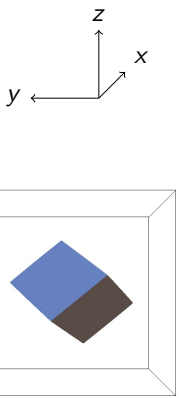


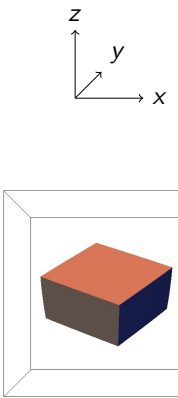


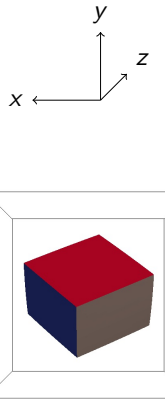


Desired Tensor $\mathbf{B} = \mathbf{T}\text{diag}(0.9, 0.88, 0.86)\mathbf{T}^T$, Initial Guess $[-0.15, 0.15]^3$, Iterations: 14.

Numerical Examples: Cube

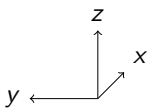


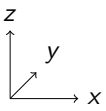


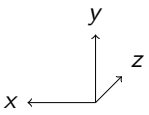


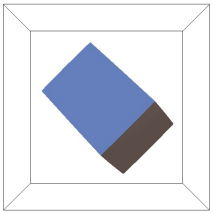
Desired Tensor $\mathbf{B} = \text{diag}(0.9, 0.88, 0.86)$, Initial Guess $\mathbf{T}[-0.15, 0.15]^3$, Iterations: 15.

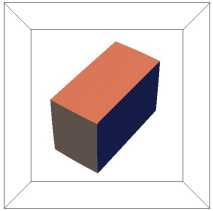
Numerical Examples: Cube

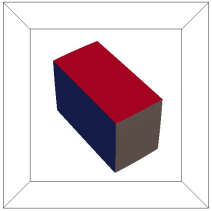












Desired Tensor $\mathbf{B} = \mathbf{T}\text{diag}(0.9, 0.88, 0.86)\mathbf{T}^T$, Initial Guess $\mathbf{T}[-0.15, 0.15]^3$, Iterations: 25.

Numerical Examples: Sphere and Cube

In the following examples, we use the initial guess

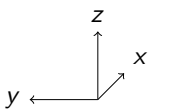
$$\mathcal{B}_{0.15}\left(\begin{bmatrix}-0.25\\-0.25\\-0.25\end{bmatrix}\right) \cup [0.175,\ 0.325]^3.$$

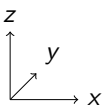
As the desired tensor, we use

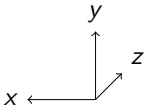
$$\mathbf{B} = \operatorname{diag}(1,\ 0.995,\ 0.99).$$

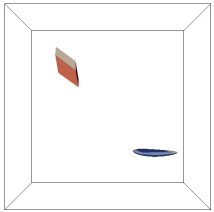
We also use a correlation length ℓ different from 1. If ℓ is small, the correlation is small.

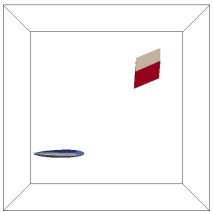
Numerical Examples: Sphere and Cube

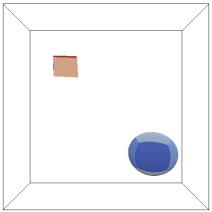






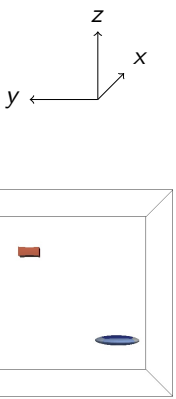


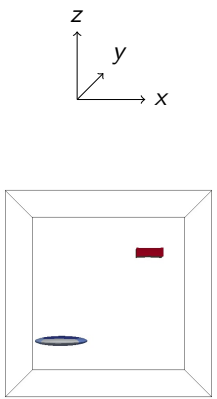


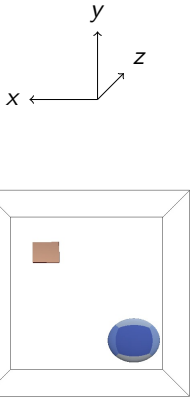


$\ell = 1$, Iterations: 12, Deformation Functions: 16.

Numerical Examples: Sphere and Cube







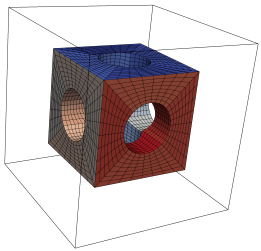
$\ell = \frac{1}{4}$, Iterations: 8, Deformation Functions: 50.

Numerical Examples: Toy

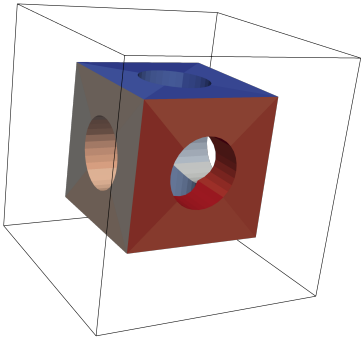
These calculations can be extended to higher-order ansatz spaces and more complex geometries.
In the following example, the initial toy box is contained in $[-0.3, 0.3]^3$. The desired tensor is

$$\mathbf{B} = \mathrm{diag}(0.82,\ 0.78,\ 0.74).$$

The calculations were performed with 200 piecewise (bi-)quadratic ansatz functions.

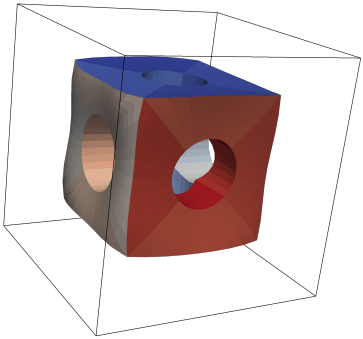


Numerical Examples: Toy



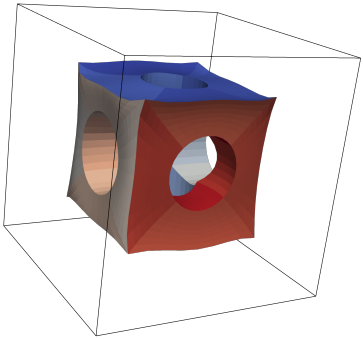
Iteration: 0, $J(\Omega) = 1.92\text{e}{-3}$, Step Size: 1.

Numerical Examples: Toy



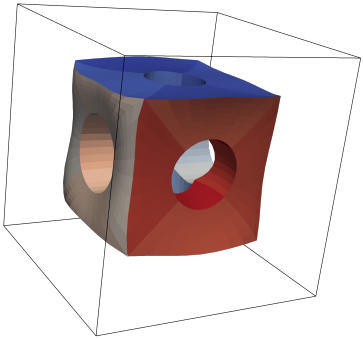
Iteration: 1, $J(\Omega) = 1.69\text{e}{-3}$, Step Size: 1.

Numerical Examples: Toy



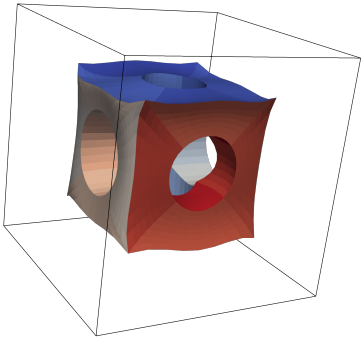
Iteration: 2, $J(\Omega) = 1.40\text{e}{-3}$, Step Size: 1.

Numerical Examples: Toy



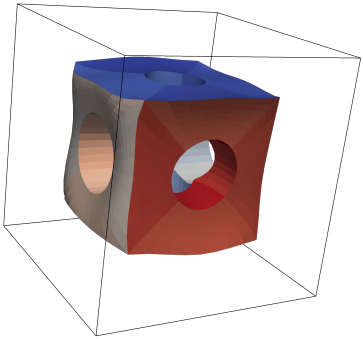
Iteration: 3, $J(\Omega) = 1.34\text{e}{-3}$, Step Size: 1.

Numerical Examples: Toy



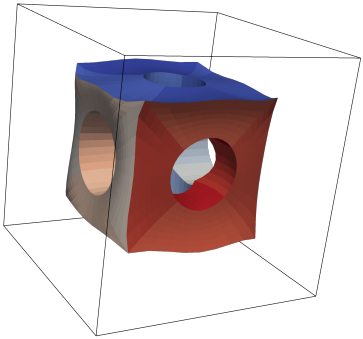
Iteration: 4, $J(\Omega) = 1.26\text{e}{-3}$, Step Size: 1.

Numerical Examples: Toy



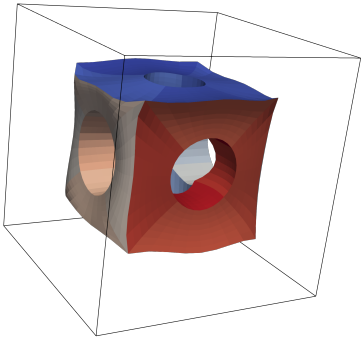
Iteration: 5, $J(\Omega) = 1.21\text{e}{-3}$, Step Size: 1.

Numerical Examples: Toy



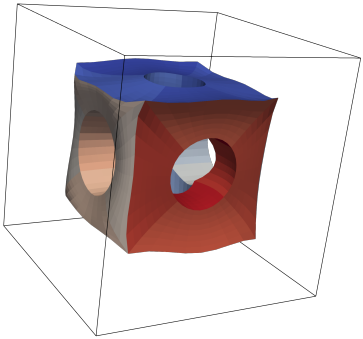
Iteration: 6, $J(\Omega) = 3.38\text{e}{-5}$, Step Size: 0.49.

Numerical Examples: Toy



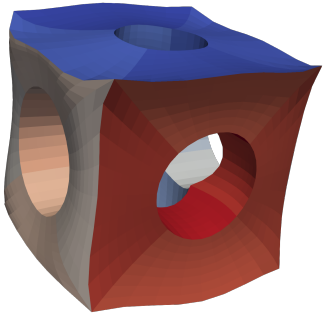
Iteration: 7, $J(\Omega) = 1.41\text{e}{-5}$, Step Size: 0.10.

Numerical Examples: Toy

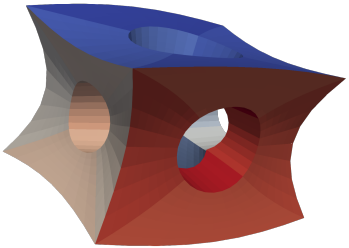


Iteration: 8, $J(\Omega) = 8.53\text{e}{-6}$, Step Size: 0.03.

Numerical Examples: Toy



200 deformation functions



50 deformation functions

Conclusion

- The final shape is not unique, but depends on the choice of the deformation functions and the initial shape.
- The shape optimisation procedure was successfully implemented with the boundary element method library **BEMBEL**.
- Boundary elements are useful for shape optimisation problems, as no mesh volume mesh has to be updated.
- The calculations can be extended to higher-order ansatz functions.
- The shape optimisation can be performed with a reference shape of an arbitrary topology.

Thank you for your attention!

M. Dambrine and H. Harbrecht. Shape optimization for composite materials and scaffold structures. *Multiscale Modeling & Simulation*, 18:1136–1152, 2020.

J. Dölz, H. Harbrecht, S. Kurz, M. Multerer, S. Schöps, and F. Wolf. Bembel: The fast isogeometric boundary element C++ library for Laplace, Helmholtz, and electric wave equation. *SoftwareX*, 11:100476, 2020.

H. Harbrecht, M. Multerer, and R. von Rickenbach. Isogeometric shape optimization for scaffold structures. ArXiv, May 2021. `https://arxiv.org/abs/2105.15158`.