An introduction to shape and topology optimization

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Part V

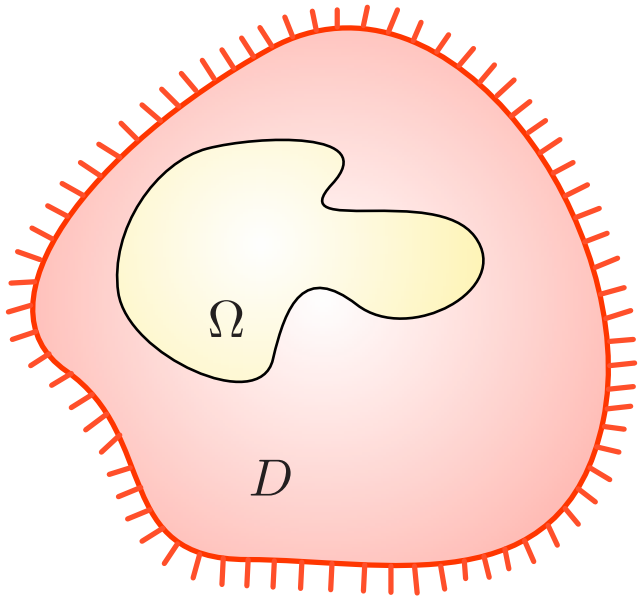
Density-based topology optimization techniques

A short reminder: homogenization-based topology optimization (I)

- Let us consider the following shape optimization problem, in the two-phase conductivity setting:

$$\min_{\Omega \subset D} J(\Omega), \text{ where } J(\Omega) := \int_D j(u_\Omega)\,\mathrm{d}x, \qquad (\mathrm{SO})$$

and $j : \mathbb{R} \to \mathbb{R}$ is a given, smooth function.



- Here, the temperature $u_\Omega \in H^1_0(D)$ is the solution to:

$$\begin{cases} -\mathrm{div}(\gamma_\Omega \nabla u_\Omega) &= f & \text{in } D, \\ u_\Omega &= 0 & \text{on } \partial D, \end{cases}$$

where the conductivity γ_Ω is of the form:

$$\gamma_\Omega(x) = \alpha + \chi_\Omega(x)(\beta - \alpha), \quad x \in D.$$

- This problem does not have a solution in general: minimizing sequences tend to create "microstructures".

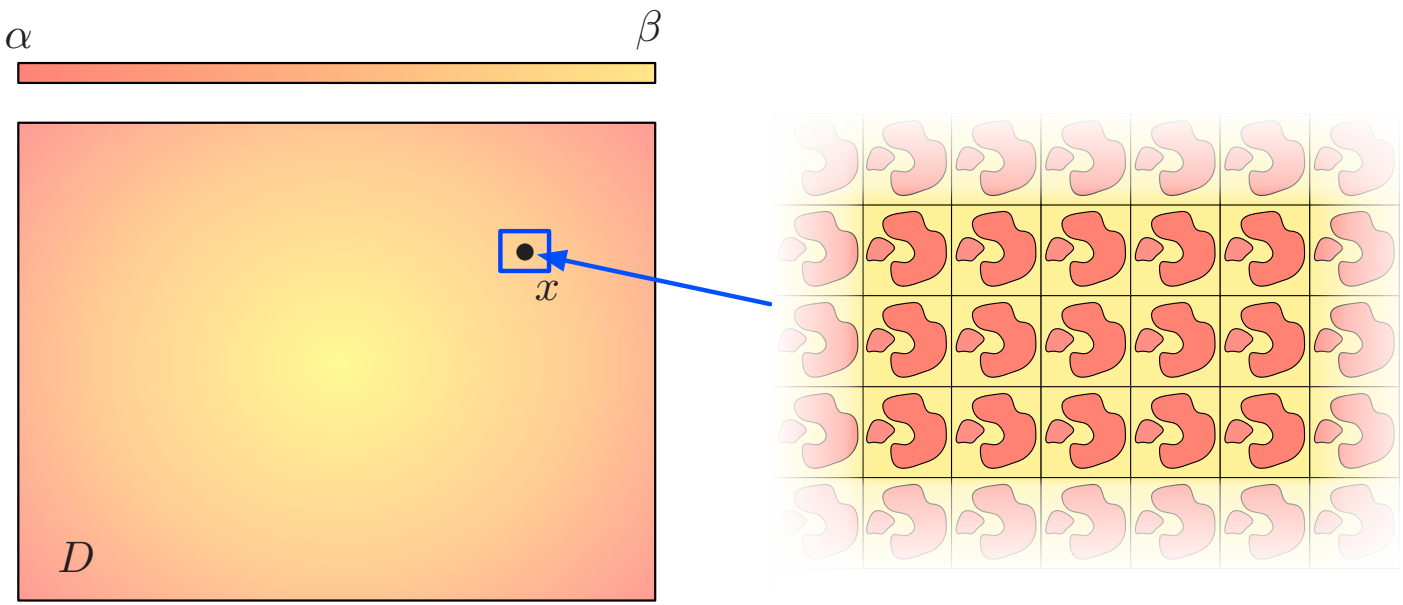
A short reminder: homogenization-based topology optimization (II)

The homogenized formulation of the problem extends the set of designs to composite structures:

$$(\theta, A) \in \mathcal{CD} := \left\{ \theta \in L^\infty(D, [0,1]),\ \ A(x) \in G_{\theta(x)} \text{ a.e. } x \in D \right\},$$

where:

- $\theta(x) \in [0,1]$ is the local density of material β around $x \in D$;
- $A(x) \in \mathbb{R}^{d \times d}$ is the microstructure tensor, in the set $G_{\theta(x)}$ of all the tensors obtained by homogenizing materials α, β in proportions $(1 - \theta(x))$ and $\theta(x)$.



A short reminder: homogenization-based topology optimization (III)

The relaxed version of the original problem is:

$$\min_{(\theta,A)\in\mathcal{CD}} J(\theta,A) := \int_D j(u_{\theta,A})\,\mathrm{d}x, \tag{H}$$

where the temperature $u_{\theta,A}$ induced by the composite structure (θ, A) satisfies:

$$\begin{cases} -\mathrm{div}(A\nabla u_{\theta,A}) = f & \text{in } D, \\ u_{\theta,A} = 0 & \text{on } \partial D. \end{cases}$$

Under suitable hypotheses, the following facts hold true:

- The problem (H) has at least one global minimizer (θ^*, A^*).
- Every such global minimizer is the limit, in the sense of homogenization, of a sequence of "classical designs" $\Omega^n \subset D$.
- Every minimizing sequence Ω^n of the original problem (SO) converges in the sense of homogenization to a global minimizer of the relaxed problem (H).

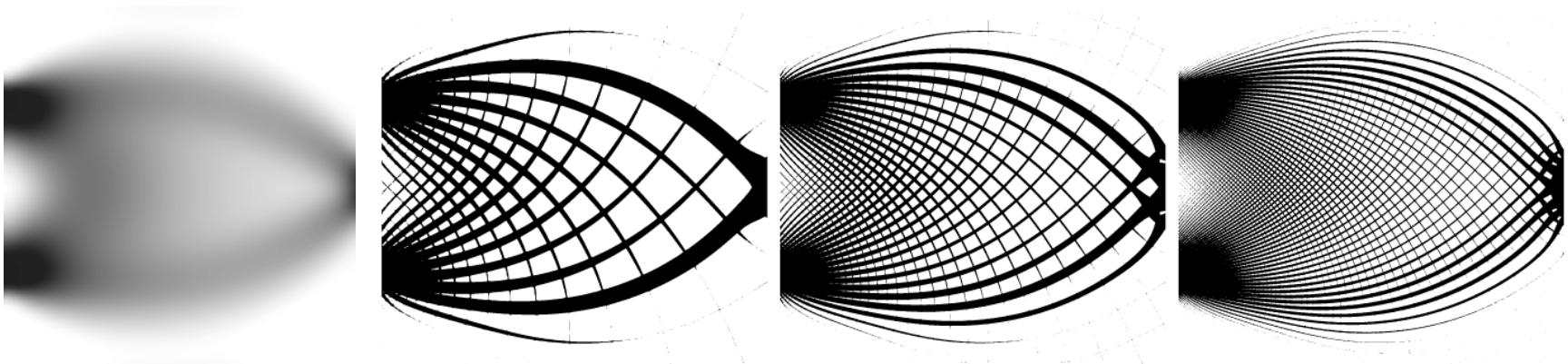
A short reminder: homogenization-based topology optimization (IV)

- From the optimal composite design $(\theta^*, A^*) \in \mathcal{CD}$, a true, "black-and-white" shape Ω is easily recovered by thresholding:

$$\Omega := \{x \in D,\ \ \theta^*(x) > c\}\,,$$

where $c \in [0,1]$ is chosen so that, e.g. Ω satisfies a desired volume constraint.

- More elaborate strategies are available, which do use the optimal microstructure tensor A^* to generate minimizing sequences Ω^n for $J(\Omega)$; see for instance the deshomogenization method from [PanTra, GroSig].



The "deshomogenization" method allows to infer minimizing sequences for the shape functional $J(\Omega)$ from the datum of the optimal composite design (θ, A^*) (picture from [AllGeoPan]).

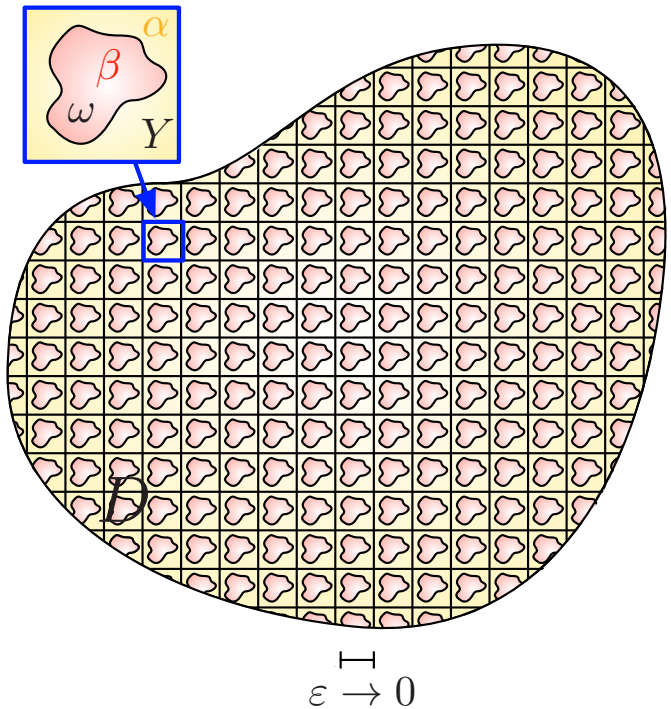
From homogenization to density-based methods (I)

- A pattern $\omega \subset Y := (0,1)^d$ induces a periodic distribution of the two conductive phases α and β at any scale ε within D:

$$A_\omega^\varepsilon(x) = A_\omega\left(\frac{x}{\varepsilon}\right), \quad x \in D,$$

where for $y \in Y$,

$$A_\omega(y) := \begin{cases} \beta & \text{if } x \in \omega, \\ \alpha & \text{if } x \notin \omega. \end{cases}$$



- The effective conductivity inside D as $\varepsilon \to 0$ is the matrix A_ω^* with entries:

$$(A_\omega^*)_{i,j} = \int_Y A_\omega(y)(e_i + \nabla w_i(y)) \cdot (e_j + \nabla w_j(y))\, \mathrm{d}y,$$

where the $w_i \in H^1_\#(Y)$ are the cell functions:

$$\begin{cases} -\mathrm{div}(A_\omega(y)(e_i + \nabla w_i)) = 0 & \text{in } Y, \\ y \mapsto w_i(y) & \text{is } Y - \text{periodic}. \end{cases}$$

From homogenization to density-based methods (II)

- The set G_θ is made of all the effective conductivities A^*_ω of periodic arrangements of the phases α and β induced by patterns $\omega \subset Y$ with volume fraction $|\omega| = \theta$.

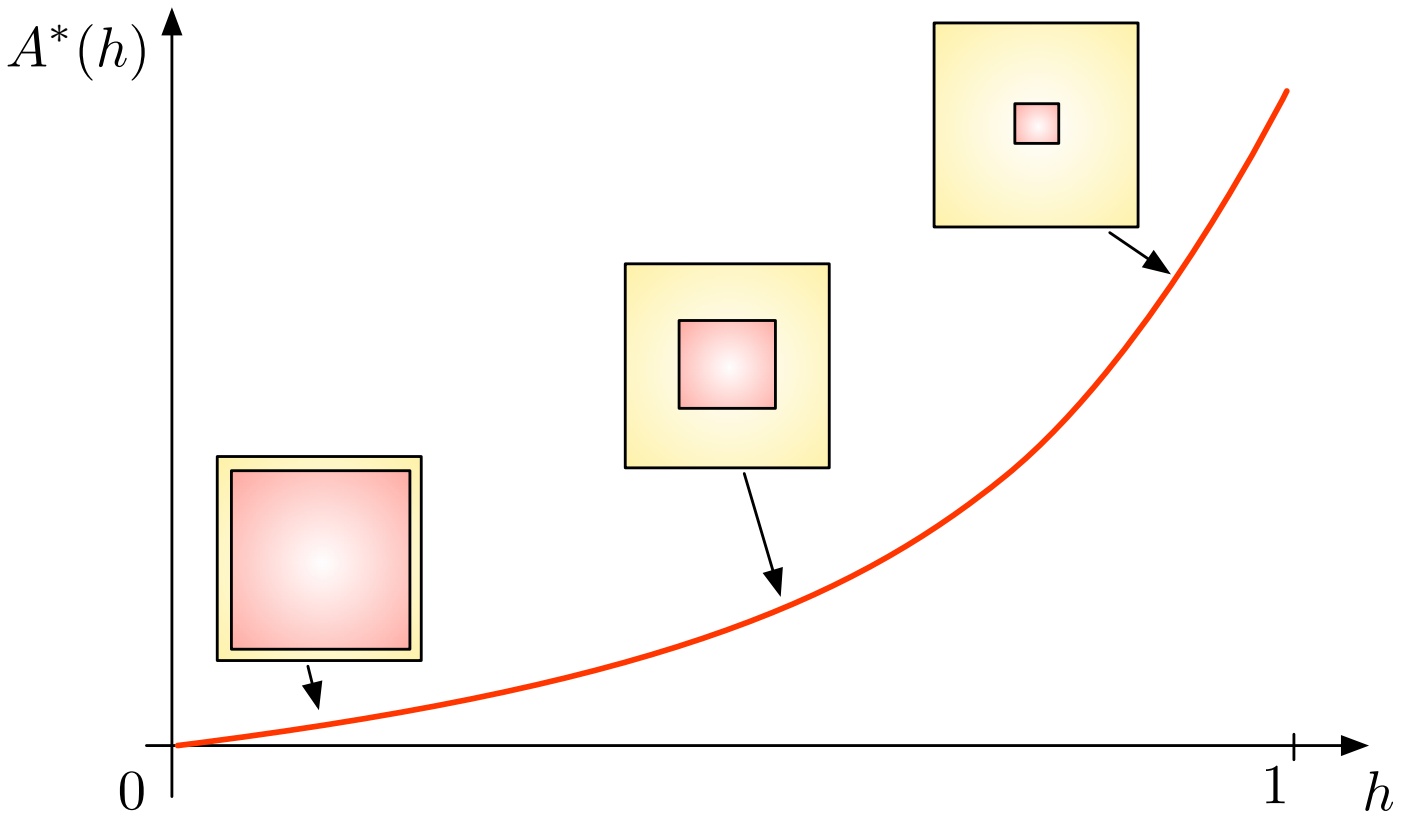
- This set can be characterized explicitly in the present two-phase conductivity setting, but this characterization is difficult to handle in practice.

- In general, only bounds are known about G_θ: the Hashin-Shtrikman bounds.

From homogenization to density-based methods (III)

One early simplification proposition [BenKik]:

- Only one microstructure pattern (e.g. a square inclusion) is retained for a given value $h \in [0, 1]$ of the volume fraction, or density.
- The homogenization tensor $A^*(h)$ is completely parametrized by h.



From homogenization to density-based methods (III)

- In numerical practice, a continuous expression $h \mapsto A^*(h)$ is constructed by:
  - Calculating $A^*(h_i)$ from the homogenization formulas, using the finite element method on the unit cell Y, for sample values $0 \leq h_1 < \ldots < h_N \leq 1$.
  - Interpolating the quantities $A^*(h_i)$ using e.g. polynomial functions (splines).

- The density-based version of the problem reads:

$$\min_{h \in L^\infty(D,[0,1])} J(h), \quad J(h) = \int_D j(u_h)\,\mathrm{d}x,$$

  where $u_h \in H_0^1(D)$ is the solution to:

$$\begin{cases} -\mathrm{div}(A^*(h)\nabla u_h) = f & \text{in } D, \\ u_h = 0 & \text{on } \partial D. \end{cases}$$

  The problem falls in the setting of parametric optimization.

- One step further in this direction consists in dropping completely the requirement that the material law $h \mapsto A^*(h)$ be "physical"...

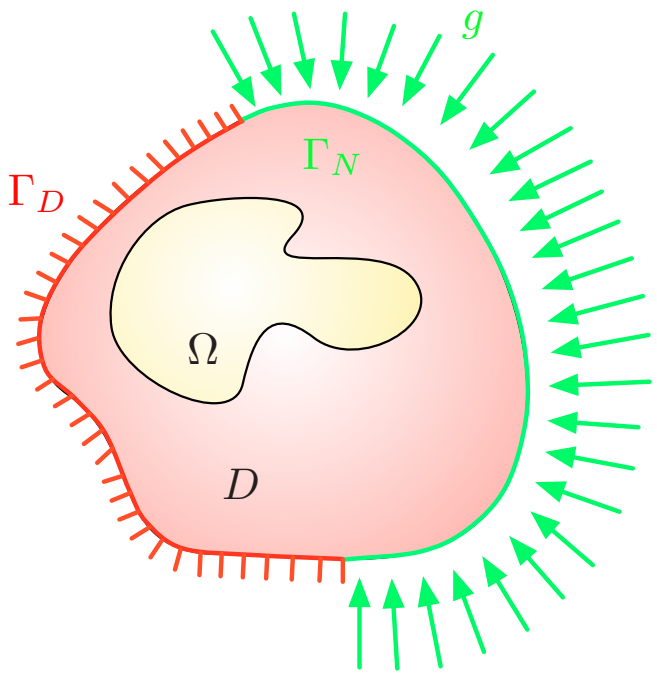
Part V

Topology optimization

Density-based topology optimization (I)

- We take again the two-phase conductivity setting:

$$\min_{\Omega \subset D} J(\Omega), \text{ where } J(\Omega) = \int_D j(u_\Omega)\,\mathrm{d}x. \qquad \text{(SO)}$$



- In here, the temperature u_Ω is the solution to:

$$\begin{cases} -\mathrm{div}(\gamma_\Omega \nabla u_\Omega) &= f & \text{in } D, \\ u_\Omega &= 0 & \text{on } \Gamma_D, \\ \gamma_\Omega \frac{\partial u_\Omega}{\partial n} &= g & \text{on } \Gamma_N, \end{cases}$$

  where the conductivity γ_Ω reads:

$$\gamma_\Omega = \alpha + \chi_\Omega(\beta - \alpha).$$

- The ideas that we now present extend to the contexts of linearized elasticity and fluid mechanics.

Density-based topology optimization (II)

- The (sought) "black-and-white" characteristic function $\chi_\Omega : D \to \{0,1\}$ of the shape Ω, is replaced by a "grayscale" density function $h : D \to [0,1]$.
- The properties (diffusion) of a region with intermediate density $h(x) \in (0,1)$ are described via an empirical isotropic interpolation law $\zeta(h)$ between α and β:

$$\zeta(0) = \alpha, \text{ and } \zeta(1) = \beta.$$

- The problem rewrites:

$$\min_{h \in \mathcal{U}_{\text{ad}}} J(h), \text{ where } \mathcal{U}_{\text{ad}} = L^\infty(D,[0,1]), \quad J(h) = \int_D j(u_h)\,\mathrm{d}x,$$

and $u_h \in H^1(D)$ is the solution to:

$$\begin{cases} -\mathrm{div}(\zeta(h)\nabla u_h) = f & \text{in } D, \\ u_h = 0 & \text{on } \Gamma_D, \\ \zeta(h)\frac{\partial u_h}{\partial n} = g & \text{on } \Gamma_N. \end{cases}$$

- It is a heuristic simplification of the homogenized problem (H), where the microstructure tensor A^* is omitted.

Density-based topology optimization (III)

The resulting density-based problem is within the realm of parametric optimization!

Theorem 1.

The objective function

$$J(h) = \int_D j(u_h)\,\mathrm{d}x$$

is Fréchet differentiable at any $h \in \mathcal{U}_{\mathrm{ad}}$, and its derivative reads

$$\forall \widehat{h} \in L^\infty(D),\ \ J'(h)(\widehat{h}) = \int_D \zeta'(h)(\nabla u_h \cdot \nabla p_h)\widehat{h}\,\mathrm{d}x,$$

where the adjoint state $p_h \in H^1(D)$ is the unique solution to the system:

$$\begin{cases} -\mathrm{div}(\zeta(h)\nabla p_h) = -j'(u_h) & \text{in } D, \\ p_h = 0 & \text{on } \Gamma_D, \\ \zeta(h)\frac{\partial p_h}{\partial n} = 0 & \text{on } \Gamma_N. \end{cases}$$

The interpolation profile

- The interpolation profile $\zeta(h)$ prescribes material properties (diffusion, etc.) to regions with (fictitious) intermediate densities.
- In the practice of the Solid Isotropic Method with Penalization (SIMP), a power law of the form
$$\zeta(h) = \alpha + h^p(\beta - \alpha)$$
is used (often, $p = 3$).
- This has the effect to penalize the presence of "grayscale" intermediate regions, and to steer the optimized density towards a "black-and white" function.
- This interpolation law is empirical: there is no guarantee that a material with such properties does exist!
- In the article [Am2], other choices for $\zeta(h)$ are discussed, which are more consistent from the physical viewpoint.

Part V

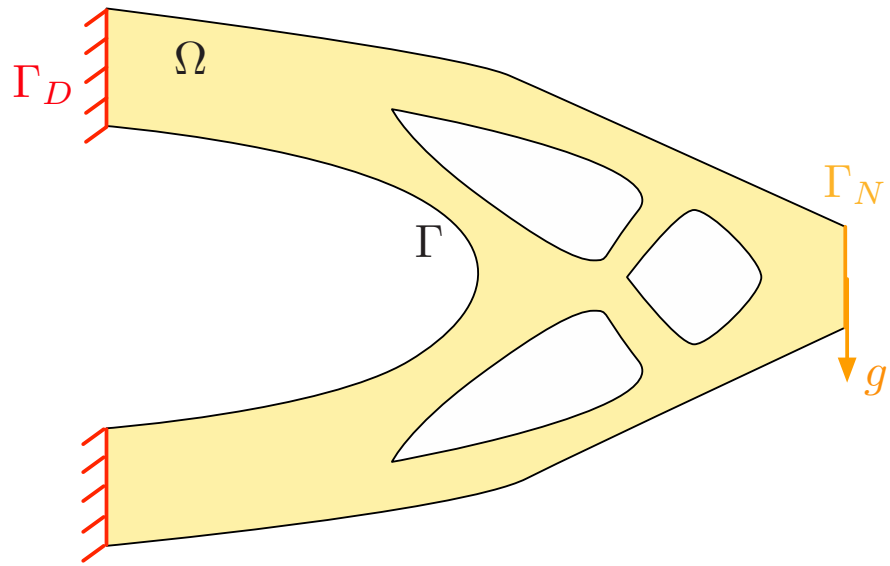
Topology optimization

The linearized elasticity setting (I)

- We consider the optimal design problem:

$$\min_{\Omega} J(\Omega), \text{ where } J(\Omega) = \int_{\Omega} j(u_\Omega)\,\mathrm{d}x,$$

and $j : \mathbb{R}^d \to \mathbb{R}$ is a smooth function.



- The displacement u_Ω is the unique solution to the linearized elasticity system:

$$\begin{cases} -\mathrm{div}(Ae(u_\Omega)) = 0 & \text{in } \Omega, \\ u_\Omega = 0 & \text{on } \Gamma_D, \\ Ae(u_\Omega)n = g & \text{on } \Gamma_N, \\ Ae(u_\Omega)n = 0 & \text{on } \Gamma, \end{cases} \tag{E}$$

where the optimized boundary Γ is traction-free.

The linearized elasticity setting (II)

The state equation for u_Ω is approximated by the Ersatz material method:

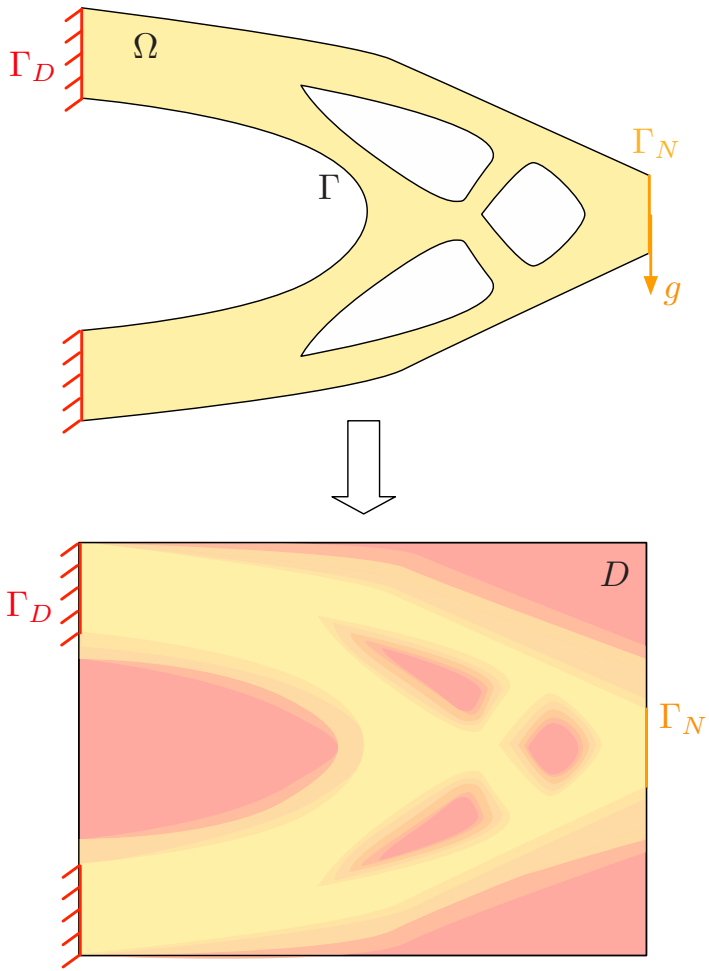
- A large computational box D is considered.
- The void $D \setminus \overline{\Omega}$ is filled with a very soft material, with Hooke's tensor εA, $\varepsilon \ll 1$.
- The solution u_Ω to (E) is replaced by that u_ε to:

$$\begin{cases} -\mathrm{div}(A_\Omega e(u_\varepsilon)) = 0 & \text{in } D, \\ u_\varepsilon = 0 & \text{on } \Gamma_D, \\ A_\Omega e(u_\varepsilon) n = g & \text{on } \Gamma_N, \\ A_\Omega e(u_\Omega) n = 0 & \text{on } \partial D \setminus (\overline{\Gamma_D} \cup \overline{\Gamma_N}), \end{cases}$$

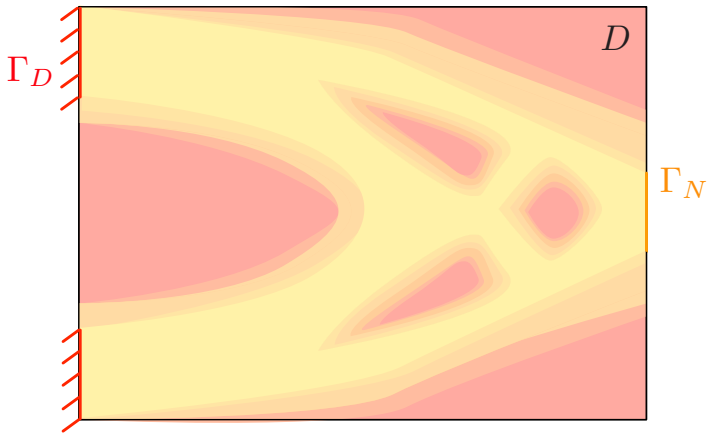
with:

$$A_\Omega = \varepsilon A + \chi_\Omega (1 - \varepsilon) A.$$

- This is only possible because the boundary Γ in contact with void is traction-free.



The linearized elasticity setting (III)



- The density-based version of the problem is:

$$\min_h J(h), \text{ where } J(h) = \int_D j(u_h)\,\mathrm{d}x.$$

- The approximate displacement u_h is the solution to:

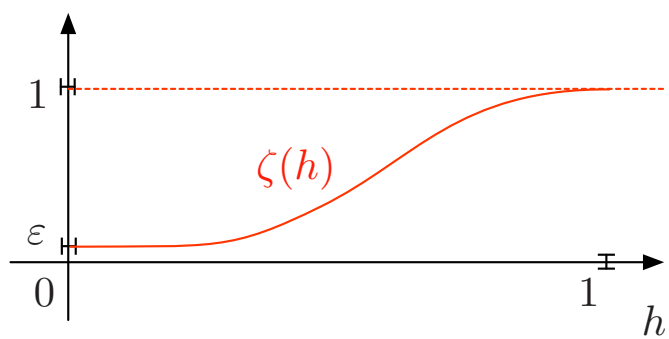
$$\begin{cases} -\mathrm{div}(\zeta(h)Ae(u_h)) = 0 & \text{in } D, \\ u_h = 0 & \text{on } \Gamma_D, \\ \zeta(h)Ae(u_h)n = g & \text{on } \Gamma_N, \\ \zeta(h)Ae(u_h)n = 0 & \text{on } \partial D \setminus (\overline{\Gamma_D} \cup \overline{\Gamma_N}). \end{cases}$$

- The transition between the soft and bulk materials is realized by a smooth interpolation profile:

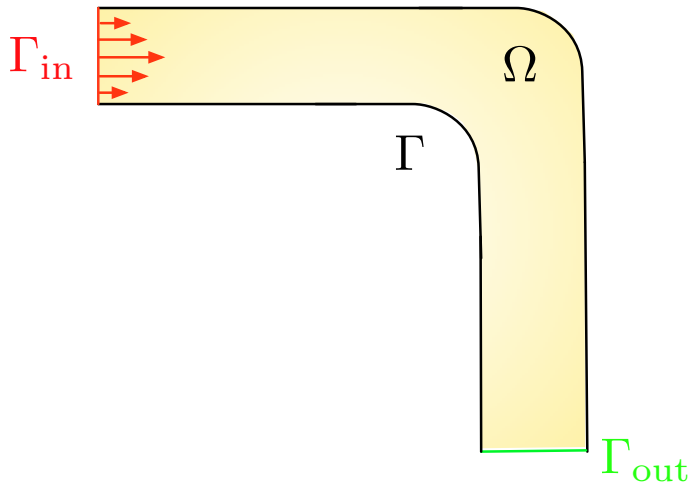
$$\zeta : [0,1] \to [0,1], \quad \zeta(0) = \varepsilon, \text{ and } \zeta(1) = 1.$$

For instance:

$$\zeta(h) = \varepsilon + h^3(1-\varepsilon).$$



Treatment of fluid mechanics by the artifical porosity method (I)



- We consider the optimal design problem:

$$\min_{\Omega} J(\Omega), \text{ where } J(\Omega) = \int_{\Omega} j(u_\Omega)\,\mathrm{d}x,$$

and $j : \mathbb{R}^d \to \mathbb{R}$ is a smooth function.

- The velocity and pressure $u_\Omega : \Omega \to \mathbb{R}^d$, $p_\Omega : \Omega \to \mathbb{R}$ are solutions to the incompressible Stokes equations:

$$\begin{cases} -2\nu \mathrm{div}(D(u_\Omega)) + \nabla p_\Omega = 0 & \text{in } \Omega, \\ \mathrm{div}(u_\Omega) = 0 & \text{in } \Omega, \\ u_\Omega = u_{\text{in}} & \text{on } \Gamma_{\text{in}}, \\ \sigma(u_\Omega, p_\Omega)n = -p_{\text{out}} n & \text{on } \Gamma_{\text{out}}, \\ u_\Omega = 0 & \text{on } \Gamma, \end{cases} \tag{S}$$

where no-slip boundary conditions are imposed on the optimized boundary Γ.

Treatment of fluid mechanics by the artifical porosity method (II)

The state equation on a shape Ω is approximated by the artificial porosity method:

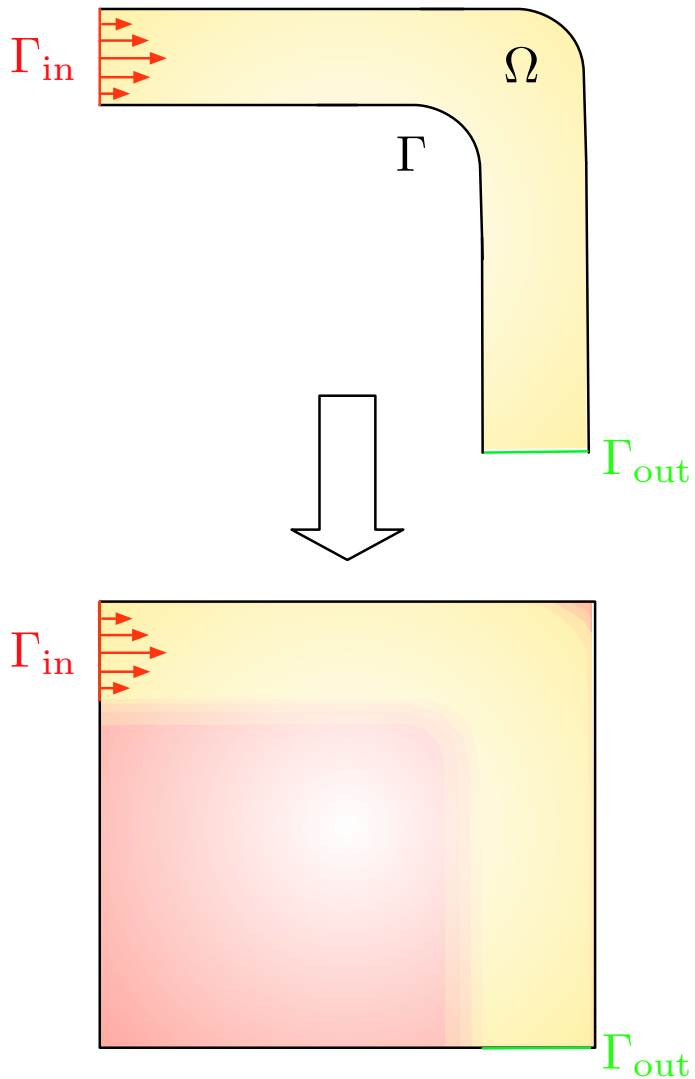
- A large computational box D is considered.
- The void $D \setminus \overline{\Omega}$ is filled with a solid material with very small porosity $\varepsilon \ll 1$.
- The velocity u_Ω and pressure p_Ω are approximated by the solutions u_ε, p_ε to the Brinkman equation:

$$\begin{cases} -2\nu \mathrm{div}(D(u_\varepsilon)) + \nabla p_\varepsilon + \alpha_\Omega u_\varepsilon = 0 & \text{in } D, \\ \mathrm{div}(u_\varepsilon) = 0 & \text{in } \Omega, \\ u_\varepsilon = u_{\mathrm{in}} & \text{on } \Gamma_{\mathrm{in}}, \\ \sigma(u_\varepsilon, p_\varepsilon) n = -p_{\mathrm{out}} n & \text{on } \Gamma_{\mathrm{out}}, \\ u_\varepsilon = 0 \quad \text{on } \partial D \setminus (\overline{\Gamma_D} \cup \overline{\Gamma_N}), \end{cases}$$

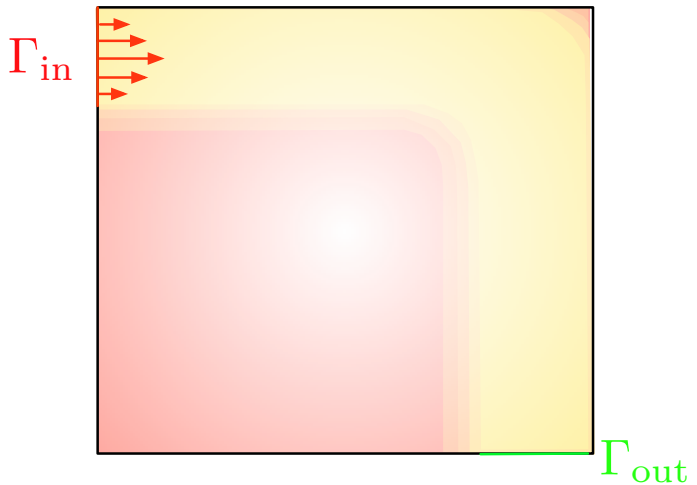
where α_Ω takes very large values in the "void":

$$\alpha_\Omega := \frac{1}{\varepsilon}(1 - \chi_\Omega).$$

- This approximation is only possible because the boundary Γ bears no slip boundary conditions.



Treatment of fluid mechanics by the artifical porosity method (III)



- The density-based version of this problem reads:

$$\min_h J(h), \text{ where } J(h) = \int_D j(u_h)\,\mathrm{d}x.$$

- The velocity u_h and pressure p_h are the solutions to the Brinkman equations:

$$\begin{cases} -2\nu\mathrm{div}(D(u_h)) + \nabla p_h + \alpha(h)u_h = 0 & \text{in } D, \\ \mathrm{div}(u_h) = 0 & \text{in } D, \\ u_h = u_{\text{in}} & \text{on } \Gamma_{\text{in}}, \\ \sigma(u_h)n = -p_{\text{out}}n & \text{on } \Gamma_{\text{out}}, \\ u_h = 0 & \text{on } \partial D \setminus (\overline{\Gamma_{\text{in}}} \cup \overline{\Gamma_{\text{out}}}). \end{cases}$$

- The artificial porosity coefficient $\alpha(h)$ is of the form:

$$\alpha(h) = \alpha_{\max} + (\alpha_{\min} - \alpha_{\max})h\frac{1+q}{h+q},$$

where q is a parameter (e.g. $q = 3$), $\alpha_{\max}$ is typically 10^6 and $\alpha_{\min} \approx 0$.

Part V

Topology optimization

Density-based relaxation (I)

- The density-based formulation of our model problem reads:

$$\min_{h \in L^\infty(D,[0,1])} J(h), \text{ where } J(h) := \int_D j(u_h)\,\mathrm{d}x$$

and $u_h \in H^1(D)$ is the solution to:

$$\begin{cases} -\mathrm{div}(\zeta(h)\nabla u_h) = f & \text{in } D, \\ u_h = 0 & \text{on } \Gamma_D, \\ \zeta(h)\frac{\partial u_h}{\partial n} = g & \text{on } \Gamma_N. \end{cases}$$

This boils down to a parametric optimization problem!

- As we have seen, the simple parametric setting allows for the use of basic gradient algorithms, but also more advanced optimization algorithms, such as:
  - The Method of Moving Asymptotes (MMA);
  - The quasi-Newton BFGS method;
  - Conjugate gradient algorithms.

Density-based relaxation (II)

- As the result of a density-based topology optimization process, a density function h is obtained, which may present grayscale values.
- However, in general, a real "black-and-white" design $\Omega \subset D$ is expected.
- Hence there is the need to threshold the density h, i.e. for an adequate value $c \in (0,1)$, Ω is obtained as:

$$\Omega = \{x \in D,\ \ h(x) > c\}\,, \text{ that is,}$$

  - Regions where $0 \leq h(x) \leq c$ are considered to be "void";
  - Regions where $c < h(x) \leq 1$ are considered to be "full of material".

- Like in the homogenization setting, one simple method is to proceed by dichotomy, so that Ω satisfies a volume target.
- "Minimizing sequences" of shapes Ω^n, showing features at scales $\frac{1}{n} \to 0$ can also be obtained from h by a variant of the deshomogenization method [GroSig].

Part V

Topology optimization

Density filters (I)

- Often, desired properties of the density h (regularity, etc.) are enforced by filtering: h appears in the state (and adjoint) equations via the quantity Lh, where

$$L : L^\infty(D, [0,1]) \to L^\infty(D, [0,1])$$

  is the filter operator.

- The problem rewrites:

$$\min_{h \in \mathcal{U}_{\mathrm{ad}}} J(h), \text{ where } J(h) = \int_D j(u_h)\, dx,$$

  and u_h is the solution to:

$$\begin{cases} -\mathrm{div}(\zeta(Lh)\nabla u_h) = f & \text{in } D, \\ u_h = 0 & \text{on } \Gamma_D, \\ (\zeta(Lh)\nabla u_h)n = g & \text{on } \Gamma_N. \end{cases}$$

- The calculation of the derivative of $J(h)$ now reads:

$$\begin{aligned} J'(h)(\widehat{h}) &= \int_D \zeta'(h)(\nabla u_h \cdot \nabla p_h)(L\widehat{h})\, \mathrm{d}x, \\ &= \int_D L^T \left(\zeta'(h)(\nabla u_h \cdot \nabla p_h)\right) \widehat{h}\, \mathrm{d}x. \end{aligned}$$

Density filters (II)

Here are some examples of regularizing filters:

- *Convolution-based filter:* For ε 'small' ($\varepsilon \approx$ mesh size), one defines:

$$L_\varepsilon h = h * \eta_\varepsilon,$$

where η_ε is a mollifying kernel; i.e. $\eta_\varepsilon(x) = \frac{1}{\varepsilon^d}\eta(\frac{x}{\varepsilon})$,

$$\eta \in \mathcal{C}_c^\infty(\mathbb{R}^d),\ \operatorname{supp}(\eta) \subset B(0,1),\ \text{and}\ \int_{\mathbb{R}^d} \eta \, \mathrm{d}x = 1.$$

- *PDE-based filter:* For small ε,

$$L_\varepsilon h = q,$$

where q is the unique solution in $H^1(D)$ to the problem:

$$\begin{cases} -\varepsilon^2 \Delta q + q = h & \text{in } D, \\ \frac{\partial q}{\partial n} = 0 & \text{on } \partial D. \end{cases}$$

Density filters (III)

Morphological filters are often useful to express the idea of geometric robustness:

- The *dilation filter*

$$D_\delta h(x) = \frac{1}{\beta} \log \left(\frac{1}{|B(x,\delta)|} \int_{B(x,\delta)} e^{\beta h(z)} \, \mathrm{d}z \right)$$

interpolates between the average and the maximum of h on $B(x,\delta)$:

$$D_\delta h(x) \xrightarrow{\beta \to 0} \frac{1}{|B(x,\delta)|} \int_{B(x,\delta)} h(z) \, \mathrm{d}z, \text{ and } D_\delta h(x) \xrightarrow{\beta \to \infty} \max_{z \in B(x,\delta)} h(z).$$

- The *erosion filter*

$$E_\delta h(x) = 1 - \frac{1}{\beta} \log \left(\frac{1}{|B(x,\delta)|} \int_{B(x,\delta)} e^{\beta(1-h(z))} \, \mathrm{d}z \right)$$

interpolates between the average and the minimum of h on $B(x,\delta)$:

$$E_\delta h(x) \xrightarrow{\beta \to 0} \frac{1}{|B(x,\delta)|} \int_{B(x,\delta)} h(z) \, \mathrm{d}z, \text{ and } D_\delta h(x) \xrightarrow{\beta \to \infty} \min_{z \in B(x,\delta)} h(z).$$

Density filters (III)

The Heaviside filter allows to steer the optimized density towards values 0 and 1 during the optimization:

$$\widetilde{H_{\beta,\eta}h} = \frac{\tanh(\beta\eta) + \tanh(\beta(h-\eta))}{\tanh(\beta\eta) + \tanh(\beta(1-\eta))},$$

where β and η are user-defined parameters which may be updated in the course of the process.

- All these filters can be combined (i.e. composed), up to some tuning.

- See for instance [WanSig] for other examples of filters.

Sensitivity filters

- As in the parametric optimization context, the expression of the derivative

$$\forall \widehat{h} \in L^\infty(D),\ \ J'(h)(\widehat{h}) = \int_D \zeta'(h)(\nabla u_h \cdot \nabla p_h)\widehat{h}\,\mathrm{d}x$$

  lends itself to a straightforward choice of a descent direction:

$$\widehat{h} = -\zeta'(h)(\nabla u_h \cdot \nabla p_h),$$

  that is, $\widehat{h}$ is the (negative) $L^2(D)$ gradient of $J'(h)$.

- Other choices are possible (and often more adequate) by changing inner products:

$$\widehat{h} = -V,$$

  where V solves:

$$\forall w \in \mathcal{H},\quad \langle V, w\rangle_{\mathcal{H}} = J'(h)(w),$$

  for an adapted choice of Hilbert space and inner product $\mathcal{H}$ and $\langle\cdot,\cdot\rangle_{\mathcal{H}}$.

- This stage is often called sensitivity filtering in density-based methods.

Part V

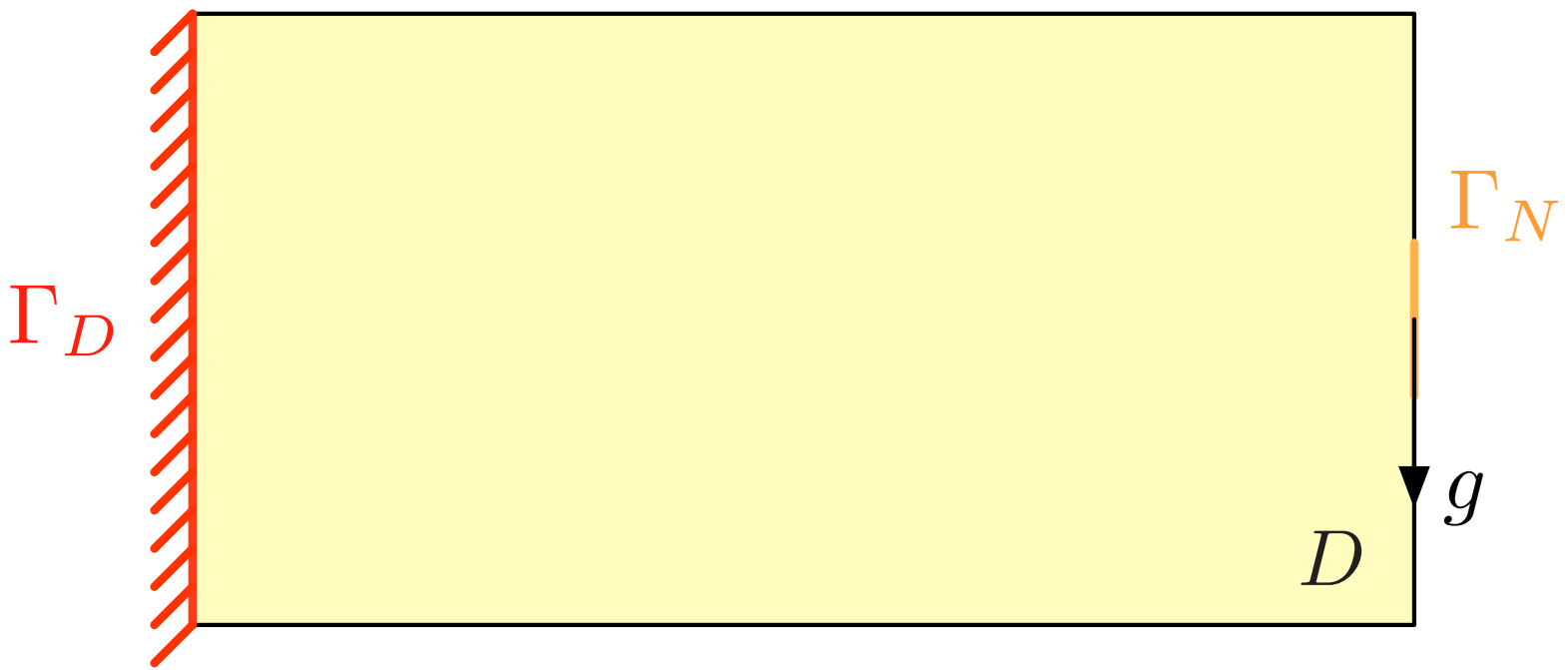
Topology optimization

Example: the cantilever benchmark

- In the context of linearized elasticity, the compliance of a cantilever beam is minimized:

$$C(h) = \int_D \zeta(h) A e(u_h) : e(u_h)\, dx.$$

- A constraint on the volume $\mathrm{Vol}(h) = \int_D h\, dx$ of the structure is added.

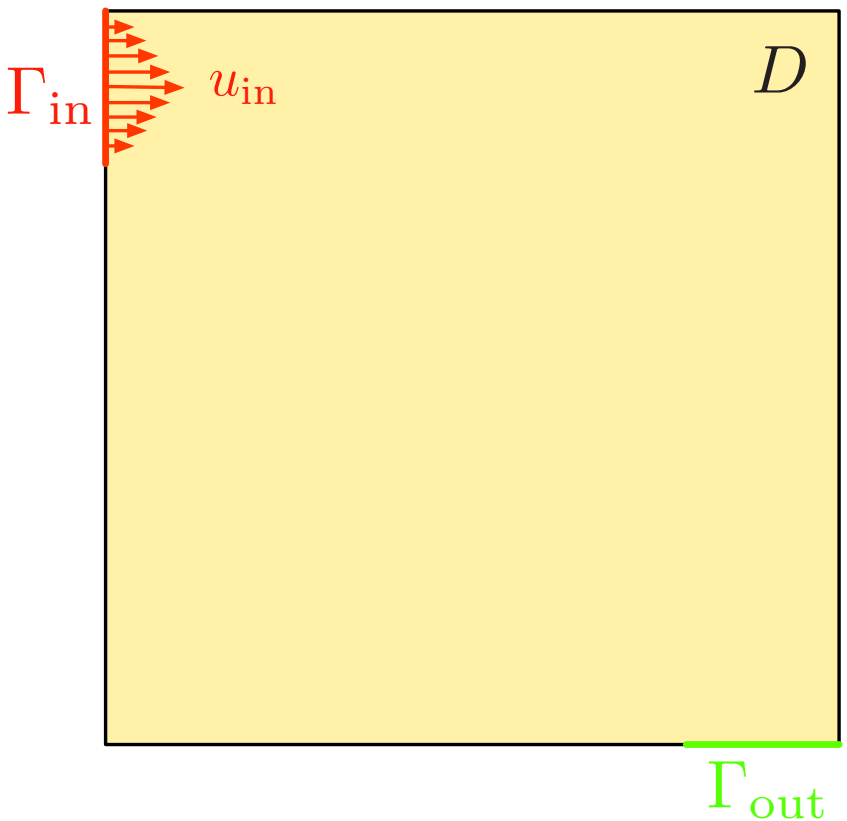


Example: the pipe benchmark

- In the context of fluid mechanics, the viscous dissipation within a pipe is minimized:

$$C(h) = \int_D \zeta(h) Ae(u_h) : e(u_h)\, dx.$$

- A constraint on the volume $\mathrm{Vol}(h) = \int_D h\, dx$ of the pipe is added.



A brief summary

Assets of density-based methods

- Simplicity of the mathematical analysis (calculation of derivatives, etc).
- They allow for the use of efficient mathematical programming routines.
- Robustness of the implementation: everything takes place on a fixed mesh, no mesh deformation is required.

Drawbacks

- Need to reformulate and approximate the physical equations.
- The geometry of shapes is lost, which may make it difficult to formulate, e.g. geometric constraints.

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