

# Null Space Gradient Flows for Shape Optimization of Multiphysics Systems

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New trends in PDE constrained optimization  
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1. Shape derivatives for a weakly coupled multiphysics system
2. Null space gradient flows for constrained optimization
3. Numerical illustrations on 2-d and 3-d test cases

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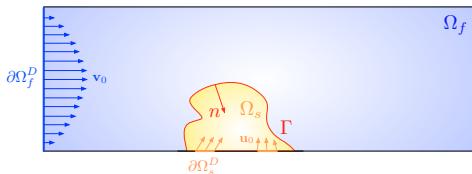
We are interested in multiphysics systems featuring

- ▶ fluids: velocity–pressure  $(\mathbf{v}, p)$
- ▶ thermal exchanges: temperature field  $T$ , convected by  $\mathbf{v}$
- ▶ mechanical structures: displacement  $\mathbf{u}$ , subjected to fluid-structure interaction with  $\mathbf{v}$  and thermoelasticity with  $T$ .



# 1. Shape derivatives for a multiphysics system

Proposed system

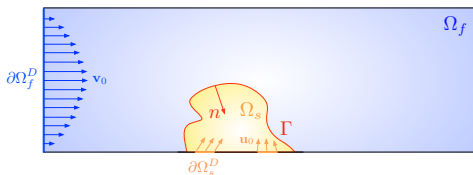


- Incompressible Navier-Stokes equations for  $(\mathbf{v}, p)$  in  $\Omega_f$

$$-\operatorname{div}(\sigma_f(\mathbf{v}, p)) + \rho \nabla \mathbf{v} \mathbf{v} = \mathbf{f}_f \text{ in } \Omega_f$$

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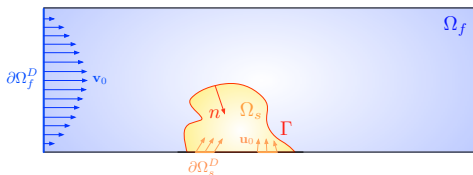
- Steady-state convection-diffusion for  $T_f$  and  $T_s$  in  $\Omega_f$  and  $\Omega_s$ :

$$-\operatorname{div}(k_f \nabla T_f) + \rho \mathbf{v} \cdot \nabla T_f = Q_f \quad \text{in } \Omega_f$$

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- ▶ Linearized thermoelasticity with fluid-structure interaction for  $\mathbf{u}$  in  $\Omega_s$ :

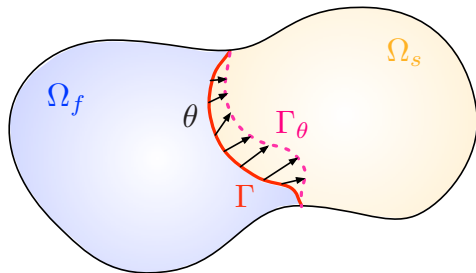
$$-\operatorname{div}(\sigma_s(\mathbf{u}, T_s)) = \mathbf{f}_s \quad \text{in } \Omega_s$$

$$\sigma_s(\mathbf{u}, T_s) \cdot \mathbf{n} = \sigma_f(\mathbf{v}, p) \cdot \mathbf{n} \quad \text{on } \Gamma.$$

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The method of Hadamard

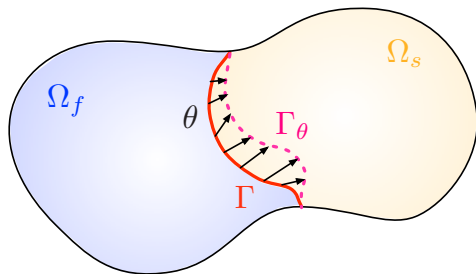
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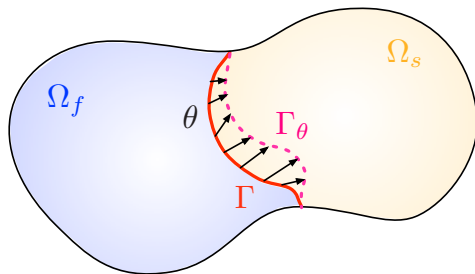


$$\Gamma_\theta = (I + \theta)\Gamma, \text{ where } \theta \in W_0^{1,\infty}(D, \mathbb{R}^d), \|\theta\|_{W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)} < 1.$$

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$$J(\Gamma_{\theta}) = J(\Gamma) + \frac{dJ}{d\theta}(\theta) + o(\theta), \quad \text{where } \frac{|o(\theta)|}{\|\theta\|_{W^{1,\infty}(D, \mathbb{R}^d)}} \xrightarrow{\theta \rightarrow 0} 0.$$

# Shape derivatives for a multiphysics system

## Shape derivative of arbitrary functionals

### Proposition

*Let  $J(\Gamma, \mathbf{u}, T, \mathbf{v}, p)$  an arbitrary functional with continuous partial derivatives and  $\mathbf{u}(\Gamma), T(\Gamma), \mathbf{v}(\Gamma), p(\Gamma)$  the above state variables. Then, if these are smooth enough,  $\Gamma \mapsto J(\Gamma, \mathbf{u}(\Gamma), T(\Gamma), \mathbf{v}(\Gamma), p(\Gamma))$  is shape differentiable and the derivative reads:*

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$\mathfrak{J}$  is a “transported” functional:

$$\mathfrak{J}(\boldsymbol{\theta}, \hat{\mathbf{v}}, \hat{p}, \hat{T}, \hat{\mathbf{u}}) := J(\Gamma_{\boldsymbol{\theta}}, \hat{\mathbf{v}} \circ (I + \boldsymbol{\theta})^{-1}, \hat{p} \circ (I + \boldsymbol{\theta})^{-1}, \hat{T} \circ (I + \boldsymbol{\theta})^{-1}, \hat{\mathbf{u}} \circ (I + \boldsymbol{\theta})^{-1}).$$

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Partial derivative for  $J$  with respect to the shape.

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Three “adjoint” terms for each of the three physics.

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Adjoint variables  $\mathbf{w}, q, S_f, S_s, \mathbf{r}$  are solved in a reversed cascade.

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## 2. Null space gradient flows for constrained optimization

- ▶ Our goal: solve constrained shape optimization problems

$$\min_{\Gamma} J(\Gamma, \mathbf{v}(\Gamma), \rho(\Gamma), T(\Gamma), \mathbf{u}(\Gamma))$$

$$\text{s.t. } g_i(\Gamma, \mathbf{v}(\Gamma), \rho(\Gamma), T(\Gamma), \mathbf{u}(\Gamma)) = 0, 1 \leq i \leq p.$$

$$h_i(\Gamma, \mathbf{v}(\Gamma), \rho(\Gamma), T(\Gamma), \mathbf{u}(\Gamma)) \leq 0, 1 \leq i \leq q$$

with *arbitrary* functionals  $J, g_i, h_i$ ;

- ▶ if possible, no fine tunings of optimization algorithm parameters;
- ▶ must deal with unfeasible initializations.



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For the exposure of our method, let us consider

$$\begin{aligned} \min_{x \in V} \quad & J(x) \\ \text{s.t.} \quad & \begin{cases} \mathbf{g}(x) = 0 \\ \mathbf{h}(x) \leq 0, \end{cases} \end{aligned}$$

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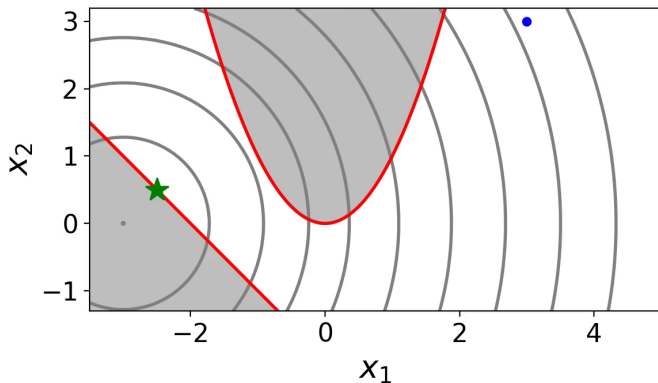
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- ▶  $V$  a Hilbert space equipped with a scalar product  $(\cdot, \cdot)_V$ .

## 2. Null space gradient flows for constrained optimization

$$\begin{aligned} \min_{(x_1, x_2) \in \mathbb{R}^2} \quad & J(x_1, x_2) = x_1^2 + (x_2 + 3)^2 \\ \text{s.t.} \quad & \begin{cases} h_1(x_1, x_2) = -x_1^2 + x_2 & \leq 0 \\ h_2(x_1, x_2) = -x_1 - x_2 - 2 & \leq 0 \end{cases} \end{aligned}$$



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$$\dot{x} = -\alpha_J(I - D\mathbf{g}^T(D\mathbf{g}D\mathbf{g}^T)^{-1}D\mathbf{g})\nabla J(x) - \alpha_C D\mathbf{g}^T(D\mathbf{g}D\mathbf{g}^T)^{-1}\mathbf{g}(x)$$

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(gradient flow on  $V = \{x \in V \mid \mathbf{g}(x) = 0\}$ ) Then Yamashita (1980) added a Gauss-Newton direction:

$$\dot{x} = -\alpha_J(I - D\mathbf{g}^T(D\mathbf{g}D\mathbf{g}^T)^{-1}D\mathbf{g})\nabla J(x) - \alpha_C D\mathbf{g}^T(D\mathbf{g}D\mathbf{g}^T)^{-1}\mathbf{g}(x)$$

$\mathbf{g}(x(t)) = \mathbf{g}(x(0))e^{-\alpha_C t}$  and  $J(x(t))$  decreases if  
 $\mathbf{g}(x(t)) = 0$ .



## 2. Null space gradient flows for constrained optimization

For *both* equality constraints  $\mathbf{g}(x) = 0$  and inequality constraints  $\mathbf{h}(x) \leq 0$ , we consider:

$$\dot{x} = -\alpha_J \xi_J(x(t)) - \alpha_C \xi_C(x(t))$$

with

$$\xi_J(x) := (I - \text{DC}_{\hat{I}(x)}^T (\text{DC}_{\hat{I}(x)} \text{DC}_{\hat{I}(x)}^T)^{-1} \text{DC}_{\hat{I}(x)}) (\nabla J(x))$$

$$\xi_C(x) = \text{DC}_{\tilde{I}(x)}^T (\text{DC}_{\tilde{I}(x)} \text{DC}_{\tilde{I}(x)}^T)^{-1} \mathbf{C}_{\tilde{I}(x)}(x),$$

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$\tilde{I}(x)$  the set of violated constraints:

$$\tilde{I}(x) = \{i \in \{1, \dots, q\} \mid h_i(x) \geq 0\}.$$

$$\mathbf{C}_{\tilde{I}(x)} = \left[ \mathbf{g}(x) \mid (h_i(x))_{i \in \tilde{I}(x)} \right]^T$$

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$$\xi_C(x) = \text{DC}_{\tilde{I}(x)}^T (\text{DC}_{\tilde{I}(x)} \text{DC}_{\tilde{I}(x)}^T)^{-1} \mathbf{C}_{\tilde{I}(x)}(x),$$

$\hat{I}(x) \subset \tilde{I}(x)$  is an “optimal” subset of the active or violated constraints which can be computed by mean of a dual subproblem.

$$\hat{I}(x) := \{i \in \tilde{I}(x) \mid \mu_i^*(x) > 0\}.$$

$$\mathbf{C}_{\hat{I}(x)} = \left[ \mathbf{g}(x) \mid (h_i(x))_{i \in \hat{I}(x)} \right]^T$$

## 2. Null space gradient flows for constrained optimization

### Definition

Let  $(\boldsymbol{\lambda}^*(x), \boldsymbol{\mu}^*(x)) \in \mathbb{R}^p \times \mathbb{R}^{\text{Card}\tilde{I}(x)}$  the solutions of the following dual minimization problem:

$$(\boldsymbol{\lambda}^*(x), \boldsymbol{\mu}^*(x)) := \arg \min_{\substack{\boldsymbol{\lambda} \in \mathbb{R}^p \\ \boldsymbol{\mu} \in \mathbb{R}^{\tilde{q}(x)}, \boldsymbol{\mu} \geq 0}} \|\nabla J(x) + D\mathbf{g}(x)^T \boldsymbol{\lambda} + D\mathbf{h}_{\tilde{I}(x)}(x)^T \boldsymbol{\mu}\|_V.$$

Define  $\hat{I}(x)$  the set obtained by collecting the non zero components of  $\boldsymbol{\mu}^*(x)$ :

$$\hat{I}(x) := \{i \in \tilde{I}(x) \mid \mu_i^*(x) > 0\}.$$

## 2. Null space gradient flows for constrained optimization

### The dual subproblem

The best descent direction  $-\xi_J(x)$  must be proportional to

$$\begin{aligned} \xi^* = & \arg \min_{\xi \in V} DJ(x)\xi \\ \text{s.t.} & \begin{cases} D\mathbf{g}(x)\xi = 0 \\ D\mathbf{h}_{\tilde{I}(x)}(x)\xi \leq 0 \\ \|\xi\|_V \leq 1. \end{cases} \end{aligned}$$

where  $\mathbf{h}_{\tilde{I}(x)}(x) = (h_i(x))_{i \in \tilde{I}(x)}$

## 2. Null space gradient flows for constrained optimization

The dual subproblem

### Proposition

$\xi^*(x)$  is explicitly given by:

$$\xi^*(x) = -\frac{\Pi_{\mathcal{C}_{\hat{\Gamma}(x)}}(\nabla J(x))}{\|\Pi_{\mathcal{C}_{\hat{\Gamma}(x)}}(\nabla J(x))\|_V},$$

with

$$\Pi_{\mathcal{C}_{\hat{\Gamma}(x)}}(\nabla J(x)) = (I - D\mathcal{C}_{\hat{\Gamma}(x)}^T (D\mathcal{C}_{\hat{\Gamma}(x)} D\mathcal{C}_{\hat{\Gamma}(x)}^T)^{-1} D\mathcal{C}_{\hat{\Gamma}(x)})(\nabla J(x))$$

## 2. Null space gradient flows for constrained optimization

The dual subproblem

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whence our definition

$$\begin{aligned}\dot{x} &= -\alpha_J \xi_J(x(t)) - \alpha_C \xi_C(x(t)) \\ \xi_J(x) &:= (I - D\mathcal{C}_{\hat{\Gamma}(x)}^T (D\mathcal{C}_{\hat{\Gamma}(x)} D\mathcal{C}_{\hat{\Gamma}(x)}^T)^{-1} D\mathcal{C}_{\hat{\Gamma}(x)}) (\nabla J(x)) \\ \xi_C(x) &= D\mathcal{C}_{\tilde{\Gamma}(x)}^T (D\mathcal{C}_{\tilde{\Gamma}(x)} D\mathcal{C}_{\tilde{\Gamma}(x)}^T)^{-1} \mathcal{C}_{\tilde{\Gamma}(x)}(x),\end{aligned}$$

## 2. Null space gradient flows for constrained optimization

We can prove:

1. Constraints are asymptotically satisfied:

$$\mathbf{g}(x(t)) = e^{-\alpha c t} \mathbf{g}(x(0)) \text{ and } \mathbf{h}_{\tilde{I}(x(t))} \leq e^{-\alpha c t} \mathbf{h}(x(0))$$



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2.  $J$  decreases as soon as the violation  $\mathbf{C}_{\tilde{I}(x(t))}$  is sufficiently small
3. All stationary points  $x^*$  of the ODE are KKT points

## 2. Null space gradient flows for constrained optimization

For shape optimization

$$\dot{x} = -\alpha_J \xi_J(x(t)) - \alpha_C \xi_C(x(t))$$

works the same with

$$\xi_J(x) := (I - \text{DC}_{\hat{I}(x)}^{\mathcal{T}} (\text{DC}_{\hat{I}(x)} \text{DC}_{\hat{I}(x)}^{\mathcal{T}})^{-1} \text{DC}_{\hat{I}(x)}) (\nabla J(x))$$

$$\xi_C(x) = \text{DC}_{\tilde{I}(x)}^{\mathcal{T}} (\text{DC}_{\tilde{I}(x)} \text{DC}_{\tilde{I}(x)}^{\mathcal{T}})^{-1} \mathbf{C}_{\tilde{I}(x)}(x),$$

where the transpose  $\mathcal{T}$  and the gradient  $\nabla$  must be computed with respect to  $\langle, \rangle_V$  thanks to an identification problem.

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This encompasses the celebrated [regularization and extension](#) step of the shape derivative in numerical algorithms.

1. Shape derivatives for a weakly coupled multiphysics system
2. Null space gradient flows for constrained optimization
3. Numerical illustrations on 2-d and 3-d test cases

### 3. Numerical applications

Lift-drag minimization:

$$\begin{aligned} \min \quad & -\text{Lift}(\Gamma, \mathbf{v}(\Gamma), p(\Gamma)) \\ \text{s.t.} \quad & \left\{ \begin{array}{l} \text{Drag}(\Gamma, \mathbf{v}(\Gamma), p(\Gamma)) \leq \text{DRAG}_0 \\ \text{Vol}(\Omega_f) = V_0 \\ \mathbf{X}(\Omega_s) := \frac{1}{|\Omega_s|} \int_{\Omega_s} \mathbf{x} dx = \mathbf{x}_0, \end{array} \right. \end{aligned}$$

$$\text{Lift}(\Gamma, \mathbf{v}(\Gamma), p(\Gamma)) := - \int_{\Gamma} \mathbf{e}_y \cdot \sigma_f(\mathbf{v}, p) \mathbf{n} ds,$$

$$\text{Drag}(\Gamma, \mathbf{v}(\Gamma), p(\Gamma)) := \int_{\Omega_f} \sigma_f(\mathbf{v}, p) : \nabla \mathbf{v} dx.$$

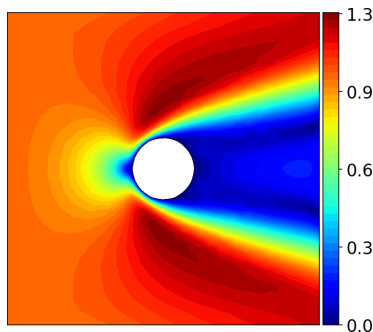


Figure: Optimized 2-d lift-drag flow profile.

### 3. Numerical applications

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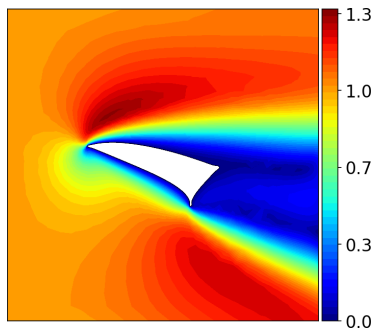
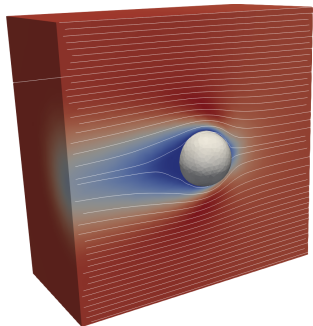


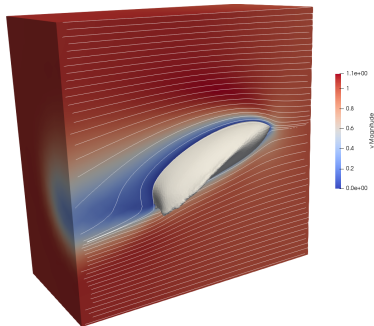
Figure: Optimized 2-d lift-drag flow profile.

### 3. Numerical applications

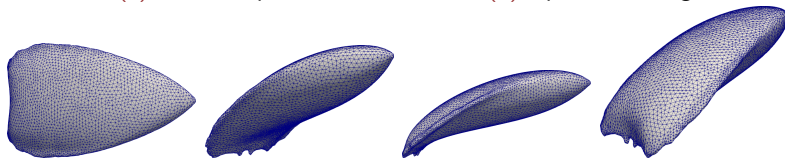
Lift-drag minimization in 3-d:



(a) Initial shape



(b) Optimized design

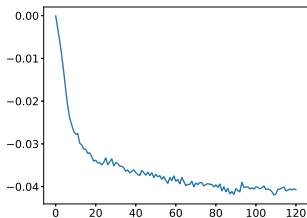


(c) Optimized design (other 3-d views)

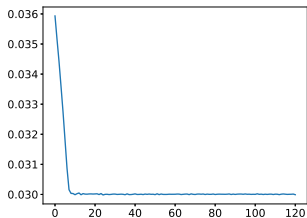


### 3. Numerical applications

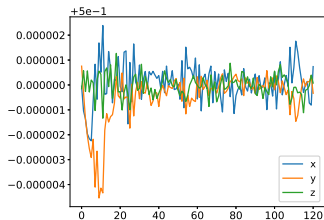
Lift-drag minimization in 3-d, convergence histories.



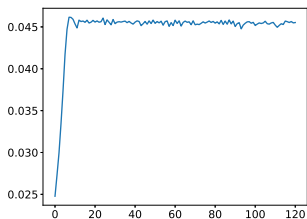
(a) Objective function.



(b) Volume constraint.



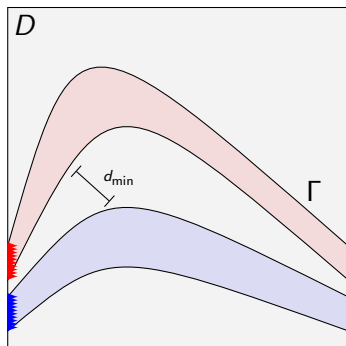
(c) Center of mass constraint.



(d) Drag constraint.

### 3. Numerical applications

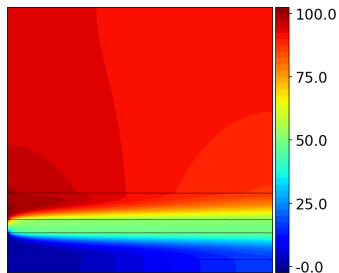
Bi-tube heat exchanger with non penetrating constraint



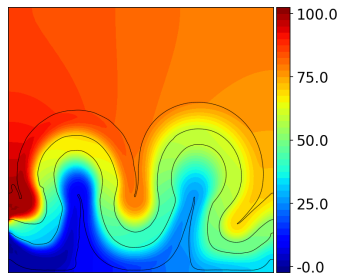
$$\begin{aligned} \min_{\Omega_f \subset D} \quad & J(\Omega_f) = - \left( \int_{\Omega_{f,cold}} \rho c_p \mathbf{v} \cdot \nabla T dx - \int_{\Omega_{f,hot}} \rho c_p \mathbf{v} \cdot \nabla T dx \right) \\ \text{s.t.} \quad & \left\{ \begin{aligned} DP(\Omega_f) &= \int_{\partial\Omega_f^D} p ds - \int_{\partial\Omega_f^N} p ds \leq DP_0 \\ Q_{hot \leftrightarrow cold}(\Omega_f) &\geq d_{min} \cdot \end{aligned} \right. \end{aligned}$$

### 3. Numerical applications

Bi-tube heat exchanger with non penetrating constraint



(a) Initial temperature field



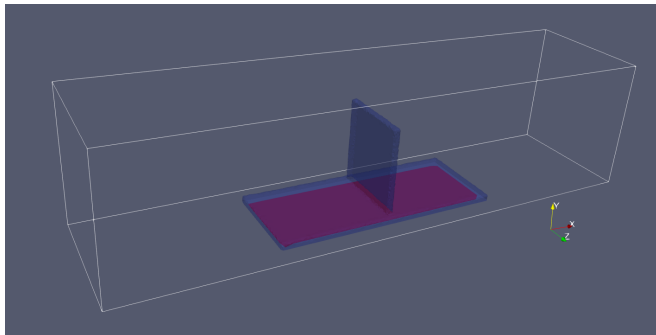
(b) Final temperature field.



(c) Intermediate iterations

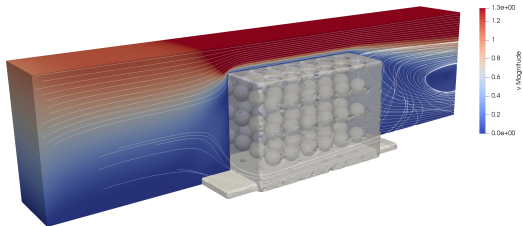
### 3. Numerical applications

3-d compliance minimization problem with fluid-structure interaction

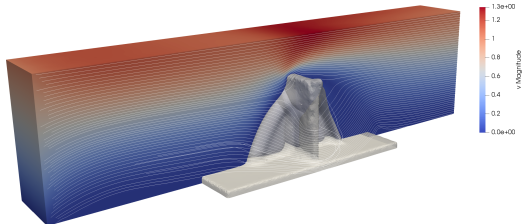


### 3. Numerical applications

3-d compliance minimization problem with fluid-structure interaction



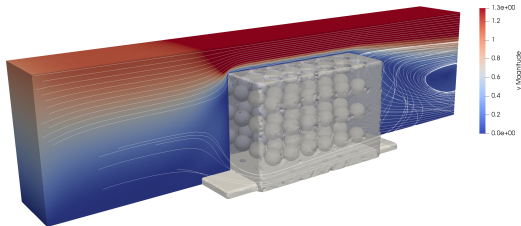
(a) Initial shape



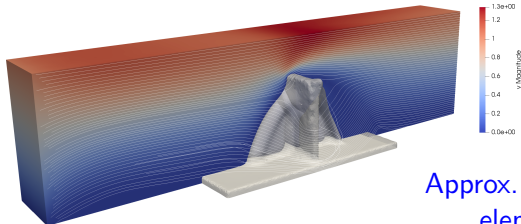
(b) Final design

### 3. Numerical applications

3-d compliance minimization problem with fluid-structure interaction



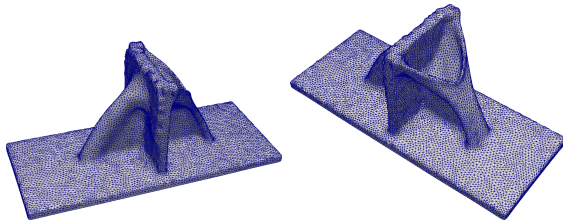
(a) Initial shape



(b) Final design

Approx. 2 millions  
elements.

### 3. Numerical applications



(a) Final design.

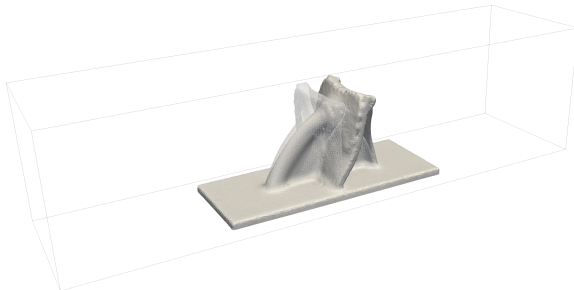
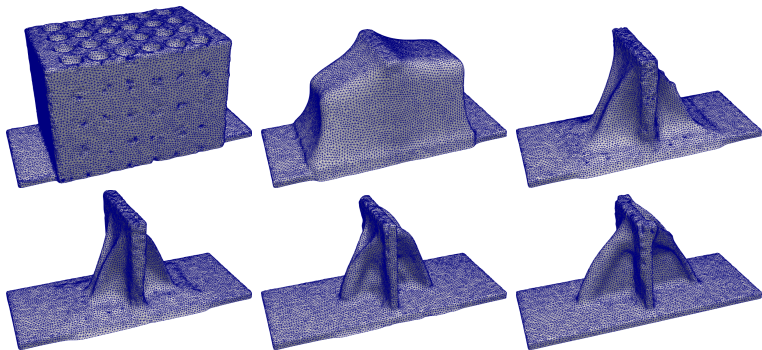


Figure: Linear elastic deformation.




### 3. Numerical applications

3-d compliance minimization problem with fluid-structure interaction



**Figure:** Intermediate iterations 0, 40, 100, 125, 175 and 300.



-  FEPPON, F., ALLAIRE, G., BORDEU, F., CORTIAL, J., AND DAPOGNY, C. Shape optimization of a coupled thermal fluid-structure problem in a level set mesh evolution framework.  
*SeMA Journal* (2019).
-  FEPPON, F., ALLAIRE, G., AND DAPOGNY, C. Null space gradient flows for constrained optimization with applications to shape optimization.  
*HAL preprint hal-01972915* (2019).
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*HAL preprint hal-01879571* (2019).

Many thanks for your  
attention.