Taking into account thermal residual stresses in topology optimization of structures built by additive manufacturing

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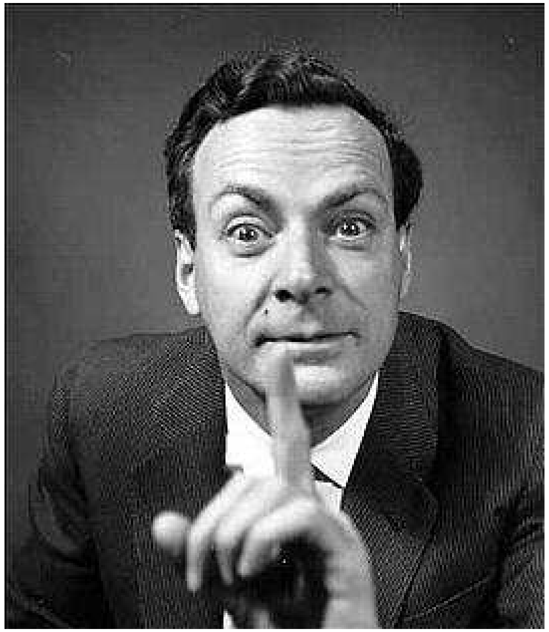
CMAP, Ecole Polytechnique

Séminaire Mathériaux, 15 Janvier 2018, Grenoble

CONTENTS

There is plenty of room for modelling...

Paraphrasing the famous punch line of Richard Feynman...



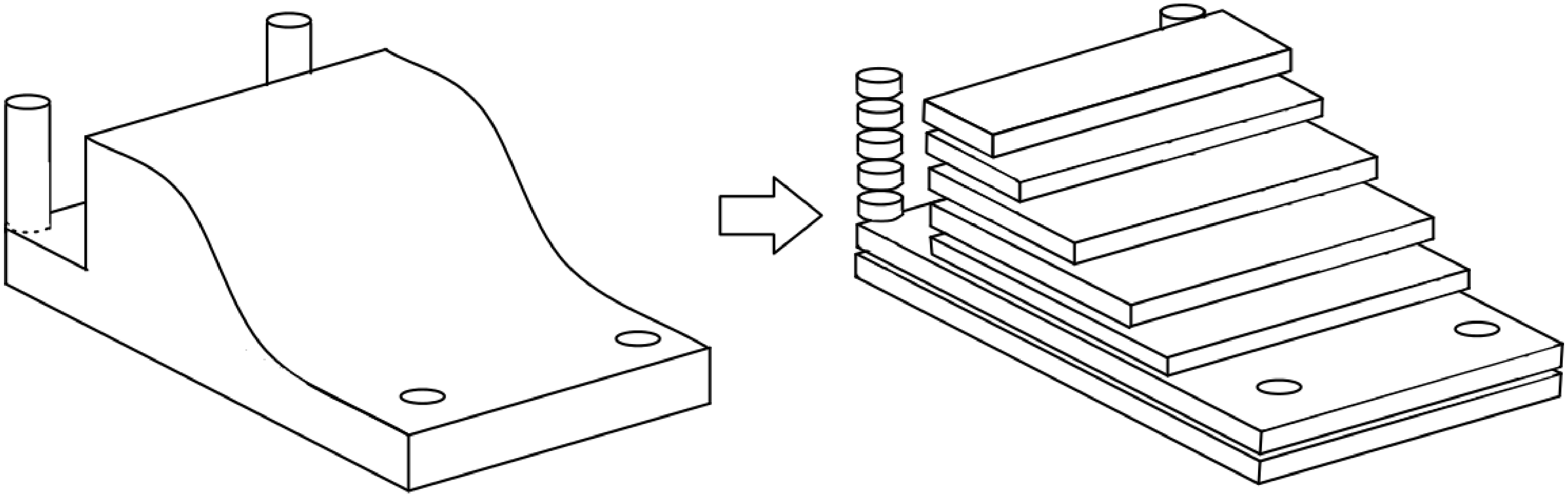
There is plenty of room at the bottom.

The dilemma of modelling

- ☞ A very precise model is usually computationally expensive.
- ☞ A computationally cheap model is usually not very precise.

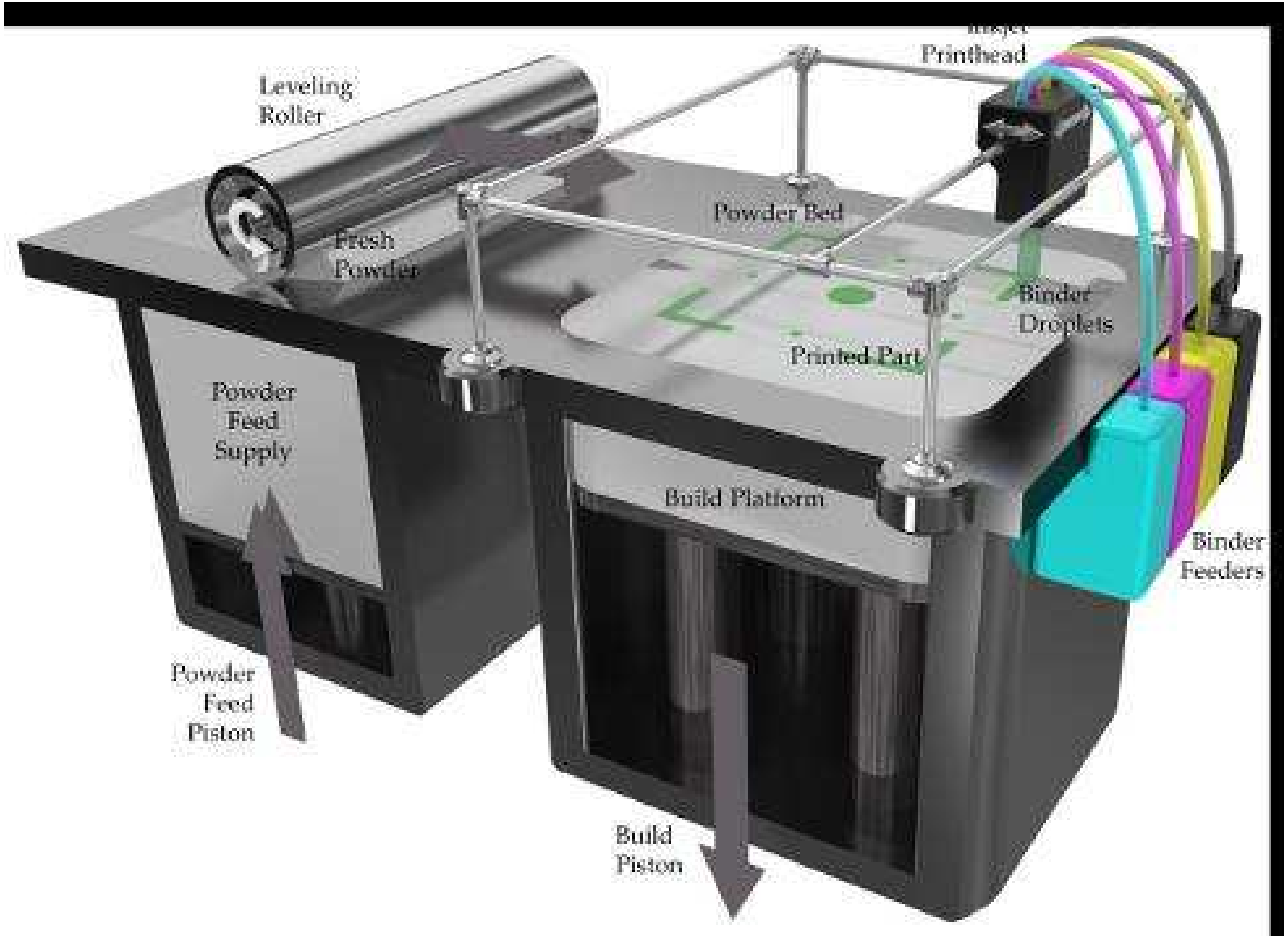
In an optimization loop, with many calls to the model, we must reach a compromise between cost and precision.

-I- INTRODUCTION



Additive manufacturing: structures built layer by layer.

Metallic powder melted by a laser or an electron beam.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Leveling
Roller
Powder Bed
Fresh
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Feed
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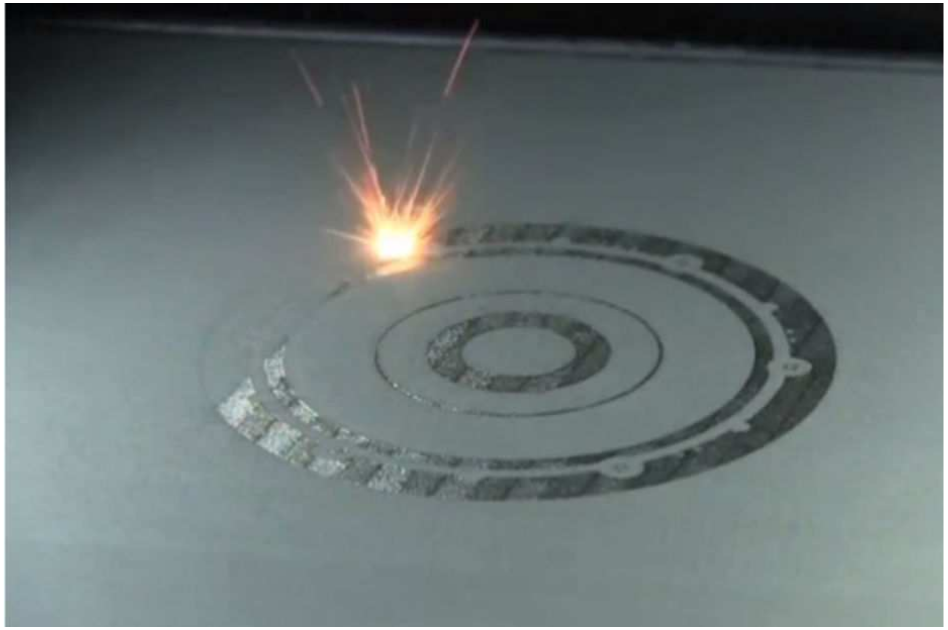
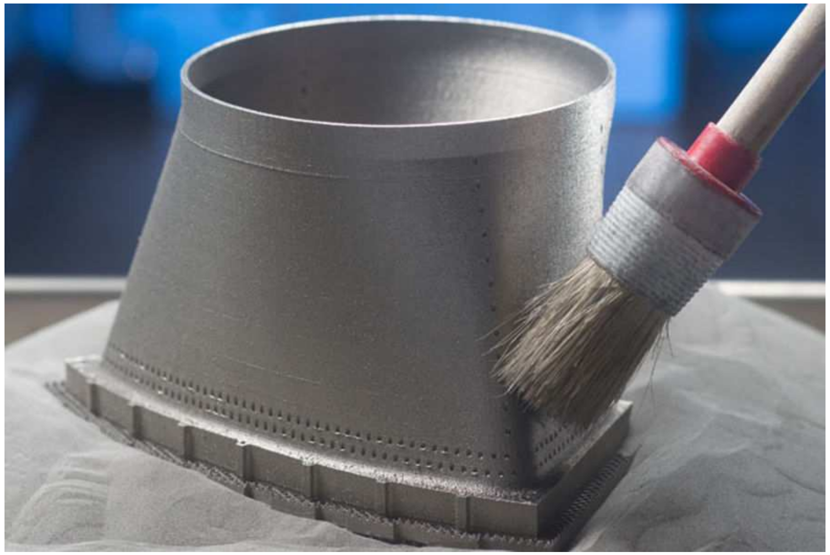
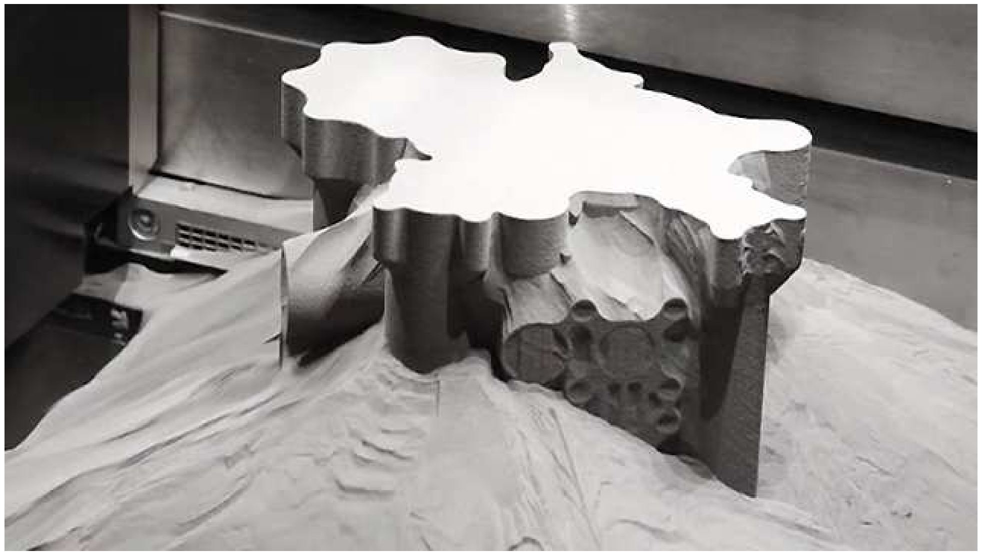
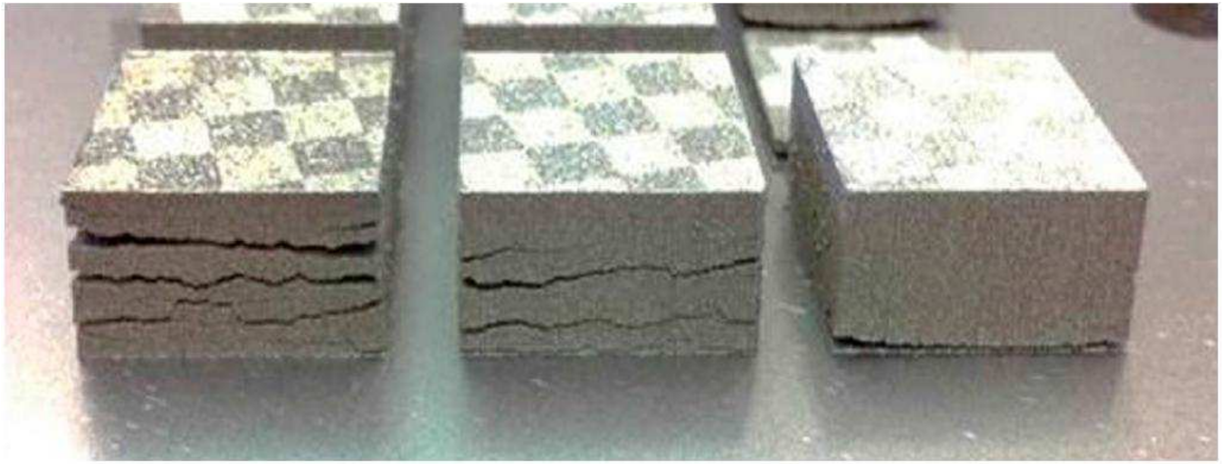


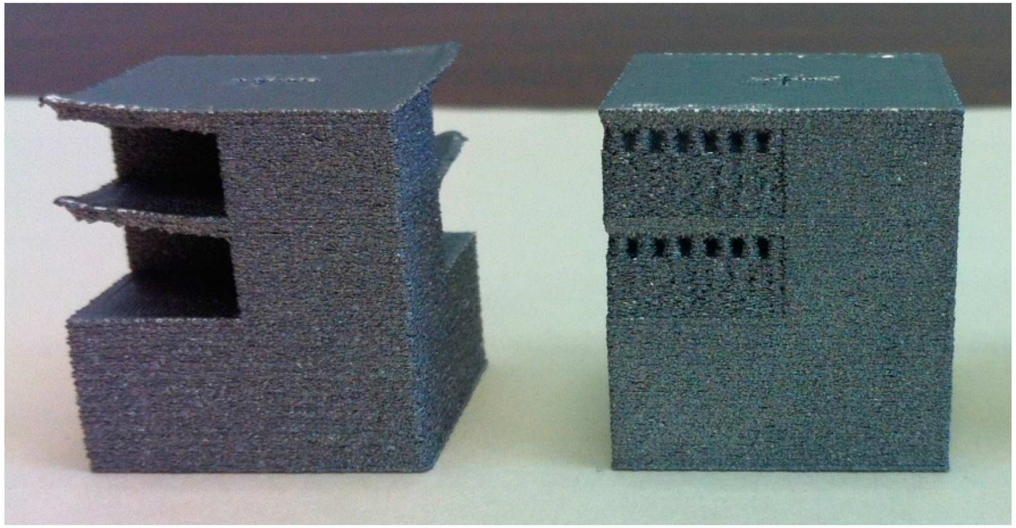


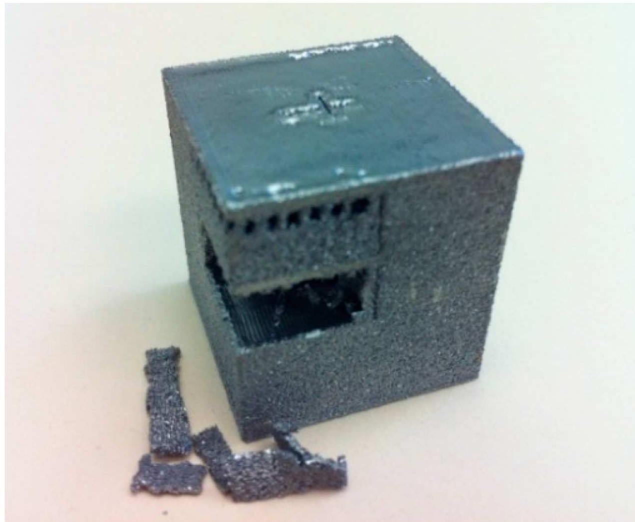


Some failures...

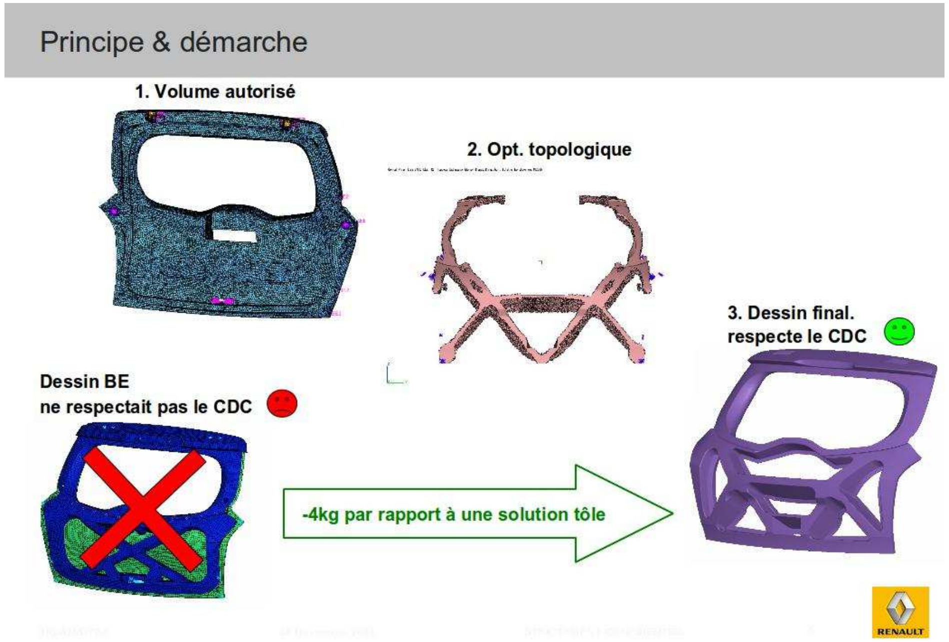


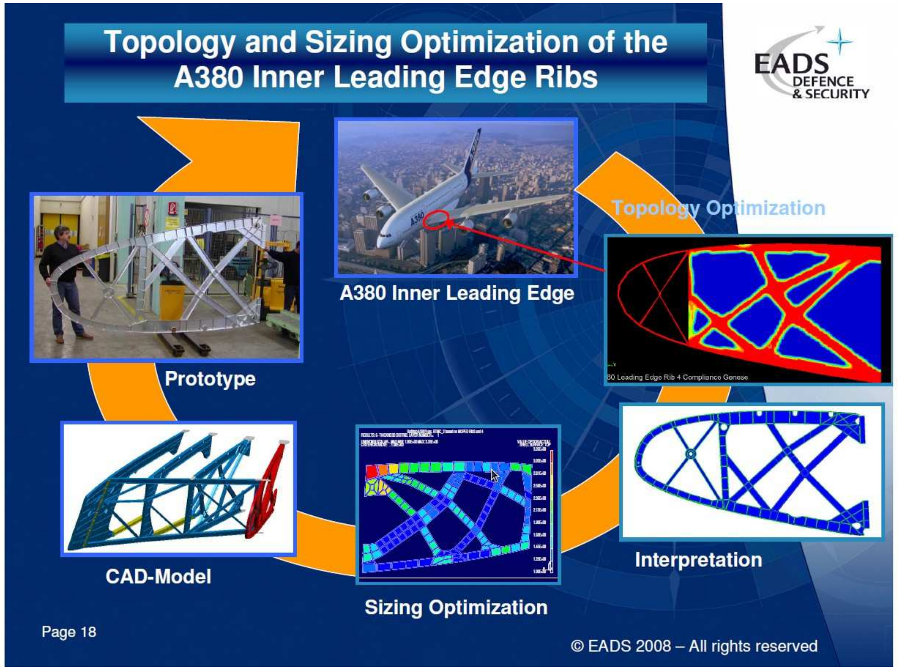
Some failures...





Shape and topology optimization





- ☞ Tremendous progresses were achieved on academic research about shape and topology optimization.
- ☞ Many commercial softwares which are heavily used by industry.
- ☞ Pending issue: manufacturability.

Shape and topology optimization

Minimize an objective function $J(\Omega)$ over a set $\mathcal{U}_{ad}$ of admissibles shapes Ω (including possible topology changes)

$$\inf_{\Omega\in\mathcal{U}_{ad},P(\Omega)\leq 0} J(\Omega)$$

with a (possible) constraint $P(\Omega)$

$$J(\Omega) = \int_\Omega j(u_\Omega)\,dx\,, \quad P(\Omega) = \int_\Omega c(u_\Omega)\,dx$$

where u_Ω is the solution of a partial differential equation (state equation)

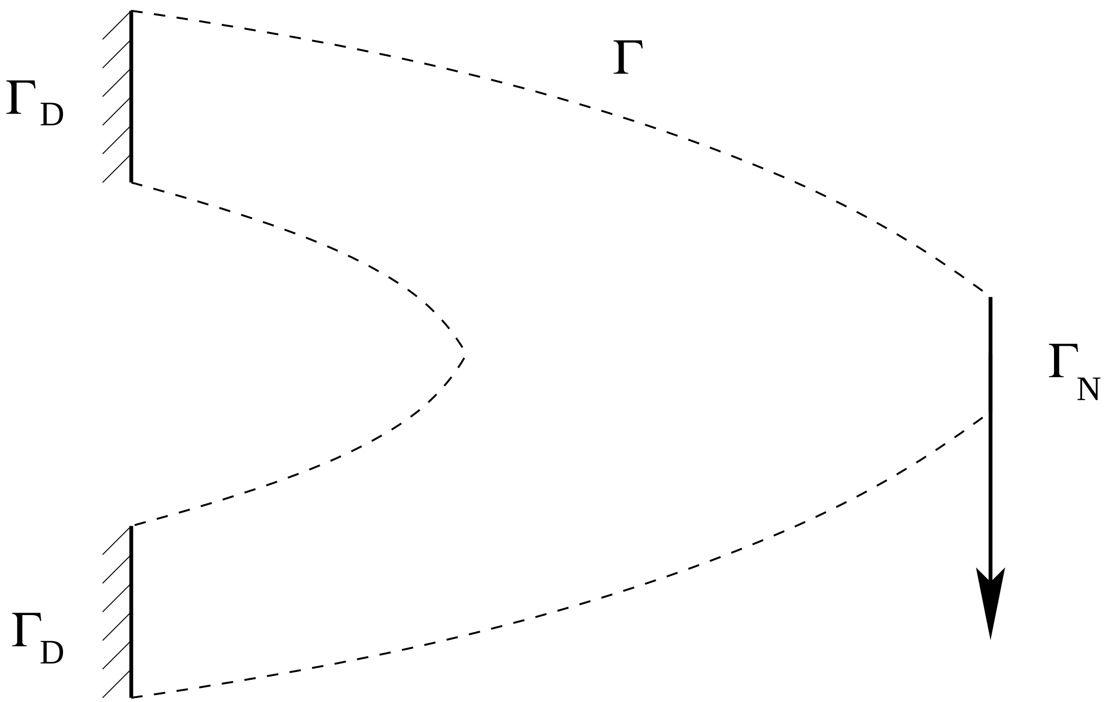
$$PDE(u_\Omega) = 0 \quad \text{in} \quad \Omega$$

Model problem

Shape $\Omega \subset \mathbb{R}^d$ with boundary $\partial\Omega = \Gamma \cup \Gamma_N \cup \Gamma_D$, where Γ_D and Γ_N are fixed.

$$\mathcal{U}_{ad} = \left\{ \Omega \subset D \text{ open set such that } \Gamma_D \bigcup \Gamma_N \subset \partial\Omega \text{ and } \int_\Omega dx = V_0 \right\},$$

with $D \subset \mathbb{R}^d$, a given “working domain” and V_0 a prescribed volume.



The model of linearized elasticity

For a given load $g : \Gamma_N \to \mathbb{R}^d$, the displacement $u : \Omega \to \mathbb{R}^d$ is the solution of

$$\begin{cases} -\operatorname{div}(A\,e(u)) = 0 & \text{in } \Omega \\ u = 0 & \text{on } \Gamma_D \\ \big(A\,e(u)\big)n = g & \text{on } \Gamma_N \\ \big(A\,e(u)\big)n = 0 & \text{on } \Gamma \end{cases}$$

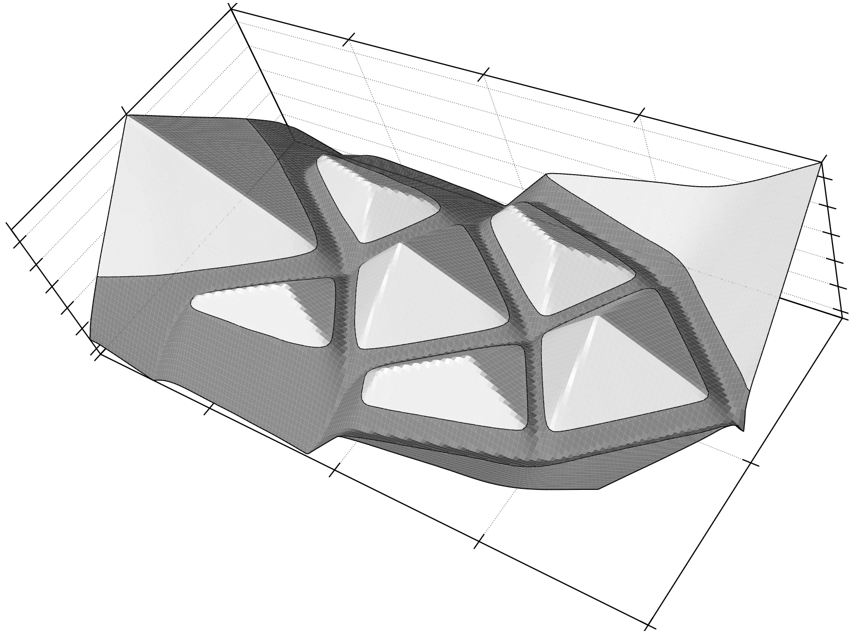
with the strain tensor $e(u) = \frac{1}{2}\left(\nabla u + (\nabla u)^T\right)$, the stress tensor $\sigma = Ae(u)$, and A an homogeneous isotropic elasticity tensor.

Typical objective function: compliance

$$J(\Omega) = \int_{\Gamma_N} g \cdot u\,dx,$$

where u depends on Ω.

LEVEL SET METHOD (Osher and Sethian)



A shape Ω is parametrized by a **level set** function

$$\psi(x) = 0 \Leftrightarrow x \in \partial\Omega \cap D, \quad \psi(x) < 0 \Leftrightarrow x \in \Omega, \quad \psi(x) > 0 \Leftrightarrow x \in (D \setminus \Omega)$$

Assume that the shape $\Omega(t)$ evolves in time t with a normal velocity $V(t,x)$. Then its motion is governed by the following Hamilton Jacobi equation

$$\frac{\partial \psi}{\partial t} + V|\nabla_x \psi| = 0 \quad \text{in } D.$$

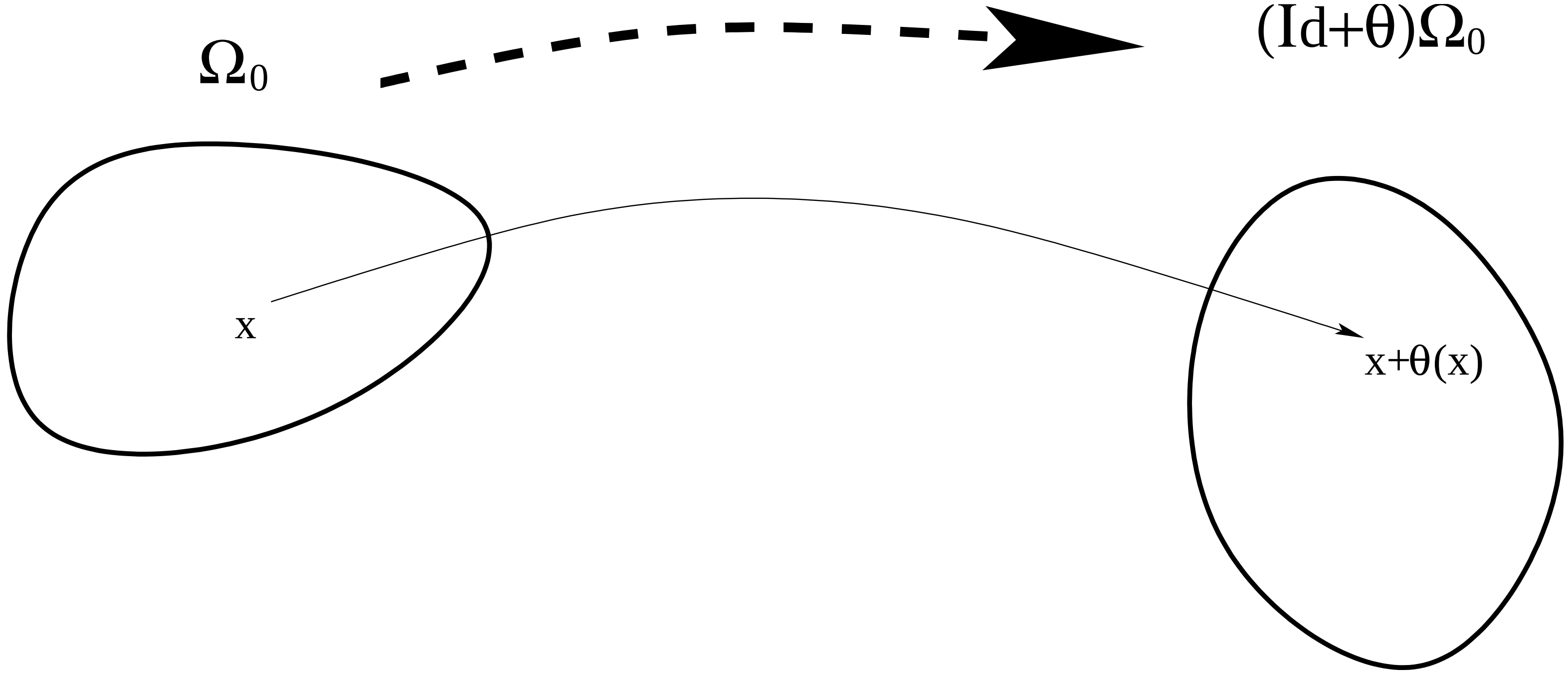
Advection velocity = shape gradient

The velocity V is deduced from the shape gradient of the objective function.

To compute this shape gradient we recall Hadamard's method.

Let Ω_0 be a reference domain. Shapes are parametrized by a vector field θ

$$\Omega = (\,\mathrm{Id} + \theta)\Omega_0 \quad \text{with} \quad \theta \in C^1(\mathbb{R}^d; \mathbb{R}^d).$$



Shape derivative

Definition: the shape derivative of $J(\Omega)$ at Ω_0 is the Fréchet differential of $\theta \to J\big((\,\mathrm{Id} + \theta)\Omega_0\big)$ at 0.

Hadamard structure theorem: the shape derivative of $J(\Omega)$ can always be written (in a distributional sense)

$$J'(\Omega_0)(\theta) = \int_{\partial\Omega_0} \theta(x) \cdot n(x)\, j(x)\, ds$$

where $j(x)$ is an integrand depending on the state u and an adjoint p.

We choose the normal velocity $V = \theta \cdot n$ such that $J'(\Omega_0)(\theta) \leq 0$.

Simplest choice: $V = \theta \cdot n = -j$ but other ones are possible.

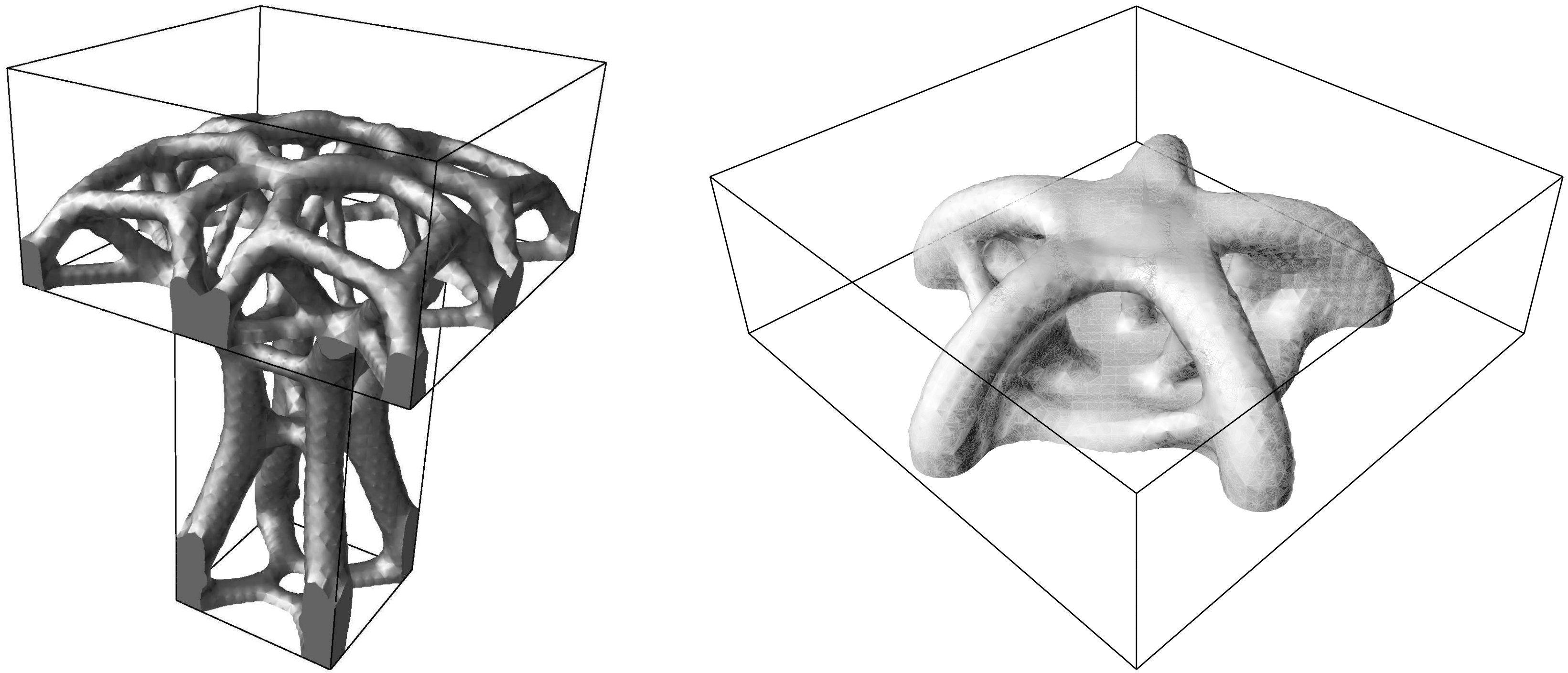
NUMERICAL ALGORITHM

1. Initialization of the level set function ψ_0 (including holes).
2. Iteration until convergence for $k \geq 1$:
   (a) Compute the elastic displacement u_k for the shape ψ_k.
   Deduce the shape gradient = normal velocity = V_k
   (b) Advect the shape with V_k (solving the Hamilton Jacobi equation) to obtain a new shape ψ_{k+1}.

Optimization algorithms:

1. Lagrangian (possibly augmented) algorithm,
2. SLP (sequential linear programming).

Examples of results with complex topologies



Hard to manufacture with traditional technologies (e.g. casting).

☞ Either, add geometrical constraints.

☞ Or, go for additive manufacturing.

-II- Mechanical constraints for additive manufacturing

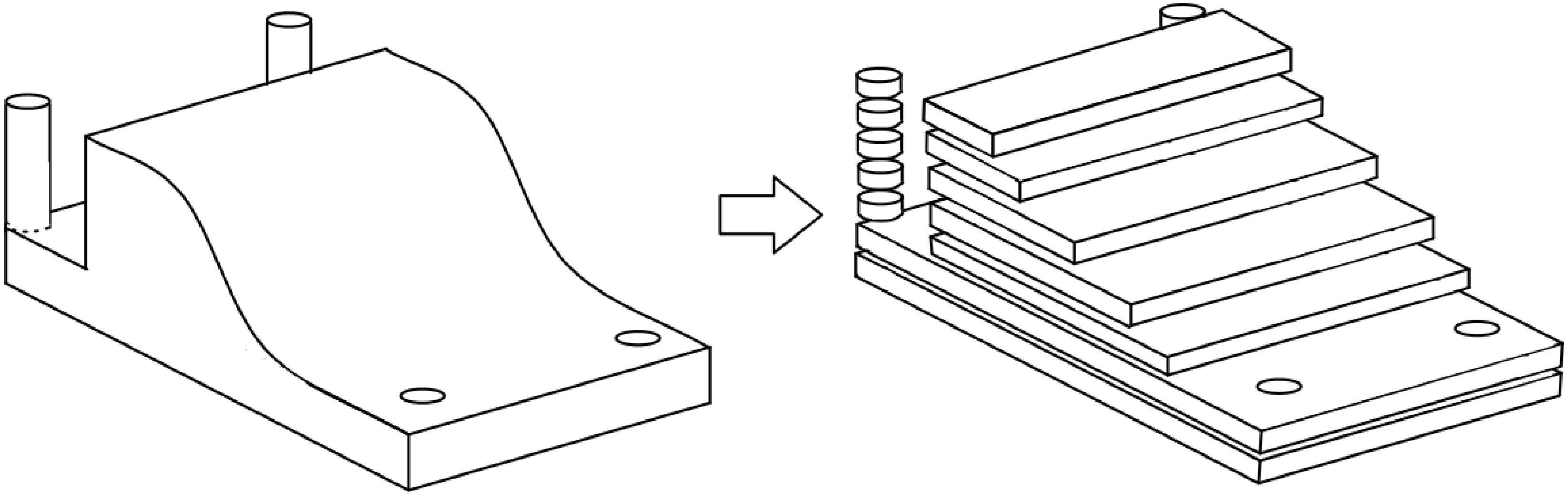
Although there are less constraints than for casting, here is a partial list of constraints for additive manufacturing:

- **overhang limitation,**
- **thermal residual stress,**
- preferred orientation of thin and slender structures,
- minimal time (or energy) for completion,
- removing the powder (no closed holes),
- adding (and removing) supports.

We discuss the two first issues.

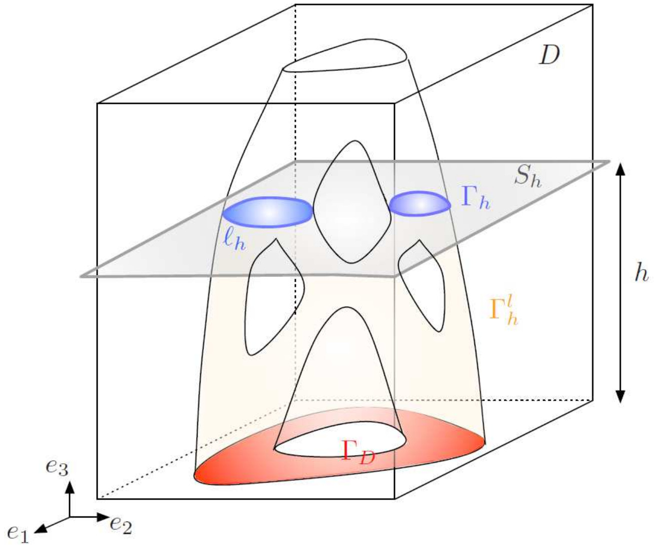
Many works on overhang limitations: Leary et al. (2014), Gaynor and Guest (2016), Langelaar (2016, 2017).

Layer by layer modelling



Additive manufacturing involves a layer by layer process.

Layer by layer modelling



For a final shape Ω, define **intermediate shapes** Ω_i of increasing height h_i

$$\Omega_i = \{x \in \Omega \text{ such that } x_d \leq h_i\} \quad 1 \leq i \leq n.$$

Two different state equations:

1. for the objective function of the final shape Ω, evaluated for its final use,
2. for the additive manufacturing constraint on the intermediate shapes Ω_i.

Overhang limitations

A **first example** is proposed in

G. Allaire, Ch. Dapogny, A. Faure, G. Michailidis, *Shape optimization of a layer by layer mechanical constraint for additive manufacturing*, C. R. Math. Acad. Sci. Paris, 355, no. 6, 699-717 (2017).

G. Allaire, C. Dapogny, R. Estevez, A. Faure and G. Michailidis, *Structural optimization under overhang constraints imposed by additive manufacturing technologies*, J. Comput. Phys. 351, pp.295-328 (2017).

1st state equation for the final shape

For a given applied load $f : \Gamma_N \to \mathbb{R}^d$,

$$\begin{cases} -\operatorname{div}(A\,e(u)) = 0 & \text{in } \Omega \\ u = 0 & \text{on } \Gamma_D \\ \big(A\,e(u)\big)n = f & \text{on } \Gamma_N \\ \big(A\,e(u)\big)n = 0 & \text{on } \Gamma \end{cases}$$

Objective function: compliance

$$J(\Omega) = \int_{\Gamma_N} f \cdot u\,dx,$$

2nd state equation for the intermediate shapes

Apply self-weight (gravity g) to the top layer of intermediate shapes Ω_i:

$$\begin{cases} -\operatorname{div}\left(A\, e(u_i)\right) &= \rho g_\delta & \text{in } \Omega_i, \\ u_i &= 0 & \text{on } \Gamma_D, \\ \big(A\, e(u_i)\big) n &= 0 & \text{on } \Gamma_i, \end{cases}$$

$$\text{with} \quad g_\delta(x) = \begin{cases} g & \text{if } h_i - \delta < x_d < h_i, \\ 0 & \text{otherwise,} \end{cases}$$

The boundary conditions are different from the first state equation.

Total self-weight compliance constraint:

$$P(\Omega) = \sum_{i=1}^{n} \int_{\Omega_i} Ae(u_i) : e(u_i)\, dx = \sum_{i=1}^{n} \int_{\Omega_i} \rho g_\delta \cdot u_i\, dx$$

Self-weight compliance constraint

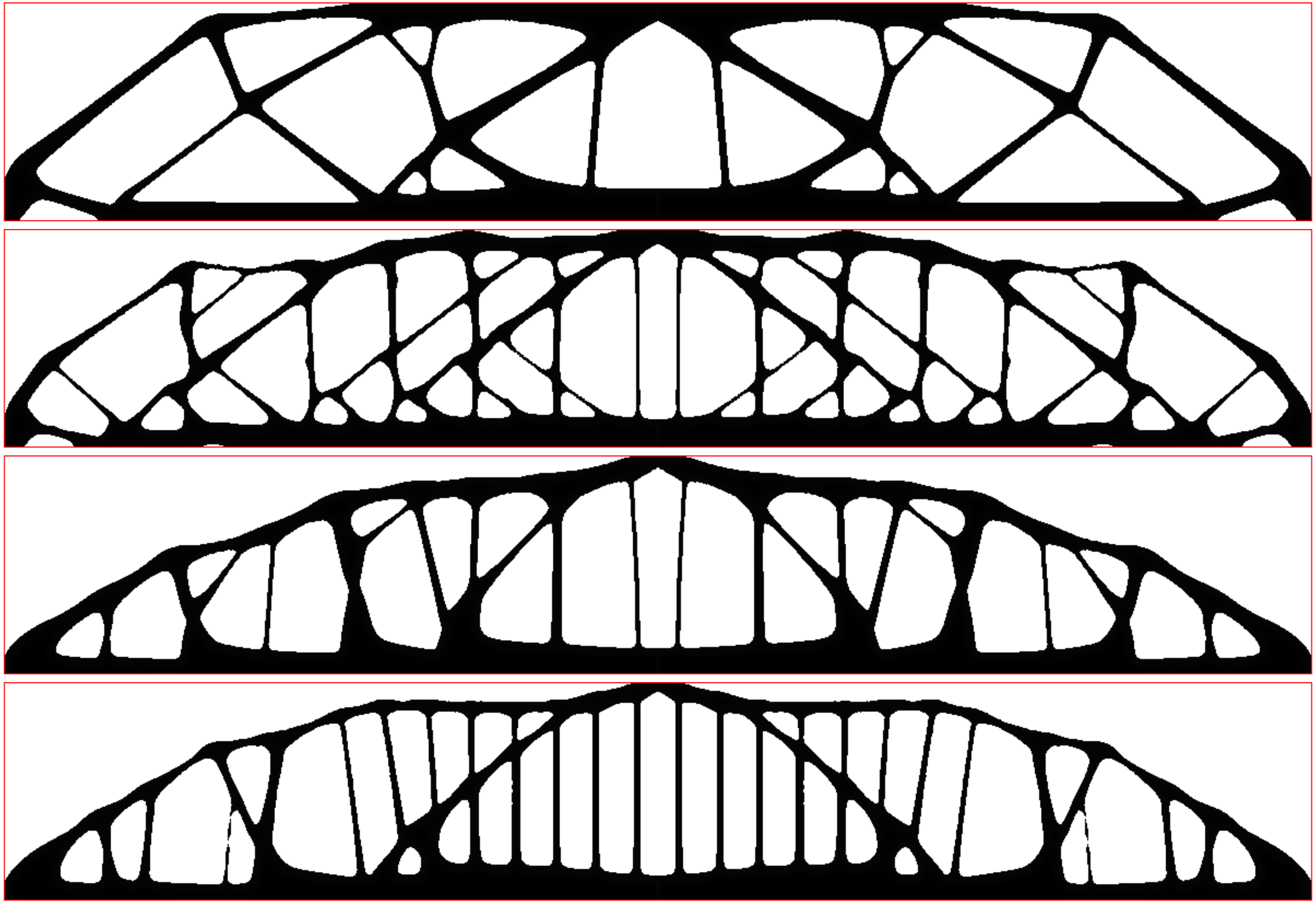
We solve the optimization problem:

$$\begin{aligned} \min_{\Omega \subset D} \quad & J(\Omega) \\ \text{s.t.} \quad & V(\Omega) \leq 0.20|D| \\ & P(\Omega) \leq \alpha P(\Omega_{ref}),\ \alpha \in (0,1). \end{aligned}$$

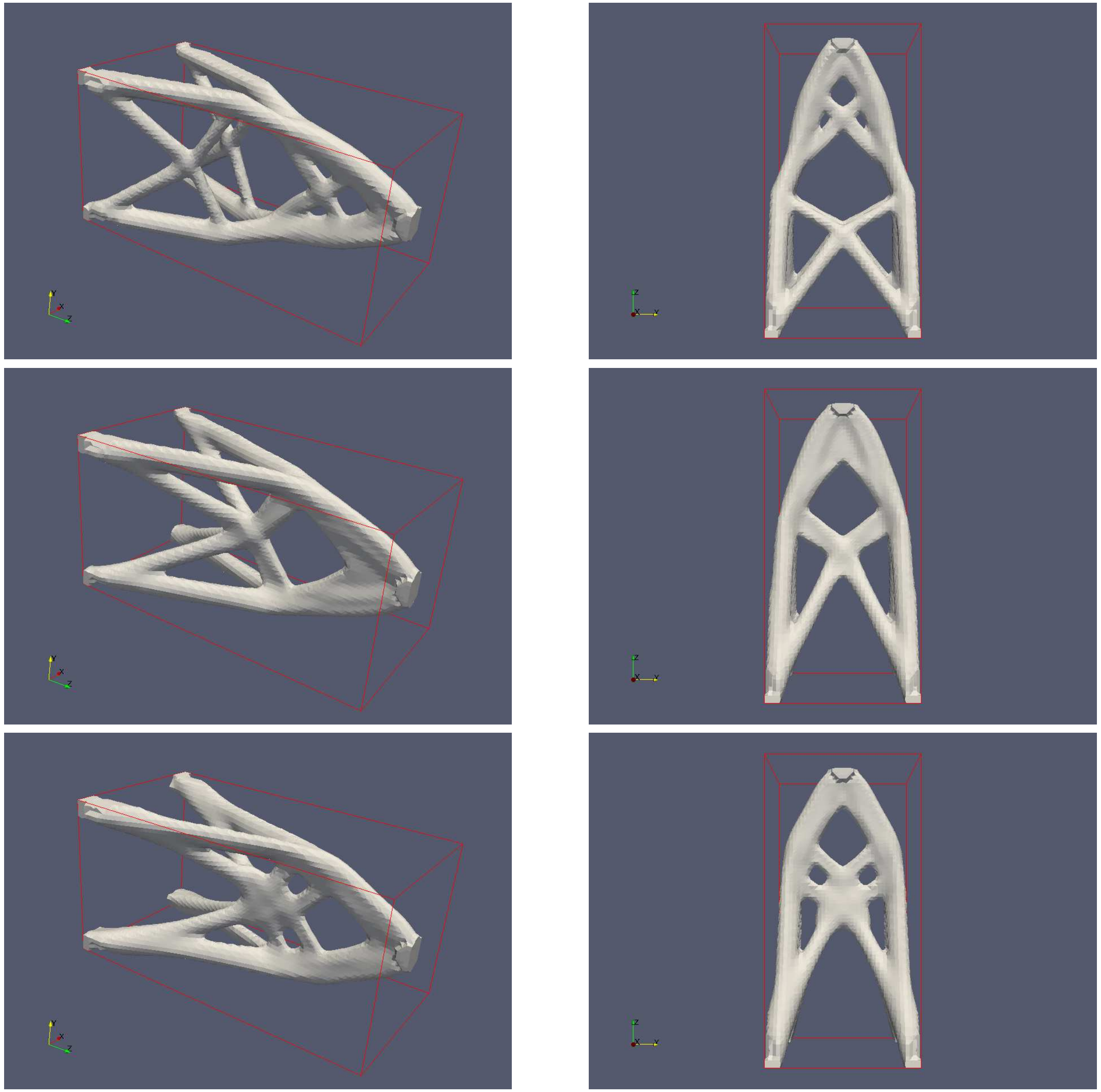
where Ω_{ref} is the optimal design without constraint and α is a parameter of the method.

Recall that $J(\Omega)$ is the compliance for the final shape and $P(\Omega)$ is the self-weight constraint for the intermediate shapes.

Self-weight compliance constraint



Self-weight compliance constraint in 3-d



-III- Thermal residual stresses

Same idea with a more involved model:

☞ Keep the intermediate **"layer by layer"** shapes Ω_i, $1 \leq i \leq n$.

☞ Each layer i is built between time t_{i-1} and t_i.

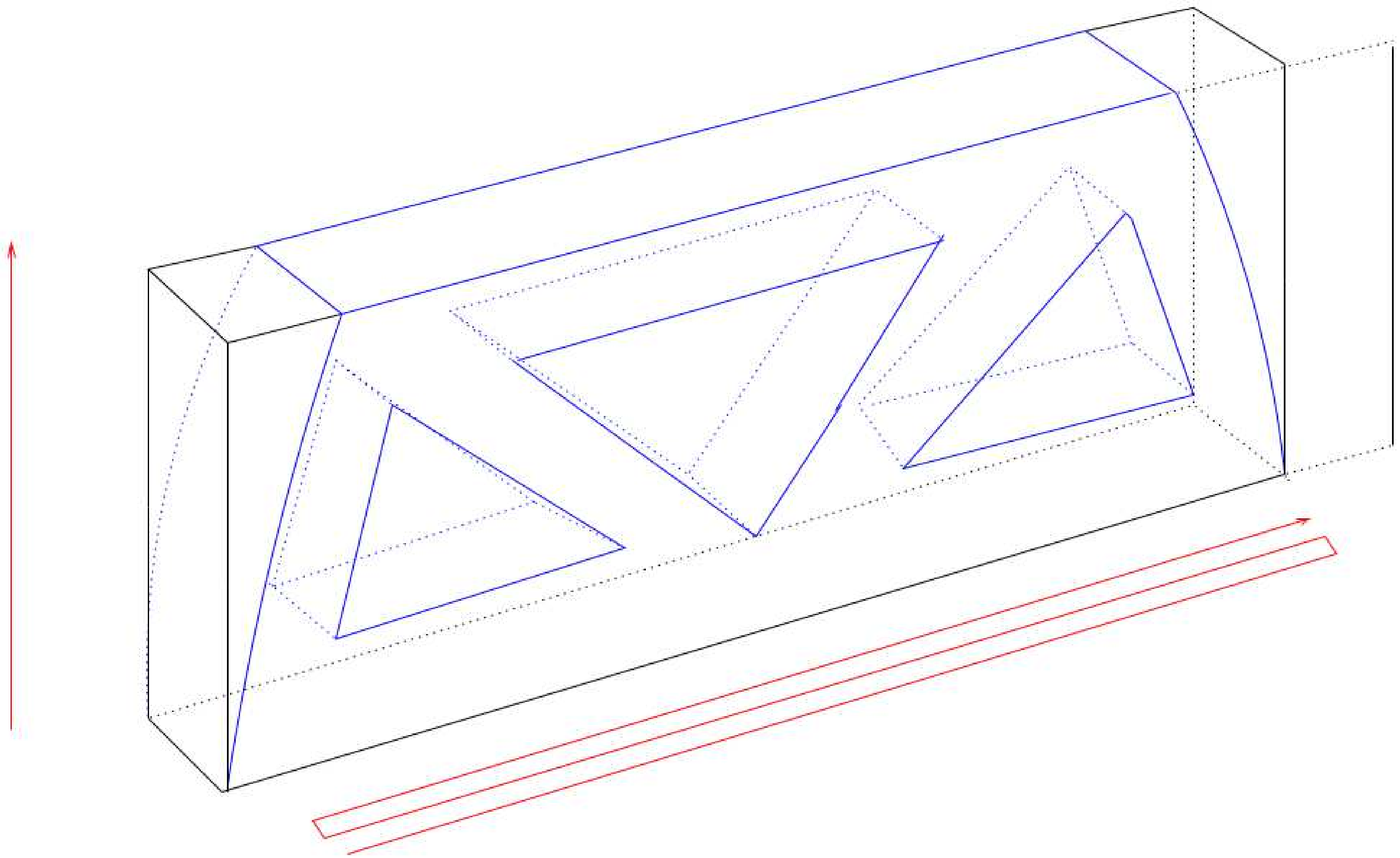
☞ Holes are now **filled by a metallic powder**.

☞ Thermal residual stress computed by a model as in

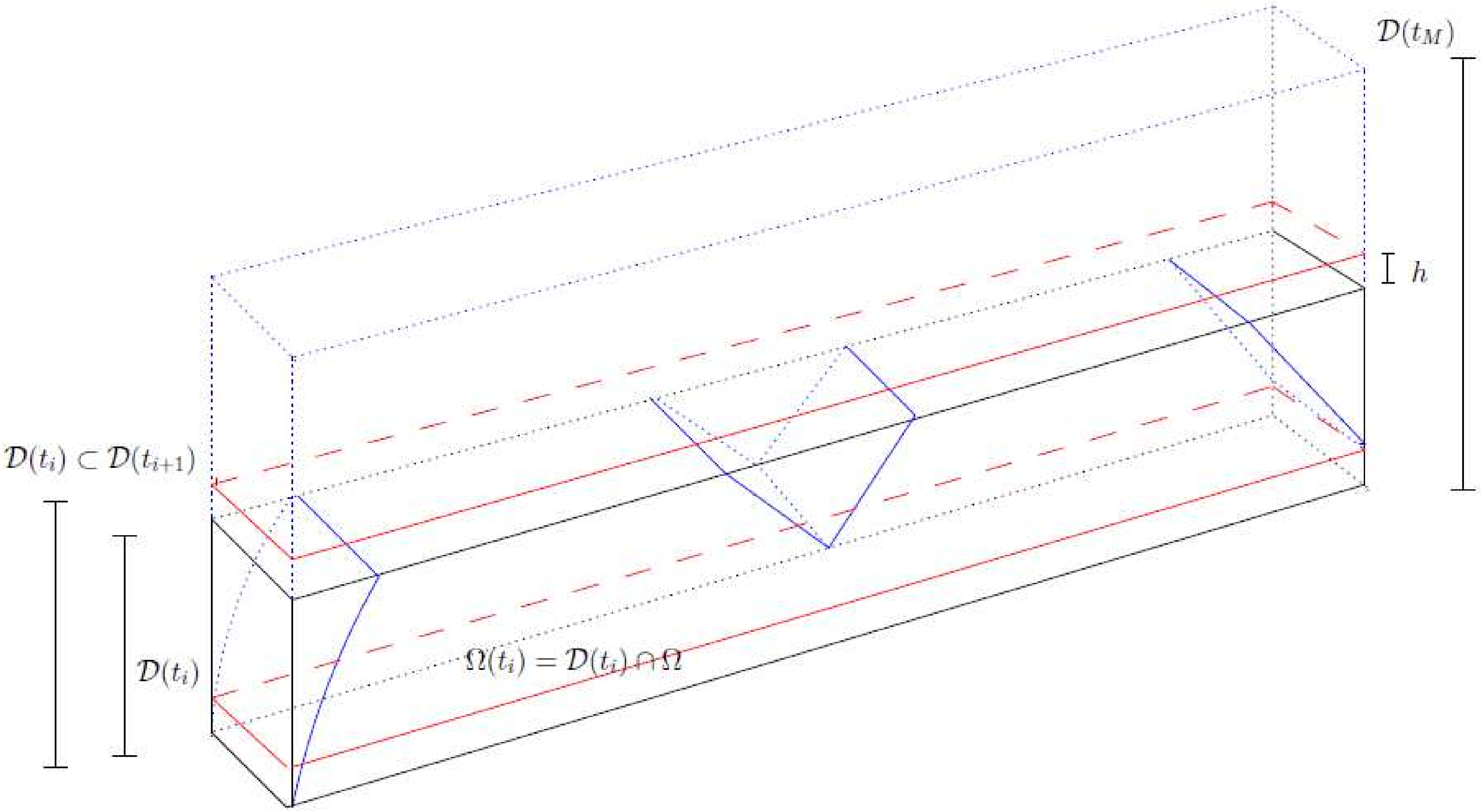
L. Van Belle, J.-C. Boyer, G. Vansteenkiste, *Investigation of residual stresses induced during the selective laser melting process*, Key Engineering Materials, 1828-2834 (2013).

M. Megahed, H.-W. Mindt, N. NâDri, H. Duan, O. Desmaison, *Metal additive-manufacturing process and residual stress modeling*, Integrating Materials and Manufacturing Innovation, 5:4, (2016).

Final shape in the build chamber



Intermediate shape at height h



Notations

- ☞ Each layer i is built between time t_{i-1} and t_i, $1 \leq i \leq n$.
- ☞ Build chamber D, vertical build direction e_d.
- ☞ Intermediate domains $D_i = \{x \in D \text{ such that } x_d \leq h_i\}$.
- ☞ Final shape Ω and intermediate shapes $\Omega_i = \Omega \cap D_i$.
- ☞ Mixture $D_i = \Omega_i \cup P_i$ of solid and powder.

Thermo-mechanical model

Heat equation:

$$\begin{cases} \rho \dfrac{\partial T}{\partial t} - \mathrm{div}(\lambda \nabla T) = Q(t) & \text{in } (t_{i-1}, t_i) \times D_i \\ T = T_{init} & \text{on } (t_{i-1}, t_i) \times \Gamma_{base} \\ \lambda \nabla T \cdot n = -H_e (T - T_{init}) & \text{on } (t_{i-1}, t_i) \times (\partial D_i \setminus \Gamma_{base}) \\ T(t = t_{i-1}) = T_{init} & \text{in } D_i \setminus D_{i-1} \end{cases}$$

Thermoelastic quasi-static equation:

$$\begin{cases} -\mathrm{div}(\sigma) = 0 \quad \text{and } \sigma = \sigma^{el} + \sigma^{th} & \text{in } (t_{i-1}, t_i) \times D_i, \\ \sigma^{el} = Ae(u) \quad \text{and } \sigma^{th} = K(T - T_{init}) \, \mathrm{Id}, & \end{cases}$$

The material parameters ρ, λ, A, K are different for the solid and the powder.

The source term $Q(t)$ is the beam spot, traveling on the upper layer.

Weak coupling: **first**, solve the heat equation, **second**, thermoelasticity.

Thermo-mechanical objective

The objective (or constraint) function is

$$J(\Omega) = \int_\Omega f \cdot u_{final}\, dx + \beta \sum_{i=1}^{n} \int_{t_{i-1}}^{t_i} \int_{D_i} j(u,\sigma,T)\, dx\, dt$$

where u_{final} is the elastic displacement for the **final shape**, (u,σ,T) is the displacement, stress and temperature fields for the **intermediate shapes** and β is a Lagrange multiplier.

- ☞ Static linearized elasticity for the **final shape**

$$-\operatorname{div}\left(A\, e(u_{final})\right) = f \quad \text{in } \Omega$$

- ☞ We compute the shape derivative of $J(\Omega)$ by an adjoint method.
- ☞ The adjoints are backward in time (huge cost and storage !).
- ☞ The shape boundary $\partial\Omega$ is an interface Γ (between metal and powder) for the **intermediate domains** D_i.

Adjoint problems

Example for an objective $j(u)$ without temperature and stress (for simplicity).

Elasticity adjoint equation: no "backward effect"

$$-\operatorname{div}(e(\eta)) = -j'(u) \quad \text{in } (t_{i-1}, t_i) \times D_i$$

Adjoint heat equation: backward in time, from $i = n$ to 1,

$$\begin{cases} \rho \dfrac{\partial p}{\partial t} + \operatorname{div}(\lambda \nabla p) = K \operatorname{div}\eta & \text{in } (t_{i-1}, t_i) \times D_i \\ p = 0 & \text{on } (t_{i-1}, t_i) \times \Gamma_{base} \\ \lambda \nabla p \cdot n = -H_e p & \text{on } (t_{i-1}, t_i) \times (\partial D_i \setminus \Gamma_{base}) \\ p(t = t_n) = 0 & \text{in } D_n \end{cases}$$

Reversed order of coupling: **first**, solve the adjoint elasticity, **second**, the adjoint heat equation.

Shape derivative

Denote by Γ the interface between solid and powder and by $[\cdot]$ the jump through the interface Γ.

$$
\begin{aligned}
J'(\Omega)(\theta) \quad = \quad & -\int_\Gamma \theta\cdot n\, Ae(u_{final}) : e(u_{final})\, ds \\
+ \quad & \beta \sum_{i=1}^{n} \int_{t_{i-1}}^{t_i} \int_\Gamma \theta\cdot n \left\{ [\rho]\frac{\partial T}{\partial t} p + [\lambda]\nabla T\cdot\nabla p - [Q]p \right\} ds\, dt \\
+ \quad & \beta \sum_{i=1}^{n} \int_{t_{i-1}}^{t_i} \int_\Gamma \theta\cdot n \left\{ ([A]e(u) + [K](T - T_{init})\,\mathrm{Id}) : e(\eta) \right\} ds\, dt \\
+ \quad & \beta \sum_{i=1}^{n} \int_{t_{i-1}}^{t_i} \int_{(\partial D_i\setminus\Gamma_{base})\cap\partial\Gamma} \theta\cdot\tau\, [H](T - T_{init}) p\, dL\, dt
\end{aligned}
$$

where τ is a unit vector, tangent to Γ and normal to $\partial\Gamma$.

Technical assumption: the direct solutions (u, T) and adjoint ones (η, p) are discretized (say by FEM).

Two objective functions

☞ Minimize the deviatoric part of the stress $\sigma_D = 2\mu e(u)_D$

$$J_1(\Omega) = \sum_{i=1}^{n} \int_{t_{i-1}}^{t_i} \int_{D_i} |\sigma_D|^2 \, dx \, dt$$

☞ Minimize the top vertical displacement (to allow the rake or roller to coat a new powder layer)

$$J_2(\Omega) = \sum_{i=1}^{n} \int_{t_{i-1}}^{t_i} \int_{D_i \setminus D_{i-1}} \left|\max(0, u \cdot e_d - u_{max})\right|^2 \, dx \, dt$$

Simplified model

Ideas:

1. forget the layer by layer construction,
2. forget the moving source term.

Consequences:

☞ apply the thermo-mechanical model only at the final shape Ω,

☞ take a source term $Q(t,x)$ constant in time and in the solid (zero in the powder),

☞ perform just a few time steps,

☞ simpler and faster ! (More simplification are possible...)

Material parameters

Solid: $E_1 = 200$ GPa, $\nu_1 = 0.3$, $\rho_1 = 8000$ kg.m^{-3}, $\lambda_1 = 15\ W.m^{-1}C^{-1}$, $K_1 = 0.000015\ C^{-1}$, $H_e^1 = 10\ Wm^{-2}C^{-1}$

Powder: $E_2 = 1.6$ GPa, $\nu_2 = 0.3$, $\rho_2 = 4000$ kg.m^{-3}, $\lambda_2 = 0.25\ W.m^{-1}C^{-1}$, $K_2 = 0.000001\ C^{-1}$, $H_e^2 = 10\ Wm^{-2}C^{-1}$

Source term: $Q_1 = 76800$ J, $Q_2 = 10^{-3}Q_1$

Heat capacity: $C_p^1 = C_p^2 = 450\ J.kg^{-1}C^{-1}$

Computational parameters: $\Delta t = 0.01$ s, mesh with 5359 nodes in 2-d and 108840 nodes in 3-d.

(Some further dimensionalization is required in 2-d...)

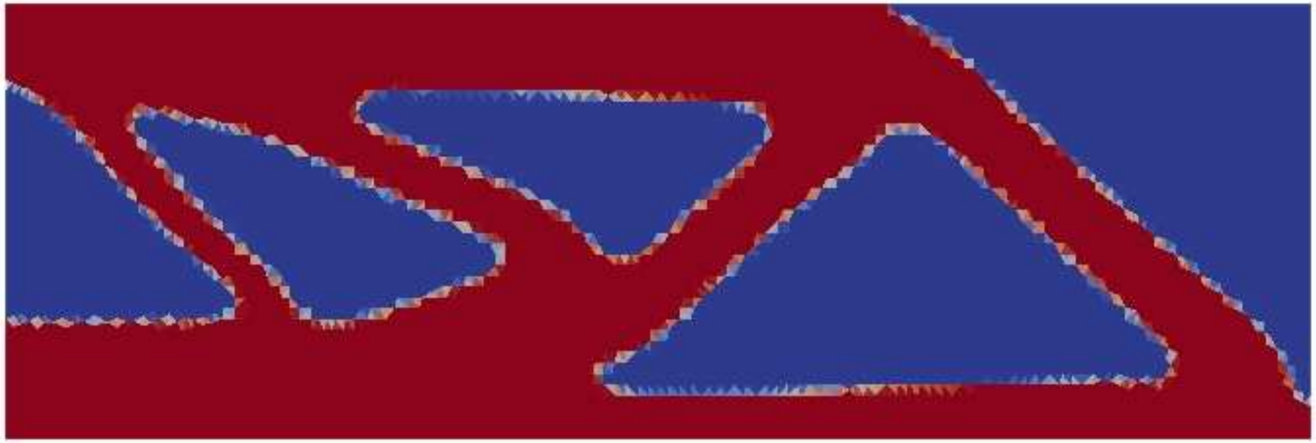
Test case 1

- Half MBB beam (2-d).
- Simplified model with $n = 5$ time steps.
- Minimize the deviatoric part of the stress $\sigma_D = 2\mu e(u)_D$

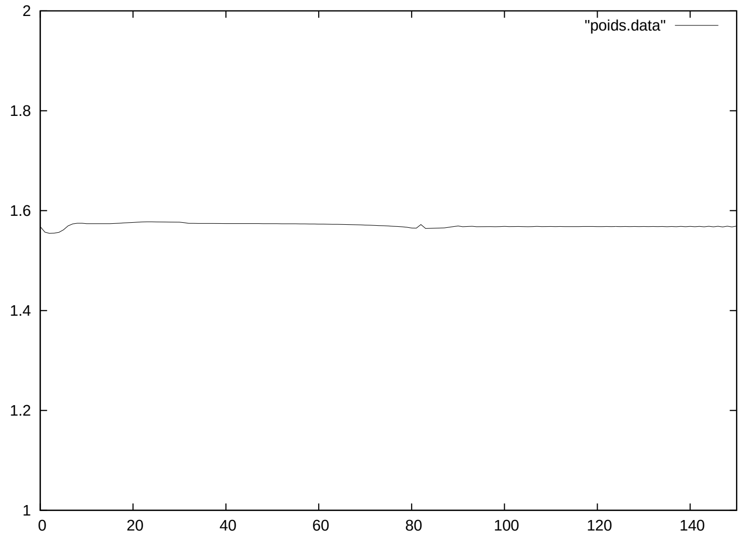
$$J_1(\Omega) = \sum_{i=1}^{n} \int_{t_{i-1}}^{t_i} \int_D |\sigma_D|^2 \, dx \, dt$$

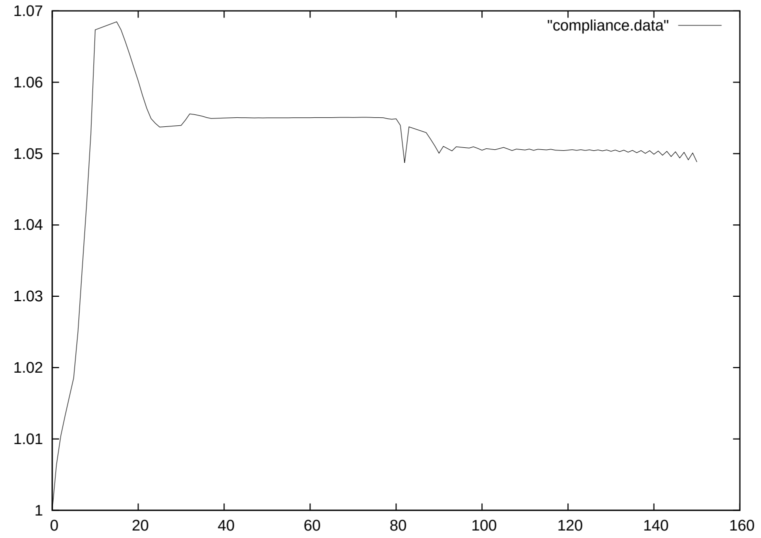
- Constraints on volume (fixed) and compliance.
- Initial design: optimal design for compliance minimization.

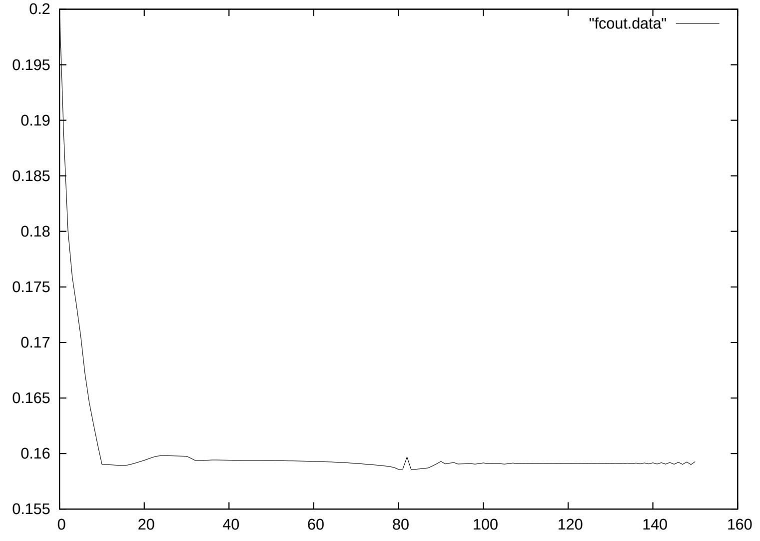
Initial and final shape



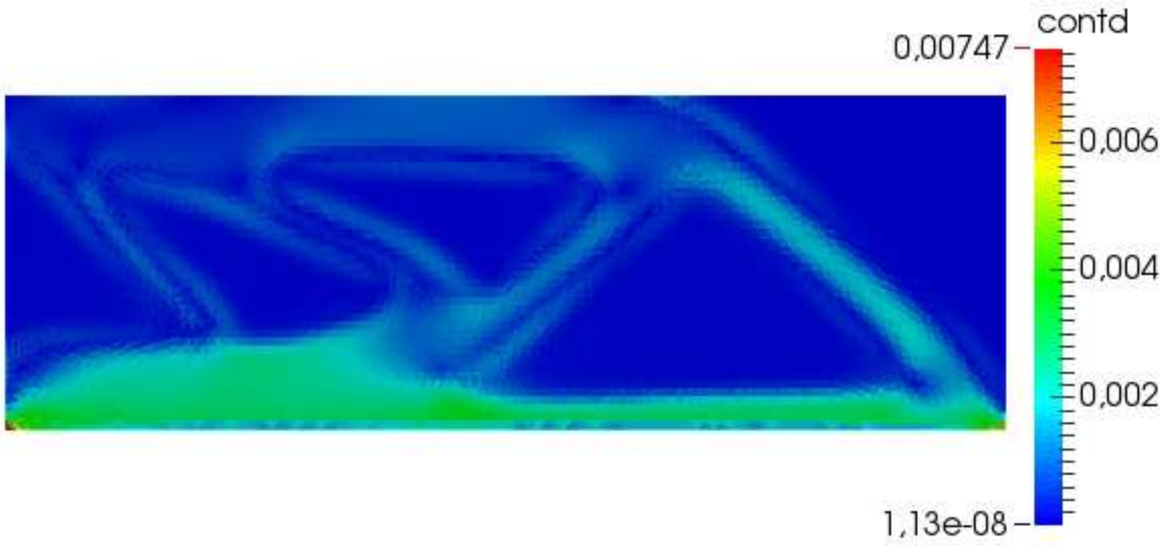
Convergence history (weight, compliance, thermal stress)

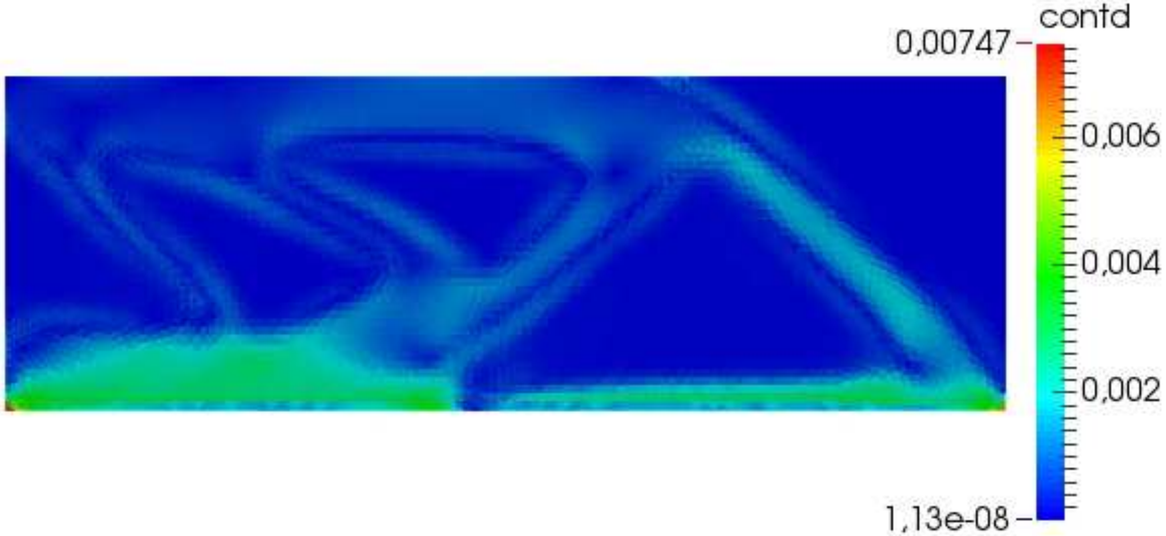






Plot of thermal stress $\sqrt{\int_0^T |\sigma^D|^2(x)\,dt}$





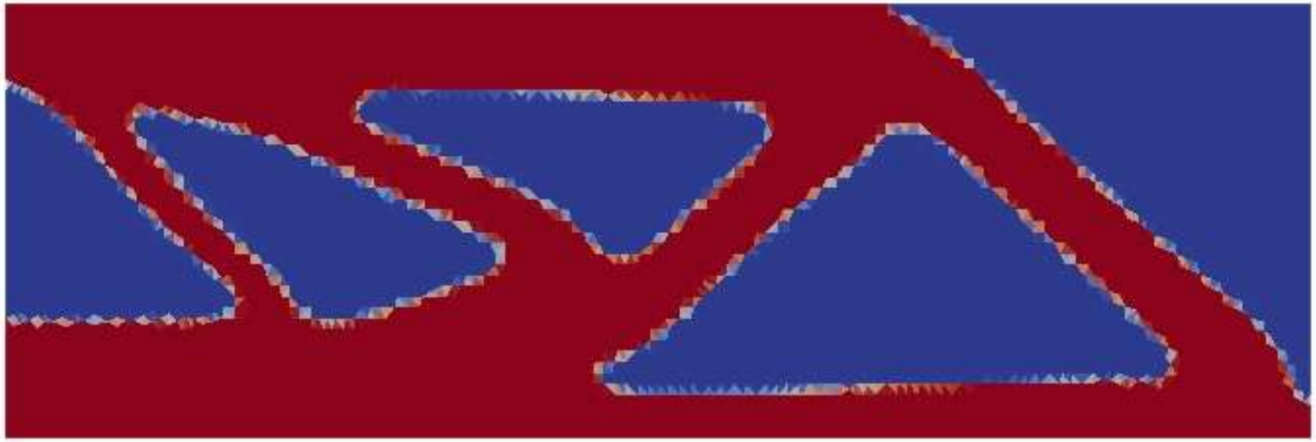
Test case 2

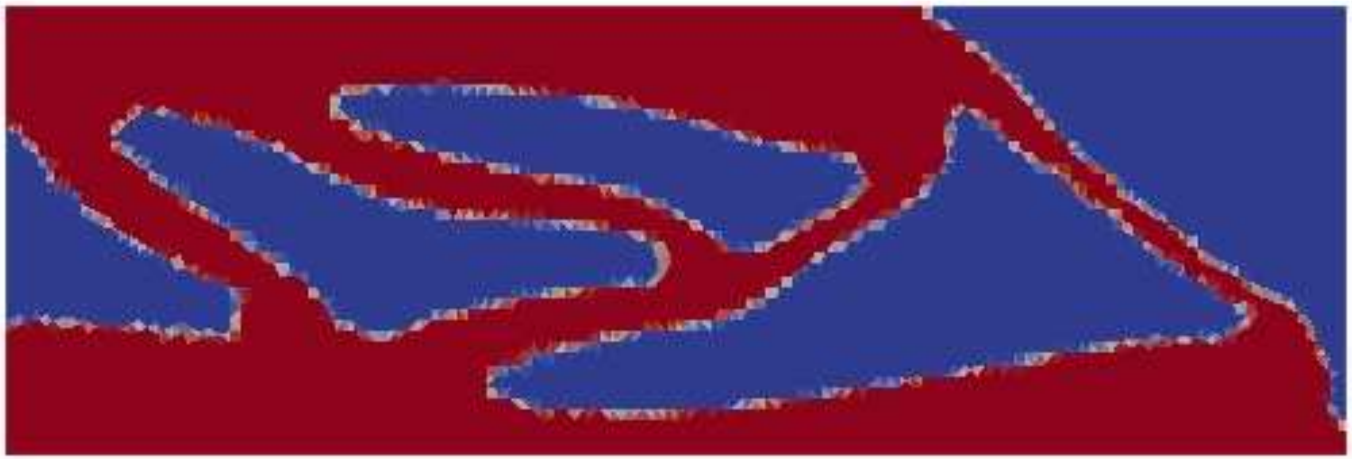
- Half MBB beam (2-d).
- Simplified model with 5 time steps.
- Minimize the vertical displacement (to allow the rake or roller to coat a new powder layer)

$$J_2(\Omega) = \sum_{i=1}^{n} \int_{t_{i-1}}^{t_i} \int_D \left|\max(0, u \cdot e_d - u_{max})\right|^2 \, dx \, dt$$

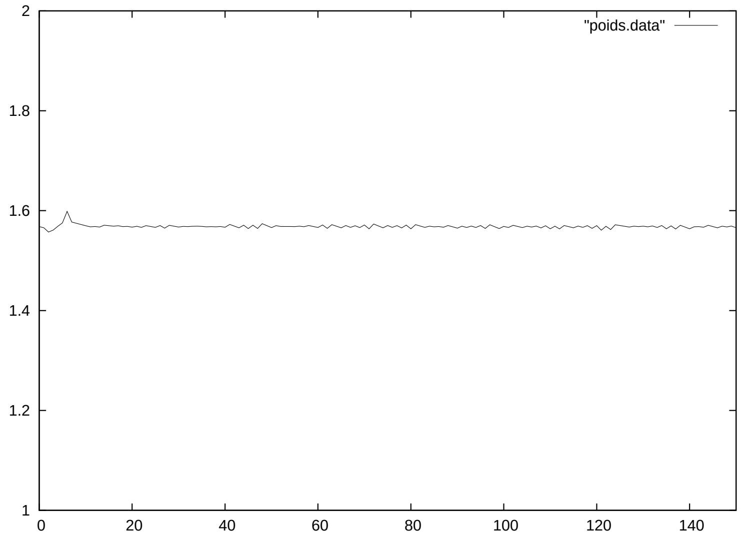
- The value u_{max} is guessed from the initial design.
- Constraints on volume (fixed) and compliance.
- Initial design: optimal design for compliance minimization.

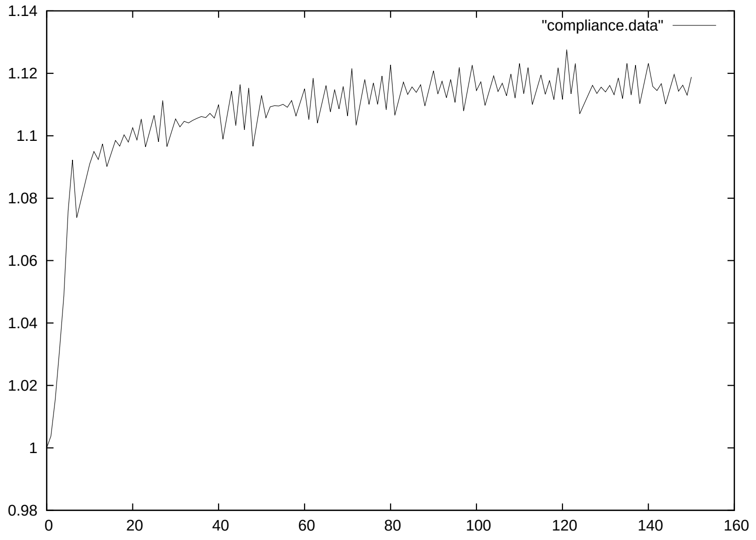
Initial and final shape

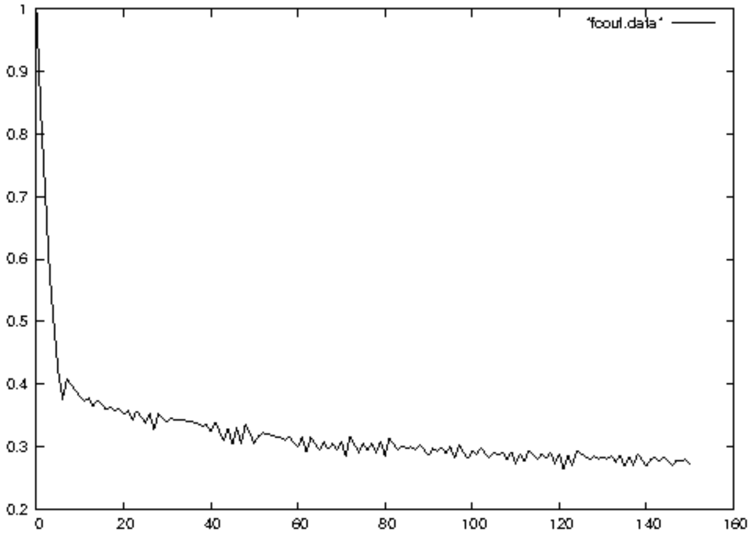




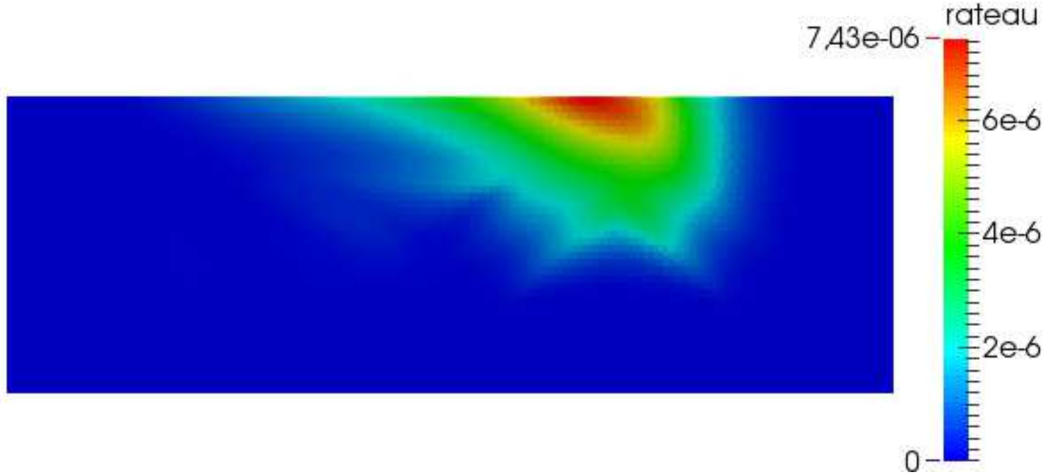
Convergence history (weight, compliance, thermal stress)

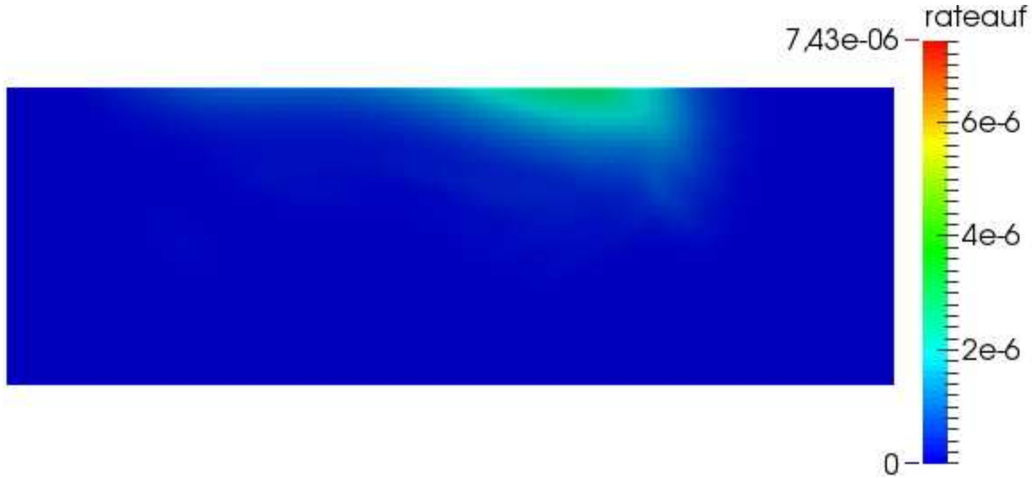






Initial and final constraint on the vertical displacement



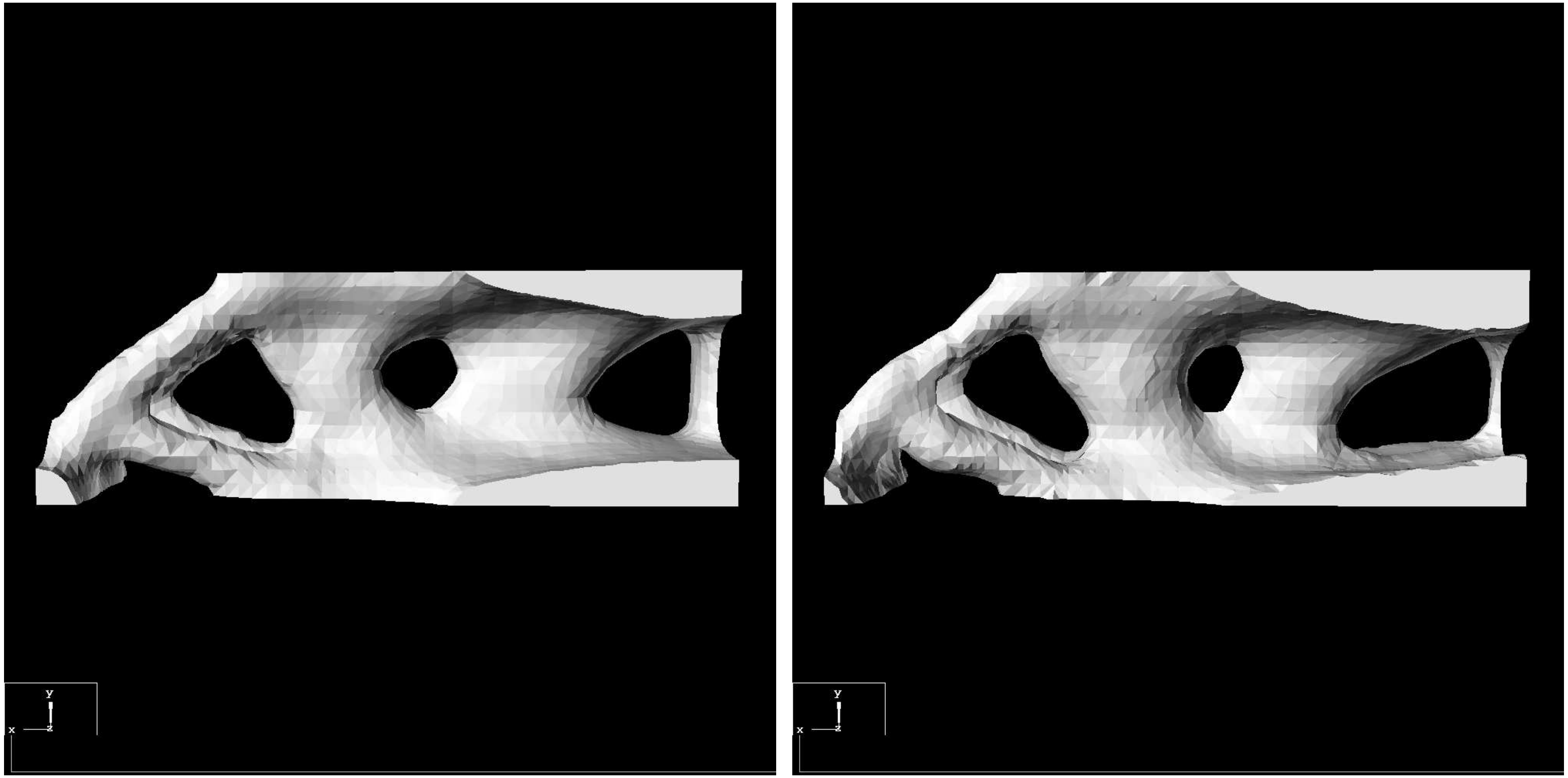


Test case 3

- Half MBB beam (3-d).
- Simplified model with 10 time steps.
- Minimize the deviatoric part of the stress $\sigma_D = 2\mu e(u)_D$

$$J_1(\Omega) = \sum_{i=1}^{n} \int_{t_{i-1}}^{t_i} \int_D |\sigma_D|^2 \, dx \, dt$$

- Constraints on volume (fixed) and compliance.
- Initial design: optimal design for compliance minimization.



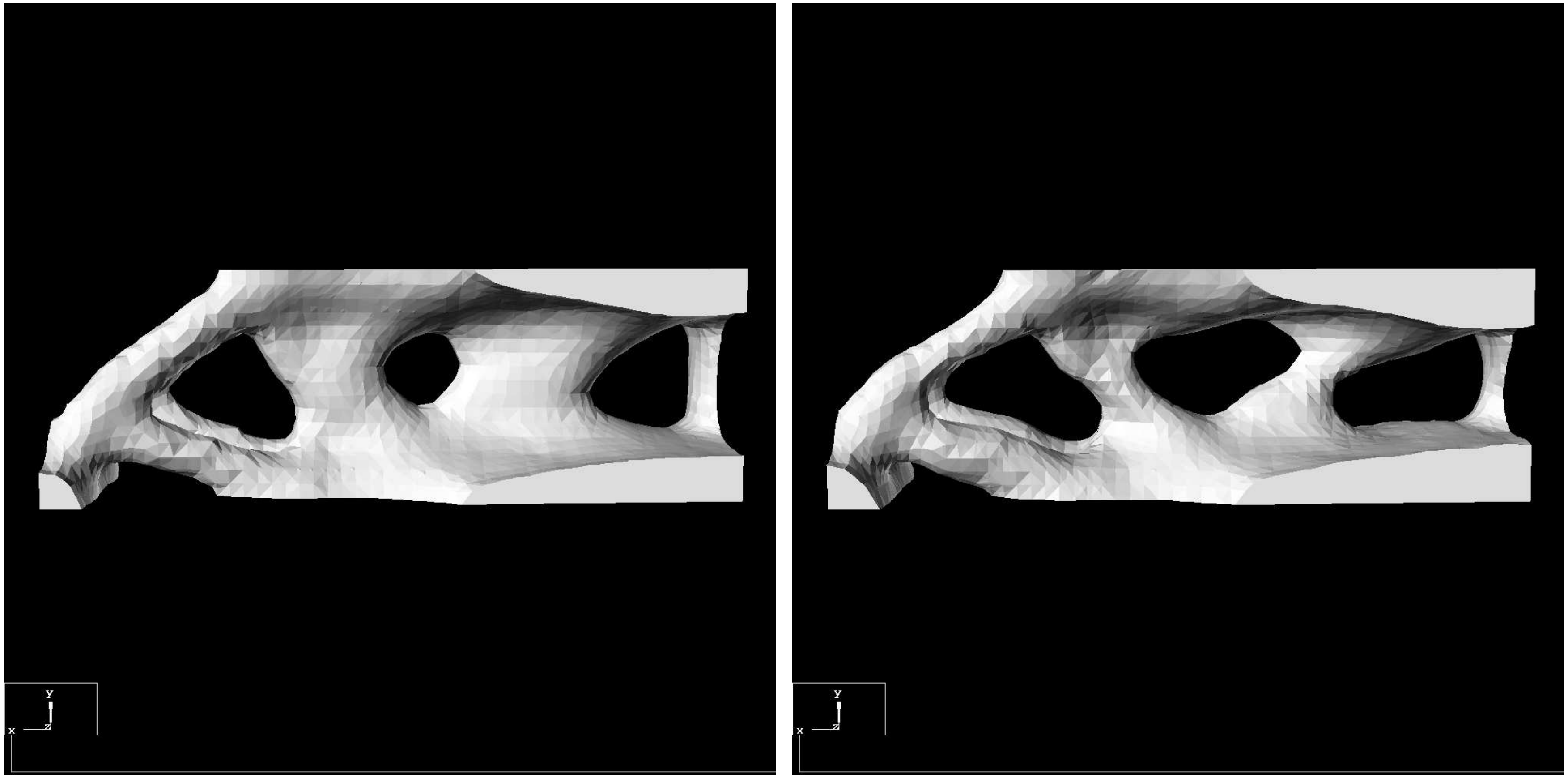
Test case 3bis

- Half MBB beam (3-d).
- Simplified model with 10 time steps.
- Minimize the vertical displacement (to allow the rake or roller to coat a new powder layer)

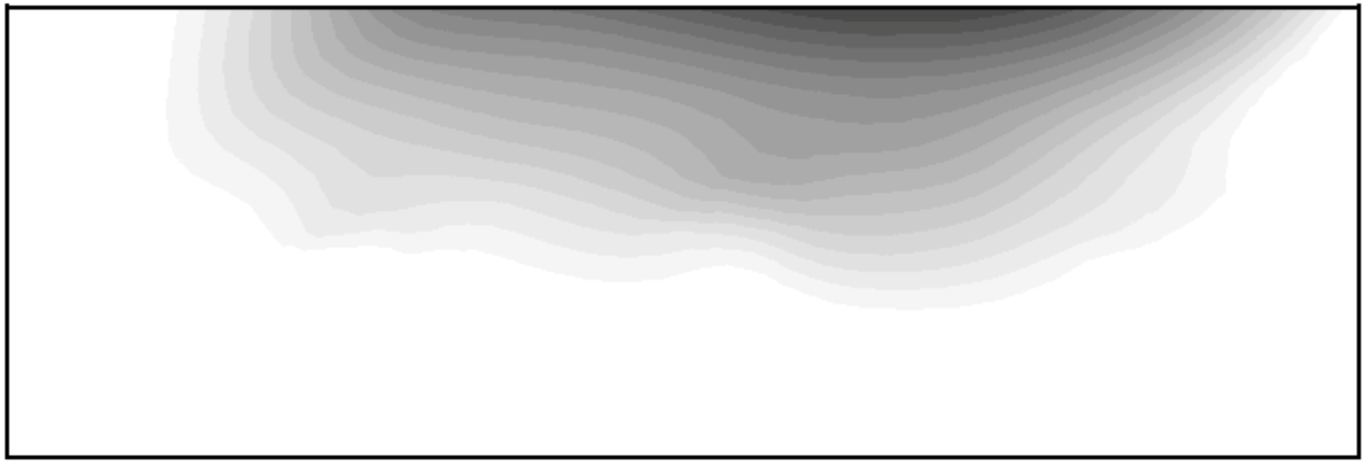
$$J_2(\Omega) = \sum_{i=1}^{n} \int_{t_{i-1}}^{t_i} \int_D |\max(0, u \cdot e_d - u_{max})|^2 \, dx \, dt$$

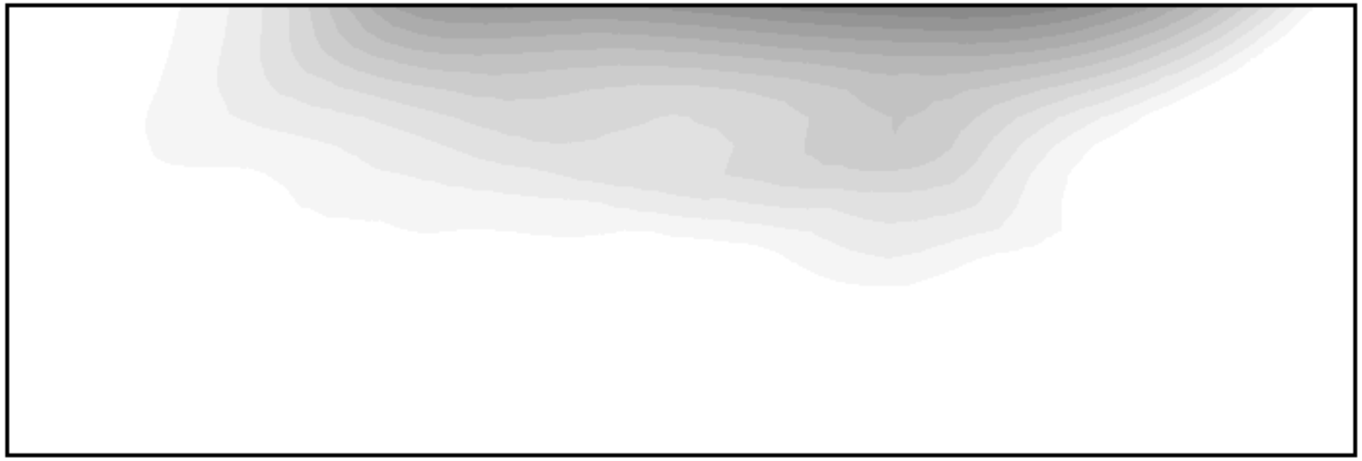
- Constraints on volume (fixed) and compliance.
- Initial design: optimal design for compliance minimization.

Initial (left) and final (right) shapes



Vertical cut of the vertical displacement





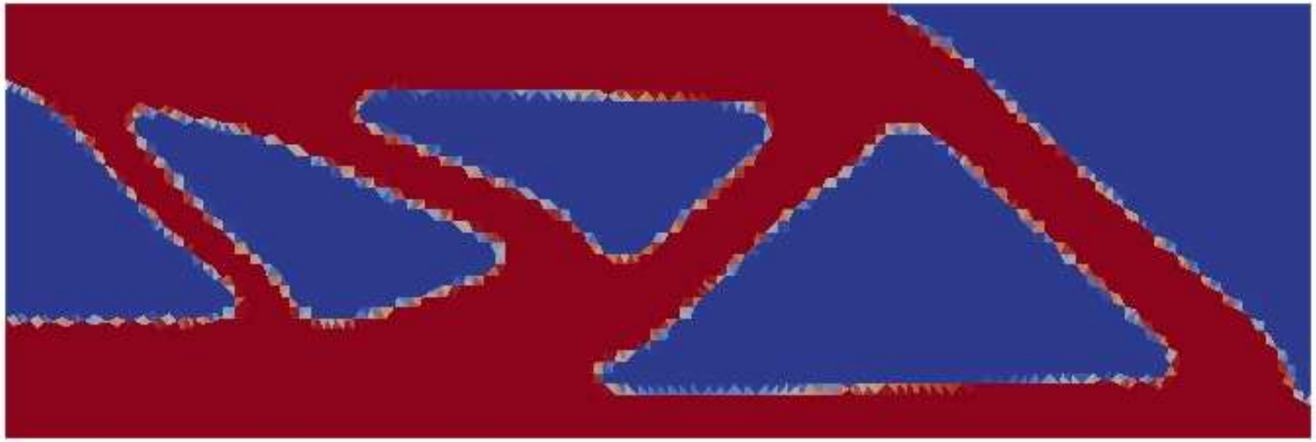
Test case 4

- Half MBB beam (2-d).
- Full model with 20 layers and 5 time steps per layer.
- Minimize the deviatoric part of the stress $\sigma_D = 2\mu e(u)_D$

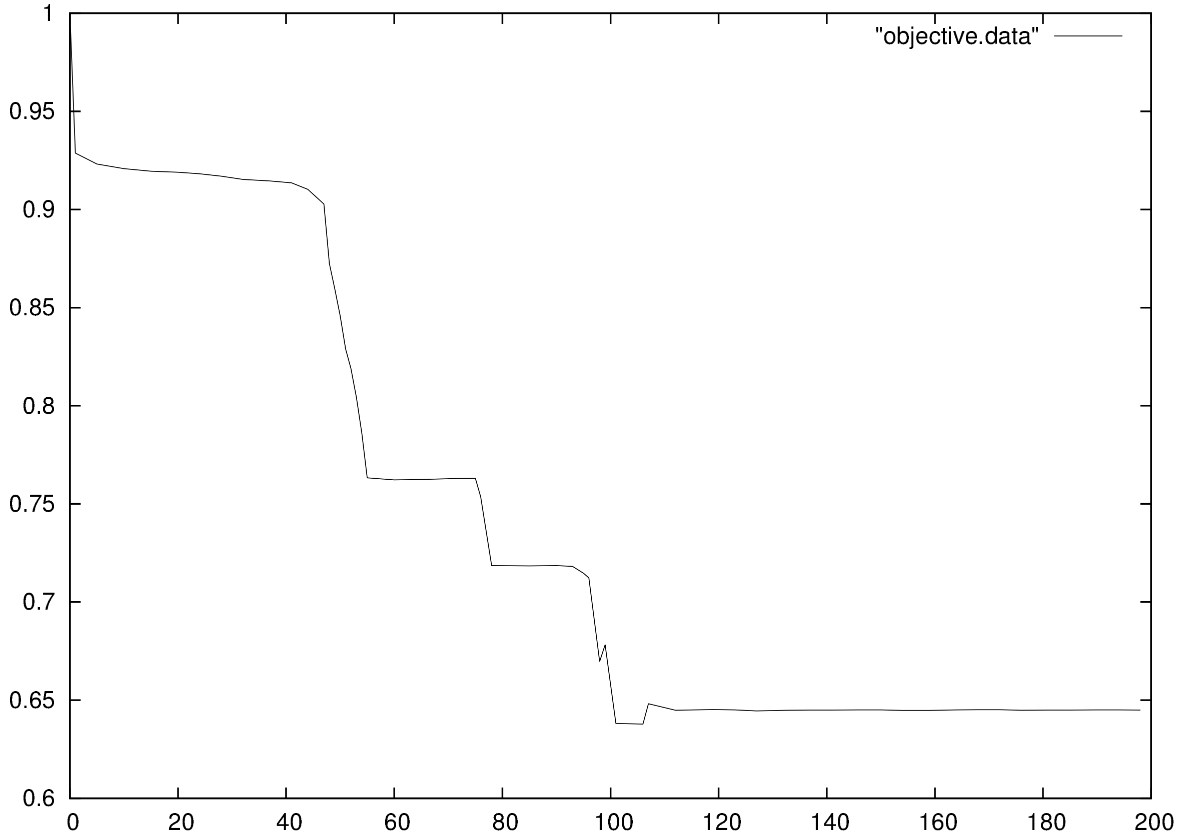
$$J_1(\Omega) = \sum_{i=1}^{n} \int_{t_{i-1}}^{t_i} \int_D |\sigma_D|^2 \, dx \, dt$$

- The value u_{max} is guessed from the initial design.
- Constraints on volume (fixed) and compliance.
- Initial design: optimal design for compliance minimization.

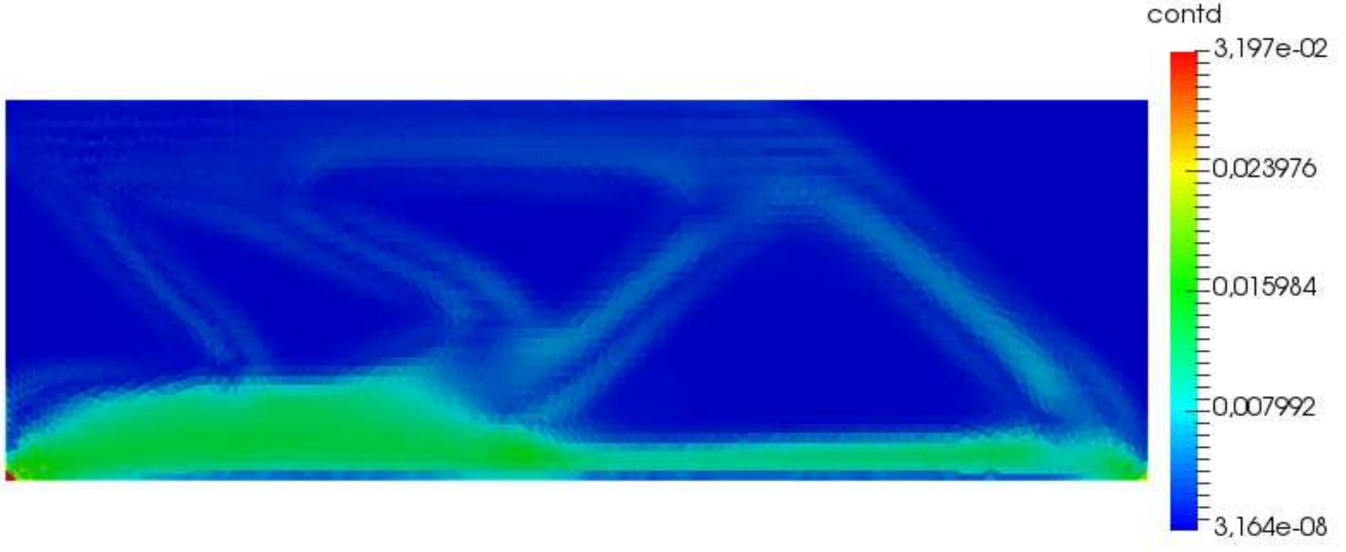
Initial and final shape

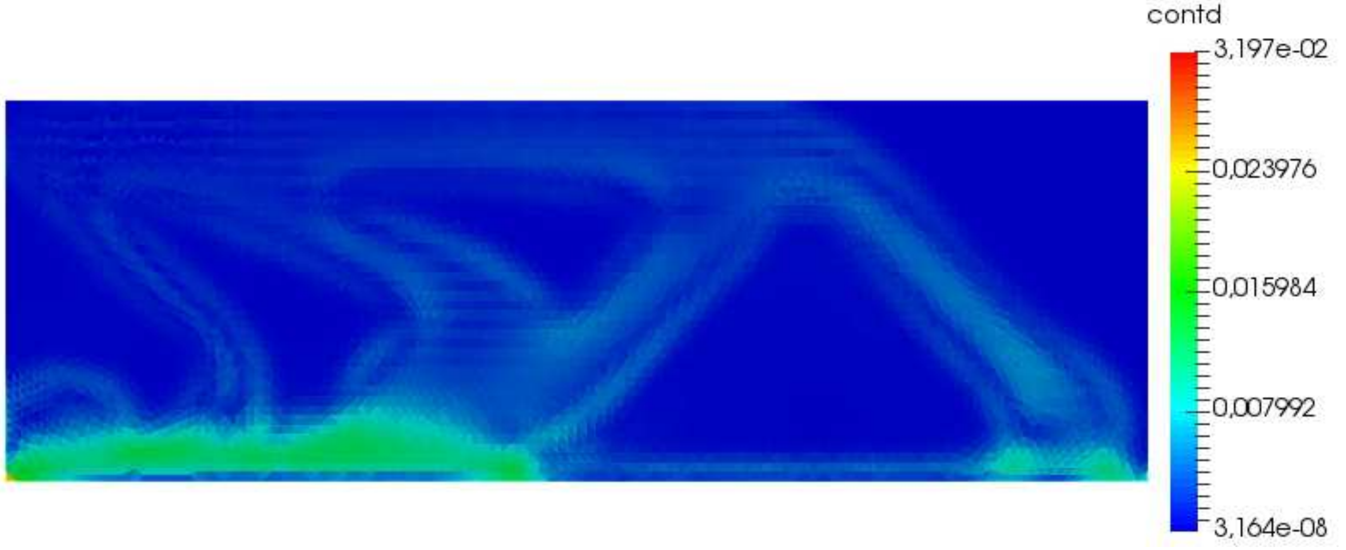


Convergence history (thermal stress)



Plot of thermal stress $\sqrt{\int_0^T |\sigma^D|^2(x)\, dt}$





Conclusions and perspectives

1. Work still going on.
2. Need to calibrate the model and assess the objective and constraints.
3. Add plasticity.
4. Could a simplified modeling be enough ?
5. More material issues: porosity, phase change, hardening, etc.

G. Allaire, L. Jakabcin, *Taking into account thermal residual stresses in topology optimization of structures built by additive manufacturing*, HAL preprint: hal-01666081 (2017).