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CONCURRENT SHAPE OPTIMIZATION OF THE PART AND SCANNING PATH FOR POWDER BED FUSION ADDITIVE MANUFACTURING

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Abstract: This paper investigates the concurrent path planning optimization and the built part structural optimization for powder bed fusion additive manufacturing processes. The state of the art studies rely on existing patterns for trajectories for a fixed built shape. The shape is often optimized for its mechanical performance but rarely in a combined way with its path planning building process. In this work, a two dimensional model (in the layer plane) of the process is proposed under a steady state assumption. Then a systematic path optimization approach, free from a priori restrictions and previously developed in [1], is coupled to a structural optimization tool, both of them based on shape optimization theory. This multiphysics optimization leads to innovative and promising results. First, they confirm that it is essential to take into account the part shape in the scanning path optimization. Second, they also give hints to some design recipes: the material and the source parameters must be related to the thickness of the bars that compose the structure. Indeed, the thickness of a bar is a key ingredient which determines the type of path pattern to scan it: straight line, Omega-pattern and Wave-pattern.

Keywords. Path planning and control, additive manufacturing, metallic powder bed fusion, structural optimization.

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1 Introduction

Among the several existing additive manufacturing (AM) processes [2], this work focuses on powder bed fusion (PBF) [3, 4, 5, 6]. This method consists in building metallic parts layer by layer: for each layer, metallic powder is regularly distributed on top of the already built part. A heat source (laser or electron beam) is then travelled along a prescribed path, melting the powder in specific areas. Finally, the part solidifies while cooling down and a new layer of powder is coated to repeat the process. This technology features several advantages [2, 7] as reducing traditional building constraints and thus allowing to manufacture complex parts (like the ones produced by topology optimization softwares), etc.

Despite its promises, there are still some issues in additive manufacturing which require technological improvements. A first issue is the appearance of quality defects such as porosities, residual stresses, rough

surfaces or anisotropy [8, 9, 5, 6, 10, 11]. They are the result of an intricate multi-physics process, involving several phenomena (mechanical, metallurgical, thermal). These defects can partly be accomodated by post treatments [5, 6] but avoiding them is nevertheless crucial. A high-fidelity numerical prediction of these defects must involve four metal states (powder, solid, fluid, gas) and thus nonlinear equations making the computations very expensive [5, 12, 13]. Simplified models have thus been set [14] and specific parameters identified to increase the final structure's quality [10, 15]. A second issue is the building time. Additive manufacturing is known to be a slow process: optimizing the scanning path is one way of reducing the manufacturing time.

In automated production, improving the path is a classical issue, already considered for traditional machining such as milling or welding [16, 17, 18, 19]. For powder bed fusion technologies the path directly impacts the heat distribution and thus both the scanning time [20, 21] and the creation of quality defects [22, 23, 24]. Departing from the literature (see [25] for a review of the existing strategies), where paths are based upon fixed strategies, it is chosen here to consider a systematic optimization approach, as initiated in [1] (see also the PhD thesis of the first author [26]). In this approach, the path is optimized without a priori given strategy and its pattern is thus expected to be varying when applied to different part shapes. The path is optimized in order to have a precise control of the temperature during the building process. On the other hand, the shape is optimized both for temperature control and for its final mechanical performance. This allows for the development of path optimization algorithms under a steady state assumption. This type of systematic optimization of the scanning path is recent with only a limited literature: the works [27, 28] give theoretical results on an optimal control approach of the problem; the works, initiated by [29] on anisotropy and further developed in [30, 31], model the scanning path connected components as the level sets of a function controlling the residual stresses using an inherent strain method, under a steady state assumption.

The originality of this article is to go beyond the sole path optimization, as in the just cited references, and to develop a concurrent optimization algorithm aimed at determining both the scanning path and the part shape and topology. To do so, two design variables are considered: the path Γ and the part shape Ω . The literature on topology optimization for metal additive manufacturing is extremely large [32, 33], with a majority of articles taking into account manufacturability constraints either through geometric constraints (like limiting overhangs) or by introducing additional supports (in a purely mechanical context). There are less papers which address the issue of the thermal effects of additive manufacturing through topology optimization (some examples are provided by [34, 35, 36, 37, 38]). Eventually, very few works consider both optimizing the scanning path and the shape [1, 30]. Building on these topology optimization works, we include in the shape and topology optimization algorithm for the part shape Ω some constraints about the scanning path Γ , which yield a compromise between the mechanical performance of the part structure and the efficiency of the building process.

In Section 2, the model elaborated for this study is presented. This is a multiphysics problem: a mechanical problem of compliance minimization under fixed volume constraint is set concerning the final use of the part, and a simplified two dimensional thermal problem, modeled under a steady state assumption, is defined for the scanning path efficiency. The scanning path being included in each layer plane, the model is limited to a single layer in two space dimensions. The optimization objectives and constraints resulting from each physics are precisely defined for the concurrent optimization problem.

For efficiency reasons, gradient-based descent algorithms are used. They require the determination of gradients related to the optimization problem, thanks to an adjoint method. In both cases, path and shape optimization, we rely on the Hadamard method of geometrical sensitivity [39, 40, 41]. Section 3 is concerned with the computation of these derivatives with respect to the path and to the shape.

Section 4 explains our numerical implementation. The path is parametrized by a collection of nodes, connected by straight lines. The shape is represented by a level set function. An augmented Lagrangian algorithm for optimization is presented.

Finally, Section 5 is devoted to numerical results for assessing our optimization approach. Two mechanical test cases (a small and a large cantilever) and two physical test cases (with the metal considered being successively aluminium and titanium) are considered for several strategies of coupled optimization. This leads to several observations from which we draw some conclusions.

2 Modelling and optimization problem

In this work, both the part to build and the associated scanning path are simultaneously optimized in the powder bed fusion context. In this section, a model of this process is proposed and an optimization problem is defined. The focus here is on a single layer and thus on a two dimensional problem. In this layer, the part shape is actually a two dimensional section of the 3-d part to build and the path is chosen to melt this part shape, a subset of the the layer (see Figure 1). The working or computational domain $D \subset \mathbb{R}^2$ is the cross-section of the build chamber containing this layer, thus a rectangle in practice. The mechanical problem, related to the part optimization, is first described. Then, a model for the building process is given, featuring the path of the heat source.

2.1 Mechanical model governing the part optimization

Before being manufactured, the part to build is designed for a specific use. Typically, for a linearized elasticity model, the part compliance is minimized under a volume constraint.



Figure 1: Layer plane: Ω part to build and Γ scanning path in the build chamber D

Definition 1. The space \mathcal{U}_{Ω} of admissible shapes is made of open bounded sets $\Omega \subset D$ with a C^2 boundary, $\partial \Omega$, composed of three disjoints parts (see Figure 1): $\partial \Omega_N$ on which a load $h \in L^2(\partial \Omega_N)^2$ is applied (Neumann boundary condition), $\partial \Omega_D$ on which the elastic displacement is prescribed (Dirichlet boundary condition) and $\partial \Omega_F$ which is traction-free. Only the boundary $\partial \Omega_F$ is optimized and the boundary $\partial \Omega_D$ is assumed to be not empty. The exterior normal to the boundary $\partial \Omega$ is denoted by n_{Ω} .

We assume that any shape $\Omega \in \mathcal{U}_{\Omega}$ is filled by an isotropic elastic material with a Hooke's tensor *A*, relating the elastic stress and strain tensors, defined, for any symmetric matrix ξ , by

$$A\xi = \left(\frac{E}{1+\nu}\right)\xi + \left(\frac{E\nu}{(1+\nu)(1-2\nu)}\right)\operatorname{Tr}(\xi)I_2,\tag{1}$$

with E the Young modulus and v the Poisson ratio. The elastic displacement u is the solution of the linear elasticity system

$$\begin{cases}
-\operatorname{div} \left(A\varepsilon(u)\right) = 0 & \operatorname{in} \Omega, \\
A\varepsilon(u).n_{\Omega} = h & \operatorname{on} \partial\Omega_{N}, \\
A\varepsilon(u).n_{\Omega} = 0 & \operatorname{on} \partial\Omega_{F}, \\
u = 0 & \operatorname{on} \partial\Omega_{D},
\end{cases}$$
(2)

with the strain tensor $\varepsilon(u) = \frac{1}{2} (\nabla u + \nabla u^T)$. Setting

$$H_D^1(\Omega, \mathbb{R}^2) = \{ v \in H^1(\Omega, \mathbb{R}^2), \text{ such that } v = 0 \text{ on } \partial\Omega_D \},$$
(3)

the set of functions in $H^1(\Omega, \mathbb{R}^2)$ vanishing on $\partial \Omega_D$, the variational formulation of (2) is to find $u \in H^1_D(\Omega, \mathbb{R}^2)$ such that

$$\int_{\Omega} A\varepsilon(u) : \varepsilon(\varphi) dx - \int_{\partial \Omega_N} h \cdot \varphi ds = 0, \qquad \forall \varphi \in H^1_D(\Omega, \mathbb{R}^2).$$
(4)

The optimization problem consists in minimizing the compliance

$$\min_{\Omega \in \mathcal{U}_{\Omega}} C_{\mathrm{ply}}(\Omega) = \int_{\Omega} A\varepsilon(u) : \varepsilon(u) dx$$

under a given volume constraint $V = \int_{\Omega} dx = V^{\text{target}}$.

2.2 Thermal model governing the path feasibility

Here, we rely on a simplified model to simulate the building process. Indeed, an accurate description of the process (taking into account all phase changes, metallurgical and mechanical aspects) would require a too complicated and CPU expensive model for optimization purposes. Therefore, the focus is rather on a simplified model [5, 12] that involves a thermal problem only. In this context, the control on the fabrication of the part, as well as on the appearance of residual stresses [42], is performed solely through the temperature. To keep a simple numerical resolution, the model is chosen two-dimensional, in the layer plane. This is obviously a huge simplification [43] but it is just a firs step and it allows us to explore optimization issues in a simplified setting. Adding the hypothesis of an infinite scanning speed, the model is further simplified by getting rid of the time dependence of the problem (see [44] for an unsteady model). Note that some of the heat sources used in the powder bed fusion context (and especially electron beams) can move very fast along the path: if the steady state property of our model is obviously a restrictive assumption [45], the results can nevertheless be physically interpreted. For further information on how to derive such a model, on its advantages and on its limits, the interested reader is referred to [26, 1].

Definition 2. The space \mathcal{U}_{Γ} of admissible paths is made of \mathcal{C}^2 oriented curves $\Gamma \subset D$, with end points denoted by A and B (depending on Γ) and unit tangent vector τ_{Γ} . The unit normal n_{Γ} is defined such that, for all $x \in \Gamma$, $(\tau_{\Gamma}(x), n_{\Gamma}(x))$ is a direct orthonormal basis. The (mean) curvature is given at each point by $\kappa_{\Gamma}(x) = div(n_{\Gamma}(x))$ where the normal has been extended to a neighborhood of Γ . Note that this curvature is well defined since the curves $\Gamma \in \mathcal{U}_{\Gamma}$ are \mathcal{C}^2 .

In the following, it is assumed that the path is switched on at once leading to the following heat equation:

$$\begin{cases} -\nabla (\lambda \nabla y) + \beta (y - y_{\text{ini}}) = P \chi_{\Gamma} & \text{in } D, \\ \lambda \partial_n y = 0 & \text{on } \partial D. \end{cases}$$
(5)

with λ the conductivity, *P* the constant source power, Γ the scanning path and $\chi_{\Gamma}(x)$ the Dirac function supported by the path. This heat equation models the conduction effects in the layer plane as well as in the building direction, through the introduction of a temperature loss term with coefficient β . Since $\chi_{\Gamma} \in H^{-1}(D)$, the variational formulation of (5) consists in finding $y \in H^1(D)$ such that

$$\int_{D} \left(\lambda \nabla y \cdot \nabla \phi + \beta \left(y - y_{\text{ini}} \right) \phi \right) dx = \int_{\Gamma} P \phi ds, \qquad \forall \phi \in H^1(D).$$
(6)

Controlling the feasibility of the part with respect to the path Γ is monitored by three different constraints which should vanish:

Control of the solid region. The part Ω ⊂ D must solidify (Figure 1). Thus, at each point x ∈ Ω, the temperature, y, must be above a change of state temperature y_φ, namely y(x) ≥ y_φ. Therefore, with (.)⁺ = max(.,0), this pointwise constraint can be translated into only one constraint, referred to as "phase constraint" in the following,

$$C_{\phi} = \int_{\Omega} \left[\left(y_{\phi} - y(x) \right)^{+} \right]^{2} dx.$$
⁽⁷⁾

• Control of the powder region. The part $D \setminus \Omega$ must remain powder. Thus, at each point $x \in D \setminus \Omega$, the temperature, y, must remain under a maximum temperature $y_{M, pow.} \leq y_{\phi}$, namely $y(x) \leq y_{M, pow.}$. A constraint, referred to as "maximum temperature constraint out of the part" in the following, can then be introduced

$$C_{M,D\setminus\Omega} = \int_{D\setminus\Omega} \left[\left(y(x) - y_{\mathrm{M, pow.}} \right)^+ \right]^2 dx.$$
(8)

• Control of the defects. To avoid the appearance of defects in the part during its building (especially residual stresses and deformations), the maximum temperature is required to stay below a fixed threshold. Thus, at each point $x \in \Omega$, the temperature y must remain below a maximum temperature $y_{M, \text{ sol.}}$, namely $y(x) \le y_{M, \text{ sol.}}$. The choice of the maximal temperature $y_{M, \text{ sol.}}$ is somehow arbitrary and obviously impacts the optimization results. For further details, the reader can refer to [26] and especially to Chapter 6. The "maximum temperature constraint in the part" is the defined by

$$C_{M,\Omega} = \int_{\Omega} \left[\left(y(x) - y_{\mathrm{M, \, sol.}} \right)^+ \right]^2 dx.$$
(9)

The optimization problem is to minimize the path length

$$\min_{\Gamma\in\mathcal{U}_{\Gamma}}L_{\Gamma}=\int_{\Gamma}ds,$$

under the constraints that $C_{\phi} = 0$, $C_{M,D\setminus\Omega} = 0$, $C_{M,\Omega} = 0$.

2.3 Concurrent optimization problem

The concurrent or simultaneous optimization problem gathers both optimization problems of Subsections 2.1 and 2.2. It is a multiphysics problem with two state equations (one mechanical for the final use of the part, one thermal for the building process of the part). It reads

$$\min_{\Omega \in \mathcal{U}_{\Omega}, \Gamma \in \mathcal{U}_{\Gamma}} J(\Omega, \Gamma) = l_{cply} C_{ply}(\Omega) + l_L L_{\Gamma}(\Gamma),$$
such that
$$\begin{cases}
V(\Omega) = V^{target}, \\
C(\Omega, \Gamma) = C_{\phi}(\Omega, \Gamma) + l C_{M,\Omega}(\Omega, \Gamma) + C_{M,D \setminus \Omega}(\Omega, \Gamma) = 0,
\end{cases}$$
(10)

where the various objectives and constraints are computed with the states $u \in H^1(D, \mathbb{R}^2)$, solution of the elasticity equation (2), $y \in H^1(D, \mathbb{R})$, solution of the heat equation (5), and $l_{cply}, l_L \in \mathbb{R}$ are some weighting coefficients. Some details about the chosen numerical values are given in Section 4.2.2.

Remark 1. In this work, we choose the path Γ and the shape Ω to be independent variables. This is a modelling choice. The truth is that they are not independent in practice but their relationship is not obvious. A first possibility is to assume that the shape depends on the path: indeed the shape could be automatically deduced from the path by considering it as a tubular neighbourhood of the path (the melted zone around the laser path). A second possibility is to assume that the path depends on the shape by some manufacturability rule: a pattern of the path is associated to some local characteristics of the shape geometry. Of course, reality lies between these two extreme cases. We believe our modeling choice to make Γ and Ω independent variables is a good compromise: in such a case, they are related to one another only through the satisfaction of temperature constraints.

Remark 2. Note that the constraint *C* corresponds to the sum of the constraints related to the control of the solid region, to the control of the powder region and to the control of the defects. Each of them is considered with equal importance. Yet, it is possible to choose differently the constraint *C*, especially by introducing weights in the sum.

3 Gradient with respect to the path Γ and the shape Ω

The optimization method is based on a gradient descent algorithm. It thus requires the computation of the gradient of each objective and constraint functions with respect to the path Γ and shape Ω . In this work, the shape optimization method (also called Hadamard method) is chosen and the gradients are computed using the Lagrangian method of Céa [46]. The proofs of the propositions are simply sketched and the interested reader is referred to [39, 40, 47, 41] for more mathematical details.

3.1 Differentiation with respect to the shape Ω

Proposition 1 details the differentiation with respect to the shape Ω .

Proposition 1. Let $\Omega \in \mathcal{U}_{\Omega}$ and $\Gamma \in \mathcal{U}_{\Gamma}$ (see Definitions 1 and 2). Then, C_{ply} , L_{Γ} , V and C are differentiable at Ω and for any perturbation $\theta_{\Omega} \in C^{2}(\overline{D}, \mathbb{R}^{2})$ such that for all $x \in \partial \Omega_{N} \cup \partial \Omega_{D}$, $\theta_{\Omega}(x) = 0$, their derivatives are

$$D_{\Omega}C_{ply}(\Omega)(\theta_{\Omega}) = \int_{\partial\Omega_F} \left(-A\varepsilon(u):\varepsilon(u)\right)\theta_{\Omega}(s)\cdot n_{\Omega}(s)ds,\tag{11}$$

$$D_{\Omega}L_{\Gamma}(\Gamma)(\theta_{\Omega}) = 0, \qquad (12)$$

$$D_{\Omega}V(\Omega)(\theta_{\Omega}) = \int_{\partial\Omega_F} \theta_{\Omega}(s) \cdot n_{\Omega}(s) ds, \qquad (13)$$

and

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$$D_{\Omega}C(\Omega,\Gamma)(\theta_{\Omega}) = \int_{\partial\Omega_{F}} \left(\left[\left(y_{\phi} - y \right)^{+} \right]^{2} + \left[\left(y - y_{M, sol.} \right)^{+} \right]^{2} - \left[\left(y - y_{M, pow.} \right)^{+} \right]^{2} \right) \theta_{\Omega}(s) \cdot n_{\Omega}(s) ds.$$
(14)

Remark 3. Note that, following the Hadamard structure theorem [40, 41, 39], for all the considered functions (denoted $G \in \{C_{ply}, L_{\Gamma}, V, C\}$ in the following), the derivative can be written, with $g_{\Omega} \in C^{0}(\overline{D}, \mathbb{R})$.

$$D_{\Omega}G(\Omega)(\theta_{\Omega}) = \int_{\partial\Omega_F} g_{\Omega}\theta_{\Omega} \cdot n_{\Omega}ds.$$
(15)

For the proof of Proposition 1 we need the following classical result [40, 41, 39] which is recalled for the sake of completeness.

Lemma 1. Let $\Omega \subset \mathbb{R}^2$ be a \mathcal{C}^2 open bounded set. Let $f \in \mathcal{C}^1(D,\mathbb{R})$. The function $J(\Omega) = \int_{\Omega} f(x) dx$ is differentiable at Ω and for all $\theta \in \mathcal{C}^2(\overline{D},\mathbb{R}^2)$,

$$D_{\Omega}J(\Omega)(\theta) = \int_{\partial\Omega} f(s)\theta(s) \cdot n_{\Omega}(s)ds.$$
(16)

Proof. First of all, the path does not depend on the shape Ω (see Remark 1) which gives (12). Lemma 1 is then used to compute the derivatives of the compliance, volume and temperature constraint.

Lemma 1 can apply directly for the volume. Since the integrand of the temperature constraint only depends on the temperature and thus on the path and not on the shape, Lemma 1 also apply. Finally, recalling that only the part of boundary $\partial \Omega_F$ is optimizable, the derivatives given by (13) and (14) are finally found.

As for the compliance, the integrand actually depends on the elastic displacement which itself depends on the shape Ω . A differentiation of this displacement with respect to Ω would then be required. To avoid such computations, the method of Céa [46] is here applied and an extended functional is introduced (recall that $H_D^1(\Omega, \mathbb{R}^2)$ is defined by (3))

$$\mathcal{G}: \begin{cases} \mathcal{U}_{\Omega} \times H_D^1(\Omega, \mathbb{R}^2) \times H_D^1(\Omega, \mathbb{R}^2) & \to & \mathbb{R} \\ (\Omega, p, q) & \mapsto & \int_{\Omega} A\varepsilon(p) : \varepsilon(p) + \int_{\Omega} A\varepsilon(p) : \varepsilon(q) dx - \int_{\partial \Omega_N} h \cdot p ds \end{cases}$$

Then, for all $q \in H_D^1(\Omega, \mathbb{R}^2)$, $\mathcal{G}(\Omega, u, q) = C_{\text{ply}}(\Omega)$. Differentiating with respect to the shape Ω then leads to

$$D_{\Omega}C_{\rm ply}(\Omega)(\theta) = \partial_{\Omega}\mathcal{G}(\Omega, u, q)(\theta) + \partial_{u}\mathcal{G}(\Omega, u, q)\left(\partial_{\Omega}u(\Omega)(\theta)\right)$$

Choosing $q = u_{adj}$ such that for all $\phi \in H_D^1(\Omega, \mathbb{R}^2)$, $\partial_u \mathcal{G}(\Omega, u, u_{adj})(\phi) = 0$ leads to choosing $u_{adj} \in H^1(\Omega, \mathbb{R}^2)$ solution of

$$\begin{cases} -\operatorname{div} \left(A \varepsilon(u_{\mathrm{adj}}) \right) = 0 & \text{in } \Omega \\ A \varepsilon(u) \cdot n_{\Omega} = -2h & \text{on } \partial \Omega_N \\ A \varepsilon(u) \cdot n_{\Omega} = 0 & \text{on } \partial \Omega_F \\ u = 0 & \text{on } \partial \Omega_D \end{cases}$$

This is equivalent to choosing $u_{adj} = -2u$. This leads to

1

$$D_{\Omega}C_{\text{ply}}(\Omega)(\theta) = \partial_{\Omega}\mathcal{G}(\Omega, u, -2u)(\theta)$$

and Lemma 1 concludes the proof.

3.2 Differentiation with respect to the path Γ

Proposition 2 details the differentiation with respect to the path Γ . To compute the derivative, an adjoint function $y_{adj} \in H^1(D)$ is introduced as

$$\begin{cases} -\nabla \left(\lambda \nabla y_{adj}\right) + \beta y_{adj} = 2 \left\lfloor \left(y_{\phi} - y\right)^{+} \mathbb{1}_{\Omega_{0}} - \left(y - y_{M, \text{ sol.}}\right)^{+} \mathbb{1}_{\Omega_{0}} - \left(y - y_{M, \text{ pow.}}\right)^{+} \mathbb{1}_{D \setminus \Omega_{0}} \right\rfloor & \text{in } D, \\ \lambda \partial_{n} y_{adj} = 0 & \text{on } \partial D. \end{cases}$$
(17)

The right hand side in equation (17) belongs to $L^2(D)$ since the temperature y, solution of (5), belongs to $H^1(D)$). Thus the adjoint equation (17) admits a unique solution $y_{adj} \in H^1(D)$.

Proposition 2. Let $\Gamma \in \mathcal{U}_{\Gamma}$ and $\Omega_0 \in \mathcal{U}_{\Omega}$ (see Definitions 1 and 2). Then, C_{ply} , L_{Γ} , V and C are differentiable at Γ and, for any perturbation $\theta_{\Gamma} \in C^2(\overline{D}, \mathbb{R}^2)$, their derivatives are as follow:

$$D_{\Gamma}C_{ply}(\Omega)(\theta_{\Gamma}) = 0, \tag{18}$$

$$D_{\Gamma}L_{\Gamma}(\Gamma)(\theta_{\Gamma}) = \int_{\Gamma} \kappa_{\Gamma}(s)\theta_{\Gamma}(s) \cdot n_{\Gamma}(s)ds + \theta_{\Gamma}(B) \cdot \tau_{\Gamma}(B) - \theta_{\Gamma}(A) \cdot \tau_{\Gamma}(A),$$
(19)

$$D_{\Gamma}V(\Omega)(\theta_{\Gamma}) = 0, \tag{20}$$

and

$$D_{\Gamma}C(\Omega_{0},\Gamma)(\theta_{\Gamma}) = \int_{\Gamma} \left(-P\left[\partial_{n}y_{adj}(s) + \kappa_{\Gamma}(s)y_{adj}(s)\right] \theta_{\Gamma}(s) \cdot n_{\Gamma}(s) \right) ds -Py_{adj}(B)\theta_{\Gamma}(B) \cdot \tau_{\Gamma}(B) + Py_{adj}(A)\theta_{\Gamma}(A) \cdot \tau_{\Gamma}(A),$$
(21)

where $y_{adj} \in H^1(D, \mathbb{R})$ is defined by (17).

Remark 4. Note that, for both the path length and the constraint (denoted $F \in \{C_{ply}, L_{\Gamma}, V, C\}$), following Hadamard structure theorem [40, 41, 39], the derivative can be written

$$D_{\Gamma}F(\Gamma)(\theta_{\Gamma}) = \int_{\Gamma} f_{n_{\Gamma}}\theta_{\Gamma} \cdot n_{\Gamma}ds + f_{\tau_{\Gamma}}(B)\theta_{\Gamma}(B) \cdot \tau_{\Gamma}(B) - f_{\tau_{\Gamma}}(A)\theta_{\Gamma}(A) \cdot \tau_{\Gamma}(A),$$
(22)

with $f_{n_{\Gamma}}, f_{\tau_{\Gamma}} \in \mathcal{C}^0(\overline{D}, \mathbb{R}).$

For the proof of Proposition 2 we need the following result, which is classical, at least when Γ is a closed curve, meaning that its end points A and B coincide (see [40, 35, 41, 48]). When Γ is not a closed loop, the classical proof can be generalized and, due to an integration by parts, the two additional terms on the line endpoints appear (see e.g. a proof in [26]).

Lemma 2. Let $\Gamma \in \mathcal{U}_{\Gamma}$, $g \in W^{2,1}(D,\mathbb{R})$. The function $J(\Gamma) = \int_{\Gamma} g(s)ds$ is differentiable at Γ and for all $\theta \in C^2(\overline{D},\mathbb{R}^2)$,

$$D_{\Gamma}J(\Gamma)(\theta) = \int_{\Gamma} (\kappa_{\Gamma}(s)g(s) + \partial_{n_{\Gamma}}g(s))\,\theta(s) \cdot n_{\Gamma}(s)ds + g(B)\theta(B) \cdot \tau_{\Gamma}(B) - g(A)\theta(A) \cdot \tau_{\Gamma}(A).$$
(23)

Proof. First of all, the compliance and volume do not depend on the shape Ω (see Remark 1) which give (18) and (20). Lemma 2 is then used to compute the derivatives of the length and temperature constraint. Lemma 2 can apply directly for the length. As for the temperature constraint, it does not depend explicitly on the path. The dependence is in the temperature, requiring, as for Proposition 1, the use of the method of Céa. The extended functional is

$$\mathcal{G}: \begin{cases} \mathcal{U}_{\Gamma} \times H^{1}(D,\mathbb{R}) \times H^{1}(D,\mathbb{R}) \rightarrow \mathbb{R} \\ (\Gamma,w,z) \qquad \mapsto \int_{\Omega} \left[\left(y_{\phi} - w \right)^{+} \right]^{2} + \left[\left(w - y_{\mathrm{M, sol.}} \right)^{+} \right]^{2} dx + \int_{D \setminus \Omega} \left[\left(w - y_{\mathrm{M, pow.}} \right)^{+} \right]^{2} \\ + \int_{D} \lambda \nabla w \cdot \nabla z dx - \int_{\Gamma} Pz ds. \end{cases}$$

Then, for all $z \in H^1(\Omega, \mathbb{R}^2)$, $\mathcal{G}(\Gamma, y, z) = C(\Gamma)$. Differentiating with respect to the shape Ω then leads to

 $D_{\Gamma}C(\Gamma)(\theta) = \partial_{\Gamma}\mathcal{G}(\Gamma, y, z)(\theta) + \partial_{y}\mathcal{G}(\Gamma, y, z)(\partial_{\Gamma}y(\Gamma)(\theta)).$

Choosing $z = y_{adj}$ such that for all $\phi \in H^1(D, \mathbb{R})$, $\partial_y \mathcal{G}(\Gamma, y, y_{adj})(\phi) = 0$ leads to define $y_{adj} \in H^1(D, \mathbb{R})$ as the solution of (17). This leads to

$$D_{\Gamma}C(\Gamma)(\theta) = \partial_{\Gamma}\mathcal{G}(\Gamma, y, y_{\mathrm{adj}})(\theta),$$

and Lemma 2 concludes the proof.

3.3 Transformation of the derivative into gradients: regularization-extension process

In order to apply a gradient descent algorithm, a gradient must be deduced from the derivatives given by Propositions 1 and 2. For $X = \Omega$ or $X = \Gamma$, a Hilbert space H_X is chosen together with its scalar product $(.,.)_X$ and the gradient J'_X of a function J corresponds to the Riesz representative of the derivative (which is a linear form) in the Hilbert space.

$$D_X J(X)(\theta) = (J'_X, \theta)_X.$$
(24)

This gradient determination process is classical and can be used as a regularization or regularization-extension process (extension of the shape gradient away from the boundary) [40, 49, 50, 51][52]. Note that the direction $\theta = -J'_X$ is then a descent direction. Indeed, this leads to $D_X J(X)(\theta) = -||J'_X||_X^2 \le 0$.

The gradient with respect to the shape is first considered choosing the gradient of each function $G \in \{C_{\text{ply}}, L_{\Gamma}, V, C\}$ as the Riesz representative of the derivative in the Hilbert space $H^1(D, \mathbb{R}^2)$ which amounts to compute $G' = G'_{n_0} n_\Omega \in H^1(D, \mathbb{R}^2)$ such that for all $Q \in H^1(D, \mathbb{R})$,

$$\int_{D} \left(\mathbf{v}_{\Omega}^2 \nabla G'_{n_{\Omega}} \cdot \nabla Q + G'_{n_{\Omega}} Q \right) dx = \int_{\partial \Omega_F} g_{\Omega} Q ds.$$
⁽²⁵⁾

The coefficient $v_{\Omega} > 0$ is a regularization coefficient in this "regularization-extension" process.

The Hilbert space $H^1(D, \mathbb{R}^2)$ cannot be used to regularize the gradient with respect to a curve $\Gamma \in \mathcal{U}_{\Gamma}$ (with two end points *A* and *B*), since any function in $H^1(D, \mathbb{R}^2)$ is not necessarily defined at points A and B. Thus, the gradient with respect to the path of each function $F \in \{C_{\text{ply}}, L_{\Gamma}, V, C\}$ is the Riesz representative of the derivative in $H^1(\Gamma, \mathbb{R}^2)$ (Laplace-Beltrami choice) which amounts to compute $F' = F'_{\tau_{\Gamma}}\tau_{\Gamma} + F'_{n_{\Gamma}}n_{\Gamma} \in H^1(\Gamma, \mathbb{R}^2)$ such that for all $W = W_{\tau_{\Gamma}}\tau_{\Gamma} + W_{n_{\Gamma}}n_{\Gamma}, W_{\tau_{\Gamma}}, W_{n_{\Gamma}} \in H^1(\Gamma, \mathbb{R})$,

$$D_{\Gamma}F(\Gamma)(W) = \int_{\Gamma} (f_{n_{\Gamma}}W_{n_{\Gamma}}) ds + f_{\tau_{\Gamma}}(B)W_{\tau_{\Gamma}}(B) - f_{\tau_{\Gamma}}(A)W_{\tau_{\Gamma}}(A),$$

$$= \int_{\Gamma} \left[v_{\Gamma}^{2} \left(\nabla_{\tau_{\Gamma}}F_{\tau_{\Gamma}}' \cdot \nabla_{\tau_{\Gamma}}W_{\tau_{\Gamma}} + \nabla_{\tau_{\Gamma}}F_{n_{\Gamma}}' \cdot \nabla_{\tau_{\Gamma}}W_{n_{\Gamma}} \right) + F_{\tau_{\Gamma}}'W_{\tau_{\Gamma}} + F_{n_{\Gamma}}'W_{n_{\Gamma}} \right] ds.$$
(26)

This regularization process is controlled by the coefficient $v_{\Gamma} > 0$.

4 Numerical algorithm

The optimization method chosen is a double loop algorithm. The outer loop is related to the part shape Ω whereas the inner loop focuses on the path Γ , both of them corresponding to gradient descent algorithms. The number of iterations in each loop determines the balance between the optimization of both variables. The following subsections detail the differentiation process, the discretization and the algorithm related to each loop.

4.1 Inner loop: path optimization

The inner loop focuses on path optimization. Let D be the working domain and Ω_0 a fixed shape that the optimized path must build. The optimization problem related to the inner loop is then

$$\min_{\Gamma \in \mathcal{U}_{\Gamma}} L_{\Gamma}(\Gamma),$$
such that $C = C_{\phi}(\Omega_{0}, \Gamma) + C_{M,\Omega}(\Omega_{0}, \Gamma) + C_{M,D \setminus \Omega}(\Omega_{0}, \Gamma) = 0,$
(27)

where $y \in H^1(D, \mathbb{R})$ solution to the heat equation (5). To numerically solve this optimization problem, the strategy is the following: first define a discretization of the problem; and then, choose an optimization algorithm and determine the corresponding numerical gradient from the gradients computed in Subsection 3.2.

4.1.1 Discretization of the optimization problem

Along the inner loop iterations, the path Γ is modified leading to re-evaluations of the temperature *y*. The numerical representation of each object is crucial since impacting both the computational time and accuracy. Among the several works related to interface representation [53, 54, 55, 56], we follow [57] and choose a front tracking approach. The working domain is discretized with a "(physical) mesh" fixed along the iterations. On this mesh, the finite element functions are defined and the temperature computed. The path is also discretized as a broken line defined by its nodal points $(x_i)_{i \in [\![1,N_x]\!]}$, N_x the number of points. This discretized path (and especially its nodal points) is modified at each iteration (Figure 2). The resulting line is re-discretized to ensure each segment length to be in the range $[d_{\text{lower}}, d_{\text{upper}}]$ such that $d_{\text{upper}} = 2d_{\text{lower}} = 0.7\Delta x$, with Δx the characteristic physical mesh size. The broken line representation of the path implies the definition of discrete tangent $(\tau_{\Gamma,i})_{i \in [\![1,N_x-1]\!]}$, normal $(n_{\Gamma,i})_{i \in [\![1,N_x-1]\!]}$ and curvature $(\kappa_{\Gamma,i})_{i \in [\![1,N_x-1]\!]}$. Their definitions follow [26] Chapter 5, in which all the details of the discretization process can be found. Finally, all the algorithmic details related to the information mapping from the line to the physical mesh (heat source definition on the physical mesh for example) can be found in [26] Chapter 5.

This representation is very convenient because it keeps the mesh fixed, thereby considerably reducing the computational costs. Moreover, the discretized path allows for a full control of the line topology (no uncontrolled changes in the number of connected components). In this work, only one connected component of the path is allowed (the path topology is fixed). An optimization to modify the path topology has been proposed in [26].



Figure 2: Front-tracking approach: fixed physical mesh and moving broken line path discretization



Figure 3: Path description as a broken line

The gradients of the path length and constraint are the solutions of (26) in their continuous version. To get them in a discretized version, compatible with the numerical problem, the gradient equation is discretized. Let *F* be the function to which the numerical gradient must be computed. Then, for all $i \in [[1, N_x]]$, its numerical gradient at point x_i , $F'_i = F'_{\tau_{\Gamma,i}} \tau_{\Gamma,i} + F'_{n_{\Gamma,i}} n_{\Gamma,i}$ is such that

$$\begin{cases} \sum_{i=1}^{N_{x}-1} l_{i} \left[v_{\Gamma}^{2} \left(\frac{F_{\tau_{\Gamma},i+1}' - F_{\tau_{\Gamma},i}'}{l_{i}} \frac{W_{i+1} - W_{i}}{l_{i}} \right) + \frac{F_{\tau_{\Gamma},i+1}'W_{i+1} + F_{\tau_{\Gamma},i}'W_{i}}{2} \right] - f_{\tau_{\Gamma},N_{x}}W_{N_{x}} + f_{\tau_{\Gamma},1}W_{1} = 0, \\ \sum_{i=1}^{N_{x}-1} l_{i} \left[v_{\Gamma}^{2} \left(\frac{F_{\Gamma,n_{\Gamma},i+1}' - F_{\Gamma,n_{\Gamma},i}'}{l_{i}} \frac{W_{i+1} - W_{i}}{l_{i}} \right) + \frac{F_{\Gamma,n_{\Gamma},i+1}'W_{i+1} + F_{\Gamma,n_{\Gamma},i}'W_{i}}{2} - \frac{f_{n_{\Gamma},i+1}W_{i+1} + f_{n_{\Gamma},i}W_{i}}{2} \right] = 0. \end{cases}$$

$$(28)$$

4.1.2 Inner loop optimization algorithm

In order to include the constraint C into the optimization algorithm, an augmented Lagrangian method is chosen [58, 26]. The optimization problem (27) is modified into

$$\max_{l_{C,\Gamma} \in \mathbb{R}} \min_{\Gamma \in \mathcal{U}_{\Gamma}} \mathcal{L}_{\Gamma}(\Omega_{0}, \Gamma, l_{C,\Gamma}; c_{C,\Gamma}) = \frac{L_{\Gamma}(\Gamma)}{L_{\Gamma}^{0}} + l_{C,\Gamma} \frac{C(\Omega_{0}, \Gamma)}{C^{0}} + \frac{c_{C,\Gamma}}{2} \left(\frac{C(\Omega_{0}, \Gamma)}{C^{0}}\right)^{2},$$
(29)

with $L_{\Gamma}^0 = \Gamma_{\Omega_0}^0$ the initial path length and $C^0 = C\left(\Omega_0, \Gamma_{\Omega_0}^0\right)$ the initial constraint. Here, the shape Ω_0 is fixed and not subject to optimization. An iterative algorithm is set. At each iteration k > 0, the Lagrange multiplier $l_{C,\Gamma}$ and the path nodal points $(x_i)_{i \in [1,N_x]}$ are updated reading

$$\begin{cases} l_{C,\Gamma}^{k+1} = l_{C,\Gamma}^{k} + c_{C,\Gamma}C(\Omega_0, \Gamma_{\Omega_0}^{k+1}), \\ \forall i \in \llbracket 1, N_x \rrbracket, x_i^{k+1} = x_i^k - s_{\Gamma}^k \mathcal{L}_{\Gamma,i}^{\Gamma}(\Omega_0, \Gamma_{\Omega_0}^k, l_{C,\Gamma}^k; c_{C,\Gamma}), \end{cases}$$
(30)

with $\mathcal{L}_{\Gamma}^{\Gamma}(\Omega_0,\Gamma,l_{C,\Gamma};c_{C,\Gamma}) = \frac{L_{\Gamma}^{\prime\Gamma}}{L_{\Gamma}^0} + \left(\frac{l_{C,\Gamma}}{C^0} + \frac{c_{C,\Gamma}}{(C^0)^2}C(\Omega_0\Gamma)\right)C^{\prime\Gamma}(\Omega_0,\Gamma).$ The step s_{Γ}^k is given by:

$$s_{\Gamma}^{k} = \frac{\operatorname{Coef}_{\Gamma}^{k}\Delta x}{\max_{i}(\|\mathcal{L}_{\Gamma,i}^{\prime\Gamma}(\Omega_{0}, \Gamma_{\Omega_{0}}^{k}, l_{C,\Gamma}^{k}; c_{C,\Gamma})\|)}$$

with Δx the characteristic physical mesh size. The coefficient $\operatorname{Coef}_{\Gamma}^{k}$ is initialized to 1 and updated at each iteration so that (line search strategy),

The tolerance is set to $tol_{\Gamma}^{0} = 1$ in the inner loop.

Finally, if some points are outside the domain D, they are orthogonally projected back to D making the algorithm a projected Augmented Lagrangian detailed by Algorithm 1.

Note that in this work, all the numerical tests have been run with $c_{C,\Gamma}$ fixed to 1.

the part shape is fixed to Ω_0 $k_{\Gamma} = 0$, initialization of the path $\Gamma_{\Omega_0}^0$ and multiplier $l_{C,\Gamma}^0$ resolution of the heat equation and computation of the objective function and constraints computation of the derivatives while $\operatorname{Coef}_{\Gamma}^{k_{\Gamma}} \ge 10^{-8}$ and $k_{\Gamma} \le N_{\Gamma}$ do update of the tolerance path variation such that $\Gamma_{\Omega_0}^{k_{\Gamma}+1} = \Gamma_{\Omega_0}^{k_{\Gamma}} - s_{\Gamma}^{k_{\Gamma}} \mathcal{L}_{\Gamma}'(\Omega_0, \Gamma_{\Omega_0}^{k_{\Gamma}}, l_{C,\Gamma}^{k_{\Gamma}}; c_{C,\Gamma})$ re-discretization of the path $\Gamma_{\Omega_0}^{k_{\Gamma}+1}$ resolution of the heat equation, computation of the objective function and constraint if $\mathcal{L}_{\Gamma}(\Omega_0, \Gamma_{\Omega_0}^{k_{\Gamma}+1}, l_{C,\Gamma}^{k_{\Gamma}}; c_{C,\Gamma}) < \mathcal{L}_{\Gamma}(\Omega_0, \Gamma^{k_{\Gamma}}, l_{C,\Gamma}^{k_{\Gamma}}; c_{C,\Gamma}) * \operatorname{tol}_{\Gamma}^{k_{\Gamma}}$ then iteration accepted Lagrange multiplier $l_{C,\Gamma}$ updated: $l_{C,\Gamma}^{k_{\Gamma}+1} = l_{C,\Gamma}^{k_{\Gamma}} + c_{C,\Gamma}C^{k_{\Gamma}+1}(\Omega_0, \Gamma_{\Omega_0}^{k_{\Gamma}+1})$ step increased update of the variables computation of the derivatives else iteration rejected step decreased end if end while Algorithm 1: Inner loop algorithm

Remark 5. The augmented Lagrangian method is one approach to deal with the constraints, in which their satisfaction is ensured at convergence only. This final convergence may not be reached in a finite (reasonable) number of iterations. In the numerical results, the algorithm has been stopped after a finite number of iterations and the constraint final value are thus not exactly zero. Improving the saturation of the constraints is one of our perspectives. Among the different possibilities, a first idea would be to switch to a better constrained optimization algorithm like, for example, the one in [59].

Remark 6. The constraint C, defined in (27), lumps together three elementary constraints on the phase change and the maximal temperature. These elementary constraints are weighted by 1 while it would have been possible to use different weights. This is done for simplicity but, of course, each constraint could be dealt with separately. This could especially be interesting to truly enforce the blue print of the built part. From an industrial point of view, the main objective is to build the part shape and minimizing the residual stresses is a secondary issue.

4.2 Outer loop: part optimization

The outer loop focuses on part optimization. A descent gradient is set in which at each iteration, the part is first modified before the inner loop algorithm to update the path is applied. The optimization problem corresponding to this outer loop is

$$\min_{\Omega \in \mathcal{U}_{\Omega}} J(\Omega, \Gamma) = l_{\text{cply}} C_{\text{ply}}(\Omega) + L_{\Gamma}(\Gamma),$$
such that
$$\begin{cases}
V(\Omega) = V^{\text{target}}, \\
C(\Omega, \Gamma) = C_{\phi}(\Omega, \Gamma) + C_{M,\Omega}(\Omega, \Gamma) + C_{M,D\setminus\Omega}(\Omega, \Gamma) = 0,
\end{cases}$$
(32)

where $y \in H^1(D, \mathbb{R})$ solution to the heat equation (5) and $u \in H^1(D, \mathbb{R}^2)$ solution to the elasticity equation (2). The precise values of the constants l_{cply} and l_L will be given in Section 4.2.2. The strategy to solve this problem is the same than for the path: define a discretization of the problem and then choose an optimization algorithm and determine the corresponding numerical gradients.

4.2.1 Discretization of the optimization problem

The shape is numerically represented by the level set of a function ψ defined on the whole working domain *D* [47, 60] such that

$$\begin{cases} \Psi(x) < 0 \quad x \in \Omega, \\ \Psi(x) = 0 \quad x \in \partial \Omega \cup D, \\ \Psi(x) > 0 \quad x \in D \setminus \overline{\Omega}. \end{cases}$$
(33)

In this context, the update of the level set is given by the Hamilton Jacobi equation, with t representing the evolution with respect to the iterations and $d_{\Omega}^{n_{\Omega}}(t,x)$ the update direction on the normal,

$$\partial_t \Psi(t,x) + d_{\Omega}^{n_{\Omega}}(t,x) |\nabla \Psi(t,x)| = 0, \quad \forall t, \forall x \in D.$$
(34)

In numerical applications, the processes described in [61, 62, 63] are used. Along the iterations, the advection equation tends to flatten the level set function values thus "blurring" the results. A redistancing algorithm is thus applied based on the signed distance equation [40, 47, 64]. In numerical applications, this function is provided by Freefem++ [65].

4.2.2 Outer loop optimization algorithm

To deal with both the volume and temperature constraints, an augmented Lagrangian method is used, coupled with a dichotomy algorithm on the volume Lagrange multiplier to better satisfy the volume constraint. Introducing the multipliers l_V and l_C , the penalizers c_V and c_C , the effective objective function is then

$$\mathcal{L}_{\Omega}(\Omega, \Gamma, l_V, l_C; c_V, c_C) = \mathcal{L}_{\Omega, A}(\Omega, \Gamma, l_C; c_V, c_C) + l_V \mathcal{L}_{\Omega, B}(\Omega, \Gamma, l_C; c_V, c_C),$$
(35)

with

$$\begin{cases} \mathcal{L}_{\Omega,A}(\Omega,\Gamma,l_{C};c_{V},c_{C}) = \frac{C_{\text{ply}}(\Omega)}{\overline{C_{\text{ply}}}^{0}} + \frac{L_{\Gamma}(\Gamma)}{\overline{L_{\Gamma}}^{0}} + \frac{c_{V}}{2} \left(\frac{V(\Omega) - V^{\text{target}}}{\overline{V}^{0}}\right)^{2} \\ + l_{C} \frac{C(\Omega,\Gamma)}{\overline{C}^{0}} + \frac{c_{C}}{2} \left(\frac{C(\Omega,\Gamma)}{\overline{C}^{0}}\right)^{2}, \\ \mathcal{L}_{\Omega,B}(\Omega) = \frac{V(\Omega) - V^{\text{target}}}{\overline{V}^{0}} \end{cases}$$
(36)

where $\overline{C_{\text{ply}}}^0 = C_{\text{ply}}(\Omega^0)$, $\overline{L_{\Gamma}}^0 = L_{\Gamma}(\Gamma^0)$, $\overline{V}^0 = V(\Omega^0)$, $\overline{C}^0 = C(\Omega^0, \Gamma^0)$ and Ω^0 is the initial shape. In the sequel, the coefficients l_{cply} and l_L in (10) and (32) are set to

$$l_{\mathrm{cply}} = rac{1}{\overline{C_{\mathrm{ply}}}^0}, \quad l_L = rac{1}{\overline{L_\Gamma}^0}.$$

The gradient to this effective objective function is then computed as $\mathcal{L}_{\Omega}^{'\Omega} = \mathcal{L}_{\Omega,A}^{'\Omega} + l_V \mathcal{L}_{\Omega,B}^{'\Omega}$, with

$$\begin{cases} \mathcal{L}_{\Omega,A}^{\prime\Omega}(\Omega,\Gamma,l_{C};c_{V},c_{C}) = \frac{C_{\text{ply}}^{\prime\Omega}(\Omega)}{\overline{C_{\text{ply}}}^{0}} + \frac{c_{V}}{\left(\overline{V}^{0}\right)^{2}}V^{\prime\Omega}(\Omega) \\ + \left(\frac{l_{C}}{\overline{C}^{0}} + \frac{c_{C}}{\left(\overline{C}^{0}\right)^{2}}C(\Omega,\Gamma)\right)C^{\prime\Omega}(\Omega,\Gamma), \\ \mathcal{L}_{\Omega,B}^{\prime\Omega}(\Omega) = \frac{V^{\prime\Omega}(\Omega)}{\overline{V}^{0}} \end{cases}$$
(37)

The descent direction $d_{\Omega}^{n_{\Omega}}$ involved in the Hamilton Jacobi equation (34) is related to this gradient and the following advection step (see Algorithm 2):

$$s_{\Omega}^{k} = \operatorname{Coef}_{\Omega}^{k} \frac{\Delta x}{\|d_{\Omega}^{n_{\Omega}}\|_{L^{\infty}}},$$
(38)

with $\operatorname{Coef}_{\Omega}^{k}$ initialized to 5 and updated so that

initialize the shape and path Ω^0 , Γ^{-1} , $c_V = 1$, $l_C^0 = 1$, $c_C = 1$, compute the optimal path Γ^0 (application of Algorithm 1 initialized by Γ^{-1} with N_{Γ}^0), initialize of l_V , for $it_{\Omega} \in [0, N_{\Omega}]$ do determine by a dichotomy l_V^{test} such that $|V(\Omega^{\text{test}}) - V^{\text{target}}| \leq \varepsilon_{\text{dicho}}$, compute the new compliance $C_{ply}(\Omega)$ and volume $V(\Omega)$, determination of the optimal Γ (application of Algorithm 1 initialized by $\Gamma^{i_{\Omega}}$ with $N_{\Gamma}^{i_{\Omega}}$), $L_{\Gamma}(\Gamma)$, $C(\Omega, \Gamma)),$ if $\mathcal{L}_{\Omega}(\Omega, \Gamma, l_{V}^{it_{\Omega}}, l_{C}^{it_{\Omega}}; c_{V}, c_{C}) \leq \operatorname{tol}_{\Omega} \mathcal{L}_{\Omega}(\Omega^{it_{\Omega}}, \Gamma^{it_{\Omega}}, l_{V}^{it_{\Omega}}, l_{C}^{it_{\Omega}}; c_{V}, c_{C})$ then iteration accepted: $\Omega^{it_{\Omega}+1} = \Omega, \Gamma^{it_{\Omega}+1} = \Gamma,$ update the Lagrange multiplier $l_V^{it_{\Omega}+1} = l_V^{test} + c_V V^{it_{\Omega}+1}$ update the Lagrange multiplier $l_C^{it_{\Omega}} + c_C C^{it_{\Omega}+1}$, compute the new objective function and gradients, increase the step coefficient related to the shape: $\text{Coef}_{\Omega} = \min(1.2 \text{Coef}_{\Omega}, 5)$ else iteration rejected (shape and path rejected), decrease the step coefficient related to the shape: $\text{Coef}_{\Omega} = 0.6 \text{Coef}_{\Omega}$. end if end for Algorithm 2: Iterative double loop algorithm to optimize the shape and the path.

The tolerance tol_{Ω} is initialized to 1.6 and multiplied by 0.9 every 50 iterations. The final algorithm is given by Algorithm 2 with further details in [26] Chapter 9.

The coefficient ε_{dicho} is initialized to 0.05 and multiplied by 0.95 at each iteration during the 120 first ones. The volume tolerance is then fixed to $\varepsilon_{dicho} = 1.1 \, 10^{-4}$.

Remark 7. In this outer loop, the augmented Lagrangian algorithm is supplemented by a dichotomy on the volume Lagrange multiplier. Indeed, as stated in Remark 5, the augmented Lagrangian ensures the fulfilment of the constraints at convergence only. However, it cannot be guaranteed that the volume constraint is satisfied at each iteration which can be problematic in some cases and explains why we favor this second method. Note that if this method can be very easily adapted to the volume, it could not be implemented at such a cheap cost for the temperature contraint. Indeed, modifying the volume does not involve any partial differential equation whereas the temperature constraint not only involves a heat equation but also the resolution of an inner loop, drastically increasing the computational costs of a dichotomy on its coefficients.

5 Numerical results

5.1 Algorithm settings

An initialization state INI is defined with a shape Ω^{INI} and a path Γ^{INI} (subfigure (a) in each Figure). To really understand the significance of a concurrent optimization, different tests are run using Algorithm 4, summed up in Figure 4:

- SONLY: shape optimized path fixed, without any consideration of the temperature constraints ($l_C = 0$ and $c_C = 0$). This test is initialized with $\Omega^0 = \Omega^{INI}$.
- STEMP: shape optimized path fixed, taking into consideration the temperature constraints $(l_C^0 = 1, c_C = 1, \text{ for all } it_\Omega \in [\![0, N_\Omega]\!], N_\Gamma^{it_\Omega} = 0)$. This test is initialized with $\Omega^0 = \Omega^{INI}$ and the fixed path used for the temperature computations is Γ^{INI} .
- SP-fromINI: shape optimized path optimized. This test optimizes both variables taking into account temperature constraints ($l_C^0 = 1$, $c_C = 1$). The number of inner loop iterations follows Table 1. Recall that the inner loop is also broken when the inner loop step coefficient is smaller than 10^{-8} . This test is initialized with $\Omega^0 = \Omega^{INI}$ and $\Gamma^0 = \Gamma^{INI}$.

it _Ω	$[\![0,24]\!]$	25	$[\![26,44]\!]$	45	$[\![46, 49]\!]$	50	[[51,54]]	55	56	57	58	59	[[60,300]]
$N_{\Gamma}^{it_{\Omega}}$	0	50	0	45	0	40	0	35	30	25	20	15	10

Table 1: Number of iterations N_{Γ} in the inner loop depending on the outer loop iteration it_{Ω} .

- PONLY: **shape fixed path optimized**. This test is initialized by $\Gamma^0 = \Gamma^{\text{INI}}$ and the fixed shape to build is Ω^{SONLY} resulting from the optimization test SONLY. This test only involves the inner loop and in this case only, the tolerance of the inner loop is initialized to 2 and multiplied by 0.9 every 50 iterations. The result could be interpreted as, starting from INI, the optimization of the part shape independently from the temperature first, followed by the optimization of the scanning path only.
- SP-fromPONLY: shape optimized path optimized. This test optimizes both variables taking into account temperature constraints ($l_C^0 = 1$, $c_C = 1$). The number of inner loop iterations follows Table 1. Recall that if the inner loop is also broken when the inner loop step coefficient is smaller than 10^{-8} . This test is initialized with the shape $\Omega^0 = \Omega^{\text{SONLY}}$ resulting from the optimization test SONLY and with the path $\Gamma^0 = \Gamma^{\text{PONLY}}$ resulting from the optimization test PONLY.



Figure 4: Recap scheme of the different tests

For all these tests, the regularization coefficients are $v_{\Omega} = 5\Delta x$ and $v_{\Gamma} = 15d_{\text{lower}}$. For each of these tests, the final shape, path and temperature are given. A table sums up the final compliance, volume, path length and non-dimensionalized temperature constraints defined by:

$$\overline{C_{\phi}} = \frac{C_{\phi}}{|\Omega| y_{\phi}^2}, \quad \overline{C_{M,\Omega}} = \frac{C_{M,\Omega}}{|\Omega| y_{M, \text{ sol.}}^2}, \quad \overline{C_{M,D\setminus\Omega}} = \frac{C_{M,D\setminus\Omega}}{|D\setminus\overline{\Omega}| y_{M, \text{ pow.}}^2}.$$
(40)

A final radar chart sums up the quantitative results. Note that in these graphs, for each of the functions represented (compliance and temperature constraints), the axes are reversed so that the best solutions correspond to the curve with the biggest area.

5.2 Cantilever test case

The numerical results presented in this section are aimed at showing the relevance of the proposed algorithm. In this work, we discuss a small cantilever test case and the interested reader can find further results in [26]. A symmetry condition is applied and the working domain is $D = [-1.4, 1.4] \times [0, 0.7]$ given in *mm* (full domain corresponding to $[-1.4, 1.4] \times [-0.7, 0.7]$, see Figure 5). This working domain is meshed with 12800 triangular elements. As only half of the working domain is considered for symmetry reasons, the point of the path initially belonging to the (Ox)-axis is constrained to remain on this axis. This constraint comes from the will, in this work, to focus on a path composed of only one connected component. Allowing this feature to be modified would impact the numerical results and is part of the perspectives. As for the volume constraint, the volume ratio is fixed to $V^{\text{target}} = 1.1V^0$ with $V^0 = 1.157e - 06m^2$.

Two different physical cases are consider in the following: the aluminium and the titanium. In both cases, the Poisson ratio is set to v = 0.3, the Young's modulus to $E = 1k_g m^{-1}s^{-2}$ and the loading to h = (0, -2) in $k_g m s^{-2}$. These values do not correspond to real values but, because there exists a linear relation between the displacement and the Young's modulus, and because the compliance is rescaled in the objective function, the results are unchanged. As for the parameters involved in the heat equation, they are summed up in Table 2.

The power *P* and the coefficient β are determined using a calibration process detailed in [26] Chapter 4. In both cases, the initial temperature is fixed to $y_{ini} = 773K$.

Metal	$\lambda(Wm^{-1}K^{-1})$	$P(Ws^{-1}m^{-1})$	$\beta(WK^{-1}m^{-3})$	$y_{\phi}(K)$	$y_{\mathrm{M, sol.}}(K)$	$y_{\mathrm{M, pow.}}(K)$
Aluminium	130	$400*5.45*10^{6}$	$\frac{\lambda}{2.21*10^{-9}}$	870	1670	870
Titanium	15	$300 * 5.45 * 10^6$	$\frac{\lambda}{2.21*10^{-9}}$	1900	3400	1800

Table 2: Numerical values chosen in the aluminium and titanium test cases.



Figure 5: Cantilever test case with the symmetry conditions for the mechanical and heat problems

In most of the following Figures, only half of the cantilever is shown. Indeed, for symmetry reasons, the optimization is run on half the working domain only. To get the full result, the Figures should be symmetrized with respect to the horizontal lower axis.

All the simulations have been run on a MacBook laptop equipped with 2,3 GHz Intel Corei5 and a RAM of 16GB. No specific efforts for optimizing the Python code have been made. Running 300 iterations requires roughly one to two hours of CPU time, depending on the chosen metal and test case.

5.3 Results

For aluminium, the results of the five tests are presented in Figures 6 and Table 3. The convergence plots for the compliance, the volume, the path length and the temperature constraint are respectively given by Figures 7, 8, 9, 10. For the titanium, the the results are presented in Figures 11 and Table 4. The convergence graphs being very similar to the aluminium case, they have been replaced by the radar chart shown in Figure 12.



Figure 6: Initialization and shape optimization for different tests, aluminium, half cantilever, $V^{\text{target}} = 1.1V^0$

case	$\frac{V}{V^0}$	$C_{\mathrm{ply}}\left(k_{g}ms^{-2}\right)$	$L_{\Gamma}(m)$	$\overline{C_{igoplus}}$	$\overline{C_{M,\Omega}}$	$\overline{C_{M,D\setminus\Omega}}$
INI	1.00	$5.67 imes 10^{-6}$	4.38×10^{-3}	4.88×10^{-3}	0.00	$7.30 imes 10^{-3}$
SONLY	1.10	$1.92 imes 10^{-6}$	$4.38 imes 10^{-3}$	2.47×10^{-3}	0.00	$1.40 imes10^{-5}$
STEMP	1.10	$2.00 imes 10^{-6}$	$4.38 imes 10^{-3}$	2.22×10^{-3}	0.00	0.00
SP-fromINI	1.10	$1.92 imes10^{-6}$	$9.57 imes10^{-3}$	$9.98 imes10^{-6}$	0.00	$1.39 imes10^{-5}$
PONLY	1.10	$1.92 imes 10^{-6}$	$8.85 imes 10^{-3}$	$1.66 imes 10^{-5}$	0.00	$1.99 imes10^{-5}$
SP-fromPONLY	1.10	$1.92 imes 10^{-6}$	$9.34 imes 10^{-3}$	$1.10 imes 10^{-5}$	0.00	$1.48 imes 10^{-5}$

Table 3: Quantitative results for the different tests, aluminium, half cantilever, $V^{\text{target}} = 1.1V^0$



Figure 7: Evolution of the compliance C_{ply} with respect to shape iterations, aluminium, half cantilever, $V^{target} = 1.1V^0$ (note that the scales of the graphs are different)



Figure 8: Evolution of the volume V with respect to shape iterations, aluminium, half cantilever, $V^{\text{target}} = 1.1V^0$ (note that the scales of the graphs are different)



Figure 9: Evolution of the length L with respect to shape iterations, aluminium, half cantilever, $V^{\text{target}} = 1.1V^0$ (note that the scales of the graphs are different)



Figure 10: Evolution of the constraint *C* with respect to shape iterations, aluminium, half cantilever, $V^{\text{target}} = 1.1V^0$ (note that the scales of the graphs are different)



Figure 11: Initialization and shape optimization for different tests, titanium, half cantilever, $V^{\text{target}} = 1.1V^0$

case	$rac{V}{V^0}$	$C_{ m ply}(k_gms^{-2})$	$L_{\Gamma}(m)$	$\overline{C_{\phi}}$	$\overline{C_{M,\Omega}}$	$\overline{C_{M,D\setminus\Omega}}$
INI	1.00	5.67×10^{-6}	4.38×10^{-3}	$1.69 imes 10^{-1}$	$2.79 imes 10^{-5}$	$2.29 imes 10^{-2}$
SONLY	1.10	$1.92 imes 10^{-6}$	$4.38 imes 10^{-3}$	$1.13 imes 10^{-1}$	$1.26 imes 10^{-4}$	0.00
STEMP	1.10	$2.12 imes 10^{-6}$	$4.38 imes 10^{-3}$	$1.08 imes10^{-1}$	$1.26 imes 10^{-4}$	0.00
SP-fromINI	1.10	$2.14 imes10^{-6}$	$1.02 imes 10^{-2}$	$3.05 imes 10^{-3}$	$1.41 imes 10^{-4}$	$6.08 imes10^{-5}$
PONLY	1.10	$1.92 imes 10^{-6}$	$1.00 imes 10^{-2}$	$1.39 imes 10^{-3}$	$9.73 imes10^{-5}$	$3.67 imes10^{-4}$
SP-fromPONLY	1.10	$1.92 imes 10^{-6}$	$1.00 imes 10^{-2}$	$1.20 imes 10^{-3}$	$9.74 imes10^{-5}$	$5.01 imes10^{-5}$

Table 4: Quantitative results for the different tests, titanium, half cantilever, $V^{\text{target}} = 1.1V^0$



Figure 12: Radar chart of the values given in Table 4, titanium, half cantilever, $V^{\text{target}} = 1.1V^0$

The results satisfy the different observations. Let start with the optimization of the shape only, corresponding to Figure 6(b) and (c) for the aluminium and Figure 11(b) and (c) for the titanium (note that 6(b) and 11(b) are exactly the same since the temperature is not taken into account in the "Shape only" test). These optimizations make clear that the introduction of a temperature constraint impacts the part's shape. Indeed, in Figure 6(b) and Figure 11(b), the optimization is run to minimize the compliance under the volume constraints only. This especially leads to a thin middle bar. In Figure 6(c) and Figure 11(c), a path has been fixed and the temperature constraint is also considered. In both the aluminium and titanium cases, the part's shape is thus modified. Indeed, the results found in (b) are not adapted to the fixed path and the temperature constraints are not met. In particular, the maximum temperature constraint out of the part's shape leads to a thickening of the middle bar whereas the other bars are made slightly thinner to better satisfy the phase constraint. Both cases make very clear how fixing the volume impacts the optimization: the shape cannot exactly adapt to the path and reduce the phase constraint since this would require decreasing the volume which is prevented by the dichotomy (see Tables 3 and 4).

The optimizations of the path only (shape fixed to the result from SONLY, Figure (b)) presented by Figure 6(e) for the aluminium and Figure 11(e) for the titanium are also very informative. Going further than the results shown in [1], they highlight a connection between the part's shape thickness and the path pattern. In Figure 6(e), the metal used is the aluminium which conductivity is high and two patterns arise. First, in the middle bar of the cantilever, the path chosen is a straight line. Indeed, the conductivity and source power make the melted thread's width close to the bar's thickness. Note that if the middle bar had been thinner, the existence of a solution to the path optimization would have been proscribed. As for the other bars, since they are thicker, a straight line pattern is not enough to satisfy the phase constraint. A pattern called in the following "Omega-shape" pattern is found, its width adapting to the part's shape. It is very interesting to see that the results obtained with the titanium corroborate these observations in spite of the conductivity differences. In Figure 11(e), the "Omega-shape" pattern also arises in the upper bar and in the middle bar. The titanium's conductivity is lower than the aluminium's and the melted thread corresponding to this metal and the source power chosen has a lower width. Thus, a straight line pattern is not appropriate to build the middle bar and an "Omega-shape" pattern.

Note that besides the respect of the constraints, the path shown on Figure 6 (e) presents a cross-over. Preventing these auto-intersections could come from a better formulation of the maximum temperature constraint within the part Ω but remains part of the perspectives. Note also that this path optimization could give different results if more than one path connected component were allowed. While some methods allowing this feature in path optimization have been developed (see [26] Chapter 8), including them in concurrent path and part optimization remains part of the perspectives.

Finally, coupled optimizations are run starting from two different initializations: from Figure(a) (INI) to Figure(d) (SP-fromINI) and from Figure(e) (PONLY) to Figure(f) (SP-fromPONLY). In the aluminium test case (Figure 6), the results between both concurrent optimizations (Figures(d,f)) remain similar with only slight

adaptations of the bars' thicknesses and the "Omega-shape" patterns. Yet Table 3 shows that the solutions found by the concurrent optimization are better than PONLY. This is natural for SP-fromPONLY since the initialization to this test is PONLY. However, this also shows that, starting from the initialization INI, the concurrent optimization result (SP-fromINI) is better than optimizing first the part's shape without any temperature consideration and then the scanning path (PONLY).

In the titanium test case (Figure 11), the results from both concurrent optimizations are different and the satisfaction of the minimum temperature constraint in the part is far from being respected (the low conductivity of this metal complicating the optimization, see [26, 1]). Starting the concurrent optimization from INI (result given by Figure(d)), the "Omega-shape" and "Wave-shape" patterns still arise but the part's shape and the scanning path are very different from PONLY (Figure(e)). It is very interesting to notice how in (d), the boundaries of the part's shape adapt to the scanning path in order to better fit the phase constraint. Yet, as shown in Figure 12, the numerical results for SP-fromINI are not as goos as for PONLY. As for the concurrent optimization given by (f) and starting from PONLY (e), it brings a significant improvement in the satisfaction of the constraints of the maximum temperature out of the part by modifying the shape of the inner hole (see Table 4 and Figure 12).

Eventually we comment the convergence histories (aluminium case) provided in Figures 7, 8, 9, 10. Note first that, but for the path length history, the graphs for STEMP and SP-fromINI are very similar (with better results for SP-fromINI). Indeed, the optimization is a lot harder for the shape than for the path : for most of the intermediary shapes, the path optimization leads to good results. Thus, since both STEMP and SP-fromINI start from the same initialization, the shape's evolution is very similar leading to similar convergence histories. As for SP-fromPONLY, it starts from an already very good initial guess, thus the scale of variations is much smaller. The convergence graphs are less regular than the previous ones but the seemingly large variations are actually smaller in scale.

Remark 8. Obviously, the choice of the path initialization is crucial for the quality of the resulting optimized design. It was already pointed out in our previous work [1]. We do not discuss this issue further here and we refer the PhD thesis of the first author [26] for more details.

Remark 9. In this work, the best result is SP-fromPONLY, initialized by the result of a sequential optimization of the shape first and then the path. This is quite surprising since optimizing with respect to both variables together usually leads to better optimal results. Thus we could have expected SP-fromINI to be the best. However, in the present setting, shape optimization is a much harder problem than path optimization. Indeed, there are many optimal paths in practice which satisfy the temperature constraints, (almost) whatever the shape. Thus, dealing first with the "more complex (shape) optimization" leads to a better result. Note that adding constraints on the path optimization (for example adding manufacturing constraints related to the machine kinematics) could lead to different results, with SP-fromINI being better than SP-fromPONLY.

Remark 10. In the test cases presented here, the shapes to melt are very small which is quite restrictive in practice. In real applications, the domain to melt is divided into several cells with a scanning path for each of them : indeed, the number of possible solutions being so large, it is easier, cheaper and not worse to optimize locally the path in each cell. Moreover, working locally helps preventing residual constraints [66, 23, 67, 42]. Therefore, a generalization of the present work for large domains could be to optimize, not a single path for the whole domain, but rather a family of paths for each cell.

6 Conclusion and perspectives

In this work, the path optimization algorithm developed in [26, 1] has been adapted to handle concurrent optimization of the path and the part's shape and topology in the steady state case. The concurrent algorithm relies on alternate optimization of the shape and topology and the path at each iteration.

The model remains here very simplistic. Indeed, it is two-dimensional and does not take into account any time dependency. Moreover, the mechanical assumptions relating the temperature to the final mechanical quality of the built shapes are very simple. But despite its simplicity, this work has interesting features and yields promising results. The most important one is the clear relation between scanning path and part's shape and topology: the shape really adapts to the temperature constraints coming from path optimization and it is often crucial in their satisfaction. This is well illustrated by the relation between thickness, material properties and scanning parameters: too thin, the bar cannot be accurately built; thicker, it induces an Omega-pattern strategy of the path; even thicker, Wave-pattern arises. A first design optimization criterion could thus be the thickness of the bars to build and an interesting perspective would be to compare the results obtained for design under thickness constraints (see [64]) to the concurrent design of shape and scanning path.

These promising results open up perspectives. First of all, keeping this simple model, an in-depth study of the impact of the part's thickness (typically the bars thickness) on the scanning path has to be conducted. For this purpose, more tests are required, mostly for different mechanical loadings but also for different metals. Then, as mentioned in Section 5, the scanning path optimization itself should be further developed, to allow for path splitting or prevent self-intersections for example. To end up with this simple model, the provided designs, especially the Omega-pattern and Wave-pattern, will be tested on real machines to get experimental information on their relevance and efficiency. The model could then be enriched by including a thermo-mechanical analysis to better control the residual stresses, using for example an inherent strain method [30, 31]. Of course, the steady-state assumption can be removed. Not only this would allow more realistic mechanical considerations but it would open the way to the addition of kinematics constraints on the path. Indeed, all paths cannot be traveled along at constant speed and taking into account the kinematics is important to really assess the quality of the built part. To further involve the kinematics, a time dependent model, such as the one developed in [26], could then be adapted to the present algorithm. In this unsteady setting it would also be possible to take into account three-dimensional effects, at least by taking into account the previous layers in the optimization of a new layer.

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