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A reduced order model to assist welding parameter setup

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Abstract. This article demonstrates the time saving in industrial process setup using numerical reduced order modelling (ROM). The numerical simulations may supply useful information to design manufacturing processes but are often time consuming and then not suited with multi-query study such as inverse problem. ROM aims at replacing the original simulation (so-called high-fidelity (HF)) by a low rank model that will run fast according to the HF simulation time. Multi-query studies will use the ROM instead of the HF simulation to save time and deliver a solution consistent with industrial timeline. To validate the solution, the HF simulation will be used. In this paper, a problem of calibration of TIG welding parameter will illustrate this approach.

Keywords: Reduced order modelling / optimization / multi-physics simulation / welding / WAAM / modelling

1 Introduction

Numerical simulation is increasingly integrated in the design of industrial manufacturing processes. It may indeed provide fruitful information on the state of the system and on the effects of the variations of processing parameters or manufacturing strategies to help decision making. The setup of welding parameters for a new material or a new application is often manual and experimental, leading to long development time. Assistance using numerical simulation may then be highly effective in this case. Recent developments demonstrate that High-Fidelity (HF) numerical simulation aims at mimicking closely the behaviour of physical experiments [1]. It is then possible to use such numerical models to find welding parameters that supply a desired behaviour in term of physical properties of the welding seams. In [2], the numerical simulation models the behaviour of metal deposit of a titanium allow weld seam through electrical arc on a plate. Inverse problem may help to find welding parameters that ensure to reach given dimensions of the melt pool. That inverse problem may be solved coupling the numerical simulation and optimization algorithm [3].

Despite the relevance of the HF model, it is difficult to use it directly to solve inverse problems due to the number of runs to reach optimal point (usually ten times the number of parameters) and the computation time of a single run of the HF model (typically several dozen hours). To alleviate this issue, research has been conducted to replace the original HF model with a fast substitution model. In [4], authors investigate the use of equivalent heat sources to replace multi-physics simulations to address large-scale models. In [5], a reference 1D model of temperature distribution induced by a laser welding is replaced by a Taylor expansion to illustrate the implementation of a digital twin. It is demonstrated that the Digital Twin might efficiently replace the reference model to solve optimization or other decision-making problem. In [6], artificial neural networks are used to identify welding parameter setup. Contrarily to the previous studies, only experimental data are used and no data coming from computational model are considered. Nevertheless, such approaches might be useful to investigate when several sources of data exist such as sensor data, numerical models of different accuracies. For instance, in [7], a numerical pipeline is investigated to merge data from such various sources. The idea investigated in the present paper is to replace the time-consuming HF computations in the inverse problem by a reduced order model (ROM). The ROM supplies rapidly an estimation of the state of the system for a new parametric configuration and supply results of the same nature as the HF model. This paper will demonstrate that solving the inverse problem with an optimization algorithm coupled with a ROM is much faster and more suitable with industrial timescale.

ROM types are numerous and applied to various domains. Originally, intrusive and physic dependent ROM were developed such as Guyan condensation [8] for static mechanics or Craig-Bampton reduction [9] for dynamic system. Generic approach to adapt more easily to other physics were also developed based on Karhunen Loève decomposition [10] such as well-known Proper Orthogonalized Decomposition (POD) [11]. Proper Generalized Decomposition (PGD) [12] were developed to parameterize

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the ROM to have fast estimation for any values of the parameters in addition to time or spatial position. The latter aims to seek a separate representation of the solutions with some precomputed computations of a parameterized simulation model. The parametric separate form is found by solving a greedy optimization problem. Methods from POD become inefficient when dealing with non-linearities. To mitigate this limitation, approaches like Discrete Empirical Interpolation Method [13] or A priori Hyper Reduction Method [14] add non-linear terms to the reduced order model from selected points in the space-time-parameter domain.

Coupling between ROM and welding simulation has been implemented using high-order PGD [15]. Alternatively, in [16] the POD is used to build the ROM. In [17,18], authors propose to use hyper-reduced model applied to the estimation of the residual welding stresses. In [19], the stochastic ROMs are investigated to propagate uncertainties induced by a laser welding process to the force-displacement curves. The methodology aims to limit the number of HF computations to estimate a reliability factor. It is relevant in this case but seams barely transposable to other engineering problem such as optimization problem.

POD and PGD based techniques have the limitation to require numerous computations to build the ROM. Recently, the ReCUR model has been developed as an attempt to circumvent this drawback in the case of solving optimization problem [20]. It may be initially built with few computations and, despite the loss of accuracy according to HF simulation, supplies fruitful information to conduct optimization toward an interesting solution. It has been successfully applied to optimization study using crash simulation [21] and hot stamping of metal sheet [22]. The present paper will investigate its use to solve optimization problem involving welding simulation.

In this paper, the next part is dedicated to the presentation of the ReCUR ROM from the justification of its use according to industrial requirements to the method of construction, and the coupling between optimization and ROM is outlined. Finally, the industrial application is introduced as well as the results of the approach with a special emphasis on the time saving in comparison to classical approaches.

2 ReCUR reduced order model

The ReCUR ROM is chosen to replace the time-consuming HF simulation. The next section highlights industrial needs that led to this choice. After, some aspects of the mathematical formulation of the ROM are outlined, and finally the coupling between optimization problem and the ROM is highlighted.

2.1 Industrial requirements

To enhance the use of numerical simulation to help design of manufacturing process, several key points exist. The first is to be able to supply answer based on numerical estimations of new process configurations in a time scale suitable with those dedicated to the process definitions. To be able to perform several estimations on a range of the process parameters, the numerical model must be parameterized according to the parameters of the physical process. Another point is the capitalization of existing computations of HF numerical model depicting the process of interest. Those computations might indeed be useful to build the ROM that supplies the estimation of the process configuration. Last, interactions with the numerical estimation such as display, post-treatment, should be possible using regular tools of the engineers. To that end, the format of the estimations must be as close as possible to the format of the HF computations.

The solution explored in this paper is the ReCUR ROM. The ReCUR name stands for **Re**gression **CUR**. The regression denotes the parametric dependency and CUR denotes the method to build the space and time basis. This is a non-intrusive ROM. This feature indicates that it does not require call to the HF solver to have an estimation for a parametric configuration. It does not require as well access to the physical modelling of the system. Drawbacks may be a loss of accuracy because the ROM is not tailored especially for the application, but it has the advantage to adapt easily to a new process or domain of application. Moreover, it is relevant regarding the use of existing computations as it relies on the existing computations to be built.

As an input, it only requires access to results of existing computations corresponding to some parametric configurations. Those computations are gathered into a pool that can be considered as a training pool to build the ROM. Consequently, it means that it does not require initial specific design of experiment to be constructed. It may be initialized with a very small number of computations, typically the number of different parameters in the model. The estimation will be poor quality, but it could be improved by adding more computations in the training pool of the ROM where it is necessary in the parametric domain. It therefore limits the number of computations to deliver an answer to an industrial demand.

ReCUR model is parametric as it depends on predefined inputs considered as parameters. The dependency according to the parameters is specified by the user. The regression aspect of the model lies in this feature.

The ROM is a low rank approximation of the HF model. It is then possible to have an estimation using the ROM very quickly compared to a time-consuming HF solver (as it the welding simulation). Another advantage of the low rank approximation is the stability in extrapolation that will reduce the overfitting issues.

Finally, ReCUR's estimation may be cast in the same format as the HF computation. It may be then manipulated and exploited using the usual tools of the engineers. It is a clear advantage in comparison to the approach that rely on metamodelling of some quantities from the requirements solely [23].

2.2 Mathematical formulation

As mentioned previously, the bases of the ROM are build using the CUR method. CUR [24] method is an alternative to the classical SVD decomposition. In CUR, the vectors of the space basis are directly the state of the system at every position for some selected instants, and the vectors of the time basis are directly the history of the system for all the time steps at selected positions. By convention in this paper, the space vectors are rows in the HF results and time vectors are columns. They may be concatenated into respectively $\boldsymbol{R}$ and $\boldsymbol{C}$ tensors.

From a mathematical point of view an estimation with the ReCUR ROM may be written as:

$$F^s_{\boldsymbol{ROM}_{tx}} = \boldsymbol{X}^s_{tx}.\boldsymbol{U} \tag{1}$$

where, $F^s_{\boldsymbol{ROM}_{tx}}$, stands for the ROM's estimation at a location x and instant t and simulation $s, X^x_{tx} = \mathbf{Ce}_t \bigotimes \mathbf{Re}^T_x \bigotimes \mathbf{P}^s \mathbf{e_t e_x}$, the regression tensor of the ROM, and $\boldsymbol{U}$ contains the coefficients of the ROM. The bases are built selecting columns and rows in the HF computations with a k-means clustering approach [25]. In this method, the number of clusters are chosen by the user. Rows and columns are selected to be the closest from the centres of each cluster. They allow to have bases representative of the HF computations while limiting their sizes. It is possible to add members to the bases to refine the approximation. It is the approach adopted here and it will be outlined in the following. The $\boldsymbol{P^s}$ tensor is constituted by the regression function related to the parameters.

The coefficients in $\boldsymbol{U}$ are calculated to minimize differences between HF data and corresponding ROM's estimations. Also, the number of non-zero coefficients defines the degree of reduction of the ROM. The more of them, the compacter is the ROM. It is possible to minimize both L_∞ interpolation errors between the HF data $\boldsymbol{F}_{HF\mathrm{tx}}$ and the interpolation given by (1) and number of non-zero coefficients solving the following linear problem:

$$\text{find } \varepsilon_{max}, U_j = \alpha^+_j - \alpha^-_j, \varepsilon_{max}, \alpha^+_j, \alpha^-_j \in \mathbb{R}^+,$$

$$\min \quad \varepsilon_{max} + \lambda \sum\nolimits_{j-i}^{n_{RM}} a^+_j + a^-_j \tag{2}$$

Such that $\forall s \in 1 \ldots n_s,\ x,\ t \in List$,

$$-\varepsilon_{max} \leq F^s_{HF_{tx}} - \boldsymbol{X}^s_{tx}.\boldsymbol{U} \leq \quad \varepsilon_{max},$$

where λ is to weight the number of non-zero coefficients according to the maximal error, it is typically small as more importance is given to the minimization of the error. Remark that ε_{max} might also be set to an arbitrary value that represent an acceptable error. As the amount of data in the HF computations may be very large, the linear problem is solved using only some of them that are concatenate in *List*. An iterative process has been setup to select the most relevant data and to refine the space and time bases:

1. Initialization	
11	Set the maximum error to $\varepsilon = \infty$, the iteration number to $ite = 0$
12	Randomly choose the data to be inserted in the linear program in *List*.
13	Perform the clustering to extract the matrices C and R, and define the polynomial dependances gathered in the matrix P
2 Coefficients loop: While $\varepsilon > 1e-8$, or $ite \leq ite\_max$	
21	Solve the linear problem (2).
22	Compute the estimation of the current ROM using (1), set $\varepsilon = \max(\lvert \boldsymbol{F}_{ROM} - \boldsymbol{F}_{HF} \rvert)$
23	Update *List* with the N worst predicted values of each HF matrices
24	Update R with the rows corresponding to the worst predicted value in each the HF matrices
25	Update C with the columns corresponding to the worst predicted values in each HF matrices

To sum-up, ReCUR model takes as input existing computations and deliver estimations for new parametric configurations in the same format than HF computations. The construction of the ROM has been developed to take advantage of the data available and to be as efficient as possible regarding construction time and accuracy.

2.3 Coupling ROM and optimization

Solving optimization problem aims at finding the solution of the following problem:

$$\min_{\boldsymbol{x}} \ J(\boldsymbol{x}),$$

$$such\,that\ \boldsymbol{f}(\boldsymbol{x}) \leq 0,$$

where $\boldsymbol{J}(\boldsymbol{x})$ is an objective function depending on the parameters $\boldsymbol{x}$ and $\boldsymbol{f}(\boldsymbol{x})$ is a set of constraint function that should be enforced. Note that bounds of $\boldsymbol{x}$ might be considered as constraints.

As stated before, the use of HF numerical modelling to solve such problem is barely achievable with time consuming HF simulation. The strategy investigated in this paper is to replace the time-consuming HF simulation with its ReCUR ROM counterpart. Initially, the ROM is

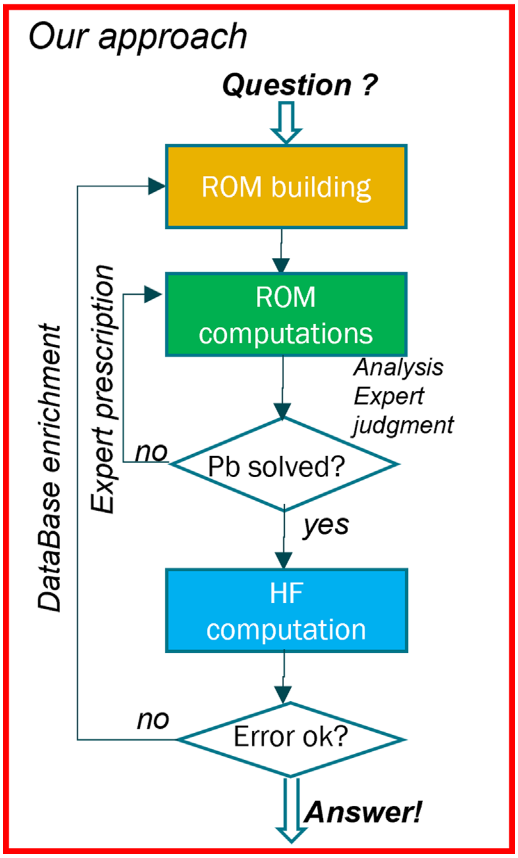

Fig. 1. Schematic view of the active learning process.

built with few existing computations, typically as many as the number of parameters. The optimization problem is solved using this ROM to compute the quantities of interest. As it is fast enough, optimization algorithm can launch a lot of runs to explore exhaustively the parametric domain and reach an interesting optimum. After, a unique HF computation corresponding to that optimum is launched with the HF solver. If the result of that configuration is satisfactory according to the optimization problem, then it is considered as solved. Otherwise, the HF computation corresponding to the optimum is added in the training pool and another ROM will be built using this enriched pool, and the optimization problem solved again. The process is repeated until a satisfactory point is reached. That methodology is like active learning in the machine learning [26]. With this approach, the precision of the ROM is improved in the areas of interest. Consequently, it allows to limit the number of HF computations to solve the optimization problem. Moreover, the ROM and the existing computations, can still be used in subsequent optimization studies or for further post-treatments. A schematic view of the process is proposed on Figure 1.

3 Numerical results

In this section, the aforementioned strategy will be applied to the setup of welding parameters. The HF simulation is a multi-physic welding simulation. This simulation supplies a fruitful information but is time-consuming as it takes several dozen hours to be solved. Then the use of ROM approach is relevant in this case.

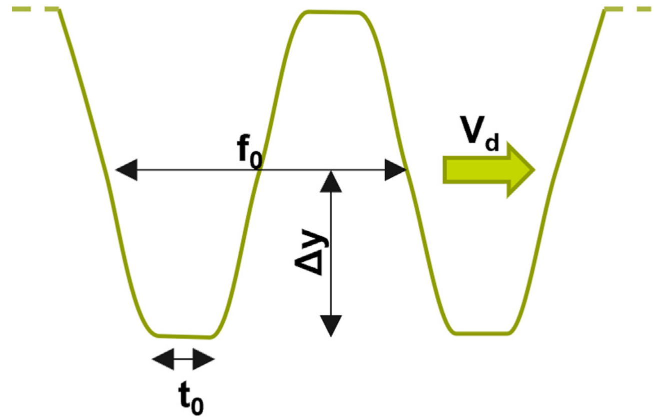

Fig. 2. Parametrization of the weaving trajectory. From [2].

3.1 Optimization problem

The methodology is applied on a metal deposit by a TIG process [2]. The trajectory of the welding follows a weaving pattern. The weaving is parameterized with respect to 4 parameters that are:
- The pause time t_0 in second
- The linear speed V_d in cm/min
- The frequency f_0 in Hz
- The half-magnitude Δy in mm

Each of these quantities are illustrated on Figure 2.

The corresponding HF simulation is a thermo-hydro-magnetic model with material feed. A single run for one parametric configuration takes from 3 to 5 days using Comsol software on 32 multi-core devices. The HF model supplies a lot of information and is representative of the physics on a wide range of parameters. Then it may be used to study the effect of the parameters on the dimensions of the welded pool. Those dimensions are key information in the development of new applications. The dimensions of the melt pool are:
- The penetration P
- The height H
- The half width $l_1/_2$
- The length L

They are depicted on Figure 3.

Given desired dimensions, it is possible to solve an inverse problem using optimization algorithm to find corresponding weaving parameters. The optimization problem reads:

$$\min_{t_0,v_d,\Delta y,f_0} \lambda_p \frac{|P-P_t|}{P_t} + \lambda_H \frac{|H-H_t|}{H_t} + \lambda_l \frac{|l_{1/2}-l_{1/2t}|}{l_{1/2t}} + \lambda_L \frac{|L-L_t|}{L_t} \tag{3}$$

$$such\,that, a_{\min} \leq a \leq a_{max}, where\, a = t_{0,} y_{d,} \Delta y, f_0.$$

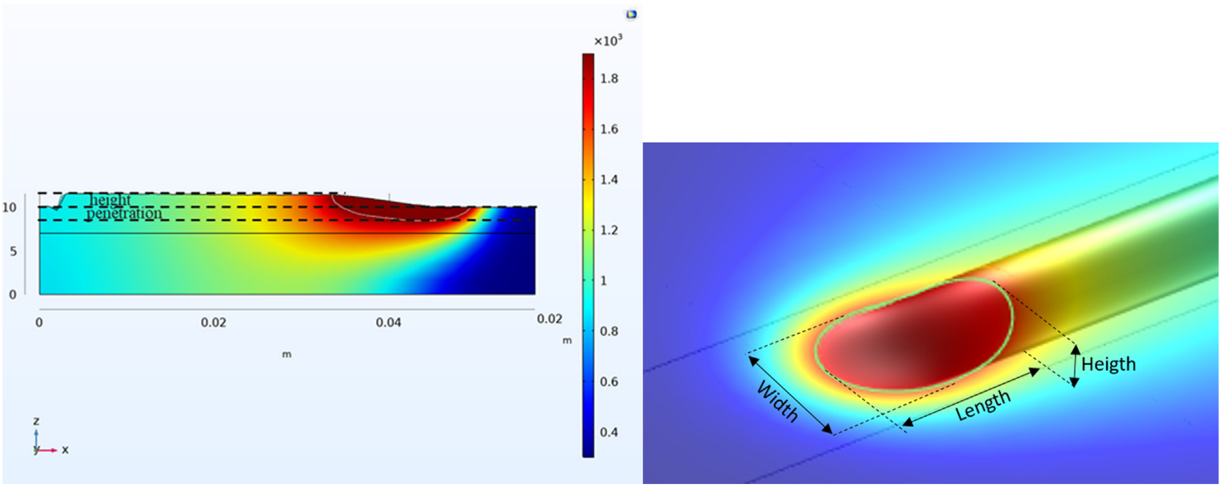

Fig. 3. Illustration of a HF result and the dimensions of the melt pool. The colour corresponds to the temperature in Kelvin.

The first line stands for the minimization of the objective function. It is a concatenation of gaps between target dimensions (designed by a_t), and dimensions obtained from post-treatment of the computations. The λ_α depicts the weights of the dimension α in the objective. The higher it is, the more important is considered the dimension. The optimization algorithm will tend to minimize the dimension with a high weight before the other. Such optimization strategy is so-called lexicographic optimization [27]. The second line stands for the bound constrains of the parameters.

An example of HF results is displayed on Figure 4. The values of the parameters for this simulation are: linear velocity 17 cm/min, half-magnitude 3 mm, 0.5 Hz for the frequency and 0.54 s for the pause time.

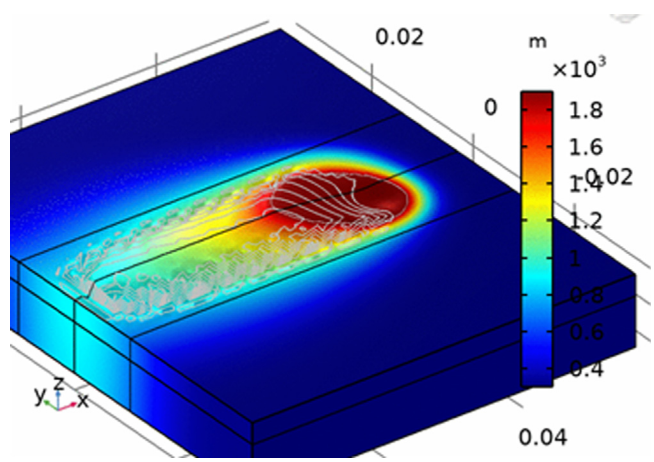

Fig. 4. HF results featuring the effect of weaving on the shape of the metal deposit. Colouring is the temperature in Kelvin.

3.2 ReCUR ROM of the melting pool

To solve the optimization problem, ReCUR ROM is used. It has been built from the previous HF simulation of the melt pool. The ROM is built on the maximum temperature at each node of the mesh. Consequently, the size of the HF results that will be used to train the model will be 1 row by the number of nodes in the mesh. To be assimilated in the ROM construction, all the HF results are projected on the same mesh. That mesh has 78,597 nodes and 505,670 tetrahedral elements. It is displayed on Figure 5.

The parametric dependency is introduced in the ROM through Legendre polynomials.

3.3 Optimization results

The target dimensions of the melt pool are displayed in Table 1.

The weights in the objective function (3) have been set to 1e12 for the penetration, 1e8 for the height, 1e4 for the half width, and 1e0 for the length. It means that optimization algorithm will look first for good penetration and height.

A first ROM is built on the maximal temperature using order 1 Legendre polynomial depending on the weaving parameters. The training pool consisted in computations with the parametric configurations exposed in Table 2.

The optimization algorithm is AGS of the Nlopt toolbox [28,29] with 1000 iterations. It is a derivative free and global algorithm dedicated to nonlinear mono-objective and nonlinear constraints. The construction time of the ROM was about 20 min and the resolution time of the optimization were about 1 hour.

Running this optimization algorithm with the first ROM leads to the results exposed on Table 3.

The right part of Table 3 gives the dimensions measured on the HF computation that corresponds to the optimal point supplied by the optimization algorithm using the ROM.

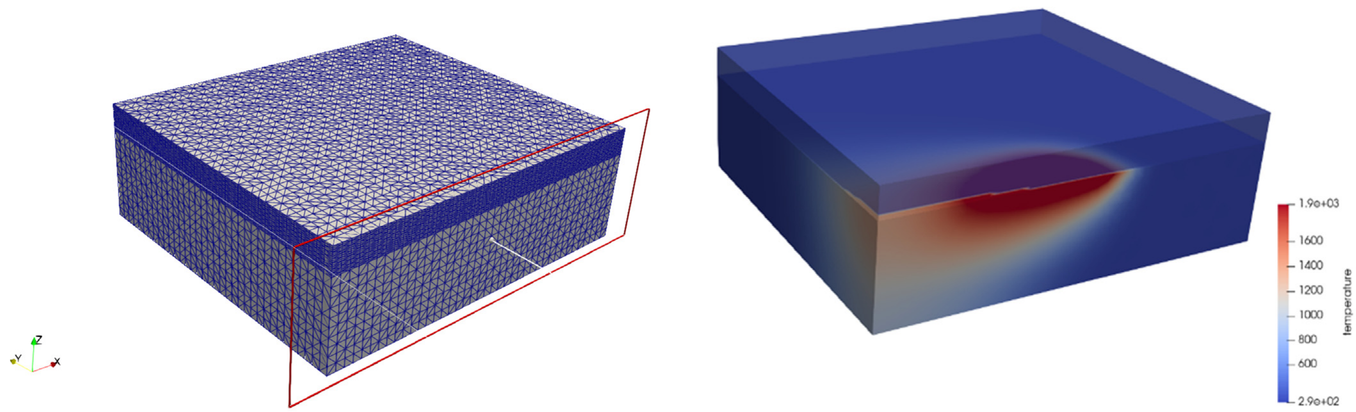

Fig. 5. Visualization of the mesh on the left. Example of a maximal temperature field on the right. A clip on the half of the domain has been made.

Table 1. Target dimensions.

Penetration	1.1 mm
Height	1.6 mm
Half-width	8.1 mm
Length	16.6 mm

Table 2. Parametric values of the initial training pool.

#	V_d (cm/min)	t_0(s)	Δy(mm)	f_0(Hz)
1	17.5	0.25	6	2
2	14.4	0.31	1.5	1.5
3	26.9	0.063	7.5	3.5
4	22.4	0.47	0.75	2.3

This point is considered far from the target, especially regarding the penetration and the height. Following the active learning strategy exposed previously, the HF computation corresponding to this weaving configuration has been added to the training pool and a new ROM has been build. This new ROM is then used to solve the optimization problem (3). The optimal point and the HF dimensions are given in Table 4.

The result is closer to the target regarding the penetration and the half width but further for the height. It means that the training pool is not complete enough to describe the molten bed on the entire parametric range. The HF result corresponding to this parametric configuration has been added to the training set of the ROM.

The next ROM are then built using 6 computations. Regarding the increase of computations in the training set, the order 1 polynomials were turned into order 2 polynomials with interactions between parameters. The optimum point is given in Table 5.

For that attempt, the penetration perfectly matches the target. The height and the half width are close to the targets. It is considered as satisfactory.

Table 3. First optimal point (weaving parameters on the left, HF dimensions of the optimal point on the right).

Pause time	0.32 s	Penetration	1.9 mm
Half-magnitude	3.34 mm	Height	2.0 mm
Frequency	1.44 Hz	Half-width	8.9 mm
Linear speed	8.69 cm/min	Length	18.5 mm

Table 4. Second optimal point (weaving parameters on the left, HF dimensions of the optimal point on the right).

Pause time	0.37 s	Penetration	1.8 mm
Half-magnitude	1.85 mm	Height	2.8 mm
Frequency	0.79 Hz	Half-width	7.7 mm
Linear speed	7.92 cm/min	Length	20.5 mm

Table 5. Fifth optimal point (weaving parameters on the left, HF dimensions of the optimum on the right).

Delay time	0.27 s	Penetration	1.1 mm
Half-magnitude	5.83 mm	Height	1.3 mm
Frequency	2.2 Hz	Half-width	9.4 mm
Linear speed	23.3 cm/min	Length	9.1 mm

A last iteration of the optimization process has been performed but without improving the results and not detailed in this paper. It could suggest that more than one iteration should be performed to improve the results. Considering the computation time of the HF model compared to the potential gain on the target, it has been considered not relevant to perform further HF computations and optimization loops. Another improvement could be to modify the ROM to be more accurate. The use of neural network instead of linear programming are ongoing research that aims for this goal. It could indeed introduce non-linearities in the ROM that could help to catch complex behaviour of the molten bed.

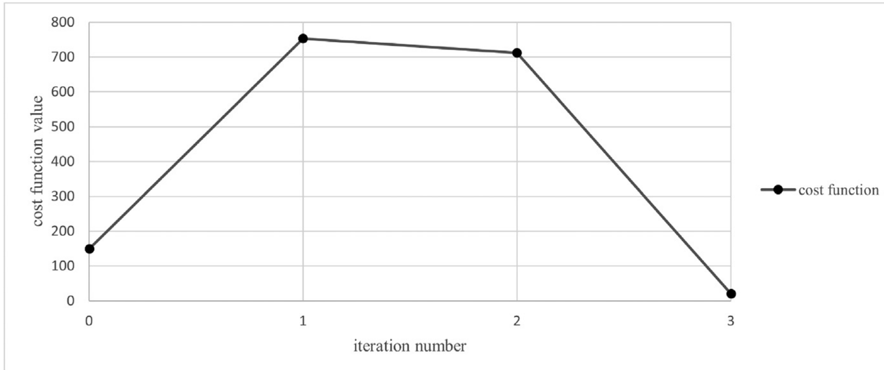

Fig. 6. Evolution of the cost function (3) according to the iteration of the ROM based optimization process.

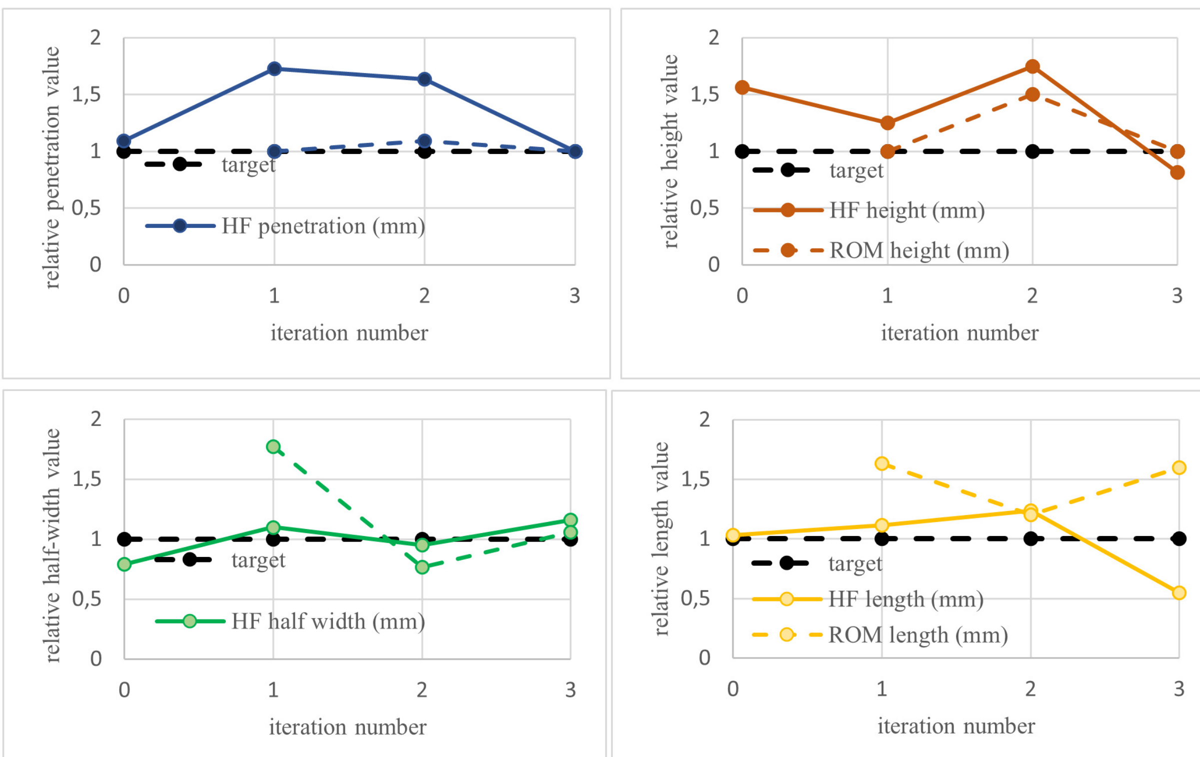

Fig. 7. Convergence of the optimization for each dimension of the molten bed. Thin dashed colour lines stand for the ROM estimations, solid lines stand for the HF dimensions.

Finally, the overall numerical process was performed using 7 HF computations. In comparison, a classic optimization approach directly using the HF computations, would require at least ten times the number of parameters, that is 40 computations. The time saving is then tremendous by using the ROM-based approach. The convergence of the optimization is displayed on Figure 6. and by component on Figure 7. All the values are normalized according to the respective target values. At iteration 0 only the HF dimensions are available as no ROM exists initially. At iteration 0, the best computation among the initial pool regarding the objective function (3) is chosen. The ROM estimations and the HF dimensions may be compared. It shows that the dimensions with the highest importance in the cost function (3) converge to the target values for the ROM estimation and the HF computations.

The comparison of the ROM estimation and the HF results for the last optimal point is displayed on Figure 8. One may observe differences between ROM and HF results, especially in the tail of the melt pool. It is both the fact of lacks in the construction of the ROM and not rich enough training set. But it must be kept in mind that the HF result remains the reference and that the ROM replaces the HF

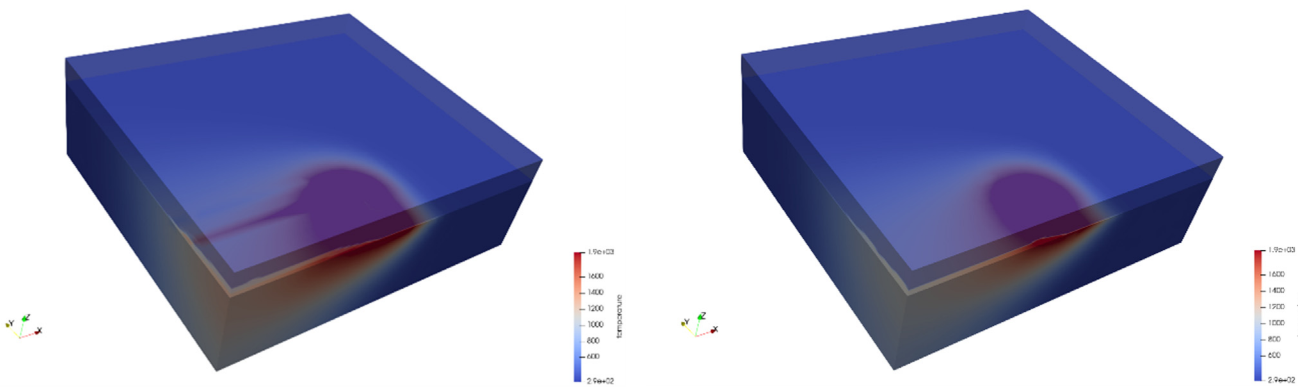

Fig. 8. Optimal results of the last iteration. On the left, the ROM's estimation, and on the right, the HF computation. Colour depicts the temperature in Kelvin.

computation only in the optimization algorithm. The ROM is useful to guide the optimization algorithm toward interesting solutions, not to provide very accurate estimations.

4 Conclusions and perspectives

The relevance of the ROM-based approach to solve optimization problem has been demonstrated on the example of weaving parameter setup for metal deposit.

The goal was to find weaving parameters that lead to desired dimensions of melt pool. A non-intrusive and parametric ROM called ReCUR was built from a pool of HF computations. The HF computations comes from a thermo-hydro-magnetic modelling with material feed. They take from 3 to 5 days. The ROM's estimation takes few seconds and are suitable with multi-query optimization process to solve the inverse problem. Using an active learning strategy for the updating of the ROM, a satisfactory solution was found with 7 computations. That must be compared with the classical optimization approach that would require 40 computations. Moreover, the ROM estimations may be visualized using classical engineer software for further post-treatments.

One lead of improvement would be to investigate another optimization algorithm than AGS to solve the inverse problem. AGS is indeed a general-purpose algorithm, and develop an algorithm dedicated to pairing with ROM could potentially be more efficient. It may indeed suggest optimum points that consider confidence of the ROM, as in the Efficient Global Optimization [30] or Bayesian optimization for instance. A second outlook is to improve the accuracy of the ROM using Neural network or Random Forest [31] instead of linear programming. This is the subject of ongoing work. That work strengthens the link between the ROM approaches and the field of machine learning [32]. Finally, experimental validation of the found optimum could be beneficial to consolidate the method. It would also be the opportunity to study data assimilation techniques to consider both simulation and sensor data in the ROM.

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