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A MULTISCALE METHOD WITH CONTINUOUS MATTER ADDITION IN DED ADDITIVE MANUFACTURING PROCESSES

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Summary. Additive manufacturing (AM) is a production method with great potential for creating complex geometries and reducing material and energy waste. Numerical simulations are crucial to minimize fabrication failures and optimize designs. Nevertheless, the high computational cost of simulating the multi-scale behaviour of AM processes is a challenge. To address this, an Arlequin-based method is proposed, which uses two distinct meshes to capture the high thermal gradients near the melt pool: a coarse mesh for the entire domain and a fine mesh that moves with the heating source. Additionally, a change of variable simplifies calculations on each time step by transforming the moving fine mesh into a fixed mesh. The proposed methodology has the potential to reduce computational costs and improve the efficiency of AM simulations.

1 INTRODUCTION

Additive manufacturing (AM) is a new production method based on material addition. AM brings new possibilities in geometries and shapes, as well as reduction on material and energy wastage, which places it in an advantageous position for a sustainable industry. AM is based on a heat source melting metal in order to form the desired geometry. Direct

energy deposition (DED) methods are a type of AM procedures, based on continuous addition of material powder as the heat source melts it. DED methods do not need a closed environment to work so the size of products is only limited by the range of the robotic tools. These processes have two main physical behaviours, each at different scales:

The micro scale refers to the behaviour near the heat source. The heat source creates a melt pool that moves along the piece adding new material to it. This coupled fluid-thermal physics takes place in a short time period in a small area.

The macro scale refers to the thermo-mechanical behaviour of the full piece. As the piece is being fabricated, high thermal gradients can produce deformations. This thermo-mechanical behaviour takes place in a long period of time and over the whole piece.

Numerical simulations are required by the AM industry in order to reduce failures in fabrications. Simulations, both in advance and in real time, simulations can save time and money in the design and fabrication of pieces by AM processes. The main challenge that AM DED processes simulations pose is their computational cost, due to the intrinsic multi-scale of the processes and the continuously growing physical domain.

The state of the art in numerical procedures for dealing with the material addition is the use of the quiet element method or the inactive element method [1]. Both methods use a unique mesh for the planned end piece and activate elements as the heat source moves above them. The main disadvantage of these methods is the mesh size. As the critical micro scale behaviours go over the whole domain, changing the zone depending on the advance of the heat source, the mesh must be fine enough to capture them. But, away from the heat source, there is no need for a fine mesh, so it could be coarser, what will lead to remeshing and its subsequent problems.

To reduce the computational costs, an Arlequin [2, 3] based method is presented. To deal with the multi-scale of the problem, the Arlequin method uses two distinct meshes: A coarse mesh of the whole domain and a fine mesh that moves along with the heating source to capture the high thermal gradients near the melt pool. In addition to the Arlequin method, a change of variable is introduced to transform the moving fine mesh in a fixed mesh so the calculations on each time step are simplified.

2 MATHEMATICAL MODEL

AM processes are driven by the effect of a strong heat source, which melts the material in powder or wire form. The molten material cools down to solidify and forms the desired shape. In DED processes, material and heat are supplied at the same time. This feature brings new possibilities, as a container to build the piece is unnecessary.

The heat source affects directly to a small part of the piece, heating and forming a melt pool. As the source moves, the melted material cools down and solidifies. In these scales, the main physics involved in the process are heat conduction, convection and radiation, fluid dynamics and phase change phenomena.

In a greater scale, the heat introduced by the source spreads by conduction to the whole piece and it dissipates through its surface. This phenomenon produces heat variations throughout time that induces deformations in shape. This mechanical behaviour coupled with the heat variation are the main physics to consider in the macro scale of the problem.

Different combinations of the physics involved in the process can be chosen to make a model of the AM process. Its objective is to simulate the behaviour of a full piece over a long time period. The multi-scale, both physical and temporal, make these simulations very computationally expensive. To do affordable simulations, a simplified model is needed.

For this macro model, only the thermo-mechanical behaviours will be taken into account. In addition to that, the thermal and mechanical problems can be decoupled. As a starting point, only the thermal model will be considered, as the main challenges of the problem are already faced by the thermal problem.

The partial differential equation for the thermal model can be written as follows:

$$\rho C_p \frac{\partial u}{\partial t} - \nabla \cdot (k \nabla u) = Q, \tag{1}$$

where ρ, C_p and k are the material density, heat capacity and conductivity, u is the temperature distribution solution and Q is the supplied heat source distribution. To model heat lose through the surface of the piece by radiation and convection, the boundary condition for the differential equation is set as:

$$\begin{aligned} -k \frac{\partial u}{\partial \overrightarrow{n}} &= (h_{rad} + h_{conv})(u - u_{ext}), \\ h_{rad} &= \sigma \epsilon (u + u_{ext})(u^2 + u_{ext}^2), \end{aligned} \tag{2}$$

where h_{conv} is the coefficient for convection, ϵ is the emissivity of the material and σ is the Stefan-Boltzmann constant, $\overrightarrow{n}$ is the outwards normal vector and u_{ext} is the temperature in the exterior. Although the term h_{rad} depend on the solution of the problem, a classical linear approximation will be done using the previous time step temperatures to compute it.

Let $\Omega(t)$ be the temporal dependent domain of the piece and $\Gamma(t)$ its boundary. The weak formulation for the thermal problem (1)-(2) can be written as follows: For each time $t \in (T_0, T_{fin}]$, find $u^t \in H^1(\Omega(t))$, such that, $\forall v \in H^1(\Omega(t))$,

$$\int_{\Omega(t)} \rho C_p \frac{\partial u^t}{\partial t} v \mathrm{d}x + \int_{\Omega(t)} k \nabla u^t \cdot \nabla v \mathrm{d}x + \int_{\Gamma(t)} (h_{rad} + h_{conv})(u^t - u_{ext}) v \mathrm{d}\Gamma = \int_{\Omega(t)} Q^t v \mathrm{d}x, \tag{3}$$

where the superscript t denotes de temporal dependency and with initial condition $u^{T_0} = u_{ini}$ for the initial time T_0.

3 MATHEMATICAL PROCEDURE

The methodology that will be described in this section was developed to address the multi-scale problem. Firstly, the Arlequin method will be considered. It will allow the use of different mesh configurations to capture the different areas (even small and evolving) with different AM process behaviours. Secondly, the other main challenge of these processes is the continuously growing domain. To deal with it, a change of variable will be proposed, simplifying the calculations in each time step.

3.1 Arlequin method

For each time t, only a small part of the domain $\Omega(t)$ has a critical behaviour. This part moves with time, following the heat source. The use of the Arlequin method allows to use two different mesh refinements without remeshing after each time step. This method will be introduced hereafter for a fixed time step t. So, to simplify the notation, while describing the Arlequin method, the temporal dependency of the domains will not be written.

The whole domain is divided into two overlapping domains, Ω_0 and Ω_1, called the global and local domains, respectively. From a function $u \in H^1(\Omega)$, a pair of functions can be univocally defined, $u_0 := u_{|\Omega_0} \in H^1(\Omega_0)$ and $u_1 := u_{|\Omega_1} \in H^1(\Omega_1)$, such that $u_0 = u_1$ in $\Omega_0 \cap \Omega_1$. Given the last condition, this process can be reversed so a function $u \in H^1(\Omega)$ is obtained from $u_0 \in H^1(\Omega_0)$ and $u_1 \in H^1(\Omega_1)$, such that $u_0 = u_1$ in $\Omega_0 \cap \Omega_1$.

The Arlequin coefficients, α_0 and α_1, are functions on the whole domain such that $\alpha_i \geq 0$ in Ω_i, $\alpha_i = 1$ in $\Omega_i \backslash (\Omega_0 \cap \Omega_1)$ and $\alpha_0 + \alpha_1 = 1$ in Ω.

Using the ingredients introduced before, and to simplify notation, the following bilinear and linear forms are defined:

$$\mathcal{A}_i(u,v) := \int_{\Omega_i} \alpha_i \rho C_p \frac{\partial u}{\partial t} v \mathrm{d}x + \int_{\Omega_i} \alpha_i k \nabla u \cdot \nabla v \mathrm{d}x + \int_{\partial\Omega_i \cap \Gamma} \alpha_i (h_{rad} + h_{conv}) u v \mathrm{d}\Gamma, \quad (4)$$

$$\mathcal{L}_i(v) := \int_{\Omega_i} \alpha_i Q v \mathrm{d}x + \int_{\partial\Omega_i \cap \Gamma} \alpha_i (h_{rad} + h_{conv}) u_{ext} v \mathrm{d}\Gamma. \quad (5)$$

The weak form (3) can be written as:

$$\mathcal{A}_0(u_0, v) + \mathcal{A}_1(u_1, v) = \mathcal{L}_0(v) + \mathcal{L}_1(v), \quad \forall v \in H^1(\Omega), \quad (6)$$

as $\alpha_0 + \alpha_1 = 1$ and $\alpha_i = 0$ outside Ω_i, and maintaining the condition $u_0 = u_1$ in the intersection $\Omega_0 \cap \Omega_1$.

This equality condition will be ensured weakly by using Lagrange multipliers. As the solution is inside a H^1 space, seems natural to also use a coupling in H^1 sense. The coupling takes place in the intersection, so the space $H^1(\Omega_0 \cap \Omega_1)$ will be used as the multipliers functional space. For this coupling a new bilinear form is introduced:

$$\mathcal{C}(u, \lambda) = \int_{\Omega_0 \cap \Omega_1} u\lambda + \nabla u \cdot \nabla \lambda \mathrm{d}x. \quad (7)$$

With all these ingredients, the classic Arlequin formulation can be presented: Find $(u_0, u_1, \lambda) \in H^1(\Omega_0) \times H^1(\Omega_1) \times H^1(\Omega_0 \cap \Omega_1)$, such that:

$$\begin{aligned} \mathcal{A}_0(u_0, v_0) + \mathcal{C}(v_0, \lambda) &= \mathcal{L}_0(v_0), && \forall v_0 \in H^1(\Omega_0), \\ \mathcal{A}_1(u_1, v_1) - \mathcal{C}(v_1, \lambda) &= \mathcal{L}_1(v_1), && \forall v_1 \in H^1(\Omega_1), \\ \mathcal{C}(u_0, v_\lambda) - \mathcal{C}(u_1, v_\lambda) &= 0, && \forall v_\lambda \in H^1(\Omega_0 \cap \Omega_1). \end{aligned} \quad (8)$$

The previous formulation is the classic one and it can be refined. For more information about the topic see [3]. As an intuitive clarification, the idea is to only couple on the boundary of the intersection so the coupling in the interior comes as the result of solving the same PDE with the same boundary conditions, saving computations in the coupling.

3.2 Finite material addition

This method uses two meshes to capture distinct scale behaviours: a coarse mesh for the whole piece and a local, finer moving mesh. To ensure efficiency, wise mesh selection is essential. In this section, the use of the global mesh will be explained, while the treatment of the moving mesh will be addressed in a subsequent section. The physical domain of the problem grows continuously from the critical zone, allowing the local mesh to handle the growing domain without depending on the global mesh. However, the local mesh fixed size cannot handle the growing behaviour of the entire problem as the grown parts will be larger than the mesh itself.

The idea to solve this challenge is to divide the full problem into a finite number of shorter subproblems, $\mathcal{P}^1, \ldots, \mathcal{P}^N$. In each of them, the local mesh will be able to deal with the growth of the domain, so the global domain will be static. Let $[T_0, T_{end}]$ be the time interval for the full problem, we introduce the time divisions $T^0, \ldots, T^N \in [T_0, T_{end}]$ so the subproblem $\mathcal{P}^n$ is defined over the time interval $[T^{n-1}, T^n]$. The length of these intervals is given by the velocity of the heat source. This length is the travel time of the source to go over the initial intersection between meshes. In figure 1 a representation of this division is shown.

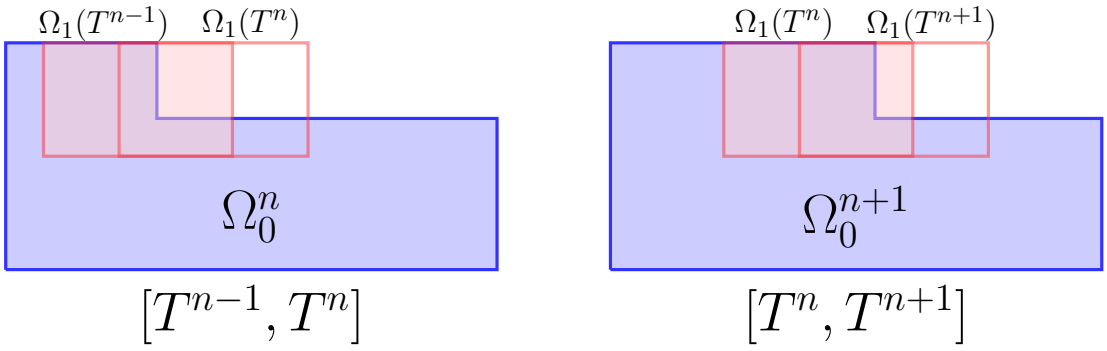

Figure 1: Representation of the position of the meshes for two consecutive subproblems.

As the global domain will be static on each subproblem, it will be denoted as $\Omega_0^n = \Omega_0(t)$, $\forall t \in [T^{n-1}, T^n]$. $\forall n \in \{1, \ldots, N\}$ and $\forall t \in [T_0, T_{end}]$, the bilinear forms $\mathcal{A}_0^n$ and $\mathcal{A}_1^t$ and the linear forms $\mathcal{L}_0^n$ and $\mathcal{L}_1^t$ are defined from the non temporal dependent definitions of $\mathcal{A}_i$ and $\mathcal{L}_i$, (4)-(5), by changing the domains Ω_0 and Ω_1 for its corresponding domains Ω_0^n and $\Omega_1(t)$ in the definitions. In the same way, $\forall t \in [T_0, T_{end}]$, the couplings $\mathcal{C}^t$ are defined from the static definition of $\mathcal{C}$, (7), by changing the intersection of Ω_0 and Ω_1 for its corresponding intersection of $\Omega_0(t)$ and $\Omega_1(t)$:

$$\mathcal{A}_i^n(u,v) := \int_{\Omega_0^n} \alpha_0 \rho C_p \frac{\partial u}{\partial t} v \mathrm{d}x + \int_{\Omega_0} \alpha_0 k \nabla u \cdot \nabla v \mathrm{d}x + \int_{\partial\Omega_0^n \cap \Gamma} \alpha_0 (h_{rad} + h_{conv}) uv \mathrm{d}\Gamma, \quad (9)$$

$$\mathcal{L}_i^n(v) := \int_{\Omega_0^n} \alpha_0 Q v \mathrm{d}x + \int_{\partial\Omega_0^n \cap \Gamma} \alpha_0 (h_{rad} + h_{conv}) u_{ext} v \mathrm{d}\Gamma, \quad (10)$$

$$\mathcal{A}_1^t(u,v) := \int_{\Omega_1(t)} \alpha_1 \left(\rho C_p \frac{\partial u}{\partial t} v + k \nabla u \cdot \nabla v \right) \mathrm{d}x + \int_{\partial\Omega_1(t) \cap \Gamma} \alpha_1 (h_{rad} + h_{conv}) uv \mathrm{d}\Gamma, \quad (11)$$

$$\mathcal{L}_1^t(v) := \int_{\Omega_1(t)} \alpha_1 Q v \mathrm{d}x + \int_{\partial\Omega_1(t) \cap \Gamma} \alpha_1 (h_{rad} + h_{conv}) u_{ext} v \mathrm{d}\Gamma, \quad (12)$$

$$\mathcal{C}^t(u,\lambda) := \int_{\Omega_0(t) \cap \Omega_1(t)} u\lambda + \nabla u \cdot \nabla \lambda \mathrm{d}x. \quad (13)$$

The subproblem $\mathcal{P}^n$ can be written as follows: For every $t \in (T^{n-1}, T^n]$ find $(u_0^t, u_1^t, \lambda^t) \in H^1(\Omega_0^n) \times H^1(\Omega_1(t)) \times H^1(\Omega_0^n \cap \Omega_1(t))$, such that:

$$\begin{aligned} \mathcal{A}_0^n(u_0^t, v_0) + \mathcal{C}^t(v_0, \lambda^t) &= \mathcal{L}_0^n(v_0), && \forall v_0 \in H^1(\Omega_0^n), \\ \mathcal{A}_1^t(u_1^t, v_1) - \mathcal{C}^t(v_1, \lambda^t) &= \mathcal{L}_1^t(v_1), && \forall v_1 \in H^1(\Omega_1(t)), \\ \mathcal{C}^t(u_0^t, v_\lambda) - \mathcal{C}^t(u_1^t, v_\lambda) &= 0, && \forall v_\lambda \in H^1(\Omega_0^n \cap \Omega_1(t)), \end{aligned} \quad (14)$$

setting for $t = T^{n-1}$ as initial condition the solution for the same time in $\mathcal{P}^{n-1}$ and the initial condition of the full problem for $\mathcal{P}^1$ and where the superscript t indicates the time dependency.

As the growth of the domain is supposed to be known a priori, the domains of the consecutive subproblems is known too. This fact makes possible to plan the structure of the mesh for the final piece such that the mesh used in each subproblem is a submesh of it. This feature makes the computation of the initial condition of each subproblem trivial in the already constructed part and an easy projection from the finer local mesh in the new added elements.

3.3 Change of variable

As the strategy for the global domain is already explained, in this section the focus will be the local domain and its corresponding temporal dependency. As it was mentioned before, the mesh selected for this domain is a fixed in size moving mesh. The reason for this is to follow the heat source and the growing boundary as it moves. To do so, the spatial position of this mesh will change, following a known a priori path.

As the local mesh moves out from the global mesh of each subproblem, the total computational domain grows. To solve a time dependent problem, a discretization of the temporal derivative will be needed. Usually, this discretization involves the state of the variable in previous time steps. When working with moving meshes or growing domains, knowing the state of a variable on the previous time step becomes a challenge. Obtaining the value of a variable on a node in the previous time step can become a challenge when that position was not a node before. This is especially troublesome in points that were not part of the domain in the previous time step.

To solve this issue, a change of variable is introduced in this method before the time discretization. A fixed position for the local mesh, $\hat{\Omega}_1$, is defined. Between this static position and the real time dependent one there is a unique translation, $f(\hat{x}; t)$, which transforms

each point of the fixed domain $\hat{x} \in \hat{\Omega}_1$ into the correspondent one of the temporal dependent domain, $f(\hat{x};t) = x \in \Omega_1(t)$. In the figure 2 a scheme of the transformation is shown.

Although the possibilities for the movement of the heat source is wide, it usually moves with constant velocity, $\overrightarrow{v}$. In this case the transformation would be $f(\hat{x};t) = \hat{x} + \overrightarrow{r} + \overrightarrow{v}t$, being $\overrightarrow{r}$ the initial displacement between $\hat{\Omega}_1$ and $\Omega_1(T_0)$.

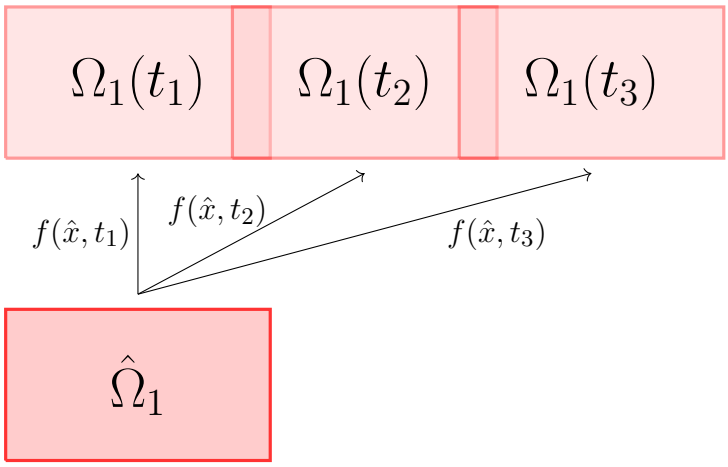

Figure 2: Scheme of the transformation throughout time.

This transformation, continuous in time, can be used as a change of variable in the integrals over $\Omega_1(t)$ in (14). Functions defined over the fixed domain will be denoted with a hat, so that $\hat{u}(\hat{x}) = u(f(\hat{x}))$. The bilinear forms $\mathcal{A}_1^t$ and $\mathcal{C}^t$ and the linear forms $\mathcal{L}_1^t$ are transformed by the change of variable into $\hat{\mathcal{A}}_1$, $\hat{\mathcal{C}}^t$ and $\hat{\mathcal{L}}_1$. The temporal dependency of the transformation introduce a convective behaviour in the bilinear form $\hat{\mathcal{A}}_1$. After the transformation, only the coupling bilinear form is time dependent (coupling over $f^{-1}(\Omega_0(t);t) \cap \hat{\Omega}_1$) as the relative real position of the meshes changes over time.

The new formulation of the subproblem $\mathcal{P}^n$, using this change, can be written as follows: For every $t \in (T^{n-1}, T^n]$, find $(u_0^t, \hat{u}_1^t, \lambda^t) \in H^1(\Omega_0^n) \times H^1(\hat{\Omega}_1) \times H^1(\Omega_0^n \cap \Omega_1(t))$, such that:

$$\begin{aligned} \mathcal{A}_0^n(u_0^t, v_0) + \mathcal{C}^t(v_0, \lambda^t) &= \mathcal{L}_0^n(v_0), && \forall v_0 \in H^1(\Omega_0^n), \\ \hat{\mathcal{A}}_1(\hat{u}_1^t, \hat{v}_1) - \hat{\mathcal{C}}^t(\hat{v}_1, f^{-1}(\lambda^t;t)) &= \hat{\mathcal{L}}_1(\hat{v}_1), && \forall \hat{v}_1 \in H^1(\hat{\Omega}_1), \\ \mathcal{C}^t(u_0^t, v_\lambda) - \hat{\mathcal{C}}^t(\hat{u}_1^t, f^{-1}(v_\lambda;t)) &= 0, && \forall v_\lambda \in H^1(\Omega_0^n \cap \Omega_1(t)), \end{aligned} \tag{15}$$

where the initial condition for T^{n-1} is obtained form the previous subproblem and the initial condition for $\mathcal{P}^1$ is the initial condition of the whole problem.

By doing the changes, both of the domains become static in each subproblem and only the coupling varies with time. As a result, the computations needed for each time step decreases and no remeshing is necessary.

Finally, partial numerical results will be given during the conference.

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