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Reduced Order Modeling via PGD for Highly Transient Thermal Evolutions in Additive Manufacturing

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Abstract

In this paper, a highly performing model order reduction technique called Proper Generalized Decomposition (PGD) is applied to the numerical modeling of highly transient non-linear thermal phenomena associated with additive manufacturing (AM) powder bed fabrication (PBF) processes. The manufacturing process allows for unprecedented design freedom but fabricated parts often suffer from lower quality mechanical properties associated with the fast transients and high temperature gradients during the localized melting-solidification process. For this reason, an accurate numerical model for the thermal evolutions is a major necessity. This work focuses on providing a low-cost/high accuracy prediction of the high gradient thermal field occurring in a material under the action of a concentrated moving laser source, while accounting for phase changes, material non-linearities and time and space-dependent boundary conditions. An extensive numerical simulation campaign shows that the use of PGD in this context enables a remarkable reduction in the total number of global matrix inversions (5 times less or better) compared to standard techniques when simulating realistic AM PBF scenarios.

Keywords: AM Process Simulation, Powder Bed Fabrication, Reduced Order Modeling, Proper Generalized Decomposition

¹ 1. Introduction

² Since their inception, selective laser melting (SLM) and electron beam ³ melting (EBM) powder bed fabrication (PBF), as prime examples in addi-

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 tive manufacturing (AM), proved to be a paradigm shift for manufacturing processes. They consist in selective melting of superposed layers of metal powder using a machine-controlled moving high energy source. Due to their nature, these processes allow unprecedented freedom in designing, personal- ization and optimization of mechanical parts. Moreover, they are particularly suited for software-hardware integration when the desired geometry is con- ceived with a Computer Assisted Design (CAD) tool and directly produced by an automated process, removing many of the intermediate steps between the designer's vision and the physical world.

 Effective numerical methods capable of predicting final characteristics of the part, spotting critical points during the process and helping the design process itself are often invaluable in gaining insight in the process. Since SLM and EBM encompass complex multiphysics (thermal, mechanical, phase change, metallurgic) and pose a gigantic multi-scale problem in both space ¹⁸ and time, special consideration is required in numerical analysis (see $[1, 2, 3]$) 3])including fast executing AM-specialized approaches (see [4]).

 This work focuses on the highly non-linear thermal phenomena occurring in the immediate proximity of the fast moving heat source where temper- ature evolution rates, phase changes and thermal gradients are the most intense, all happening on a very small scale (see [5]). The goal is to provide a lower-cost / high accuracy simulation of this important region. To provide this solution, a technique belonging to Reduced Order Model (ROM) fam- $_{26}$ ily (see [6, 7, 8, 9, 10, 11]) called Proper Generalized Decomposition (PGD) $_{27}$ (see [12, 13, 14, 15, 16, 17]) has been adapted for this problem to consider temperature-dependent material properties and latent heat associated with phase change. Heating is accomplished via a laser model that moves rapidly along the path while heat removal is modeled via temperature dependent thermal conductivity and rapidly evolving Neumann boundary conditions. This model order reduction technique allows computing a reduced base for each variable without solving the full eigenvalue problem. In order to prop- erly keep into account the non-linearities and the boundary condition of highly transient thermal evolutions, a dedicated PGD algorithm and method- ology have been developed, representing the main contributions of this work. Thanks to it, computational cost is significantly reduced and variable separa- tion is achieved enabling a highly meaningful reduced basis. Benchmarking against the full transient finite element solutions are performed. For the purpose of benchmarking, a linear finite element full integration formulation was chosen. An in-depth study on PGD controls (number of modes, number

⁴² of iterations, etc.) and on how they can be best selected for efficient com-⁴³ putations is included and accuracy and performance findings are carefully ⁴⁴ tabulated.

⁴⁵ 2. Problem description

⁴⁶ For the purpose of this study, a patch of material of unit thickness is ⁴⁷ subjected to intense heating from a heat source moving over its surface (see Figure 1). While the heating is three-dimensional in nature and the build

Figure 1: Problem under study

48

⁴⁹ direction involves a very important heat transport mechanism, for simplicity, $\frac{1}{50}$ we have modeled it as a 2D problem in the xy plane (all units are modified ⁵¹ accordingly). Despite this simplification, all core non-linearities associated ⁵² with additive manufacturing heat transfer computations including material ⁵³ properties, high temperature gradients and high heating and cooling rates are ⁵⁴ included and therefore the setup serves the core purpose of the paper. The 55 patch is a square region of given length (L) made of Ti-6Al-4V, a popular ⁵⁶ Titanium-based alloy used widely in powder bed fabrication additive manu-⁵⁷ facturing (see [18]). The material definition includes temperature-dependent 58 properties (such as the density (ρ) , the heat capacity (C_p) and the thermal \mathfrak{so} conductivity (k) ; the heat source is a laser beam with prescribed power ω density input (P) in the form of a Gaussian distribution initially centered 61 at point (X_0, Y_0) relative to a $(0, x, y)$ coordinate system aligned with the ϵ_2 plate edges with origin at the lower left corner of the plate. The heat source 63 is moving over the patch in the negative x-direction with a given speed (v) . ⁶⁴ The patch loses heat to the surrounding environment at temperature (T_{env}) ⁶⁵ through its surface according to a film condition with heat transfer coeffi- ϵ cient (h). In addition heat is also lost through its boundaries according to a

 σ prescribed outward flux $(\overline{q}^{out}(x, y, t))$, where t denotes the time. The values ⁶⁸ of all these parameters are subject to change depending on the particular ⁶⁹ test scenario presented in the Results and Discussion section.

 This problem can be formulated as a boundary value problem governed by a parabolic partial differential equation (PDE) for the scalar temperature τ_1 field $T(x, y, t)$, with material non-linearities and a non-linear varying source, ⁷³ in a 2D domain $\Omega = [0, L] \times [0, L]$ over a time interval $I = [0, t_{end}]$, with prescribed Neumann boundary conditions and uniform initial conditions. In its most general form, the boundary value problem is formulated as follows:

$$
\begin{cases}\n\frac{\partial(\rho C_p(T)T(x,y,t))}{\partial t} + \nabla \cdot (-k(T)\nabla T(x,y,t)) = Q^{in}(x,y,t) - Q^{out}(T) \text{ in } \Omega \times I \\
-k(T)\nabla T(x,y,t) \cdot \mathbf{n}^{out} = \overline{q}^{out}(x,y,t) \text{ on } \partial \Omega \times I \\
T(x,y,0) = T_0 \text{ in } \Omega\n\end{cases}
$$
\n(1)

⁷⁶ where

$$
\begin{cases}\nQ^{in}(x, y, t) = \frac{2P}{\pi R_0^2} \exp\left(\frac{-2}{R_0^2}((x - x_0(t))^2 + (y - y_0(t))^2)\right) \\
Q^{out}(T) = h(T - T_{env})\n\end{cases} (2)
$$

 \mathbb{R}^n Here \mathbf{n}^{out} represents the outer unit normal to the domain boundary, T_0 τ ⁸ represents the prescribed uniform initial temperature field, R_0 represents a ⁷⁹ characteristic radius for the Gaussian distribution and

$$
\begin{cases}\nx_0(t) = X_0 + f_x(t) \\
y_0(t) = Y_0 + f_y(t)\n\end{cases} (3)
$$

⁸⁰ represent the prescribed energy source motion. A description of the Gaussian ⁸¹ source model can be found in [19].

82 3. Methods and Algorithms

 Since the PGD results are compared to Finite Element Method (FEM) ⁸⁴ results (both in terms of accuracy and performance), the FEM and PGD methods will be described in parallel, for each new simulation capability added in order to solve the proposed problem.

⁸⁷ We start by describing the linear case, then move to comprehensive non- linear cases, including temperature-dependent properties and latent heat as- sociated with phase changes, fast moving time-dependent heat sources and temperature-dependent Neumann boundary conditions.

⁹¹ 3.1. Linear case

⁹² The FEM and PGD approaches are first briefly reviewed in the context of 93 a linear problem (parameters such as ρ , C_p and k are considered independent ⁹⁴ of the temperature) with zero Neumann boundary conditions (insulated) ⁹⁵ and a stationary and temperature independent heat source. Consequently, ⁹⁶ $\overline{q}^{out} = Q^{out} = f_x = f_y = 0 \,\forall t \in I$, and Q^{in} is independent of time:

$$
Q^{in}(x,y) = \frac{2P}{\pi R_0^2} \exp\left(\frac{-2}{R_0^2}((x - X_0)^2 + (y - Y_0)^2)\right).
$$
 (4)

⁹⁷ So, for the linear problem, Equation (1) can be reformulated as:

$$
\begin{cases}\n\rho C_p \frac{\partial T}{\partial t} - k \nabla^2 T = Q^{in}(x, y) \text{ in } \Omega \times I \\
k \nabla T \cdot \mathbf{n}^{out} = 0 \text{ on } \partial \Omega \times I \\
T(x, y, 0) = T_0 \text{ in } \Omega\n\end{cases}
$$
\n(5)

⁹⁸ The problem is solved by classical FEM (see [20]). A backward-Euler ⁹⁹ finite difference scheme is used for implicit time integration in an incremental ¹⁰⁰ approach.

¹⁰¹ For PGD, the temperature field is assumed to be decomposable in the ¹⁰² form of a finite sum of products between space and time functions:

$$
T(x, y, t) \approx \sum_{i=1}^{N_{mod}} \Phi_i(x, y) \lambda_i(t)
$$
\n(6)

103 where N_{mod} is the number of products, determined based on a convergence 104 criterion. The space functions are discretized according to $\Phi_i(x, y) \approx \mathbb{N}(x, y)\Phi_i$, ¹⁰⁵ where Φ_i represents the ith nodal solution vector and $\mathbb{N}(x, y)$ represents a set ¹⁰⁶ of interpolation functions. In a way, this is similar to the FEM approach, 107 where the solution field is discretized as $T(x, y, t) \approx \mathbb{N}(x, y)\mathbf{T}(t)$, with $\mathbf{T}(t)$ ¹⁰⁸ representing the solution vector at the nodes of the FEM mesh.

¹⁰⁹ The nodal solution vector is thus expressed as a separated representation 110 of the form $\mathbf{T}(t) \approx \sum_{i=1}^{N_{mod}} \Phi_i \lambda_i(t)$, where the vectors Φ_i can be viewed as ¹¹¹ "basis vectors" and the time functions $\lambda_i(t)$ can be viewed as coefficients ¹¹² in a linear combination analogous to FEM-based eigenmode superposition. 113 Alternatively, each couple $(\mathbf{\Phi}_i, \lambda_i(t))$ can be viewed as a "mode" in this ¹¹⁴ superposition. This terminology will be used in the Results and Discussion ¹¹⁵ section.

 In contrast to usual methods (which include FEM eigenmode analysis and other order reduction methods such as the Proper Orthogonal Decomposition - POD method), in which the projection basis is known a priori, the PGD basis vectors and time functions are both unknown and will be computed on the fly, for the particular problem at hand.

121 The basis is progressively enriched by the addition, at stage $n < N_{mod}$, of 122 a new couple $(\Phi_n, \lambda_n(t))$ which can be viewed as a correction to the previous 123 result $\mathbf{T}_{n-1}(t)$:

$$
\mathbf{T}_n(t) = \sum_{i=1}^n \mathbf{\Phi}_i \lambda_i(t) = \sum_{i=1}^{n-1} \mathbf{\Phi}_i \lambda_i(t) + \mathbf{\Phi}_n \lambda_n(t) = \mathbf{T}_{n-1}(t) + \mathbf{\Phi}_n \lambda_n(t). \tag{7}
$$

¹²⁴ The basis computation proceeds in successive stages. At each stage there 125 are two steps (see [15]):

- ¹²⁶ An enrichment step: a new couple consisting of a basis vector and a 127 time function $(\Phi_n, \lambda_n(t))$ is computed;
- ¹²⁸ An update step: all time functions are recomputed.

¹²⁹ PGD Enrichment step (addition of a new couple)

130 Assuming that the first $n-1$ couples $(\mathbf{\Phi}_i, \lambda_i(t))_{i=1,\dots,n-1}$ have been previ-¹³¹ ously obtained, the current approximation of the field is written in the form $T_n(t) = T_{n-1}(t) + \Phi_n \lambda_n(t)$, with the new couple $(\Phi_n, \lambda_n(t))$ unknown.

133 The new couple $(\Phi_n, \lambda_n(t))$ is obtained by applying an alternating direc- tions fixed point iterations method , which is the standard choice for PGD algorithms (see [15]). In contrast with the FEM, the time marching incre- ment has less influence on convergence. Other factors, such as a bad choice of the initialization function (for example a null function) can have a more detrimental effect.

139 The process starts with the initialization of the time function $\lambda_n^{(0)}(t)$. This choice is arbitrary, since several functions can result in converged results. We opted for using a linear time function. This was determined on physical grounds, based on the fact that in the absence of transients the solution of the boundary value problem with constant source and no Neumann boundary conditions behaves as an unbounded growth of the temperature field.

¹⁴⁵ After the initialization, the fixed-point iterations consist in computing ¹⁴⁶ in sequence: $\Phi_n^{(1)}$ and $\lambda_n^{(1)}(t)$ (first iteration), then $\Phi_n^{(2)}$ and $\lambda_n^{(2)}(t)$ (second 147 iteration), etc., until convergence to the couple $(\Phi_n, \lambda_n(t))$.

 148 At the k^{th} iteration, consistently with the basic premise of separation of ¹⁴⁹ variables, one thus solves in sequence:

- **•** A space problem for $\Phi_n^{(k)}$ (with $\lambda_n^{(k-1)}(t)$ known);
- ¹⁵¹ A time problem for $\lambda_n^{(k)}(t)$ (with $\Phi_n^{(k)}$ known).
- ¹⁵² Space problem

Assuming that $\lambda_n^{(k-1)}(t)$ is known, one obtains $\mathbf{\Phi}_n^{(k)}$ by assuming that ¹⁵⁴ $\mathbf{T}_n(t) = \mathbf{T}_{n-1}(t) + \mathbf{\Phi}_n^{(k)} \lambda_n^{(k-1)}(t)$ and by choosing a test function for the weak ¹⁵⁵ formulation of the problem in the form $\mathbf{T}^*(t) = \mathbf{\Phi}^* \lambda_n^{(k-1)}(t)$.

 $Based$ on the work of Nouy (see [15]) and Néron (see [16]), by employing ¹⁵⁷ the virtual work machinery, the space problem is then given by the equation:

$$
\left(\int_{I} \lambda_n^{(k-1)}(t) \dot{\lambda}_n^{(k-1)}(t) dt \mathbb{M} + \int_{I} \lambda_n^{(k-1)^2}(t) dt \mathbb{K}\right) \Phi_n^{(k)} =
$$

$$
\int_{I} \lambda_n^{(k-1)}(t) \mathbf{F}_{Q_{in}} dt - \sum_{i=1}^{n-1} \left(\int_{I} \lambda_n^{(k-1)}(t) \dot{\lambda}_i(t) dt \mathbb{M} + \int_{I} \lambda_n^{(k-1)}(t) \lambda_i(t) dt \mathbb{K}\right) \Phi_i
$$
\n(8)

¹⁵⁸ where

$$
\begin{cases} \mathbb{M} = \int_{\Omega} \mathbb{N}^{T}(x, y) \rho C_{p} \mathbb{N}(x, y) dS \\ \mathbb{K} = \int_{\Omega} (\nabla \mathbb{N})^{T}(x, y) k \nabla \mathbb{N}(x, y) dS \\ \mathbf{F}_{Q_{in}} = \int_{\Omega} \mathbb{N}^{T}(x, y) Q^{in}(x, y) dS \end{cases}
$$
(9)

¹⁵⁹ Letting:

$$
\begin{cases}\na_i = \int_I \lambda_n^{(k-1)}(t) \dot{\lambda}_i(t) dt \\
b_i = \int_I \lambda_n^{(k-1)}(t) \lambda_i(t) dt\n\end{cases}
$$
\n(10)

160 for $i = 1, ..., n - 1$ and

$$
\begin{cases}\na = \int_I \lambda_n^{(k-1)}(t) \dot{\lambda}_n^{(k-1)}(t) dt \\
b = \int_I \lambda_n^{(k-1)^2}(t) dt \\
\mathbf{c} = \int_I \lambda_n^{(k-1)}(t) \mathbf{F}_{Q_{in}} dt - \sum_{i=1}^{n-1} (a_i \mathbb{M} + b_i \mathbb{K}) \Phi_i\n\end{cases}
$$
\n(11)

¹⁶¹ this problem takes the form:

$$
(a\mathbb{M} + b\mathbb{K})\Phi_n^{(k)} = \mathbf{c}.\tag{12}
$$

¹⁶² Time problem

 $\Lambda_{\text{as}} \qquad \text{Assuming that } \boldsymbol{\Phi}_n^{(k)} \text{ is known, one obtains } \lambda_n^{(k)}(t) \text{ by assuming that } \mathbf{T}_n(t) = 0.$ $T_{n-1}(t) + \Phi_n^{(k)}(t) \lambda_n^{(k)}(t)$ and by choosing a test function for the weak formu-¹⁶⁵ lation of the problem in the form $\mathbf{T}^*(t) = \mathbf{\Phi}_n^{(k)} \lambda^*(t)$.

 $Based$ again on the work of Nouy (see [15]) and Ladevèze (see [21]), the ¹⁶⁷ time problem is then given by the equation:

$$
\boldsymbol{\Phi}_n^{(k)}^T \mathbb{M} \boldsymbol{\Phi}_n^{(k)} \dot{\lambda}_n^{(k)}(t) + \boldsymbol{\Phi}_n^{(k)}^T \mathbb{K} \boldsymbol{\Phi}_n^{(k)} \lambda_n^{(k)}(t) =
$$
\n
$$
\boldsymbol{\Phi}_n^{(k)}^T \mathbf{F}_{Q_{in}} - \sum_{i=1}^{n-1} (\boldsymbol{\Phi}_n^{(k)}^T \mathbb{M} \boldsymbol{\Phi}_i \dot{\lambda}_i(t) + \boldsymbol{\Phi}_n^{(k)}^T \mathbb{K} \boldsymbol{\Phi}_i \lambda_i(t)).
$$
\n(13)

¹⁶⁸ Letting:

$$
\begin{cases}\na_i' = \boldsymbol{\Phi}_n^{(k)}^T \mathbb{M} \boldsymbol{\Phi}_i \\
b_i' = \boldsymbol{\Phi}_n^{(k)}^T \mathbb{K} \boldsymbol{\Phi}_i\n\end{cases}
$$
\n(14)

169 for $i = 1, ..., n - 1$ and

$$
\begin{cases}\na' = \boldsymbol{\Phi}_n^{(k)}^T \mathbb{M} \boldsymbol{\Phi}_n^{(k)} \\
b' = \boldsymbol{\Phi}_n^{(k)}^T \mathbb{K} \boldsymbol{\Phi}_n^{(k)} \\
c'(t) = \boldsymbol{\Phi}_n^{(k)}^T \mathbf{F}_{Q_{in}} - \sum_{i=1}^{n-1} (a_i' \dot{\lambda}_i(t) + b_i' \lambda_i(t))\n\end{cases}
$$
\n(15)

¹⁷⁰ this problem takes the form:

$$
a'\dot{\lambda}_n^{(k)}(t) + b'\lambda_n^{(k)}(t) = c'(t). \tag{16}
$$

¹⁷¹ This standard ordinary differential equation in time is solved here for ¹⁷² $\lambda_n^{(k)}(t)$ by numerical integration in time making use of Backward-Euler finite 173 difference scheme with large time increments.

¹⁷⁴ Convergence criterion

175 The new couple $(\boldsymbol{\Phi}_n, \lambda_n(t))$ is obtained after convergence of the fixed point ¹⁷⁶ iterations for the sequence $\Phi_n^{(k)}$, $\lambda_n^{(k)}(t)$, based on the relative error criterion ¹⁷⁷ chosen as:

$$
\epsilon = \frac{2\int_I \left(\lambda_n^{(k)}(t) - \lambda_n^{(k-1)}(t)\right)^2 dt}{\int_I \left(\lambda_n^{(k)}(t) + \lambda_n^{(k-1)}(t)\right)^2 dt} < tol_{PGD}
$$
(17)

¹⁷⁸ where tol_{PGD} is a small tolerance. The optimal value of tol_{PGD} is case- dependent. On one hand, a small tolerance will lead to few PDG modes at the price of many fixed point iterations. On the other hand, a large value of $_{181}$ tol_{PGD} will need fewer fixed point iterations but more PDG couples in order to reach convergence. An in-depth analysis of this behavior will be presented in Section 4.

¹⁸⁴ PGD Update step (re-computation of all time functions)

185 Based again on [15], once the new couple $(\Phi_n, \lambda_n(t))$ has been computed, ¹⁸⁶ all time functions $\{\lambda_i(t)\}_{i=1,\dots,n}$ are updated based on all currently known 187 space vectors $\{\mathbf{\Phi}_i\}_{i=1,\dots,n}$ by requiring that:

$$
\sum_{i=1}^{n} \mathbf{\Phi}_{j}^{T} \mathbb{M} \mathbf{\Phi}_{i} \dot{\lambda}_{i}(t) + \sum_{i=1}^{n} \mathbf{\Phi}_{j}^{T} \mathbb{K} \mathbf{\Phi}_{i} \lambda_{i}(t) = \mathbf{\Phi}_{j}^{T} \mathbf{F}_{Q_{in}} \text{ for } j=1,...,n .
$$
 (18)

¹⁸⁸ Letting:

$$
\begin{cases}\n a'_{j,i} = \mathbf{\Phi}_j^T \mathbb{M} \mathbf{\Phi}_i \\
 b'_{j,i} = \mathbf{\Phi}_j^T \mathbb{K} \mathbf{\Phi}_i \\
 c'_j = \mathbf{\Phi}_j^T \mathbf{F}_{Q_{in}}\n\end{cases}
$$
\n(19)

¹⁸⁹ this problem takes the form:

$$
\sum_{i=1}^{n} a'_{j,i} \dot{\lambda}_i(t) + \sum_{i=1}^{n} b'_{j,i} \lambda_i(t) = c'_j \text{ for } j = 1,...,n .
$$
 (20)

¹⁹⁰ This coupled ordinary differential equations system in time is solved for $\{\lambda_1(t),...,\lambda_n(t)\}\;$ by numerical integration making use of Backward-Euler fi-¹⁹² nite difference scheme with large time increments over the entire time interval ¹⁹³ $I = [0, t_{end}]$. For the purpose of this study, the interval I was always dis-¹⁹⁴ cretized via 100 equally sized increments.

¹⁹⁵ 3.2. Extension to the non-linear case - non-linear materials

 The extension of the FEM and PGD approaches to the non-linear case is briefly described next. PDG has seen applications in non-linear cases, mainly by the use of linearization schemes or of asymptotic numerical methods as in [22], [23] and [24] . Nevertheless, the PGD algorithm and methodology pro- posed in this section are an original adaptation of PGD for highly transient 201 thermal evolution. The material parameters ρ , C_p and k are now assumed

²⁰² to be prescribed functions of the temperature. Since the capacitance ma-203 trix depends on the product $\rho C_P(T)$, it becomes a function of temperature $\mathbb{M}(T)$. Likewise, since the conductivity matrix depends on $k(T)$, it becomes 205 a function of temperature $\mathbb{K}(T)$.

²⁰⁶ For the FEM, the equation becomes:

$$
\mathbb{M}(T)\dot{\mathbf{T}}(t) + \mathbb{K}(T)\mathbf{T}(t) = \mathbf{F}_{Q_{in}},
$$
\n(21)

²⁰⁷ which is solved incrementally using implicit time integration with Backward- $_{208}$ Euler finite differences and Newton iterations (where a small tolerance Tol_{FEM} ²⁰⁹ must be used) at each time increment. More details can be found in [20].

²¹⁰ For the PGD, the non-linearities are taken into account at each stage by ²¹¹ using all the known information about the current content of the solution. 212 The computation of each new couple $(\Phi_n, \lambda_n(t))$ takes place again in two ²¹³ steps.

²¹⁴ PGD Enrichment step

²¹⁵ This step proceeds again by fixed point iterations.

²¹⁶ Since

$$
\mathbf{T}_n(t) = \sum_{i=1}^n \mathbf{\Phi}_i \lambda_i(t) = \mathbf{T}_{n-1}(t) + \mathbf{\Phi}_n \lambda_n(t), \qquad (22)
$$

217 where $\mathbf{T}_{n-1}(t)$ is not known for the first couple, one proceeds by using all ²¹⁸ the available information at each iteration.

219 To compute the first couple $(\Phi_1, \lambda_1(t))$, the temperature field $T(x, y, t)$ $_{220}$ is initialized to T_0 and used to compute initial values for the capacitance ²²¹ and conductivity matrices $\mathbb{M}_0^{(0)} = \mathbb{M}(\rho C_p(T_0))$ and $\mathbb{K}_0^{(0)} = \mathbb{K}(k(T_0))$. These matrices are then used to compute the first iterate $\{\mathbf{\Phi}_1^{(1)}\}$ ²²² matrices are then used to compute the first iterate $\{\mathbf{\Phi}_1^{(1)}, \lambda_1^{(1)}(t)\}\$. After each ²²³ new iteration, these matrices are updated with the temperature field of the ²²⁴ current iteration.

Thus, after the k^{th} iteration, yielding $(\boldsymbol{\Phi}_1^{(k)})$ ²²⁵ Thus, after the k^{th} iteration, yielding $(\boldsymbol{\Phi}_1^{(k)}, \lambda_1^{(k)}(t))$, the matrices are up-²²⁶ dated according to

$$
\begin{cases} \mathbb{M}_0^{(k)}(t) = \mathbb{M}(\rho C_p(\Phi_1^{(k)} \lambda_1^{(k)}(t))) \\ \mathbb{K}_0^{(k)}(t) = \mathbb{K}(k(\Phi_1^{(k)} \lambda_1^{(k)}(t))) \end{cases}
$$
(23)

and used to compute the next iterate $(\boldsymbol{\Phi}_1^{(k+1)})$ ²²⁷ and used to compute the next iterate $(\mathbf{\Phi}_1^{(k+1)}, \lambda_1^{(k+1)}(t))$. This process con-²²⁸ tinues until convergence of the first pair.

229 To compute the other couples $\{(\mathbf{\Phi}_i, \lambda_i(t))\}_{i=2,\dots,n-1}$, the temperature vec-²³⁰ tor is replaced by the sum of the products of the currently known terms ²³¹ and the capacitance and conductivity matrices are pre-computed once based ²³² on all previous information and then stored. Thus, for the computation of the n^{th} 233 \sum ²³³ the *n*th pair (Φ_n , $\lambda_n(t)$), **T**(*t*) is replaced by the known quantity **T**_{*n*-1}(*t*) = $\sum_{i=1}^{n-1} \Phi_i \lambda_i(t)$, where all the time functions have been updated, and the ca-²³⁵ pacitance and conductivity matrices are updated via:

$$
\begin{cases} \mathbb{M}_{n-1}(t) = \mathbb{M}(\rho C_p(\mathbf{T}_{n-1}(t))) \\ \mathbb{K}_{n-1}(t) = \mathbb{K}(k(\mathbf{T}_{n-1}(t))) \end{cases} . \tag{24}
$$

²³⁶ Aside from the special treatment for the first couple, the process is repet-²³⁷ itive.

238 After initializing the process for the n^{th} couple $(\Phi_n, \lambda_n(t))$ with an arbitrary time function $\lambda_n^{(0)}(t)$, each iteration consists of solving in sequence:

240 • A space problem for $\Phi_n^{(k)}$ (with $\lambda_n^{(k-1)}(t)$ known). Letting:

$$
\begin{cases}\n\mathbb{A}_{i} = \int_{I} \lambda_{n}^{(k-1)}(t) \mathbb{M}_{n-1}(t) \dot{\lambda}_{i}(t) dt \\
\mathbb{B}_{i} = \int_{I} \lambda_{n}^{(k-1)}(t) \mathbb{K}_{n-1}(t) \lambda_{i}(t) dt\n\end{cases}
$$
\n(25)

241 for $i = 1, ..., n - 1$ and

$$
\begin{cases}\n\mathbb{A} = \int_{I} \lambda_{n}^{(k-1)}(t) \mathbb{M}_{n-1}(t) \dot{\lambda}_{n}^{(k-1)}(t) dt \\
\mathbb{B} = \int_{I} \lambda_{n}^{(k-1)^{2}}(t) \mathbb{K}_{n-1}(t) dt, \\
\mathbf{c} = \int_{I} \lambda_{n}^{(k-1)}(t) \mathbf{F}_{Q_{in}} dt - \sum_{i=1}^{n-1} ([\mathbb{A}_{i}] + [\mathbb{B}_{i}]) \mathbf{\Phi}_{i}\n\end{cases}
$$
\n(26)

²⁴² the space problem takes the form:

$$
(\mathbb{A} + \mathbb{B})\Phi_n^{(k)} = \mathbf{c};\tag{27}
$$

• A time problem for $\lambda_n^{(k)}(t)$ (with $\Phi_n^{(k)}$ known). Letting:

$$
\begin{cases}\na_i'(t) = \boldsymbol{\Phi}_n^{(k)}^T \mathbb{M}_{n-1}(t) \boldsymbol{\Phi}_i \\
b_i'(t) = \boldsymbol{\Phi}_n^{(k)}^T \mathbb{K}_{n-1}(t) \boldsymbol{\Phi}_i\n\end{cases}
$$
\n(28)

244 for $i = 1, ..., n - 1$ and

$$
\begin{cases}\na'(t) = {\boldsymbol{\Phi}_n^{(k)}}^T \mathbb{M}_{n-1}(t) {\boldsymbol{\Phi}_n^{(k)}} \\
b'(t) = {\boldsymbol{\Phi}_n^{(k)}}^T \mathbb{K}_{n-1}(t) {\boldsymbol{\Phi}_n^{(k)}} \\
c'(t) = {\boldsymbol{\Phi}_n^{(k)}}^T \mathbf{F}_{Q_{in}} - \sum_{i=1}^{n-1} (a_i'(t)\dot{\lambda}_i(t) + b_i'(t)\lambda_i(t))\n\end{cases} (29)
$$

²⁴⁵ the time problem takes the form:

$$
a'(t)\dot{\lambda}_n^{(k)}(t) + b'(t)\lambda_n^{(k)}(t) = c'(t).
$$
\n(30)

²⁴⁶ PGD Update step

²⁴⁷ This step re-computes all time functions. The capacitance and conductiv-²⁴⁸ ity matrices are first updated in terms of all current information $\{(\boldsymbol{\Phi}_i, \lambda_i(t))\}_{i=1,\dots,n}$, ²⁴⁹ by assuming that $\mathbf{T}_n(t) = \sum_{i=1}^n \mathbf{\Phi}_i \lambda_i(t)$ according to:

$$
\begin{cases} \mathbb{M}_n(t) = \mathbb{M}(\rho C_p(\mathbf{T}_n(t))) \\ \mathbb{K}_n(t) = \mathbb{K}(k(\mathbf{T}_n(t))) \end{cases} .
$$
 (31)

²⁵⁰ Letting:

$$
\begin{cases}\na'_{j,i}(t) = \boldsymbol{\Phi}_j^T \mathbb{M}_n(t) \boldsymbol{\Phi}_i \\
b'_{j,i}(t) = \boldsymbol{\Phi}_j^T \mathbb{K}_n(t) \boldsymbol{\Phi}_i \\
c'_{j} = \boldsymbol{\Phi}_j^T \mathbf{F}_{Q_{in}}\n\end{cases}
$$
\n(32)

²⁵¹ the update problem takes the form:

$$
\sum_{i=1}^{n} a'_{j,i}(t)\dot{\lambda}_i(t) + \sum_{i=1}^{n} b'_{j,i}(t)\lambda_i(t) = c'_j \text{ for } j=1,...,n .
$$
 (33)

²⁵² 3.3. Extension to phase change by latent heat capacity, time- and temperature-²⁵³ dependent source, time and space-dependent boundary conditions

 The next step is to build a model that includes the latent change of phase of the patch material located in the close vicinity of the laser source which is now allowed to move inside the patch. Realistic Neumann boundary conditions at the patch edges and a convective heat loss throughout the patch surface are also taken into account.

²⁵⁹ In SLM processes, phase changes from raw materials (e.g. powder) to ²⁶⁰ liquid followed by solidification occur at very high speed $(10^{-6} - 10^{-3} s)$. Upon melting, the local internal energy increases significantly while the tem-₂₆₂ perature typically increases over a small range between T_S (solidus) and T_L (liquidus). Upon solidification, the opposite takes place: a large amount of energy is conducted/convected/radiated away from the "action" zone while temperatures decrease over the same range between liquidus and solidus. These high temperature cooling/heating rates and large temperature gradi- ents are the dominant factors in determining at microstructural level grain morphologies and are the primary driver behind metallurgical phase transfor- mations upon solidification. These have a direct influence on the mechanical properties of the finished product, and therefore it is critical to capture rea-sonably well these highly transient events (see [19]).

²⁷² The change in internal energy as function of temperature can then be ²⁷³ interpreted as a rather very non-linear specific heat relationship given by ²⁷⁴ $C_p(T) = dU/dT$ as illustrated in Figure 2. Only for the sake of simplifying ²⁷⁵ the illustration of this relationship, we have considered that otherwise the 276 specific heat is independent of temperature outside of range T_L-T_S , a premise ₂₇₇ that is not considered in the results shown in the following section.

²⁷⁸ If the source is time-dependent, i.e. the laser source is no longer station-²⁷⁹ ary, the the right-hand side of the FEM equation for the problem becomes:

$$
\mathbf{F}_{Q_{in}}(t) = \int_{\Omega} \mathbf{N}^{T}(x, y) Q^{in}(x, y, t) \, dS. \tag{34}
$$

 With the impetus of global-local FEM-based modeling techniques, the ability of robustly handling arbitrary Neumann boundary conditions on lo- cal models (like the ones illustrated in this work) is mandatory. While it is not the purpose of this work to dive into the global-local coupling algo- rithms, if time-dependent non-homogeneous Neumann boundary conditions are imposed (on this local model), an additional term must be added to the right-hand side of the FEM equation:

$$
\mathbf{F}_{\overline{q}^{out}}(t) = \int_{\partial \Omega} \mathbb{N}^T(x, y) \overline{q}^{out}(x, y, t) \, dl. \tag{35}
$$

²⁸⁷ Furthermore, if an additional temperature-dependent source, represent-²⁸⁸ ing an outward convective flux similar to a 3D film condition is taken into ²⁸⁹ account:

$$
Q^{out}(T) = h (T - T_{env})
$$
\n(36)

Figure 2: Internal energy for phase change and equivalent non-linear specific heat

²⁹⁰ a convective conductivity matrix must be added to the non-linear conductiv-²⁹¹ ity matrix:

$$
\mathbb{K}_h = \int_{\Omega} \mathbb{N}^T(x, y) \ h \ \mathbb{N}(x, y) \, dS \tag{37}
$$

²⁹² and a convective source term must be added to the right-hand side of the ²⁹³ FEM equation:

$$
\mathbf{F}_{\mathbf{h}}(T_{env}) = \int_{\Omega} \mathbb{N}^{T}(x, y) \ h \ T_{env} \ dS. \tag{38}
$$

²⁹⁴ The FEM equation finally becomes:

$$
\mathbb{M}(T)\dot{\mathbf{T}}(t) + (\mathbb{K}(T) + \mathbb{K}_h)\mathbf{T}(t) = \mathbf{F}_{Q_{in}}(t) - \mathbf{F}_{\overline{q}^{out}}(t) + \mathbf{F}_{\mathbf{h}}(T_{env}).
$$
 (39)

²⁹⁵ The FEM formulation remains incremental, with Newton iterations at ²⁹⁶ each time increment as described in Section 3.2.

²⁹⁷ The PGD formulation also remains a succession of stages consisting of an ²⁹⁸ enrichment step followed by an update step, as described in Section 3.2, but ²⁹⁹ some terms are modified, as presented below.

³⁰⁰ PGD Enrichment step

301 In the enrichment step, a new couple $(\Phi_n, \lambda_n(t))$ is again obtained with ³⁰² fixed point iterations by alternating sequentially between:

³⁰³ • The space problem, consisting of solving the algebraic system:

$$
(\mathbb{A} + \mathbb{B})\Phi_n^{(k)} = \mathbf{c}
$$
 (40)

³⁰⁴ with:

$$
\begin{cases}\n\mathbb{A}_{i} \text{ and } \mathbb{A} \text{ unchanged} \\
\mathbb{B}_{i} = \int_{I} \lambda_{n}^{(k-1)}(t) (\mathbb{K}_{n-1}(t) + \mathbb{K}_{h}) \lambda_{i}(t) dt & \text{for } i = 1, ..., n-1 \\
\mathbb{B} = \int_{I} \lambda_{n}^{(k-1)^{2}}(t) (\mathbb{K}_{n-1}(t) + \mathbb{K}_{h}) dt \\
\mathbf{c} = \int_{I} \lambda_{n}(t) (\mathbf{F}_{Q_{in}}(t) - \mathbf{F}_{\overline{q}^{out}}(t) + \mathbf{F}_{h}(T_{env})) dt - \sum_{i=1}^{n-1} (\mathbb{A}_{i} + \mathbb{B}_{i}) \Phi_{i} \tag{41}\n\end{cases}
$$

³⁰⁵ • The time problem, consisting of integrating the ordinary differential ³⁰⁶ equation:

$$
a'(t)\dot{\lambda}_n^{(k)}(t) + b'(t)\lambda_n^{(k)}(t) = c'(t)
$$
\n(42)

³⁰⁷ with:

$$
\begin{cases}\na_i'(t) \text{ and } a'(t) \text{ unchanged} \\
b_i'(t) = \boldsymbol{\Phi}_n^{(k)^T}(\mathbb{K}_{n-1}(t) + \mathbb{K}_h)\boldsymbol{\Phi}_i \quad \text{for } i = 1, \dots, n-1 \\
b'(t) = \boldsymbol{\Phi}_n^{(k)^T}(\mathbb{K}_{n-1}(t) + \mathbb{K}_h)\boldsymbol{\Phi}_n^{(k)} \\
c'(t) = \boldsymbol{\Phi}_n^T(\mathbf{F}_{Q_{in}}(t) - \mathbf{F}_{\overline{q}^{out}}(t) + \mathbf{F}_h(T_{env})) - \sum_{i=1}^{n-1} (a_i'(t)\dot{\lambda}_i(t) + b_i'(t)\lambda_i(t)).\n\end{cases}
$$
\n(43)

³⁰⁸ PGD Update step

309 In the update step, the set of time functions $\{\lambda_1(t),...,\lambda_n(t)\}\$ is again ³¹⁰ simultaneously updated by integrating the ordinary differential system:

$$
\sum_{i=1}^{n} a'_{j,i} \dot{\lambda}_i(t) + \sum_{i=1}^{n} b'_{j,i} \lambda_i(t) = c'_j(t) \text{ for } j = 1, ..., n
$$
 (44)

³¹¹ with:

$$
\begin{cases}\na'_{j,i}(t) \text{ unchanged} \\
b'_{j,i}(t) = \boldsymbol{\Phi}_j^T (\mathbb{K}_n(t) + \mathbb{K}_h) \boldsymbol{\Phi}_i \\
c'_{j}(t) = \boldsymbol{\Phi}_j^T (\mathbf{F}_{Q_{in}}(t) - \mathbf{F}_{\overline{q}^{out}}(t) + \mathbf{F}_{\mathbf{h}}(T_{env})).\n\end{cases}
$$
\n(45)

312 The computations for stage $n(> 1)$ in this most general case are summa-³¹³ rized in Algorithm 1.

³¹⁴ 4. Results and Discussion

 In this Section, the most relevant results are shown in order to compare PGD with FEM. All the simulations were done in Matlab. To assure the correct answers, Abaqus was used to verify FEM Matlab results. Meshes 318 were generated by Gmsh. The coefficients a, b, c (see Equation (11)) and A, \mathbb{B} , **c** (see Equations (26) and (41)) were calculated by numerical integration using a rectangular method with 100 discretization points in all the following examples.

$322 \quad 4.1.$ Example 1: linear case

³²³ Even though no computational gain is expected in the linear case, it is a ³²⁴ good starting point to better understand the PGD behavior when applied to ³²⁵ an additive manufacture problem.

326 The domain to be analyzed consists of a 2 $mm \times 2$ mm square plate 327 made of Ti-6Al-4V. The laser is stationary and heats the plate during 0.1 s. ³²⁸ The walls are insulated and there are no Dirichlet boundary conditions. A ³²⁹ non-uniform triangular mesh with 1894 degrees of freedom was used, with 330 an element size of 10^{-6} m in the laser region and 10^{-4} m in the edges.

³³¹ Further information is presented in Table 1 and in Figure 3.

³³² Some of the cases tested are presented in Table 2 and Figure 4. Note ³³³ that in all cases the temperature is analyzed at the node where the laser is ³³⁴ located.

Algorithm 1 Non-linear PGD

Require: $\mathbb{M}_{n-1}(t)$, $\mathbb{K}_{n-1}(t)$, \mathbb{K}_h , $\mathbf{F}_{Q^{in}}(t)$, $\mathbf{F}_{\bar{q}^{out}}(t)$, $\mathbf{F}_h(T_{env})$, tol_{PGD} , $(\mathbf{\Phi}_{n-1}, \lambda_{n-1}(t))$ for $n = 2$ to N_{mod} do Enrichment step (Fixed-point iterations) to Compute $(\Phi_n, \lambda_n(t))$ Initialize $\lambda_n^{(k=0)}(t)$ while $\epsilon = \frac{\int_I \left(\lambda_n^{(k)}(t) - \lambda_n^{(k-1)}(t)\right)^2 dt}{\int_I \left(\frac{1}{k}\right)^2 dt}$ $\frac{1}{2}\int_I \left(\lambda_n^{(k)}(t)+\lambda_n^{(k-1)}(t)\right)^2 dt > tol_{PGD}$ $k = k + 1$ **Space problem:** Compute $\Phi_n^{(k)}$ from a known $\lambda_n^{(k-1)}(t)$

$$
\begin{cases} \mathbb{A}_i = \int_I \lambda_n^{(k-1)}(t) \mathbb{M}_{n-1}(t) \dot{\lambda}_i(t) dt \\ \mathbb{B}_i = \int_I \lambda_n^{(k-1)}(t) (\mathbb{K}_{n-1}(t) + \mathbb{K}_h) \lambda_i(t) dt \end{cases}
$$

for $i = 1, \ldots, n-1$ and

$$
\begin{cases}\n\mathbb{A} = \int_I \lambda_n^{(k-1)}(t) \mathbb{M}_{n-1}(t) \dot{\lambda}_n^{(k-1)}(t) dt \\
\mathbb{B} = \int_I \lambda_n^{(k-1)^2}(t) (\mathbb{K}_{n-1}(t) + \mathbb{K}_h) dt, \\
\mathbf{c} = \int_I \lambda_n^{(k-1)}(t) (\mathbf{F}_{Q_{in}}(t) - \mathbf{F}_{\overline{q}^{out}}(t) + \mathbf{F}_{\mathbf{h}}(T_{env})) dt - \sum_{i=1}^{n-1} ([\mathbb{A}_i] + [\mathbb{B}_i]) \Phi_i\n\end{cases}
$$

Solve for $\mathbf{\Phi}_n^{(k)}$: $(\mathbb{A} + \mathbb{B})\mathbf{\Phi}_n^{(k)} = \mathbf{c}$ **Time problem:** Compute $\lambda_n^{(k)}(t)$ from a known $\Phi_n^{(k)}$

$$
\begin{cases} a_i'(t) = {\bf \Phi}_n^{(k)}^T \mathbb{M}_{n-1}(t) {\bf \Phi}_i \end{cases}
$$

$$
\left\{\quad b_i'(t) = {\bf \Phi}_n^{(k)}^T (\mathbb{K}_{n-1}(t) + \mathbb{K}_h) {\bf \Phi}_i\right\}
$$

for $i = 1, \ldots, n-1$ and

$$
\begin{cases}\n a'(t) = {\boldsymbol{\Phi}_n^{(k)}}^T \mathbb{M}_{n-1}(t) {\boldsymbol{\Phi}_n^{(k)}}\\ \n b'(t) = {\boldsymbol{\Phi}_n^{(k)}}^T (\mathbb{K}_{n-1}(t) + \mathbb{K}_h) {\boldsymbol{\Phi}_n^{(k)}}\\ \n c'(t) = {\boldsymbol{\Phi}_n^{(k)}}^T (\mathbf{F}_{Q_{in}}(t) - \mathbf{F}_{\overline{q}^{out}}(t) + \mathbf{F}_{\mathbf{h}}(T_{env})) - \sum_{i=1}^{n-1} (a_i'(t)\dot{\lambda}_i(t) + b_i'(t)\lambda_i(t))\n\end{cases}
$$

Solve for $\lambda_n^{(k)}(t)$: $a'(t)\dot{\lambda}_n^{(k)}(t) + b'(t)\lambda_n^{(k)}(t) = c'(t)$ Check ϵ if $\epsilon \leq tol_{PGD}$ then $\textbf{Set: } (\boldsymbol{\Phi}_{n}, \lambda_{n}(t)) = (\boldsymbol{\Phi}_{n}^{(k)}, \lambda_{n}^{(k)}(t))$

end if

end while

Update step (Re-computation of all time functions $\{\lambda_1(t), ..., \lambda_n(t)\}\)$

$$
\begin{cases}\na'_{j,i}(t) = \boldsymbol{\Phi}_j^T \mathbb{M}_n(t) \boldsymbol{\Phi}_i & \text{for } i = 1, \dots, n \\
b'_{j,i}(t) = \boldsymbol{\Phi}_j^T (\mathbb{K}_n(t) + \mathbb{K}_h) \boldsymbol{\Phi}_i & \text{for } i = 1, \dots, n \\
c'_{j}(t) = \boldsymbol{\Phi}_j^T (\mathbf{F}_{Q_{in}}(t) - \mathbf{F}_{\overline{q}^{out}}(t) + \mathbf{F}_{\mathbf{h}}(T_{env})).\n\end{cases}
$$

Solve for $\{\lambda_1(t), ..., \lambda_n(t)\}\colon a'_{j,i}\dot{\lambda}_i(t) + b'_{j,i}\lambda_i(t) = c'_{j}(t)$ for $i=1,...,n$ end for

Figure 3: Representative schema of Example 1

General properties	Values
Density (ρ)	4500 kg/m^2
Conductivity (k)	$12\ W/K$
Heat capacity (C_p)	700 $J/K/kg$
Laser power (P)	100~kW
Laser radius (R_0)	$5 \cdot 10^{-5}$ m
Total time (t_{end})	0.1 s
Time increment (Δt)	$0.001 \; s$

Table 1: General properties for Example 1

(c) PGD 5 modes, 1 iteration per mode

Figure 4: Comparison between PGD and FEM at the laser node for Example 1

Table 2: PGD performance at the laser node for Example 1

Simulation				
Type	Modes	Error	Criterion	Solve Total
PGD	4		0.0327 1 iteration/mode	4
PGD	4	0.0280	$tol_{PGD} = 0.01$	8
PGD	5		0.0098 1 iteration/mode	5
PGD	5	0.0092	$tol_{PGD}=0.01$	9
PGD	10		$3.31 \cdot 10^{-5}$ $tol_{PGD} = 10^{-8}$	

³³⁵ Here:

$$
Error = \frac{\|T_{FEM} - T_{PGD}\|_{L^{2}(\Omega \times [0, t_{end}])}}{\|T_{FEM}\|_{L^{2}(\Omega \times [0, t_{end}])}}
$$
(46)

³³⁶ is the expression used to compute the error. It measures the difference be-³³⁷ tween FEM and PGD results according to the L^2 norm, normalized by the 2^{338} L^2 norm of the FEM answer. Solve Total represents the number of times a ³³⁹ linear system was solved by matrix inversion.

 Comparing the accuracy of the PGD results for various numbers of re- tained modes and for various numbers of iterations per mode, we can make some observations. First, very few iterations are needed per mode. The error criterion can be replaced by a strategy with 1 iteration per mode. This shows that the method is self-correcting. Besides, since each iteration requires the resolution of a potentially large algebraic system (along with the integration of an ODE), for a given number of matrix factorizations, it is more advanta- geous to increase the number of modes with just a few (one or two) iterations per mode than to increase the number of iterations per mode with a lower number of computed modes. This is illustrated by comparing Figures 4b 350 (PGD 4 modes, $tol_{PGD}=0.01$) and 4c (PGD 5 modes, 1 iteration per mode). Both represent an improvement of the PGD 4 modes, 1 iteration per mode solution. But, in the first case, it is necessary 8 iterations for an error equals to 0.028, while for the second one, less iterations (5) give better result (error $_{354}$ = 0.0098).

³⁵⁵ Furthermore, Figure 4a confirms that as the number of modes increases, ³⁵⁶ the PGD solution converges to the FEM solution.

³⁵⁷ Finally, to illustrate the principle of the PGD, a few couples of basis ³⁵⁸ vectors and time functions are presented in Figure 5. The basis vectors have

 been normalized with respect to the capacitance matrix in order to maintain consistent orders of magnitude for the time functions. The time functions

were initialized by assuming a linear time dependence.

(c) Space and time functions for the tenth PGD mode

Figure 5: PGD space and time functions

³⁶² 4.2. Example 2: non-linear materials

³⁶³ As expected, the PGD-computed response is very accurate in the linear ³⁶⁴ cases. So, in order to increase the complexity of the model, non-linearities must be introduced. First, we will consider material non-linearities, i.e. temperature-dependent conductivity and heat capacity. These values were obtained in [25] and they are shown in Figure 6.

(b) Thermal capacity as function of the temperature

Figure 6: Non-linear material properties for Ti-6Al-4V

 Several tests were run, varying the number of modes and convergence criterion. The results are presented in Figure 7 and Table 3, again at the node where the laser is located.

 The PGD error measure is the same as in Equation (46). The FEM tolerance, on the other hand, is chosen so as to yield a reference FEM solution of the same precision when compared to Abaqus. The reported Speed-up Factor is the ratio of the total number of solves needed for our FEM solution by the total number of solves needed for our PGD solution. Due to the fact that Abaqus requires only roughly half the number of solves per increment, a more conservative way to measure the PGD gain would be to divide the reported Speed-up Factor by two.

 First of all, the 50 modes PGD solution (Figure 7a) is very accurate, confirming the assumption that if the number of PGD modes is large enough,

(b) PGD 7 modes, 2 iterations in the 1^{st} mode and 1 iteration in the others

Figure 7: Performance comparison between PGD and FEM at the laser node for Example 2

³⁸¹ the PGD solution tends towards the reference solution, even when some non-³⁸² linearities are introduced.

 Moreover, regarding the modes convergence criterion, the same conclu- sions as in the linear case can be applied here. It is possible, and preferable, to impose a fixed number of iterations per mode instead of using a tolerance. 386 For example, one can compare PGD 6 modes with $tol_{PGD}=0.01$ and PGD 7 modes with 2 iterations for the first mode and 1 iteration for the others. In the first case, the total number of iterations is not known a priori. The error ϵ from Equation (17) must be smaller than 0.01 in order to calculate the next mode. In the second case, the number of iterations of a specific mode is imposed, and Equation (17) is ignored. One concludes that a few iterations suffice, since the first case has more iterations (meaning larger computational

	Simulation			Solve	
Type	Modes	Error	Criterion	Total	Speed-up Factor
FEM		$\omega_{\rm{eff}}$	$Tol_{FEM} = 0.0001$	658	
PGD	$\overline{5}$	0.0168	2 it. in the first mode and 1 it. in the others	6	109.67
PGD	6	0.0077	$tol_{PGD}=0.01$	17	38.71
PGD	6	0.0083	2 it. in the first mode and 1 it. in the others	$\overline{7}$	94.00
PGD	7	0.0070	$tol_{PGD} = 0.01$	19	34.63
PGD	7	0.0063	2 it. in the first mode and 1 it. in the others	8	82.25
PGD	8	0.0059	2 it. in the first mode and 1 it. in the others	9	73.11
P(1)	50	0.0025	$tol_{PGD} = 0.01$	105	6.26

Table 3: Performance comparison between PGD and FEM at the laser node for example 2

 costs) and its results are less accurate. 2 iterations for the first mode and 1 iteration for the others is the minimum necessary number of iterations, since the first mode has a larger contribution to the final result - so it must have a special treatment - and each new mode seems to correct partially the flaws of previous modes. If a given result is not precise enough, it is preferable to add an extra mode (with just one iteration) than to perform more iterations. Finally, PGD has responded well to the non-linear case. Satisfactory results were obtained with just a few iterations, as shown for instance in Figure 7b.

 4.3. Example 3: non-linear material properties, latent heat and moving laser From Example 2, it was observed that PGD responded well to the first non-linearities. So, one can increase the sources of non-linearities to investi- gate the limits of PGD. The idea is to introduce a moving torch for the laser and to take into account the latent heat and the melting pools.

⁴⁰⁷ The properties for this problem are shown in Table 4 and in Figures 9 and ⁴⁰⁸ 6a. Some modifications were made in the domain as illustrated in Figure 8.

409 It is still a 2 $mm \times 2 mm$ square patch, with the origin located at the bottom ⁴¹⁰ left corner and with the laser starting at point 5 located at position (1.5,1) 411 mm. However, new points were introduced (points 6 to 10) to represent the 412 path of the moving laser. At the instant $t = 0$ s (beginning of the simulation), ⁴¹³ the laser is at point 5 and starts moving during 1 ms with a speed of 0.5 $_{414}$ m/s in the direction of point 10, located at position $(0.5,1)$ mm. Afterwards, ⁴¹⁵ the laser is turned off $(Q_{in} = 0)$, and cooling takes place during 1 ms. With ⁴¹⁶ this approach, it is possible to see the latent heat effects when the material ⁴¹⁷ undergoes phase transitions both from solid to liquid and from liquid to solid.

Figure 8: Representative schema of Example 3

Table 4: General properties for Example 3

General properties Values	
Density (ρ)	4500 kg/m^2
Laser power (P)	460~kW
Laser radius (R_0)	$5 \cdot 10^{-5}$ m
Torch speed (v)	$0.5 \; m/s \; (v_x = -0.5 \; m/s \; , \; v_y = 0 \; m/s)$
Laser initial position	$X_0 = 1.5$ mm and $Y_0 = 1.0$ mm
Total time (t_{end})	$2 \; ms \; (1 \; ms \; with \; the \; laser \; on \; and \; 1 \; ms \; of \; cooling)$
Time increment (Δt)	$2 \cdot 10^{-5} s$

⁴¹⁸ In addition, a non-uniform mesh is used. It has 1208 degrees of freedom,

419 with an element size of 10^{-4} m at the edges and 10^{-5} m along the laser path. The element size must be smaller than the laser radius in the path region, otherwise the heating effect caused by the laser is not well captured. Nevertheless, far from the laser path, there is no need to have a refined mesh, so it is possible to have coarser elements to save computational time.

$4.3.1.$ Latent heat

⁴²⁵ The approach used for modeling latent heat is explained in Section 3.3. The phase transformation from solid to liquid and vice-versa occurs for Ti- 6Al-4V over a narrow range of temperatures (of about 50 K) centered around 1920 K. In the finite element formulation, in order to achieve reasonable convergence when traversing this strong non-linearity, we chose to widen the phase transformation interval using the parameters presented in Table 5. Previous studies (see [26], [19]) suggest that such choice has almost no detrimental effect when numerical results are a compared to physical tests including melt pool in plane dimensions and depth. For consistency a similar approach is adopted in the PGD formulation.

Parameter	Value
\mathcal{L} (latent heat)	440 kJ/kg
T_S (modified solid temperature)	1653 K
T_L (modified liquid temperature) 2153 K	

Table 5: Latent heat parameters

⁴³⁵ In order to obtain a smooth variation of the total heat capacity, the latent 436 heat capacity (henceforth C_{λ}) is interpolated using a fourth order degree ⁴³⁷ polynomial:

$$
C_{\lambda} = \begin{cases} 30\left(\frac{T-T_S}{T_L-T_S}\right)^2 \left(1 - \left(\frac{T-T_S}{T_L-T_S}\right)\right)^2 \frac{\mathcal{L}}{T_L-T_S} & \text{if } T_S < T < T_L\\ 0 & \text{otherwise} \end{cases} \tag{47}
$$

438 Adding the C_{λ} values from Equation (47) to the previous C_p defined in $_{439}$ Figure 6b, one obtains the total C_p which will be used in the current analysis ⁴⁴⁰ (Figure 9).

⁴⁴¹ 4.3.2. Moving source

⁴⁴² The source is now allowed to move within the patch in the negative x-443 direction with speed $v = v_x$, so that $f_x(t) = v_x$ and $f_y(t) = 0$ (see Equations

Figure 9: Total heat capacity (including latent heat) as a function of the temperature for Ti-6Al-4V

⁴⁴⁴ (2) and (3)). Consequently, the moving source expression becomes:

$$
Q^{in}(x, y, t) = \frac{2P}{\pi R_0^2} \exp\left(\frac{-2}{R_0^2}((x - (X_0 + v_x t))^2 + (y - Y_0)^2)\right).
$$
 (48)

⁴⁴⁵ As the source travels along the horizontal direction, the regions of high ⁴⁴⁶ temperature are expected to follow its motion.

⁴⁴⁷ 4.3.3. Results and Discussion for Example 3

 Before comparing PGD and FEM results, it is interesting to better un- derstand the effects of the latent heat. Figure 10 shows how the latent heat leads to a significant reduction of the temperature. Both curves (with and 451 without latent heat) coincide as long as $T < T_S$. When the temperature ϵ_{452} reaches the value $T = T_S$, there is a decrease in the slope of the curve with 453 latent heat, and the curves no longer coincide. However, when $T > T_L$, the slope of the curve with latent heat increases again and the curves become nearly parallel.

⁴⁵⁶ The results of the simulation are illustrated in Figure 11 and 12 and in ⁴⁵⁷ Table 6.

Figure 10: Comparison between FEM with latent heat and FEM without latent heat

(b) PGD 20 modes, 2 iterations per mode

Figure 11: Comparison between PGD and FEM for Example 3 for a low number of modes

(b) PGD 100 modes, 3 iterations in the 1^{st} mode and 1 iteration in the others

Figure 12: Comparison between PGD and FEM for Example 3 for a high number of modes

	Simulation					Solve
Type	Modes	Error 1	Error 2	Criterion	Total	Speed-up Factor
FEM				$Tol_{FEM} = 0.0001$	994	
PGD	10	0.0999	0.0642	2 it./mode	20	49.70
PGD	15	0.0685	0.0434	2 it./mode	30	33.13
PGD	20	0.0299	0.0190	2 it./mode	40	24.85
PGD	25	0.0264	0.0168	2 it./mode	50	19.88
PGD	30	0.0196	0.0125	2 it./mode	60	16.57
PGD	50	0.0070	0.0045	2 it./mode	100	9.94
PGD	100	0.1795	0.1206	3 it. in the 1st mode and 1 it. in the others	102	9.75

Table 6: Performance comparison between PGD and FEM for Example 3

⁴⁵⁸ Here:

$$
\text{Error 1} = \frac{\|T_{FEM} - T_{PGD}\|_{L^{2}(\Omega \times [0, t_{end}/2])}}{\|T_{FEM}\|_{L^{2}(\Omega \times [0, t_{end}/2])}}
$$
(49)

⁴⁵⁹ is the error for the first half time of the simulation, where the laser is turned ⁴⁶⁰ on and travels from point 5 to point 10, and

$$
\text{Error } 2 = \frac{\|T_{FEM} - T_{PGD}\|_{L^{2}(\Omega \times [0, t_{end}])}}{\|T_{FEM}\|_{L^{2}(\Omega \times [0, t_{end}])}}
$$
(50)

 is the error for the total duration of the simulation, i.e., the laser on and the cooling (laser off) phases. Notice that the temperature gradients are higher in the laser "on" scenario than in the cooling scenario, meaning that relative global discrepancies between PGD and FEM results are expected to be larger in the first half of the simulation . This justifies the fact that Error 1 will always be larger than Error 2 in this example.

⁴⁶⁷ As can be seen from these curves, the response behavior is in accordance ⁴⁶⁸ with expectations and shows good correlation between FEM and PGD results ⁴⁶⁹ provided the number of retained modes is sufficient.

 Important points can be highlighted from this example. First of all, in contrast with the case of a stationary source, the solution requires more than 1 iteration per mode, even when using several modes. For example, using 100 modes with 3 iterations in the first mode and 1 iteration in the others (Figure 12b), the result is very different from the FEM answer and totally unacceptable. Nevertheless, when using 50 modes with 2 iterations per mode (Figure 12a), the result accuracy is excellent. In both cases, there are about 100 iterations in total, but in the first case, although more modes are used, the result is worse than in the second case. This might seem contradictory with the previous results and with the PGD assumptions. However, in the case of a moving laser, the higher modes have an important contribution to the response due to the non-separability of time and space. As the new 482 expression for Q_{in} is such that it is not possible to separate time and space -483 due to the terms $v_x t$ and $v_y t$ in the exponential - the higher order modes are no longer mere corrections, but contribute as importantly to the solution as the lower ones. Since higher modes are very relevant for the solution in this new case, the convergence criterion needs to be more strict in order to obtain an accurate PGD solution. This explains the difference between 50 and 100 modes PGD solutions. Besides, it establishes that at least 2 iterations are necessary for each mode to have an acceptable solution. In fact, one can consider that 2 iterations per mode is the ideal mode convergence criterion for this example, and a larger number of iterations could add numerical pollution . Adding an extra mode is again better than adding more iterations per mode.

 Moreover, the number of modes and iterations required to correctly cap- ture the diffusion effect is much larger than for a stationary source, even though, with 20 modes, PGD represents a performance gain of 24.85 times compared to FEM. Qualitatively the result is quite acceptable as the very large temperature gradients, peak temperatures and overall temperature dis-tributions are captured reasonably well, as shown in Figure 13.

Figure 13: Temperature field in all the domain at $t=1$ ms for FEM and PGD

 Summarizing the results of Sections 4.3 and 4.2, one can observe the influence of the latent heat with a moving laser on the solution in Figure 14. Figures 14a and 14b support the verification of PGD, showing it is able to handle problems with moving source and latent heat, and the larger the number of modes, the better the solution (here 50 modes and 2 iterations per mode were used). One can note that the PGD solution without latent heat is more accurate than the one with latent heat. This is consistent, since the latent heat introduces a very strong non-linearity to the problem.

(a) Comparison between FEM and PGD without latent heat

(b) Comparison between FEM and PGD with latent heat

Figure 14: FEM and PGD behaviors for problems with and without latent heat

⁵⁰⁸ 4.4. Example 4: non-linear material properties, latent heat, moving laser, ⁵⁰⁹ time and space-dependent Neumann boundary conditions and convection

 This is the final example that encompasses most different types of non- $_{511}$ linearities a thermal problem in the field of additive manufacturing can have, by adding a film condition and time and space-dependent Neumann boundary conditions to the previous example. The notable exception is radiative heat loss which will be subject of future work.

 The properties for this problem are the same as in Example 3, so they can be found in Table 4 and in Figures 9 and 6a. However, it was again necessary to modify the domain (to be explained later). The patch is now represented by a 1 mm x 0.1 mm rectangular uniform mesh (this region will be also called the small patch), with the origin at the bottom left corner and μ ₅₂₀ with triangular elements of size 10^{-5} m, totalizing 1378 degrees of freedom. The source motion is the same as in the previous case: at the beginning of μ_{522} the simulation (t=0), the laser is at point 5 (now located at (0.85,0.05) mm). Then it starts moving towards point 10, traveling a distance of 0.5 mm with a constant speed of 0.5 m/s . Once arrived at point 10, the laser is turned off, and the cooling phenomenon is observed during 1 ms.

The previous description is illustrated in Figure 15.

Figure 15: Representative schema of Example 4

4.4.1. Neumann Boundary Conditions

 In all previous examples, it was considered that the domain was ther- mally insulated, so the Neumann boundary conditions were zero everywhere. However, in reality, not all the laser heat received remains inside the model. A fraction of the heat is lost through the edges due to non-homogeneous Neumann boundary conditions. In order to determine realistic Neumann boundary conditions (to be applied to our model in Example 4), a specific approach was used.

 The procedure starts with the computation of the non-linear problem ϵ_{536} response (i.e., non-linear k, non-linear C_p , latent heat, convection, moving laser and insulated boundaries) in a larger patch. A 2 mm x 2 mm square domain (henceforth the super-patch), totally overlapping the small patch was created and used in a first simulation. It was assumed that the influence of the diffusion of the laser heat on the edges of the super-patch during the first 2 ms is negligible, so the insulated walls assumption is more realistic for this super-patch.

 The second step was the extraction of the space and time-dependent out- flux, that is represented in Figure 16. 30 points at and near the boundaries of the small patch (labeled "point 11" to "point 41") were created. For each pair of points (for example points 12 and 13), the heat flux was computed at each time increment. The result is a vector containing the time evolution of the heat flux for a specific point in space. With this methodology, one can

 extract the time and space-dependent Neumann boundary conditions for the small patch. The criterion for choosing the width of the small patch equal 551 to 0.1 mm was that 0.1 $Q_{in} < Q_{out} < 0.5 Q_{in}$, so the influence of non-zero Neumann boundary conditions is significant.

 The final step was to apply at the boundaries of the small patch the previously computed flux and to compute the new response.

Figure 16: Approach to extract the space and time-dependent Neumann boundary conditions

 The small patch is represented by the red rectangle and is exactly the same as in Figure 15. The green arrow is the laser trajectory. The super- patch is represented by the black square which contains the red rectangle. To save computation time, the super-patch was meshed non-uniformly. The ⁵⁵⁹ element sizes are 10^{-4} m near the black edges, $2.5 \cdot 10^{-5}$ m near the red edges $_{560}$ and 10^{-5} m along the laser path.

4.4.2. Surface convection (film condition)

 In order to take into account heat exchanges between the model and the surrounding environment (air), a film condition was applied to the entire 564 surface Ω - (not only redat the edges $(\partial \Omega)$). Thus, the film condition was treated as a body source rather than as a boundary condition. Its expression

⁵⁶⁶ is given by:

$$
-\mathbf{n}^{out} \cdot k \nabla T = h(T - T_{env})\tag{51}
$$

 $_{567}$ where $h= 18$ $W/K/m$ (see [27]) is the heat transfer coefficient for the air-568 titanium interaction and $T_{env}= 293 K$ is the air temperature, here considered ⁵⁶⁹ the same as the room temperature.

⁵⁷⁰ This approach is an attempt to be as realistic as possible, since we are ⁵⁷¹ representing a 2D top view model of a 3D problem.

⁵⁷² 4.4.3. Results and Discussion

 The simulation was done for FEM and for PGD with different numbers of modes (always with 2 iterations per mode). The results are shown in Figure 17 and in Table 7. Points 5 to 10 were chosen in order to analyze the temperature behavior. Because the laser crosses these points, the changes in temperature are highly transient, and so they are good candidates for comparing FEM with PGD.

Table 7: Performance comparison between PGD and FEM for Example 4

	Simulation				Solve	
Type	Modes			Error 1 Error 2 Criterion	Total	Speed-up Factor
FEM				$Tol_{FEM} = 0.0001$	880	
PGD	10	0.0827	0.0519	2 it./mode	20	44.00
PGD	15	0.0427	0.0274	2 it./mode	30	29.33
PGD	20	0.0355		$0.0223 \quad 2 \text{ it.} / \text{mode}$	40	22.00
PGD	25	0.0170	0.0121	2 it./mode	50	17.60
PGD	30	0.0147	0.0105	2 it./mode	60	14.67
PGD	50	0.0105	0.0098	2 it./mode	100	8.80

⁵⁷⁹ Here, Error 1 and Error 2 are the same as defined in Equations (49) and ⁵⁸⁰ (50), respectively.

 As expected, at least 2 iterations are needed per mode, because higher modes are important to correctly capture the effect of the traveling laser and time-varying Neumann boundary conditions. The result with 50 modes (Figure 17c) is extremely accurate, however the performance gain is not very high in this case. 10 or 15 modes (Figure 17a) are not sufficient, because the accuracy in the high temperature zone is poor. 20 modes (Figure 17b)

(c) PGD 50 modes, 2 iterations per mode

Figure 17: Performance comparison between PGD 50 modes and FEM for Example 4

⁵⁸⁷ seems a good compromise, even though there are some oscillations at the ⁵⁸⁸ beginning of the simulation for the PGD response. The accuracy in the most important regions (such as high temperatures or cooling) is acceptable and the number of matrix inversions in this case is reduced by 22 compared to the FEM. As the out-flux represents a considerable percentage of the laser energy, there is a remarkable drop in the temperature when compared to Example 3. However, this does not seem to be a problem for PGD. Adding the time and space-dependent Neumann boundary conditions and the film convection does not change the number of modes necessary for a reasonable PGD response. Previously, with 20 modes and 2 iterations per mode one obtained an error $\frac{597}{1}$ = 0.0299 and an error 2 = 0.0190. Thus, although the errors have slightly increased, the choice of 20 modes seems a reasonable compromise. Finally, this example proves that PGD can handle highly non-linear and complex problems.

5. Conclusion

 In this paper, a PGD model order reduction technique has been applied to the numerical model of highly transient non-linear thermal phenomena as- sociated with melt pools in additive manufacturing powder bed fabrication. In previous work we have found that with minimal calibration, parabolic PDEs associated with transient heat transfer equations are sufficiently accu-rate/predictive and hence we have focused this work in that context.

 After a brief introduction and setting the objectives in Section 1, the specific problem benchmark in this work is outlined in Section 2. Linear and non-linear PGD theory for transient heat transfer equations has been carefully described in Section 3. To develop a realistic AM thermal model, most relevant non-linearities associated with the parabolic PDE, such as ma- terial property non-linearities, phase change by latent heat, time-dependent source, temperature-dependent source and time and space-dependent bound- ary conditions have been introduced. Finally, Section 4 presents an extensive numerical campaign to validate the PDG-based approach against traditional FEM while thoroughly assessing the execution performance gains.

 As demonstrated by these tests, model order reduction techniques such as PGD appear to be a very promising lead when tackling highly non-linear nu- $\epsilon_{0.00}$ merical simulation challenges in AM. Two key aspects should be highlighted: ϵ_{621} 1) the possibility to considerer several high complexity non-linearities in PGD (key for realistic models in AM process simulation) in this highly transient thermal analysis, and; 2) the remarkable computational time savings.

 Short term perspectives of this work will cover implementation, validation ₆₂₅ and performance assessment of a 3D model, development of an *ad-hoc* PGD algorithm to further improve computational gains and implementation in commercial codes to solve complex industrial cases. On a broader long-term scale, future work should address the gigantic multi-physics and the multi- scale nature of the problem which could take great advantage from model order reduction techniques at both local (melt pool level) and global (part level) scales.

6. References

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