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▶ To cite this version:

B. Favoretto, C.A. de Hillerin, O. Bettinotti, V. Oancea, Andrea Barbarulo. Reduced order modeling via PGD for highly transient thermal evolutions in additive manufacturing. Computer Methods in Applied Mechanics and Engineering, 2019, 10.1016/j.cma.2019.02.033. hal-02062582

HAL Id: hal-02062582 https://hal.science/hal-02062582

Submitted on 28 Mar 2019

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

B. Favoretto^{a,b}, C.A. de Hillerin^b, O. Bettinotti^c, V. Oancea^c, A. Barbarulo^a

^a Laboratoire MSSMat, CentraleSupélec/CNRS UMR 8579/ Université Paris Saclay, 91190 Gif-sur-Yvette, France

^b Dassault Systèmes SIMULIA Corp., Vélizy-Villacoublay, France ^c Dassault Systèmes SIMULIA Corp., Johnston, RI, USA

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

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

Preprint submitted to CMAME https://doi.org/10.1016/j.cma.2019.02.033March 28, 2019

tive manufacturing (AM), proved to be a paradigm shift for manufacturing 4 processes. They consist in selective melting of superposed layers of metal 5 powder using a machine-controlled moving high energy source. Due to their 6 nature, these processes allow unprecedented freedom in designing, personalization and optimization of mechanical parts. Moreover, they are particularly 8 suited for software-hardware integration when the desired geometry is con-9 ceived with a Computer Assisted Design (CAD) tool and directly produced 10 by an automated process, removing many of the intermediate steps between 11 the designer's vision and the physical world. 12

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 and time, special consideration is required in numerical analysis (see [1, 2,]) including fast executing AM-specialized approaches (see [4]).

This work focuses on the highly non-linear thermal phenomena occurring 20 in the immediate proximity of the fast moving heat source where temper-21 ature evolution rates, phase changes and thermal gradients are the most 22 intense, all happening on a very small scale (see [5]). The goal is to provide 23 a lower-cost / high accuracy simulation of this important region. To provide 24 this solution, a technique belonging to Reduced Order Model (ROM) fam-25 ily (see [6, 7, 8, 9, 10, 11]) called Proper Generalized Decomposition (PGD) 26 (see [12, 13, 14, 15, 16, 17]) has been adapted for this problem to consider 27 temperature-dependent material properties and latent heat associated with 28 phase change. Heating is accomplished via a laser model that moves rapidly 29 along the path while heat removal is modeled via temperature dependent 30 thermal conductivity and rapidly evolving Neumann boundary conditions. 31 This model order reduction technique allows computing a reduced base for 32 each variable without solving the full eigenvalue problem. In order to prop-33 erly keep into account the non-linearities and the boundary condition of 34 highly transient thermal evolutions, a dedicated PGD algorithm and method-35 ology have been developed, representing the main contributions of this work. 36 Thanks to it, computational cost is significantly reduced and variable separa-37 tion is achieved enabling a highly meaningful reduced basis. Benchmarking 38 against the full transient finite element solutions are performed. For the 39 purpose of benchmarking, a linear finite element full integration formulation 40 was chosen. An in-depth study on PGD controls (number of modes, number 41

42 of iterations, etc.) and on how they can be best selected for efficient com43 putations is included and accuracy and performance findings are carefully
44 tabulated.

45 2. Problem description

For the purpose of this study, a patch of material of unit thickness is
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

direction involves a very important heat transport mechanism, for simplicity, 49 we have modeled it as a 2D problem in the xy plane (all units are modified 50 accordingly). Despite this simplification, all core non-linearities associated 51 with additive manufacturing heat transfer computations including material 52 properties, high temperature gradients and high heating and cooling rates are 53 included and therefore the setup serves the core purpose of the paper. The 54 patch is a square region of given length (L) made of Ti-6Al-4V, a popular 55 Titanium-based alloy used widely in powder bed fabrication additive manu-56 facturing (see [18]). The material definition includes temperature-dependent 57 properties (such as the density (ρ) , the heat capacity (C_p) and the thermal 58 conductivity (k); the heat source is a laser beam with prescribed power 59 density input (P) in the form of a Gaussian distribution initially centered 60 at point (X_0, Y_0) relative to a (O, x, y) coordinate system aligned with the 61 plate edges with origin at the lower left corner of the plate. The heat source 62 is moving over the patch in the negative x-direction with a given speed (v). 63 The patch loses heat to the surrounding environment at temperature (T_{env}) 64 through its surface according to a film condition with heat transfer coeffi-65 cient (h). In addition heat is also lost through its boundaries according to a 66

prescribed outward flux $(\overline{q}^{out}(x, y, t))$, where t denotes the time. The values of all these parameters are subject to change depending on the particular 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 field T(x, y, t), with material non-linearities and a non-linear varying source, 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:

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

76 where

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

Here \mathbf{n}^{out} represents the outer unit normal to the domain boundary, T_0 represents the prescribed uniform initial temperature field, R_0 represents a represents the Gaussian distribution and

$$\begin{cases} x_0(t) = X_0 + f_x(t) \\ y_0(t) = Y_0 + f_y(t) \end{cases}$$
(3)

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

⁸² 3. Methods and Algorithms

Since the PGD results are compared to Finite Element Method (FEM) 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.

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

91 3.1. Linear case

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

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

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

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

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

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

The nodal solution vector is thus expressed as a separated representation 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 "basis vectors" and the time functions $\lambda_i(t)$ can be viewed as coefficients in a linear combination analogous to FEM-based eigenmode superposition. Alternatively, each couple $(\Phi_i, \lambda_i(t))$ can be viewed as a "mode" in this superposition. This terminology will be used in the Results and Discussion 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.

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

$$\mathbf{T}_{n}(t) = \sum_{i=1}^{n} \mathbf{\Phi}_{i}\lambda_{i}(t) = \sum_{i=1}^{n-1} \mathbf{\Phi}_{i}\lambda_{i}(t) + \mathbf{\Phi}_{n}\lambda_{n}(t) = \mathbf{T}_{n-1}(t) + \mathbf{\Phi}_{n}\lambda_{n}(t).$$
(7)

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

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

129 PGD Enrichment step (addition of a new couple)

Assuming that the first n-1 couples $(\Phi_i, \lambda_i(t))_{i=1,...,n-1}$ have been previously obtained, the current approximation of the field is written in the form $\mathbf{T}_n(t) = \mathbf{T}_{n-1}(t) + \Phi_n \lambda_n(t)$, with the new couple $(\Phi_n, \lambda_n(t))$ unknown.

The new couple $(\Phi_n, \lambda_n(t))$ is obtained by applying an alternating directions fixed point iterations method, which is the standard choice for PGD algorithms (see [15]). In contrast with the FEM, the time marching increment 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.

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.

After the initialization, the fixed-point iterations consist in computing in sequence: $\Phi_n^{(1)}$ and $\lambda_n^{(1)}(t)$ (first iteration), then $\Phi_n^{(2)}$ and $\lambda_n^{(2)}(t)$ (second iteration), etc., until convergence to the couple ($\Phi_n, \lambda_n(t)$). At the k^{th} iteration, consistently with the basic premise of separation of variables, one thus solves in sequence:

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

• 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 $\mathbf{T}_n(t) = \mathbf{T}_{n-1}(t) + \mathbf{\Phi}_n^{(k)} \lambda_n^{(k-1)}(t)$ and by choosing a test function for the weak 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 the virtual work machinery, the space problem is then given by the equation:

$$\left(\int_{I} \lambda_{n}^{(k-1)}(t) \dot{\lambda}_{n}^{(k-1)}(t) dt \ \mathbb{M} + \int_{I} \lambda_{n}^{(k-1)^{2}}(t) dt \ \mathbb{K}\right) \mathbf{\Phi}_{n}^{(k)} = \int_{I} \lambda_{n}^{(k-1)}(t) \mathbf{F}_{Q_{in}} dt - \sum_{i=1}^{n-1} \left(\int_{I} \lambda_{n}^{(k-1)}(t) \dot{\lambda}_{i}(t) dt \ \mathbb{M} + \int_{I} \lambda_{n}^{(k-1)}(t) \lambda_{i}(t) dt \ \mathbb{K}\right) \mathbf{\Phi}_{i}$$

$$\tag{8}$$

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:

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

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

$$\begin{cases} a = \int_{I} \lambda_{n}^{(k-1)}(t) \dot{\lambda}_{n}^{(k-1)}(t) dt \\ b = \int_{I} \lambda_{n}^{(k-1)^{2}}(t) dt \\ \mathbf{c} = \int_{I} \lambda_{n}^{(k-1)}(t) \mathbf{F}_{Q_{in}} dt - \sum_{i=1}^{n-1} (a_{i}\mathbb{M} + b_{i}\mathbb{K}) \mathbf{\Phi}_{i} \end{cases}$$
(11)

¹⁶¹ this problem takes the form:

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

162 Time problem

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

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

$$\Phi_{n}^{(k)T} \mathbb{M} \Phi_{n}^{(k)} \dot{\lambda}_{n}^{(k)}(t) + \Phi_{n}^{(k)T} \mathbb{K} \Phi_{n}^{(k)} \lambda_{n}^{(k)}(t) = \Phi_{n}^{(k)T} \mathbf{F}_{Q_{in}} - \sum_{i=1}^{n-1} (\Phi_{n}^{(k)T} \mathbb{M} \Phi_{i} \dot{\lambda}_{i}(t) + \Phi_{n}^{(k)T} \mathbb{K} \Phi_{i} \lambda_{i}(t)).$$
(13)

168 Letting:

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

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

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

170 this problem takes the form:

$$a'\dot{\lambda}_{n}^{(k)}(t) + b'\lambda_{n}^{(k)}(t) = c'(t).$$
 (16)

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

174 Convergence criterion

The new couple $(\Phi_n, \lambda_n(t))$ is obtained after convergence of the fixed point iterations for the sequence $\Phi_n^{(k)}, \lambda_n^{(k)}(t)$, based on the relative error criterion 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)

where tol_{PGD} is a small tolerance. The optimal value of tol_{PGD} is casedependent. 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 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)

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

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

189 this problem takes the form:

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

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 finite difference scheme with large time increments over the entire time interval $I = [0, t_{end}]$. For the purpose of this study, the interval I was always discretized via 100 equally sized increments.

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

¹⁹⁶ The extension of the FEM and PGD approaches to the non-linear case is ¹⁹⁷ briefly described next. PDG has seen applications in non-linear cases, mainly ¹⁹⁸ by the use of linearization schemes or of asymptotic numerical methods as in ¹⁹⁹ [22], [23] and [24]. Nevertheless, the PGD algorithm and methodology pro-²⁰⁰ 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 to be prescribed functions of the temperature. Since the capacitance matrix 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 a function of temperature $\mathbb{K}(T)$.

²⁰⁶ For the FEM, the equation becomes:

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

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

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

214 PGD Enrichment step

This step proceeds again by fixed point iterations.

216 Since

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

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

To compute the first couple $(\Phi_1, \lambda_1(t))$, the temperature field T(x, y, t)is initialized to T_0 and used to compute initial values for the capacitance 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 $\{\Phi_1^{(1)}, \lambda_1^{(1)}(t)\}$. After each new iteration, these matrices are updated with the temperature field of the current iteration.

Thus, after the k^{th} iteration, yielding $(\mathbf{\Phi}_1^{(k)}, \lambda_1^{(k)}(t))$, the matrices are updated according to

$$\begin{cases} \mathbb{M}_{0}^{(k)}(t) = \mathbb{M}(\rho C_{p}(\mathbf{\Phi}_{1}^{(k)}\lambda_{1}^{(k)}(t))) \\ \mathbb{K}_{0}^{(k)}(t) = \mathbb{K}(k(\mathbf{\Phi}_{1}^{(k)}\lambda_{1}^{(k)}(t))) \end{cases}$$
(23)

and used to compute the next iterate $(\Phi_1^{(k+1)}, \lambda_1^{(k+1)}(t))$. This process continues until convergence of the first pair. To compute the other couples $\{(\Phi_i, \lambda_i(t))\}_{i=2,...,n-1}$, the temperature vector is replaced by the sum of the products of the currently known terms and the capacitance and conductivity matrices are pre-computed once based on all previous information and then stored. Thus, for the computation of the n^{th} pair $(\Phi_n, \lambda_n(t))$, $\mathbf{T}(t)$ is replaced by the known quantity $\mathbf{T}_{n-1}(t) =$ $\sum_{i=1}^{n-1} \Phi_i \lambda_i(t)$, where all the time functions have been updated, and the capacitance and conductivity matrices are updated via:

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

Aside from the special treatment for the first couple, the process is repetitive.

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

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

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

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

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

the space problem takes the form:

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

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

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

244

245

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

$$\begin{cases} a'(t) = {\mathbf{\Phi}_{n}^{(k)}}^{T} \mathbb{M}_{n-1}(t) {\mathbf{\Phi}_{n}^{(k)}} \\ b'(t) = {\mathbf{\Phi}_{n}^{(k)}}^{T} \mathbb{K}_{n-1}(t) {\mathbf{\Phi}_{n}^{(k)}} \\ c'(t) = {\mathbf{\Phi}_{n}^{(k)}}^{T} \mathbf{F}_{Q_{in}} - \sum_{i=1}^{n-1} (a_{i}'(t) \dot{\lambda}_{i}(t) + b_{i}'(t) \lambda_{i}(t)) \end{cases}$$
(29)

the time problem takes the form:

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

²⁴⁶ PGD Update step

This step re-computes all time functions. The capacitance and conductivity matrices are first updated in terms of all current information $\{(\Phi_i, \lambda_i(t))\}_{i=1,...,n}$, by assuming that $\mathbf{T}_n(t) = \sum_{i=1}^n \Phi_i \lambda_i(t)$ 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:

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

²⁵¹ the update problem takes the form:

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

In SLM processes, phase changes from raw materials (e.g. powder) to liquid followed by solidification occur at very high speed $(10^{-6} - 10^{-3} \text{ s})$.

Upon melting, the local internal energy increases significantly while the tem-261 perature typically increases over a small range between T_S (solidus) and T_L 262 (liquidus). Upon solidification, the opposite takes place: a large amount of 263 energy is conducted/convected/radiated away from the "action" zone while 264 temperatures decrease over the same range between liquidus and solidus. 265 These high temperature cooling/heating rates and large temperature gradi-266 ents are the dominant factors in determining at microstructural level grain 267 morphologies and are the primary driver behind metallurgical phase transfor-268 mations upon solidification. These have a direct influence on the mechanical 260 properties of the finished product, and therefore it is critical to capture rea-270 sonably well these highly transient events (see [19]). 271

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

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

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

With the impetus of global-local FEM-based modeling techniques, the ability of robustly handling arbitrary Neumann boundary conditions on local 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 algorithms, 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:

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

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

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



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

a convective conductivity matrix must be added to the non-linear conductivity 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:

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

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

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

300 PGD Enrichment step

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

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

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

304 with:

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

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

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

•

307 with:

$$\begin{aligned} a_{i}'(t) & and \ a'(t) \ unchanged \\ b_{i}'(t) &= \Phi_{n}^{(k)^{T}} (\mathbb{K}_{n-1}(t) + \mathbb{K}_{h}) \Phi_{i} \quad \text{for } i = 1, \dots, n-1 \\ b'(t) &= \Phi_{n}^{(k)^{T}} (\mathbb{K}_{n-1}(t) + \mathbb{K}_{h}) \Phi_{n}^{(k)} \\ c'(t) &= \Phi_{n}^{T} (\mathbf{F}_{Q_{in}}(t) - \mathbf{F}_{\bar{q}^{out}}(t) + \mathbf{F}_{\mathbf{h}}(T_{env})) - \sum_{i=1}^{n-1} (a_{i}'(t)\dot{\lambda}_{i}(t) + b_{i}'(t)\lambda_{i}(t)) \\ (43) \end{aligned}$$

308 PGD Update step

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

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

311 with:

$$a'_{j,i}(t) \text{ unchanged}$$

$$b'_{j,i}(t) = \mathbf{\Phi}_{j}^{T}(\mathbb{K}_{n}(t) + \mathbb{K}_{h})\mathbf{\Phi}_{i}$$

$$c'_{j}(t) = \mathbf{\Phi}_{\mathbf{j}}^{T}(\mathbf{F}_{Q_{in}}(t) - \mathbf{F}_{\overline{q}^{out}}(t) + \mathbf{F}_{\mathbf{h}}(T_{env})).$$
(45)

The computations for stage n(>1) in this most general case are summarized 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 were generated by Gmsh. The coefficients a, b, c (see Equation (11)) and A, \mathbb{B}, \mathbf{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 4.1. Example 1: linear case

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

The domain to be analyzed consists of a 2 $mm \times 2 mm$ square plate made of Ti-6Al-4V. The laser is stationary and heats the plate during 0.1 s. The walls are insulated and there are no Dirichlet boundary conditions. A non-uniform triangular mesh with 1894 degrees of freedom was used, with 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.

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

Algorithm 1 Non-linear PGD

$$\begin{split} & \textbf{Require: } \mathbb{M}_{n-1}(t), \, \mathbb{K}_{n-1}(t), \, \mathbb{K}_{h}, \, \textbf{F}_{Q^{in}}(t), \, \textbf{F}_{\bar{q}^{out}}(t), \, \textbf{F}_{h}(T_{env}), \, tol_{PGD}, \, (\boldsymbol{\Phi}_{n-1}, \lambda_{n-1}(t)) \\ & \textbf{for } n = 2 \text{ to } N_{mod} \text{ do} \\ & \textbf{Enrichment step (Fixed-point iterations) to Compute } (\boldsymbol{\Phi}_{n}, \lambda_{n}(t)) \\ & \textbf{Initialize } \lambda_{n}^{(k=0)}(t) \\ & \textbf{while } \epsilon = \frac{\int_{I} (\lambda_{n}^{(k)}(t) - \lambda_{n}^{(k-1)}(t))^{2} dt}{\frac{1}{2} \int_{I} (\lambda_{n}^{(k)}(t) + \lambda_{n}^{(k-1)}(t))^{2} dt} > tol_{PGD} \text{ do} \\ & k = k + 1 \\ & \textbf{Space problem: Compute } \boldsymbol{\Phi}_{n}^{(k)} \text{ from a known } \lambda_{n}^{(k-1)}(t) \end{split}$$

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

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

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

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 $\mathbf{\Phi}_n^{(k)}$

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

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

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

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 Set: $(\Phi_n, \lambda_n(t)) = (\Phi_n^{(k)}, \lambda_n^{(k)}(t))$

end if

end while

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

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

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

Simu	lation			
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	$3.31 \cdot 10^{-5}$	$tol_{PGD} = 10^{-8}$	40

335 Here:

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

is the expression used to compute the error. It measures the difference between FEM and PGD results according to the L^2 norm, normalized by the L^2 norm of the FEM answer. Solve Total represents the number of times a linear system was solved by matrix inversion.

Comparing the accuracy of the PGD results for various numbers of re-340 tained modes and for various numbers of iterations per mode, we can make 341 some observations. First, very few iterations are needed per mode. The error 342 criterion can be replaced by a strategy with 1 iteration per mode. This shows 343 that the method is self-correcting. Besides, since each iteration requires the 344 resolution of a potentially large algebraic system (along with the integration 345 of an ODE), for a given number of matrix factorizations, it is more advanta-346 geous to increase the number of modes with just a few (one or two) iterations 347 per mode than to increase the number of iterations per mode with a lower 348 number of computed modes. This is illustrated by comparing Figures 4b 349 (PGD 4 modes, $tol_{PGD}=0.01$) and 4c (PGD 5 modes, 1 iteration per mode). 350 Both represent an improvement of the PGD 4 modes, 1 iteration per mode 351 solution. But, in the first case, it is necessary 8 iterations for an error equals 352 to 0.028, while for the second one, less iterations (5) give better result (error 353 = 0.0098). 354

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

Finally, to illustrate the principle of the PGD, a few couples of basis vectors and time functions are presented in Figure 5. The basis vectors have ³⁵⁹ been normalized with respect to the capacitance matrix in order to maintain³⁶⁰ consistent orders of magnitude for the time functions. The time functions

³⁶¹ 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

As expected, the PGD-computed response is very accurate in the linear 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 371 tolerance, on the other hand, is chosen so as to yield a reference FEM solution 372 of the same precision when compared to Abaqus. The reported Speed-up 373 Factor is the ratio of the total number of solves needed for our FEM solution 374 by the total number of solves needed for our PGD solution. Due to the fact 375 that Abaque requires only roughly half the number of solves per increment, 376 a more conservative way to measure the PGD gain would be to divide the 377 reported Speed-up Factor by two. 378

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 $\,$

the PGD solution tends towards the reference solution, even when some nonlinearities are introduced.

Moreover, regarding the modes convergence criterion, the same conclu-383 sions as in the linear case can be applied here. It is possible, and preferable, 384 to impose a fixed number of iterations per mode instead of using a tolerance. 385 For example, one can compare PGD 6 modes with $tol_{PGD}=0.01$ and PGD 7 386 modes with 2 iterations for the first mode and 1 iteration for the others. In 387 the first case, the total number of iterations is not known a priori. The error 388 ϵ from Equation (17) must be smaller than 0.01 in order to calculate the 389 next mode. In the second case, the number of iterations of a specific mode is 390 imposed, and Equation (17) is ignored. One concludes that a few iterations 391 suffice, since the first case has more iterations (meaning larger computational 392

Simu	lation			Solve	
Type	Modes	Error	Criterion	Total	Speed-up Factor
FEM	-	-	$Tol_{FEM} = 0.0001$	658	-
PGD	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	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
PGD	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 1 393 iteration for the others is the minimum necessary number of iterations, since 394 the first mode has a larger contribution to the final result - so it must have 395 a special treatment - and each new mode seems to correct partially the flaws 396 of previous modes. If a given result is not precise enough, it is preferable to 397 add an extra mode (with just one iteration) than to perform more iterations. 398 Finally, PGD has responded well to the non-linear case. Satisfactory 399 results were obtained with just a few iterations, as shown for instance in 400 Figure 7b. 401

402 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 investigate 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.

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

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



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	$X_0 = 1.5 \ mm \text{ and } Y_0 = 1.0 \ mm$
Total time (t_{end})	2 ms (1 ms with the laser on and 1 ms of cooling)
Time increment (Δt)	$2 \cdot 10^{-5} s$

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

418

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.

424 4.3.1. Latent heat

The approach used for modeling latent heat is explained in Section 3.3. 425 The phase transformation from solid to liquid and vice-versa occurs for Ti-426 6Al-4V over a narrow range of temperatures (of about 50 K) centered around 427 1920 K. In the finite element formulation, in order to achieve reasonable 428 convergence when traversing this strong non-linearity, we chose to widen 429 the phase transformation interval using the parameters presented in Table 430 5. Previous studies (see [26], [19]) suggest that such choice has almost no 431 detrimental effect when numerical results are a compared to physical tests 432 including melt pool in plane dimensions and depth. For consistency a similar 433 approach is adopted in the PGD formulation. 434

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

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

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

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

441 4.3.2. Moving source

The source is now allowed to move within the patch in the negative xdirection 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

(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)

As the source travels along the horizontal direction, the regions of high 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-448 derstand the effects of the latent heat. Figure 10 shows how the latent heat 449 leads to a significant reduction of the temperature. Both curves (with and 450 without latent heat) coincide as long as $T < T_S$. When the temperature 451 reaches the value $T = T_S$, there is a decrease in the slope of the curve with 452 latent heat, and the curves no longer coincide. However, when $T > T_L$, the 453 slope of the curve with latent heat increases again and the curves become 454 nearly parallel. 455

The results of the simulation are illustrated in Figure 11 and 12 and in 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

Simu	lation					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:

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)

is the error for the first half time of the simulation, where the laser is turnedon and travels from point 5 to point 10, and

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

⁴⁶¹ is the error for the total duration of the simulation, i.e., the laser on and the ⁴⁶² cooling (laser off) phases. Notice that the temperature gradients are higher ⁴⁶³ in the laser "on" scenario than in the cooling scenario, meaning that relative ⁴⁶⁴ global discrepancies between PGD and FEM results are expected to be larger ⁴⁶⁵ in the first half of the simulation. This justifies the fact that Error 1 will ⁴⁶⁶ always be larger than Error 2 in this example.

As can be seen from these curves, the response behavior is in accordance
with expectations and shows good correlation between FEM and PGD results
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 474 unacceptable. Nevertheless, when using 50 modes with 2 iterations per mode 475 (Figure 12a), the result accuracy is excellent. In both cases, there are about 476 100 iterations in total, but in the first case, although more modes are used, 477 the result is worse than in the second case. This might seem contradictory 478 with the previous results and with the PGD assumptions. However, in the 479 case of a moving laser, the higher modes have an important contribution 480 to the response due to the non-separability of time and space. As the new 481 expression for Q_{in} is such that it is not possible to separate time and space -482 due to the terms $v_x t$ and $v_y t$ in the exponential - the higher order modes are 483 no longer mere corrections, but contribute as importantly to the solution as 484 the lower ones. Since higher modes are very relevant for the solution in this 485 new case, the convergence criterion needs to be more strict in order to obtain 486 an accurate PGD solution. This explains the difference between 50 and 100 487 modes PGD solutions. Besides, it establishes that at least 2 iterations are 488 necessary for each mode to have an acceptable solution. In fact, one can 489 consider that 2 iterations per mode is the ideal mode convergence criterion 490 for this example, and a larger number of iterations could add numerical 491 pollution. Adding an extra mode is again better than adding more iterations 492 per mode. 493

⁴⁹⁴ Moreover, the number of modes and iterations required to correctly cap-⁴⁹⁵ ture the diffusion effect is much larger than for a stationary source, even ⁴⁹⁶ though, with 20 modes, PGD represents a performance gain of 24.85 times ⁴⁹⁷ compared to FEM. Qualitatively the result is quite acceptable as the very ⁴⁹⁸ large temperature gradients, peak temperatures and overall temperature dis-⁴⁹⁹ 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 500 influence of the latent heat with a moving laser on the solution in Figure 14. 501 Figures 14a and 14b support the verification of PGD, showing it is able 502 to handle problems with moving source and latent heat, and the larger the 503 number of modes, the better the solution (here 50 modes and 2 iterations 504 per mode were used). One can note that the PGD solution without latent 505 heat is more accurate than the one with latent heat. This is consistent, since 506 the latent heat introduces a very strong non-linearity to the problem. 507



(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 nonlinearities 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 $mm \ge 0.1 mm$ rectangular uniform mesh (this region will be also called the small patch), with the origin at the bottom left corner and 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 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.

⁵²⁶ The previous description is illustrated in Figure 15.



Figure 15: Representative schema of Example 4

527 4.4.1. Neumann Boundary Conditions

In all previous examples, it was considered that the domain was thermally 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 535 response (i.e., non-linear k, non-linear C_p , latent heat, convection, moving 536 laser and insulated boundaries) in a larger patch. A 2 mm x 2 mm square 537 domain (henceforth the super-patch), totally overlapping the small patch was 538 created and used in a first simulation. It was assumed that the influence of 539 the diffusion of the laser heat on the edges of the super-patch during the first 540 2 ms is negligible, so the insulated walls assumption is more realistic for this 541 super-patch. 542

The second step was the extraction of the space and time-dependent outflux, 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 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 superpatch is represented by the black square which contains the red rectangle. To save computation time, the super-patch was meshed non-uniformly. The element sizes are 10^{-4} m near the black edges, $2.5 \cdot 10^{-5}$ m near the red edges and 10^{-5} m along the laser path.

⁵⁶¹ 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 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:

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

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

This approach is an attempt to be as realistic as possible, since we are 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

Simu	lation					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	2 it./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

Here, Error 1 and Error 2 are the same as defined in Equations (49) and (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

seems a good compromise, even though there are some oscillations at the beginning of the simulation for the PGD response. The accuracy in the most

important regions (such as high temperatures or cooling) is acceptable and 589 the number of matrix inversions in this case is reduced by 22 compared to the 590 FEM. As the out-flux represents a considerable percentage of the laser energy, 591 there is a remarkable drop in the temperature when compared to Example 3. 592 However, this does not seem to be a problem for PGD. Adding the time and 593 space-dependent Neumann boundary conditions and the film convection does 594 not change the number of modes necessary for a reasonable PGD response. 595 Previously, with 20 modes and 2 iterations per mode one obtained an error 596 1 = 0.0299 and an error 2 = 0.0190. Thus, although the errors have slightly 597 increased, the choice of 20 modes seems a reasonable compromise. Finally, 598 this example proves that PGD can handle highly non-linear and complex 599 problems. 600

601 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 associated 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 accurate/predictive and hence we have focused this work in that context.

After a brief introduction and setting the objectives in Section 1, the 608 specific problem benchmark in this work is outlined in Section 2. Linear 609 and non-linear PGD theory for transient heat transfer equations has been 610 carefully described in Section 3. To develop a realistic AM thermal model, 611 most relevant non-linearities associated with the parabolic PDE, such as ma-612 terial property non-linearities, phase change by latent heat, time-dependent 613 source, temperature-dependent source and time and space-dependent bound-614 ary conditions have been introduced. Finally, Section 4 presents an extensive 615 numerical campaign to validate the PDG-based approach against traditional 616 FEM while thoroughly assessing the execution performance gains. 617

As demonstrated by these tests, model order reduction techniques such as PGD appear to be a very promising lead when tackling highly non-linear numerical simulation challenges in AM. Two key aspects should be highlighted: 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 624 and performance assessment of a 3D model, development of an ad-hoc PGD 625 algorithm to further improve computational gains and implementation in 626 commercial codes to solve complex industrial cases. On a broader long-term 627 scale, future work should address the gigantic multi-physics and the multi-628 scale nature of the problem which could take great advantage from model 629 order reduction techniques at both local (melt pool level) and global (part 630 level) scales. 631

632 6. References

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