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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. Introduction

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

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

13 Effective numerical methods capable of predicting final characteristics of
14 the part, spotting critical points during the process and helping the design
15 process itself are often invaluable in gaining insight in the process. Since
16 SLM and EBM encompass complex multiphysics (thermal, mechanical, phase
17 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,
19 3])including fast executing AM-specialized approaches (see [4]).

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

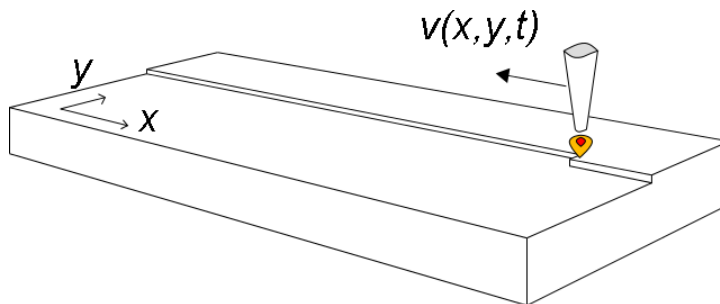


Figure 1: Problem under study

48 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

67 prescribed outward flux ($\bar{q}^{out}(x, y, t)$), 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.

70 This problem can be formulated as a boundary value problem governed
 71 by a parabolic partial differential equation (PDE) for the scalar temperature
 72 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
 74 prescribed Neumann boundary conditions and uniform initial conditions. In
 75 its most general form, the boundary value problem is formulated as follows:

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

76 where

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

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

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

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

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

87 We start by describing the linear case, then move to comprehensive non-
 88 linear cases, including temperature-dependent properties and latent heat as-
 89 sociated with phase changes, fast moving time-dependent heat sources and
 90 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 $\bar{q}^{out} = Q^{out} = f_x = f_y = 0 \forall t \in I$, and Q^{in} is independent of time:

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

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

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

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:

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

103 where N_{mod} is the number of products, determined based on a convergence
 104 criterion. The space functions are discretized according to $\Phi_i(x, y) \approx \mathbb{N}(x, y) \mathbf{\Phi}_i$,
 105 where $\mathbf{\Phi}_i$ represents the i^{th} 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 $\mathbf{T}(t) \approx \sum_{i=1}^{N_{mod}} \mathbf{\Phi}_i \lambda_i(t)$, where the vectors $\mathbf{\Phi}_i$ 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.

116 In contrast to usual methods (which include FEM eigenmode analysis and
 117 other order reduction methods such as the Proper Orthogonal Decomposition
 118 - POD method), in which the projection basis is known a priori, the PGD
 119 basis vectors and time functions are both unknown and will be computed on
 120 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 $\mathbf{T}_{n-1}(t)$:

$$\mathbf{T}_n(t) = \sum_{i=1}^n \Phi_i \lambda_i(t) = \sum_{i=1}^{n-1} \Phi_i \lambda_i(t) + \Phi_n \lambda_n(t) = \mathbf{T}_{n-1}(t) + \Phi_n \lambda_n(t). \quad (7)$$

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 $(\Phi_i, \lambda_i(t))_{i=1, \dots, n-1}$ have been previ-
 131 ously obtained, the current approximation of the field is written in the form
 132 $\mathbf{T}_n(t) = \mathbf{T}_{n-1}(t) + \Phi_n \lambda_n(t)$, 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-
 134 tions fixed point iterations method, which is the standard choice for PGD
 135 algorithms (see [15]). In contrast with the FEM, the time marching incre-
 136 ment has less influence on convergence. Other factors, such as a bad choice
 137 of the initialization function (for example a null function) can have a more
 138 detrimental effect.

139 The process starts with the initialization of the time function $\lambda_n^{(0)}(t)$. This
 140 choice is arbitrary, since several functions can result in converged results.
 141 We opted for using a linear time function. This was determined on physical
 142 grounds, based on the fact that in the absence of transients the solution of
 143 the boundary value problem with constant source and no Neumann boundary
 144 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:

- 150 • 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*

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

156 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:

$$\left(\int_I \lambda_n^{(k-1)}(t) \dot{\lambda}_n^{(k-1)}(t) dt \mathbb{M} + \int_I \lambda_n^{(k-1)2}(t) dt \mathbb{K} \right) \Phi_n^{(k)} = \int_I \lambda_n^{(k-1)}(t) \mathbf{F}_{Q_{in}} dt - \sum_{i=1}^{n-1} \left(\int_I \lambda_n^{(k-1)}(t) \dot{\lambda}_i(t) dt \mathbb{M} + \int_I \lambda_n^{(k-1)}(t) \lambda_i(t) dt \mathbb{K} \right) \Phi_i \quad (8)$$

158 where

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

159 Letting:

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

160 for $i = 1, \dots, n-1$ and

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

161 this problem takes the form:

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

162 *Time problem*

163 Assuming that $\Phi_n^{(k)}$ is known, one obtains $\lambda_n^{(k)}(t)$ by assuming that $\mathbf{T}_n(t) =$
 164 $\mathbf{T}_{n-1}(t) + \Phi_n^{(k)}(t)\lambda_n^{(k)}(t)$ and by choosing a test function for the weak formu-
 165 lation of the problem in the form $\mathbf{T}^*(t) = \Phi_n^{(k)}\lambda^*(t)$.

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

$$\begin{aligned} & \Phi_n^{(k)T} \mathbb{M} \Phi_n^{(k)} \dot{\lambda}_n^{(k)}(t) + \Phi_n^{(k)T} \mathbb{K} \Phi_n^{(k)} \lambda_n^{(k)}(t) = \\ & \Phi_n^{(k)T} \mathbf{F}_{Q_{in}} - \sum_{i=1}^{n-1} (\Phi_n^{(k)T} \mathbb{M} \Phi_i \dot{\lambda}_i(t) + \Phi_n^{(k)T} \mathbb{K} \Phi_i \lambda_i(t)). \end{aligned} \quad (13)$$

168 Letting:

$$\begin{cases} a_i' = \Phi_n^{(k)T} \mathbb{M} \Phi_i \\ b_i' = \Phi_n^{(k)T} \mathbb{K} \Phi_i \end{cases} \quad (14)$$

169 for $i = 1, \dots, n-1$ and

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

170 this problem takes the form:

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

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 $(\Phi_n, \lambda_n(t))$ 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:

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

178 where tol_{PGD} is a small tolerance. The optimal value of tol_{PGD} is case-
 179 dependent. On one hand, a small tolerance will lead to few PDG modes at
 180 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
 182 to reach convergence. An in-depth analysis of this behavior will be presented
 183 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 $\{\Phi_i\}_{i=1,\dots,n}$ by requiring that:

$$\sum_{i=1}^n \Phi_j^T \mathbb{M} \Phi_i \dot{\lambda}_i(t) + \sum_{i=1}^n \Phi_j^T \mathbb{K} \Phi_i \lambda_i(t) = \Phi_j^T \mathbf{F}_{Q_{in}} \text{ for } j=1,\dots,n . \quad (18)$$

188 Letting:

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

189 this problem takes the form:

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

190 This coupled ordinary differential equations system in time is solved for
 191 $\{\lambda_1(t), \dots, \lambda_n(t)\}$ 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

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

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
 204 $\mathbb{M}(T)$. 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:

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

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

$$\mathbf{T}_n(t) = \sum_{i=1}^n \Phi_i \lambda_i(t) = \mathbf{T}_{n-1}(t) + \Phi_n \lambda_n(t), \quad (22)$$

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
 222 matrices are then used to compute the first iterate $\{\Phi_1^{(1)}, \lambda_1^{(1)}(t)\}$. After each
 223 new iteration, these matrices are updated with the temperature field of the
 224 current iteration.

225 Thus, after the k^{th} iteration, yielding $(\Phi_1^{(k)}, \lambda_1^{(k)}(t))$, the matrices are up-
 226 dated according to

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

227 and used to compute the next iterate $(\Phi_1^{(k+1)}, \lambda_1^{(k+1)}(t))$. This process con-
 228 tinues until convergence of the first pair.

229 To compute the other couples $\{(\Phi_i, \lambda_i(t))\}_{i=2, \dots, n-1}$, 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
 233 the n^{th} pair $(\Phi_n, \lambda_n(t))$, $\mathbf{T}(t)$ is replaced by the known quantity $\mathbf{T}_{n-1}(t) =$
 234 $\sum_{i=1}^{n-1} \Phi_i \lambda_i(t)$, where all the time functions have been updated, and the ca-
 235 pacitance and conductivity matrices are updated via:

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

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 arbi-
 239 trary 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:

$$\begin{cases} \mathbb{A}_i = \int_I \lambda_n^{(k-1)}(t) \mathbb{M}_{n-1}(t) \dot{\lambda}_i(t) dt \\ \mathbb{B}_i = \int_I \lambda_n^{(k-1)}(t) \mathbb{K}_{n-1}(t) \lambda_i(t) dt \end{cases} \quad (25)$$

241 for $i = 1, \dots, n-1$ and

$$\begin{cases} \mathbb{A} = \int_I \lambda_n^{(k-1)}(t) \mathbb{M}_{n-1}(t) \dot{\lambda}_n^{(k-1)}(t) dt \\ \mathbb{B} = \int_I \lambda_n^{(k-1)2}(t) \mathbb{K}_{n-1}(t) dt, \\ \mathbf{c} = \int_I \lambda_n^{(k-1)}(t) \mathbf{F}_{Q_{in}} dt - \sum_{i=1}^{n-1} ([\mathbb{A}_i] + [\mathbb{B}_i]) \Phi_i \end{cases} \quad (26)$$

242 the space problem takes the form:

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

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

$$\begin{cases} a_i'(t) = \Phi_n^{(k)T} \mathbb{M}_{n-1}(t) \Phi_i \\ b_i'(t) = \Phi_n^{(k)T} \mathbb{K}_{n-1}(t) \Phi_i \end{cases} \quad (28)$$

244 for $i = 1, \dots, n - 1$ and

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

245 the time problem takes the form:

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

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 $\{(\mathbf{\Phi}_i, \lambda_i(t))\}_{i=1, \dots, n}$,
249 by assuming that $\mathbf{T}_n(t) = \sum_{i=1}^n \mathbf{\Phi}_i \lambda_i(t)$ according to:

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

250 Letting:

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

251 the update problem takes the form:

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

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

254 The next step is to build a model that includes the latent change of
255 phase of the patch material located in the close vicinity of the laser source
256 which is now allowed to move inside the patch. Realistic Neumann boundary
257 conditions at the patch edges and a convective heat loss throughout the patch
258 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).

261 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
 263 (liquidus). Upon solidification, the opposite takes place: a large amount of
 264 energy is conducted/convected/radiated away from the “action” zone while
 265 temperatures decrease over the same range between liquidus and solidus.
 266 These high temperature cooling/heating rates and large temperature gradi-
 267 ents are the dominant factors in determining at microstructural level grain
 268 morphologies and are the primary driver behind metallurgical phase transfor-
 269 mations upon solidification. These have a direct influence on the mechanical
 270 properties of the finished product, and therefore it is critical to capture rea-
 271 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:

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

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

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

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:

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

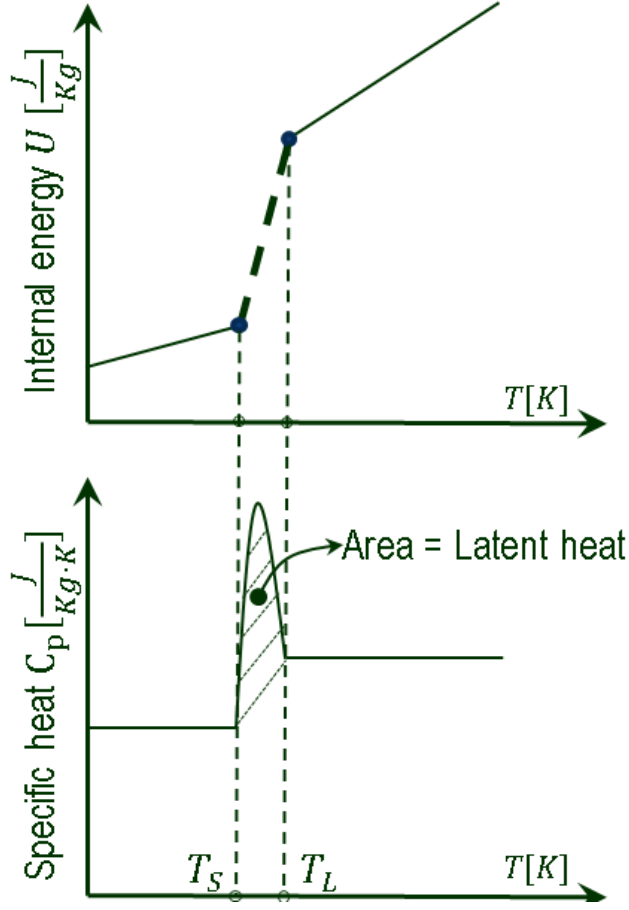


Figure 2: Internal energy for phase change and equivalent non-linear specific heat

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

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

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

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

294 The FEM equation finally becomes:

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

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:

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

304 with:

$$\left\{ \begin{array}{l} \mathbb{A}_i \text{ and } \mathbb{A} \text{ unchanged} \\ \mathbb{B}_i = \int_I \lambda_n^{(k-1)}(t)(\mathbb{K}_{n-1}(t) + \mathbb{K}_h)\lambda_i(t) dt \quad \text{for } i = 1, \dots, n-1 \\ \mathbb{B} = \int_I \lambda_n^{(k-1)2}(t)(\mathbb{K}_{n-1}(t) + \mathbb{K}_h) dt \\ \mathbf{c} = \int_I \lambda_n(t)(\mathbf{F}_{Q_{in}}(t) - \mathbf{F}_{\bar{q}^{out}}(t) + \mathbf{F}_h(T_{env})) dt - \sum_{i=1}^{n-1} (\mathbb{A}_i + \mathbb{B}_i)\Phi_i \end{array} \right. \quad (41)$$

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

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

307 with:

$$\left\{ \begin{array}{l} a_i'(t) \text{ and } a'(t) \text{ unchanged} \\ b_i'(t) = \Phi_n^{(k)T}(\mathbb{K}_{n-1}(t) + \mathbb{K}_h)\Phi_i \quad \text{for } i = 1, \dots, n-1 \\ b'(t) = \Phi_n^{(k)T}(\mathbb{K}_{n-1}(t) + \mathbb{K}_h)\Phi_n^{(k)} \\ c'(t) = \Phi_n^T(\mathbf{F}_{Q_{in}}(t) - \mathbf{F}_{\bar{q}^{out}}(t) + \mathbf{F}_h(T_{env})) - \sum_{i=1}^{n-1} (a_i'(t)\dot{\lambda}_i(t) + b_i'(t)\lambda_i(t)). \end{array} \right. \quad (43)$$

308 *PGD Update step*

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

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

311 with:

$$\begin{cases} a'_{j,i}(t) \text{ unchanged} \\ b'_{j,i}(t) = \Phi_j^T (\mathbb{K}_n(t) + \mathbb{K}_h) \Phi_i \\ c'_j(t) = \Phi_j^T (\mathbf{F}_{Q_{in}}(t) - \mathbf{F}_{\bar{q}^{out}}(t) + \mathbf{F}_h(T_{env})). \end{cases} \quad (45)$$

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

314 4. Results and Discussion

315 In this Section, the most relevant results are shown in order to compare
 316 PGD with FEM. All the simulations were done in Matlab. To assure the
 317 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 \mathbb{A} ,
 319 \mathbb{B} , \mathbf{c} (see Equations (26) and (41)) were calculated by numerical integration
 320 using a rectangular method with 100 discretization points in all the following
 321 examples.

322 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 $2 \text{ mm} \times 2 \text{ mm}$ 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: $\mathbb{M}_{n-1}(t), \mathbb{K}_{n-1}(t), \mathbb{K}_h, \mathbf{F}_{Qin}(t), \mathbf{F}_{\bar{q}out}(t), \mathbf{F}_h(T_{env}), tol_{PGD}, (\Phi_{n-1}, \lambda_{n-1}(t))$

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 $\epsilon = \frac{\int_I (\lambda_n^{(k)}(t) - \lambda_n^{(k-1)}(t))^2 dt}{\frac{1}{2} \int_I (\lambda_n^{(k)}(t) + \lambda_n^{(k-1)}(t))^2 dt} > tol_{PGD}$ **do**

$k = k + 1$

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 $i = 1, \dots, n-1$ and

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

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

Time problem: Compute $\lambda_n^{(k)}(t)$ from a known $\Phi_n^{(k)}$

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

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

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

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 $\{\lambda_1(t), \dots, \lambda_n(t)\}$)

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

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

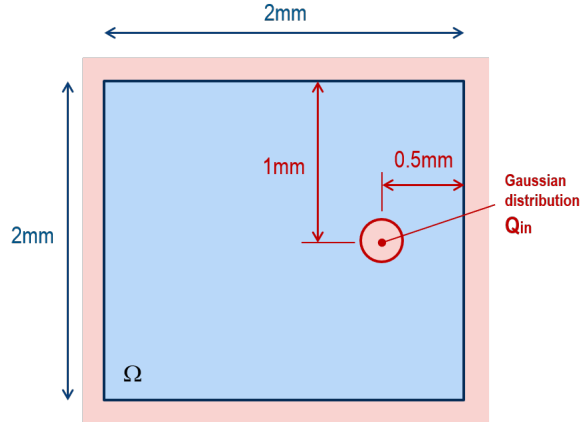
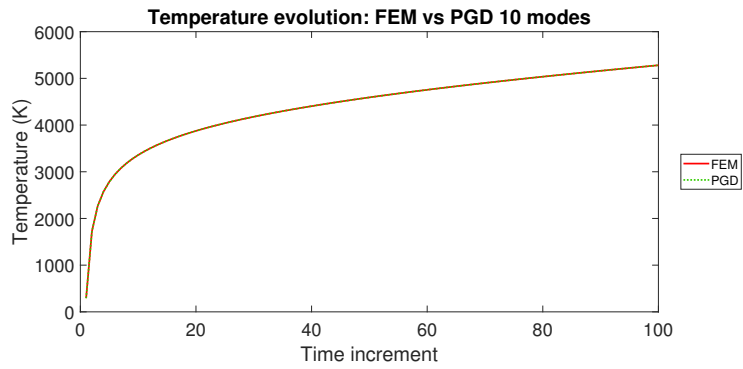


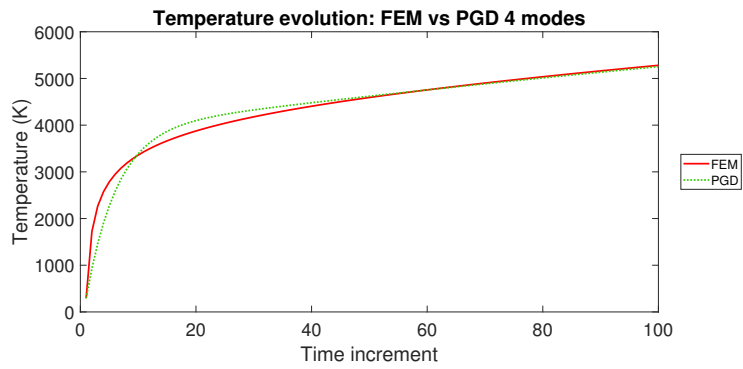
Figure 3: Representative schema of Example 1

Table 1: General properties for Example 1

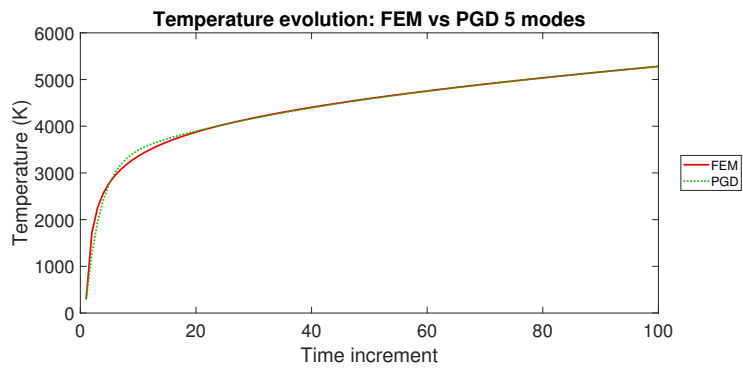
General properties	Values
Density (ρ)	4500 kg/m^2
Conductivity (k)	12 W/K
Heat capacity (C_p)	700 $J/K/kg$
Laser power (P)	100 kW
Laser radius (R_0)	$5 \cdot 10^{-5} m$
Total time (t_{end})	0.1 s
Time increment (Δt)	0.001 s



(a) PGD 10 modes, $tol_{PGD} = 10^{-8}$



(b) PGD 4 modes, $tol_{PGD} = 10^{-2}$



(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		Error	Criterion	Solve Total
Type	Modes			
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:

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

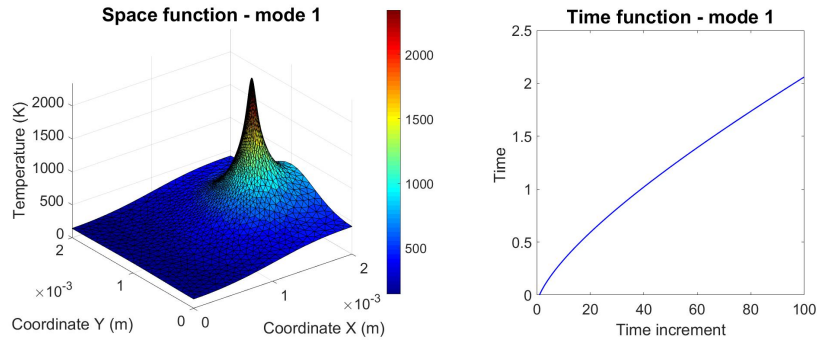
336 is the expression used to compute the error. It measures the difference be-
 337 tween FEM and PGD results according to the L^2 norm, normalized by the
 338 L^2 norm of the FEM answer. Solve Total represents the number of times a
 339 linear system was solved by matrix inversion.

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

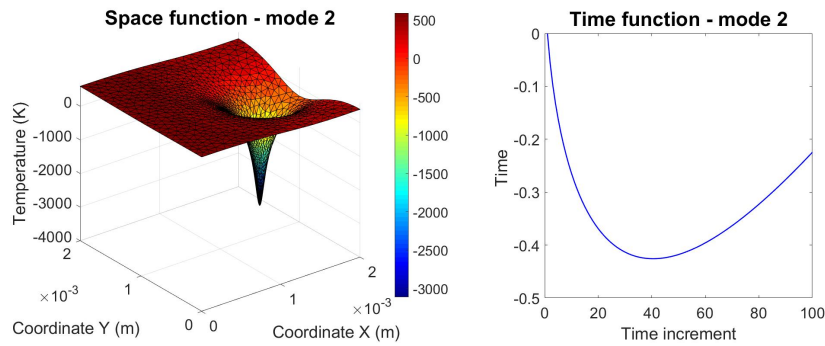
355 Furthermore, Figure 4a confirms that as the number of modes increases,
 356 the PGD solution converges to the FEM solution.

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

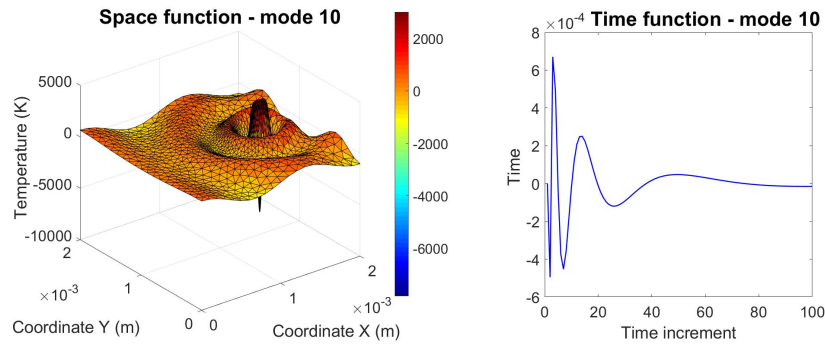
359 been normalized with respect to the capacitance matrix in order to maintain
360 consistent orders of magnitude for the time functions. The time functions
361 were initialized by assuming a linear time dependence.



(a) Space and time functions for the first PGD mode



(b) Space and time functions for the second PGD mode



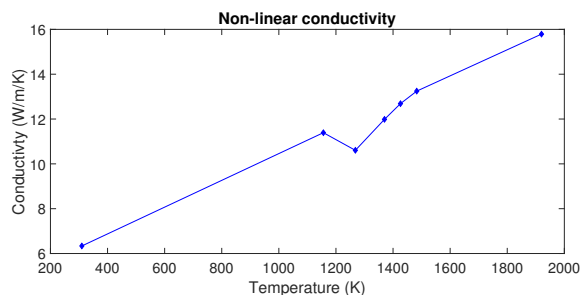
(c) Space and time functions for the tenth PGD mode

Figure 5: PGD space and time functions

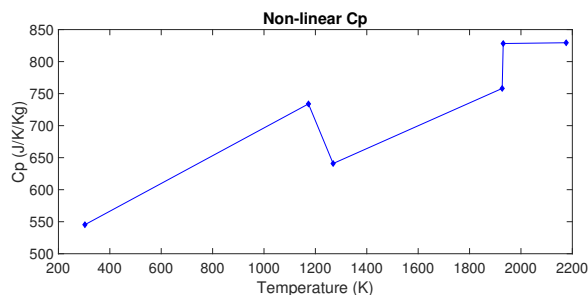
362 *4.2. Example 2: non-linear materials*

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

365 must be introduced. First, we will consider material non-linearities, i.e.
 366 temperature-dependent conductivity and heat capacity. These values were
 367 obtained in [25] and they are shown in Figure 6.



(a) Conductivity as function of the temperature



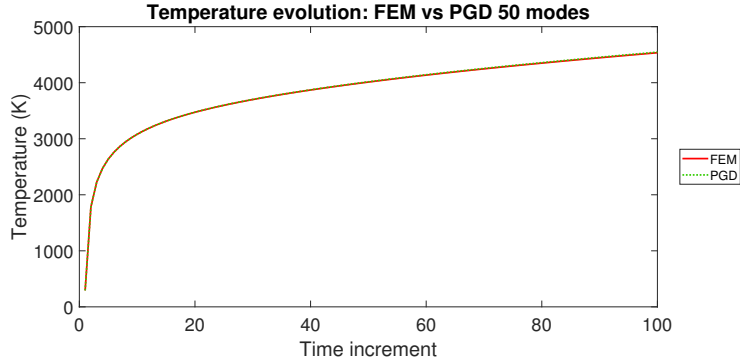
(b) Thermal capacity as function of the temperature

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

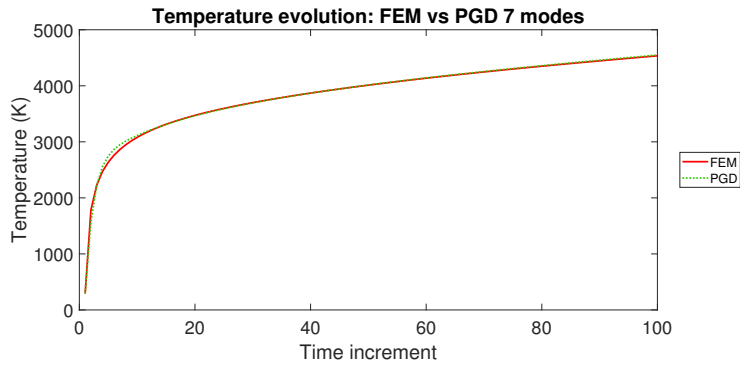
368 Several tests were run, varying the number of modes and convergence
 369 criterion. The results are presented in Figure 7 and Table 3, again at the
 370 node where the laser is located.

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

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



(a) PGD 50 modes, 2 iterations per mode



(b) PGD 7 modes, 2 iterations in the 1st 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.

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

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

Simulation		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

393 costs) and its results are less accurate. 2 iterations for the first mode and 1
 394 iteration for the others is the minimum necessary number of iterations, since
 395 the first mode has a larger contribution to the final result - so it must have
 396 a special treatment - and each new mode seems to correct partially the flaws
 397 of previous modes. If a given result is not precise enough, it is preferable to
 398 add an extra mode (with just one iteration) than to perform more iterations.

399 Finally, PGD has responded well to the non-linear case. Satisfactory
 400 results were obtained with just a few iterations, as shown for instance in
 401 Figure 7b.

402 *4.3. Example 3: non-linear material properties, latent heat and moving laser*

403 From Example 2, it was observed that PGD responded well to the first
 404 non-linearities. So, one can increase the sources of non-linearities to investi-
 405 gate the limits of PGD. The idea is to introduce a moving torch for the laser
 406 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 $2\text{ mm} \times 2\text{ mm}$ 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 $t = 0\text{ s}$ (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 $(0.5, 1)\text{ mm}$. 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.

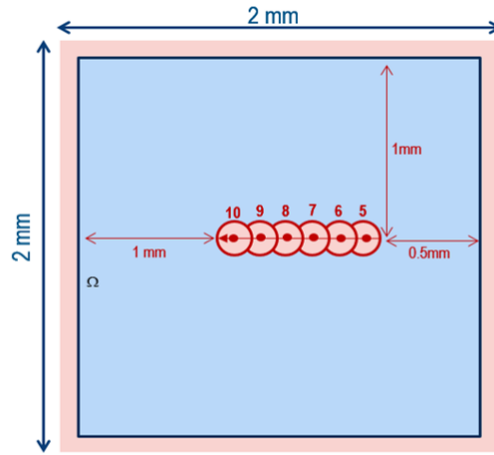


Figure 8: Representative schema of Example 3

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)	$5 \cdot 10^{-5}\text{ m}$
Torch speed (v)	0.5 m/s ($v_x = -0.5\text{ m/s}$, $v_y = 0\text{ m/s}$)
Laser initial position	$X_0 = 1.5\text{ mm}$ and $Y_0 = 1.0\text{ mm}$
Total time (t_{end})	2 ms (1 ms with the laser on and 1 ms of cooling)
Time increment (Δt)	$2 \cdot 10^{-5}\text{ s}$

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
 420 path. The element size must be smaller than the laser radius in the path
 421 region, otherwise the heating effect caused by the laser is not well captured.
 422 Nevertheless, far from the laser path, there is no need to have a refined mesh,
 423 so it is possible to have coarser elements to save computational time.

424 4.3.1. Latent heat

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

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

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

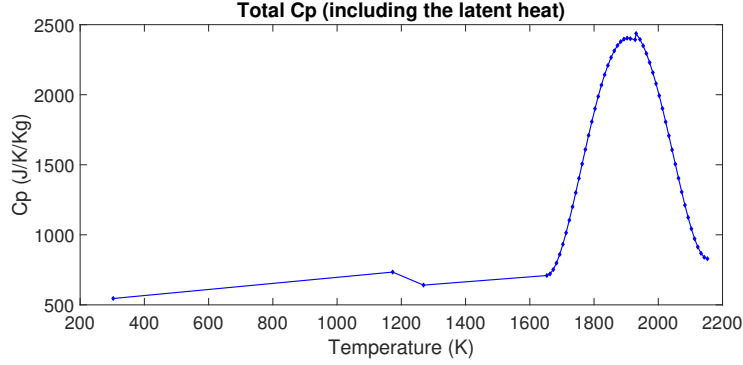


Figure 9: Total heat capacity (including latent heat) as a function of the temperature for Ti-6Al-4V

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

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

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

448 Before comparing PGD and FEM results, it is interesting to better un-
449 derstand the effects of the latent heat. Figure 10 shows how the latent heat
450 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
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
454 slope of the curve with latent heat increases again and the curves become
455 nearly parallel.

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

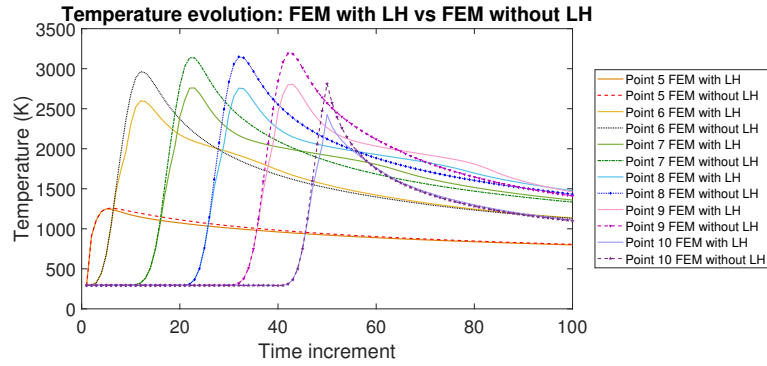
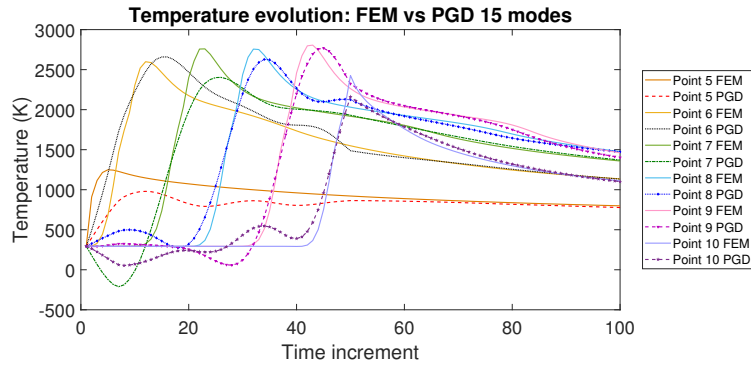
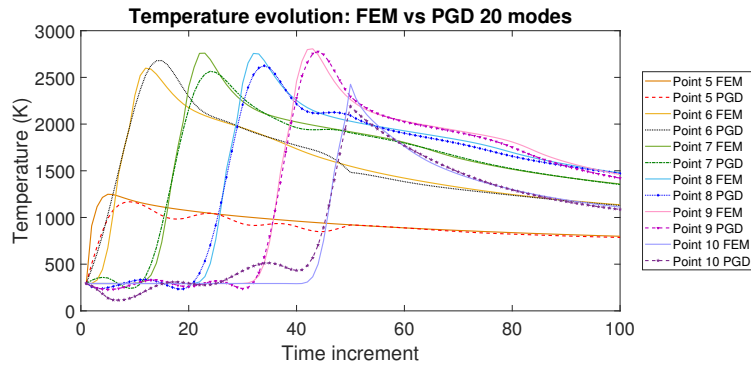


Figure 10: Comparison between FEM with latent heat and FEM without latent heat

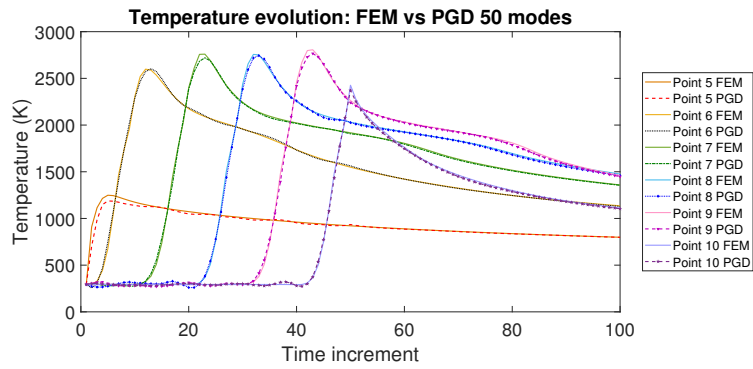


(a) PGD 15 modes, 2 iterations per mode

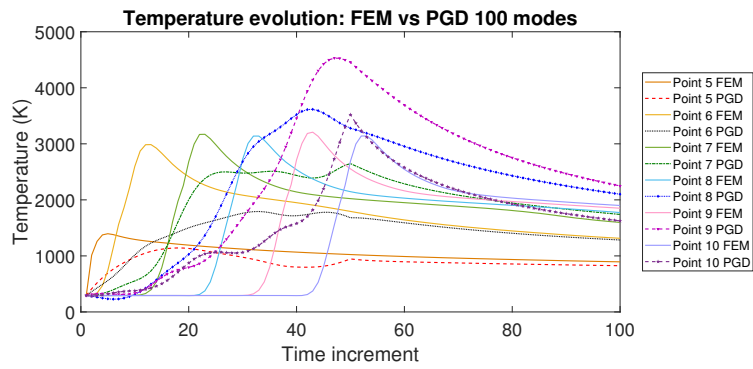


(b) PGD 20 modes, 2 iterations per mode

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



(a) PGD 50 modes, 2 iterations per mode



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

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

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

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

458 Here:

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

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

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

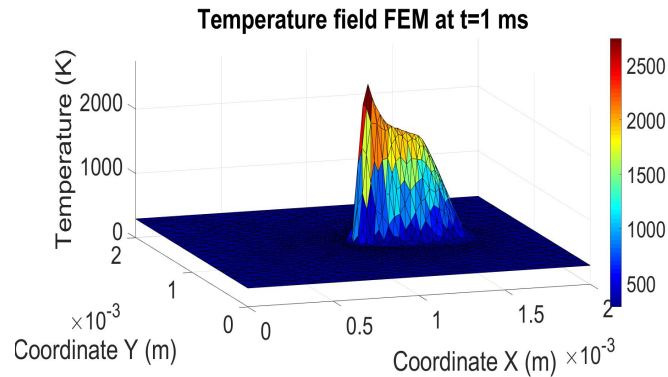
461 is the error for the total duration of the simulation, i.e., the laser on and the
462 cooling (laser off) phases. Notice that the temperature gradients are higher
463 in the laser "on" scenario than in the cooling scenario, meaning that relative
464 global discrepancies between PGD and FEM results 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.

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.

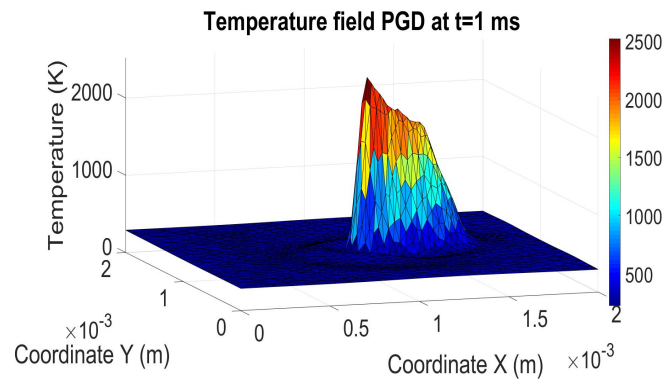
470 Important points can be highlighted from this example. First of all, in
471 contrast with the case of a stationary source, the solution requires more than
472 1 iteration per mode, even when using several modes. For example, using
473 100 modes with 3 iterations in the first mode and 1 iteration in the others

474 (Figure 12b), the result is very different from the FEM answer and totally
475 unacceptable. Nevertheless, when using 50 modes with 2 iterations per mode
476 (Figure 12a), the result accuracy is excellent. In both cases, there are about
477 100 iterations in total, but in the first case, although more modes are used,
478 the result is worse than in the second case. This might seem contradictory
479 with the previous results and with the PGD assumptions. However, in the
480 case of a moving laser, the higher modes have an important contribution
481 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
484 no longer mere corrections, but contribute as importantly to the solution as
485 the lower ones. Since higher modes are very relevant for the solution in this
486 new case, the convergence criterion needs to be more strict in order to obtain
487 an accurate PGD solution. This explains the difference between 50 and 100
488 modes PGD solutions. Besides, it establishes that at least 2 iterations are
489 necessary for each mode to have an acceptable solution. In fact, one can
490 consider that 2 iterations per mode is the ideal mode convergence criterion
491 for this example, and a larger number of iterations could add numerical
492 pollution . Adding an extra mode is again better than adding more iterations
493 per mode.

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.



(a) FEM

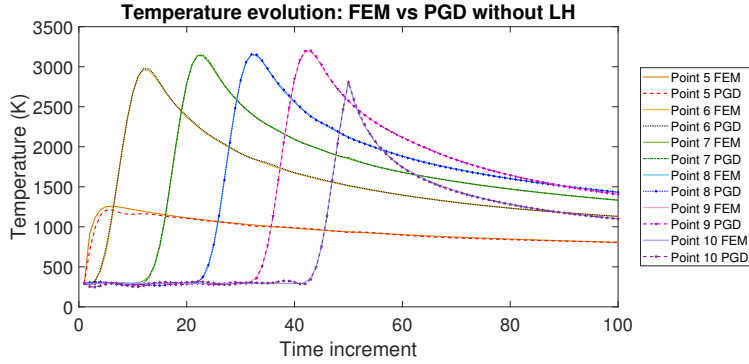


(b) PGD 20 modes 2 iterations per mode

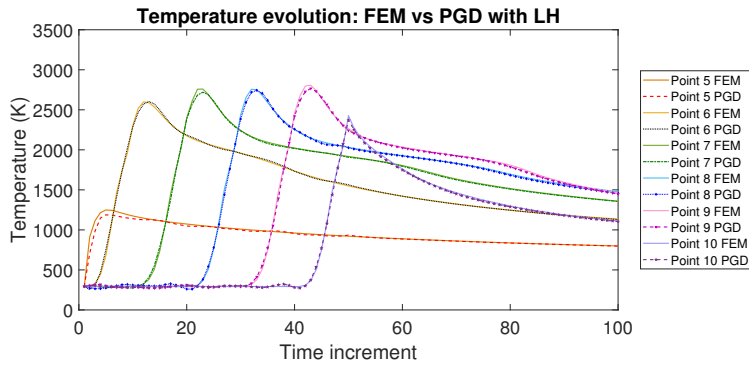
Figure 13: Temperature field in all the domain at $t=1$ ms for FEM and PGD

500 Summarizing the results of Sections 4.3 and 4.2, one can observe the
 501 influence of the latent heat with a moving laser on the solution in Figure 14.

502 Figures 14a and 14b support the verification of PGD, showing it is able
 503 to handle problems with moving source and latent heat, and the larger the
 504 number of modes, the better the solution (here 50 modes and 2 iterations
 505 per mode were used). One can note that the PGD solution without latent
 506 heat is more accurate than the one with latent heat. This is consistent, since
 507 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*

510 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,
 512 by adding a film condition and time and space-dependent Neumann boundary
 513 conditions to the previous example. The notable exception is radiative heat
 514 loss which will be subject of future work.

515 The properties for this problem are the same as in Example 3, so they
 516 can be found in Table 4 and in Figures 9 and 6a. However, it was again
 517 necessary to modify the domain (to be explained later). The patch is now
 518 represented by a 1 mm x 0.1 mm rectangular uniform mesh (this region will
 519 be also called the small patch), with the origin at the bottom left corner and
 520 with triangular elements of size 10^{-5} m, totalizing 1378 degrees of freedom.

521 The source motion is the same as in the previous case: at the beginning of
 522 the simulation ($t=0$), the laser is at point 5 (now located at $(0.85,0.05)$ mm).
 523 Then it starts moving towards point 10, traveling a distance of 0.5 mm with
 524 a constant speed of 0.5 m/s . Once arrived at point 10, the laser is turned
 525 off, and the cooling phenomenon is observed during 1 ms .
 526 The previous description is illustrated in Figure 15.

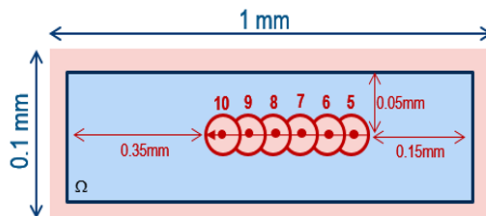


Figure 15: Representative schema of Example 4

527 4.4.1. Neumann Boundary Conditions

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

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

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

549 extract the time and space-dependent Neumann boundary conditions for the
 550 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
 552 Neumann boundary conditions is significant.

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

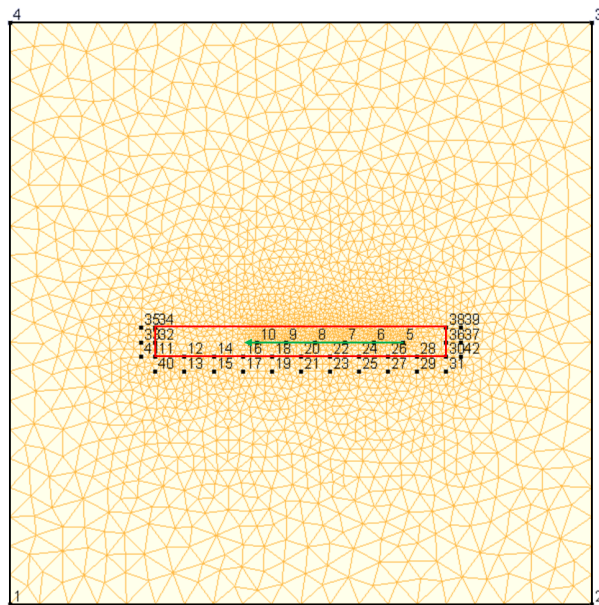


Figure 16: Approach to extract the space and time-dependent Neumann boundary conditions

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

561 4.4.2. Surface convection (film condition)

562 In order to take into account heat exchanges between the model and the
 563 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
 565 treated as a body source rather than as a boundary condition. Its expression

566 is given by:

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

567 where $h= 18 \text{ W/K/m}$ (see [27]) is the heat transfer coefficient for the air-
 568 titanium interaction and $T_{env}= 293 \text{ K}$ 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

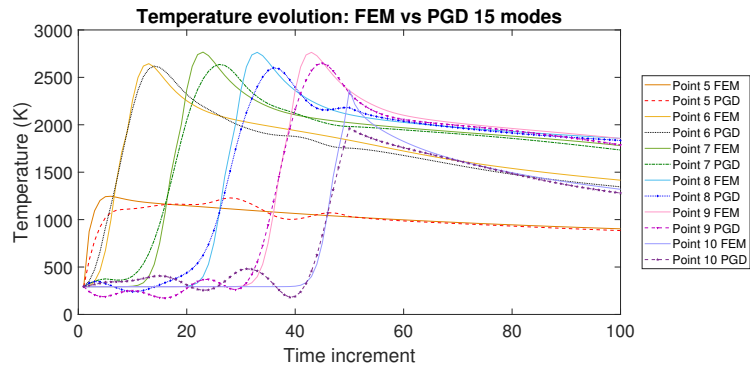
573 The simulation was done for FEM and for PGD with different numbers
 574 of modes (always with 2 iterations per mode). The results are shown in
 575 Figure 17 and in Table 7. Points 5 to 10 were chosen in order to analyze the
 576 temperature behavior. Because the laser crosses these points, the changes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

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

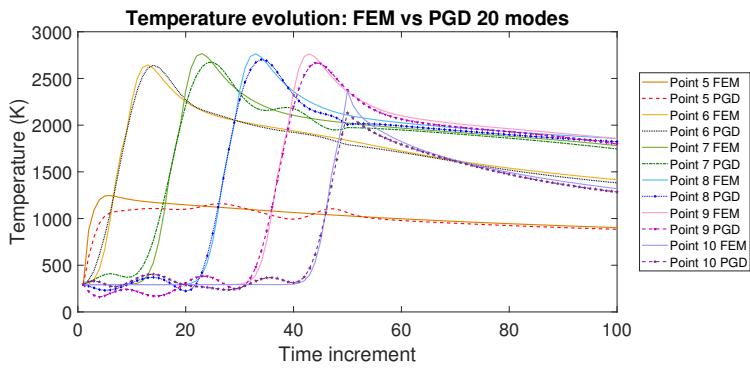
Simulation		Solve					
Type	Modes	Error 1	Error 2	Criterion	Total	Speed-up	Factor
FEM				$Tol_{FEM}=0.0001$	880		
PGD	10	0.0827	0.0519	2 it./mode	20		44.00
PGD	15	0.0427	0.0274	2 it./mode	30		29.33
PGD	20	0.0355	0.0223	2 it./mode	40		22.00
PGD	25	0.0170	0.0121	2 it./mode	50		17.60
PGD	30	0.0147	0.0105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

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

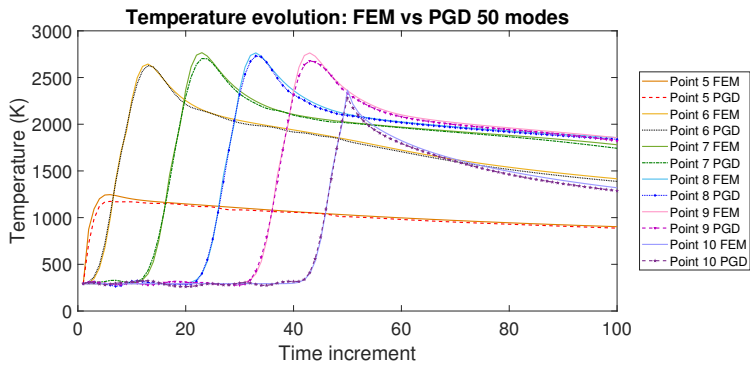
581 As expected, at least 2 iterations are needed per mode, because higher
 582 modes are important to correctly capture the effect of the traveling laser
 583 and time-varying Neumann boundary conditions. The result with 50 modes
 584 (Figure 17c) is extremely accurate, however the performance gain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



(a) PGD 15 modes, 2 iterations per mode



(b) PGD 20 modes, 2 iterations per mode



(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

589 important regions (such as high temperatures or cooling) is acceptable and
590 the number of matrix inversions in this case is reduced by 22 compared to the
591 FEM. As the out-flux represents a considerable percentage of the laser energy,
592 there is a remarkable drop in the temperature when compared to Example 3.
593 However, this does not seem to be a problem for PGD. Adding the time and
594 space-dependent Neumann boundary conditions and the film convection does
595 not change the number of modes necessary for a reasonable PGD response.
596 Previously, with 20 modes and 2 iterations per mode one obtained an error
597 $\epsilon_1 = 0.0299$ and an error $\epsilon_2 = 0.0190$. Thus, although the errors have slightly
598 increased, the choice of 20 modes seems a reasonable compromise. Finally,
599 this example proves that PGD can handle highly non-linear and complex
600 problems.

601 5. Conclusion

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

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

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

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

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