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A priori hyperreduction method: an adaptive approach

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Model reduction methods are usually based on preliminary computations to build the shape function of the reduced order model (ROM) before the computation of the reduced state variables. They are a posteriori approaches. Most of the time these preliminary computations are as complex as the simulation which we want to simplify by the ROM. The reduction method we propose avoids such preliminary computations. It is an a priori approach based on the analysis of some state evolutions, such that all the state evolutions needed to perform the model reduction are described by an approximate ROM. The ROM and the state evolution are simultaneously improved by the method, thanks to an adaptive strategy. Obviously, an initial set of known shape functions can be used to define the ROM to adapt. But it is not necessary. The adaptive procedure includes extensions of the subspace spanned by the shape functions of the ROM and selections of the most relevant shape functions in order to represent the state evolution. The hyperreduction is achieved by selecting a part of the integration points of the finite element model to forecast the evolution of the reduced state variables. Hence both the number of degrees of freedom and the number of integration points are reduced. To perform the adaptive procedure, different computational strategies can be developed. In this paper, we propose an incremental algorithm involving adaptive periods. During these adaptive periods the incremental computation is restarted until a quality criterion is satisfied. This approach is compatible with classical formulations of the equations.

Keywords: Model reduction; Karhunen–Loève expansion; Proper orthogonal decomposition; Krylov subspace; Adaptive strategy; Singular value decomposition; Learning strategy; Hyperreduction

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1. Introduction

The purpose of model reduction methods is to provide few shape functions in order to represent the spatially distributed state of a system. The reduced order models (ROMs) are interesting to reduce the cost of parametric studies on the state evolution of the system [1–4]. Moreover, if we assume that a ROM is convenient to perform a simulation and if the same ROM is used for another simulation corresponding to a modification of the values of the parameter of the system, then the less this modification have influence on the state evolution of the system the better should be the interest of the ROM. Obviously, the simplest way to use a ROM for two different simulations is to use the same shape functions during all the state evolution. Thus the shape functions of a ROM should enable to forecast large evolutions of the state variables.

In this paper, we focus on numerical simulations of problems described by a finite element model, which provides the reference model. The problems we are interested in are non-linear and time dependent thermomechanical problems. The purpose of this paper is not to present an extension of the modal superposition method which is convenient to linear and time independent systems [5]. An analysis of tangent spectrum methods can be found in [6]. For non-linear time dependent problems two main approaches are used the Karhunen–Loève expansion and the balance truncation approach. Interesting overviews of these methods can be found in [7–10]. The main point we want to address is the following: what kind of model reduction method do we need to enable fast influence analysis corresponding to large variations of the parameters of the reference model? This is a key point in the frame work of optimization of thermomechanical systems. The answer we propose is an adaptive strategy. The method we are developing provides an estimated state evolution and builds an adapted ROM to perform this estimation.

The tangent spectrum approaches and the Karhunen–Loève one have a common pattern: they are a posteriori approaches. The shape function of the ROM is built before the computation of the reduced state variables thanks to preliminary problems. Moreover, the complexity of these problems and the complexity of the reference problem are quite the same. In case of modal approaches, an eigenproblem involving all the degrees of freedom of the reference model has to be solved in order to get the shape functions of the ROM. In case of the Karhunen–Loève expansion several state evolutions must be forecast thanks to the full reference model with different values of system parameters. Then a signal processing [11] of all the forecast state evolutions allows to defined shape functions corresponding to the most significant events involved in these evolutions.

The adaptive strategy we propose allows to avoid the preliminary construction of the shape functions before the computation of the reduced state variables. It is an extension of the Karhunen–Loève expansion to obtain an a priori approach. Obviously, an initial set of known shape functions can be used, but it is not necessary. All the state evolutions needed to perform the model reduction are described by approximate ROMs. The adaptive procedure includes extensions of the subspace spanned by the shape functions of the ROM and selections of the most significant shape functions in order to represent the state evolution. These selections are obtained by the Karhunen–Loève expansion applied on the reduced state variables.

Finally, the classical Galerkin formulation is not the best way to define some governing equations that the reduced state variables must satisfy. The Garlerkin procedure provides orthogonality conditions that must be fulfilled by the residuals of the balance conditions of the reference model. But for non-linear time dependent problems no orthogonal condition has a strong physical meaning. The reason is that there is no unique definition of an inner product between two state evolutions. Otherwise, in the framework of the control of complex systems, it is sufficient to observe only few state variables for the automatic control of a system. The choice of control variables leads to the study of observability criterion [12] and balanced truncation approaches in the framework of model reduction methods [8,9]. The same kind of control variables are also used to study the correlation between experimental eigenmodes and computed eigenmodes. In such cases, the inner products are defined only on a part of the state variables of the system. The choice of the control variables among the state variables of the reference problem and the Galerkin projection leads to

the hyperreduction. We then obtain a number of governing equation equal to the number of the reduced state variables. But only the integration points connected to the control variables have a contribution in these governing equations. So, both the number of degrees of freedom and the number of integration points are reduced to forecast the state evolution.

Despite the a priori hyperreduction method (APHR method) can be applied to various kind of non-linear problems we illustrate its implementation with a simple non-linear thermal problem. Different ROM adaptive strategies can be developed with the APHR method. The common items of such strategies are:

- a ROM always defined over the entire time interval;
- an extension of the subspace spanned by the shape functions of the ROM;
- a selection of shape functions based on a Karhunen–Loève expansion of the evolution of reduced state variables;
- and a formulation of balance equations restricted to few control variables in order to compute the reduced state variables.

The simplest way to present the strategy is to consider that no ROM is known to initialize the adaptive strategy. A general formulation of the non-linear time dependent problems is chosen to describe the APHR method. An example of such problem, a transient thermal problem, allows to illustrate the capabilities of the reduction method we proposed. After some examples of profits in terms of floating point operations (FLOPs), a learning strategy is presented. This strategy corresponds to the previous strategy used with a previously identified ROM to initialize the adaptive procedure. Other examples of profits illustrate the interest of this learning strategy.

2. Finite element model and reduced state variables

2.1. The formulation of the reference model

The purpose of this section is to define the equations of the reference model. In the framework of thermomechanic simulations, the state variable s could be a displacement field or a temperature field defined over the structure Ω. The finite element method allows to describe this state variable thanks to shape functions N_i and nodal degrees of freedom q_i such that:

$$s(x, t) = \sum_{i=1}^{i=\tilde{n}} N_i(x)\, q_i(t) \quad \forall x \in \Omega, \ \forall t. \tag{1}$$

The physical meaning of the shape function N_i is quite poor. The state evolution is described by the value of the degrees of freedom at different time instants $t_j \in \{t_1,\ldots,t_m\}$ such that:

$$q_i(t) = q_i(t_j)\,\frac{t_{j+1} - t}{t_{j+1} - t_j} + q_i(t_{j+1})\,\frac{t - t_j}{t_{j+1} - t_j}. \tag{2}$$

A column $\underline{q}_j$ of state variables at the time instant t_j can be define such that the ith component of $\underline{q}_j$ is $q_i(t_j)$. Let us assume that a numerical scheme is used for the time integration of the balance equations. Then the following formulation of the balance conditions is obtained:

$$\underline{q}_1 = q_{\text{ini}}, \tag{3}$$

$$\underline{F}_{\text{int}}\left(\underline{q}_{j+1}, \underline{q}_j\right) = \underline{F}_{\text{ext}}\left(\underline{q}_{j+1}, \underline{q}_j, t_{j+1}\right) \quad \forall j = 1 \ldots m-1, \tag{4}$$

$\underline{F}_{\text{int}}$ corresponds to the Galerkin formulation of the internal generalized forces and $\underline{F}_{\text{ext}}$ corresponds to the loading and the boundary conditions applied on the structure Ω. $\underline{F}_{\text{int}}$, $\underline{F}_{\text{ext}}$ and $\underline{q}$ have the same size. Each line of the system of Eq. (4) corresponds to a local balance condition. A step by step approach is used: we forecast $\underline{q}_{j+1}$ for a known $\underline{q}_j$.

Each current ROM considered in this paper is defined over all the time interval. The prediction $(\underline{q}_j^{(n)})_{j=1\ldots m}$ is the one obtained with the nth ROM proposed by the reduction method. If an implicit and iterative algorithm is used to resolve (4), we only consider the last result obtained by this iterative algorithm. This iterative algorithm could be a fixed point algorithm, a Newton algorithm, an Usawa algorithm or a LATIN one. The way the balance conditions are fulfilled can be checked with the residual $\underline{R}_{j+1}(\underline{q}_{j+1}^{(n)})$ defined by:

$$\underline{R}_{j+1}\left(\underline{q}_{j+1}^{(n)}\right) = \underline{F}_{\text{int}}\left(\underline{q}_{j+1}^{(n)}, \underline{q}_j^{(n)}\right) - \underline{F}_{\text{ext}}\left(\underline{q}_{j+1}^{(n)}, \underline{q}_j^{(n)}, t_{j+1}\right). \tag{5}$$

An estimated state evolution $(\underline{q}_j^{(n)})_{j=1\ldots m}$ is convenient if the following quality criterion is satisfied:

$$\left\|\underline{R}_{j+1}\left(\underline{q}_{j+1}^{(n)}\right)\right\| < \epsilon_R \max_{p\leq j}\left(\left\|\underline{F}_{\text{ext}}\left(\underline{q}_{j+1}^{(n)}, \underline{q}_j^{(n)}, t_{j+1}\right)\right\|\right) \quad \forall j = 1\ldots m-1, \tag{6}$$

where the norm $\|\cdot\|$ is the euclidian norm such that $\|\underline{q}\|^2 = \underline{q}^{\mathrm{T}}\underline{q}$. If a tangent matrix $\underline{\underline{K}}_{j+1}$ can be defined the following property is fulfilled:

$$\lim_{\epsilon\to 0} \underline{R}_{j+1}\left(\underline{q}_{j+1}^{(n)} + \epsilon\,\delta\underline{q}\right) = \underline{R}_{j+1}\left(\underline{q}_{j+1}^{(n)}\right) + \epsilon\,\underline{\underline{K}}_{j+1}\,\delta\underline{q} \quad \forall\delta\underline{q}. \tag{7}$$

The shape functions $(\phi_k^{(n)})_{k=1\ldots r}$ of the nth ROM are deduced from the shape functions of the reference model thanks to a basis reduction matrix $\underline{\underline{A}}^{(n)}$. The kth shape function $\phi_k^{(n)}$ is a field of the same kind as s and it is defined by the kth column of $\underline{\underline{A}}^{(n)}$ such that:

$$\phi_k^{(n)}(x) = \sum_{i=1}^{i=\widetilde{n}} N_i(x)\,A_{ik}^{(n)}. \tag{8}$$

The variables $a_k^{(n)}(t)$ are the reduced state variables of the reduced problem such that:

$$q_i^{(n)}(t) = \sum_{k=1}^{k=r} A_{ik}^{(n)}\,a_k^{(n)}(t), \tag{9}$$

which leads to:

$$\underline{q}_j^{(n)} = \underline{\underline{A}}^{(n)}\,\underline{a}_j^{(n)} \quad \forall j. \tag{10}$$

Since the current ROM is always defined over the entire time interval it is easy to define a prediction over the entire time interval even if the incremental computation of the state evolution has been done only over the time interval $[t_1, t_{j+1}]$. To do so we can choose:

$$\underline{a}_p^{(n)} = \underline{a}_{j+1}^{(n)} \quad \forall p > j+1. \tag{11}$$

Obviously it is not the best estimation of the state evolution.

2.2. A simple transient thermal problem

To illustrate the implementation of the APHR method, a simple transient thermal problem is studied. The temperature is the state variable. We consider a bar with a fiber inside (Fig. 1). On the face Γ_c of the bar (Fig. 1) the heat transfer is governed by conductivity coefficient $h = 800$ and a given temperature

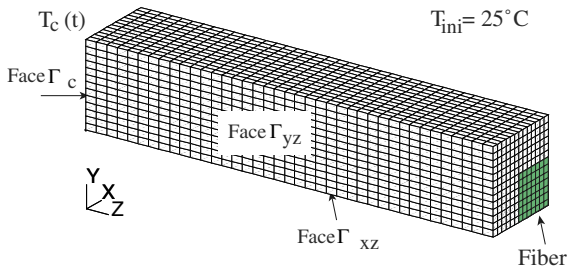

Fig. 1. Transient thermal problem: a bar with a fiber (7840 FE degrees of freedom and 6691 elements).

$T_c(t)$. On the other faces of the bar the heat flux is equal to zero. Around the fiber the material has properties close to the properties of steel 42CrMo4. The thermal capacity C and the conductivity k are temperature dependent.

The time interval is regularly split into 50 time steps. The time integration scheme is the implicit forward Euler scheme. The elements chosen for the mesh are hexagonal ones with eight nodes and one integration point. The column $\underline{q}$ contains the nodal temperatures of the considered mesh.

Thanks to a classical Galerkin projection we can define $\underline{F}_{\text{int}}$ and $\underline{F}_{\text{ext}}$ such that:

$$\underline{q}^{*\,\mathrm{T}}\,\underline{F}_{\text{int}}\left(\underline{q}_{j+1},\,\underline{q}_j\right) = \int_{\Omega} T^*\,\rho\,C(T)\,\dot{T}\,\mathrm{d}\Omega + \int_{\Omega} \overrightarrow{Grad}(T^*)\,k(T)\,\overrightarrow{Grad}(T)\,\mathrm{d}\Omega \quad \forall \underline{q}^*, \tag{12}$$

$$\underline{q}^{*\,\mathrm{T}}\,\underline{F}_{\text{ext}}\left(\underline{q}_{j+1},\,\underline{q}_j,\,t_{j+1}\right) = -\int_{\Gamma_c} T^*\,h\,(T - T_c)\,\mathrm{d}\Gamma \quad \forall \underline{q}^* \tag{13}$$

with $t = t_{j+1}$, $T(x,t) = \sum_{i=1}^{i=n} N_i(x)\,q_i(t)$ and $T^*(x) = \sum_{i=1}^{i=n} N_i(x)\,q_i^*$.

3. An adaptive strategy

3.1. From the mesh adaptivity to the ROM adaptivity

The adaptive strategy must precise when the state variables should be computed, when the quality of the forecast state should be checked and when the model should be adapted. The ROM adaptation is a shape function adaptation as well as a mesh adaptation. There are various adaptive strategies proposed in the framework of mesh adaptivity in order to master the quality of the finite element shape functions $N_i(x)$. The same strategies can be applied to perform the ROM adaptivity in order to master the quality of the shape functions ϕ_k. Since the finite element model remains unchanged during the reduction procedure, we only adapt the basis reduction matrix $\underline{\underline{A}}$.

In the framework of adaptive strategies, only a posteriori approaches are used to check the quality of shape functions. This means that the quality criterion is applied on a known state evolution. This state evolution can be forecast over several time steps $[t_\alpha, t_{\alpha+\beta}]$ before the quality is checked. If the quality of the estimation of the state evolution is convenient the step by step computation of the state variables can be pursued without any adaptation. But, if it is not the case, t_α is the beginning of an adaptation period and different decisions are possible. Each choice leads to define an adaptive strategy (Fig. 2).

- Strategy Str1: β is small, the shape functions are adapted, the state description at time instant $t_{\alpha+\beta}$ is updated and the step by step computation is pursued on $t_{\alpha+\beta+1}$.

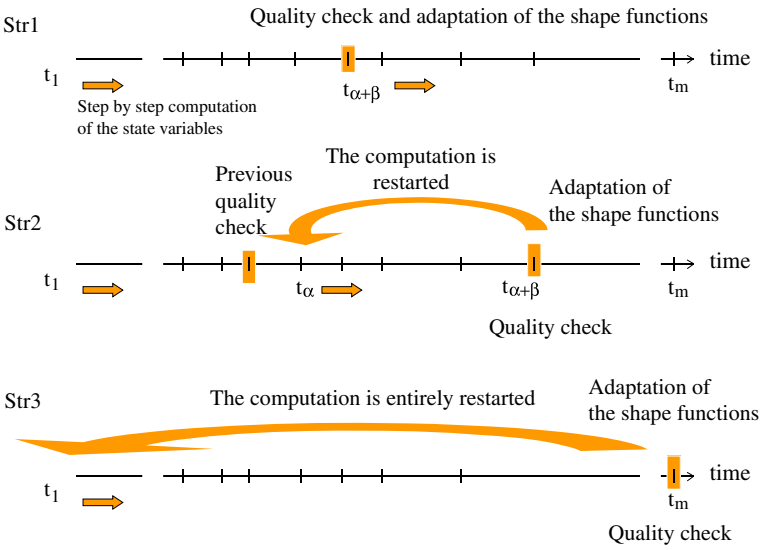

Fig. 2. Adaptive strategies.

- Strategy Str2: whatever β is, the shape functions are adapted, the state description at time instant $t_{\alpha-1}$ is updated and the step by step computation is restarted on $t = t_\alpha$;
- Strategy Str3: $\alpha = 1$ and $\beta = m$, the shape functions are adapted and the step by step computation is restarted on $t = t_1$.

The strategy Str3 is implemented in [13] for explicit computations. It is also very convenient for non-incremental computations thanks to the LATIN method [14]. An example of mesh adaptivity procedure based on the LATIN method and the strategy Str3 can be found in [15] for viscoplastic problems. As shown in [16] the LATIN method can be considered as an a priori method for model reduction which can be optimized thanks to the Karhunen–Loève expansion. Moreover, the hyperreduction can be applied on such an approach. But an important drawback of this kind of non-incremental approach is the formulation of the balance conditions, which is not a classical one. So the tangent stiffness matrix does not correspond to tangent stiffness matrix of the classical incremental formulation.

The first strategy is convenient for explicit time integration scheme. A recent example can be found in [17] for transformations involving large elastoplastic deformations with damage (simulation of orthogonal cutting). An other example of implementation of such a strategy can be found in [18]. It is applied to strain localization phenomena with an ALE analysis and an explicit dynamics scheme. But it does not allow to master the quality of the forecast state evolution because some errors at time instant $t_{\alpha+\beta}$ could not be reduced by any adaptation of the shape functions on further time instants.

Thanks to the strategy Str2 we tend to really master the quality of the shape functions as β decreases. We choose this strategy to master the quality of the ROM. Between two quality check the state evolution is forecast thanks to the current ROM and thanks to reduced number of integration points. To reduce the number of computation of the residuals (5) on all the integration points, β should be as large as possible. In practice, for the first computation of the reduced state variables during the current adaptation period $[t_\alpha, t_{\alpha+\beta}]$, we choose $\beta = 4$. Then the computation is restarted for the first time with β changed into 2. And after $\beta = 0$ until the quality criterion (6) is fulfilled at $j + 1 = \alpha + \beta$. For the example of thermal problem, two convergence curves of residuals are shown in Fig. 3:

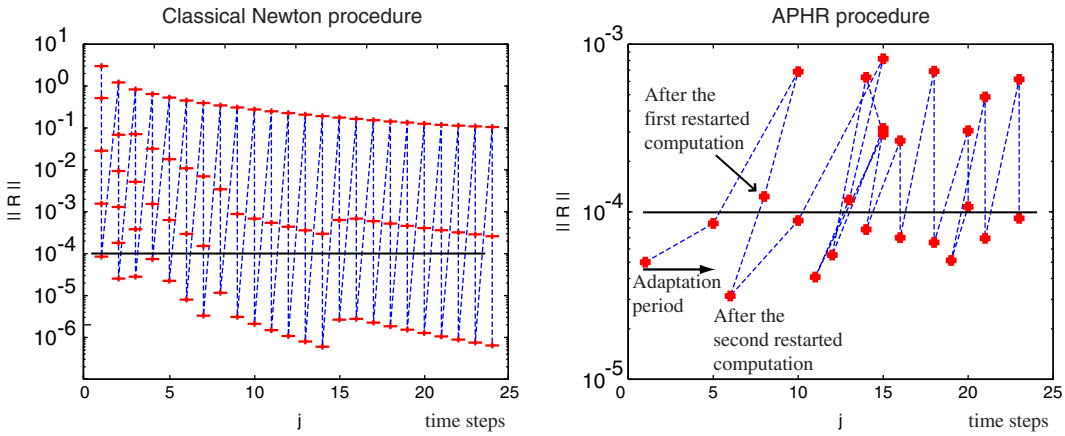

Fig. 3. Examples of computations of the residuals of all the balance conditions of the reference model.

- one obtained by a classical Newton–Raphson incremental resolution of the finite element problem;
- and an other one obtained by the APHR method with very convenient initial shape functions.

During the APHR resolution the residuals of all the balance equations are checked only for the quality control. Thanks to the adaptation of the shape functions of the ROM these residuals decrease.

When the shape functions of the ROM are adapted such that $\underline{\underline{A}}^{(n)}$ becomes $\underline{\underline{A}}^{(n+1)}$, then we can define an intermediate update of the reduced state variables $\underline{a}_j^{(n+1/2)}$ such that the estimation of the state evolution tends to be unchanged. This intermediate update is not the best one according to the equations of the reference problem. In the framework of mesh adaptation it corresponds to the projection of the state variables defined on the old mesh, onto the new adapted mesh. If the computation is restarted on the interval $[t_\alpha, t_{\alpha+\beta}]$ then we obtain new updated reduced state variables $\underline{a}_j^{(n+1)}$ for any j such that $\alpha \leq j \leq \alpha + \beta$. But over $[t_1, t_{\alpha-1}]$ the updated reduced state variables $\underline{a}_j^{(n+1)}$ are equal to the intermediate ones $\underline{a}_j^{(n+1/2)}$. If the computation is not restarted then: $\underline{a}_j^{(n+1)} = \underline{a}_j^{(n+1/2)}\ \forall j \leqslant \alpha + \beta$.

3.2. The subspace expansion by Krylov subspaces

A Krylov subspace is defined by a matrix, a vector and the size of this subspace. Usually, the vector and the matrix. respectively, correspond to a residual of balance equations and a tangent stiffness matrix. Let us denote $\underline{Y}_1$ this vector and $\underline{\underline{K}}$ the matrix. A Krylov subspace is spanned by the vectors $(\underline{Y}_i)_{i=1\ldots\nu}$ such that $\underline{Y}_i = \underline{\underline{K}}\,\underline{Y}_{i-1}$ for $i > 1$.

We choose:

$$\underline{Y}_1 = \underline{R}_{j+1}\left(\underline{q}_{j+1}^{(n)}\right). \tag{14}$$

And, as proposed in [19,20], the following difference provides the vectors $\underline{Y}_{i+1}$ with a matrix-free approach:

$$\underline{Y}_{i+1} = \underline{R}_{j+1}\left(\underline{q}_{j+1}^{(n)} + \epsilon_Y \frac{\left\|\underline{q}_{j+1}^{(n)}\right\|}{\|\underline{Y}_i\|}\underline{Y}_i\right) - \underline{R}_{j+1}\left(\underline{q}_{j+1}^{(n)}\right). \tag{15}$$

If a tangent stiffness matrix exists and if ϵ_Y is small enough, then the vectors $(\underline{Y}_i)_{i=1\ldots\nu}$ tend to span a Krylov subspace. In practice, we choose $\epsilon_Y = 0.01$ and $\nu = 3$.

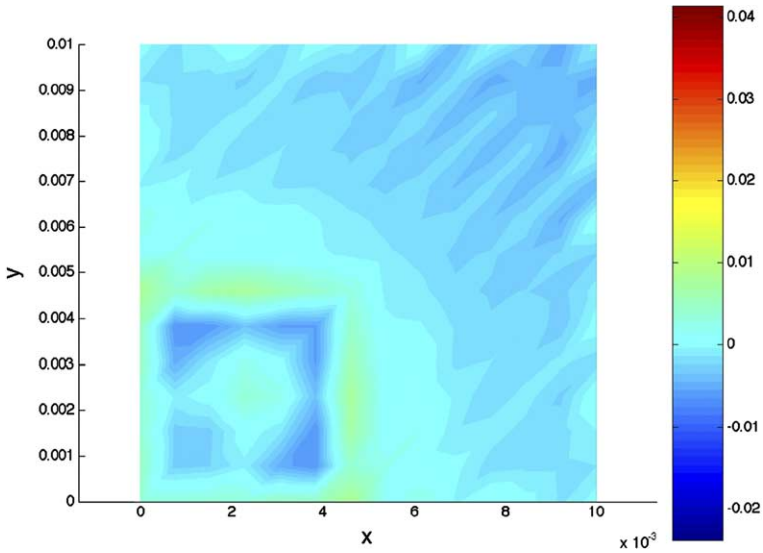

Fig. 4. Example of a residual field on the face Γ_c of Ω for the thermal problem.

The shape functions corresponding to the vectors $(\underline{Y}_i)_{i=1\ldots v}$ are rarely smooth. In Fig. 4 an example of such a shape function is shown in the case of the 3D transient thermal problem. The state evolution we want to forecast with the ROM is smoother than the shape functions corresponding to the vectors $(\underline{Y}_i)_{i=1\ldots v}$. So, how can we obtain smoother shape functions?

Krylov subspaces are widely used for reduction methods. But none of them directly uses the vectors $(\underline{Y}_i)_{i=1\ldots v}$ to define the shape functions. For example, in the case of the modal superposition methods where the eigenmodes are computed by the Lanczos algorithm [21], the shape functions are the eigenmodes. And these shape functions are defined thanks to Krylov subspaces according to the Lanczos algorithm. An example of such an approach applied to linear or non-linear problems can be found in [22]. In the framework of non-linear time dependent problems, some extended conjugate gradient methods were proposed to represent the forecast state evolution by a superposition of shape functions defined thanks to Krylov subspaces [20,23]. For these methods too, the shape functions do not directly correspond to the vectors defining the Krylov subspaces. An orthogonalization procedure is used to build them. In other cases of reduction method the shape functions are defined by some Arnoldi vectors [24,25].

In the framework of non-linear problems we do not expect any orthogonal property, or any uncoupled governing equations. The reduced state variables can be forecast even if the reduced governing equations are coupled. So, even if the vectors $(\underline{Y}_i)_{i=1\ldots v}$ are not smooth enough, we propose to use them directly to define new shape functions for the adapted ROM. We expect from the Karhunen–Loève expansion to improve the shape of theses shape functions.

Few remarks:

- If the vectors $(\underline{Y}_i)_{i=1\ldots v}$ are not independent we recommend to use $v = 1$. We have never met this problem yet with the APHR method.
- All the integration points are needed to compute each residual but this subspace creation is highly parallelizable [23].
- The Krylov subspaces allow to take into account coupling terms in an easy way, even if we consider multiphysic simulations. In this case the residuals define multiphysic shape functions.

- The incremental approach based on Krylov subspaces proposed in [23,20] are more computational methods than model reduction methods, and they are proposed as computational methods.

3.3. The selection of the most relevant shape functions

The Karhunen–Loève expansion [26,27], named also the proper orthogonal decomposition [1], is widely used for a posteriori model reduction of non-linear time dependent problems. The first works about this approach deal with weather prediction [28] thanks to a statistical analysis of experimental data (pressures and temperatures). The most popular approach seems to be the snapshot POD proposed in [29] because it is based on smaller eigenproblem than the classical Karhunen–Loève expansion.

The main advantage of the Karhunen–Loève expansion is to provide shape functions corresponding to the main events contained in known state evolutions. Usually the state evolutions used for the Karhunen–Loève expansion are computed thanks to the reference model with different values of parameters. Let us note $s_i(x,t)$ the state variable corresponding to the ith study of the influence of some parameters. Let us consider an inner product of two fields $u(M)$ and $v(M)$ defined over Ω: $\langle u,v\rangle$. Thanks to this inner product the Karhunen–Loève expansion can be defined by a problem of optimization where a field ϕ must maximize its projection $\lambda(\phi)$ on all the fields spanned by the state variables $s_i(x,t)$. $\lambda(\phi)$ is defined such that:

$$\lambda(\phi) = \sum_i \int_0^{t_f} \frac{\langle s_i,\, \phi\rangle^2}{\langle \phi, \phi\rangle}\, \mathrm{d}t. \tag{16}$$

This optimization problem leads to an eigenproblem. There are several solutions: the empirical eigenvectors ϕ_k. To each ϕ_k corresponds the eigenvalue $\lambda_k = \lambda(\phi_k)$. The empirical eigenvectors ϕ_k are sorted according to the magnitude of the projections λ_k such that: $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_k \cdots$. An approximate state $\widehat{s}_i(x,\, t)$ is provided with a truncated decomposition involving the first empirical eigenvectors such that:

$$\widehat{s}_i(x,\, t) = \Sigma_{k=1}^{k=\eta} \alpha_{k\,i}(t)\, \phi_k(x) \quad \text{with} \quad \alpha_{k\,i}(t) = \frac{\langle s_i,\, \phi_k\rangle}{\langle \phi_k,\, \phi_k\rangle}. \tag{17}$$

The higher is η, the better is the approximation of $s_i(x,\, t)$ and the distance between $\widehat{s}_i$ and s_i can be estimated by $\sqrt{\sum_{k=\eta+1}^{k=\inf} \lambda_k}$.

To perform other state predictions corresponding to unstudied values of the parameters a ROM is built by selecting a set of first empirical eigenvectors $(\phi_k)_{k=1\ldots\eta}$ as shape functions of the ROM. The smaller the difference between the new values of the parameters, and the ones used for the Karhunen–Loève expansion is, the better the quality of the ROM should be. But this method is not convenient for any adaptation of a known ROM to any modification of some parameters of the reference model. Moreover, it is based on several full finite element computations.

According to us, an approximate ROM can provide informations on what is significant on a state evolution. Then the Karhunen–Loève expansion can be applied on the reduced state variables of such a ROM. So, for the APHR method, the state variables we propose to consider are the reduced state variables of the current ROM: $\underline{a}^{(n)}$. Then the Rayleigh quotient we use is:

$$\lambda(\underline{\Phi}) = \sum_{j=1}^{j=m} \frac{\left(\underline{a}_j^{(n)\,\mathrm{T}}\, \underline{\Phi}\right)^2}{\underline{\Phi}^{\mathrm{T}}\, \underline{\Phi}}. \tag{18}$$

The eigenproblem is the following:

$$\underline{\underline{H}}^{(n)}\, \underline{\Phi}_k^{(n)} = \lambda_k^{(n)}\, \underline{\Phi}_k^{(n)}, \tag{19}$$

where $\underline{\underline{H}}^{(n)}$ is the following covariance matrix:

$$\underline{\underline{H}}^{(n)} = \sum_{j=1}^{j=m} \underline{a}_j^{(n)} \, \underline{a}_j^{(n)\,\mathrm{T}}. \tag{20}$$

The empirical eigenvectors $\underline{\Phi}_k^{(n)}$ belong to the space of the reduced state variables of the current ROM. A set of first empirical eigenvectors defines a selection matrix $\underline{\underline{V}}^{(n)}$ such that:

$$\underline{\underline{V}}^{(n)} = \left[\underline{\Phi}_1^{(n)}, \underline{\Phi}_2^{(n)}, \ldots, \underline{\Phi}_\eta^{(n)}\right]. \tag{21}$$

To get the main significant part of the empirical eigenvectors, η, is such that:

$$\lambda_\eta^{(n)} \geqslant 10^{-8} \, \lambda_1^{(n)}. \tag{22}$$

The selection matrix defines a subspace of the space of the reduced state variables. The shape functions corresponding to this subspace are obtained by the following product: $\underline{\underline{A}}^{(n)} \, \underline{\underline{V}}^{(n)}$. We think that thanks to the Karhunen–Loève expansion these shape functions have a better physical meaning than the shape function of the current ROM.

Few remarks:

- As for the snapshot POD the size of the covariance matrix is small. It is less than 100 in practice.
- Obviously, since $\underline{\underline{H}}^{(n)}$ is a real symmetric matrix, the matrix $\underline{\underline{V}}^{(n)\,T}\underline{\underline{V}}^{(n)}$ is diagonal.
- Thanks to the link between the eigenvectors of the covariance matrix $\underline{\underline{H}}$ and the singular value decomposition of the state matrix $[\underline{a}_1^{(n)}, \underline{a}_2^{(n)}, \ldots, \underline{a}_m^{(n)}]$ [30], it can be proved that η is lower than m which is assumed to be lower than the number of the finite element degrees of freedom. So, the size of the ROM depends on the complexity of the state evolution and does not depend on number of degrees of freedom of the reference model (if $\tilde{n}$ is higher than m).
- The correlations between the shape functions of the ROM are not explicitly taken into account with the proposed Karhunen–Loève expansion, but the computation of the reduced state variables takes into account the non-linear coupling between these shape functions.

3.4. Adaptation of the shape functions

The adapted ROM is defined thanks to the new vectors $(\underline{Y}_i)_{i=1\ldots v}$ and thanks to the selection matrix $\underline{\underline{V}}^{(n)}$ such that:

$$\underline{\underline{A}}^{(n+1)} = \left[\underline{\underline{A}}^{(n)} \, \underline{\underline{V}}^{(n)}, \frac{1}{\|\underline{Y}_1\|} \underline{Y}_1, \ldots, \frac{1}{\|\underline{Y}_v\|} \underline{Y}_v\right]. \tag{23}$$

The intermediate updated variables are chosen such that each contribution of the new shape functions $(\frac{1}{\|\underline{Y}_k\|} \underline{Y}_k)_{k=1..v}$ is equal to zero. This way, we obtain:

$$\underline{a}_j^{(n+1/2)} = \begin{bmatrix} \left(\underline{\underline{V}}^{(n)\,\mathrm{T}} \underline{\underline{V}}^{(n)}\right)^{-1} \underline{\underline{V}}^{(n)\,\mathrm{T}} \underline{a}_j^{(n)} \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{24}$$

The norms of the empirical eigenvectors are such that the norms of the columns of the matrix $\underline{\underline{A}}^{(n+1)}$ remain equal to 1. The vectors $(\underline{Y}_i)_{i=1\ldots v}$ are going to be modified by the next selection matrix $\underline{\underline{V}}^{(n+1)}$ of the next ROM adaptation.

4. The hyperreduction of the balance conditions

The purpose of this section is to define control variables for the formulation of the governing equations of the ROM. According to the Galerkin projection, the balance equations can be formulated with test functions corresponding to test columns $\underline{q}^*$ such that:

$$\underline{q}^{*\,\mathrm{T}}\,\underline{F}_{\mathrm{int}}\left(\underline{q}_{j+1},\underline{q}_j\right) = \underline{q}^{*\,\mathrm{T}}\,\underline{F}_{\mathrm{ext}}\left(\underline{q}_{j+1},\,\underline{q}_j,\,t_{j+1}\right) \quad \forall \underline{q}^*,\ \ \forall j = 1\ldots m-1. \tag{25}$$

For the current ROM the Galerkin projection provides the following balance equations:

$$\underline{\underline{A}}^{(n)\,\mathrm{T}}\,\underline{F}_{\mathrm{int}}\left(\underline{\underline{A}}^{(n)}\,\underline{a}^{(n)}_{j+1},\,\underline{\underline{A}}^{(n)}\,\underline{a}^{(n)}_{j}\right) = \underline{\underline{A}}^{(n)\,\mathrm{T}}\,\underline{F}_{\mathrm{ext}}\left(\underline{\underline{A}}^{(n)}\,\underline{a}^{(n)}_{j+1},\,\underline{\underline{A}}^{(n)}\,\underline{a}^{(n)}_{j},\,t_{j+1}\right) \quad \forall j = 1\ldots m-1. \tag{26}$$

This means that the residuals $\underline{R}_{j+1}(\underline{\underline{A}}^{(n)}\,\underline{a}^{(n)}_{j+1})$ must be orthogonal to the space spanned by the shape functions of the current ROM. Obviously all the balance conditions are not checked if the number of shape functions of the ROM is lower than the number of shape functions of the reference model. Moreover, each shape function of the ROM is a global field defined over all the structure Ω. So to a line of the system of equations (26) corresponds a global balance equation. But we want to satisfy all the local balance conditions of the reference problem according to the criterion (6). This is possible only if the shape functions of the ROM are convenient ones.

In the frame work of linear problems with a symmetric definite and positive matrix, the Galerkin projection corresponds to an optimization of the reduced state variables according to a global energy criterion. And this optimization leads to an orthogonal property. But no orthogonal condition has a strong physical meaning for the problems we are interested in. The same lack of orthogonal property of global fields appears in the frame work of correlation studies between an experimental modal analysis and an analytical modal analysis. Let us consider a linear mechanical system. Two analytical eigenmodes $\underline{\Psi}_k$ and $\underline{\Psi}_p$ are orthogonal vectors such that:

$$\underline{\Psi}_k^{\mathrm{T}}\,\underline{\underline{M}}\,\underline{\Psi}_p = \delta_{k\,p}, \tag{27}$$

where $\underline{\underline{M}}$ is the mass matrix of the finite element model of the mechanical system and $\delta_{k\,p}$ is the delta Kronecker. The experimental analysis leads to define the experimental values corresponding to the degrees of freedom of any experimental eigenmode k: $\underline{\Psi}_{k\,\mathrm{exp}}$. Let us imagine that sensors allow to observe all the accelerations corresponding to the degrees of freedom of the model. Then the modal assurance criteria (MAC) [31] based on the mass matrix $\underline{\underline{M}}$ is very convenient to perform the correlation analysis, such that:

$$\mathrm{MAC}_{k\,p} = \underline{\Psi}_{k\,\mathrm{exp}}^{\mathrm{T}}\,\underline{\underline{M}}\,\underline{\Psi}_p. \tag{28}$$

But in practice it is not possible to observe the acceleration corresponding to all the degrees of freedom of the finite element model. Let us assume that a restricted part of these degrees of freedom is observed. This observed part, $\underline{\widehat{\Psi}}_{k\,\mathrm{exp}}$, is defined by a matrix $\underline{\underline{P}}$ such that:

$$\underline{\widehat{\Psi}}_{k\,\mathrm{exp}} = \underline{\underline{P}}\,\underline{\Psi}_{k\,\mathrm{exp}}. \tag{29}$$

Then, in practice, the MAC can be:

$$\widehat{\mathrm{MAC}}_{k\,p} = \frac{1}{\left\|\underline{\underline{P}}\,\underline{\Psi}_{k\,\mathrm{exp}}\right\|\,\left\|\underline{\underline{P}}\,\underline{\Psi}_p\right\|}\,\underline{\Psi}_{k\,\mathrm{exp}}^{\mathrm{T}}\,\underline{\underline{P}}^{\mathrm{T}}\,\underline{\underline{P}}\,\underline{\Psi}_p. \tag{30}$$

If there are enough sensors at convenient places, then the correlation analysis can be achieved [32]. The more $|\widehat{MAC}_{k\,p}|$ is close to 1, the better the correlation is. As a conclusion, the inner product is defined by the matrix $\underline{\underline{P}}^{\mathrm{T}}\,\underline{\underline{P}}$ instead of the mass matrix. Moreover, the key point of this approach is not the orthogonality condition but concerns the recognition of the shape of global fields thanks to few control variables.

For the non-linear problems, we are interested in, we can consider that we must "recognize" the state of the system thanks to a linear combination of global shape functions according to balance conditions. So, we choose to check only few balance equations to find the reduced state variables of the current ROM. These checked equations are obtained by a matrix $\underline{\underline{P}}$ such that a restricted part of test variables $\underline{\widehat{q}}^*$ is considered as control variables:

$$\underline{q}^* = \underline{\underline{P}}^{\mathrm{T}}\,\underline{\widehat{q}}^* \quad \forall \underline{\widehat{q}}^*, \tag{31}$$

where $\underline{\underline{P}}$ is full of zeros excepted a one per line such that $\underline{\widehat{q}}^*$ is a part of $\underline{q}^*$ with:

$$\underline{\widehat{q}}^* = \underline{\underline{P}}\,\underline{q}^*. \tag{32}$$

In practice, we choose more checked balance equations than shape functions of the current ROM. But finally the number of reduced balance conditions and the number of reduced state variables are the same by choosing:

$$\underline{q}^* = \underline{\underline{P}}^{\mathrm{T}}\,\underline{\underline{P}}\,\underline{\underline{A}}\,\underline{a}^* \quad \forall \underline{a}^*. \tag{33}$$

We then obtain the following balance conditions:

$$\underline{\underline{A}}^{\mathrm{T}}\,\underline{\underline{P}}^{\mathrm{T}}\,\underline{\underline{P}}\,\underline{F}_{\mathrm{int}}\left(\underline{\underline{A}}\,\underline{a}_{j+1}, \underline{\underline{A}}\,\underline{a}_j\right) = \underline{\underline{A}}^{\mathrm{T}}\,\underline{\underline{P}}^{\mathrm{T}}\,\underline{\underline{P}}\,\underline{F}_{\mathrm{ext}}\left(\underline{\underline{A}}\,\underline{a}_{j+1}, \underline{\underline{A}}\,\underline{a}_j, t_{j+1}\right) \quad \forall j = 1 \ldots m-1. \tag{34}$$

The control variables are the finite element degrees of freedom of control nodes. Only few elements are directly connected to these control nodes. Let us Ω_{R} be the reduced integration domain defined by these elements. The other elements of the mesh do not have any contribution to the formulation (34). So, we only use the integration points of Ω_{R} to perform the hyperreduction. The list of control nodes is defined after each adaptation of the ROM by a loop on the shape functions. First, we compute a local average of the norm of the gradient of each shape function on each node of the mesh. Then, for each shape function, we add to the list a node which does not belong to this list, where the maximum of the norm of the gradient is reached. Thanks to this procedure all the shape functions should be observable with the control variables.

Few remarks:

- In practice, the product $\underline{\underline{P}}\,\underline{F}$ is implemented as a selection of lines of $\underline{F}$.
- The tangent stiffness matrix $\underline{\underline{K}}_{Aj+1}$ (35) of the reduced governing equations is not symmetric and it is a full matrix. But in practice its size is lower than 100.

$$\underline{\underline{K}}_{A\,j+1} = \underline{\underline{A}}^{\mathrm{T}}\,\underline{\underline{P}}^{\mathrm{T}}\,\underline{\underline{P}}\,\underline{\underline{K}}_{j+1}\,\underline{\underline{A}}. \tag{35}$$

- If $\underline{\underline{A}}^{\mathrm{T}}\underline{\underline{P}}^{\mathrm{T}}\,\underline{\underline{P}}\,\underline{F}_{\mathrm{ext}}$ is equal to zero, we must add to the list of control nodes some nodes connected to the loading conditions.

5. First examples of reduction of floating point operations

5.1. Computational savings over the reference simulation

We propose to study the influence of the number of FE degrees of freedom $\tilde{n}$ and the required precision ϵ_{R} (6) on the computational savings provided by the APHR method. Five different meshes are considered. From a mesh to another there is the same ratio of elements in the 3 directions. The number of FE degrees of freedom of each mesh, M1 M2 M3 M4 M5, are, respectively, 980, 2025, 3872, 7840, and 16,200. The mesh M3 is the one shown on Fig. 1.

An estimation of the computational savings over the reference simulation is obtained by the number of FLOPs needed to forecast the state evolution over $[t_1,t_m]$, according to the quality criterion (6) thanks to the

reference model divided by the number of FLOP needed to forecast the state evolution over same time interval according to the same quality criterion thanks to the APHR method. The FLOP reduction coefficient is denoted G:

$$G = \frac{\text{EF FLOP}}{\text{APHR FLOP}}. \tag{36}$$

Thanks to the Matlab software version 5.2.1, we are able to get the number of FLOP involved in a computation. So, both APHR method and finite element method where implemented with Matlab.

5.2. The initial ROM

We have to choose a set of initial shape functions in order to define the matrix $A^{(0)}$. It can be a unique shape function to represent the initial state of the structure. In practice, if we do not know any approximate state of the non-linear problem we want to study, we add a shape function in order to represent the state of the linearized problem at the beginning of the time interval.

5.3. Some details of the main results provided by the APHR method

Let us consider the finite element model obtained with the mesh M3 (7840 FE degrees of freedom) with material properties described by the Tables 1 and 2 such that $\widetilde{T}_1 = 25$ °C, $\widetilde{T}_2 = 700$ °C. A 3D state evolution is obtained with properties of the fiber different from the ones of the material around it (Table 2).

The initial temperature of the bar is $T_{\text{ini}} = 25$ °C. During the 25 first time steps the boundary condition T_c is equal to 700 °C and after it is equal to 25 °C. So the time interval involves two transient responses. In Fig. 5 the temperature field corresponding to the 3D problem is shown for different time instant, on the face Γ_c and on the face Γ_{xz}.

161 adaptations are performed to build the ROM and to forecast the state variables over $[t_1, t_m]$. In Fig. 6 the evolution of α and r – the number of shape functions of the current ROM – is shown at the end of each adaptation period. The Karhunen–Loève selection is not applied if $r < 7$. For $r \geqslant 7$ the size of the ROM is strongly connected to the number of computed time steps ($\alpha + \beta$) and to smoothness of the state evolution. The more important the state evolution is during an adaptation period the more important is the number of

Table 1
Thermal capacity and conductivity

	$T < \widetilde{T}_1$	$\widetilde{T}_1 \leqslant T \leqslant \widetilde{T}_2$	$T > \widetilde{T}_2$
$C(T)$	C_1	$C_1 \dfrac{\widetilde{T}_2 - T}{\widetilde{T}_2 - \widetilde{T}_1} + C_2 \dfrac{T - \widetilde{T}_1}{\widetilde{T}_2 - \widetilde{T}_1}$	C_2
$k(T)$	k_1	$k_1 \dfrac{\widetilde{T}_2 - T}{\widetilde{T}_2 - \widetilde{T}_1} + k_2 \dfrac{T - \widetilde{T}_1}{\widetilde{T}_2 - \widetilde{T}_1}$	k_2

Table 2
Material parameters

	C_1 (J kg^{-1} K^{-1})	C_2 (J kg^{-1} K^{-1})	k_1 (W m^{-1} K^{-1})	k_2 (W m^{-1} K^{-1})
Around the fiber	500	700	50	25
In the fiber	570	707	110	85

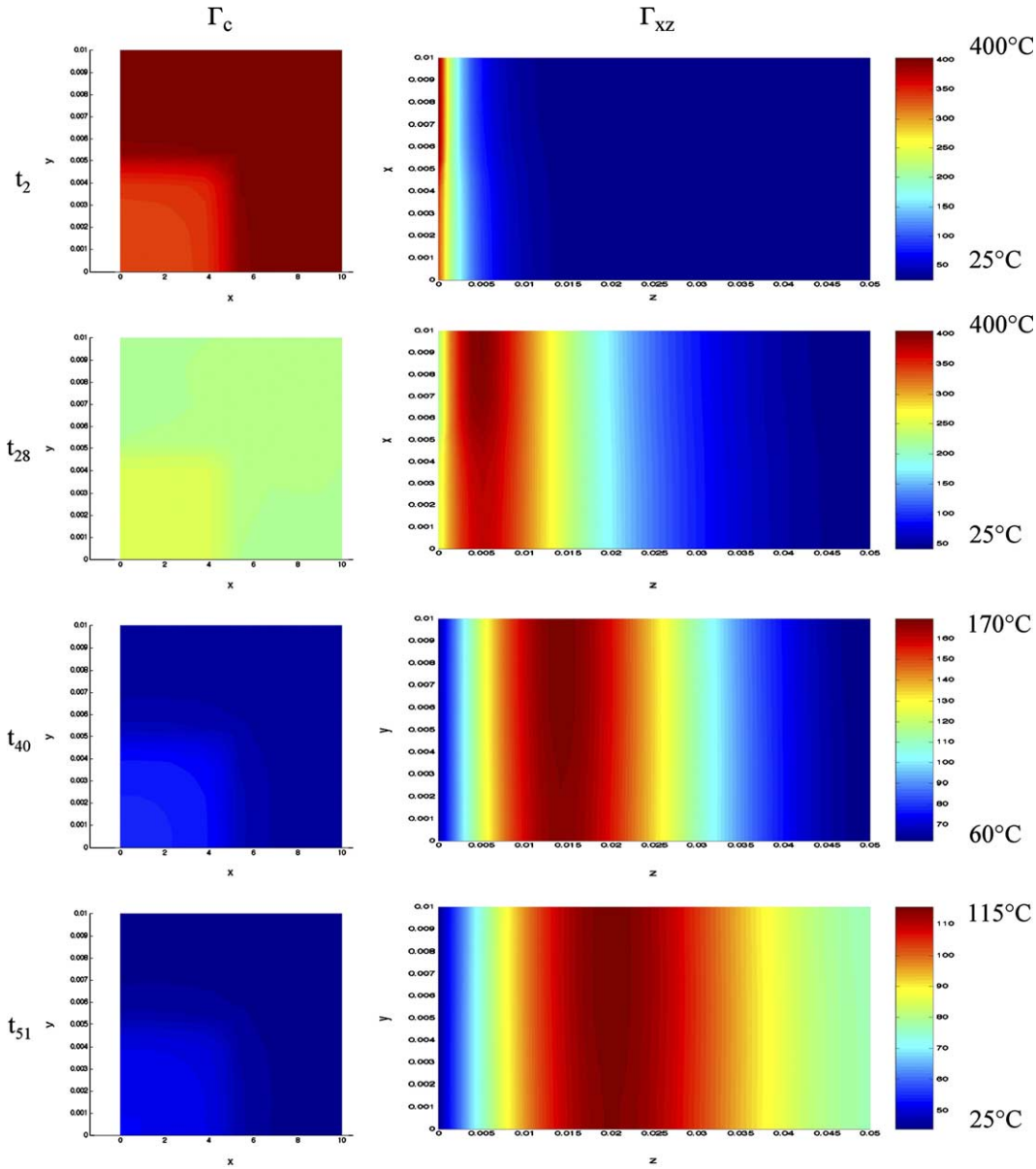

Fig. 5. Temperature fields at different time instants obtained by the APHR method.

adaptations of the ROM during this period and the higher are the norms of the residuals. Fig. 7 represents the evolution of $\|\underline{R}_{\alpha+\beta}(\underline{q}^{(n)}_{\alpha+\beta})\|$ at the end of each quality check.

For this example, the size of the matrix $\underline{\underline{H}}^{(n)}$ and the number of equilibrium conditions (34) are always lower than 35. When quality criterion is fulfilled on the entire time interval, the ROM is defined by only 32 shape functions in stead of 7840 finite element ones. As expected, in Fig. 8 we can see that the shape functions are global. Moreover, the first ones are as smooth as the temperature field despite the residuals are not. This means that the Karhunen–Loève selection improves the shape functions of the ROM. The other shape functions allow to take into account local events.

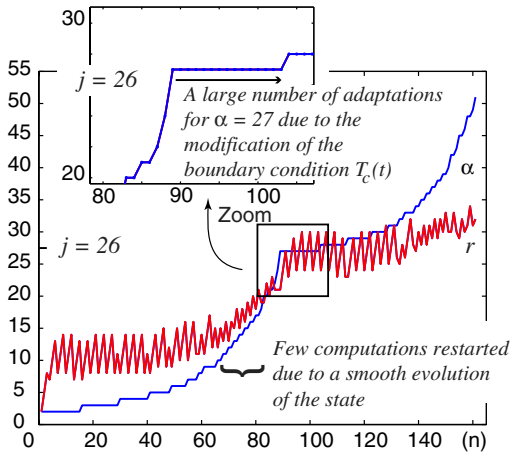

Fig. 6. Size of the ROM (r) and evolution of α during the APHR procedure.

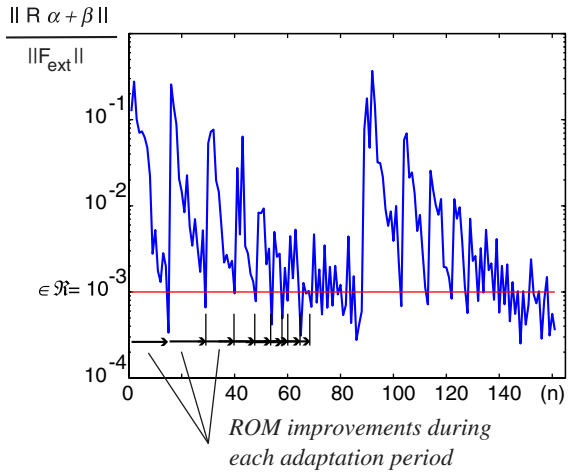

Fig. 7. Evolution of the norm of the residuals during the APHR procedure.

During the last adaptation period the reduced integration domain Ω_R involved only a selection of 326 elements (Fig. 9) instead of 6691 elements for the full finite element model. The spatial distribution of the elements of Ω_R seems to correspond to the position of the main transformations.

Finally, the FLOP reduction is: $G = 24$. Despite the reference model is not a large one (only 7840 unknowns) the reduction of floating point operations is really interesting.

For the next numerical results, a 1D state evolution has been also considered. It is obtained by the 3D model with the properties shown in Table 3.

5.4. Numerical analysis of the complexity of the APHR method

What we expect from a model reduction method is to provide increasing computational savings while the size of the reference model increases. Since there is 50 time steps, according to the Karhunen–Loève selection the number of shape function of the ROM must be lower than 53 ($m = 50$ and $v = 3$) for any mesh. This

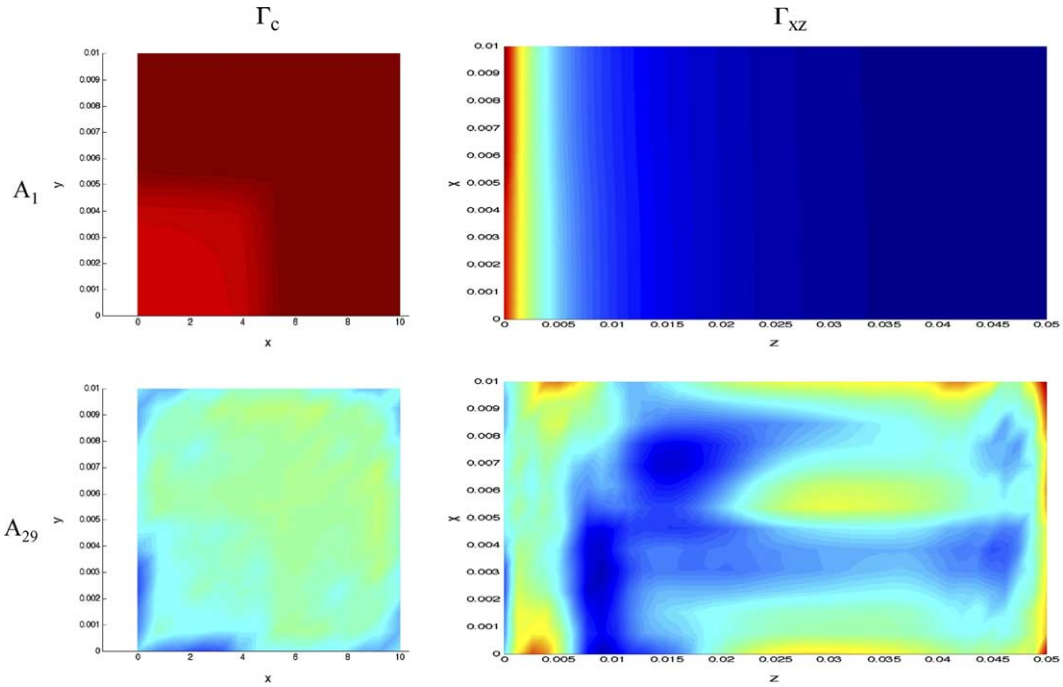

Fig. 8. First and 29th shape functions obtained by the APHR method.

is confirmed by Fig. 10 for the five meshes M1, M2,. . .,M5. More shape functions are needed to represent the state estimated with $\epsilon_R = 10^{-2}$ than the one obtained with $\epsilon_R = 10^{-4}$ because the selection criterion does not depend on ϵ_R and the state evolution if smother for the second case than for the other one. For this thermal problem there is no influence of the size of the reference model on the size of the ROM. The number of elements of the reduced integration domain is also independent of the size of the reference model.

The study of the FLOP reduction confirms what we could expect. This FLOP reduction increases as the number of degrees of freedom of the finite element model increases (Fig. 11). Moreover, the APHR method seems to be interesting even if the reference model is a small one (about 2000 degrees of freedom).

The previous results were obtained thanks to an optimal resolution of the different FE linear systems involved in the incremental Newton procedure. In Fig. 12 there is a comparison between the number of FLOP for the APHR estimation of the state evolution over $[t_1,t_m]$ with $\epsilon_R = 10^{-3}$ and one linear resolution corresponding to the finite element model, for the five different meshes. As the size of the reference model increases the contribution to the number of FLOP of the initialization thanks to a linear finite element problem becomes more important.

6. A learning strategy

6.1. The initial ROM

On the previous section we observed that the contribution to the number of FLOP of the initialization increases as the size of the mesh increases. In some cases, a previous ROM construction could provide interesting shape functions that could be convenient to describe the state evolution during the current compu-

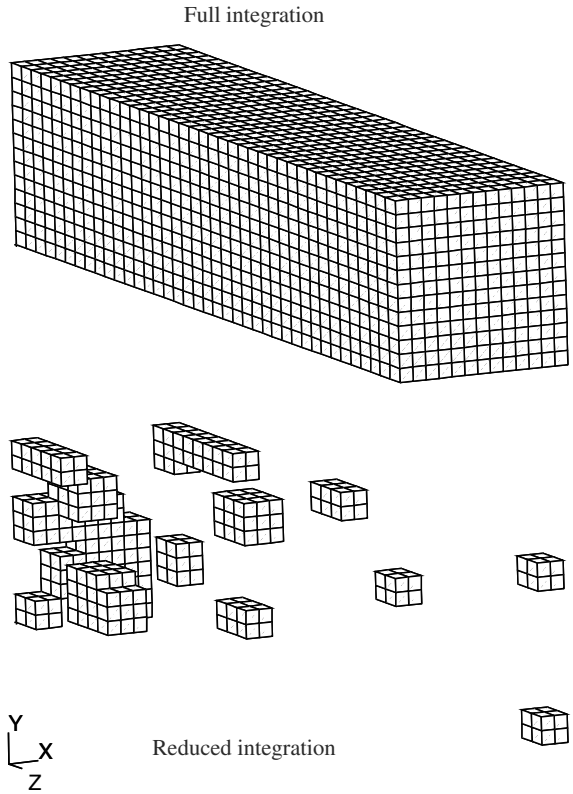

Fig. 9. Elements of the full FE model and elements of the reduced integration domain.

Table 3
Material parameters

	C_1 (J kg^{-1} K^{-1})	C_2 (J kg^{-1} K^{-1})	k_1 (W m^{-1} K^{-1})	k_2 (W m^{-1} K^{-1})
Around the fiber	500	700	50	25
In the fiber	500	700	50	25

tation. Thus, the current ROM construction should be initialized with a matrix $\underline{\underline{A}}^{(0)}$ that contains the shape functions of this previous ROM construction. Then any resolution of linear finite element problem can be avoided.

But since the method we proposed is an adaptive strategy, we must take care of the information involved in the matrix $\underline{\underline{A}}^{(0)}$. If the strategy proposed above is not modified, we can loose some of these informations. Let us consider that the current ROM has been adapted over $[t_1, t_{\alpha+\beta}]$. The previous strategy is based on a selection of the shape functions with a state extrapolation such that:

$$\underline{a}_p^{(n)} = \underline{a}_{\alpha+\beta}^{(n)} \quad \forall p > \alpha + \beta. \tag{37}$$

Then if some shape functions of the current ROM are only relevant to describe events happening at t_j such that $t_j > t_{\alpha+\beta}$, then these shape function are not going to be selected. Thus, they are going to be removed to the current ROM. To avoid this, we just have to replace the extrapolation of the state by a description of

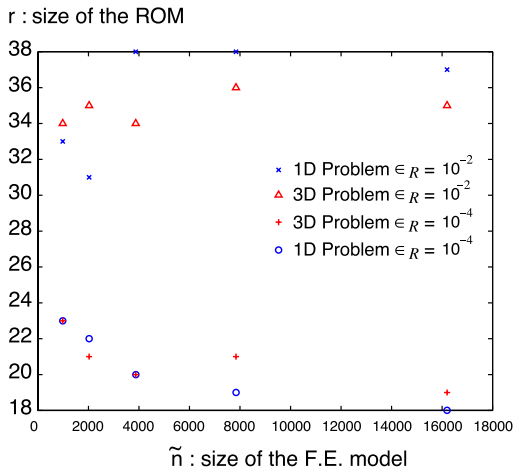

Fig. 10. Influence of number of the degrees of freedom of the FE model and influence of ϵ_R on the number of shape functions of the ROM.

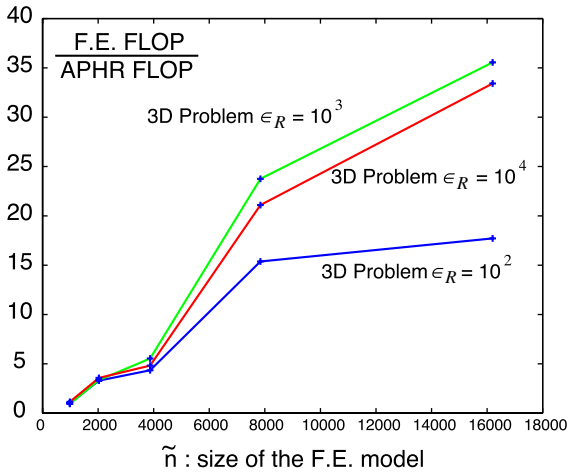

Fig. 11. Influence of number of degrees of freedom of the FE model and influence of ϵ_R on the FLOP reduction.

the state obtained during the previous ROM construction. But these description has to be compatible with the current ROM. Let us denote $(\underline{b}_j^{(0)})_{j=1\ldots m}$ the reduced state variables such that the product $\underline{\underline{A}}^{(0)}\,\underline{b}_j^{(0)}$ is the state estimation at $t = t_j$ obtained during the previous ROM construction. During the adaptation of the current ROM the reduced state variables $(\underline{b}_j^{(0)})_{j=1\ldots m}$ have to be updated just like the current reduced state variables are updated:

$$\underline{b}_j^{(n+1)} = \begin{bmatrix} \left(\underline{\underline{V}}^{(n)\,\mathrm{T}}\,\underline{\underline{V}}^{(n)}\right)^{-1}\underline{\underline{V}}^{(n)\,\mathrm{T}}\,\underline{b}_j^{(n)} \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad \forall j. \tag{38}$$

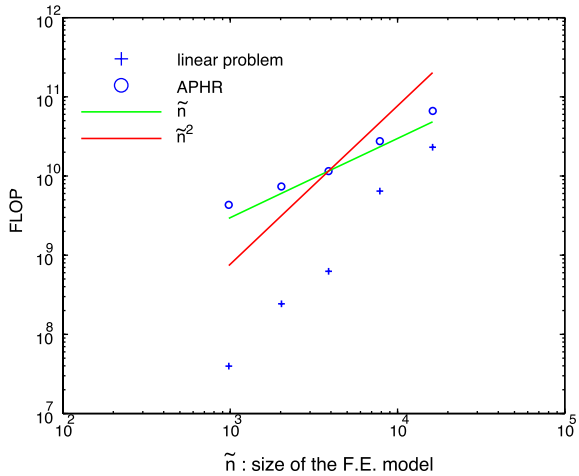

Fig. 12. Influences of the number of degrees of freedom of the reference model on the number of FLOP (mesh M3, $\epsilon_R = 10^{-3}$).

The block of zeros correspond to the vectors $(\underline{Y}_i)_{i=1\ldots v}$. So, to keep the shape functions that are relevant during the time steps where the current computation have not been done, we just have to replace the extrapolation by this one (Fig. 13):

$$\underline{a}_p^{(n)} = \underline{b}_p^{(n)} \quad \forall p > \alpha + \beta. \tag{39}$$

Thus, the selection matrix $\underline{\underline{V}}^{(n)}$ allows to keep shape functions corresponding to events that are not yet forecast with the current ROM construction. Moreover, if previous shape functions are not interesting, the Karhunen–Loève selection eliminates them as $\alpha + \beta$ increases thanks to this approach, we obtain a strategy that takes into account a previous ROM construction and current reference model equations. This is a learning strategy.

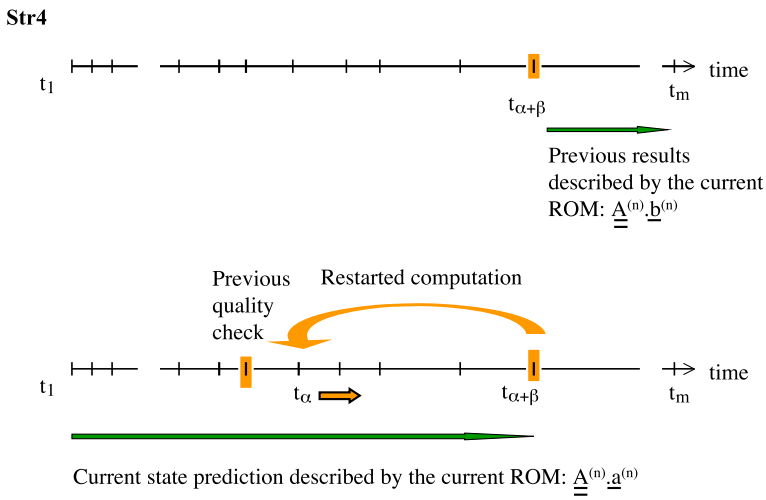

Fig. 13. The learning strategy.

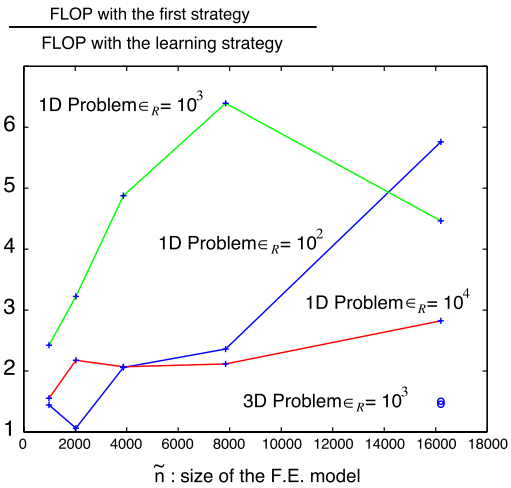

Fig. 14. More cost reduction obtained with the learning strategy.

6.2. Numerical analysis of the complexity of the learning strategy

Let us consider the 1D problem to build a first ROM thanks to the first adaptive strategy. Thus, we obtain a convenient initialization for the 3D problem studied above. Moreover, this initialization has to be very convenient for the same 1D problem.

In Fig. 14 is shown the ratio between two numbers of FLOP for the 1D problem. On the numerator there is the number of FLOP corresponding to the first strategy and on the denominator there is the number of FLOP corresponding to the learning strategy. As expected, this ratio is always greater than one.

If the ROM of the 1D problem is used to initialize the ROM construction of the 3D problem, we divide the number of FLOP by 1.5 (Fig. 14).

The learning strategy really takes into account the previous results. But should we take into account all the shape function of the previous ROM to build $\underline{\underline{A}}^{(0)}$? Certainly not. This learning strategy has to be optimized.

7. Conclusions

We propose an algorithm which builds a reduced-order model from a finite element model. No previous estimation of what are the main events forecast by the finite element model is needed. Only a model of what could happen is necessary. This algorithm is based on an adaptive strategy. This approach is therefore convenient to update the reduced-order model when the finite element model is modified. To do so a learning strategy is proposed. The reduction of the number of unknowns is important. On one of the proposed example, this number is divided by almost 1000. This is obtained by studying the time correlation between the reduced state variables. The computational savings increase as the size of the reference model increases, and the APHR method starts to be interesting for small problem (about 2000 FE degrees of freedom). The proposed algorithm can be applied on different non-linear time dependent problems.

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