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Multidimensional *a priori* hyper-reduction of mechanical models involving internal variables

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ABSTRACT

Modeling large systems usually requires metamodels or response surfaces (RSs) of sub-systems. These metamodels are using sampling points in a parameter domain and related responses provided by the solution of parametric partial differential equations (PDEs). Between sampling points the responses are interpolated. We propose to incorporate the RS approximation into the weak form of parametric partial differential equations (PDEs). Hence a multidimensional model-reduction can be achieved. RSs provide very fast predictions. But their enrichment, by adding new sampling points, requires new response evaluations, and therefore new solutions of PDEs. Although it is off-line computations, their complexity does not facilitates the study of large-scale non-linear problems involving a large number of parameters. Reduced-order models can facilitate the solution of the PDEs used to enrich the RSs. We propose a multidimensional *a priori* model-reduction method to generate or to enrich RSs. It is coined multidimensional because the fields to forecast are defined over an augmented domain in terms of dimension. They are functions of both space variables and parameters that simultaneously evolve in time. This changes the functional space related to the weak form of the PDEs and the definition of the reduced-bases. It has a significant impact on the proposed model-reduction method. In particular, the variable interpolation in the framework of reduced-basis approximations has to be reconsidered. Moreover, a multidimensional reduced integration domain (MRID) is proposed to reduce the complexity of the reduced formulation. It is a subdomain of the full multidimensional domain. The multidimensional hyper-reduction method extracts from the MRID truncated equilibrium equations, truncated residuals and a truncated error indicator. This work is an extension of the *a priori* hyper-reduction (APHR) method to parametric PDEs coupled to a design of experiments (DOE) method. In this paper, the outputs of the metamodels are the elastic stiffness and the damping coefficient of non-linear mechanical sub-systems that could be incorporated in the model of aircrafts or cars subjected to vibrations. The proposed method has been designed to account for various recent and ongoing research on mathematical formulation of mechanical constitutive equations in material science. Here, we are using a constitutive model proposed by Qi and Boyce for polymers.

The three following issues are addressed: Is the multidimensional APHR method more efficient than the APHR method applied individually on separated simulations? What is the efficiency of the proposed approach when adding sampling points in the current parameter domain? What is the efficiency of the method when adding a new dimension to the parameter domain, i.e. when adding a new parameter to enrich a former parametric study?

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1. Introduction

In the field of large-scale system structural-dynamics, substituting complex non-linear models of sub-systems by meta-models, or response surfaces (RSs) should make the numerical simulations easier and faster ([1,2]). The response surface methodology aims to model an unknown relation between inputs $\boldsymbol{\mu}$ and outputs $s(\boldsymbol{\mu})$ by a metamodel $s_{RS}\left(\boldsymbol{\mu}; \{\boldsymbol{\mu}_p\}_{p=1}^{\mathcal{P}}, \{s(\boldsymbol{\mu}_p)\}_{p=1}^{\mathcal{P}}\right)$. Here $\boldsymbol{\mu}$ is a vector of parameters. We denote by $\mathcal{D}$ the parametric domain such that: $\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^{\mathcal{Q}}$. The metamodel is defined by a set of sampling points denoted by $\mathcal{F}_{\mathcal{D}}$, $\mathcal{F}_{\mathcal{D}} = \{\boldsymbol{\mu}_p\}_{p=1}^{\mathcal{P}}$, and the related responses. Usually s_{RS} is based on an interpolation technique. Various interpolation functions are available. They are denoted by ξ_p. For instance it can be polynomial functions, moving least-squares interpolation functions or radial basis functions. The interpolation of responses reads:

$$s_{RS}(\boldsymbol{\mu}; \{\boldsymbol{\mu}_p\}_{p=1}^{\mathcal{P}}, \{s(\boldsymbol{\mu}_p)\}_{p=1}^{\mathcal{P}}) = \sum_{p=1}^{\mathcal{P}} \xi_p(\boldsymbol{\mu}) s(\boldsymbol{\mu}_p) \quad \forall \boldsymbol{\mu} \in \mathcal{D}. \tag{1}$$

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Most of the time, a large number of expensive simulations is required to provide the set of responses $\{s(\boldsymbol{\mu}_p)\}_{p=1}^{\mathcal{P}}$. In case of full factorial sampling, $\mathcal{P}$ grows exponentially with respect to the dimension of $\mathcal{D}$. This exponential growth is often mentioned as the curse of dimensionality. Convenient sampling points are provided by design of experiments (DOE) methods. The Monte Carlo sampling, the Latin hypercube sampling, the moving least-squares metamodels and the Kriging method are very popular. In this paper, the responses of interest are extracted from the solution of physically-based differential equations. This extraction procedure reads:

$$s(\boldsymbol{\mu}) = \ell(\mathbf{u}, \boldsymbol{\alpha}; \boldsymbol{\mu}). \tag{2}$$

Here, $\mathbf{u}$ is a displacement field, $\boldsymbol{\alpha}$ is a field of internal variables (more details are given below) and $\boldsymbol{\mu}$ is a vector of model parameters. $\mathbf{u}$ and $\boldsymbol{\alpha}$ are functions of space variable and time variables, and their dependence on $\boldsymbol{\mu}$ has to be enlightened. We assume that the interpolation functions $\{\xi_p\}_{p=1}^{\mathcal{P}}$ are relevant to approximate the variables $\mathbf{u}$ and $\boldsymbol{\alpha}$ between sampling points. The response-surface approximation reads:

$$\mathbf{u}_{RS}(\mathbf{x}, \boldsymbol{\mu}, t) = \sum_{p=1}^{\mathcal{P}} \xi_p(\boldsymbol{\mu}) \mathbf{u}(\mathbf{x}, \boldsymbol{\mu}_p, t), \quad \mathbf{x} \in \Omega \ \boldsymbol{\mu} \in \mathcal{D} \ t \in]0, T], \tag{3}$$

$$\boldsymbol{\alpha}_{RS}(\mathbf{x}, \boldsymbol{\mu}, t) = \sum_{p=1}^{\mathcal{P}} \xi_p(\boldsymbol{\mu}) \boldsymbol{\alpha}(\mathbf{x}, \boldsymbol{\mu}_p, t), \quad \mathbf{x} \in \Omega \ \boldsymbol{\mu} \in \mathcal{D} \ t \in]0, T]. \tag{4}$$

Here, $\mathbf{x}$ and Ω are respectively the spatial variable and the spatial domain, t is the time variable; T is the last time of the time interval.

We propose a multidimensional-APHR method that accounts for this approximation to generate the solutions of the PDEs required to forecast the sampling-point responses $\{s(\boldsymbol{\mu}_p)\}_{p=1}^{\mathcal{P}}$. As proposed in [3] the parameters are considered as additional coordinates, as if the responses were defined with coupled PDEs, although the PDEs related to two different vectors of parameters are not coupled. This paper focuses on the off-line simulations that provide $\{\ell(\mathbf{u}, \boldsymbol{\alpha}; \boldsymbol{\mu}_p)\}_{p=1}^{\mathcal{P}}$. The proposed method is an *a priori* reduction method involving both partial residual-estimations and an interpolation technique defined over the parametric domain. To highlight the added value of the proposed method we recall how, in the existing approaches, (i) the parameters are taken into account when doing reduced order modeling, (ii) how the main salient feature of the state evolutions can be discovered by *a priori* model reduction methods and the PGD method, and (iii) and why the full residual-estimation must be avoided in case of non-linear problems.

Model-reduction methods aim to propose alternative approaches to the $\mathcal{P}$ high-fidelity simulations, such as finite-element simulations, involved in the prediction of the responses $\{\ell(\mathbf{u}, \boldsymbol{\alpha}; \boldsymbol{\mu}_p)\}_{p=1}^{\mathcal{P}}$. They reduce the dimension of the functional space of the high-fidelity model, and a reduction of the computational complexity is expected. Usually, a reduced-basis approximation has the following form:

$$\mathbf{u}(\mathbf{x}, \boldsymbol{\mu}, t) = \mathbf{u}_o(\mathbf{x}, \boldsymbol{\mu}, t) + \sum_{k=1}^{N} \boldsymbol{\phi}_k(\mathbf{x}) \varphi_k(t, \boldsymbol{\mu}),$$
$$\mathbf{x} \in \Omega \ \boldsymbol{\mu} \in \mathcal{D} \ t \in]0, T], \tag{5}$$

$$\boldsymbol{\phi}_k(\mathbf{x}) = \sum_{i=1}^{\mathcal{N}} \mathbf{N}_i(\mathbf{x}) A_{ik}, \quad k = 1, \ldots, N. \tag{6}$$

Here $\mathbf{u}_o$ is a given parametrized field related to a Dirichlet boundary condition $\mathbf{u} = \mathbf{u}_c$ prescribed over a part $\partial_u\Omega$ of the boundary of the spatial domain. $\{\mathbf{N}_i\}_{i=1}^{\mathcal{N}}$ are the shape functions of the finite-element model which is considered to be the high-fidelity model. A_{ik} for $i = 1 \ldots \mathcal{N}$ and $j = 1 \ldots N$ are the matrix entries of the matrix $\mathbf{A}$. This matrix is termed reduction matrix. $\{\boldsymbol{\phi}_k\}_{k=1}^{N}$ are the vectors of the reduced-basis. $\{\varphi_k\}_{k=1}^{N}$ are the reduced state variables. Here, the vector of parameters plays a role similar to the time variable: if a unique core is used to perform the simulations, the responses are evaluated one after another by a sequential approach (obviously the reduced equations for the different parameter values can also be solved in parallel, but parallel computing is a specific topic that is not an issue of this paper). Although the set of sampling points can be optimal in order to capture the response-surface variations, remaining common salient features among the forecasted state variables $\mathbf{u}$ and $\boldsymbol{\alpha}$ make reduced-order models efficient for the approximate solution of the physically-based equations.

In the scientific literature, many authors proposed to replace some finite-element simulations by reduced-order simulations in the framework of parametrized evaluation problems. In non-linear mechanics, the proper orthogonal decomposition (POD) [4,5] and the snapshot POD [6] are the foremost methods used to extract a reduced basis (RB) from a set of fields (displacement fields or velocity fields) provided by simulations using classical approximation methods (i.e. finite-element method, backward Euler scheme, Runge–Kutta time integrators,...). Given a POD reduced basis, a POD-Galerkin formulation can be introduced to state a reduced form of the weak formulation of the differential equations, as proposed in [7]. When solving the Navier–Stokes equations by using POD approximations, the stability of the method can to be improved by a Petrov–Galerkin formulation as proposed in [8,9]. The POD and the snapshot POD method proposed in [6,7] are *a posteriori* approaches. High-fidelity simulations (i.e. full-basis simulations) have to be performed prior to constructing a RB. The POD and the snapshot POD methods aim to extract the salient features of various predictions to create the RB. The accuracy of the POD RB depends both on: (1) the basis truncation related to the POD method, and (2) the similarity of the training trajectories to the high-fidelity trajectories that will be approximated by the reduced-order model during the deployed stage. Therefore, a trust-region framework has been introduced in [10–12] to avoid undue use of approximate simulations instead of the full-basis simulations. It turns out that RB can differ between points of the parameter domain. In most cases, the best reduced basis of fixed dimension is input-parameter-dependent, especially when its dimension is low. Various interpolation methods have been proposed, the direct interpolation of RB in [13], the subspace angle interpolation method in [14] and methods based manifolds [15,16]. Therefore, the reduced-basis approximation reads:

$$\mathbf{u}(\mathbf{x}, \boldsymbol{\mu}, t) = \mathbf{u}_o(\mathbf{x}, \boldsymbol{\mu}, t) + \sum_{k=1}^{N} \boldsymbol{\phi}_k(\mathbf{x}, \boldsymbol{\mu}) \varphi_k(t, \boldsymbol{\mu}),$$
$$\mathbf{x} \in \Omega \ \boldsymbol{\mu} \in \mathcal{D} \ t \in]0, T], \tag{7}$$

$$\boldsymbol{\phi}_k(\mathbf{x}, \boldsymbol{\mu}) = \sum_{i=1}^{\mathcal{N}} \mathbf{N}_i(\mathbf{x}) A_{ik}(\boldsymbol{\mu}), \quad k = 1, \ldots, N. \tag{8}$$

The interpolation methods enable to update RB according to parameter variations but they do not really answer to the question regarding the adaptivity by considering error estimators. They provide multifidelity models, accuracy and efficiency of which are in-between the response surface model and the high-fidelity model. But these methods do not match the expectation to discover the salient feature of the responses during the solution of the underlining physically-based equations.

The aforementioned reduction methods are *a posteriori* methods because they require preliminary high-fidelity simulations that provide snapshots related to given sampling points in $]0, T] \times \mathcal{D}$. Unfortunately, the accuracy of the reduced-order model depends on the relevance of the sampling points. *A priori* model-reduction methods create a reduced representation during the solution of the differential equations. The accuracy of the reduced-approximation provided by *a priori* reduction methods is not affected by the initial choice of sampling points. During the approximate solution of the differential equations, the reduced-approximation is adapted according to an error estimator, or an error indicator having a less

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