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A priori model reduction through Proper Generalized Decomposition for solving time-dependent partial differential equations

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ABSTRACT

Over the past years, model reduction techniques have become a necessary path for the reduction of computational requirements in the numerical simulation of complex models. A family of *a priori* model reduction techniques, called Proper Generalized Decomposition (PGD) methods, are receiving a growing interest. These methods rely on the *a priori* construction of separated variables representations of the solution of models defined in tensor product spaces. They can be interpreted as generalizations of Proper Orthogonal Decomposition (POD) for the *a priori* construction of such separated representations. In this paper, we introduce and study different definitions of PGD for the solution of time-dependent partial differential equations. We review classical definitions of PGD based on Galerkin or Minimal Residual formulations and we propose and discuss several improvements for these classical definitions. We give an interpretation of optimal decompositions as the solution of pseudo-eigenproblems. We also introduce a new definition of PGD, called Minimax PGD, which can be interpreted as a Petrov–Galerkin model reduction technique, where test and trial reduced basis functions are related by an adjoint problem. This new definition improves convergence properties of separated representations with respect to a chosen metric. It coincides with a classical POD for degenerate time-dependent partial differential equations. For the numerical construction of each PGD, we propose algorithms inspired from the solution of eigenproblems. Several numerical examples illustrate and compare the different definitions of PGD on transient advection–diffusion–reaction equations.

1. Introduction

The numerical simulation of physical models takes today an important place in numerous branches of science and engineering. Due to the increasing complexity of models, more and more refined discretizations and robust numerical solution techniques are needed in order to obtain reliable predictions of their responses. Furthermore, in the context of optimization, model identification, or parametric and stochastic analyses, the aim is not to predict the response of a unique model but of a family of models. In order to achieve these analyses, traditional solution techniques require the optimal use of constantly evolving computational resources. However, for many applications, innovative methodologies, alternative to the brute force approach, are obviously necessary to access numerical predictions.

The concept of model reduction seems to be a path for solving these computational issues. Model reduction methods exploit the fact that the response of complex models (or of a family of models) can often be approximated with a reasonable precision by the response of a surrogate model, which is the projection of the initial model on a low dimensional reduced basis. The dimension of reduced bases may be of several orders of magnitude lower than the dimension of the classically used numerical models. Model reduction methods distinguish themselves by the way of defining and constructing the reduced bases of functions. Among these methods, model reduction methods based on separation of variables are receiving a growing interest in various fields of scientific computing. In the context of the solution of evolution problems, a separated representation of the solution $u(x,t)$ defined on a space–time domain consists of a sum of products of scalar functions of the time variable by functions of the space variable:

$$u(x,t) \approx u_m(x,t) = \sum_{i=1}^{m} w_i(x)\lambda_i(t). \tag{1}$$

When the solution u is known (or at least an approximation of it), an optimal order m (or rank m) separated representation (1) — also known as tensor product approximation or finite sums decomposition — can be classically defined as the one which minimizes the distance to the solution with respect to a particular norm. This separated representation is optimal in the sense that it minimizes this distance for a given order m of decomposition. Under some

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assumptions on the chosen norm, this is the basic definition of the classical Proper Orthogonal Decomposition (POD), also known as Karhunen–Loève decomposition [18,26], Singular Value Decomposition or Principal Component Analysis in other contexts. This decomposition is classically used as an *a posteriori* model reduction technique for long-time simulations or parametric analyses of evolution problems [5,4,19,20,16,36,24,10,15,3].

In this paper, we focus on the more challenging problem of the *a priori* construction of such separated representations. The aim is to introduce different strategies for the construction of an approximate separated representation (1) of the solution, without *a priori* knowing the solution nor an approximation of it. This requires to adopt another definition of the separated representation and then to propose dedicated algorithms for its construction. The different methods introduced in this article can be interpreted as generalizations of the POD for the *a priori* construction of separated representations. The resulting decompositions have been recently called *Proper Generalized Decompositions* (PGD).[1] This type of methods has been first introduced by Ladevèze in the context of the LATIN method [21] (LArge Time INcrement method) for reducing computational costs (memory requirements and computational times) associated with the solution of multiple linear evolution problems resulting from a nonlinear iterative strategy which is global in time. In this context, separated representation (1) was called "radial approximation". In the literature, two variants of PGD have been proposed for the progressive construction of (1), respectively based on a Galerkin formulation [21,12,22,9] or a Minimal Residual formulation [31,23] of the evolution problem. PGD methods have also been introduced in other contexts: separation of physical variables and parameters (or random variables) in the context of parametrized (or stochastic) PDEs [27,28,32,29],[2] with a possible additional separation of parameters [11,30],[3] separation of coordinate variables in multi-dimensional PDEs [6,1,2,8].[4]

In this paper, we introduce and study different definitions of PGD for the solution of time-dependent partial differential equations. We review classical definitions of PGD based on Galerkin or Minimal Residual formulations and we propose and discuss several improvements for these classical definitions. We give an interpretation of decompositions as the solution of pseudo-eigenproblems and propose algorithms inspired from the solution of eigenproblems for the construction of these decompositions. We also introduce an innovative definition, called Minimax PGD, which allows us to improve convergence properties of decomposition (1) with respect to a chosen metric. This new PGD can be interpreted as an *a priori* Petrov–Galerkin model reduction technique, where test and trial reduced basis functions are related by an adjoint problem involving the chosen metric. For degenerate time-dependent partial differential equations, this new definition coincides with a classical POD with respect to the chosen metric.

The outline of the paper is as follows: In Section 2, we introduce an abstract weak formulation of a class of time-dependent partial differential equations. In Section 3, we recall the principles of model reduction methods with a particular focus on *a posteriori* model reduction methods based on the POD. In Section 4, we focus on PGD methods. We present classical progressive definitions of these decompositions, based on Galerkin or minimal residual formulations. We give an interpretation of these decompositions as the solutions of pseudo-eigenproblems and we propose possible improvements. In Section 5, we introduce and analyze a non-classical definition of PGD, called Minimax PGD. In Section 6, several numerical examples illustrate the behavior of the Proper Generalized Decomposition methods introduced in this article.

2. Time-dependent partial differential equation and discretization

2.1. Model problem: advection–diffusion–reaction equation

As a problem model, we consider a transient advection–diffusion–reaction equation defined on a spatial domain $\Omega \subset \mathbb{R}^d$ and a time interval $I = (0,T)$. The solution $u(x,t)$, with $(x,t) \in \Omega \times I$, solves:

$$\dot{u} - \nabla \cdot (\mu \nabla u) + c \cdot \nabla u + \sigma u = f \quad \text{on } \Omega \times I, \tag{2a}$$

$$u = 0 \quad \text{on } \partial\Omega \times I, \tag{2b}$$

$$u = u_0 \quad \text{on } \Omega \times \{0\}, \tag{2c}$$

where $\dot{u} = \frac{\partial u}{\partial t}$, $u_0(x)$ is the initial condition, $f(x,t)$ is a volumic source, and $\mu(x,t)$, $c(x,t)$ and $\sigma(x,t)$ are diffusion, advection and reaction parameters which are eventually space and time-dependent.

2.2. Space weak formulation

We identify u with a function defined on I with values in Hilbert space $\mathcal{V} = H_0^1(\Omega)$, with $u(t) : x \in \Omega \mapsto u(t)(x) \simeq u(x,t)$. A weak formulation of (2c) writes: find $u : I \to \mathcal{V}$ such that

$$m(\dot{u}(t), v) + a(u(t), v; t) = \ell(v; t) \quad \forall v \in \mathcal{V}, \tag{3a}$$

$$u(0) = u_0, \tag{3b}$$

where $m(\cdot,\cdot)$ and $a(\cdot,\cdot;t)$ are bilinear forms on $\mathcal{V}$ and where $\ell(\cdot;t)$ is a linear form on $\mathcal{V}$, defined by:

$$m(u,v) = \int_\Omega uv\,dx = \langle u, v\rangle_{L^2(\Omega)}, \quad \ell(v;t) = \int_\Omega f(t)v\,dx, \tag{4}$$

$$a(u,v;t) = \int_\Omega \mu(t)\nabla u \cdot \nabla v\,dx + \int_\Omega c(t)\cdot\nabla u v\,dx + \int_\Omega \sigma(t) u v\,dx. \tag{5}$$

2.3. Space–time weak formulation

A space–time weak formulation of (2c) is now introduced [25]. We introduce the following function space

$$L^2(I;\mathcal{V}) = \{v : I \to \mathcal{V}; \int_I \|v(t)\|_{\mathcal{V}}^2\,dt < +\infty\}, \tag{6}$$

where $\|\cdot\|_{\mathcal{V}}$ is a norm on $\mathcal{V}$. We denote $\mathcal{T} = L^2(I;\mathbb{R}) := L^2(I)$ and identify the space $L^2(I;\mathcal{V})$ with the tensor product space $\mathcal{V}\otimes\mathcal{T}$. We denote by $\mathcal{V}' = H^{-1}(\Omega)$ the dual space of $\mathcal{V}$. A weak solution of problem (3b) can then be defined by the following problem: find $u \in \mathcal{V}\otimes\mathcal{T}$ such that $\dot{u} \in L^2(I;\mathcal{V}')$ and[5]

$$B(u,v) = L(v) \quad \forall v \in \mathcal{V}\otimes\mathcal{T}, \tag{7}$$

where B and L are bilinear and linear forms defined by

$$B(u,v) = \int_I m(\dot{u}(t), v(t))dt + \int_I a(u(t), v(t); t)dt + m(u(0^+), v(0^+)), \tag{8}$$

$$L(v) = \int_I \ell(v(t);t)dt + m(u_0, v(0^+)) \tag{9}$$

with $v(0^+) = \lim_{s\downarrow 0} v(s)$. The solution of problem (7) verifies the initial condition in a weak sense.

[1] Roughly speaking, PGD methods introduce different definitions of the separated representation (1) which require only the operator and right-hand side of the PDE, and not the solution itself as in the definition of the POD. With dedicated algorithms, it then allows to build the separated representation without knowing the solution a priori.

[2] $u(x,t,\xi) \approx \sum_{i=1}^m w_i(x,t)\lambda_i(\xi)$, with ξ the (random) parameters. In this context, PGD has been named Generalized Spectral Decomposition as a generalization of spectral decomposition of random processes.

[3] $u(x,t,\xi) \simeq u(x,t,\xi_1,\ldots,\xi_d) \approx \sum_{i=1}^m w_i(x,t)\lambda_i^1(\xi_1)\cdots\lambda_i^d(\xi_d)$.

[4] $u(x_1,\ldots,x_d) \approx \sum_{i=1}^m w_i^1(x_1)\cdots w_i^d(\xi_d)$.

[5] Let us note that $\dot{u}(t) \in \mathcal{V}'$ is assimilated with its Riesz representation in $\mathcal{V}$ in the notation $m(\dot{u}(t), v(t))$.