Available online at www.sciencedirect.com
ScienceDirect
Mathematics and Computers in Simulation 81 (2010) 791–810
MATHEMATICS AND COMPUTERS IN SIMULATION
www.elsevier.com/locate/matcom

Original article

On the deterministic solution of multidimensional parametric models using the Proper Generalized Decomposition

E. Pruliere [a,*], F. Chinesta [b,c], A. Ammar [d]

[a] *Arts et Métiers ParisTech, Esplanade des Arts et Métiers, 33405 Talence Cedex, France*
[b] *GeM: UMR CNRS, Centrale Nantes, 1 rue de la Noë, BP 92101, F-44321 Nantes Cedex 3, France*
[c] *EADS Corporate Foundation Internantional Chair, GeM, Centrale Nantes, France*
[d] *Arts et Métiers ParisTech, 2 boulevard du Ronceray, BP 93525, 49035 Angers Cedex 01, France*

Received 4 June 2009; received in revised form 18 June 2010; accepted 16 July 2010
Available online 24 July 2010

Abstract

This paper focuses on the efficient solution of models defined in high dimensional spaces. Those models involve numerous numerical challenges because of their associated curse of dimensionality. It is well known that in mesh-based discrete models the complexity (degrees of freedom) scales exponentially with the dimension of the space. Many models encountered in computational science and engineering involve numerous dimensions called configurational coordinates. Some examples are the models encountered in biology making use of the chemical master equation, quantum chemistry involving the solution of the Schrödinger or Dirac equations, kinetic theory descriptions of complex systems based on the solution of the so-called Fokker–Planck equation, stochastic models in which the random variables are included as new coordinates, financial mathematics, etc. This paper revisits the curse of dimensionality and proposes an efficient strategy for circumventing such challenging issue. This strategy, based on the use of a Proper Generalized Decomposition, is specially well suited to treat the multidimensional parametric equations.

Keywords: Multidimensional models; Curse of dimensionality; Parametric models; Proper Generalized Decompositions; Separated representations

1. Introduction: revisiting the Proper Generalized Decomposition

The efficient solution of complex models involving an impressive number of degrees of freedom could be addressed by performing high performance computing (in general making use of parallel computing platforms) or by speeding up the calculation by using preconditioning, domain decomposition, etc.

In the case of transient models the use of model reduction can alleviate significantly the solution procedure. The main ingredient of model reduction techniques based on the use of proper orthogonal decompositions – POD – consists of extracting a reduced number of functions able to represent the whole time evolution of the solution, that could be then used to make-up a reduced model. This extraction can be performed by invoking the POD. The reduced model can be then used for solving a similar model, i.e. a model slightly different to the one that served to extract the reduced approximation basis, or for solving the original model in a time interval larger than the one that served for constructing the reduced basis. The main issue in this procedure consists in the evaluation of the reduced basis quality when it applies

* Corresponding author.
E-mail address: etienne.pruliere@lamef.bordeaux.ensam.fr (E. Pruliere).

0378-4754/$36.00
doi:10.1016/j.matcom.2010.07.015

in conditions beyond its natural interval of applicability. In order to ensure the solution accuracy one should proceed to enrich the reduced approximation basis, and the definition of optimal, or at least efficient, enrichment procedures is a difficult task that remains at present an open issue.

Such model reduction strategies were successfully applied, in some of our former works, to solve kinetic theory models [5,23] allowing impressive computing-time savings. The main conclusion of our former works was the fact that an accurate description of a complex system evolution can, in general, be performed from the linear combination of a reduced number of space functions (defined in the whole space domain). The coefficients of that linear combination evolve in time. Thus, during the resolution of the evolution problem, an efficient algorithm has to compute the approximation coefficients and to enrich the approximation basis at the same time. An important drawback of one such approach is the fact that the approximation functions are defined in the space domain. Until now, the simplest form to represent one such function is to give its values in some points of the domain of interest, and to define its values in any other point by interpolation. However, sometimes models are defined in multidimensional spaces and in this case the possibility of describing functions from their values at the nodes of a mesh (or a grid in the domain of interest) can become prohibitory.

Many models encountered in computational science and engineering involve numerous dimensions called configurational coordinates. Some examples are the models encountered in biology making use of the chemical master equation, quantum chemistry involving the solution of the Schrödinger or Dirac equations, kinetic theory descriptions of complex materials and systems based on the solution of the so-called Fokker–Planck equation, stochastic models in which the random variables are included as new coordinates, financial mathematics modeling credit risk in credit markets (multi-dimensional Black and Scholes equation). The numerical solution of those models introduces some specific challenges related to the impressive number of degrees of freedom required because of the highly dimensional spaces in which those models are defined. Despite the fact that spectacular progresses have been accomplished in the context of computational mechanics in the last decades, the treatment of those models, as we describe in the present work, requires further developments.

The brut force approach cannot be considered as a possibility for treating this kind of models. Thus, in the context of quantum chemistry, the Nobel Prize laureate R.B. Laughlin, affirmed that no computer existing, or that will ever exist, can break the barriers found in the solution of the Schrödinger equation in multi-particle systems, because of the multidimensionality of this equation [15].

We can understand the catastrophe of dimension by assuming a model defined in a hyper-cube in a space of dimension D, $\Omega =]-L, L[^D$. In fact, if we define a grid to discretize the model, as it is usually performed in the vast majority of numerical methods (finite differences, finite elements, finite volumes, spectral methods, etc.), consisting of N nodes on each direction, the total number of nodes will be N^D. If we assume that for example $N \approx 10$ (an extremely coarse description) and $D \approx 80$ (much lower than the usual dimensions required in quantum or statistical mechanics), the number of nodes involved in the discrete model reaches the astronomical value of 10^{80} that represents the presumed number of elementary particles in the universe! Thus, progresses on this field need the proposal of new ideas and methods in the context of computational physics.

A first solution is the use of sparse grids methods [8], however as argued in [1], this strategy fails when it applies for the solutions of models defined in spaces whose dimension are about 20.

Another possible alternative for circumventing, or at least alleviating the curse of dimensionality issue, consists of using separated representations within the context of the so-called Proper Generalized Decomposition. We proposed recently a technique able to construct, in a completely transparent way for the user, the separated representation of the unknown field involved in a partial differential equation. This technique, originally described and applied to multi-bead-spring FENE models of polymeric systems in [3], was extended to transient models of such complex fluids in [4]. Other more complex models (involving different couplings and non-linearities) based on the reptation theory of polymeric liquids were analyzed in [17]. This technique was also applied in the fine description of the structure and mechanics of materials [11], including quantum chemistry [2], and in materials homogenization [12]. Some numerical results concerning this kind of approximation were addressed in [22] and [7].

Basically, the separated representation of a generic function $u(x_1, \ldots, x_D)$ (also known as finite sums decomposition) writes:

$$u(x_1, \ldots, x_D) \approx \sum_{i=1}^{i=N} F_1^i(x_1) \times \cdots \times F_D^i(x_D) \tag{1}$$