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An overview of the proper generalized decomposition with applications in computational rheology

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ABSTRACT

We review the foundations and applications of the proper generalized decomposition (PGD), a powerful model reduction technique that computes *a priori* by means of successive enrichment a separated representation of the unknown field. The computational complexity of the PGD scales linearly with the dimension of the space wherein the model is defined, which is in marked contrast with the exponential scaling of standard grid-based methods. First introduced in the context of computational rheology by Ammar et al. [3,4], the PGD has since been further developed and applied in a variety of applications ranging from the solution of the Schrödinger equation of quantum mechanics to the analysis of laminate composites. In this paper, we illustrate the use of the PGD in four problem categories related to computational rheology: (i) the direct solution of the Fokker-Planck equation for complex fluids in configuration spaces of high dimension, (ii) the development of very efficient non-incremental algorithms for transient problems, (iii) the fully three-dimensional solution of problems defined in degenerate plate or shell-like domains often encountered in polymer processing or composites manufacturing, and finally (iv) the solution of multidimensional parametric models obtained by introducing various sources of problem variability as additional coordinates.

1. Introduction

The direct solution of many problems in scientific computing has long been thought intractable in view of the so-called curse of dimensionality. Consider for example the quantum-mechanical description of a physical system made of N particles. The evolution of the associated wavefunction is governed by the Schrödinger equation (or its relativistic Dirac counterpart). This defines a transient problem to be solved in a space of dimension $d = 3N + 1$. A typical grid-based discretization with M nodes for each coordinate would yield a total number of discrete unknowns of order M^d. A rather coarse discretization ($M = 10^3$) of a modest atomic system ($d = 30$) would thus involve 10^{90} unknowns. This is a gigantic number indeed, larger than the presumed number 10^{80} of elementary particles in the universe, according to the estimate put forward in the 1920s by the famous astronomer A.S. Eddington.

Problems defined in high-dimensional spaces abound. For example, the atomistic and mesoscopic models of theoretical rheology usually involve a large number of configurational coordinates. They thus also constitute a rich source of mathematical problems defined in high-dimensional spaces. In particular, coarse-grained models of kinetic theory result in a Fokker-Planck equation for the distribution function that must be solved in both configuration space, physical space and temporal domain. Until recently, the *direct* numerical solution of the Fokker-Planck equation has been limited to models having but few (2 or 3) configurational degrees of freedom (see e.g. the review [22]).

In two recent papers [3,4], we have proposed a technique able to circumvent, or at least alleviate, the curse of dimensionality. This method is based on the use of separated representations. It basically consists in constructing by successive enrichment an approximation of the solution in the form of a finite sum of N functional products involving d functions of each coordinate. In contrast with the shape functions of classical methods, these individual functions are unknown *a priori*. They are obtained by introducing the approximate separated representation into the weak formulation of the original problem and solving the resulting non-linear equations. If M nodes are used to discretize each coordinate, the total number of unknowns amounts to $N \times M \times d$ instead of the M^d degrees of free-

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dom of classical mesh-based methods. Thus, the complexity of the method grows linearly with the dimension d of the space wherein the problem is defined, in vast contrast with the exponential growth of classical mesh-based techniques.

In [3], for example, this new technique has allowed us to compute solutions of the Fokker-Planck equation in configuration spaces of dimension 20 using the multi-bead-FENE spring model of dilute polymer solutions.

The method was later coined proper generalized decomposition (or PGD), as in many cases the number N of terms in the separated representation needed to obtain an accurate solution is found to be close to that of the optimal decomposition obtained by applying *a posteriori* the proper orthogonal decomposition to the problem solution.

The goal of the present review paper is twofold. First, we wish to describe the PGD with sufficient detail and generality in order to allow the interested reader to grasp its main features and to implement it for her or his particular application. Second, we illustrate recent developments of the PGD for the solution of four problem categories that are typical of computational rheology: (1) the direct solution of the Fokker-Planck equation for complex fluids in configuration spaces of high dimension, (2) the development of very efficient non-incremental algorithms for transient problems, (3) the fully three-dimensional solution of problems defined in degenerate plate or shell-like domains often encountered in polymer processing or composites manufacturing, and finally (4) the solution of multidimensional parametric models obtained by introducing various sources of problem variability as additional coordinates. We also point to the recent literature where other applications of the PGD have been reported.

Use of the PGD is by no means restricted to computational rheology. In fact, each of the above problem categories instantiates a significant challenge in scientific computing that the PGD can address efficiently whereas standard techniques either cannot be used at all or are computationally very expensive indeed:

(1) Quantum mechanics and molecular modeling of complex fluids are not the only branches of science that suffer from the curse of dimensionality. Consider for example a chemical process involving so few molecules of the reacting species that use of the continuum concept of concentration is not valid. This situation is often found in genetic processes such as expression of genes. The state of such a discrete system is given by a probability distribution for the number of individual molecules of each one of the d coexisting species. The balance equation governing the evolution of the system, the so-called master equation, is again defined in a high-dimensional space that prevents direct solution by means of standard grid-based techniques. There are of course alternative methods to address these high-dimensional problems indirectly, stochastic simulations being one of the foremost approaches. Stochastic techniques have their own challenges, however. While variance reduction is always an issue, it is impossible with a stochastic technique to implement parametric or sensitivity studies that go beyond the brute force approach of computing a large number of expensive, individual simulations.

(2) The second problem category involves time-dependent problems not necessarily defined in high-dimensional spaces, but whose spectrum of characteristic times is so wide that standard incremental time discretization techniques cannot be applied. In such cases, the time step is extremely small as a consequence of numerical stability requirements. Thus, simulations over the much larger time interval of interest, which typically requires the solution of a large linear algebraic system at each time step, simply become impossible. Multiscale models involving a wide range of characteristic times abound in many fields. Reaction-diffusion models of the degradation of plastic materials, for example, describe chemical reactions occurring within microseconds coupled to diffusion of chemical substances that takes place over years.

(3) Problems of the third category are defined in degenerate geometrical domains. By this we mean that at least one of the characteristic dimensions of the domain is smaller by several orders of magnitude than the others. This is the case of bar, plate or shell-like domains typical of materials processing applications. In simple situations, such problems are readily transformed into reduced, one or two-dimensional approximate theories (e.g. the classical elastic plate theory). When geometrical or material non-linearities are present, however, it is usually impossible to derive lower-dimensional models of sufficient validity. Standard grid-based discretization methods then quickly become impractical, in view of the compulsory discretization of the small length scales that yield extremely fine meshes.

(4) Finally, many problems in process control, parametric modeling, inverse identification, and process or shape optimisation, usually require, when approached with standard techniques, the direct computation of a very large number of solutions of the concerned model for particular values of the problem parameters. Consider for example the optimization of a pultrusion process where optimal parameter values must be determined for process operating conditions (e.g. pultrusion speed, position and temperature of heaters) and material properties (e.g. thermal and rheological properties of the resin). Clearly, it would be useful to be able to simulate this process *at once* for *all* values of these parameters within a prescribed interval, and then perform data mining within this rather general solution to identify optimal values. As we shall see, this can be achieved with the PGD by viewing all sources of problem variability as additional coordinates of a higher-dimensional problem.

The paper is organized as follows. We begin with a brief discussion of model reduction and illustrate the use of the standard POD technique to build a reduced-order model *a posteriori*. The PGD is then described at a glance in Section 3. Technical details are given in Section 4 for the solution of a parametric heat transfer problem. The four problem categories are further discussed in Section 5, and their individual PGD treatment is illustrated in the four subsequent sections.

2. Model reduction: information versus relevant information

Consider a mesh having M nodes, and associate to each node an approximation function (e.g. a shape function in the framework of finite elements), we implicitly define an approximation space wherein a discrete solution of the problem is sought. For a transient problem, one must thus compute at each time step M values (the nodal values in the finite element framework). For non-linear problems, this implies the solution of at least one linear algebraic system of size M at each time step, which becomes computationally expensive when M increases.

In many cases, however, the problem solution lives in a subspace of dimension much smaller than M, and it makes sense to look for a reduced-order model whose solution is computationally much cheaper to obtain. This constitutes the main idea behind the proper orthogonal decomposition (POD) reduced modeling approach, which we revisit in what follows.