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Proper Generalized Decomposition based dynamic data-driven control of thermal processes ☆

Ch. Ghnatios [a], F. Masson [a], A. Huerta [b], A. Leygue [a], E. Cueto [c,*], F. Chinesta [a]

[a] EADS Corporate Foundation International Chair, GEM, UMR CNRS-Centrale Nantes, 1 rue de la Noe, BP 92101, F-44321 Nantes cedex 3, France
[b] Laboratori de Calcul Numeric, Universitat Politècnica de Catalunya, Jordi Girona, 1 Campus Nord, C2, E-08034 Barcelona, Spain
[c] Aragon Institute of Engineering Research, Universidad de Zaragoza, María de Luna, 7, E-50018 Zaragoza, Spain

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ABSTRACT

Dynamic Data-Driven Application Systems—DDDAS—appear as a new paradigm in the field of applied sciences and engineering, and in particular in Simulation-based Engineering Sciences. By DDDAS we mean a set of techniques that allow to link simulation tools with measurement devices for real-time control of systems and processes. In this paper a novel simulation technique is developed with an eye towards its employ in the field of DDDAS. The main novelty of this technique relies in the consideration of parameters of the model as new dimensions in the parametric space. Such models often live in highly multidimensional spaces suffering the so-called curse of dimensionality. To avoid this problem related to mesh-based techniques, in this work an approach based upon the Proper Generalized Decomposition—PGD—is developed, which is able to circumvent the redoubtable curse of dimensionality. The approach thus developed is composed by a marriage of DDDAS concepts and a combination of PGD “off-line” computations, linked to “on-line” post-processing. In this work we explore some possibilities in the context of process control, malfunctioning identification and system reconfiguration in real time, showing the potentialities of the technique in real engineering contexts.

1. Introduction: Dynamic Data-Driven Application Systems (DDDAS)

Traditionally, Simulation-based Engineering Sciences (SBES) relied on the use of static data inputs to perform the simulations. These data could be parameters of the model(s) or boundary conditions, outputs at different time instants, etc., traditionally obtained through experiments. The word static is intended here to mean that these data could not be modified during the simulation.

A new paradigm in the field of applied sciences and engineering has emerged in the last decade. Dynamic Data-Driven Application Systems (DDDAS) constitute nowadays one of the most challenging applications of SBES. By DDDAS we mean a set of techniques that allow the linkage of simulation tools with measurement devices for real-time control of simulations and applications. As defined by the US National Science Foundation, “DDDAS entails the ability to dynamically incorporate additional data into an executing application, and in reverse, the ability of an application to dynamically steer the measurement process” [37].

The term Dynamic Data-Driven Application System was coined by Darema in a NSF workshop on the topic in 2000 [36]. The document that initially put forth this initiative stated that DDDAS constitute “application simulations that can dynamically accept and respond to ‘online’ field data and measurements and/or control such measurements. This synergistic and symbiotic feedback control loop among applications, simulations, and measurements is a novel technical direction that can open new domains in the capabilities of simulations with a high potential pay-off, and create applications with new and enhanced capabilities. It has the potential to transform the way science and engineering are done, and induces a major beneficial impact in the way many functions in our society are conducted, such as manufacturing, commerce, transportation, hazard prediction/management, and medicine, to name a few” [14].

The importance of DDDAS in the forthcoming decades can be noticed from the NSF Blue Ribbon Panel on SBES report [33], that in 2006 included DDDAS as one of the five core issues or challenges in the field for the next decade (together with multiscale simulation, model validation and verification, handling large data and visualization). This panel concluded that “Dynamic Data-Driven Application Systems will rewrite the book on the validation and

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* Corresponding author.
E-mail addresses: antonio.huerta@upc.es (A. Huerta), ecueto@unizar.es (E. Cueto), Francisco.Chinesta@ec-nantes.fr (F. Chinesta).

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verification of computer predictions" and that "research is needed to effectively use and integrate data-intensive computing systems, ubiquitous sensors and high-resolution detectors, imaging devices, and other data-gathering storage and distribution devices, and to develop methodologies and theoretical frameworks for their integration into simulation systems" [33]. Moreover, the NSF believes that "...The DDDAS community needs to reach a critical mass both in terms of numbers of investigators, and in terms of the depth, breadth and maturity of constituent technologies..." [37].

A DDDAS includes different constituent blocks:

(1) A set of (possibly) heterogeneous simulation models.
(2) A system to handle data obtained from both static and dynamic sources.
(3) Algorithms to efficiently predict system behaviour by solving the models under the restrictions set by the data.
(4) Software infrastructure to integrate the data, model predictions, control algorithms, etc.

Almost a decade after the establishment of the concept, the importance of the challenge is better appreciated. As can be noticed, it deals with very different and transversal disciplines: from simulation techniques, numerical issues, control, modelling, software engineering, data management and telecommunications, among others. The three different blocks of interactions concern: (i) the one between human systems and the simulation, (ii) the simulation interaction with the physical system and (iii) the simulation and the hardware/ data infrastructure. Physical systems operate at very different time scales: from 10^{-20} Hz for cosmological systems to 10^{20} Hz for problems at the atomic scales. Humans, however, can be considered as a system operating at rates from 3 Hz to 500 Hz in haptic devices for instance to transmit realistic touch sensations. A crucial aspect of DDDAS is that of real-time simulation. This means that the simulations must run at the same time (or faster) than data are collected. While this is not always true (as in weather forecasting, for instance, where collected data are usually incorporated to the simulations after long time periods), most applications require different forms of real-time simulations. In haptic surgery simulators, for instance, the simulation result, i.e., forces acting on the surgical tool, must be translated to the peripheral device at a rate of 500 Hz, which is the frequency of the free hand oscillation. In other applications, such as some manufacturing processes, the time scales are much bigger, and therefore real-time simulations can last for seconds or minutes.

As can be noticed from the introduction above, DDDAS can revolutionize the way in which simulation will be done in the next decades. No longer a single run of a simulation will be considered as a way of validating a design on the basis of a static data set [33].

While research on DDDAS should involve applications, mathematical and statistical algorithms, measurement systems, and computer systems software methods, see for instance [16,17,21,28,29], our work focuses on the development of mathematical and statistical algorithms for the simulation within the framework of such a system. In brief, we intend to incorporate a new generation of simulation techniques into the field, allowing to perform faster simulations, able to cope with uncertainty, multiscale phenomena, inverse problems and many other features that will be discussed. This new generation of simulation techniques has received the name of Proper Generalized Decomposition—PGD—and has received an increasing level of attention by the SBES community. PGD was initially introduced for addressing multidimensional models encountered in science and engineering (see [1,2] and the references therein) and was then extended to address general computational mechanics models [10]. We are revisiting the motivation and the key ideas of such technique in the next sections.

1.1. When the solution of many direct problems is needed

An important issue encountered in DDDAS, related to process control and optimization, inverse analysis, etc., lies in the necessity of solving many direct problems. Thus, for example, process optimization implies the definition of a cost function and the search of optimum process parameters, which minimize the cost function. In most engineering optimization problems the solution of the model is the most expensive step. Real-time computations with zero-order optimization techniques can not be envisioned except for very particular cases. The computation of sensitivity matrices and adjoint approaches also hampers fast computations. Moreover, global minima are only ensured under severe conditions, which are not (or cannot be) verified in problems of engineering interest. There are many strategies for updating the set of design parameters and the interested reader can find most of them in books focusing on optimization procedures. Our interest here is not the discussion on optimization strategies, but pointing out that standard optimization strategies need numerous direct solutions of the problem that represents the process, one solution for each tentative choice of the process parameters, plus those required for sensitivity.

As we discussed in the previous paragraphs, the solution of the model is a tricky task that demands important computational resources and usually implies extremely large computing times. Usual optimization procedures are inapplicable under real-time constraints because they need numerous solutions. The same issues are encountered when dealing with inverse analysis in which material or process parameters are expected to be identified from numerical simulation, by looking for the unknown parameters such that the computed fields agree in minute with the ones measured experimentally. However, some previous references exist on the treatment of problems that require extensive solution procedures for different parameter values. The interested reader can consult, for instance [6,7,20].

1.2. Towards generalized parametric modelling

One possibility for solving many problems very fast consists of using some kind of model order reduction based on the use of reduced bases [18,34]. In these works authors proved the capabilities of performing real time simulation even using light-computing devices, as smartphones for example. The tricky point in such approaches is the construction of such reduced bases and the way of adapting them when the system explores regions far from the ones considered in the construction of the reduced model. Solutions to this issue exist and others are been developed to fulfil with real time requirements.

Multidimensionality offers an alternative getaway to avoid too many direct solutions. In our opinion it could represent a new paradigm in computational mechanics. For the sake of clarity, the use of multidimensional modelling in an academic physical problem is illustrated and motivated.

Imagine for example that we are interested in solving the heat equation but the material's thermal conductivity is not known, because it has a stochastic nature or simply because prior to solve the thermal model it is necessary to measure it experimentally. Three possibilities arise: (i) wait to know the conductivity before solving the heat equation (a conservative solution); (ii) solve the equation for many values of the conductivity (a sort of Monte Carlo method); or (iii) solve the heat equation only once for any value of the conductivity.

Obviously the third alternative is the most appealing one. To compute this quite general solution it suffices to introduce the conductivity as an extra independent coordinate, taking values in a certain interval and playing a similar role as standard space and