**Theme:** BRICKS

**Axis:** Processes

**Project:** Advanced simulation of processes

**Summary:** PGD-based model reduction - Understanding physics and controlling processes from robust numerical simulation performed in real-time on deployed platforms.

**Project code:** B/P/3

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**Context:**

Many problems in science and engineering remain intractable, in spite of the impressive progress made in mechanical modelling, numerical analysis, discretization techniques and computer science during the past decade, because their numerical complexity is simply unimaginable.

We can distinguish different challenging scenarios for efficient numerical simulations concerning by the five year research project that we are proposing:

- The first one concerns models that are defined in high dimensional spaces, usually encountered in quantum chemistry and kinetic theory descriptions of complex fluids [B/P/3-1]. Model defined in high dimensional spaces suffer from the so-called curse of dimensionality. If one proceeds to the solution of a model defined in a space of dimension *N*, by using a standard mesh based discretization technique, where *M* nodes are used for discretizing each space coordinate, the resulting number of nodes reaches the astronomical value of . With (a very coarse description in practice) and (a very simple model) the numerical complexity results . It is important at this point to remember that is the presumed number of elementary particles in the universe! But 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 that involves so few molecules from the reacting species that the use of the continuum concept of concentration is not valid. The state of such a discrete system is given by a probability distribution for the number of individual molecules of each one of the coexisting species. The balance equation governing the evolution of the system, the so-called chemical master equation, is again defined in a high-dimensional space that prevents direct solution by means of standard grid-based techniques.
- 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 with the diffusion of chemical substances taking place over years. In processes involving microwaves, ultrasounds, etc. or materials exhibiting different relaxation times, the difficulty related to time integration is crucial.

- Real-time simulators are needed in many applications, like when we consider haptic devices, where forces must be translated to the peripheral device at a rate of 500 Hz. Control, malfunctioning identification and reconfiguration of malfunctioning systems also need to run in real-time.
- Problems of the fourth category are defined in degenerate geometrical domains. By this we mean to say 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 that are 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. Consequently, standard grid-based discretization methods quickly become impractical, in view of the compulsory discretization of the small length scales that yield extremely fine meshes.
- Many problems in process control, parametric modeling, inverse identification and process or shape optimization, 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 process where optimal parameter values must be determined for process operating conditions (e.g. speed, position and the temperature of heaters) and material properties (e.g. thermal and rheological properties of the materials). 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.
- Traditionally, Simulation-based Engineering Sciences – SBES- relied on the use of *static* data inputs to perform the simulations. This data could be parameters of the model(s) or boundary conditions. The word *static* is intended to mean here that this 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. Nowadays, *Dynamic Data-Driven Application Systems* (DDDAS) constitute one of the most challenging applications of simulation-based Engineering Sciences. By DDDAS we mean a set of techniques that allow the linkage of simulation tools with measurement devices for real-time control of simulations. 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 [B/P/3-2-B/P/3-5].
- Augmented reality is another area in which efficient (fast and accurate) simulation is urgently needed. The idea is to supply appropriate information in real-time to the reality perceived by the user. Augmented reality could be an excellent tool in many branches of science and engineering.
- Light computing platforms are appealing alternatives to heavy computing platforms that in general are expensive and whose use requires technical knowledge. One can imagine that the *off-line* parametric solution of many models will make the *on-line* manipulation of those general solutions possible by using very light computing platforms like smartphones.

**Research project:**

The main objective of the present research project is to address the modeling and simulation of “real” models encountered in material forming processes with all their complexity from the geometrical and constitutive points of view, some of which have not, at present, been solved because their computational complexity. These models should be solved very fast, in some cases in real time, by using light computing platforms. Classical simulation techniques fail to fulfill the above requirements. An appealing alternative consists in considering *off-line* solutions of parametric models, in which all the sources of variability – loads, boundary conditions, material parameters, geometrical parameters, etc. - will be considered as extra-coordinates. Thus, by solving the resulting multidimensional model only once, we have access to the solution of the model for any value of the parameters considered as extra-coordinates. Now, from this general solution computed only once and off-line we could perform on-line real time post-processing, optimization, inverse analysis, analysis of sensibilities, stochastic analysis … by using very light computing platforms like smartphones. We could also adapt the model on-line while its simulation is running within the framework of dynamic data-driven application systems – DDDAS. The price to be paid is the solution of parametric models defined in high dimensional spaces that could involve hundreds of coordinates. The use of the Proper Generalized Decomposition that we recently proposed and we are intensively developing, allows such a solution, because thanks to the separated representation of the unknown fields the computational complexity scales linearly with the dimensionality, instead of growing exponentially which is characteristic of mesh-based discretization techniques. This off-line-on-line Proper Generalized Decomposition Based Dynamic Data-Driven Application Systems could constitute a new paradigm in computational sciences. Some progress in these directions has already been achieved (see [B/P/3-6-B/P/3-14] and the references therein) constituting the starting point of the proposed research project.

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