S20. Model Order Reduction and Highly Demanding Applications

Organizers:

- Ferdinando Auricchio (University of Pavia, Italy)
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Speakers:

1. Pedro Díez (UPC-BarcelonaTech, Spain)
   Reduced order modeling of parametrized geometrical boundaries and internal interfaces
2. David González (Universidad de Zaragoza, Spain)
   Real-time direct integration of reduced solid dynamics equations
3. Gerard J. Gorman (Imperial College, London, UK)
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4. Elie Hachem (MINES ParisTech, Sophia-Antipolis, France)
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Proper Generalized Decomposition of geometrical parametrization of boundaries and internal interfaces: multidimensional parametric problems for inverse problems and uncertainty quantification

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Inverse problems to identify the geometry of internal interfaces are very common in geophysics but also in many other disciplines. For instance, aiming at identifying geological structures from surface thermal measurements. Facing this problem requires having the possibility of testing a very large number of geometric configurations combined with a variety of different material parameters (thermal diffusivity). The number of problems explodes with number of free parameters, suggesting the use of reduced order models. We explore the use of PGD in this context, introducing the separable approximations in both the geometric and the material parameters. The PGD approach results extremely efficient in this context, producing a computational vademecum that transforms the inverse problem into a simple functional exploration.

Real-time direct integration of reduced solid dynamics equations: A PGD-POD framework

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Using a model order reduction technique, like Proper Generalized Decomposition (PGD), and with a traditional discretization in time of dynamics equations we obtain a very efficient method for real-time direct integration of reformulated solid dynamics equations in a multidimentsional form.

We pre-compute a meta-model of the system for any initial values and for any type of force in an off-line previous stage. With this PGD solution we obtain the system response for very large time intervals without lost of accuracy and in a real time (on-line stage). In order to alleviate the degrees of freedom of the system, a combination methodology between PGD-POD is proposed in this work.

The behaviour of the technique is tested in several examples, focused on the number of modes of the POD approximation used, for optimal accuracy.

In our webpage, `http://amb.unizar.es/beamdyn.htm`, it is possible to play with a cantilever beam under dynamic behaviour for any posible location of the load.

Fast scalable mesh coarsening for geometric multigrid preconditioning

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Computing hardware is currently undergoing a rapid transformation from the historical trend of increasingly complex single processing units operating at ever increasing clock frequency, towards high numbers of low power processing units where computing throughput is achieved by increasing concurrency. The consequence for models is that their constituent algorithms must be amenable to parallelization, otherwise the (quasi-)serial section will quickly become the dominant computational cost. In short, algorithms without a high degree of parallelism will rapidly become impractical. Luckily many algorithms, such as matrix-vector multiplication, are readily parallelizable on many levels and lots of effort is going into optimal strategies on a range of different types of architectures. However, other key algorithms, such as many preconditioners in iterative solvers, have complex data interdependencies and access patterns and the overhead associated with parallelization can easily outweigh the gains.

In this work we investigate the challenges with parallelizing unstructured mesh coarsening as part of a geometric multi-grid preconditioner. Geometric (and algebraic) multigrid methods are highly effective at accelerating solver convergence in systems exhibiting multiple scales of behavior. Previous work in this field has mostly been limited to domain decomposition methods implemented using MPI. The disadvantage with this is that the work on the multi-core or many-core host is still essentially serial - and therefore a performance bottleneck in applications already capable of exploiting multi-/many-core architectures. We present a number of parallel strategies and their implementation in C++ for mesh coarsening that exploit both domain decomposition methods with MPI and thread-parallelism. Performance analysis shows that fast scalable performance is achieved but there is still room for improvement. We will consider what novel trends in parallel programming models and hardware might create new opportunities for further performance and efficiency gains.

Computational Fluid Dynamics with high performance parallel computing

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Aerodynamic characteristics of various 3D geometries are predicted using a parallel finite element code coupled with several numerical techniques to ensure stability and accuracy. First, an edge based error estimator and dynamic anisotropic parallel mesh adaptation are used for detecting sharp gradients, inner and boundary layers under the constraint of a fixed number of elements, thus controlling the computational cost. Then a Variational MultiScale (VMS) stabilized finite element method is employed to solve the incompressible Navier-Stokes equations [1]. The basic idea is to consider that the unknowns can be split in two components, coarse and fine, corresponding to different scales or levels of resolution. By solving first the fine scales and then replacing their effect into the large scales, we obtain a new system that acts as an implicit Large Eddy Simulation (ILES). However, it requires tuning of the stabilization coefficients in both the convective and diffusive terms to take into account highly stretched elements with an anisotropic ratio of the order of $O(1 : 1000)$.

Finally, the interested part of this talk, we want to verify how accurate the Parallel Programming and Computing Platform may become combining anisotropic unsteady mesh adaptation with the ILES method and how the solution behaves in particular near the boundary layers when compared to DNS results. Therefore, several test cases and confrontation with literature are proposed. The simulation of flows past a 3D F1 car, a large scale airship, a wind turbine and a drone with complex geometries will highlight the capability of the proposed techniques.

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Stochastic parameters estimation in dynamical systems from observations: general framework and applications

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Stochastic ordinary and partial differential equations are of a great interest to describe random phenomena in dynamical systems in different applicative fields, from physics to engineering and biology. Randomness can be considered in different parts of the differential equation, i.e., coefficients, forcing terms, initial and boundary conditions. Moreover, their use for reverse engineering problems, i.e., problems where available measurements are converted into knowledge of parameters of the physical system that are not directly observable, is also important.

In this talk, I present a Bayesian approach to estimate the posterior probability density functions of model parameters given observations of the state variables, and to generate latent data for missed measurements of some state variables at some time instants. Briefly, the ordinary or partial differential equation or system is discretized, and the conditioned density of each state variable at each time instant given the previous instant is obtained. Then, the likelihood function is derived from the conditioned densities, and the posterior distribution of parameters is obtained by means of the Bayes' theorem (analytically or with an iterative Gibbs sampler). In the case that latent data are also generated, an iterative Metropolis-Hastings algorithm is included to simulate data at each time instant, based on a proposal density function and an acceptance/rejection mechanism. I also present some applications of the approach and the results in several fields: biomechanics (non-invasive estimation of the aortic stiffness given computed tomography angiography images, and inertance estimation in a mock loop system that in-vitro replicates human vasculature), heat transfer (procedure coupled with an experimental layout to jointly estimate the thermal conductivity of a specimen and to reproduce the entire temperature profile evolution over time by means of generated latent temperatures), dialysis (estimation of patient-specific clinical parameters to optimize dialysis treatments), and manufacturing (estimation of energy consumption in machining and definition of the experiments to get a significant dataset for the estimation).

A separated representation of the discretization error under the Proper Generalized Decomposition framework

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A powerful method to deal with high dimensional problems is the Proper Generalized Decomposition (PGD) [1], based on the use of a separated representation strategy. The PGD technique requires of verification procedures in order to guarantee the quality of the solution. However, we are facing two main sources of error. The first one is due to the truncation of the separate representation of the solution. The second one is due to the discretization used to evaluate each mode of the solution. Each mode is obtained via a numerical approach, i.e. the Finite Element Method (FEM).

In this contribution we propose a technique which is able to provide a local error indicator into each discretization space, separately, for locally adapt the mesh. In this case, the quantity to estimate is the error, in L_2-norm, between an improved flux field and the flux obtained with the numerical approach, using the ideas presented by Zienkiewicz and Zhu [2]. The improved solution will be obtained with a smoothing process applied to the flux provided by the FEM solution.

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One-dimensional surrogate models generated via a Hi-Mod reduction approach

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Many applications in scientific computing demand for surrogate models, i.e., simplified models which are expected to be computationally affordable and reliable from a modeling viewpoint. In this presentation we focus on surrogate models fitted to deal with problems characterized by an intrinsic directionality, with transverse components relevant locally. Well-established examples are the modeling of the blood flow in arteries, of the air pressure forces in internal combustion engines, of the water flow in a river network.

The idea of Hierarchical Model (Hi-Mod) reduction is essentially to discretize the full model via a combination of a standard 1D finite element approximation along the leading direction combined with a modal expansion for the transverse dynamics [**?**]. This leads to a hierarchy of 1D models solved along the mainstream, whose coefficients are suitably tuned to include the possible presence of significant local transverse information. The models of the hierarchy differ essentially for the level of detail in describing the transverse dynamics, i.e., for the number of modal functions included in the modal expansion. The type (sinusoidal functions, Legendre polynomials, suitable eigenfunctions) as well as the number of the modal functions to be included in a Hi-Mod expansion represent a crucial issue of this approach. In [**?**], we propose an automatic procedure to select the number of transverse modes, moving from a modeling *a posteriori* error estimator. The appropriate selection of the modal functions in 3D problems (in slabs as well as cylindrical domains) is a crucial issue in view of CFD applications and it is currently under investigation.

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Model reduction for parameter estimation in computational hemodynamics

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With the progressive inclusion of numerical simulations in medical research and clinical practice, accuracy and reliability of a patient-specific computational analysis need to be properly certified. This raises new challenges when estimating patient-specific parameters that may be too difficult or even impossible to measure in practice. Data assimilation techniques are required to merge available data and numerical models to assess the reliability of a quantitative analysis [1]. In this talk, variational procedures will be considered to estimate (a) vascular compliance from available measures of displacement [2, 3]; (b) cardiac conductivities from available measures of cardiac potentials [4]. In particular, we pursue variational techniques based on a constrained minimization approach, the constraint being represented by the fluid-structure interaction vascular problem or by the Bidomain equations for electrocardiology. In general, these techniques lead to high computational costs and proper methods for the sake of computational efficiency need to be adopted. We consider in particular both methods based on simplified models for the forward problem (like the Monodomain equation) or on surrogate solutions obtained on the basis of the offline/online paradigm, like the Proper Orthogonal Decomposition method (POD).

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