

IHP QUARTER ON NUMERICAL METHODS FOR PDES

ME3 RECENT DEVELOPMENTS IN NUMERICAL METHODS FOR MODEL REDUCTION

IHP, Paris, France, 7-10 November 2016

Workshop Organizers:

Tony Lelièvre (ENPC PariTech, CERMICS),

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Steering committee: D. A. Di Pietro, A. Ern, L. Formaggia

IHP QUARTER ON NUMERICAL METHODS FOR PDES

Numerical Analysis applied to the approximate solution of PDEs is a key discipline in Applied Mathematics.

Over the last few years, several new paradigms have appeared, leading to entire new families of discretization methods and solution algorithms. Simultaneously, the increased complexity of the underlying physical problems and the need to use simulators in many-query scenarios has prompted the study of model reduction techniques. Finally, a whole new approach to solution algorithms and adaptivity has been made possible by the recent advances in the context of a posteriori error analysis. The goal of this thematic quarter is to provide an opportunity to bring together leading scientists in the field of Numerical Analysis to discuss and disseminate the latest results and envisage new challenges in traditional and new application fields.

IHP QUATER ORGANIZATION

Steering committee: D. A. Di Pietro (coordinator), A. Ern, L. Formaggia

Scientific committee: R. Herbin, Y. Maday, D. Marini, R. Verfürth

Organizing committee: P. F. Antonietti, S. Cordier, J. Droniou, R. Eymard, R. Fontanges, T. Lelièvre, B. Mohammadi, S. Perotto, G. Rozza.

ME3

INVITED SPEAKERS

(Ordered according the programme)

Model Order Reduction in the factory of the future: from data to knowledge

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Abstract

Big Data has bursted in our lives in many aspects, ranging from e-commerce to social sciences, mobile communications, healthcare, etc. However, very little has been done in the field of scientific computing, despite some very promising first attempts. Engineering sciences, however, and particularly Integrated Computational Materials Engineering (ICME), seem to be a natural field of application. In the past, models were more abundant than data, too expensive to be collected and analyzed at that time. However, nowadays, the situation is radically different, data is much more abundant (and accurate) than existing models, and a new paradigm is emerging in engineering sciences and technology. Advanced clustering techniques, for instance, not only help engineers and analysts, they become crucial in many areas where models, approximation bases, parameters, etc. are adapted depending on the local state (in space and time senses) of the system. They make possible to define hierarchical and goal-oriented modeling. Machine learning needs frequently to extract the manifold structure in which the solution of complex and coupled engineering problems is living. Thus, uncorrelated parameters can be efficiently extracted from the collected data, coming from numerical simulations or experiments. As soon as uncorrelated parameters are identified (constituting the information level), the solution of the problem can be predicted at new locations of the parametric space, by employing adequate interpolation schemes. On a different setting, parametric solutions can be obtained within an adequate framework able to circumvent the curse of dimensionality for any value of the uncorrelated model parameters. This unprecedented possibility of directly determine knowledge from data or, in other words, to extract models from experiments in a automated way, is being followed with great interest in many fields of science and engineering. In the present work we will assume that all the needed data is available. We will not address all the difficulties related to data generation from adequate experiments. This is a topic that, of course, remains open. On the contrary, we develop a method in which this stream of data plays the role of a constitutive equation, without the need of a phenomenological fitting to a prescribed model.

Reduced-order modeling for deterministic and stochastic anomalous diffusion problems

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Nonlocal models arise in a large number of applications such as the peridynamics model for solid mechanics, anomalous diffusion in subsurface flows, image processing, and machine learning. We consider a class of nonlocal models for diffusion having random input data, a model that includes fractional Laplacian equations as a special case. We briefly review the theory and approximation of the nonlocal models we employ. An important observation is that reduced-order modeling is even more useful for nonlocal models, compared to PDE models, due the reduced sparsity of the discrete systems corresponding to the former. We then use a reduced basis method for spatial approximation coupled to sparse grid stochastic collocation methods for stochastic approximation. Two reduced basis methods are constructed using a greedy algorithm. The well posedness of the problem and convergence results for numerical approximations are given and the efficiency of the methods developed are studied. Particular attention is paid to the effects of nonlocality on the complexity of the discretized systems. Numerical experiments are used to illustrate the theoretical results. (Joint work with Qingguang Guan, Clayton Webster, and Guannan Zhang.)

Localized Model Reduction Beyond Offline-Online Splitting

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Many physical, chemical, biological or technical processes can be described by means of partial differential equations. Due to nonlinear dynamics, interacting processes on different scales, and possible parametric or stochastic dependencies, an analysis and prediction of the complex behavior is often only possible – if at all – with severe simplifications. This is in particular true if not only single forward problems are considered, but beyond that uncertainty quantification, parameter estimation or optimization in engineering applications are investigated. A mathematical key ingredient to achieve "optimal" numerical methods is error control via rigorous a posteriori error estimates. Such error estimates can not only be used to certify approximate solutions, but rather are the essential building block in the construction of problem adapted optimal solution spaces and related adaptive numerical methods. Examples of such optimal methods are e.g. particularly tuned mesh-adaptive finite element schemes for the approximation of PDEs or reduced basis methods (week greedy algorithms) for the approximation of parameterized PDEs. In this talk we will address error control for localized model reduction methods and its usage for the construction of efficient numerical schemes for parameterized single and multiscale PDEs. Thereby we overcome the classical paradigm of offline-online splitting by allowing for arbitrary local modifications and local basis enrichment in the so called online-phase [1, 2, 3]. We also refer to [5, 6] for an alternative approach based on discontinuous global approximation spaces. Several numerical examples and applications will be shown to demonstrate the efficiency of the resulting adaptive approaches. The numerical results were obtained with the newly developed model reduction algorithms implemented in pyMOR (see <http://pymor.org> and [4]).

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Uncertainty Quantification cascade in optimization.

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We present an original framework for uncertainty quantification (UQ) in optimization. It is based on a cascade of ingredients with growing computational complexity for both forward and reverse uncertainty propagation. The approach is merely geometric. It starts with a complexity-based splitting of the independent variables and the definition of a parametric optimization problem. Geometric characterization of global sensitivity spaces through their dimensions and relative positions by the principal angles between global search subspaces bring a first set of information on the impact of uncertainties on the functioning parameters on the optimal solution. Joining the multi-point descent direction and the quantiles on the optimization parameters permits to define the notion of Directional Extreme Scenarios (DES) without a sampling of large dimension design spaces. One goes beyond DES with Ensemble Kalman Filters (EnKF) after the multi-point optimization algorithm is cast into an ensemble simulation environment. The UQ cascade ends with the joint application of the EnKF and DES leading to the concept of Ensemble Directional Extreme Scenarios (EDES) which provides more exhaustive possible extreme scenarios knowing the Probability Density Function of the optimization parameters. The presentation also makes the link with moment-based formulations considering the four first moments of the functionals. Sampling issues are also discussed and the procedure is shown to permit a quantification of our confidence level on the robustness of the design. The proposed algorithm is fully parallel and the time-to-solution is comparable to mono-point deterministic situations. The different ingredients are illustrated on aircraft shape design in the presence of operational and geometrical uncertainties. This is a data analytic ensemble and it can be applied to direct and reverse uncertainty quantifications for any complex system.

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Generalized parametric solutions in Stokes flow and complex domains

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Abstract

Design optimization and uncertainty quantification, among other applications of industrial interest, require fast or multiple queries of some parametric model. The Proper Generalized Decomposition (PGD) provides a separable solution, explicitly dependent on the parameters, efficiently computed with a greedy algorithm combined with an alternated directions scheme and compactly stored. This strategy has been successfully employed in many problems in computational mechanics. The application to problems with saddle point structure raises some difficulties requiring further attention. Here, a PGD formulation is proposed for the Stokes problem, one of the simplest equations with saddle point structure. The various possibilities of the separated forms of the PGD solutions are discussed and analyzed, selecting the more viable option. The efficacy of the proposed methodology is demonstrated in numerical examples for both Stokes and Brinkmann models. Moreover, complex geometries are also taking into account.

No equations, no variables, no parameters, no space, no time: Data and the computational modeling of complex/multiscale systems

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Abstract

Obtaining predictive dynamical equations from data lies at the heart of science and engineering modeling, and is the linchpin of our technology. In mathematical modeling one typically progresses from observations of the world (and some serious thinking!) first to equations for a model, and then to the analysis of the model to make predictions. Good mathematical models give good predictions (and inaccurate ones do not) - but the computational tools for analyzing them are the same: algorithms that are typically based on closed form equations.

While the skeleton of the process remains the same, today we witness the development of mathematical techniques that operate directly on observations -data-, and appear to circumvent the serious thinking that goes into selecting variables and parameters and deriving accurate equations. The process then may appear to the user a little like making predictions by "looking into a crystal ball". Yet the "serious thinking" is still there and uses the same -and some new- mathematics: it goes into building algorithms that "jump directly" from data to the analysis of the model (which is now not available in closed form) so as to make predictions. Our work here presents a couple of efforts that illustrate this "new path from data to predictions. It really is the same old path, but it is travelled by new means.

Structure preserving reduced order models

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Abstract

Reduced basis methods have emerged as a powerful approach for the reduction of the intrinsic complexity of parametrized partial differential equations. However, standard formulations of reduced models do not generally guarantee preservation of symmetries, invariants, and conservation laws of the original system. This questions the validity of such models and has a number of unfortunate consequences, e.g., lack of stability of the reduced model.

In this talk we discuss the recent development of reduced methods that ensures the conservation of chosen invariants. We shall pay particular attention to the development of reduced models for Hamiltonian problems and propose a greedy approach to build the basis. The performance of the approach is demonstrated for both ODEs and PDEs.

We subsequently discuss the extension of these techniques to ABC flows and, time permitting, outline an approach to develop structure preserving reduced models for nonlinear PDEs endowed with constraints.

Data assimilation, parameter estimation and reduced modeling

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This talk will address some recent mathematical advances on two problems which occur in parameter estimation in PDEs from observed data. The first one concerns the identifiability of the scalar diffusion coefficient a in the elliptic equation $-\operatorname{div}(a\nabla u) = f$ from the observation of the full solution u for a given right hand side f . Our main results show that for strictly positive right hand side, and a belonging in certain smoothness classes, identification is possible with Hölder dependence of a on u , and that Lipschitz dependence does not generally hold. The second problem concerns the recovery of the full solution u from a finite number of linear measurements representing the observed data. Motivated by reduced modeling, the a-priori additional information about u is in the form of how well it can be approximated by a certain known subspace of given dimension (reduced bases, POD). Algorithms that yield near optimal recovery bounds are proposed.

These results were obtained in collaborations with Peter Binev, Andrea Bonito, Wolfgang Dahmen, Ronald DeVore, Guergana Petrova, Gerrit Welper and Przemyslaw Wojtaszczyk.

On a goal-oriented formulation for model reduction methods

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The talk will deal with the development of a mathematical formulation aiming at constructing reduced-order models tailored for the approximation of quantities of interest. The main idea is to formulate a minimization problem subjected to an inequality constraint on the error in the goal functional so that the resulting model be capable of delivering predictions on the quantity of interest within some prescribed tolerance. The formulation will be applied to the so-called proper generalized decomposition (or a low-rank approximation) method. Such a paradigm represents a departure from classical goal-oriented approaches where the reduced model is first derived by minimization of the energy, or the residual functional, and subsequently adapted via a greedy approach by controlling a posteriori error estimates measured in terms of quantities of interest using dual-based error estimates. Numerical examples will be presented in order to demonstrate the efficiency of the proposed approach.

Large Eddy Simulation Reduced Order Models

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This talk proposes several large eddy simulation reduced order models (LES-ROMs) based on the proper orthogonal decomposition (POD). To develop these models, explicit POD spatial filtering is introduced. Two types of spatial filters are considered: A POD projection onto a POD subspace and a POD differential filter. These explicit POD spatial filters allow the development of two types of ROM closure models: phenomenological and approximate deconvolution. Furthermore, the explicit POD spatial filters are used to develop regularized ROMs in which various ROM terms are smoothed (regularized). The new LES-ROMs are tested in the numerical simulation of a three-dimensional flow past a circular cylinder at a Reynolds number $Re = 1000$.

Parametrized Model Order Reduction for Component-to-System Synthesis

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Abstract

In this talk we describe and demonstrate a model order reduction methodology for efficient treatment of large engineering systems with many (spatially distributed) parameters. The approach is relevant in many-query, real-time, and interactive contexts such as design, shape and topology optimization, parameter estimation, monitoring, reconditioning, and education.

The numerical approach comprises four principal ingredients: component-to-system synthesis, formulated as a static-condensation procedure; model order reduction, informed by evanescence arguments at component interfaces (port reduction) and low-dimensional parametric manifolds in component interiors (reduced basis techniques); offline-online computational decomposition strategies; and parallel calculation, implemented in a cloud environment. We provide examples in acoustics, linear elasticity, and also nonlinear elasticity.

Reduced-basis residual-minimization for parametrized PDEs in Banach-space settings

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7 Oct. 2016

We consider the reduced-basis approximation of parametrized solutions to linear operator equations in general (non-Hilbert) Banach-space settings. Such a setting is useful for PDEs with rough data or nonsmooth solutions.

To guarantee stable discretizations of the operator equation, we consider the recently introduced (nonstandard) nonlinear Petrov–Galerkin finite element method [1]. This method builds on ideas of residual minimization in dual spaces and the recent theory of optimal Petrov–Galerkin methods [2–4].

We demonstrate how a reduced-order model can be obtained, which is useful for solving the problem for many parameter values, by extending the reduced-basis approach [5,6] to this class of nonstandard discretizations.

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Hierarchical Model Reduction Methods for Incompressible Fluids: Basics, IsoGeometric formulation, Applications

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Abstract

Reduction of computational costs is becoming mandatory as scientific computing progressively becomes an important decision-making tool in engineering and practical daily activities. We mention in particular computational hemodynamics that has been incorporated in medical research and clinical practice and it is becoming an important part of Clinical Trials (CACT-Computer Aided Clinical Trials) and Surgical Planning (SP). In this respect, a possible way for reducing computational costs is to take advantage of the specific features of the problem at hand - as opposed to general purpose strategies. Specifically, we can devise methods for incompressible fluids in pipe-like domains. *Hierarchical Model-Reduction* (HiMod) is an approach [3] where the solution is properly split into mainstream and transverse components. The former is solved with finite elements [3, 5, 1] or iso-geometric analysis [4], to be versatile in following the centerline of the pipe; the latter is solved with spectral methods, to be able of capturing the significant features of the dynamics with relatively few (and adaptively) degrees of freedom [5]. We will present the basic features of this method at both the theoretical and practical level (selection of spectral basis, interplay with IGA, accuracy, etc.) and some preliminary results from cardiovascular applications that point out the excellent effectiveness of the approach [2]. This work is supported by the US National Science Foundation, DMS 1419060 in collaboration with *M. Aletti, L.A. Mansilla Alvarez, P.J. Blanco, S. Guzzetti, S. Perotto, A.Reali,P. Rusconi*

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ME3

CONTRIBUTED SPEAKERS

(Ordered according the programme)

Reduced Order Model Stabilization for Partial Differential Equations based on Lyapunov Theory and Extremum Seeking with Applications to the Burgers' and Boussinesq equations

Mouhacine Benosman

Abstract

The problem of reducing a partial differential equation (PDE) to a system of finite dimensional ordinary differential equations (ODE), is of paramount importance in engineering and physics where solving PDE models is often too time consuming. The idea of being able to reduce the PDE model to a simple ODE model, without losing the main characteristics of the original model, such as stability and prediction precision, is appealing for any real-time model-based estimation and control applications. However, this problem remains challenging since model reduction can introduce stability loss and prediction degradation. To remedy these problems many methods have been developed aiming at what is known as stable model reduction. In this talk, we focus on the so-called closure models and their application in reduced order model (ROM) stabilization. We present some results on robust stabilization for reduced order models (ROM) of partial differential equations using Lyapunov theory. Stabilization is achieved via closure models for ROMs where we use Lyapunov theory to design a new closure model, which is robust with respect to model structured uncertainties. Furthermore, we use an extremum-seeking algorithm to optimally tune the closure models' parameters for optimal ROM stabilization. The Burgers' equation and a 3D Boussinesq equation examples are employed as a test-bed for the proposed stabilization method.

New trends for advanced reduced order methods in CFD: applications to parametric cardiovascular flows

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Abstract

We present new trends for parametric computing based on advanced reduced order methods for applications in computational fluid dynamics, with a special interest in problems related with cardiovascular flows. These problems are of particular interest due to the fact that they bring a certain complexity related with the geometry of biological structures to be reconstructed and parametrized for the simulation, medical data subject to uncertainty and noise. In addition the numerical approximation of complex nonlinear parametric systems needs proper stabilization also at the reduced order level. Few examples from real-life problems are introduced as proof-of-concept to introduce a complete computational pipeline in an advanced reduced order setting. Multi-physics is accounted in considering fluid and structure interaction between flows and arterial walls, and optimal flow control is accounted for the solution of inverse problems (defective boundary conditions, parameter estimation, data assimilation) as well as for interfacing network components.

Simulation-Based Classification; a Model-Order-Reduction Approach for Structural Health Monitoring

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Abstract

We present a Model-Order-Reduction approach to Simulation-Based classification, with particular application to Structural Health Monitoring. The approach exploits (i) synthetic results obtained by repeated solution of a parametrized mathematical model for different values of the parameters, (ii) machine-learning algorithms to generate a classifier that monitors the damage state of the system, and (iii) a Reduced Basis method to reduce the computational burden associated with the model evaluations.

Our approach is based on an offline/online computational decomposition. In the offline stage, the field associated with many different system configurations, corresponding to different states of damage, are computed and then employed to teach a classifier. Model reduction techniques, ideal for this many-query context, are employed to reduce the computational burden associated with the parameter exploration. In the online stage, the classifier is used to associate measured data to the relevant diagnostic class.

We propose a mathematical formulation which integrates the partial differential equation model within the classification framework and clarifies the influence of model error on classification performance. We prove that, given upper bounds for the model error related to the assumed damage configurations, we can provide upper bounds for the misclassification error associated with the classifier.

We illustrate our approach and we demonstrate its effectiveness through the vehicle of a particular physical companion experiment, a harmonically excited microtruss. We show that the use of simulations allows us to drastically reduce the number of physical experiments needed during the offline stage, and also to improve the design of the experiment

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Title: Dynamical model reduction method for solving parameter-dependent dynamical systems

Abstract: This talk is concerned with the solution of parameter-dependent dynamical systems under the form

$$\begin{cases} u'(t, \xi) = f(u(t, \xi), t, \xi), \\ u(0, \xi) = u^0(\xi), \end{cases} \quad (1)$$

where the flux f and initial condition depend on some parameters ξ with values in a parameter set Ξ . Here, the state $u(t, \xi)$ belongs to the high-dimensional space $X = \mathbb{R}^d$. For solving (1), we propose a projection-based model order reduction method onto a time-dependent low-dimensional reduced space $X_r(t)$ of X , which results in a low-rank approximation u_r of u under the form

$$u_r(t, \xi) = \sum_{i=1}^r v_i(t) \alpha_i(t, \xi), \quad (2)$$

with $X_r(t) = \text{span}\{v_1(t), \dots, v_r(t)\}$. The proposed approach can be interpreted as a dynamical low-rank approximation method but with a subspace point of view and providing a uniform control of the error over the parameter set. In that sense, it is closer to a Reduced Basis method with time-dependent reduced spaces $X_r(t)$ generated from evaluations of the solution of the full-order model (1) at some selected parameters values. The approximation u_r is obtained by Galerkin projection leading to a reduced dynamical system with a modified flux which takes into account the time dependency of the reduced spaces. An a posteriori error estimate is derived and a greedy algorithm using this error estimate is proposed for the adaptive selection of parameters values. The applicability of our method is illustrated through numerical experiments on both linear and non-linear test cases.

Selected event for submission: *Conference (ME3)* : Recent developments in numerical methods for model reduction, 7-10 November 2016, IHP (Paris)

Projection-based model order reduction for the estimation of vector-valued variable of interest

Olivier Zahm,^{*} Anthony Nouy,[†] Marie Billaud-Friess[‡]

Conference (ME3), Paris 7-10 November 2016:

Recent Developments in Numerical Methods for Model Reduction

Abstract

We propose and compare goal-oriented projection-based model order reduction methods for the estimation of vector-valued functionals of the solution of parameter-dependent equations. The first projection method is a generalization of the classical primal-dual strategy to the case of vector-valued variables of interest. The second approach is based on a saddle-point problem which involves three reduced spaces: the approximation space and the test space associated to the primal variable, and the approximation space associated to a dual variable. In the spirit of the Reduced Basis method, we propose greedy algorithms for the construction of these reduced spaces.

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Geometric Methods for the Approximation of High-dimensional Dynamical Systems

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Abstract

We discuss a geometry-based statistical learning framework for performing model reduction and modeling of stochastic high-dimensional dynamical systems. We consider two complementary settings. In the first one, we are given long trajectories of a system, e.g. from molecular dynamics, and we discuss new techniques for estimating, in a robust fashion, an effective number of degrees of freedom of the system, which may vary in the state space of then system, and a local scale where the dynamics is well-approximated by a reduced dynamics with a small number of degrees of freedom. We then use these ideas to produce an approximation to the generator of the system and obtain, via eigenfunctions of an empirical Fokker-Planck question, reaction coordinates for the system that capture the large time behavior of the dynamics. We present various examples from molecular dynamics illustrating these ideas. In thesecond setting we only have access to a (large number of expensive) simulators that can return short simulations of high-dimensional stochastic system, and introduce a novel statistical learning framework for learning automatically a family of local approximations to the system, that can be (automatically) piecedtogether to form a fast global reduced model for the system, called ATLAS. ATLAS is guaranteed to be accurate (in the sense of producing stochastic paths whose distribution is close to that of paths generated by the original system) not only at small time scales, but also at large time scales, under suitable assumptions on the dynamics. We discuss applications to homogenization of rough diffusions in low and high dimensions, as well as relatively simple systems with separations of time scales, and deterministic chaotic systems in high-dimensions, that are well-approximated by stochastic differential equations.

A minimal subspace rotation approach for extreme model reduction in fluid mechanics

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ME3 Conference: Recent Developments in Numerical Methods for Model Reduction (Nov,7-11, 2016, Paris)

High-fidelity modeling (HFM) and simulation is critical in many science and engineering applications; however, high-fidelity simulations remain prohibitive for parametric, time-critical and many-query applications (e.g., design optimization, control, uncertainty quantification). Model reduction seeks to circumvent this difficulty and achieve near real-time prediction by approximately solving the state equations of the HFM via projection onto a low-dimensional subspace. This subspace is “learned” offline from a small set of high-fidelity snapshots, and constructed using data compression and truncation: the removal of modes deemed unimportant in representing the problem solution. Truncation is usually based on an energy criterion: modes with low energy are discarded, so that the reduced basis subspace consists of the highest energy modes. In most realistic applications, e.g., nonlinear compressible fluid flow, a basis that captures 99% or more of the snapshot energy is required for a reduced order model (ROM) to accurately reproduce the snapshots from which it was constructed. Capturing 99% of snapshot energy is only possible for toy problems and/or low-fidelity models, however. Moreover, higher order modes are in general unreliable for prediction, so including them in the basis is unlikely to improve the predictive capabilities of a ROM.

This talk presents an *a priori* approach for creating stable and accurate projection-based compressible flow ROMs of extremely low order based on an approach known as minimal subspace rotation. Of particular interest is stability and accuracy of fluid ROMs for long-time simulations. The proposed approach is based on the idea that, although low-energy modes are negligible from a data compression point of view, they are actually crucial for representing solutions to dynamical flow equations. Traditionally, low-dimensional ROMs of fluid flows are stabilized and enhanced using empirical turbulence models. These approaches have several downsides, e.g., they destroy consistency between the ROM and the HFM. In the minimal subspace rotation method, we model the modal truncation *a priori* by “rotating” the projection subspace into a more dissipative regime rather than through the addition of an ad hoc empirical turbulence term to the ROM equations. The minimal rotation is determined in a goal-oriented fashion through the formulation and offline numerical solution of small-scale quadratic matrix program on the Stiefel manifold. The proposed approach can be interpreted as an *a priori* consistent formulation of the eddy-viscosity turbulence modeling approach: because only the projection subspace is modified, consistency between the ROM and the Navier-Stokes equations is retained. The reproductive as well as predictive capabilities of POD/Galerkin ROMs stabilized via the proposed method are evaluated on several nonlinear compressible flow problems of extremely low order (e.g. $O(10)$). Recent extensions of the method to minimum-residual-based nonlinear compressible flow ROMs are described and evaluated numerically.

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ADVANCED FINITE ELEMENT TOOLS FOR MULTIPHYSICS SIMULATION OF A HYDRAULIC FRACTURING PROBLEM USING A REDUCED BASIS APPROACH

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A hydraulic fracturing problem in porous media is considered, where a 3D elastic structure interacts with the fluid flow inside the planar fracture [1]. The fracture opening is the result of the fluid pressure acting on the fracture walls, which enters as boundary Neumann condition of the elastic model for the structure displacement. Conversely, the normal displacement to the fracture plane enters in the composition of the fracture.

This coupled problem is implemented in a multiphysics context by using H^1 -conforming spaces for the fluid pressure, and approximation spaces spanned by elastic response to piecewise constant pressure on fracture walls are adopted for the structure displacement. This reduced basis approach combined with a dynamic refinement remeshing technique, applied at each fracture propagation step, guaranties a substantial reduction of computational time.

The multiphysics framework considered in the present work has been developed in [1], and it is implemented within NeoPZ¹, an open-source object-oriented computational environment. NeoPZ already incorporates a variety of element geometries (in one, two and three dimensions), variational formulations, and approximation spaces. In addition to the usual conforming and non-conforming spaces, now spaces spanned by reduced basis can be used as well. The users of NeoPZ can implement arbitrary high order approximations, and apply hp-strategies, without limitations on hanging sides and distribution of approximation orders. NeoPZ is integrated with pthreads and thread building blocks for efficient execution on multi core computers.

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¹ <http://github.com/labmec/neopz>

Model reduction for verification and updating of Computational Mechanics models

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Abstract

A permanent issue in science and engineering activities is the verification and validation (V&V) of mathematical and numerical models, which nowadays can attain very high levels of complexity. We focus here on the Constitutive Relation Error (CRE) concept which has been widely used over the last 40 years for robust verification [4] and validation [3] of Computational Mechanics models, in which the constitutive relation is a major component. The objective of this research work is to present new numerical tools, based on Proper Generalized Decomposition (PGD) and an offline-online strategy, that can be coupled to the CRE concept to make this latter fully implementable and exploitable for practical industrial applications [1]. The PGD is a model reduction technique that has been extensively applied over the last decade to solve multi-parametric problems [2]. Its use into the CRE concept enables to decrease the computational cost and technicality associated with the construction of so-called admissible fields, leading to faster and cheaper V&V procedures. Numerical illustrations, addressing both model verification and model updating, are presented to assess the performances of the proposed approach.

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POD-Based Bicriterial Optimal Control by the Reference Point Method

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Abstract

In the talk bicriterial optimal control problem governed by a parabolic partial differential equation (PDE) and bilateral control constraints is considered. For the numerical optimization the reference point method is utilized. The PDE is discretized by a Galerkin approximation utilizing the method of proper orthogonal decomposition (POD). POD is a powerful approach to derive reduced-order approximations for evolution problems. Numerical examples illustrate the efficiency of the proposed strategy.

Dictionary data assimilation for recovery problems

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Abstract

The approximation of physical systems by coupling measurement data and parametric PDE models has led to a new class of problems in optimal recovery. The setup is the following. Let \mathcal{M} be a compact set of a Hilbert space \mathcal{H} and let V be a finite dimensional subspace of \mathcal{H} which approximates the elements of \mathcal{M} at ε accuracy. Given a function $u \in \mathcal{M}$, the goal is to find the optimal reconstruction of u with the knowledge of V and of m measurements of u , $\ell_i(u)$, $i = 1, \dots, m$, where the ℓ_i are linear functionals of \mathcal{H}' . Physically speaking the ℓ_i should be understood as sensors to install in the real system.

In this setting, the optimal map understood in a sense described in [1] was first found in [2]. However, its stability strongly depends on the measurement subspace $W = \text{span}\{w_1, \dots, w_m\} \subset \mathcal{H}$, where the w_i are the Riesz representations of the ℓ_i . In this talk, we first discuss whether the use of subspaces of W could help stabilize the approximation and retrieve better accuracy. Since there are many physical situations in which there is some freedom to choose the sensors, we present a greedy strategy to select appropriate ones from a dictionary and measure its “deviation” from the optimal choice via convergence rate results.

This is an ongoing work in collaboration with P. Binev from the University of South Carolina.

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PGD for solving parametrized nonlinear time-dependent structural problems

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The numerical simulation of very large multiscale models is becoming increasingly important because of the need to describe realistic scenarios and to derive tools to facilitate the virtual design of new structures. In this context, model reduction methods have a huge potential to develop innovative tools for intensive computations and allow a “real time” interaction between the user and the simulations, which gives the opportunity to investigate a large number of scenarios in the design office.

Among others, the PGD model reduction technique consists in building progressively an approximation of the solution of a given problem by assuming a separated variables form and using a greedy algorithm. It allows to solve easily parametrized problems and then to build virtual charts of solutions that can be reused in a very convenient and inexpensive way to explore the influence of parameters such as material characteristics, dimensions of a structure or loading amplitude ...

The LATIN method, originally introduced to solve time-dependent problems encountered in computational mechanics, allows to solve, combined with the PGD technique, nonlinear problems with a strong decrease of the computational cost. In the first part of this talk, its capabilities will be exemplified for the simulation of the response of a concrete structure to an accidental phenomenon, such as an earth-quake, over a short time lapse. This type of problem presents a highly nonlinear behavior, including damage that usually leads to high CPU costs.

The second part of this talk will focus on a major limitation of reduced modeling which concerns the number of the parameters that can be involved (about 10 to 20). Some preliminary works to deal with large number of parameters in solid mechanics will be presented. The proposed strategy is an extended PGD approach based on an iterative computational technique with conditioners. First illustrations will show its performances and also its present limits.

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Reduced order method combined with domain decomposition applied to biomechanics problems

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The complexities and nonlinearity of the PDEs in biomechanics and the requirement for rapid solution pose significant challenges for the biomedical applications. For these reasons, different methods for reducing the complexity and solving efficiently have been investigated in the last 15 years. At the state-of-art, due to spatial different behaviours and highly accurate simulation required, a decomposition of physical domain is deeply investigated in reduced basis element method approaches.

In this talk, the main focus is devoted to present suitable reduction strategy which combines a domain decomposition approach and a proper interface management with a proper orthogonal decomposition.

We provide numerical tests implemented in DOLFIN[4] using SLEPc [3] and PETSc [1, 2] that show a speed up in forward runtime on a two-dimensional and three-dimensional non-linear hyperelastic model.

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Reduced-order models from data: Eigensystem Realization Algorithm

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Abstract

Subspace-based system identification for dynamical systems is a sound, system-theoretic way to obtain linear, time-invariant system models from data. The interplay of data and systems theory is reflected in the Hankel matrix, a block-structured matrix whose factorization is necessary for system identification. For systems with many inputs, many outputs, or large time-series of system-response data, established methods based on the singular value decomposition (SVD)—such as the eigensystem realization algorithm (ERA)—are prohibitively expensive.

In this talk, we present two approaches to circumvent the computational expense of the eigensystem realization algorithm when faced with a large amount of data. When the system has a large number of inputs and outputs, we use tangential interpolation based ideas to project the original impulse response sequence onto suitably chosen directions. This reduces the computational cost of the standard ERA algorithm, and we give error bounds for the obtained reduced-order models. We present a second algorithm in a more general setting, replacing the SVD with a CUR decomposition that directly seeks a low-rank approximation of the Hankel matrix. The CUR decomposition is obtained by selecting a small number rows and columns using a maximum-volume-based cross approximation scheme. We also give a worst-case error bound for our resulting model-reduction algorithm. We demonstrate the computational advantages and accuracy of both algorithms on a numerical example.

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SIMULTANEOUS EMPIRICAL INTERPOLATION AND REDUCED BASIS METHOD FOR NON-LINEAR PROBLEMS

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Key words: *SER Methods, Reduced Basis Methods, Non-linear Multi-Physics, High Performance Computing.*

In this talk, we will focus on the reduced basis methodology in the context of non-linear and non-affinely parametrized partial differential equations in which affine decomposition necessary for the reduced basis methodology is not obtained. To deal with this issue, it is now standard to apply the Empirical Interpolation Method (EIM) methodology [1, 4] before deploying the Reduced Basis (RB) methodology. The EIM building step can be costly and requires many (hundreds) finite element solutions when the terms are non-linear that forbids its application to large non-linear problems.

In this talk, we will introduce a Simultaneous EIM Reduced basis algorithm (SER) [2] based on the use of reduced basis approximations into the EIM building step. Enjoying the efficiency offered by reduced basis approximation, this method provides a huge computational gain and can require as little as $N + 1$ finite element solves where N is the dimension of the RB approximation and allows to recover the approximation properties when using the standard approach.

We will start this talk with a brief overview of the EIM and RB methodologies applied to non-linear problems. The identification of the main issue, discussing the changes to be made in the EIM offline step for such problems will then introduce the SER method detailed in the first part of the talk with some of its variants.

The second part of the talk will first illustrate our method with results obtained on a benchmark introduced in [4]. We will then present its performances for large scale problems it is designed for, through a 3D non-linear multi-physics reduced model used in high field magnet optimization context introduced in [3].

The SER method is now available in the generic and seamlessly parallel reduced basis framework of the opensource library Feel++ (Finite Element method Embedded Language in C++, <http://www.feelpp.org>). An online demonstrations will be done.

Acknowledgements the authors would like to thank Romain Hild (U. Strasbourg) and Christophe Tropheime (LNCMI) for fruitful discussions on various aspects of this work.

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Greedy algorithms for the electronic many-body Schrödinger equation

Virginie Ehrlacher, Eric Cancès, Tony Lelièvre, Filippo Lipparini,
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Abstract

In this talk, a greedy algorithm will be presented in order to compute the lowest eigenvalue and an associated eigenstate for high-dimensional problems and its numerical behaviour will be illustrated for the computation of the ground-state electronic wave function of a molecule, solution of the many-body Schrödinger equation. Usually, these algorithms are implemented in practice using the Alternating Least-Square algorithm, which leads to some computational difficulties in this particular situation due to the antisymmetry of the ground state wavefunction. A computational strategy to overcome this difficulty will be presented and illustrated on several molecules.

A HJB-POD approach to the control of the level set equation

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We consider an optimal control problem where the dynamics is given by the propagation of a one-dimensional graph controlled by its normal speed, which has been proposed in [3]. A target corresponding to the final configuration of the front is given and we want to minimize the cost to reach the target. We want to solve this optimal control problem via the dynamic programming approach but it is well known that this method suffers of the “curse of dimensionality” so that we can not apply the method to the semi-discrete version of the dynamical system. However, this is made possible by a reduced-order model for the level set equation which is based on Proper Orthogonal Decomposition (see [4]). This results in a new low-dimensional dynamical system which is sufficient to track the dynamics. By the numerical solution of the Hamilton-Jacobi-Bellman equation related to the POD approximation we can compute the feedback law and the corresponding optimal trajectory for the nonlinear front propagation problem (see [1] and the reference therein for the HJB-POD approach). In particular for solving the Bellman equation we will use the accelerated policy iteration algorithm proposed in [2]. We will present some numerical tests to show the efficiency of the proposed method.

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GNAT-FV: Structure-preserving model reduction for finite-volume discretizations of conservation laws

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Finite-volume discretizations are commonly used for numerically solving systems governed by conservation laws, especially those appearing in compressible fluid dynamics. Such techniques numerically enforce conservation laws over cells by discretizing the *integral form* of the conservation laws. However, such models can become very large-scale for when high fidelity (i.e., high spatial resolution) is required, leading to simulation times that can exceed weeks on a supercomputer. As a result, these high-fidelity models are not practical for many-query and real-time scenarios such as model predictive control and uncertainty quantification.

Reduced-order models (ROMs) have been developed to mitigate this burden. However, most techniques in the literature have focused on generating ROMs for finite-element discretizations of conservation laws (e.g., Refs. [3, 2]). While some techniques like the Gauss–Newton with approximated tensors (GNAT) method [1] have been successfully applied to finite-volume models, these techniques do not guarantee that conservation laws are enforced over any subset of the computational domain. As a result, instability and inaccurate responses are common; even responses with low errors generally yield spurious generation or dissipation of quantities that should be conserved.

To address this, we propose a nonlinear model-reduction technique that *explicitly enforces* conservation laws over subdomains of the problem. This guarantees that, even when the dimensionality of the model is greatly reduced, the most important structure intrinsic to the finite-volume model—the conservation laws—are enforced over subdomains. We refer to the method as the **GNAT-finite volume** (GNAT-FV) technique, as it amounts to equipping the nonlinear least-squares GNAT formulation with *equality constraints* associated with conservation laws over subdomains. Furthermore, we equip both the objective function and constraints with hyper-reduction via gappy POD; this ensures computational efficiency in the presence of nonlinearities. Numerical results highlight the improvement in long-time behavior of GNAT-FV over existing ROMs (i.e., Galerkin, least-squares Petrov–Galerkin, and GNAT) when applied to finite-volume models.

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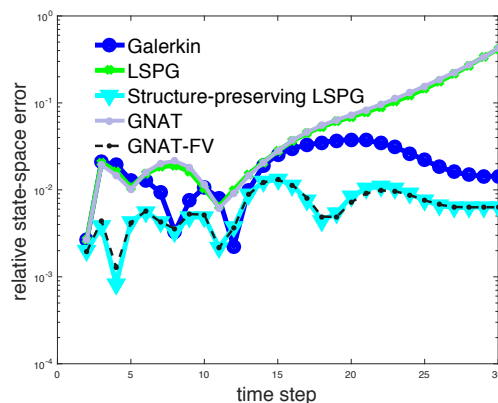


Figure 1: Results for a parameterization of Euler’s equations in one dimension. Equipping least-squares Petrov–Galerkin (LSPG) or GNAT with structure-preserving constraints reduces the error by orders of magnitude.

An adaptive dynamical tensor method for the Vlasov-Poisson system

Virginie Ehrlacher and Damiano Lombardi

Abstract

The time dependent Vlasov-Poisson system, arising in kinetic theory, is a simple yet challenging problem to be solved, due to the high dimensionality of domain (the phase space). Whereas a full eulerian approach is appealing to represent the variables, it is difficult to set up especially in realistic 3D-3D configurations. Other methods are proposed in the literature to solve the problem, namely semi-lagrangian methods and stochastic particle methods (PIC). The present work deals with an adaptive tensor method to set up parsimonious discretizations for the Vlasov-Poisson system in a full-eulerian framework. The proposed approach is not a discretization per se, instead, it introduces a systematic way to discretize the problem starting from separated discretizations in space and velocity. Moreover, the hamiltonian formulation of the Vlasov-Poisson system is considered: the tensorization allows to deal naturally with the Poisson bracket structure of the problem, inducing a splitting of the operator. A symplectic time advancing scheme is used, in order to respect, at second order, the hamiltonian structure of the problem. In order to determine the separate expansion at each time step, a modified Proper Generalised Decomposition (PGD) method is introduced. Its convergence is proved, providing some insight on the performances of the numerical method. Several numerical experiments are proposed to validate the method, including 2D-2D and 3D-3D examples.

An approach to perform shape optimisation by means of hybrid ROM-CFD simulations

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Abstract

Reduced Order Models (ROMs) represent a powerful tool to capture the most important features of a flow field by using a small number of degrees of freedom. Recently, the interest in the use of ROMs for design and optimisation purposes has increased in several different field of engineering. These applications introduce important challenges related to the training of the model and the estimation of the error in the predicted field. In particular, the different ROM procedures share the need of a training stage in which several high-fidelity simulations are performed in order to get a set of snapshots and to build a reference database. The sampling in the space of the design parameters is a critical issue since it influences directly the ability of the model to predict a wide range of configurations.

In order to optimise the sampling a possible approach is represented by the use of a recursive Voronoi algorithm which explores the design space and focuses the attention on the regions which require further investigation [1].

When a ROM is used to predict a field which corresponds to a set of parameters not included in the database particular care must be taken. Indeed, the non linear nature of the fluid dynamics equations and the high sensitivity of the flow field to some design parameters (geometry of the body, Reynolds and Mach number,...) make the direct use of ROMs particularly difficult for general purpose and industrial applications. Furthermore, the dynamics equations related to ROMs are often characterised by an unstable behaviour which requires the introduction of ad-hoc dissipation terms. In order to avoid these shortcomings, an hybrid approach can be efficiently used to deal with complex flows [2]. In particular, the computational domain can be split into two regions: a region close to the body in which the effects of the body are directly taken into account by CFD and a far-field region in which the flow is described by the ROM. The coupling between the CFD solver and the ROM requires the definition of an overlapping region on which the coefficients of the ROM are computed in order to fit the CFD solution. As a result, the size of the domain on which the expensive CFD simulation has to be performed is strongly reduced.

In this work, the previously described hybrid ROM-CFD approach is used to solve a shape optimisation problem. The POD database is trained on a set of full CFD simulations for several values of the design parameters which have been chosen according to the previously described Voronoi sampling technique. The optimisation process is driven by an evolutionary algorithm which calls the hybrid ROM-CFD simulation in order to evaluate the goal function.

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Multiscale computations based on MsFEM: model reduction and goal-oriented a posteriori error estimation

L. Chamoin and F. Legoll

Abstract

The Multiscale Finite Element Method (MsFEM) is a Finite Element type approach for multiscale PDEs, where the basis functions used to generate the approximation space are precomputed and are specifically adapted to the problem at hand. A priori bounds on the numerical error have been established for several variants of the MsFEM approach. In this work, we introduce a guaranteed and fully computable a posteriori error estimate, both for the global error and for the error on quantities of interest. We discuss the accuracy of such estimates and show how they can be used to efficiently drive an adaptive discretization. Time permitting, PGD-type approaches in the context of the MsFEM will be discussed.

Fully certified and adaptive localized model reduction for elliptic and parabolic problems

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Abstract

We are interested in efficient and reliable numerical approximations of parametric elliptic and parabolic problems, in particular in the multiscale setting. Based on the localized reduced basis (LRB) multiscale method [1] we present the fully certified and adaptive LRB method for elliptic and parabolic problems. Using (spatially) localized reduced bases, a broken reduced space and novel a posteriori error estimates, the LRB allows to control the full approximation error (including the discretization as well as the model reduction error). Using a localization of these estimates, we present recent advances in the direction of adaptivity on all levels, to obtain efficient as well as reliable approximations: grid-adaptation, adaptive reduced basis generation and adaptive local enrichment of the broken reduced space during the online phase.

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Dynamical Bases Reduced-Order modelling methods

Jean Frédéric Gerbeau and Damiano Lombardi

Abstract

Reduced-Order Modelling methods aim at obtaining a reasonable approximation of complex models solutions with a computational cost which is significantly smaller with respect to standard full-order discretization methods. They are often based on an offline and an online phase. In the offline phase, several full-order numerical simulations are performed in a meaningful number of scenarios. Then, in the online phase, the database of simulated solutions is exploited to speed up the computations. Most commonly, a basis is constructed in order to obtain, via a Galerkin, or a Petrov-Galerkin projection, a parsimonious discretisation of the original system of equations. Classical methods such as Proper Orthogonal Decomposition (POD) or Reduced-Basis method (RB) provide excellent performances in a certain number of cases. However, they are not effective when dealing with advection-dominated problems or progressive waves phenomena. To overcome these drawbacks, a dynamical basis class of parsimonious discretizations is introduced, in which the basis (that is non-necessarily obtained via an offline phase) evolve and adapt in time in order to provide, locally in time, a good representation of the solution. An Empirical Interpolation (EI) approach is adopted in order to deal with non-linear non-polynomial Partial Differential Equations. A numerical analysis of the method is proposed. Several numerical test-cases on linear and non-linear waves are presented. Moreover, some numerical experiments on reaction-diffusion equations arising in cardiac electro-physiology are shown.

ME3

POSTER ABSTRACTS

(Ordered alphabetically according to the presenting author)

A reduced order model for multi-physics problems

Matteo Aletti and Damiano Lombardi

Abstract

In the present work we focus on multi-physics systems. In particular, we consider physical phenomena where two (or more) domains interact with each other through an interface. In several cases, one is interested only in the dynamic of one of the two domains, but the solution of both systems is necessary because of the interaction. The goal of the present technique is to provide an accurate solution for the problem in the main domain, while modeling the second domain through the corresponding Steklov operator. In the applications, the finite element representation of the Steklov operator cannot be computed and stored because, even if defined only at the interface, it is a dense matrix and it would require many solutions of the secondary problem. Keeping in mind that we want to avoid or at least minimize the number of online solutions of the secondary problem, we propose to represent the Steklov operator on a few number of basis functions for which the secondary problem is solved offline. During the online phase the coupling of the two domains is enforced via a Domain Decomposition approach, but the solution of the secondary problem is reconstructed in an extremely fast way. The method will be presented on some 3D examples of fluid-porous media interaction, fluid-fluid interaction and fluid-structure interactions.

Stabilized Reduced Basis Methods for the approximation of parametrized viscous flows: increasing Reynolds number

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Abstract

Starting from the state of the art [1, 2, 3] we study stabilization techniques in different options for parametrized viscous flows. We are interested in the approximation both of the velocity and of the pressure. Offline-online computational splitting is implemented and offline-only, offline-online stabilization is compared (as well as without stabilization approach). Different test cases are illustrated and several stabilization classical approaches (SUPG, GaLS, Brezzi-Pitkaranta, Franca, Hughes, ect) are recast into a parametric reduced order setting. This approach is then compared with the supremizer approach to guarantee the approximation stability by increasing the corresponding parametric inf-sup constant. The goal is two-fold: to guarantee stable parametrized viscous flows with increasing Reynolds numbers and to look for online computational savings by reducing the dimension of the online reduced basis system.

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Image Inpainting Using finite element method with domain decomposition

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Abstract

Removing or repairing the imperfections of a digital images or videos is a very active and attractive field of research belonging to the image denoising and inpainting technique. This later has a wide range of applications, such as removing scratches in old photographic image, removing text and logos or creating cartoon and artistic effects. In this paper, we propose an efficient method to repair a damaged image based a nonlinear diffusion model with domain decomposition method. To illustrate the effective performance of our method, we present some experimental results on several images.

Keywords : image inpainting, nonlinear diffusion, decomposition method.

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Parametric Model Order Reduction: An LPV/LFT Framework

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Abstract

Rigorous models are a key tool to improve performance and to optimize process behavior. Because of the increasing complexity of mathematical models in the high-tech industry, the analysis and optimization of parameter dependent rigorous models is often a tedious and time consuming task. In recent years, parametric model order reduction has achieved a great success. Typically, the parameter subspace is sampled and model reduction is carried on each of the particular system and the reduced-order models are interpolated. When the number of parameters becomes large or the parameters vary in a considerably large range, the system behaviors are quite different for different parameter values. In order to capture these system behaviors, plenty of sampled systems are needed which makes the process time consuming and computationally expensive.

From a system theoretic point of view, parametrized system models can be reinterpreted as linear parameter-varying systems (LPV). As a unified framework, linear fractional transformation (LFT) provides a powerful tool to deal with LPV systems. We propose a model order reduction method, which is based on the LFT framework. By applying such a technique, the system parameters can be extract from the model and we only deal with a non-parametrized system with extended inputs and outputs. This approach leads to augmented inputs and outputs which makes the system more difficult to reduce. A remedy is that we partition the parameter subspace into several regions and reduce the system in each of them separately. The parameter perturbed system behavior in each region can capture the full system behavior piece-wisely. The contribution is on how to transform the system into LFT representation efficiently, how to partition the parameter subspace and how to reduce the augmented multi-input multi-output systems efficiently and accurately.

Space–time least-squares Petrov–Galerkin nonlinear model reduction

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Reduced-order models (ROMs) of nonlinear dynamical systems are essential for enabling high-fidelity computational models to be used in many-query and real-time applications such as uncertainty quantification and design optimization. Such ROMs reduce the dimensionality of the dynamical system by executing a projection process on the governing system of nonlinear ordinary differential equations (ODEs). The resulting ROM can then be numerically integrated in time. Unfortunately, many applications require resolving the model over *long time intervals*, leading to a large number of time instances at which the fully discretized model must be resolved. As such, the number of time instances required for the ROM simulation remains large, which can limit its realizable computational savings.

Space–time ROMs have been devised for computational models that have been developed using a space–time finite-element formulation [2]. Unfortunately, many practical computational models are constructed using a spatial discretization (which yields a parameterized system of ODEs) followed by time integration with a linear multi–step method or Runge–Kutta scheme; such space–time ROMs cannot be applied for these models.

To address this, we propose to apply a space–time projection to nonlinear ODE models, which are resolved in time using implicit time-integration schemes. The method adopts the least-squares Petrov–Galerkin (LSPG) formulation that underlies the Gauss–Newton with approximated tensors (GNAT) method [1]. The proposed technique executes the following steps: (1) introduce a low-dimensional (spatio–temporal) basis for the state (*over all time*), (2) apply implicit time integration to the system of nonlinear ODEs, and (3) minimize the sum of squares of discrete residuals arising *over all time steps*. The technique also introduces hyper–reduction (via collocation or gappy POD) with an attendant spatio–temporal sample mesh in order to realize computational savings.

We derive error bounds that show the method exhibits slower time-growth of the error as compared to typical spatial-projection-based ROMs. We apply it to two time dependent problems (i.e., Burger’s equation and Euler’s equation). Numerical results show that the proposed technique enables additional computational savings to be realized with similar accuracy as compared to typical spatial-projection-based ROMs. We also show that the method effectively removes spurious temporal modes (e.g., unstable growth, artificial dissipation) from the ROM response, which can significantly improve its performance in certain cases.

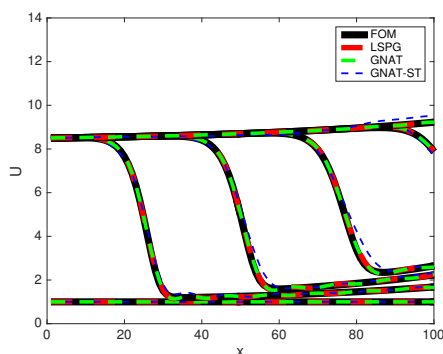


Figure 1: Solutions for Burger’s equation at multiple time steps. GNAT-ST yields a speed-up of five.

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Multi space reduced basis preconditioners for large-scale parametrized PDEs

Niccol Dal Santo, Simone Deparis, Andrea Manzoni and Alfio Quarteroni

Abstract

In this talk we present a new 2-level preconditioner for the efficient solution of large-scale linear systems arising from the discretization of parametrized PDEs. Our preconditioner combines multiplicatively a reduced basis (RB) coarse component and a non singular preconditioner, such as 1-level Additive Schwarz, Gauss-Seidel or Jacobi preconditioner. The proposed technique hinges up on the construction of a new Multi Space Reduced Basis (MSRB) method, where a reduced space is built through proper orthogonal decomposition at each iteration of the Richardson or the flexible GMRES method used to solve the large-scale linear system. As a matter of fact, each reduced space is suited to solve a particular iteration and aims at fixing the scales that have not been treated by previous iterations and the fine preconditioner yet. Not only, the RB error decays exponentially fast for each space, thus yielding to very small (compared to the dimension of the original system) reduced spaces. Since the RB accuracies obtained for each space affect the overall convergence of the iterative method in a multiplicative way, a very accurate solution of the large-scale system can be computed in very few (about 10) iterations. Numerical tests have been carried out to evaluate the performance of the preconditioner in different large-scale modeling settings related to parametrized advection-diffusion-reaction equations, up to millions of degrees of freedom, and compared with the current state-of-art algebraic multigrid preconditioners

Reduced basis method for the Smagorinsky model

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Abstract

In this work we present a reduced basis model for the Smagorinsky turbulence model. This turbulence model includes a non-linear eddy diffusion term that we have to treat in order to solve efficiently our reduced basis model. We approximate this non-linear term using the Empirical Interpolation Method [1], in order to obtain a linearised decomposition of the reduced basis Smagorinsky model.

This model is based upon an a posteriori error estimation for Smagorinsky turbulence model. The theoretical development of the a posteriori error estimation is based on [2] and [4], according to the Brezzi-Rappaz-Raviart stability theory, and adapted for the non-linear eddy diffusion term.

The reduced basis Smagorinsky turbulence model is decoupled in a Online/Offline procedure. First, in the Offline stage, we construct hierarchical bases in each iteration of the Greedy algorithm, by selecting the snapshots which have the maximum a posteriori error estimation value. To assure the Brezzi inf-sup condition on our Reduced Basis space, we have to define a supremizer operator on the pressure solution, and enrich the reduced velocity space. Then, in the Online stage, we are able to compute a speedup solution of our problem, with a good accuracy.

Finally we present a numerical test, programmed in FreeFem++ [3], in which we show the speedup the computation of a solution of a steady flow in a backward-facing step

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Model Reduction for Large-Scale Computational Simulations

Jeffrey A. Fike, Irina K. Tezaur and Kevin T. Carlberg

Abstract

High-fidelity computational simulations are routinely used for engineering analysis. However, real-world systems often differ from the idealized geometry and nominal operating conditions typically assumed for the simulations. Uncertainty quantification methods seek to assess the effects of these variations on the predicted performance of the system. This often requires very many simulations, which can be prohibitively expensive when a single high-fidelity simulation takes weeks on thousands of processors. Reduced-order models can be used as a surrogate for the high-fidelity simulations by reducing the computational cost of repeated analyses while maintaining a sufficient level of accuracy. This poster describes the reduced-order modeling capabilities that have been incorporated in two analysis codes: the computational fluid dynamics code SPARC, and the multiphysics finite-element code Albany. Albany can solve a variety of problems ranging from solid mechanics to climate modeling. This poster describes the application of the reduced-order modeling capabilities in Albany to mechanical and coupled thermal/mechanical simulations, but the capabilities can be applied to any physics set. The reduced-order modeling capabilities in SPARC are applied to unsteady, compressible, viscous flows.

A PGD SOLVER FOR THE PARAMETRIC POWER FLOW PROBLEM: MODELING ELECTRIC GRIDS WITH ACCURACY ASSESSMENT AND CONTROL

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October 18, 2016

ABSTRACT

The parametric analysis of electric grids requires carrying out a large number of Power Flow computations. The different parameters describe loading conditions and grid properties. In this framework, the Proper Generalized Decomposition (PGD) [1] provides a numerical solution explicitly accounting for the parametric dependence. Once the PGD solution is available, exploring the multidimensional parametric space is computationally inexpensive. The aim of this paper is to provide tools to monitor the error associated with this significant computational gain and to guarantee the quality of the PGD solution. In this case, the PGD algorithm consists in three nested loops that correspond to 1) iterating algebraic solver, 2) number of terms in the separable greedy expansion and 3) the alternated directions for each term. In the proposed approach, the three loops are controlled by stopping criteria based on residual goal-oriented error estimates. This allows one for using only the computational resources necessary to achieve the accuracy prescribed by the end-user. The paper discusses how to compute the goal-oriented error estimates. This requires linearizing the error equation and the Quantity of Interest to derive an efficient error representation based on an adjoint problem. The efficiency of the proposed approach is demonstrated on benchmark problems [2, 3].

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Non-Smoothness in Space and Time within Model Reduction

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Abstract

It is well-known that model reduction techniques for parameterized systems perform particularly well for problems whose solution depends smoothly on the involved parameters. In this talk, we consider the Reduced Basis Method (RBM) [1, 2] for instationary problems involving various sources of non-smoothness in space, time and parameter. In particular, we are concerned with the Hamilton Jacobi Bellman (HJB) equation, the wave equation and time-dependent obstacle problems. In all these cases, non-smooth effects may vary (travel) in space over time and the evolution is typically unknown, but of great importance.

For the corresponding analysis, we use the space-time variational formulation, in which time is treated as an additional variable within the variational formulation of the problem, [3]. In special cases, certain discretizations of such space-time problems yield time-stepping schemes. Otherwise, recent tensor product solvers may be used.

We discuss recent results in this framework concerning stability, approximation and reduced basis methods including efficient and reliable a posteriori error estimates.

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Magic Point Empirical Interpolation: Parametric Integration and Application

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Abstract

We derive analyticity criteria for explicit error bounds and an exponential rate of convergence of the magic point empirical interpolation method introduced by Barrault et al. (2004). Furthermore, we investigate its application to parametric integration. We find that the method is well-suited to Fourier transforms and has a wide range of applications in such diverse fields as probability and statistics, signal and image processing, physics, chemistry and mathematical finance. To illustrate the method, we apply it to the evaluation of recurrent option pricing problems in finance. Our numerical experiments display convergence of exponential order, even in cases where the theoretical results do not apply.

Hi-POD reduction techniques for parametrized fluid dynamics problems

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Abstract

Hi-POD reduction techniques provide a new procedure to efficiently solve parametrized PDE models featuring a leading dynamics. In more detail, Hi-POD techniques merge the computational efficiency and reliability provided by a Hierarchical Model (Hi-Mod) reduction when dealing, for instance, with fluids in pipes, with a standard Proper Orthogonal Decomposition (POD) approach, ideal for a rapid solution of parametrized settings. Thus, during the offline stage, we employ Hi-Mod reduction to build the response matrix associated with different samples of the parameter. Then, we perform the online computation by assembling the Hi-Mod matrix associated with the new value of the parameter and, successively, by projecting such a matrix onto the POD basis.

In this poster, after highlighting the main steps of the Hi-POD procedure, we assess the reliability and the efficiency of Hi-POD on multiparameter advection-diffusion-reaction tests as well as on the incompressible Navier-Stokes equations, both in a steady and in an unsteady setting. These preliminar results confirm that Hi-POD can be a useful tool in view, e.g., of variational data assimilation procedures or, more in general, inverse problems, where it is crucial to efficiently solve a parametrized problem for several choices of the parameters of interest.

The Certified Reduced-Basis Method for Darcy flows in Porous Media

Riad Sanchez, Sébastien Boyaval, Guillaume Enchery and Quang Huy Tran

Abstract

In this work we extend the Reduced Basis (RB) method [2] to efficiently solve parametrized two-phase flows problems in porous media whose high fidelity (HF) discretization falls into the gradient scheme framework. Our first step in this study is to develop an efficient reduced basis scheme for the pressure equation. Considering the oil-water flows in a highly heterogeneous porous medium simulating oil production, the water viscosity is assumed to be variable due to operational conditions. In the oil industry, a certain concentration of polymer may be added to water to reduce the contrast of mobility with the oil phase and obtain a more efficient sweeping and thus a better oil recovery. To assess numerically the potential of this strategy, our objective consists in approximating all the pressure fields obtained at the final time step according to the values of the water viscosity using a RB approach. To this end, an a posteriori error estimate is built giving an upper bound on the residual obtained when replacing the discrete solution by the RB approximation. This error estimate is used during the construction of the reduced basis (offline phase) by the so-called greedy algorithm and during the computation of new (reliable) solutions for numerous parameter values (online phase). Since our parametrized formulation does not fulfill the affine parameter dependence assumption, the empirical interpolation method is used to obtain a fast approximation in the online stage (the complexity does not depend on the size of the HF problem). Let us notice that our a posteriori error estimate also takes into account the error related to the interpolation procedure. We also show how the affine decomposition and the RB approximation can be simultaneously built. Numerical experiments performed on the SPE10 benchmark [1] are presented as an illustration.

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POD-Galerkin Reduced Order Model for the simulation of laminar and turbulent flows around a circular cylinder

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Abstract

In this contribution the development of a Reduced Order Model (ROM) using a POD-Galerkin approach for the simulation of laminar and turbulent vortex-shedding flows around a circular cylinder is investigated. The Proper Orthogonal Decomposition (POD) is used to decompose the flow fields, derived from a high-fidelity finite volume approximation, into a set of spatial modes and temporal amplitudes. The POD approach permits to create spatial bases that are optimal in terms of energy, and a Galerkin projection of the governing equations onto the spatial-modes is performed in order to obtain a system of ordinary differential equations for the evolution of the time-dependent amplitudes. The projection is performed using the incompressible Navier-Stokes equations for the laminar case and incompressible Reynolds Averaged Navier-Stokes (RANS) equations for the turbulent case. The boundary conditions are enforced on the ROM using a penalty approach. The applicability and accuracy of the present method is studied and discussed for different values of the Reynolds numbers and for different phenomena used as benchmark test cases.

Dimension reduction in heterogeneous parametric spaces: shape and drag optimization in naval engineering

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Abstract

The active subspaces approach represents one of the emerging ideas for dimension reduction in the parameter studies. The concept was introduced by Constantine and employed in different real problems. A characteristic of the active subspaces is that instead of identifying a subset of the inputs as important, they identify a set of important directions in the space of all inputs. If the simulation prediction does not change as the inputs move along a particular direction, then we can safely ignore that direction in the parameter study. After identifying an active subspace it is possible to perform different parameter studies such as response surfaces, integration, optimization and statistical inversion. We are going to introduce in details the Active Subspace Method. Moreover we present an application in naval engineering where the quantity of interest is the wave resistance. We will perform the reduction of the parameters space constructed with geometrical, structural and physical parameters. The geometrical morphing is done with the Free Form Deformation technique applied to the DTMB 5415 hull. The physical parameter is the velocity of the hull and the structural one is the load.