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of Finite Elements and Applications

14–17 June 2016

INVITED LECTURES

Abstracts in alphabetical order

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HIGH ORDER FINITE ELEMENTS: MATHEMATICIAN'S PLAYGROUND OR PRACTICAL ENGINEERING TOOL?

Mark Ainsworth

Division of Applied Mathematics,
Brown University, Providence RI 02912, USA
Mark_Ainsworth@brown.edu

High order finite element methods have been analysed extensively for a wide variety of applications and are known to be capable of producing exponential rates of convergence, even for challenging problems with singularities, sharp boundary layers and high frequency oscillations. High order polynomial approximations are commonplace in many areas of scientific computing including computer graphics, computer aided-geometric design, and spectral methods for PDEs. It is commonplace to see the spectral method used with approximation orders in the 100s or even 1000s. Yet, despite theory giving the nod to the use of very high order finite element methods, the range of polynomial degree used in practical finite element computations is rarely larger than eighth order! Few commercial codes allow the use of high order finite elements. The rather modest polynomial degrees seen in high order finite element analysis are due to efficiency considerations rather than any theoretical barriers. Bernstein-Bezier polynomials have a number of interesting properties that have led to their being the industry standard for visualisation and CAGD. We explore the use of Bernstein polynomials as a basis for finite element approximation.

COMPUTING SPECTRA WITHOUT SOLVING EIGENVALUE PROBLEMS

Douglas N. Arnold

School of Mathematics, University of Minnesota, USA
arnold@umn.edu

The puzzling and important phenonenon of wave localization arises in many physical and mathematical contexts, with applications range from the quantum mechanics of electrical conduction through the design of optical devices to the construction of noise abatement systems, to name but a few. Although studied by physicists and mathematicians for the better part of a century, localization of eigenmodes is still not fully understood nor controlled. In this talk we will describe recent major strides which have been made towards a comprehensive theory. In particular, it is now possible to predict and control the spectrum–both the eigenfunctions and the eigenvalues–of a large class of elliptic PDE, such as Schrödinger operators with random potentials. The talk will feature numerous high fidelity large scale finite element computations which have played a crucial role in guiding our understanding, validating theoretical results, and highlighting mysteries as yet unexplained.

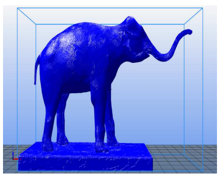
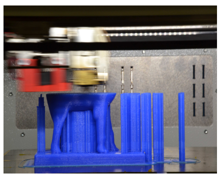
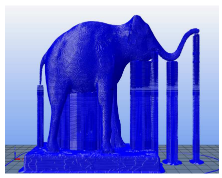
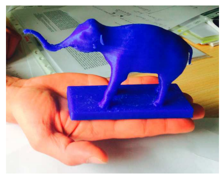
VIRTUAL MODELING AND ADDITIVE MANUFACTURING (3D PRINTING) FOR ADVANCED MATERIALS (3D@UNIPV): A NEW RESEARCH ARENA

Ferdinando Auricchio

Computational Mechanics & Advanced Materials Group,
Department of Civil Engineering and Architecture,
University of Pavia, Italy
auricchio@unipv.it

Additive manufacturing (also known as 3D printing) is becoming more and more a prominent technology, which however still requires deep investigations in terms of materials, virtual modeling, applications, as well as effective economic impact evaluation. In particular, 3D printing cuts across many different areas, involving several research subjects and allowing the development of new high-impact applications.

Aware of all these aspects, after a quick overview of 3D printing in general, as well as of the new University of Pavia strategic project entitled Virtual modeling and additive manufacturing (3D printing) for advanced materials (3D@UniPV), the talk will discuss some specific area of active research, ranging from plastic sintering to metal 3D printing, from the production of high performing materials to new civil engineering structural applications.

PREPARING FOR THE FUTURE OF COMPUTING: BRIDGING SCALES WITHIN THE EXASCALE MATERIALS CO-DESIGN CENTER

James Belak

Lawrence Livermore National Laboratory, USA
belak1@llnl.gov

The advent of Advanced/Additive Manufacturing and the Materials Genome Initiative has placed significant emphasis on accelerating the qualification of new materials for use in real applications. Within these workflows lies both the engineering scale qualification through building and testing components at scale and full-scale modeling with integrated continuum computer codes and the materials scale qualification through revolutionary methods to non-destructively measure microstructure (3DXRD) and physics specific experiments coupled with meso-scale mechanics simulations of the same physics specific experiment using the same microstructure. This Integrated Computational Materials Engineering (ICME) process is one of the use cases that drives the Exascale Materials Co-design Center (ExMatEx). The goal of the Co-design Center is very analogous to the acceleration of new materials deployment within the MGI, rather co-design accelerates the deploying of laboratory concepts for future computer components to enable a productive exascale computer system. Our science strategy applies adaptive physics refinement, whereby a coarse-scale simulation dynamically spawns fine-scale simulations as needed. This direct coupling between the continuum integrated code (continuum plasticity) and direct numerical simulation of the meso-scale phenomena (crystal plasticity) involves a coarse-scale simulation, dynamically spawned fine-scale simulation tasks, a database for storing the results of fine-scale tasks, and an adaptive sampling layer which queries the database, interpolates results, and decides when to spawn new fine-scale tasks. Here we review the ExMatEx project, and its use cases.

This was joint work with Timothy Germann (LANL) and was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DEAC52-07NA27344 and supported by Office of Science, Office of Advanced Scientific Computing Research

EFFICIENT PRECONDITIONING OF hp-FEM MATRICES BY HIERARCHICAL LOW-RANK APPROXIMATIONS

P. Gatto[a] and J.S. Hesthaven[b]

Chair of Computational Mathematics and Simulation Science (MCSS)
École Polytechnique Fédérale de Lausanne (EPFL)
Lausanne, Switzerland
[a]paolo.gatto@epfl.ch, [b]jan.hesthaven@epfl.ch

During the last decade, substantial advances have enabled the efficient construction and application of low-rank approximations to large matrices. Among many examples, matrices arising as discretizations of compact operators such a boundary integral operators, have been shown to enable very efficient compression, thus allowing for both compression and solution in linear complexity.

However, for matrices arising from unbounded operators, e.g., finite element discretizations of differential operators, progress has been slower and is often more challenging. These difficulties are further enhanced when considering linear operators originating from the hp-FEM discretizations of non-trivial operators such as highly anisotropic problems with high contrast and the wave Helmholtz problem.

In this talk, we discuss two different attempts to take advantage of low rank approximations to develop efficient preconditioners for a variety of problems arising as hp-finite element discretizations of linear problems. We discuss the development of efficient hierarchical techniques, utilizing efficient compression of the Schur complement on a hierarchical skeleton, and consider scaling behavior of the compression for both h- and p-refinement.

We illustrate the performance of the techniques of a number of challenging test cases, including highly anisotropic problems and the wave Helmholtz problem, and discuss a few open problems towards an efficient black-box preconditioner.

SELECTION, CALIBRATION, VALIDATION, AND IMPLEMENTATION OF PREDICTIVE COMPUTATIONAL MODELS IN THE PRESENCE OF UNCERTAINTY

J. Tinsley Oden

Institute for Computational Engineering and Sciences,
The University of Texas at Austin, USA

The great advances in computational engineering and sciences over the last half century, including profound advances in finite element methods initiated at the first MAFELAP conference over forty years ago, together with huge strides in high performance computing, have ushered in a new age in scientific discovery and engineering innovation. These advances have pushed computer simulation from a largely qualitative exercise to a source of quantitative information now used as a basis for important, often life–and–death decisions: predictive surgery, climate change, drug design, nano–manufacturing, design of materials, etc. However, as evidence of the true predictability of many time–honored models has come to light, the question of the reliability of all computer predictions has come under serious scrutiny. At the root of these concerns is the inevitable uncertainty in all phases of the predictive process, uncertainty in model selection, observational data, and model parameters, all contributing to the uncertainty of predictions of the target realities.

This lecture presents an overview of the foundations of predictive computational science, the discipline concerned with the quantification of uncertainty in computer predictions. It is argued that a Bayesian setting provides a logical and unifying framework for handling many of the uncertainties in model prediction. When coupled with tools from information theory, a powerful approach to predictive modeling can be formulated. We describe the Occam Plausibility Algorithm (OPAL) as an adaptive approach to model selection and validation. Applications to coarse–grained models of atomistic systems, phase–field models of tumor growth, and models of gamma wave radiation are presented as examples.

COMPUTATIONAL PHOTONICS

Jaime Peraire

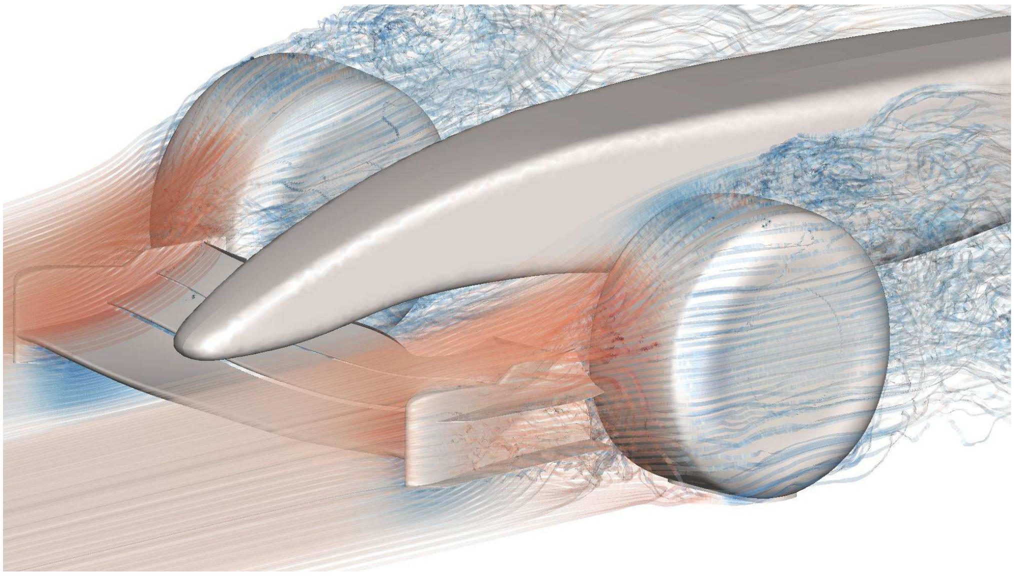
Department of Aeronautics and Astronautics,
Massachusetts Institute of Technology, USA
peraire@mit.edu

Novel photonic materials such as photonic crystals and metamaterials are scientifically engineered to interact with and control electromagnetic waves in ways that cannot be achieved with conventional materials. Photonic crystals exhibit bandgap phenomena and have proven very important as an integrated component in many optical devices including waveguides, fibers, lasers, cloaks, superlenses. At sub-wavelength scales, the interaction between electromagnetic waves and conduction electrons at metallic interfaces leads to surface plasmon polaritons and to the confinement of electrognatic fields over very small spatial dimensions with applications in heat trasnfer, energy harvesting and sensing. These and other novel applications have attracted considerable research interest. However, fundamental challenges abound about the design and fabrication of these photonic strcutures in order to yield a given set of prescribed properties. For instance, it is currently beyond the stateof- the-art to compute robust designs that exhibit prescribed properties subject to fabricability constraints. The issue of fabrication adaptivity (adapting a given computed design so that it is fabricable, without signficantly deteriorating the design quality) is particularly important in practical applications since the desired length scales and material distributions are often at the limit of our fabrication capability and hence geometric design tolerances (in relative scale) need to be larger. Another important issue to address in the design optimization is the uncertainty arising in the mathematical model since physical phenomena can rarely be modeled with complete fidelity even under the best of circumstances. We will described a range of numerical simulation and optimiation algorithms for the design of photonic structures. These will include our multi-scale high order Hybridized Discontinuos Galerkin method, including novel approaches for accurate wave propagation, our topology optimization approach via modern convex optimization techniques, particularly semi-dfinite programming (SDP) interior-point methods, and our fabrication adaptive optimization algorithrm. We will illustrate our algorithms with examples in both photonic crystal design and plasmonics.

DEVELOPMENT AND ANALYSIS OF SPECTRAL/hp ELEMENT TECHNIQUES FOR HIGH REYNOLDS NUMBER FLOW SIMULATIONS RELEVANT TO FORMULA ONE

Spencer Sherwin

McLaren Racing/RAEng Research Chair, Imperial College, London, UK
s.sherwin@imperial.ac.uk



Spectral/hp element simulation over flow past an F1 geometry

The use of computational tools in industrial flow simulations is well established. As engineering design continues to evolve and become ever more complex there is an increasing demand for more accurate transient flow simulations. It can, using existing methods, be extremely costly in computational terms to achieve sufficient accuracy in these simulations. Accordingly, advanced engineering industries, such as the Formula One (F1) industry, are looking to academia to develop the next generation of techniques which may provide a mechanism for more accurate simulations without excessive increases in cost.

This demand for modelling of accurate flow physics around complex geometries are therefore making high order methods such as spectral/hp type discretisations more attractive to industry. Nevertheless a number of challenges still exist in translating academic tools into engineering practice. As the start of the pipeline, meshing techniques for high order methods are required to handle highly complex geometries. Next many engineering problems require high Reynolds numbers leading to turbulent flow that typically are only marginally resolved. Therefore, there is a need for greater robustness in marginally resolved conditions where aliasing errors and high frequency damping are typically required. Finally maintaining computational efficiency is also obviously important.

In this presentation we will outline the demands imposed on computational aerodynamics within the highly competitive F1 sector and discuss the numerical challenges which have to be overcome to translate academic tools into this environment.

SOME ASPECTS OF MODELLING HIGH VELOCITY IMPACT ON CARBON FIBRE REINFORCED COMPOSITES

Rade Vignjevic

Brunel University London, Kingston Lane, Uxbridge UB8 3PH, UK.
v.rade@brunel.ac.uk

Carbon fibre reinforced composites (CFRP) are often exposed to the impact loading with high strain rates in the range from to (e.g. debris, hail stone, bird strike and ballistic impacts). These extreme impact loadings almost always involve generation and propagation of shock waves within the material. The material behaviour under such a complex loading needs to be accurately modelled, in order to minimise the risk of the catastrophic impact related failure. The presented research is related to development and validation of a thermodynamically consistent constitutive model for CFRP materials under high velocity impact loading. The model is capable of modelling damage, failure and formation and propagation of shock waves in non-homogeneous anisotropic material. The model has two main parts: the strength part which defines the material response to shear deformation and an equation of state (EOS) which defines the material response to isotropic volumetric deformation [1]. The constitutive model was implemented into the transient nonlinear finite element code DYNA3D [2] and our in house SPH code. Limited model validation was performed by simulating a number of high velocity material characterisation and validation impact tests.

The new damage model was developed in the framework of configurational continuum mechanics and irreversible thermodynamics with internal state variables. It is applicable to large deformations.

The damage was represented as a second order tensor, which was divided into the volume change related damage (e.g. voids, cavities) and damage related to shear deformation. The damage evolution equations were based on the modified Tuler Bucher "time to failure" [3] approach which was coupled with a thermo elastic model and the shock EOS. The failure initiation was based on a critical value of a specific dissipation function. Validated model was used for modelling of composite aircraft engine blade impacts.

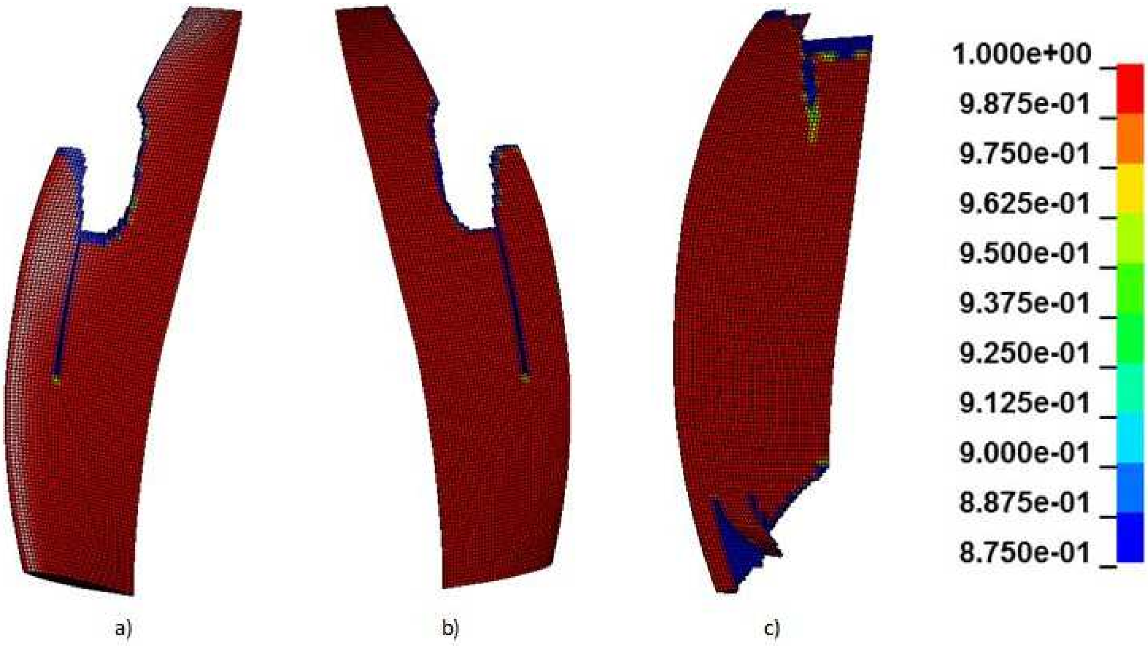


Figure: a) front and b) rear side of the impacted blade, c) released blade .

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MODEL REDUCTION TECHNIQUES IN VIBRO-ACOUSTICS

Barbara Wohlmuth[a], Thomas Horger[b] and Linus Wunderlich[c]

Department of Mathematics, Technical University of Munich, Germany
[a]wohlmuth@ma.tum.de, [b]horger@ma.tum.de,
[c]linus.wunderlich@ma.tum.de

We consider model reduction techniques for the numerical simulation of vibro-acoustics. The mathematical model is based on an eigenvalue problem for the possibly orthotropic linear elasticity equation. In addition to nine material parameters, geometrical parameters and insulation by thin elastomeric layers can be taken into account. A fine scale finite element simulation is typically expansive due to complex geometries. In this talk we cover several aspects. Firstly, weakly coupled patch-wise tensorial structured isogeometric elements are considered. These are of special interest for complex geometries with piecewise smooth but curvilinear boundaries. We discuss the well-posedness of the isogeometric Lagrange multiplier based mortar formulation. Secondly, we consider a dimension reduction technique which allows us to reformulate a layered geometry as interface equation coupling the 3D blocks by a spring. Thirdly, we provide upper bounds for the approximation of eigenvalues in a reduced basis setting. To obtain locality in the detailed system, we use the saddle point approach and do not apply static condensation techniques. However within the reduced basis context, it is natural to eliminate the Lagrange multiplier and formulate a reduced eigenvalue problem for a symmetric positive definite matrix. The selection of the snapshots is controlled by a multi-query greedy strategy taking into account an error indicator allowing for multiple eigenvalues.

As example for isogeometrical mortar methods, we consider the vibration of a violin bridge in a multi-query context and as example for dimension reduced interface couplings, we use a timber building block having thin elastomeric layers as insulation. Our numerical results illustrate several aspects such as accuracy of mortar couplings for splines, the influence of the orthotropic material and geometrical parameters on the eigenvalues and the component based decomposition for a multi-storey timber building.

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