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BASIC IDEAS ON VIRTUAL ELEMENT METHODS AND SOME RECENT DEVELOPMENTS

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The talk will be (roughly) split in two parts. The first, meant for people not familiar with Virtual Elements, will briefly recall the basic ideas: Virtual Elements Spaces are made of piecewise smooth functions (or vector valued functions) on decompositions made of very general polygons or polyhedra. They are defined as solutions of suitable (systems of) PDE equations inside each element, but "the name of the game" is that one does not solve these problems, but uses the degrees of freedom to compute suitable projections from the local VEM space to spaces of polynomials. Everything is made in such a way that the Patch-Test will always be satisfied. In the beginning VEMs were introduced for solving simple problems, as Laplace equation, but then they were extended to more complicated ones, like linear and non-linear elasticity, Stokes and Navier-Stokes equations, Plate bending problems, Magnetostatic problems, etc. Some of the more recent among such developments will be briefly hinted in the second part of the talk, to give an idea of the typical demeanor used to deal with these methods.

INVERSE PROBLEMS AND HYBRID OPTIMIZATION ALGORITHMS

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Inverse problems are classified as problems with unknown: a) shapes and sizes of the domains, b) boundary and/or initial conditions, c) singularities in /on the domain, d) physical properties of the media, and e) governing system of equations. These types of problems can be solved when additional information, such as over-specified boundary conditions, are provided and enforced. For example, unknown boundary conditions on arbitrary 3D solid objects can be accurately determined non-iteratively for linear models and iteratively for non-linear models where it requires regularization. Similarly, spatial distribution of material properties in arbitrarily shaped, multiply-connected 3D solid objects can be non-destructively determined by minimizing the sum of normalized least-squares differences between measured and calculated boundary values of the field variables. This means also accounting for measurements containing varying levels of noise. These methods can also be used to detect locations, sizes and shapes of unknown domains. The least squares differences between calculated and measured/enforced values was minimized using a cluster of optimization algorithms assembled in a hybrid optimization tool where a set of heuristic rules was used to perform automatic switching among the individual optimizers in order to avoid local minima, escape from the local minima, converge on the global minimum, and reduce the overall computing time. Examples of solved inverse problems governed by systems of ordinary and partial differential equations will be presented with applications in heat transfer, elasticity, aerodynamics, epidemiology, electro-chemistry, and electro-magneto-hydro-dynamics with solidification.

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LARGE-SCALE STOCHASTIC PDE-CONSTRAINED OPTIMIZATION

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We consider optimization problems governed by PDEs with infinite dimensional random parameter fields. Such problems arise in numerous applications: optimal design and control of systems with stochastic forcing or uncertain material properties or geometry; inverse problems with stochastic forward problems; or Bayesian optimal experimental design problems with the goal of minimizing the uncertainty or maximizing the information gain in the inferred parameters.

Monte Carlo evaluation of the objective as per the popular Sample Average Approximation (SAA) algorithm results in an optimization problem that is constrained by N PDE systems, where N is the number of samples. This results in an optimization problem that is prohibitive to solve, especially when the PDEs are "complex" (e.g., large-scale, nonlinear, coupled) and discretization of the infinite-dimensional parameter field results in a high-dimensional parameter space.

We discuss high-order derivative-based approximations of the parameter-to-objective maps that exploit the structure of these maps, in particular their smoothness, geometry, and low effective dimensionality. Their use as a basis for variance reduction, in combination with randomized linear algebra algorithms, is demonstrated to accelerate Monte Carlo sampling by up to three orders of magnitude and permit efficient solution of large scale stochastic PDE-constrained optimization problems with up to with $O(10^6)$ uncertain parameters and $O(10^6)$ optimization variables. Applications to optimal control of turbulent flow and optimal design of acoustic metamaterials are presented.

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MULTI-TRACE BOUNDARY ELEMENT METHODS

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The scattering of acoustic or electromagnetic waves at a penetrable object composed of different homogeneous materials can be modelled by means of boundary integral equations (BIE) posed on the interfaces. This approach is widely used in numerical simulations and often relies on so-called first-kind single-trace BIE [3, Sect. 2]. Their boundary element Galerkin discretization gives rise to poorly conditioned linear systems, for which the otherwise successful operator (Calderón) preconditioning approach does not seem to be available.

As a remedy we propose new multi-trace boundary integral equations; whereas the single-trace BIE feature unique Cauchy traces on sub-domain interfaces as unknowns, the multi-trace idea takes the cue from domain decomposition and tears the unknowns apart so that *local* Cauchy traces are recovered. The benefit is the possibility of straightforward Calderón preconditioning.

Multi-trace formulations come in two flavors. A first variant, the *global multi-trace approach*, is obtained from the single-trace equations by taking a "vanishing gap limit" [3, Sect. 3]. The second variant is the *local multi-trace method* and is based on local coupling across sub-domain interfaces [1, Sect. 4]. Numerical experiments for acoustic scattering demonstrate the efficacy of Calderón preconditioning.

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HIGH-ORDER DISCONTINUOUS GALERKIN METHODS ON POLYTOPIC GRIDS

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Numerical methods defined on computational meshes consisting of polytopic elements, which potentially contain many faces, have gained substantial traction in recent years for a number of important reasons. Firstly, flexibility, in terms of the shape of the elements admitted within a given mesh, is crucial in the context of the efficient approximation of localized geometrical features present in the underlying geometry. Indeed, the use of standard element shapes typically necessitates the exploitation of very fine computational meshes when the geometry possesses small details or microstructures. Furthermore, polytopic elements are naturally suited to applications in complicated/moving domains, for example, in solid mechanics, fluid-structure interaction, geophysical problems including earthquake engineering and flows in fractured porous media, and mathematical biology. Moreover, the ability to incorporate polytopic meshes offers a number of advantages also in the context of multilevel linear solvers, such as Schwarz-based domain decomposition preconditioners and multigrid.

In this talk, we present a survey of so-called composite/agglomerated discontinuous Galerkin finite element methods (DGFEMs) which employ general polytopic elements. In particular, we provide an overview of *hp* -version inverse estimates and approximation results for general polytopic elements, which are sharp with respect to element facet degeneration. On the basis of these results, *a priori* error bounds for the *hp*- DGFEM approximation of both second–order elliptic and first–order hyperbolic PDEs will be derived, cf. [1, 4]. Furthermore, the design of efficient quadrature rules for the numerical approximation of integrals of polynomial functions over general polytopic elements that do not require the explicit construction of a sub-tessellation into triangular/tetrahedral elements will be discussed, based on the work presented in our recent article [2]. Finally, we consider the application of these methods within Schwarz-type domain decomposition preconditioners; see [3] for further details.

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PATHWAYS TO GEOMETRIC SOLID MECHANICS

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Describing materials sub-continuum structures with 3-complexes, known from algebraic topology, offers multiple advantages for modelling and simulation. For example, a set of grains forming a polycrystalline material is a 3-complex of 3-celles (volumes), 2-cells (faces), 1-cells (edges) and 0-cells (vertices). Sub-grains structures down to atomic lattices can be conceptualised in a similar way, providing an opportunity to work across length scales with a single computational framework. The discrete nature of such representations is attractive, because it allows for assigning different characteristics to individual or sets of k-cells in order to capture heterogeneity at particular length scales. For example, measurable features of variable sizes or properties of variable magnitudes can be readily incorporated. Importantly for mechanical analysis, discrete representations allow for capturing explicitly micro-crack initiation, growth and coalescence. Development of analysis on such 3-complexes is essential for unlocking the potential of such representations.

Discrete Exterior Calculus (DEC) offers an efficient way to analyse 3-complexes. Currently DEC uses the de Rham complex, known from algebraic and differential topology, with Hodge star operators to form discrete analogues of gradient, curl and divergence. This approach has been successfully applied to analysis of a number of physical problems with scalar principal unknown. The few attempts to describe elasticity with DEC are limited to 2D problems and have a common problem Hodge stars couple fully material constitutive laws with metric information. As a result, such descriptions are only applicable to truss structures, and these are more conveniently analysed with 1-complexes (graphs). This talk presents the on-going project Geometric Mechanics of Solids (GEMS), which aims at developing an efficient tool for analysis on 3-complexes with representing elasticity as critical first step.

The scene is set by a brief description of the DEC theory. Several DEC based-schemes with different Hodge star operators, implemented in in-house codes, are discussed. One line of enquiry is based on a discrete analogue of the Navier-Lame equation of linear elasticity using a scalar-valued discrete differential forms: 0,1,2,3-cochains (functions on 0,1,2,3-cells). While this formulation can be seen as intrinsic, prescribing boundary conditions requires mapping between co-chains and external vector fields. Finding unique mapping is challenging because both vector fields and cochains belong to infinite dimensional function spaces before the discretization is made.

Another line of enquiry is based on vector-valued co-chains, offering direct correspondence between external vector fields and 0-cochains. Main issue with this approach is the unwanted coupling of metric and constitutive information by the Hodge star, seen in the few past works on the topic. Discussed are options for decoupling by separating the deformation component from the rotation component of the discrete displacement/deformation gradient.

A third line of enquiry is based on analysis of sub-complexes, formed by existing 1-

cells, intended to measure length changes, and a set of complimentary 1-cells (3-complex dependent), intended to measure angle changes. Examples solved with this approach are demonstrated.

Final line of enquiry is inspired by the computational attractiveness of modern tools in geometry integration. Elasticity problems are a formulated by energy functional, which for quasi-static cases uses a generalization of the Biot strain measure. The deriving schemes minimised via variational methods are structure preserving. That opens up a wide range of possibilities for robust and efficient nonlinear elastic simulation, improving on state of the art methods in geometry discretization schemes on solid mechanics.

FEMS FOR FRACTIONAL DIFFUSION: A SURVEY

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Fractional diffusion is a non-local diffusion process that accounts for long-range interactions. We review three finite element methods that build on different definitions of the fractional Laplacian in bounded domain. The first method is the integral formulation and deals with singular non-integrable kernels. The second method is a PDE approach that applies to the spectral definition and exploits the extension to one higher dimension. The third method is a discretization of the Dunford-Taylor formula. We discuss pros and cons of each method, error estimates, and document their performance with a few numerical experiments. We conclude with extensions to several nonlinear fractional diffusion problems.

IMPACT ANALYSIS AS AN INTEGRAL PART OF THE DESIGN PROCESS

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During the design and certification process for its products, Rolls-Royce has a need to solve various impact and non-linear structural dynamic problems. These include bird/ice ingestion, fan blade-off, core engine blade-off and response of aerofoils to tip rubbing to name but a few. The standard Finite Element package used during this process is LS-Dyna; suitably modified by Rolls-Royce in-house routines.

This lecture will provide some insight into the philosophy employed by Rolls-Royce in the analysis of impact and non-linear structural dynamic events and will also discuss the necessary rigour and attention to detail that is required to use Finite Elements routinely and robustly in a reliable predictive manner. Reference will be made where appropriate to test/analysis comparisons to demonstrate the points made.

Comment will be made as to progress made over recent years to develop the use of the software and large-scale computing to replace test and enable a smoother engine development process and eventual certification; this includes the prospect of certification of products by analysis only. In addition, a look forward to the likely future requirements for impact and non-linear structural dynamic analyses over the next few years is made.

EXPLOITING UNDERLYING APPROXIMATION PROPERTIES IN THE DISCONTINUOUS GALERKIN METHOD FOR IMPROVED TROUBLE CELL INDICATION

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Nonlinear hyperbolic equations are often used to describe the behaviour of a quantity of interest in many areas such as climate modeling, shallow water equations, and computational fluid dynamics. Solutions of these equations may develop discontinuities or shocks. The discontinuous Galerkin (DG) method allows for great flexibility in creating accurate and efficient simulations. However, near a discontinuity or shock, solutions may develop non-physical spurious oscillations. Areas where these occur are called "troubled cells". To counteract these oscillations, typically some stabilization is used such as limiting, filtering, or artificial dissipation. To ensure these techniques are only applied in necessary regions, an accurate troubled cell indicator is needed.

In this presentation we discuss how to exploit the underlying approximation space of the DG method. Specifically, the use of multiwavelets [1] for troubled cell indication. We explain how the DG coefficients easily relate to the multiwavelet decomposition [2]. This decomposition is written as a sum of a global average and finer details on different levels. Using such a decomposition allows the multiwavelet expansion to act as a troubled-cell indicator, where the averages of this contribution are computed on each element, [3, 4]. Additionally, we will discuss the performance of this indicator which typically relies on a problem-dependent parameter. Optimal performance of these indicators should produce an approximation that is free of spurious oscillations. In general, many tests are required to obtain this optimal parameter for each problem. However, to avoid choosing parameters, it is possible to combine the underlying approximation properties with techniques from statistics such as Tukey's boxplot approach [5]. This allows for investigating sudden increases or decreases of the indicator value with respect to the neighboring values and hence, indication basically reduces to detecting outliers. This allows for an automated algorithm that can easily be applied to various troubled-cell indication variables.

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MULTILEVEL UNCERTAINTY QUANTIFICATION WITH SAMPLE-ADAPTIVE MODEL HIERARCHIES

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Sample-based multilevel uncertainty quantification tools, such as multilevel Monte Carlo, multilevel quasi-Monte Carlo or multilevel stochastic collocation, have recently gained huge popularity due to their potential to efficiently compute robust estimates of quantities of interest (QoI) derived from PDE models that are subject to uncertainties in the input data (coefficients, boundary conditions, geometry, etc). Especially for problems with low regularity, they are asymptotically optimal in that they can provide statistics about such QoIs at (asymptotically) the same cost as it takes to compute one sample to the target accuracy. However, when the data uncertainty is localised at random locations, such as for manufacturing defects in composite materials, the cost per sample can be reduced significantly by adapting the spatial discretisation individually for each sample. Moreover, the adaptive process typically produces coarser approximations that can be used directly for the multilevel uncertainty quantification. In this talk, I will present two novel developments that aim to exploit these ideas.

In the first part I will present Continuous Level Monte Carlo (CLMC), a generalisation of multilevel Monte Carlo (MLMC) to a continuous framework where the level parameter is a continuous variable. This provides a natural framework to use sample-wise adaptive refinement strategy, with a goal-oriented error estimator as our new level parameter. We introduce a practical CLMC estimator (and algorithm) and prove a complexity theorem showing the same rate of complexity as for MLMC. Also, we show that it is possible to make the CLMC estimator unbiased with respect to the true quantity of interest. Finally, we provide two numerical experiments which test the CLMC framework alongside a sample-wise adaptive refinement strategy, showing clear gains over a standard MLMC approach with uniform grid hierarchies.

In the second part, I will show how to extend the sample-adaptive strategy to multilevel stochastic collocation (MLSC) methods providing a complexity estimate and numerical experiments for a MLSC method that is fully adaptive in the dimension, in the polynomial degrees and in the spatial discretisation.

This is joint work with Gianluca Detommaso (Bath), Tim Dodwell (Exeter) and Jens Lang (Darmstadt).