ABSTRACTS 1.2

FOR RESEARCH IN MATHEMATICAL SCIENCES

MARK AINSWORTH Strathclyde University

Hp-Finite Element Methods for Maxwell's Equations

Recently, there has been a dramatic increase in the use of high order finite element methods for the approximation of Maxwell's equations. We shall discuss some of our own work in this area. In particular, we shall present families of hierarchic basis functions for the Galerkin discretisation of the space $H(\operatorname{curl}; \Omega)$ that naturally arises in the variational formulation of Maxwell equations. The conditioning and dispersive behaviour of the elements is discussed along with approximation theory. Numerical examples are shown which demonstrate the accuracy and efficiency of the methods for computing solutions of the time-harmonic Maxwell's equations.

IVO BABUSKA University of Texas

Adaptivity problems in the solution of stochastic PDE's

The talk will elaborate on the formulation of the stochastic partial differential equations of elliptic type and on the obtaining the needed data from experiments. It will address the equations with stochastic coefficients and right hand side. The problem is transformed into deterministic problem in a high dimensional space. The adaptivity then includes dimensional reduction, shape functions (mesh) selection as well selection of the combination of various solution methods. This is in possible conjunction with the obtaining data from the experiments.

RANDOLPH E. BANK* AND JINCHAO XU University of California, San Diego and Penn State

Asymptotically Exact A Posteriori Error Estimators for General Unstructured Grids

In this talk, we analyze superconvergence for general unstructured but shape regular meshes. We develop a postprocessing gradient recovery scheme for the finite element solution u_h , inspired in part by the smoothing iteration of the multigrid method. This recovered gradient superconverges to the gradient of the true solution, and becomes the basis of a global a posteriori error estimate that is often asymptotically exact. Next, we use the superconvergent gradient to approximate the Hessian matrix of the true solution, and form local error indicators for adaptive meshing algorithms. We provide several numerical examples illustrating the effectiveness of our procedures.

ABSTRACTS 1.2

FOR RESEARCH IN MATHEMATICAL SCIENCES

RANDOLPH E. BANK AND JINCHAO XU University of California, San Diego and Penn State

Superconvergence and Asymptotically Exact A Posteriori Error Estimators

In this talk, we will report superconvergence estimates for piecewise linear finite element approximations on nonuniform triangular meshes satisfying an $O(h^2)$ parallelogram property in most part of the domain. In particular, we show the finite element solution u_h and the interpolant u_I have super close gradients and analyze a postprocessing gradient recovery scheme, showing that $Q_h \nabla u_h$ is a superconvergent approximation to ∇u . Here Q_h is the global L^2 projection. We then apply these superconvergence results to verify the asymptotic exactness of some new a posteriori error estimators as well as some existing ones. Both two and three dimensional results will be reported.

MARTIN BERZINS University of Leeds

Computational Engineering Challenges for Adaptive Mesh Refinement

Joint work with C.E. Goodyer R. Fairlie at Leeds, Chris Johnson of the SCI Institute at the University of Utah, and L.E. Scales of Shell Research and Technology Centre, Thornton, Chester, UK

The solution of real life computational engineering problems poses many challenges for adaptive Mesh Refinement (AMR). The AMR requirements of two such problems will be considered in the light of recent developments in both theory and algorithms. The two motivating problems are Elasto-Hydrodynamic Lubrication (EHL) as being modeled at Leeds and the explosive container problem currently being solved by the CSAFE centre at the University of Utah. In the case of the EHL example, although the modelling of lubrication problems extends back to the hydrodynamic equation of Reynolds, for very highly loaded cases (from 0.25 GPa) the contacts themselves deform, defining elastohydrodynamic lubrication (EHL). These cases are important to industry for the design of new oils and new components and pose a formidable computational engineering challenge. Coupling the dense matrices of the elastic deformation of the surfaces with the highly non-linear equations of the pressure distribution and lubricant rheology leads to an intensive computation requiring at least 100 million grid points to resolve micro-EHL problems (which are generally also transient) with realistic surface roughness.

Although the CSAFE problem is perhaps an order of magnitude more challenging still, both problems have a number of common characteristics:

- (i) complex multi-scale phenomena and experimental physical models
- (ii) an inherently transient nature with multiple space and time scales
- (iii) the need for parallel computing and large numbers of grid points
- (iv) accuracy requirements specified in terms of particular quantities of interest.
- (v) the need to use adaptive multigrid methods on cartesian type meshes.

FOR RESEARCH IN MATHEMATICAL SCIENCES

(vi) the end-user desire for an integrated problem solving environment

These characteristics will be described in relation to the problems under consideration and used to motivate an examination of existing techniques for transient error estimation and for determining the error in quantities of interest. The theoretical and algorithmic issues related to current AMR techniques will be considered and the techniques applied to current lubrication problems. The challenge of applying such techniques to the CSAFE problem will be considered.

ANNE BOURLIOUX University of Montreal

Some adaptive strategies in turbulent combustion

Turbulent combustion represents an enormous computational challenge because of the multiple scales involved: from the large scales of interest of engineers down to the smallest scales related to turbulence fluctuations, and the even smaller ones associated with the flame thickness. I will introduce some key ideas on how to tackle this challenge for an idealized test-case of a multiple-scale advection- reaction-diffusion equation. The first testproblem will be linked to premixed flames, where the challenge is to predict the speed of propagation and the shape of a very thin, very distorted flame front. Those overall features of the flame dynamics depend very much on resolving the detailed behavior down to the smallest scales. In a traditional adaptive mesh strategy, the pde would be discretized in a nested set of grids of increasing resolution, with the solution on the different meshes tightly coupled. An asymptotic study however reveals that tight coupling is not required: I will describe a loosely-coupled grids strategy designed to exploit the asymptotic results for greater efficiency. The second test-problem will be linked to nonpremixed flames. As in the first example, a practical strategy to deal with the computational challenge is to decouple to some extent the computation at large and small scales - this leads to the socalled steady laminar flamelet model. As indicated by the name, one major assumption is that the smallest scales behave as if the problem was steady. A test- case is set-up to validate this type of strategy in a case with extreme unsteady, intermittent behavior that reflects more realistic turbulent conditions. The validation requires a very accurate time-integrator. I will describe a very convenient approach to design a high order time integrator for advection-reaction- diffusion equation. It is a multi-implicit, split, scheme where high order is achieved via spectral deferred correction. It is built upon simple backward Euler schemes and very easy to implement; it also leads very naturally to timestep adaptation.

ABSTRACTS 1.2

FOR RESEARCH IN MATHEMATICAL SCIENCES

BERNARDO COCKBURN University of Minnesota

Adaptivity and a posteriori error estimation for Hamilton-Jacobi equations

We propose a new a posteriori error estimate for Hamilton- Jacobi equations which is independent of the Hamiltonian, the space dimension, and of the way the approximate solution is computed; moreover, it is local. This unique a posteriori error estimate allows us to construct a simple, recursive adaptive algorithm with which we can achieve a rigorous error control even in the presence of discontinuities in the derivatives. The algorithm can be applied to any explicit and stable numerical scheme; moreover, the algorithm uses a local space-time refinement strategy that does not alter the stability condition of the numerical scheme.

This is joint work with Jianliang Qian, IMA, University of Minnesota.

LESZEK DEMKOWICZ The University of Texas at Austin

Fully automatic hp-adaptive simulations

I will present an algorithm allowing for a FULLY AUTOMATIC solution of elliptic and (time-harmonic) Maxwell's equations with the hp-adaptive edge finite elements. With no interaction from the user, except for defining the problem, the algorithm delivers a sequence of optimally refined hp meshes, aimed at delivering a high quality solution (typically one percent error measured in energy norm, relative to the energy of the solution), with a minimum number of degrees-of-freedom. Construction of the meshes involves not only identifying which elements to refine, but also deciding whether to increase the order of approximation p, or break the elements, decreasing element size h. Additionally, one has to decide between ISOTROPIC or ANISOTROPIC refinements, an issue critical in capturing effectively various types of singularities and boundary layers. The algorithm (to the best of our knowledge - first of its kind), is based on identifying the optimal refinements, by minimizing the corresponding hp-interpolation error for a reference solution which is obtained by solving the problem on a mesh obtained by globally refining the current mesh in BOTH h and p. Critical to the efficiency of the method is the use of a two-grid solver for obtaining the reference solution. The method has been succesfully tested on a series of 2D test problems, delivering (known from elsewhere) optimal meshes, and exponential convergence rates. The test problems to be presented include:

a/ for H1-conforming elements: - 2D Laplace (Poisson) equation, - 2D non-homogeneous, highly anisotropic heat conduction, - 2D system of linear elaticity equations, - 3D axisymmetric problem for Maxwell equations, reduced to a 2D elliptic problem,

b/ for H(curl)-conforming elements: - 2D diffraction problem for Maxwell equations.

Additionally, I will show results on combining hp- adaptivity with a goal-oriented adaptive strategy, and (hopefully) first 3D results for 3D Fichera's corner problem.

ABSTRACTS 1.2

FOR RESEARCH IN MATHEMATICAL SCIENCES

YVON MADAY Laboratoire Jaques-Louis Lions

A posteriori bounds on outputs : applications to finite element and reduced basis approximations.

For many problems and many discretizations, a priori analysis allows to state that, if the number of degrees of freedom is large enough, the approximation of the solution will be good enough. The problem that has been the subject of many research and the subject of the current worshop is to guess and certify the right size of discrete spaces for a given accuracy.

Among the possible results that one want to certify lies some outputs, computed from the discrete solution of partial differential system. We define and explain how to get reliable and computable bounds on these outputs.

The problem will consider include the Stokes and Navier Stokes equations in fluid dynamics and the Hartree Fock problem in quantum chemistry.

The discretization we shall present will be either of classical finite element type but also of reduced basis type that, coupled with the error bounds can become reliable and serious alternative to more standard discretization methods.

This work has been done through collaborations more particularly with A. T. Patera, E. M. Ronquist, D. Rovas and G. Turinici

OLEG V. VASILYEV University of Missouri - Columbia

Adaptive Wavelet Collocation Method for the Solution of Partial Differential Equations

Today there are a number of problems in engineering and science, which share a single common computational challenge: the ability to solve and/or model accurately and efficiently a wide range of spatial and temporal scales. Different scales are often not distributed uniformly in space and time and have complex nonlinear dynamics due to different physical feedback mechanisms. In this talk we present a general framework for constructing an adaptive method that takes advantage of the multi-resolution wavelet analysis, a new mathematical concept, which allows one to represent a function in terms of special basis functions, called wavelets.

Wavelets are localized in both space and scale, and as a result functions with localized regions of sharp transition are well compressed using wavelet decomposition. This property allows us to construct an efficient adaptive numerical method, which employs wavelet compression as an integral part of the solution. The adaptation is achieved by retaining only those wavelets whose coefficients are greater than an a priory prescribed threshold. This property of the multi-level wavelet approximation allows local grid refinement up to an arbitrary small scale without a drastic increase in the number of grid points; thus

FOR RESEARCH IN MATHEMATICAL SCIENCES

ABSTRACTS 1.2

high resolution computations are carried out only in those regions where sharp transitions occur. Wavelet decomposition is used for both grid adaptation and interpolation, while a O(N) hierarchical finite difference scheme, which takes advantage of multi-level wavelet decomposition, is used for derivative calculations. The prowess and computational efficiency of the adaptive wavelet collocation method are demonstrated for the solution of a number of test problems including both evolution-type and elliptic partial differential equations. The results indicate that the computational grid and associated wavelets can very efficiently adapt to the local irregularities of the solution. Furthermore, a solution is obtained on a near optimal grid, i.e. the compression of the solution is performed dynamically as opposed to a posteriori as it is done in data analysis.

JUNPING WANG Colorado School of Mines

Interior Estimates of Superconvergence for Finite Element Solutions by Local Projections

This talk will discuss superconvergence and its application to posteriori error estimation for finite element solutions of partial differential equations. In particular, we are interested in projection methods defined locally on subdomains. The projection method is a post- processing procedure that constructs new approximations by using the method of least-squares. This procedure has been proved to produce new approximations with superconvergence on quasi-uniform meshes. The existing results rely on a global a priori regularity of the adjoint problem.

The goal of this talk is to establish some interior superconvergence estimates in the L^2 and L^{∞} norms for local projections of the Galerkin finite element solutions. The results have two prominent features. First, they are established for any quasi-uniform meshes which are of practical importance in scientific computing. Second, they are derived on the basis of local properties of the domain and the solution for the second order elliptic problem. As a result, the global a priori regularity on the adjoint problem is no longer required in the superconvergence. Therefore, the result of this paper can be employed to provide local and useful a posteriori error estimators in practical scientific computing.

This is a joint work with Professor Hongsen Chen at the University of Wyoming.