THE FIELDS INSTITUTE
FOR RESEARCH IN MATHEMATICAL SCIENCES

ABSTRACTS 1.2

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A Posteriori Error Analysis for Multi- Dimensional Hyperbolic Problems

The discontinuous Galerkin method (DGM) is an appealing approach to address problems having discontinuities, such as those that arise in hyperbolic conservation laws. The DGM uses a discontinuous finite element basis which simplifies hp adaptivity and leads to a simple communication pattern across faces that makes it useful for parallel computation. In order for the DGM to be useful in an adaptive setting, techniques for estimating the discretization errors should be available both to guide adaptive enrichment and to provide a stopping criteria for the solution process. We will show that the $p-$degree DG finite element solution for hyperbolic problems exhibits superconvergence at the roots of Radau polynomials of degree $p+1$ with the fixed endpoints selected at the downwind boundary of each quadrilateral element. We also show that the DG solution has strong superconvergence on average at the outflow boundary. We use this superconvergence results to construct asymptotically exact a posteriori error estimates for first-order hyperbolic partial differential equations. Finally, we present numerical results for several computational examples with both continuous and discontinuous solutions that show the efficiency of our a posteriori error estimator.

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Université Cadi Ayyad, Universtất Chemnitz, Université Ibn Tofail , Université de Valencienne et du Hainaut-Cambrésis

A posteriori error estimation for anisotropique finite volume meshs

In this work we develop a discretization using Finite Volume (FV) Method of vertex-centered type, for the numerical solution of a convection-diffusion equation on unstructured grids.Because such problem yield a solution which exhibits little variation in one direction, but much change in an other direction (the solution is called anisotropic), it is natural to use a small mesh size in the direction of the rapid variation of the solution and a larger mesh size in the direction of the little variation (the mesh is called anisotropic).

The aim of this work is to develop , firstly a FV scheme to approximate a convection-diffusion equation which is anisotropic and convergent, and secondly an a posteriori error estimate efficient and reliable for such scheme, in order to introduce an auto-adaptive refinement. Some numerical results will be presented to confirm the theory.

We consider the problem

$$-\epsilon\Delta u + q\cdot\nabla u + cu = f \text{ in } \Omega \subset IR^d \quad (1)$$

$$u = 0 \text{ on } \Gamma := \partial\Omega \quad (2)$$

where q, c and f are regular functions such that $q = (q_1(x), ..., q_d(x)) \geq (1, ..., 1)\ \forall x \in \Omega$, $0 < \epsilon \ll 1$ and $c + \frac{1}{2}divq \geq C_0 \geq 0$ in Ω.

M. AIFFA
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A geometrical approach to mesh : smoothing

It is well known that poorly shaped elements in a finite element mesh affect both the accuracy of the finite element solution and the stability of the process by which it is computed. Adaptive mesh refinement is one cause for the generation of highly distorted elements. In this talk we will go over some of the mesh improvement techniques such as edge swapping, node insertion, node deletion etc ... We will concentrate on node relocation, also known as mesh smoothing, where each mesh vertex v is recursively moved to a target location that minimizes a given mesh quality measure. The target location v_t is expressed as a solution to a local optimization problem that is usually solved using a line search type approach. We will describe an alternative way for solving the local optimization problem by characterizing the set of optimal locations in terms of the level sets associated with the shape quality measure in use. Modulo some assumptions on the shape quality measure, satisfied by most one in use, we completely characterize the set of optimal locations. As a consequence we are able to write explicit formulas for the optimal locations, provided the level sets are simple enough such as circles in $2D$ and spheres in $3D$. Finally we will introduce a new shape measure for tetrahedra.

JÖRN BEHRENS*, ARMIN ISKE, MARTIN KÄSER
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An adaptive mesh-free method of backward characteristics for advection equations

A mesh-free method for solving linear and nonlinear multi-dimensional transport problems is proposed. This method is essentially a combination of an adaptive semi-Lagrangian method with a mesh-free radial basis function interpolation on scattered data.

We discuss customized strategies for node placement for achieving locally optimally spaced node clusters for the approximation of PDEs. A special a posteriori error indicator is developed, in order to refine/coarsen the nodes according to approximation requirements. Some remarks on the stability of the proposed method are made.

Numerical examples in two space dimensions demonstrate the effectiveness of the mesh-free method of backward characteristics. A model problem and a near-realistic problem for linear transport are treated yielding accurate results.

The new method proves to be applicable to nonlinear equations. Examples of Burger's equation and Buckley-Leverret equation in two dimensions are given. An artificial viscosity ansatz is chosen to model shock propagation with the characteristics based method.

ALEXEI BESPALOV* AND NORBERT HEUER
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An a-posteriori error estimate for problems with strong singularities

We present an a-posteriori error estimator for a finite element scheme applied to an elliptic boundary value problem with strong point singularities. The singularities caused by singular data are such that the problem is not well-posed in H^1, but needs special weighted spaces for its variational formulation, see [1]. The corresponding finite element scheme uses standard piecewise polynomials but weighted with appropriate singular functions. The weight functions depend on the problem and the weighted energy space, see [2].

We define an a-posteriori error estimator for the special finite element scheme using a two-level hierarchical decomposition of the ansatz space. Our analysis follows Bank and Smith [3]. Main ingredient is a saturation assumption and a strengthened Cauchy-Schwarz inequality for the two-level decomposition in the weighted Sobolev spaces.

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J. DE FRUTOS* & J. NOVO
Universidad de Valladolid

Postprocessing the p version of finite element method and adaptivity in the numerical solution of nonlinear parabolic equations of dissipative type

In recent years spectral methods for the numerical solution of nonlinear parabolic equations have received increasingly attention. The p and h-p versions of finite element method allow to treat complex geometries with spectral accuracy. Spectral-type approximations have been proven to be suitable for parabolic equations due to their regularization properties. In this talk we focus on the p- version of the finite element method.

The theory of a posteriori error estimation for elliptic problems has been extensively treated in the literature. For parabolic equations much fewer results are available, see [1]. In [1], [2], it is proven that an a posteriori error estimator for evolutionary problems can be obtained by using any elliptic a posteriori error estimator. In these papers, the analysis is done in a special time-weighted energy norm in the space-time cylinder. In the present talk we propose a similar procedure that can be used for nonlinear dissipative equations. In our approach the error estimation is done at fixed times by means of only one elliptic problem with right hand side the residual of the numerical solution with time frozen. Furthermore, the main advantage of the procedure we propose is that it gives a hierarchy of corrections to the numerical solution that allow to improve the spatial accuracy (if it is needed) without increasing the computational cost of the overall time integration, including the cost of error estimation.

The results are based in the theory of the so called postprocessed Galerkin methods [3], [4]. Postprocessed methods have been used in a different context to get improved solutions of dissipative equations. The main hypothesis needed is that the solutions of the equations are smooth in time, a property that is shared for most dissipative partial differential equations including, reaction-convection-diffusion equations, Navier-Stokes equations, etc.

The computation of the a posteriori error estimator, and a fortiori the correction, is far less expensive than the computation of the numerical solution and can be carried out at every time when it is needed. The results can be used as a basis for an adaptive numerical procedure that controls adaptive enrichment through h or p version of finite element method. Some numerical results are presented.

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E. G. FILIPPENKO AND V. S. ZYUZIN
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A Posteriori Error Estimation of Gursa Problem

The method of finding coefficients of Taylor series is proposed for the solution of partial differential equations (PDEs) with initial conditions. It is used to find interval solution of Gursa problem

$$U_{xy} + a(x,y)U_x + b(x,y)U_y + c(x,y)U = f(x,y) \tag{1}$$

(a, b, c - are analytical functions in the given field) with following conditions

$$U(x_0, y) = \varphi_1(y), y_0 \leq y \leq b,$$
$$U(x, y_0) = \varphi_2(x), x_0 \leq x \leq a, \tag{2}$$

and besides $\varphi_1(y_0) = \varphi_2(x_0)$.

Functions $\varphi_1(y)$ and $\varphi_2(x)$ have continuous derivatives of the first order.

The same method of finding coefficients of Taylor series is developed for the solution of homogeneous differential equations system (HDE) [1].

The Taylor series function $f(x,y)$ in the point (x_0, y_0) is the following:

$$f(x,y) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} (f)_{ij}(x - x_0)^i (y - y_0)^j,$$

where

$$(f)_{ij} := \frac{1}{i!j!} \frac{\partial^{i+j} f}{\partial x^i \partial y^j}.$$

The following formulas are used to find coefficients of Taylor series

$$(f_x)_{ij} = (i+1)(f)_{i+1,j}; \quad (f_{xy})_{ij} = (i+1)(j+1)(f)_{i+1,j+1};$$
$$(f_{xx})_{ij} = (i+1)(i+2)(f)_{i+2,j}; \quad (f \pm g)_{ij} = (f)_{ij} + (g)_{ij};$$
$$(fg)_{ij} = \sum_{k=0}^{i} \sum_{l=0}^{j} (f)_{kl}(g)_{i-k,j-l}.$$

The recurrence formula is as follows:

$$(U_{xy})_{ij} = -(aU_x)_{ij} - (bU_y)_{ij} - (cU)_{ij} + (f)_{ij}. \tag{3}$$

The remaining member is calculated according to the formula:

$$R_{n+1} = \frac{1}{(n+1)!}(\frac{\partial}{\partial x}h_1 + \frac{\partial}{\partial y}h_2)^{n+1}U(\tau_1, \tau_2),$$

where

$$x_0 \leq \tau_1 \leq x_0 + h_1,$$
$$y_0 \leq \tau_2 \leq y_0 + h_2.$$

The polynomial to the n power is found and the remaining member of the $(n+1)$ order is evaluated. Using interval methods get guaranteed a posteriori error estimation including error calculation for the approximate problem solution (1)(2).

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JOSEPH E. FLAHERTY AND LILIA KRIVODONOVA
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Error Estimation and Limiting Techniques for Discontinuous Galerkin Method

A computationally efficient error estimator is needed to guide adaptive enrichment and to provide a measure of solution accuracy for any numerical method. Efficiency is of special importance for hyperbolic problems where solution features evolve in space and time. We develop an inexpensive a posteriori error estimation technique based on superconvergence. The superconvergence phenomena is described for one- and multi-dimensional problems and for structured and unstructured meshes. We prove that the discretization error of pth-order approximation converges at the downwind boundaries of elements as $O(h^{2p+1})$ pointwise for one-dimensional problems and on average for higher dimensions. We further prove that the global error converges at $O(h^{p+2})$ rate at the Radau points of degree $p+1$ for one-dimensional problems. In higher dimensions, point-wise superconvergence as well as Radau polynomials seize to exist. However, we demonstrate that average errors converge at a faster $O(h^{p+2})$ rate over lines (in two dimensions) parallel to the downwind boundary. The estimator requires $O(Np^{k-1})$ operations to compute relative to $O(Np^k)$ solution complexity on a mesh of N elements in k dimensions for one time step.

High-order accuracy is desirable, but difficult to achieve for hyperbolic conservation laws with discontinuous solutions. High-order approximations of such problems develop spurious oscillations near discontinuities. One possible solution is to use a limiter - a nonlinear procedure that suppresses oscillations. However, existing limiters reduce the order of accuracy near smooth extrema. By constructing an indicator that distinguishes smooth and "rough" areas, we restrict the use of the limiter to the elements containing discontinuities. As a result, we obtain sharp resolution of shocks as well as achieve the theoretical high-order rate of convergence in smooth regions.

A. FOURNIER* AND S. SUMETKIJAKAN
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Multiresolution Adaptive Spectral Elements:Application to shallow-water flow on the sphere

We present a high-order, adaptive numerical method for numerically solving advection-diffusion PDEs, and demonstrate the advantage of this method for fluid dynamics problems, especially that generate quasi-singular or coherent structures.

There are four aspects of the method that we will elucidate. First, the spatial discretization employs piecewise-polynomial spaces similar to the traditional spectral-element method; however we use orthogonal multiresolution analysis (MRA) comprising many nonconforming elements of various scales. This MRA is constructed using multiwavelets, which are orthonormal basis functions whose span efficiently describes the extra "detail" information gained in refining some of the spectral elements (Alpert et al. 1999).

Second, the adaptivity criterion for a set of elements is the norm of the projection onto the corresponding multiwavelets. Using this simple criterion, the algorithm refines and coarsens the representation of steepening or translating structures. Our criterion replaces more traditional criteria, based on local gradients or local spectra.

Third, we take advantage of the spatial discretization, to improve the time-stepping scheme. We use the "exact linear part" scheme (Beylkin et al. 1998), which amounts to using scaling and squaring to compute the exponential propagator due to the diffusive linear operator. This adaptive operator exponentiation is made feasible by our spatial discretization. It significantly improves convergence for high Reynolds numbers and large time steps.

Finally, we use block-sparse data structures to achieve efficiency.

We will demonstrate these features using the standard shallow-water test suite of Williamson et al. (1992).

VASILE CATRINEL GRADINARU
Universität Tübingen

Mixed Finite Elements on Sparse Grids

Sparse grids provide efficient approximations of smooth functions. More precisely, they are a device to describe a function up to a prescribed accuracy with very few degrees of freedom. If conventional Sobolev-norms are used to measure accuracy, sparse grids can be shown to be optimal or near optimal. A tremendous reduction of the amount of data is achieved compared to standard schemes of multivariate approximations that rely on low-order polynomials. It turns out that sparse grids are a priori adaptive grids. The crucial idea is to drop certain insignificant contributions of hierarchical representations of functions

So far, sparse grids schemes have been based on linear and higher order Lagrange polynomials for H^1 conforming finite elements. We generalize the discretization on sparse grids to discrete differential forms (Whitney forms). The extension to general l-forms in d dimensions includes mixed elements for and can be used for the Galerkin discretization of mixed boundary value problems.

The tensor product structure and the hierarchical multilevel principle provide the hierarchical decomposition of the Whitney spaces. We define the sparse grid interpolation operator relying on the hierarchical basis. The interpolation estimates generalize the known results for Lagrangian finite elements. Approximate interpolation is needed for the Galerkin method for boundary value problems on sparse grids. The combination technique and a two point quadrature rule ensure that similar error estimate as for the exact interpolation hold.

Some inherent limitations of the proposed method are given by the fact that only tensor product domains have been successfully investigated. Further, no techniques for boundary value problems with variable coefficients are available yet. However, we will discuss adaptively refined sparse grids, too.

S. HAMDI,* W. H. ENRIGHT, J.J. GOTTLIEB AND W.E. SCHIESSER
The Fields Institute, University of Toronto, University of Toronto and Lehigh University

Accurate Interpolations for Adaptive Method of Lines

The problem addressed in this paper is the accurate interpolation of numerical solutions of high order partial differential equations (PDE)s. This problem arises frequently, for example, with the static adaptive method of lines where a numerical solutions from a previous grid needs to be mapped accurately onto a new adapted grid. In most previous studies the mapping is performed using cubic splines interpolation but this can be insufficiently accurate for high order (PDE)s such as the Korteweg-de Vries equations. In this paper, we will consider three standard interpolating algorithms (based on the use of cubic splines, quintic splines and quintic B-splines) and two non-standard interpolating algorithms based on Fornberg interpolation and on almost collocation.

Accurate interpolation of a numerical solution is also frequently used in the assessment of the performance of the solution method. In such cases, accurate evaluation of the phase and amplitude errors and accurate integration of the invariants of motion of solitary waves are used as measures of the reliability of the underlying solution method of the PDE. Numerical integration using adaptive quadrature routines is not applicable in this case because it relies on the ability to automatically choose the location of the abscissas. The basic approach investigated in this study uses the exact integration

of the interpolants. Several alternatives based on different choices for the interpolation technique will be investigated and applied to problems arising from several invariants of motion for the conservation of mass, momentum and energy for the Korteweg-de Vries Burgers equations. Each of the integration algorithms is implemented in Fortran and MAPLE and is available from the authors. Several numerical examples are presented to illustrate important features of the propagation and interactions of solitary waves of the Korteweg-de Vries Burgers equations, the breakup of a Gaussian pulse into solitary waves, and the development of an undular bore.

NORBERT HEUER
Universidad de Concepción

Error indicators based on two-level decompositions for the BEM

We present error indicators for the p- and hp-version of the boundary element method for elliptic boundary value problems in two and three dimensions. Our indicators are based on local enrichments of the ansatz spaces and decompositions thereof. Key points in the analysis of reliability are a saturation assumption and stability of the subspace decompositions. For efficiency, on the other hand, just stability of the decompositions is needed. We present various types of decompositions, in two and three space dimensions, and prove stability.

For model problems, the performance of corresponding algorithms is shown and the influence of saturation on reliability is indicated.

HUNG-TSAI HUANG AND ZI-CAI LI*

The Adini's Elements for the Neumann Problems of Poisson's Equation

Co-author Ningnig Yan, Institute of System Science.

In this paper, we report some new discoveries of Adini's elements for the Neumann problems of Poisson's equation in error estimates, stability analysis and global superconvergence. It is well known that the optimal convergence rate $\|u-u_h\|_{1,S} = O(h^3)|u|_{4,S}$ can be obtained, where u_h and u are the Adini's solution and the true solution respectively. In this paper, for all kinds of boundary conditions of Poisson's equations, the superclose $\|u_I^A - u_h\|_{1,S} = O(h^{3.5})|u|_{5,S}$ can be obtained for uniform rectangles $\square_{ij}$, where u_I^A is the Adini's interpolation of the true solution u. Moreover, for the Neumann problems of Poisson's equation, new treatments adding the explicit natural constraints $(u_n)_{ij} = g_{ij}$ on ∂S are proposed to yield the Adini's solution u_h^* having superclose $\|u_I^A - u_h^*\|_{1,S} = O(h^4)|u|_{5,S}$. Hence, the global superconvergence $\|u - \Pi_p^5 u_h^*\|_{1,S} = O(h^4)|u|_{5,S}$ can be achieved, where $\Pi_p^5 u_h^*$ is an a posteriori interpolant of polynomials with order five based on the obtained solution u_h^*. New basic estimates of errors are derived for Adini's elements, and new proofs are provided to derive the optimal rate $O(h^{-2})$ of condition number for the associated matrix resulting from Adini's elements. Numerical experiments in this paper are also provided to verify perfectly the superconvergences, $O(h^{3.5})$ and $O(h^4)$, and the optimal condition number $O(h^{-2})$.

CHRISTIANE JABLONOWSKI
University of Michigan

A View of the Sphere: Adaptive Methods in Climate and Weather Modeling

Climate and weather models are amongst the many fluid dynamics applications that are characterized by multi-scale interactions. But although today's atmospheric general circulation models (GCMs), and in particular weather prediction codes, are already capable of uniformly resolving horizontal scales of order 20km, the motions of interest span many more scales than those captured in a fixed resolution model run.

Dynamically adaptive grid approaches have long been used in aerospace engineering, astrophysics, aeronautical and other computational fluid dynamics problems. In atmospheric science they were first applied approximately twelve years ago and mostly restricted to Cartesian coordinate systems. However, modeling weather phenomena on a global scale requires spherical coordinates and this new research effort aims at adaptive schemes for PDEs on the sphere.

The talk will give a design overview of an adaptive GCM that is based on NASA's next generation global climate model. This conservative model in flux form uses a local finite volume discretization that is third order accurate when applying the piecewise parabolic method (PPM). The main building block of the adaptations is a block-structured data structure that allows high performance computations with minimal changes to the preexisting PDE solvers. Blocks are refined or coarsened by a factor of two and neighboring blocks can only differ by one refinement level. This guarantees accurate influx and outflow conditions at the interface boundaries, but on the other hand can lead to cascading refinement requests. Therefore, questions concerning the optimal refinement criteria that are capable of capturing the atmospheric 'features of interest' must be discussed. Furthermore, the challenging aspects of grid adaptations on parallel computers will be addressed.

PETER K. JIMACK
University of Leeds

An Adaptive Arbitrary Lagrangian-Eulerian (ALE) Approach for Time-Dependent Free-Surface Flow Problems in 2 and 3 Dimensions

This talk will include joint work with a number of colleagues in the Schools of Computing, Mathematics and Mechanical Engineering at the University of Leeds: P.H. Gaskell, M.A. Kelmanson, R.C. Peterson, J.L. Summers, H.M. Thompson, M.A. Walkley and M.C.T. Wilson.

We describe a very general ALE algorithm, using a boundary- conforming finite-element method, for the solution of surface-tension-dominated free-surface flow problems in two and three dimensions. This algorithm combines both mesh movement, driven by the motion of the free surface, with discrete remeshing, if and when the quality of the mesh deteriorates below certain quantified thresholds. The main strength of the adaptive approach that has been adopted is that it allows the shape of the free-surface to change significantly during the course of a simulation without any *a priori* knowledge of how the geometry will evolve. Furthermore, the use of adaptivity ensures that the free-surface may be represented to a high accuracy and the ALE approach means that the computational domain is restricted to the region occupied by the fluid at any given time.

Our implementation using triangles in two dimensions, allowing both Cartesian and axisymmetric flow simulations, is well developed, whilst the three-dimensional implementation based upon tetrahedra is still ongoing. Details of the adaptive algorithms and the underlying flow solvers will be presented. In particular we will describe how the position of the free-surface is updated at each time step and then how the positions of the rest of the nodes in the mesh are moved, and the finite element equations updated, to be consistent with this. The mechanisms for triggering discrete remeshing will also be discussed, as will the remeshing algorithms themselves and the data structures required for efficient interpolation between grids after discrete remeshing has taken place.

Example simulations that will be described include the shedding of a curtain of fluid from a rotating roller, the formation of an axisymmetric drop, the breaking of a liquid bridge as two wet surfaces are pulled apart, and the viscous sintering of two cylinders or two spherical droplets of fluid. In each of these cases the geometry of the solution domain changes substantially during the course of the simulation and so the use of mesh adaptivity is essential for an efficient computation to be achieved.

SERPIL KOCABIYIK
Memorial University of Newfoundland

A Finite Difference Method for the Simulation of Flow Around

A Circular Cylinder Subject to Forced Oscillations

The problem of unsteady, laminar flow past a circular cylinder which performs rectilinear oscillations at an arbitrary angle η with respect to the oncoming uniform flow is investigated numerically for the first time. Not only do these oscillations have practical consequences relating to the design of engineering structures, but from a fundamental standpoint the forced oscillations of cylinders at an arbitrary angle with respect to the oncoming uniform flow form an important and relatively unexplored class of oscillatory flows. The flow is incompressible and two-dimensional, and the cylinder oscillations are harmonic.

The investigation is based on the solution of unsteady Navier-Stokes equations together with the mass conservation equation in the case of viscous fluids. The method of solution is based on the use of truncated Fourier series representations for the stream function and vorticity in the angular polar coordinate. A non-inertial coordinate transformation is used so that the grid mesh remains fixed relative to the accelerating cylinder. The Navier-Stokes equations are reduced to ordinary differential equations in the spatial variable and these sets of equations are solved by using finite difference methods, but with the boundary vorticity calculated using integral conditions rather than local finite-difference approximations.

The cylinder motion starts suddenly from rest at time $t = 0$. Immediately following the start of the cylinder motion, a very thin boundary-layer develops over the cylinder surface and grows with time. Accordingly, we divide the solution time into two distinct zones. First zone begins following the start of fluid motion and continues until the boundary-layer becomes thick enough to use physical coordinates. In this zone, we use boundary-layer coordinates, which are appropriate to the flow field structure, in order to obtain an accurate numerical solution. The spacing of the grid points used in this zone are such that they are spaced closer together near the surface and further apart at large distances. In addition, the adopted grid mesh continually grows in time to properly accommodate the vortex shedding process and boundary-layer development of the flow. The second zone starts following the first one and continues until the termination of calculations. The change from boundary layer coordinates to physical coordinates is made when boundary layer thickens which also ensures that the same grid points can be used in boundary-layer and actual physical space. In this way the numerical solution procedure can be started with good accuracy and continued with comparable accuracy until a periodic vortex-shedding regime is established.

The numerical method is verified for small times by comparison with the analytical results of a perturbation series solution and an excellent agreement is found. The results of this study are consistent with previous experimental predictions.

A. M. LAKHANY AND J. R. WHITEMAN
Algorithmics Inc.

A Posteriori Error Estimation Using Superconvergent Recovered Gradients

During this talk I shall be mainly discussing some of the post processing methods for the gradient of the finite element approximation that render a superconvergent approximation to the gradient of the weak solution for a variety of problems. I shall follow the historical development of this field and emphasize how the evolution of this field has been influenced by the need for a posteriori error estmates that are based on superconvergent gradient recovery. Today, the selling point for gradient recovery techniques is no longer based on obtaining a superconvergent gradient in order to substitute the gradient of finite element approximation. In fact the focus of research has been on the use of the recovered gradients to provide a posteriori error estimation. In this context I shall discuss two types of estimators where superconvergent gradients can be employed, namely,

1. the Zienkiewicz-Zhu type error estimators and
2. estimators based on interpolation error bounds.

Because of the superconvergence property, these estimators can be proved to be asymptotically exact.

This talk will follow the natural course of development in superconvergence theory. I shall start with some earlier results in this field and demonstrate how the subsequent results were mostly dedicated to addressing undesirable assumptions required by the former results. Examples include the high regularity of the weak solution, the simplicity of the problem and the regularity of the mesh. I shall focus primarily on how the regularity requirements on the mesh were relaxed as this seems essential under adaptive refinement of the finite element meshes.

I shall finish my talk by mentioning some newer results in this field and current research in which I am engaged.

SHENGTAI LI*, LINDA R. PETZOLD AND JAMES M. HYMAN
LANL, University of California Santa Barbara and University of California Santa Barbara

Implicit Implementation and Sensitivity Analysis for PDEs with Adaptive Mesh Refinement

A method of lines (MOL) approach was employed to solve the time-dependent PDE on an adaptive mesh. First the PDE system is semi-discretized in space into a DAE system. Then the DAE system is integrated by a variable order variable stepsize backward differention formula (BDF) method. The structured adaptive mesh refinement (SAMR) method was used to achieve the adaptivity when the mesh varies with time.

Most implementations of SAMR have used an explicit time integration, and refined time as well as space by taking local smaller time steps for finer grids. The explicit time integration is not efficient when solving some parabolic type PDEs or when solving for the solutions of near steady-state equations. In our implementation, SAMR was combined with an implicit time integration solver DASPK3.0, which also has the sensitivity analysis capability. An efficient transformation between the DASPK3.0 flat structure and AMR hierarchical data structure was designed and applied. To improve the computational efficiency, we used a *warm restart* technique so that the integration is continued with almost the same step size and order after remeshing as would have been used had the remeshing not taken place. Even with the warm restart, the overhead of the mesh adaptation is relatively high. The most significant cost is evaluation of the Jacobian. To further reduce the overhead of the mesh adaptation, we perform the mesh refinement after a number of time steps instead of at every time step, and replace the old mesh with the new adaptive one only when the variance is big enough. An automatic differentiation tool is also used to reduce the cost of the Jacobian evaluation.

We have applied two sensitivity analysis approaches to our adaptive solver: forward and adjoint. The forward approach can be implemented in a straightforward way with the help of the automatic differentiation. However, the adjoint approach cannot be used directly with the adaptive mesh methods due to either inadmissibility or inconsistency problems. We proposed a new adjoint approach to solve the problems.

LIPING LIU AND SHUHUA ZHANG
Lakehead University and Tianjin University of Finance and Economics

Global Superconvergence Analysis for Finite Element Methods of Integro-Differential Equations

Our talk introduces a global superconvergence in maximum norm for the derivatives of the time-continuous Galerkin finite element solutions of parabolic integro-differential equation of the form

$$
\begin{aligned}
&u_t + A(t)u + \int_0^t B(t,s)u(s)ds = f(t) \text{ in } \Omega \times J,\\
&u = 0 \text{ on } \partial\Omega \times J,\\
&u(0) = u_0(x) \ x \in \Omega,
\end{aligned}
$$

where $\Omega \subset R^2$ is an open bounded domain with smooth boundary $\partial\Omega$, $J = (0, T)$ with $T > 0$, $A(t)$ is a self-adjoint positive definite linear elliptic partial differential operator of second order, and $B(t, s)$ an arbitrary second-order linear partial differential operator, both with coefficients depending smoothly on x, t, and, for the latter, s in the closure of their respective domains.

First, we recall a regularized Green's functions with memory terms and present some estimates for them. Secondly, we consider the global superconvergence in $W^{1,\infty}$-norm by virtue of the supercloses between the finite element solution and the interpolation function of the exact solution of the problem, and between the Ritz-Volterra projection of the exact solution and its interpolant. In the end, we devote to the global superconvergence analysis in $W^{1,\infty}$-norm for hyperbolic integro-differential equations, Sobolev and viscoelasticity type equations, on the basis of which some a posteriori error estimators are presented.

MICHAEL D. MARCOZZI
University of Nevada

Approximation and valuation of derivative securities by variational methods

We consider the valuation of derivative securities by variational methods. In particular, the expectations of such processes may be represented as solutions of variational inequalities of evolutionary type typically characterized by multiple time variables, nonlocal behavior, high number of degrees of freedom, unbounded state spaces, and lack of boundary conditions. We introduce a general framework for such valuations as well as Galerkin methodologies for their constructive approximations. Results are implemented utilizing finite elements; benchmarks are provided which validate the applicability and efficiency of the method and include the valuation of options on multiple assets, options depending on path history, and options on a foreign currency.

CATHERINE MAVRIPLIS* AND HUIYU FENG
National Science Foundation and George Washington University

An Adaptive Spectral Element Method

The goal of this on-going work is to show that a high order adaptive Spectral Element Method is an effective technique for the simulation of complex physical phenomena, in particular fluid flow. Atmospheric, oceanographic, biological and other flows contain so many different features over a wide range of scales, that adaptive refinement has become a necessity in order to resolve these features efficiently. The spectral element method lends itself naturally to adaptivity by its hybrid nature of a finite element method and a spectral method. Both h- (finite element) and p- (spectral) refinement and coarsening are used in this method to improve resolution in a cost effective way. The adaptivity criteria are based on elemental *a posteriori* error estimators that analyze the quality of the solution as well as give an estimated value of the error. A tree data structure has been implemented to simplify the refinement and especially the coarsening algorithms.

Two-dimensional simulations of a thin premixed flame front wrinkled by synthetic turbulent velocity fields illustrate the resolution capabilities of the adaptive spectral element method. In the figure below, results of three cases are shown: a flame deformed by (a) a sin shear flow, (b) a periodic array of vortices, and (c) the combination of shear and vortices. The starting grid is the same for all the three cases with K =12 elements and N =4th order polynomials or 5×5 collocation points in each element.

Adaptive spectral element simulations of thin flame front deformations (closeup view). (a) Case One: a sine shear flow (K = 200, DoF=12180) (b) Case Two: a vortex flow (K = 150, DoF=10746) (c) Case Three: a flow with sine shear and vortices (K = 232, DoF=14300). Element boundaries are indicated by white lines. Red represents burnt gases, blue unburnt gases. DoF refers to the total number of degrees of freedom, while K is the number of elements.

Three-dimensional simulations of a moving heat source will also be shown. A parallel adaptive spectral element method is currently being developed. Load balancing, data movement and access are important issues that need to be resolved for unstructured dynamically adaptive methods. Some preliminary work in this area will be discussed if time permits.

WILLIAM F. MITCHELL
National Institute of Standards and Technology

Parallel Adaptive Grid Refinement in PHAML

The numerical solution of partial differential equations (PDEs) is the most compute-intensive part of most scientific computer simulations, with applications in all fields of science and engineering. Consequently, improving the methods for solving PDEs has been the focus of much research in numerical methods for several decades. In the last two decades it has been shown that the combination of adaptive grid refinement and multigrid solution, known as adaptive multilevel methods, provide effective methods on sequential computers. Adaptive grid refinement reduces the problem size by focusing the effort to the regions where higher resolution is needed. In the last decade, research has been performed on parallelizing these procedures. Effective parallelization is difficult because of the irregular nature of adaptively refined grids.

In this talk we present the coarse-grain algorithm for adaptive refinement used in the parallel adaptive multilevel program PHAML. The algorithm uses only two communication steps during an adaptive refinement phase. Adaptive refinement can be performed by each processor in parallel without communication until the very end. The algorithm is identical to the sequential algorithm except that only the elements in the partition owned by the processor, and those needed for compatibility of the grid, are candidates for refinement. This can be achieved by setting the refinement error indicator to zero outside the partition. A communication step at the end informs other processors of any elements that were refined outside the partition to insure that the owner of that element also refines it. A second communication step enforces an overlap requirement needed for fast convergence of the parallel multigrid algorithm.

Results of numerical experiments on a cluster of eight PCs will be presented. These results demonstrate 60–90% parallel efficiency.

PETER K. MOORE
Southern Methodist University

Interpolation Error-Based A Posteriori Error Estimation for Parabolic and Elliptic Equations

A new a posteriori error estimation strategy based on the Lobatto interpolant will be presented. This approach offers several advantages over other methods: i) it is easy to compute; ii) it is asymptotically exact; iii) it provides asymptotically exact estimates one order higher than the current order; iv) it provides error indicators on elements with irregular nodes. I will develop the estimates for linear two-point boundary value problems and one- dimensional parabolic equations. I will discuss extensions of the method to three dimensions and the impact of different bases on the error estimates.

JENS MÜLLER AND JAN G. KORVINK
IMTEK Institute for Microsystem Technology

An adaptive FE-method for multi-layer MEMS

Simulating the physical behavior of thin structures accurately is central to micro-electro-mechanical systems (MEMS) CAD. We have implemented an adaptive finite element method suited for multi-physically active and multi-layered thin MEMS structure simulation. We use a multi-layer Kirchhoff-Love thin structure model that also covers thermo-mechanical and piezoelectrical effects and which is implemented as an Argyris element. The adaptivity is carried out by deriving residual error estimates for the thin structure model together with recursive split patterns for triangular meshes.

Modeling thin structure MEMS

Many mechanical microsystem components are plate-like or beam-like. They are obtained from semiconductor integrated- circuit manufacturing processes as multi-layer sandwiches [1].

The bilinear or weak form for thin multi-layer structures can be expressed by means of a Kirchhoff-Love model

$$\begin{aligned} a(\boldsymbol{U},\boldsymbol{V}) & \\ &= (\hat{\boldsymbol{A}}_0 : (\nabla \boldsymbol{u})^S - \hat{\boldsymbol{A}}_1 : \nabla\nabla w + \boldsymbol{\sigma}_0^{ext}, (\nabla \boldsymbol{v})^S) \\ &-(\hat{\boldsymbol{A}}_1 : (\nabla \boldsymbol{u})^S - \hat{\boldsymbol{A}}_2 : \nabla\nabla w + \boldsymbol{\sigma}_1^{ext}, \nabla\nabla v) \\ &= (\boldsymbol{F},\boldsymbol{V}), \end{aligned} \tag{3}$$

where we have merged the in-plane displacement fields $\boldsymbol{u}$ and the out-of-plane deflection field w and their variations $\boldsymbol{v}$ and v into the fields $\boldsymbol{U}$ and $\boldsymbol{V}$ respectively. In case the externally imposed prestress $\boldsymbol{\sigma}^{ext}$ of the structure is caused by an additional temperature field or arises from a piezoelectric effect, the corresponding fields also have to be considered in the weak form. The indices i of the reduced (anisotropic) elastic and prestress tensors $\hat{\boldsymbol{A}}_i$, $\boldsymbol{\sigma}_i$ account for the dimensionally reduced solid model and represent the moment order with respect to the integration that is performed across the structure thickness. The right hand side of (3) represents the external load acting on the structure. The solution space X for this problem is some product space of sobolev spaces. We conformingly approximate this solution space by 21-noded Argyris triangle C^1 finite elements [2].

Error estimation

The bilinear form (3) induces an energy norm in which we are aiming to estimate the solution error

$$|||\boldsymbol{U}-\boldsymbol{U}_h|||^2 = a(\boldsymbol{U}-\boldsymbol{U}_h, \boldsymbol{U}-\boldsymbol{U}_h). \tag{4}$$

The starting point for residual error estimation [3] is the inequality

$$\begin{aligned} |||\boldsymbol{U}-\boldsymbol{U}_h||| &\leq \sup_{\boldsymbol{V}\in X, |||\boldsymbol{V}|||=1} a(\boldsymbol{U}-\boldsymbol{U}_h, \boldsymbol{V}) \\ &= \sup_{\boldsymbol{V}\in X, |||\boldsymbol{V}|||=1} (\boldsymbol{F}-L\boldsymbol{U}_h, \boldsymbol{V}) \end{aligned} \tag{5}$$

where L denotes the linear differential operator associated with the bilinear form (3) through

$$(L\boldsymbol{W}, \boldsymbol{V}) = a(\boldsymbol{W}, \boldsymbol{V}) \qquad \forall\, \boldsymbol{W}, \boldsymbol{V} \in X. \tag{6}$$

The term $\boldsymbol{F} - L\boldsymbol{U}_h$ in relation (5) is the residual with respect to the strong form of the multi-layer plate problem. Calculating the right-hand-side of (5) by exploiting the continuity and ellipticity of the bilinear form (3) and using Clément's interpolation estimates [4] yields an a posteriori error estimation

$$|||\boldsymbol{U}-\boldsymbol{U}_h||| \leq c \left(\sum_{T\in S} \eta_T^2(\boldsymbol{U}_h) \right)^{1/2} \tag{7}$$

where c is some constant and $\eta_T(\boldsymbol{U}_h)$ is the (local) element error estimator depending only on the computed solution and the given data. This error estimator consists of the sum of individual errors that all have a proper physical meaning and can thus be related to specific simulation and design requirements of the MEMS developper. Major error contributions consist of non physical body forces $\|\nabla(\nabla\hat{\boldsymbol{A}}_2 : \nabla\nabla w_h)\|^2_{L^2(T)} h_T^4$ and unphysical jumps of shear forces $\|[\boldsymbol{n}\nabla\hat{\boldsymbol{A}}_2 : \nabla\nabla w_h]\|^2_{L^2(E)} h_E^3$ and bending moments $\|[\boldsymbol{n}\hat{\boldsymbol{A}}_2 : \nabla\nabla w_h]\|^2_{L^2(E)} h_E$ across element interfaces (h_E and h_T are the triangle edge lengths and the triangle diameters, respectively). The number of error contributions increases in case of the structure's multi- layer arrangement or if additional fields are present. In the latter case a considerable number of terms are caused by the coupling of the various fields. The adaptivity then is carried out using a maximum refinement strategy [3] and a recursive refinement algorithm for triangles [5]. We will show the formulation of this error estimator, and demonstrate its use with computed examples from MEMS.

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MARIUS PARASCHIVOIU AND HAE-WON CHOI*
University of Toronto

Adaptive Computations of Finite Element Output Bounds for Three-Dimensional Problems

An implicit A Posteriori framework to compute the upper and lower bounds for outputs of finite element solutions is extended for adaptive mesh refinement in three space dimensions. To motivate the characteristics of this framework, termed the bound method, a two dimensional heat transfer problem in a multi-material electronic components array is analyzed. The bound method calculates very sharp lower and upper bounds for the temperature of the hottest component which is assumed to be the engineering output of interest. For this two-dimensional problem, the bound method can yields more than eighty-fold reduction in simulation time over a fine mesh calculation (330,050 d.o.f.) while still maintaining quantitative control over the accuracy of the engineering output of interest. For three dimensional problems, the bound method evaluates large bound gaps (i.e., the difference between upper and lower bounds). To achieve a desired bound gap at the lowest cost, an adaptive mesh refinement technique is used to refine the subdomain mesh only where needed. An optimal stabilization parameter is also applied to improve the sharpness of the bound gap. These techniques are applied to an output of a heat transfer problem in a rectangular duct with a given velocity field. The average temperature at one section of the duct is bounded for given inlet temperature and heat flux. For this problem, the adaptive mesh refinement strategy uses half the number of subdomain elements required by an uniform mesh refinement strategy to calculate the same bound gap.

ABANI K. PATRA* AND ANDREW C. BAUER
University at Buffalo

Parallel Adaptive hp Schemes for Elliptic and Hyperbolic Systems

We will report here on the development of parallel adaptive hp schemes for the modeling of two problems. First we will report on the problems of classical linear elastostatics. Secondly we will describe early work on hyperbolic systems arising from a class of geophysical mass flows arising from landslides, avalanches and the like. These flows often have catastrophic consequences and lead to great loss of life. Over the last few years great strides have been made in developing sound mathematical models of these phenomena (see for e.g. the work of Hutter et. al [1] or more recently Ivarson and Denlinger [2]. Accurate numerical modeling of such flows is of great importance in conducting the realistic simulations necessary for a variety of purposes ranging from public safety planning to validation of the models. Developing parallel adaptive hp finite element simulations requires development of suitable data structures (see for e.g.Laszloffy, Long and Patra [4], load balancing schemes and solvers. For the elliptic systems, we will describe some of our recent work on developing reliable and portable solvers using a variety of preconditioners. For the hyperbolic systems we will extend here the work of Bey, Patra and Oden [3], on model hyperbolic systems to create parallel adaptive approximations. The key features of our approach include integrated development of parallel data structures and partitioners using good ordering schemes. Suitable adaptive strategies and residual based error estimators are other highlights of the work. REFERENCES [1] K. Hutter, M. Siegel, S. Savage and Y. Nohguchi, Two- dimensional spreading of a granular avalance down an inclined plane Part 1 Theory, Acta Mechanica 100, 37-68, (1993). [2] R. Ivarson and R. Denlinger, Flow of variably fluidized granular masses across threedimensional terrain 1. Couloumb mixture theory Journal Geophysical Research, 106 B1, 537- 552, (2001). [3] K.S. Bey, J. T. Oden and A. Patra A Parallel hp- Adaptive Discontinuous Galerkin Method For Hyperbolic Conservation Laws, in Applied Numerical Mathematics vol. 20, 1996, pp. 321-336. [4] A. Laszloffy, J. Long and A. Patra, "Simple Data management Schemes and Scheduling Schemes For Managing the Irregularities in Parallel Adaptive hp Finite Element Simulations" Parallel Computing vol 26, 2000, pp.1765-1788.

MICHAEL PERNICE
Los Alamos National Laboratory

Newton-Krylov-FAC Methods for Problems Discretized on Locally Refined Grids

Many problems in computational science and engineering are nonlinear and time-dependent. Often, these problems have solutions that include spatially localized features, such as boundary layers or sharp fronts, that require very fine grids to resolve. Resolving these features with a globally fine grid is often impractical or prohibitively expensive, especially in three dimensions. Gridding approaches based on adaptive mesh refinement (AMR) attempt to resolve these features by using a fine grid only where it is necessary. Numerous AMR algorithms for hyperbolic problems with explicit timestepping and some classes of linear elliptic problems have been developed. However, AMR algorithms for implicit timestepping methods have received much less attention. The key to the success of such an approach is the efficient solution of large-scale systems of nonlinear equations.

Recent efforts have demonstrated the effectiveness of Newton-Krylov methods combined with multigrid preconditioners on a broad range of applications. This suggests that a hierarchical approach, such as the Fast Adaptive Composite grid (FAC) method of McCormick and Thomas, should provide effective preconditioning for problems discretized on locally refined grids. The resulting Newton-Krylov-FAC method has been implemented on structured AMR grids. The software infrastructure combines nonlinear solvers from KINSOL or PETSc with the SAMRAI framework, and includes capabilities for implicit timestepping. Convergence rates that are independent of the number of refinement levels have been obtained for simple Poisson-like problems. Additional efforts to employ this infrastructure in a variety of applications are underway. LAUR 02-0336. This work was performed under the auspices of the U.S. Department of Energy by Los Alamos National Laboratory under contract W-7405-ENG-36

P. SAUCEZ AND A. VANDE WOUWER
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Numerical investigation of existence properties of solitonic solutions of an extended fifth-order

In recent years, much interest has developed in the numerical treatment of partial differential equations (PDEs) describing nonlinear wave phenomena, and particularly solitary waves. In this study, special attention is paid to an extended fifth-order Korteweg-de Vries equation (EKdV5) used to model water waves with surface tension.

As a particular case, this equation possesses a family of explicit solitary wave solutions. In addition, the EKdV5 possesses a range of solitonic solutions whose existence properties can only be assessed numerically.

In order to efficiently compute numerical solutions to the EKdV5 with sharp spatial variations, we use an adaptive grid technique that automatically concentrates the spatial nodes in the regions of high solution activity. An adaptive mesh refinement (AMR) algorithm based on the equidistribution principle and spatial regularization is used. On the resulting highly nonuniform spatial grids, the computation of the high-order derivative terms is particularly delicate; stagewise differentiation schemes, which compute high-order derivatives by successive numerical computation of first-order derivatives, e.g., $u_{xxxxx} = ((((u_x)_x)_x)_x)_x$, produce very satisfactory solutions.

These numerical techniques are used to investigate: (a) the propagation of solitonic waves corresponding to different parameter choices in the EKdV5, and (b) the existence properties of the solutions (semi- stability with respect to perturbations, conservation of invariants). Comparison with other numerical techniques (fixed uniform grids, nonuniform grids with predefined node movements) are presented. The use of AMR allows numerical solutions to be observed and investigated where other conventional techniques perform poorly or even fail.

Some implementation details are given and the performance of the method is discussed in terms of accuracy and computational efficiency.

WILLI SCHÖNAUER* AND TORSTEN ADOLPH

Rechenzentrum der Universität Karlsruhe

Development of flexibility and selfadaptation for the FDM: From FIDISOL to S-FDEM

Usually the FDM is a second order method on a rectangular grid. In the FIDISOL (Finite Difference Solver) program package for the solution of nonlinear systems of elliptic and parabolic PDEs (black-box), see [1], Chapter 17, we have generalized the FDM to arbitrary consistency order. The access to the discretization error is by the difference of different consistency orders. We derive an error equation that makes transparent the influence of all types of discretization and linearization errors and is the key to selfadaptation of the whole solution process, e.g. to select the optimal consistency order, space and time mesh size, stopping criterion for Newton iteration and iterative linear solver.

In order to increase the geometrical flexibility we developed the CADSOL (Cartesian Arbitrary Domain Solver) package that solves the PDEs on an arbitrary domain with body-oriented grid (rectangular in index space). Here we learned how to generate difference formulas of arbitrary order on an arbitrary set of nodes by influence functions and we introduced dividing lines (DLs) that separate subdomains with different PDEs and couple the solution globally by coupling conditions (CCs). However, the body-oriented grid is a severe restriction.

In the FDEM (Finite Difference Element Method) program package, see [2], we generalize our solution method to an arbitrary 2-D/3-D domain with triangular/tetrahedral grid. The consistency order is arbitrary, the FEM grid gives only the space structure. A sophisticated algorithm has been developed to select nodes in rings (2-D) or balls (3-D) for the generation of the difference formulas. The same error equation allows mesh refinement and order selection. By DLs and CCs we treat a domain composed of subdomains with different PDEs.

Finally in the S-FDEM (Sliding FDEM) package (under development) we generalize our solution method to a domain whose subdomains may slide relative to the other subdomains, separated by S-DLs (sliding DLs). In the different domains are quite different meshes, so one has non-matching moving grids, with individual mesh refinement in the subdomains and global error estimate. These requests result from industry cooperations, e.g. if there is for a high pressure diesel injection pump the large housing, the thin lubrication gap and the rotating shaft, the whole can be solved uniformly with global error estimate (note that we have a black-box solver).

The (S-)FDEM program package is parallelized with optimal data structures for distributed memory parallel computers, see [3]. The (iterative) solution of the resulting large and sparse linear systems is made by the LINSOL program package, see [4], that has polyalgorithms with automatic method switching between generalized conjugate gradient methods of different properties. This is even a selfadaptation of the solution method.

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JAMES D. TERESCO* AND JOSEPH E. FLAHERTY
Williams College and Rensselaer Polytechnic Institute

Architecture-Aware Dynamic Load Balancing

Parallel computation is a well-established and essential tool for large-scale scientific computation. Modern three- dimensional steady and transient scientific computation problems must execute in a parallel computational environment to achieve acceptable performance. Adaptive computation has been recognized as a means of providing reliable results to demanding scientific computational problems with minimal resources. Adaptivity requires explicit parallelization and frequent dynamic load balancing, so the procedures must be fast, must provide a high-quality partitioning, and should be incremental. Our parallel adaptive software uses Sandia National Laboratories' Zoltan library for partitioning and load balancing. Zoltan provides a common interface to a number of state-of-the-art partitioning and dynamic load balancing algorithms.

Modern parallel processing is being performed on everything from the largest tightly-coupled supercomputers to clusters of workstations. Any adaptive strategy seeking optimal performance had better account for processor, memory, and communications hierarchies. Processing nodes need not be the same. Such hierarchical and heterogeneous systems are increasingly common, and present additional challenges for the development of efficient software, particularly influencing dynamic load balancing procedures.

We have been developing the *Rensselaer partition model* (RPM), which includes a hardware model to support architecture- aware load balancing. The hierarchical model represents heterogeneous processor and network speeds, and may be used to represent any parallel computing environment, including an SMP, a distributed- memory computer, a network of workstations, or some combination of these. A similar hardware model is being implemented within Zoltan to support architecture-aware load balancing for a wide variety of partitioning and load balancing algorithms, and to provide a framework for the implementation of new algorithms.

An architecture-aware load balancer can tailor partitions for a particular architecture by, for example, seeking to achieve a good balance with minimal interprocessor communication penalties when a slow interconnection network is involved. This may be achieved though appropriate selection from among existing algorithms, adjustment of parameters or weights in existing algorithms, or through entirely new algorithms. A hierarchical balancing, where different algorithms are applied at different levels of the network hierarchy, can be guided by the tree structure of the hardware model.

The hardware model is constructed when a parallel computation is initiated on a particular system. This process involves (*i*) discovering the topology of the network and constructing the model's tree structure, and (*ii*) identifying the terminal nodes of the tree and determining their relevant characteristics. Ideally, this process will be completely automatic. We are investigating network discovery approaches to automate construction of the tree, and agents, threads spawned during initialization of the library, to collect information about the computing nodes.

ERVIN J. VINCENT AND LOUIS N. NTASIN*
Clemson University

A Posteriori Error Estimation and Adaptive Computation of Viscoelastic Flows

The accuracy and quality of approximation of solutions to viscoelastic flows in complex geometries depends strongly on using numerically stable methods that are computationally costs effective. In practical applications of viscoelastic flow modeling, stress and pressure singularities arise, resulting in layers that are difficult to resolve. We present Finite Element based a posteriori error estimates for viscoelastic flows governed by differential constitutive laws. These estimates are constructed based on a general nonlinear residual-based framework for a posteriori error estimation. We examine two main discretizations: one with continuous stress approximation and another with a discontinuous stress approximation. Using these estimators as error indicators and the DEVSS formulation of the govening equations we then perform adaptive computation of viscoelastic flows.

We examine the channel flow with an obstacle using a pseudo time stepping technique (θ-method).

KUMAR VEMAGANTI
University of Cincinnati

Adaptive Model Selection for Multiscale Problems:
A Goal-Oriented Approach

In this talk, we discuss a goal-oriented methodology for the accurate simulation of certain multiscale phenomena. In virtually every simulation, there are two sources of error: (a) the use of a simplified mathematical model that does not fully capture the fine-scale physics of the phenomenon results in *modeling error*, and (b) the use of a numerical method, such as the finite element method, introduces *discretization or approximation error*. To minimize the total error in the simulation, it is necessary to estimate and control both contributions. While the estimation and control of discretization error is relatively well-explored [1, 2], there remain several unanswered questions regarding the estimation and control of modeling error.

In [3, 4], Oden and Vemaganti put forward an adaptive mechanism for choosing the most appropriate mathematical model based on the goals of the simulation. This goal-oriented approach relies on *local* a posteriori estimates of modeling error. We describe some recent work on the local estimation and control of modeling error and discuss applications to plate- and shell-shaped structures.

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RONG WANG
Dalhousie University

High Order Adaptive Collocation Code for 1-D Parabolic PDEs

A high order adaptive method-of-lines package, BACOL, is developed for solving one dimensional parabolic partial differential equations. Collocation with a B-spline basis is used for the spatial discretization. An approximate solution is calculated in a piecewise polynomial subspace of degree p, and the spatial error estimate is obtained by using a second solution computed in a degree $p+1$ piecewise polynomial subspace.

BACOL controls both the spatial error and the time error. After each time step the spatial error is estimated, and if it is larger than the spatial error tolerance, an equidistribution principle is employed to refine the mesh. At the same time, the number of mesh points employed can be changed if necessary. The time integration is done by a differential-algebraic-eqation (DAE) solver, DASSL, which uses backward differentiation formulas. Modifications made to DASSL include replacing the original linear algebraic solver by the almost block diagonal system solver, COLROW and scaling the newton iteration matrix to avoid the large condition number generated by the index-1 DAE. Computational results, comparing with D03PPF, TOMS731, EPDCOL, indicate that BACOL is reliable and extremely efficient in dealing with problems having solutions with rapid variation.

SHEN R. WU
Ford Motor Company

Application Of Adaptive Finite Element To Crash Worthiness Analysis

Accuracy, robustness and efficiency are always the fundamental requirements for engineering applications. Adaptive method of finite element analysis can serve these goals if it can efficiently deliver high accuracy solutions to the engineering problems. Crash worthiness analysis involves highly nonlinear transient dynamics problems with large deformation of thin shell structures, elastic- plasticity, surface contact, etc. This report presents case studies of crash analysis using adaptive method implemented in LSDYNA, commercial software of explicit finite element. The change of normal angle between the neighboring shell elements is used as an engineering error indicator. Examples of structural component crash simulations are used to illustrate the adaptive procedure of explicit finite element analysis and to examine the quality of adaptive refinement with comparisons to uniform refinement. It is observed that solutions by adaptive method can compare to those using a uniform mesh of the same level but use much less CPU time. For this type of transient dynamics problem, a backward loop to resume the analysis at an earlier time with a refined mesh is necessary to avoid or reduce error accumulation. A suitable time period of refinement is important for the engineering applications. The error indicator based on shell element normal rotation is found to be effective for the solutions of bending dominated crashworthiness applications.

YUESHENG XU AND QINGSONG ZOU
University of West Virginia

Adaptive Wavelet Methods for Elliptic Operator Equations with Nonlienar Terms

We will present an adaptive method for solving elliptic operator equations with nonlinear terms when the solution is in a Besov space based on wavelet approximation. We prove that this method produces an approximate solution with convergence order $O(N^{-s})$ where N is the number of operations used to compute the approximate solution.

NAIL K. YAMALEEV AND MARK H. CARPENTER
National Research Council and NASA Langley Research Center

Moving Mesh Method for Efficient Simulation of Synthetic Jet Actuators

The effects of numerical boundary conditions on the accuracy of simulation of synthetic jet actuators are analyzed. The flowfield surrounding a synthetic jet actuator located on a flat plate is simulated numerically by solving the 2-D unsteady compressible Navier-Stokes equations. Time-accurate solutions are obtained by an explicit finite difference method which is 4th-order accurate in both time and space. The numerical simulation is based on treating the actuator as a suction/blowing boundary condition imposed inside the throat of the actuator. Numerical results have shown that the conventional boundary conditions based on the normal momentum equation do not provide mass conservation. As follows from our calculations, the maximum mass rate error, which occurs during the suction stage, is of the order of 15% if the normal momentum equation is used as a boundary condition for pressure. Note that the error introduced into the numerical solution increases as the boundary condition is imposed closer to the plate surface. To overcome this problem, new characteristic boundary conditions based on the moving mesh technique are proposed. The new method simulates the 2-D actuator by solving the 1-D Euler equations on a moving grid. The simplified actuator model has several advantages. First, this approach provides conservation of not only mass, but also momentum and energy. Furthermore, the new method is much more efficient in terms of computational time compared with the full 2-D simulation of the flowfield in the actuator. Numerical examples demonstrating efficiency and accuracy of the new strategy are presented