Adaptivity and Beyond: Computational Methods for Solving Differential Equations

Celebrating the 60th Birthday of Bob Russell

TALK TITLES & ABSTRACTS

Pacific Institute for the Mathematical Sciences

MITACS

Centre for Scientific Computing
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Adaptivity & Beyond — Vancouver, August 2005

Contents

Artificial time and inverse problems

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Abstract. A typical inverse problem involves the inference of a solution from a discrete set of data through the inversion of a possibly continuous forward problem, in which case the solution algorithm invariably involves a discretization of the continuous problem. Moreover, many recent algorithmic approaches involve the construction of a differential equation model for computational purposes, typically by introducing an artificial time variable. Of course the actual computational model involves a discretization of the now time-dependent differential system: forward Euler is usually employed. The resulting dynamics of such an algorithm is then a discrete dynamics, and it is expected to be "close enough" to the dynamics of the continuous system (which is typically easier to analyze) provided that small – hence many – time steps, or iterations, are taken. Indeed, recent papers in inverse problems and image processing routinely report results requiring thousands of iterations and more. This makes one wonder if and how the computational modeling process can be improved to better reflect the actual properties sought.

In this talk I elaborate on several problem instances that illustrate the above observations. I then show how a broader computational modeling approach may possibly lead to improved algorithms.

Scale invariant moving mesh finite elements

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Abstract. The GCL method of Cao, Huang and Russell is a velocity-based moving mesh method driven by a monitor function. We present a fully discrete finite element scheme based on this idea which for a simple monitor is locally conservative, preserves scale invariance of the underlying PDE and, for the porous medium equation, reproduces key geometric properties.

For more general monitors, needed to follow distinctive features of the solution, conservation breaks down and the scale invariance property does not hold. We show how the method can be modified so that these features are restored.

Two dimensional results are shown for second and fourth order nonlinear moving boundary problems and for a hyperbolic system.

Adaptive point shifts in the linear rational pseudospectral method

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Abstract. The pseudospectral method we discuss here for solving boundary value problems on the interval consists in replacing the solution by an interpolating polynomial in Lagrangian form between well-chosen points and collocating at those same points. Due to its globality, the method cannot handle steep gradients well (Markovs inequality). We will present and discuss two means of improving upon this: the attachment of poles to the ansatz polynomial, on one hand, and conformal point shifts on the other hand, both optimally adapted to the problem to be solved.

Who put the r into r-adaptivity?

Chris Budd, University of Bath, cjb@maths.bath.ac.uk

Abstract. In an attempt to achieve the impossible, I will try to summarise Bob's immense contribution to numerical analysis in general and to adaptivity and moving meshes in particular.

Moving meshes help your digestion

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Abstract. When we eat food it passes through our stomachs into our small intestine, where nutrients are absorbed before the remaining food passes out of our bodies. The wall of the intestine moves by the action of peristaltic waves. I will construct a model for this process and then solve it numerically by using a moving mesh method to cope with the moving boundary caused by the intestinal waves. Ill show some images of how these wave act to mix up the food in the intestine and improve the absorbtion process, thus making us all digest food better.

Mathematics in Industry: Things we don't learn in Graduate School

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Abstract. In this talk I will describe what I consider to be the main differences in the way Industry and Academia go about solving problems. I will illustrate my points using example of industrial problems I have worked on in which adaptive computational methods for differential equations are essential. I will give some useful tips for Grad Students interested in a carrier as an industrial mathematician.

An interpolation error estimate in R2 based on anisotropic measure of higher order derivatives

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Abstract. In this talk, we introduce the magnitude, orientation, and anisotropic ratio for the higher order derivative $\nabla^{k+1}u$ (with $k \geq 1$) of a function u to characterize its anisotropic behavior. The magnitude of $\nabla^{k+1}u$ is equivalent to its usual Euclidean norm. The orientation is the direction along which the $k+1$-th directional derivative is about the smallest, while along its perpendicular direction it it about the largest. The anisotropic ratio measures the strength of the anisotropic behavior of $\nabla^{k+1}u$. These quantities are invariant under translation and rotation of the independent variables. They correspond to the area, orientation, and aspect ratio for triangular elements. Based on these measures, we derive an anisotropic error estimate for the piecewise polynomial interpolation over a family of triangulations that are quasi-uniform under a given Riemannian metric M. It is identified among a general class of triangulations that the interpolation error is nearly the minimum on the mesh in which all the elements are aligned with the orientation of $\nabla^{k+1}u$, their aspect ratios are about the anisotropic ratio of $\nabla^{k+1}u$, and their areas make the error evenly distributed over every element.

A Simple Moving Mesh Method for Blowup Problems

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Abstract. This talk will present a simple adaptive method in solving parabolic blowup problems numerically. The mesh will be generated directly on the physical domain as Ceniceros and Hou developed. A curvature term is added to smooth the mesh. Several numerical examples are presented by way of comparison.

Affine similar convergence theorems for collocation methods

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Abstract. In the course of his book 'Newton Methods for Nonlinear Problems. Affine Invariance and Adaptive Algorithms', the author has worked out a new 'affine similar' convergence theorem for collocation methods, a class of techniques that has attracted Bob's interest for quite a time. This theorem applies to collocation for nonlinear boundary value problems (BVPs) showing the possible existence of discrete 'ghost solutions', and therefore advocating the use of Newton methods in function space rather than discrete Newton methods – which is just the route that has been taken by the COLSYS people. From this starting point, the talk will derive further (yet unpublished) collocation theorems (a) for stiff nonlinear initial value problems (IVPs) which do not contain any undesirable Lipschitz constant of the right hand side, but only the IVP condition number (known to be moderate for stiff IVPs), and (b) for linear BVPs which are anyway the ones realized in COLSYS. The new theorems should open the door to further insight into singularly perturbed problems.

Construction of smooth SVDs with applications

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Abstract. In this talk, we will consider the singular value decomposition (SVD) of a smooth matrix valued function A. After a quick review of results guaranteeing that the factors in the SVD are themselves smooth functions, a brief discussion of algorithmic aspects of the computation of such smooth SVD will be given. As illustration, we will use the smooth SVD for computing a curve of equilibria of a dynamical system.

Krylov integrators for Hamiltonian systems

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Abstract. Viewing Hamiltonian systems in $\mathbb{C}^n$ instead of $\mathbb{R}^{2n}$ brings a useful structure, since the real and imaginary parts of the complex inner product correspond to the real inner product and the standard symplectic form, respectively. The inconveninence that the "linear part" is then not complex linear can be taken care of by using real linear operators. It turns out that complex orthonormal vectors of Arnoldi like processes become useful for Hamiltonian systems. This approach is taken and a large system is locally approximated by one living in a low-dimensional Krylov subspace. When this is applied to Hamiltonian systems, the low dimensional approximations stay Hamiltonian. Combined with some symplectic and exponential integrators the overall methods preserve the energy exactly in linear problems. In numerical experiments the behaviour in nonlinear Hamiltonian problems seems also promising.

An Inexpensive Estimate of Arc Length and its use in Automatic Mesh Refinement

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Abstract. It is well known that in the numerical solution of differential equations one must use adaptive mesh refinement to obtain reliable and efficient performance, especially on nonlinear problems. Automatic mesh refinement (AMR) is therefore a key component of methods for BVPs in ODEs and methods for PDEs that use a MOL approach. In these applications the overall performance of the method (especially on nonlinear problems or problems with boundary layers) can depend critically on the choice of an effective mesh selection scheme. In this talk we will present a mesh refinement strategy for ordinary differential equations (ODEs) based on an inexpensive estimate of the arc length of the numerical solution. We will present an overview of the technique, analyze its cost and accuracy and present numerical evidence to show its potential for use in static remeshing in the MOL solution of a nonlinear Boussinesq wave equation.

Personalized Adaptive Computational Experimentation

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Abstract. Computational discovery is facilitated by tools that enable the researcher to focus on a problem and the making sense of results obtained, rather than on the idiosyncrasies of command syntax and the bookkeeping associated with repeated variable command invocations. In a search for insight, imagination should be encouraged more than patience should be required. The *cogito* software system is described, which allows any researcher a great deal of flexibility to personalize how computational experiments are conducted and how results are visualized. The system features an application programming interface that allows it to be adapted to a wide range of uses.

Optimal Control Problems from Finance and Engineering Applications

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Abstract. In this talk we discuss two classes of optimal control problems. The first type of problems come from finance, formulated under the classical optimal consumption framework originally developed by Merton. We describe a solution procedure which combines incomplete similarity reduction and numerical PDE techniques for the HJB (Hamilton-Jacobi-Bellman) equation. Optimal consumption with restricted assets and insurance-wage-consumption problems are used as two examples to illustrate the method.

If time permits, we will also describe another type of constrained optimal control problems from engineering applications. In this case, we described a solution procedure which combines asymptotic expansion and numerical methods. Thermal stress reduction in compound crystal growth is used as an example and numerical results are also given.

A three-dimensional adaptive moving mesh method based on MMPDEs

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Abstract. A three-dimensional adaptive moving mesh method will be presented. The method is based on a moving mesh partial differential equation. Theoretical and computational issues, including formulation and computation of the monitor function, movement of boundary points, and mesh quality measure, will be addressed. Numerical results will be given to demonstrate the ability of the method to adapt the mesh according to evolutionary features of the physical solution.

Finite volume methods for partial differential equations with intrinsic constraints

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Abstract. Many partial differential equations describing evolutions have solutions which satisfy an intrinsic constraint. Examples are the Maxwell Equations, ideal MHD equations, nonlinear system for the wave equation, Einsteins Equations. Numerical schemes for such equations often freeze the transport velocity locally in time and use a scheme to perform a linear transport in each step. In order to design schemes for evolutions with inherent constraints we consider in addition to the well known linear transport equation two special linear transport equations, each satisfying an inherent condition. In one, the divergence of the transported quantity is constant, in the other the curl stays constant. As an example we mention the ideal MHD equations where the divergence of the magnetic field stays constant and the field equations in the elasticity theory, where the curl of the deformations stays constant. A general framework allows to construct numerical methods that preserve exactly the discretized constraint on arbitrary grids by special fluxdistributions. Assuming at first in two space dimensions a rectangular grid numerical upwind schemes are developed. It turns out that there is a duality between the equations preserving the divergence and the ones preserving the curl. Applications to the MHD equation are presented.

Anisotropic mesh refinement based upon sensitivity analysis of an a posteriori error estimate.

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Abstract. A posteriori error estimation is widely used to control local mesh refinement and recent advances include the development of error estimates, based upon the use of an adjoint formulation, for quantities of interest that depend upon the computed solution. This work extends the use of the discrete adjoint technique to also efficiently calculate the sensitivity of such a posteriori error estimates to the location of the nodes of the mesh. It is demonstrated that, in addition to providing the usual information about where to locally refine, this also yields guidance on how to refine (isotropically or anisotropically). The talk will also discuss possible implementations that exploit this sensitivity estimate and present some promising early numerical results.

RH-Adaptive Finite Elements

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Abstract. The purpose of this talk is to present a combination of an r-adaptive and an h-adaptive finite element method. r-adaptivity, i.e., moving grid points through the computational domain without destroying the mesh connectivity, is accomplished by a moving mesh method which has been developed by Cao, Huang, and Russell for a few years. Although moving methods have a good potential to solve non-trivial problems including free boundaries or time-dependent domains, a fixed number of grid points may become a major disadvantage. Here, h-adaptivity can be useful to insert new grid points in regions where large solution variations have to be resolved and to delete grid points where they are no longer needed. Thus, the main idea is to run the r-method until an h-method is required to keep the estimated discretization error in space below a certain tolerance.

High-Order Embedded Runge-Kutta Pairs for the Time Evolution of Hyperbolic Conservation Laws

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Abstract. This talk will deal with the construction and use of new fifth-order Runge-Kutta schemes with embedded third-order strong-stability-preserving (SSP) Runge-Kutta pairs. The motivation for such pairs is to evolve Weighted Essentially Non-Oscillatory (WENO) spatial discretizations of hyperbolic conservation laws. The third-order SSP scheme would be used near shocks or discontinuities where the SSP property is useful for minimizing spurious oscillations. The fifth-order scheme would then be used in smoother regions where WENO provides fifth-order in space and SSP properties are not necessary.

Numerical estimation of progesterone transcriptional activity in the EGFR pathway using Chemcell

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Abstract. Among several possible ways to control endometrial cell growth, it was recently found that the optimization of progesterone transcriptional activity could well be an efficient method. As simple as it may sound this method is not trivial at all: in the ERB1 pathway transcriptional activity is affected by ubiquitination, which in turn can break down molecules of dimerized active forms of progesterone receptors (PrR), transcription factor (TF) and DNA bound to TF, thus representing a bottleneck for mRNA formation.

In order to determine the ranges of concentrations of the molecular species to achieve an optimal transcriptional activity, we were aided by the use of Chemcell (Sandia National Laboratories) and considered a parametric analysis of diffusion and reaction rates.

Numerical results for simulations of the EGFR-pathway will be presented, as well as validation of simulations (comparison with experimental biological data), and partial validation through its related ODE system of reactions. We also consider verification on stochastic automata procedures, as opposed to the regular global error analysis in deterministic systems.

Adaptive Schemes for Static Hamilton-Jacobi

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Abstract. Hamilton-Jacobi PDEs arise in shortest path computations – the classical example being the Eikonal equation for wavefront time of arrival. Algorithms such as fast marching and fast sweeping have been proposed to solve these equations. I discuss implementations and modifications of these algorithms to permit solution on adaptive grids in moderate dimensions (two to six).

Wide stencil schemes for nonlinear second order elliptic equations

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Abstract. We build convergent finite difference schemes for nonlinear elliptic partial differential equations, such as the equation for motion by mean curvature, the "infinity Laplacian", which has applications to image inpainting, and the Monge-Ampere equation.

These equations are nonlinear, and possibly degenerate. We show that naive schemes can fail to converge without actually blowing up. A result of Motzkin and Wasow from the 50s shows the need for large stencil schemes, even for linear ellipitic pdes. We build monotone, wide stencil schemes for these nonlinear PDEs.

A hybrid h-refinement / p-refinement strategy

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Abstract. MMPDEs and ideas from the GCL (Geometric Conservation Law) are augmented by a levelset framework to control the location, and number of mesh nodes used to solve a physical PDE. The main advantages of using a levelset framework are: the automatic creation and deletion of grid nodes as necessary, and circumventing the problem of mesh crossing

Solving large sparse $Ax = b$: stopping criteria, and GMRES behaviour.

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Abstract. We give a gentle introduction to such strange sounding (but in fact logical and quite simple) concepts as the "normwise relative backward error" for an approximate solution y to the linear system of equations $Ax = b$ where A is a large sparse matrix, and describe its use in determining when to stop an iterative process for solving $Ax = b$. An efficient implementation of the generalized minimum residual (GMRES) method for solving $Ax = b$ uses modified Gram-Schmidt orthogonalization (MGS-GMRES). We show how, and why, this behaves so well despite loss of orthogonality, and use it to illustrate the effectiveness of the normwise relative backward error in designing stopping criteria.

Applications of mesh adaptivity in ocean modelling

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Abstract. Modelling of the oceans represents an important application area where a vast range of scales are present and need accurate numerical simulation. Currently mesh adaptivity is not employed in any ocean model, indeed the numerical technology has remained largely unchanged in three decades. Increasing interest in climate and extreme events means that there is a real need to make use of the latest techniques of numerical analysis, and in particular adaptive mesh methods which are able to accurately and efficiently resolve complex solution dynamics. In this presentation I will describe efforts underway to develop ICOM (Imperial College Ocean Model) using adaptive algorithms.

Pricing and Risk Analysis of Financial Instruments

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Abstract. This presention gives an introduction to pricing and risk analysis of financial instruments, including examples of financial instruments, mathematical models for risk factors, mathematical formulation of pricing problems and numerical methods for their solution, and Value at Risk and Potential Future Exposure risk analyis.

Shallow Waves in an Evolving Basin

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Abstract. We present an effective algorithm for the numerical simulation of shallow water waves in a basin that is composed of an erodible bed. The interactions between the water and the sandy bottom can lead to the appearance and disappearance of islands and of dramatic changes in the basin itself. Combining a Lagrangian description of the water boundary, an indicator function and standard shallow water wave equation Eulerian numerical implementations we can effectively handle the evolution of this multiphase flow even when the domain itself changes dramatically in topology.

How Efficient is Adaptive Delaunay Refinement?

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Abstract. Let $M(f, D)$ denote an unstructured triangular mesh for defining a pwlinear approximation, $f^{(pl)}(x, y)$, to a function $f(x, y)$ for (x, y) in a domain D. Adaptive refinement (AR) is a familiar technique for generating $M(f, D)$ to control the error, $err(x, y, M) = f(x, y) - f^{(pl)}(x, y)$. The primary goal of these methods is efficiency. I.e. vertices of $M(f, D)$ should be limited to locations necessary to control $err(x, y, M)$.

AR can be combined with Delaunay meshing techniques to enhance the geometric attributes of $M(f, D)$; the resulting approach is referred to as Adaptive Delaunay Refinement (ADR). Several forms of robust, geometry based, algorithms for Delaunay refinement have been developed (Chew,Ruppert, and Shewchuk), (M-C Rivara et al), (P L George et al) which can be readily extended to ADR. In this paper, we present some computations that rate the efficiency of ADR generated meshes.

On the mesh relaxation time in the moving mesh method

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Abstract. In the moving mesh method, the "physical PDE" governing the problem of interest is discretized using a set of nonuniform points whose motion is governed by a "moving mesh PDE" or MMPDE. The MMPDE contains a *mesh relaxation time*, often denoted τ, which is employed as a temporal smoothing parameter that acts to regularize the mesh motion. Most previous moving mesh simulations employ a constant value of τ even though the time scale of the mesh motion may vary significantly throughout a computation. We propose a modification to the MMPDE which includes a variable relaxation time that is chosen to adaptively smooth the mesh in time. The effectiveness of this approach is illustrated using problems involving blow-up and front propagation.

Collocation-type approximations to hypersingular integrals and hypersingular integral equations

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Abstract. Many physical problems require an efficient discrete scheme for Hadamard finite-part integral operators and an efficient quadrature rule for such integrals. In this talk, we present several collocation-type approximations to Hadamard integral operators. These discrete schemes are of Toeplitz or nearly Toeplitz structure, which gives many advantages in developing fast linear solvers for numerical solution of integral equations and intego-differential equations. Also the superconvergence of classical Newton-Cotes formulae and Gauss quadrature rules are investigated.

Adaptive Collocation for Boundary Layer Problems with Radial Basis Functions

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Abstract. An adaptive collocation method based upon radial basis functions is presented for the solution of singularly perturbed two-point boundary value problems. Using a multiquadric integral formulation, the second derivative of the solution is approximated by multiquadric radial basis functions. This approach is combined with a coordinate stretching technique. The required variable transformation is accomplished by a conformal mapping, an iterated sine-transformation. A new error indicator function accurately captures the regions of the interval with insufficient resolution. This indicator is used to adaptively add data centres and collocation points. The method resolves extremely thin layers accurately with fairly few basis functions. The proposed adaptive scheme is very robust, and reaches high accuracy even when parameters in our coordinate stretching technique are not chosen optimally. The effectiveness of our new method is demonstrated on two examples with boundary layers, and one example featuring an interior layer. It is shown in detail how the adaptive method refines the resolution.

Approximation of Lyapunov and Dichotomy Spectra

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Abstract. We will review theoretical and algorithmic aspects of QR methods to approximate Lyapunov exponents and Exponential Dichotomy spectra of dynamical systems.

Solving large Hamiltonian eigenvalue problems

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Abstract. Large, sparse eigenvalue problems with Hamiltonian structure arise in several contexts, including the study of corner singularities in anisotropic elastic solids. We show how to solve these by applying structure-preserving Krylov subspace methods of several types, including some that attack the Hamiltonian problem directly and others that make a further transformation to either skew-Hamiltonian or symplectic form. All of the structure-preserving methods are more accurate than a comparable method that ignores the structure. The fastest of the structure-preserving methods is more efficient than the method that ignores the structure.

Adaptive Grid Control for Singular BVPs

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Abstract. We describe a mesh selection strategy for the numerical solution of boundary value problems for singular ordinary differential equations. We prove that under realistic assumptions our mesh selection strategy serves to approximately equidistribute the global error of the collocation solution, thus enabling to satisfy prescribed tolerances efficiently.

This mesh adaptation procedure has been implemented in our new `Matlab` code `colimp`, a successor of `sbvp`. `colimp` is based on polynomial collocation, equipped with an a posteriori estimate for the global error of the numerical solution, and the mesh adaptation procedure. Moreover, in the present version of the code a pathfollowing strategy based on pseudo-arclength parametrization applied for the computation of solution branches with turning points of parameter-dependent equations in implicit form,

$$\begin{aligned} & f(y'(t), y(t)/t^\alpha, t, \lambda), \quad t \in (0,1], \quad \alpha \geq 1 \\ & g(y(0), y(1)) = 0, \end{aligned}$$

is available. We show that the pathfollowing procedure is well-defined under realistic assumptions, and a numerical solution is possible with a stable, high-order discretization method.

Finally, we demonstrate the performance of our code by solving a number of problems relevant in applications. These include the computation of density profiles in a non-homogeneous fluid, complex Ginzburg-Landau equation, and problems from the shell buckling.