Third Canadian Symposium in

Numerical Analysis and Scientific Computing

Organized by Alexander Bihlo, Ned Nedialkov, Sander Rhebergen

CAIMS Annual Meeting, Dalhousie University
July 17–21, 2017

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Abstracts

Handling Stiffness in Simulating and Calibrating Physics-based Soft Object Deformation

Uri Ascher
University of British Columbia

Motion simulation of soft objects such as cloth, plants and some body parts is ubiquitous in computer graphics and robotics applications. The governing elastodynamics PDE system is often discretized in space already at the variational level, using FEM. This leads to a large, expensive to assemble, ODE system in time, where the damped motion may mask highly oscillatory stiffness.

The model described by the differential system must be calibrated first. A data-driven method for this inverse problem is introduced. Many expensive simulations of the motion in time are required, and a semi-implicit time integration method using large time steps was employed. This however introduces artificial damping. I will show a simple analysis of this effect and discuss its implications. Methods for decoupling fast and slow modes are derived. Our results will be demonstrated.

This talk is based on joint works with Bin Wang, Longhua Wu, KangKang Yin, Libin Liu and Hui Huang ('15), and Edwin Chen and Dinesh Pai ('16).

The Partial Fourier Transform

John Bowman
University of Alberta

An efficient algorithm for computing the one-dimensional partial fast Fourier transform $f_j = \sum_{k=0}^{c(j)} e^{2\pi ijk/N} F_k$ is presented. This operator has applications in seismic imaging and in studies of inertial-range energy transfer in incompressible turbulence. Naive computation of the partial fast Fourier transform requires $O(N^2)$ arithmetic operations for input data of length N. Unlike the standard fast Fourier transform, the partial fast Fourier transform imposes on the frequency variable k a cutoff function $c(j)$ that depends on the space variable j; this prevents one from directly applying standard FFT algorithms. It is shown that the space–frequency domain can be partitioned into rectangular and trapezoidal subdomains over which efficient algorithms can be developed. As in the previous work of Ying and Fomel (2009), the contribution from rectangular region scan be reduced to a series of fractional-phase Fourier transforms over squares, each of which can be reduced to a convolution. In this work, we demonstrate that the partial Fourier transform over trapezoidal domains can also be reduced to a convolution. Since the computational complexity of a de-aliased convolution of N inputs is $O(N \log N)$, a fast algorithm for the partial Fourier transform is achieved, with a lower overall coefficient than obtained by Ying and Fomel.

A Well-Balanced Meshless Tsunami Propagation and Inundation Model

Rüdiger Brecht

Memorial University of Newfoundland

We present a novel mesh-less tsunami propagation and inundation model. We discretize the nonlinear shallow-water equations using a well-balanced scheme relying on radial basis function based finite differences. The inundation model relies on radial basis function generated extrapolation from the wet points closest to the wet–dry interface into the dry region. Numerical results against standard one- and two-dimensional benchmarks are presented.

This is joint work with Alexander Bihlo, Scott MacLachlan and Jörn Behrens.

Non-convex Online Robust PCA: Enhance Sparsity via lp-norm Minimization

Tien D. Bui

Concordia University

Compressive sensing, matrix rank optimization and Robust PCA-based matrix decomposition have an increasing number of non-convex approaches for optimizing the ideal l0-norm sparsity. This paper presents a novel online non-convex lp- norm based Robust PCA approach, where $0 < p < 1$. This method is developed from an offine version that uses a new objective function in the Alternating Direction Method of Multipliers (ADMM) framework to efficiently solve the Robust PCA problem. More importantly, our online method can achieve real-time performance on large-scale data without parallelizing or implementing on a graphics processing unit. We mathematically and empirically show that the computational complexity of our algorithm is linear in both the sample dimension and the number of samples. The proposed approaches are evaluated in various applications including Gaussian/non-Gaussian image denoising, face modeling, real-time background subtraction and video inpainting and compared against numerous state-of-the-art low-rank minimization methods to demonstrate the robustness of our algorithms.

Numerical Simulations of Nonlinear Dynamical-Chemical Processes in the Atmosphere

Lucy Campbell

Carleton University

A nonlinear spectral numerical model for dynamical-chemical processes in the atmosphere is presented. Internal gravity waves affect the general circulation, chemical composition and energy budget of the atmosphere. This model involves nonlinear reaction-diffusion equations for chemical transport coupled with the conservation equations that describe dynamical processes in the atmosphere, including interactions between internal gravity waves and the background fluid flow.

Numerical Algorithms for Recovery of Integer-Valued Signals

Xiao-Wen Chang

McGill University

Given the measurement vector $\mathbf{y} \in \mathbb{R}^m$ and the model matrix $\mathbf{A} \in \mathbb{R}^{m\times n}$ satisfying the following model:

$$\mathbf{y} = \mathbf{ADx} + \mathbf{v},$$

where $\mathbf{D}$ is a real parameter matrix and $\mathbf{D} \in \mathcal{D} = \{\text{diag}(\sqrt{d_1}, \cdots, \sqrt{d_n}) : \sum_{j=1}^{n} d_j = 1\}$, $\mathbf{x}$ is an integer-valued parameter vector and $\mathbf{x} \in \mathcal{B} = \{\mathbf{x} : \mathbf{x} \in \mathbb{Z}^n, l \leq x_i \leq u, i = 1, \cdots, n\}$, and $\mathbf{v}$ is a noise vector following the normal distribution $N(\mathbf{0}, \sigma^2\mathbf{I})$, one would like to recover the integer-valued signal $\mathbf{x}$. This problem arises from digit communications.

To recover $\mathbf{x}$, ideally one would like to solve the following mixed integer least squares problem:

$$\min_{\mathbf{D}\in\mathcal{D},\mathbf{x}\in\mathcal{B}} \|\mathbf{y} - \mathbf{ADx}\|_2.$$

But the computational cost for this mixed integer least squares problem may be too high if n is large, $\mathbf{A}$ is ill-conditioned or the noise variance σ^2 is large. For real time applications, one would like to find a suboptimal solution.

In this talk we will provide some efficient suboptimal algorithms to recover the integer-valued signal $\mathbf{x}$ based on some theory we have recently developed. Numerical results will be given to demonstrate the performance of those algorithms.

Variational and PDE method in reconstructing CT images.

George Chen

Cape Breton University

The talk gives a brief introduction of physical and mathematical principles of the Computed Tomography (CT). A modified minimization of total deviation constraint is introduced and a variational and PDE method in CT reconstruction is investigated. The aim of this talk is to impose an effective edge preserving and noise removing to optimize the quality of CT reconstructed images. A basic analysis of the proposed model with some other existing standard methods in literature is presented using simulated test phantom and standard digital image.

Effect of Initial Conditions Discontinuity on the Numerical Solution of Parabolic PDEs: Applications to Finance

Christina Christara

University of Toronto

In several PDE problems arising in finance or in other applications, the initial conditions exhibit either singularity (such as the Dirac-delta function), or discontinuity (such as the Heaviside function), or discontinuity of the derivative (such as the hockey-stick or ramp function), at certain points of the spatial domain, usually known in advance. These discontinuities render the standard error and convergence analysis results inapplicable, or at least not directly applicable. Furthermore, we may notice an erratic order of convergence, which makes any type of error estimation, as well as extrapolation of solution values difficult.

We present an analysis of the error arising from certain types of non-smooth initial conditions in the numerical solution of a parabolic PDE. The analysis focuses on finite difference spatial discretization and Crank-Nicolson-Rannacher timestepping. We derive an explicit relation for the lower order terms of the error, and indicate the terms corresponding to the timestepping and quantization errors, the latter depending (linearly or quadratically) on the relative position of the point of non-smoothness in the discretization grid. We show that the order of convergence does not suffer from fluctuations, when the relative position is maintained at each refinement of the grid. We also study the effect of smoothing of the initial conditions on the order of convergence.

Joint work with Nat H.C. Leung

The Bohemian Eigenvalue Project

Steven Thornton and Robert Corless

Western University

The BOunded HEight Matrix of Integers Eigenvalue project, or "Bohemian Eigenvalue Project" for short, has its original source in the work of Peter Borwein and Loki Jrgenson on visible structures in number theory (c 1995), which did computational work on roots of polynomials of bounded height (following work of Littlewood). Some time in the late 90's I realized that because their companion matrices also had bounded height entries, such problems were equivalent to a subset of the Bohemian eigenvalue problems. That they are a proper subset follows from the Mandelbrot matrices, which have elements -1, 0 but whose characteristic polynomials have coefficients that grow doubly exponentially, in the monomial basis. There are a great many families of Bohemian eigenvalues to explore: companion matrices in other bases such as the Lagrange basis (my work here dates to 2004), general Bohemian dense matrices, circulant and Toeplitz matrices, complex symmetric matrices, and many more. The conference poster contains an image from this project. This talk presents some of our recent results. Joint work with Steven Thornton, Sonia Gupta, Jonny Brino-Tarasoff, and Venkat Balasubramanian.

Massively Parallel Monte Carlo Methods in Computational Geophysics

Fabrizio Donzelli

Memorial University of Newfoundland

In this talk we discuss stochastic solutions of partial differential equations (known as Feynman–Kac–Dynkin formulas), that arise as model problems in geophysics, and their implementation via stochastic numerical algorithms (Monte Carlo simulations), which provide a discretization of the Feynman–Kac–Dynkin formulas. The advantage of Monte Carlo methods, in comparison with deterministic ones, is their natural adaptability to parallel computing architectures, resulting in a dramatic improvement of the performance.

In this talk we present two applications of Monte Carlo-based algorithms, which were executed on multi core machines at Memorial University of Newfoundland.

First, we test the performance and accuracy of Monte Carlo-based algorithms in finding solutions of the Poisson equation for the Newtonian potential, which is the model problem for gravity exploration. The first application is mainly is a test model, since the Newtonian potential, from which we recover the gravitational acceleration, admits rather general analytic formulas, and it gives us a way to test the accuracy of our model.

Second, we discuss the stochastic solution of the two-dimensional Maxwell equations, which is of higher interest since in this case we do not have analytic formulas. The two-dimensional Maxwell equations are an example of a model problem for magneto-telluric methods in geophysics.

This is a joint work with A. Bihlo and C. Farquharson.

Efficient and Reliable Tools for Investigating the Approximate Solution of Systems of PDEs

Wayne H. Enright

University of Toronto

In recent years we have developed a a class of effective software tools for visualizing approximate solutions of systems of ODEs and for performing key tasks such as identifying extreme values of the approximate solution and parameter fitting. In this talk we will discuss how some of these tools can be extended in a natural way to investigate similar properties of the approximate solution of systems of two and three dimensional PDEs.

In particular we will define the defect of an approximate solution determined by some order three and four PDE methods and use this concept to develop tools for visualizing the approximate solutions of systems of PDEs. We will then introduce software tools for identifying extreme values of the approximate solution (over the domain of interest), and subset(s) of the domain where the approximate solution exceeds a specified critical value. We will also consider how one can extend the tool for parameter fitting for ODEs to parameter fitting for PDEs.

SCRAP: Spline Collocation Rarely Applied Properly - Some Remedies

Graeme Fairweather

American Mathematical Society

During the last several decades, much attention has been devoted to the formulation, analysis and implementation of collocation methods based on smoothest splines for the approximate solution of second–order two–point boundary value problems (TPBVPs), elliptic problems and for the spatial discretization in time dependent partial differential equations. Typically, these methods employ C^2 cubic splines. While one would expect fourth order accuracy when such a space is used, de Boor proved in 1966 that C^2 nodal cubic spline collocation for TPBVPs cannot be more than second order accurate. This fact appears to have escaped the attention of many authors. Also overlooked are the fundamental works of Archer, Daniel and Swartz, who devised optimal nodal spline collocation methods based on a perturbed differential equation. Similar work was carried out by Houstis, Christara and Rice for C^1 quadratic spline collocation. In this talk, we provide a brief overview of the recent spline collocation literature for TPBVPs before describing contributions of Pat Keast which led to the formulation of collocation and collocation-like methods of optimal accuracy for TPBVPS, and to the development of software for solving the almost block diagonal linear algebraic systems to which they lead.

Scalable Bifurcation Analysis of Nonlinear Partial Differential Equations and Variational Inequalities

Patrick Farrell

University of Oxford

Computing the solutions u of an equation $f(u, \lambda) = 0$ as the parameter $\lambda \in \mathbb{R}$ is varied is a central task in applied mathematics. In this talk I will present a new algorithm, deflated continuation, for this task.

Deflated continuation has three main advantages. First, it is capable of computing disconnected bifurcation diagrams in a single pass; other algorithms only attempt to compute that part of the bifurcation diagram continuously connected to the given initial data. Second, its implementation is extremely simple: it only requires a minor modification to any existing Newton-based solver. Third, it can scale to very large discretisations if a good preconditioner is available.

Among other equations, we will apply this to a famous singularly perturbed ODE, Carrier's problem. The algorithm reveals a striking and beautiful bifurcation diagram, with an infinite sequence of alternating pitchfork and fold bifurcations as the singular perturbation parameter tends to zero. The analysis yields a novel and complete taxonomy of the solutions to the problem, and demonstrates that a claim of Bender & Orszag (1999) is not quite correct.

Methods for Computing Critical Yield Numbers

Ian Frigaard[1], Emad Chaparian[1], Ida Karimfazli[2] and Anthony Wachs[1]
[1]University of British Columbia; [2]Concordia University

Yield stress fluids do not deform unless a stress threshold is exceeded, but are otherwise viscous. The presence of the yield stress significantly alters the stability properties of these flows. In the first place, many static flows which would be mechanically unstable for simpler Newtonian fluids can now be observed. These flows are found when the ratio of yield stress to driving stresses exceeds a critical value, say $Y > Y_c$. Secondly, in the case that $Y > Y_c$ the static flows appear to be energy stable (and globally energy stable in some cases). The critical value Y_c is defined by an optimization problem that may be solved approximately by a number of methods that we outline and illustrate through examples.

High-Order Finite-Volume Method with Anisotropic Block-Based AMR

Clinton P. T. Groth[1], Lucie Freret[1] and Hans De Sterck[2]
[1]University of Toronto; [2]Monash University

A high-order central essentially non-oscillatory (CENO) finite-volume scheme combined with a block-based anisotropic adaptive mesh refinement (AMR) algorithm is proposed for the solution of hyperbolic conservation laws on three-dimensional multi-block body-fitted mesh consisting of hexahedral elements. The cell-centered CENO method uses a hybrid reconstruction approach based on a fixed central stencil. Smooth and fully resolved solution data is represented using an unlimited high-order k-exact reconstruction. In cells deemed to have under-resolved/discontinuous solution content based on a smoothness indicator, the high-order reconstruction reverts to a lower-order limited linear scheme. The high-order CENO finite-volume scheme is implemented within a flexible multi-block hexahedral grid framework. Parallel implementation and local anisotropic grid adaptivity are achieved by using a hierarchical block-based domain decomposition strategy in which the connectivity and refinement history of grid blocks are tracked using a binary tree data structure. Physics-based refinement criteria as well as criteria based on the smoothness indicator are used for directing the mesh refinement. Numerical results for several flow problems are described, including those involving solution-driven anisotropic refinement on cubed-sphere grids, in order to demonstrate the accuracy and efficiency of the proposed high-order solution method.

Polynomial Extensions in Two dimensions and its Application to Error Estimation for the p and h-p FEM

Benqi Guo

University of Manitoba

Polynomial extensions play a vital role in the analysis of the *p* and *h-p* FEM as well as the spectral element method. We construct explicitly polynomial extensions on a triangle T and a square S, which lift a polynomial defined on a side Γ or on whole boundary of T or S. The continuity of these extension operators from $H_{00}^{\frac{1}{2}}(\Gamma)$ to $H^1(T)$ or $H^1(S)$ and from $H^{\frac{1}{2}}(\partial T)$ to $H^1(T)$ or from $H^{\frac{1}{2}}(\partial S)$ to $H^1(S)$ is rigorously proved in a constructive way. Applications of these polynomial extensions to the error analysis for the *h-p* FEM are presented.

A Neural Network Approach to Efficient Valuation of Large Portfolios of Variable Annuities

Seyed Amir Hejazi[1] and Ken Jackson[2]

[1]Manulife Toronto; [2]University of Toronto

Managing and hedging the risks associated with Variable Annuity (VA) products require intraday valuation of key risk metrics for these products. The complex structure of VA products and computational complexity of their accurate evaluation have compelled insurance companies to adopt Monte Carlo (MC) simulations to value their large portfolios of VA products. Because the MC simulations are computationally demanding, especially for intraday valuations, insurance companies need more efficient valuation techniques. Recently, a framework based on traditional spatial interpolation techniques has been proposed that can significantly decrease the computational complexity of MC simulation (Gan and Lin, 2015). However, traditional interpolation techniques require the definition of a distance function that can significantly impact their accuracy. Moreover, none of the traditional spatial interpolation techniques provide all of the key properties of accuracy, efficiency, and granularity (Hejazi et al., 2015). In this talk, we present a neural network approach for the spatial interpolation framework that affords an efficient way to find an effective distance function. The proposed approach is accurate, efficient, and provides an accurate granular view of the input portfolio. Our numerical experiments illustrate the superiority of the performance of the proposed neural network approach compared to the traditional spatial interpolation schemes.

Stochastic Multi-Cloud Models for the Parameterization of Organized Tropical Convection

Boualem Khouider

University of Victoria

Tropical convection is organized on a hierarchy of scales that interact with each other and with the large-scale flow. Efforts to adequately represent these convective systems in a global climate model (GCM) has led the scientific community to think beyond conventional convective parameterization schemes. Super-paramaterized GCMs (SP-GCM) and global cloud resolving models (GCRM) are such promising approaches. While the high computational cost inhibited the widespread use of SP-GCMs and GCRMs operationally, they highlighted the importance of the representation of sub-grid scale variability collec- tively while realizing the individual behaviour of the convective elements. I will discuss a new perspective of stochastic multicloud models (SMCM), based on Markov lattice models, to represent the sub-grid scale organization of convection and its two-way interaction with large-scale tropical waves. Building up from simple models for convectively coupled waves to their implementation in GCMs, I will demonstrate the importance of three key cloud types (congestus, deep and stratiform) as a building block for organized convection. Results showing significant improvements in the capability and superiority of the SMCM to capture synoptic and intra-seasonal variability associated with tropical convection, in GCMs, including convectively coupled equatorial waves, the Madden-Julian oscillation and monsoon intraseasonal oscilla- tions, will be presented.

Preventing Race Conditions in Unstructured CFD Solvers on GPUs

Andrew Giuliani and Lilia Krivodonova

University of Waterloo

Graphics processing units (GPUs) are massively parallel platforms that have become useful in computational fluid dynamics (CFD) solvers. GPUs store data in shared memory and manipulate them by processes that solve the problem in parallel. If multiple processes, or threads, write simultaneously to the same memory location, a race condition is created and computations can have unpredictable results. Therefore, care must be taken to develop algorithms that do not lead to race conditions.

We propose an algorithm for preventing race conditions in the evaluation of the surface integral contributions in edge-based CFD solvers by coloring the faces (or edges) of the computational mesh. We use a partitioning algorithm that separates the edges of triangular elements into three groups, the faces of quadrilateral and tetrahedral elements into four groups, and the faces of hexahedral elements into six groups. Our method is also applicable to hybrid meshes. We then extend this partitioning to adaptively refined, nonconforming meshes. We use the coloring to reduce code memory requirements by eliminating buffering. The coloring is also used to renumber and reorder elemental data to optimize reading and writing to memory, thus reducing access latencies and accelerating computations.

Instability from Lack of Smoothness in Local Polynomial Interpolants

Colin Macdonald

University of British Columbia

Low-degree polynomials are commonly used to interpolate values in gridded data. An example is the Matlab/Octave "interp2" command. We show that a seemingly-reasonable choice of interpolation stencils, when used with the closest point method for solving PDEs on surfaces, results in an unstable method. We give an intuition (based on smoothness) for why this occurs and show how to fix the instability using an alternative choice of stencils.

Combining Deflation and Nested Iteration for Nonlinear Variational Problems

Scott MacLachlan[1], James Adler[2], Timothy Atherton[2], David Emerson[3] and Patrick Farrell[4]

[1]Memorial University of Newfoundland, [2]Tufts University, [3]Street Contxt, [4]Oxford University

Many physical systems support multiple equilibrium states that enable their use in modern science and engineering applications. Having the ability to reliably compute such states facilitates more accurate physical analysis and understanding of experimental behaviour. In this talk, we consider adapting and extending a deflation technique for the computation of multiple distinct solutions in the context of nonlinear systems and apply the resulting method to the modeling of equilibrium configurations of nematic and cholesteric liquid crystals. In particular, the deflation approach is interwoven with nested iteration, creating an efficient and effective method that further enables the discovery of distinct solutions. The combined methodology is applied as part of an overall free-energy variational approach within the framework of optimization of a functional with constraints imposed via Lagrange multipliers. Numerical experiments demonstrate the efficacy and accuracy of the algorithm in detecting important physical phenomena, including bifurcation and disclination behaviours.

Recent Developments in Software for the Numerical Solution of BVODEs

Paul Muir

Saint Mary's University

Two-point Boundary Value Ordinary Differential Equations (BVODEs) are systems of ordinary differential equations that have boundary conditions imposed on the solution at two distinct points. In his 1983 paper, Pat Keast (together with Diaz and Fairweather) analyzed the use of finite element methods, including collocation methods, for the numerical solution of BVODEs.

Current software for the efficient and accurate solution of BVODE systems employs an adaptive computation that controls an estimate of some measure of the quality (e.g., the global error, or the defect, or both) with respect to a user-specified tolerance. In this talk we describe recent work associated with the development of new versions of two families of software packages for the error-controlled numerical solution of BVODEs.

The first project involves the development of extensions of the MIRKDC/BVP_SOLVER software family which employs discrete and continuous mono-implicit Runge-Kutta (MIRK) methods

and (originally) defect control; the family has recently been extended to also provide a hybrid defect/global error control option. A key computational component of this family of software packages is the almost block diagonal linear system solver, COLROW, developed by Pat Keast (together with Diaz and Fairweather) also in 1983.

Current work on this project includes the development of generalizations of the MIRK methods that have higher stage order and are thus not susceptible to order reduction when applied to stiff BVODEs, the development of new CMIRK methods that lead to asymptotically correct defect control, and extensions of the software to allow for the direct treatment of mixed order BVODE systems and the treatment of BVODEs with advance or delay terms.

The second project focuses on the COLSYS/COLNEW family of BVODE collocation solvers. Current work involves the development of a Fortran95/2003 version of the software, and the implementation of what are known as superconvergent interpolants to augment the lower order collocation solution leading to much faster convergence of the computation to obtain an error-controlled continuous numerical solution.

High-Order Immersed Approach for Poisson's Equation with Discontinuous Coefficients and Jump Discontinuities

Jean-Christophe Nave
McGill University

One of the fundamental numerical challenges associated in simulating fluid flows with multiple fluids/components/phases is to obtain high-order solutions of PDEs with discontinuous coefficients and interface jump conditions.

In this talk I will present a general numerical framework, the Correction Function Method (CFM), which allows one to solve these problems with high-order convergence on a regular Cartesian grid. I will apply the CFM framework to solving a canonical problem: Poissons equation with interface jump discontinuities and discontinuous piece-wise constant coefficients. The presented algorithm is 4th-order accurate and is oblivious to the size of the jumps or to the ratio of the coefficients.

Solving Lagrangian Dynamics Directly

Ned Nedialkov
McMaster University

The DAETS solver by Nedialkov and Pryce is capable of solving systems of any order, high-index differential algebraic equations. Recently, we discovered how to combine automatic differention with the machinary already in place in DAETS to integrate systems written in a Lagrangian form. That is, the user writes a Lagrangian and possibly algebraic constraints, and DAETS performs a numerical integraion. Our approach avoids lengthy symbolic transformations of a Lagrangian into a system of ODEs: such transformations are carried out purely through automatic differentiation and invisible to the user. Similarly, we can also integrate systems directly from a Hamiltonian formulation, without writing explicitly the resulting ODE equations. We demonstrate our Lagrangian facility on a pendulum-mass-spring problem, the motion of the outer planets, and a controlled simple pendulum.

Joint work with J. Pryce, G. Tan, and Xiao Li.

The Many Uses and Surprising Accuracy of Lanczos Tridiagonalization and Golub-Kahan Bidiagonalization for Large Sparse Matrices

Chris Paige
McGill University

Cornelius Lanczos's 1952 process for tridiagonalizing a symmetric matrix $A \in \mathbb{R}^{n \times n}$ is the basis for many well known very useful large sparse matrix algorithms. Starting with a given vector v_1, $\|v_1\|_2 = 1$, each step produces a new vector v_j and column of a symmetric tridiagonal matrix T_k via a 3-term recurrence with one matrix-vector multiplication each step. Ideally after k steps

$$AV_k = V_k T_k + v_{k+1}\beta_{k+1}e_k^T, \qquad V_{k+1} = [v_1, \ldots, v_{k+1}], \qquad V_{k+1}^T V_{k+1} = I_{k+1},$$

so that it stops after n steps, and the eigenvectors and values of A, or the solution x of $Ax = v_1\beta_1$ for any scalar β_1, can be found from T_n and V_n. Golub and Kahan's 1965 bidiagonalization of a general matrix B can be framed and analyzed as a Lanczos process, and the results used to find the singular value decomposition or solutions of equations or least squares problems involving B.

These processes are mathematically simple and elegant, but their computational behaviour is far from simple. The finite precision Lanczos process can lose orthogonality immediately the first eigenvector of A has converged to machine precision, and so was largely discarded until about 1971, since many believed it did not work. But since then these processes have became the basis for some of our most powerful tools for large sparse matrix problems—even though poorly understood.

Finally we can show that the Lanczos process does eventually give all eigenvalues and vectors, or solutions of equations, with an accuracy similar to that of backward stable methods. We will not go into the gory details, but concentrate more on what the Lanczos process and Golub and Kahan bidiagonalizations actually achieve, and what to expect when using such computational algorithms.

Computation of Ground States of the Gross-Pitaevskii Functional via Riemannian Optimization

Bartosz Protas
McMaster University

This presentation concerns a novel approach to the computation of ground states in Bose-Einstein condensates, a topic which receives significant attention in theoretical physic. In the proposed approach we combine concepts from Riemannian Optimization and the theory of Sobolev gradients to derive a new conjugate gradient method for direct minimization of the Gross-Pitaevskii energy functional with rotation. The conservation of the number of particles in the system constraints the minimizers to lie on a Riemannian manifold corresponding to the unit L2 norm. The idea developed in our study is to transform the original constrained optimization problem to an unconstrained problem on this (spherical) Riemannian manifold, so that faster minimization algorithms can be applied. First, we first obtain Sobolev gradients using an equivalent definition of an H^1 inner product which takes into account rotation. Then, the Riemannian gradient (RG) steepest descent method is derived based on projected gradients and retraction of an intermediate solution back to the constraint manifold. Finally, we use the concept of the Riemannian vector transport to propose a new Riemannian conjugate gradient (RCG) method for this problem. It is derived at the continuous level based on the "optimize-then-discretize" paradigm instead of the usual "discretize-then-optimize" approach, as this ensures robustness of the method when adaptive mesh refinement is performed in computations. Numerical tests carried out in the finite-element setting based on Lagrangian piecewise quadratic space discretization demonstrate that the proposed RCG method outperforms the simple gradient descent RG method in terms of rate of convergence. The RCG method is extensively tested by computing complicated vortex configurations in rotating Bose-Einstein condensates, a task made challenging by large values of the non-linear interaction constant and the rotation rate.

Joint work with Ionut Danaila.

Computing the Minkowski Reduced Lattice Basese

Sanzheng Qiao
McMaster University

Lattice basis reduction has many applications, such as geometry of numbers, random number generators, cryptography, and wireless communications, just to name a few. Among various notions of lattice basis reduction, the Minkowski reduction is the strongest, in that it defines a basis consisting of shortest possible lattice vectors. Finding a Minkowski reduced basis for a given lattice is a process of tree search. Inspired by the alpha-beta pruning techniques for searching trees, we present an efficient algorithm for computing a Minkowski reduced basis for a given lattice. The efficiency is achieved by dynamically updating the search radius and enforcing the mutual prime constraint. We show that these tree pruning techniques can drastically reduce the search space.

Eroding Bodies in a Stokesian Fluid

Brian Quaife
Simon Fraser University

Erosion of solid material by flowing fluids plays an important role in shaping many objects in nature. For example, erosion of a porous media can be be used to describe groundwater flow. I will describe a high-order and fast method that couples a boundary integral equation method with erosion equations to simulate the erosion of multiple bodies in a Stokesian fluid.

A Hybridizable DG Method for the Navier–Stokes Equations with Pointwise Divergence-free Velocity Field

Sander Rhebergen
University of Waterloo

I will discuss a Hybridizable Discontinuous Galerkin (HDG) method for the incompressible Navier–Stokes equations for which the approximate velocity field is pointwise divergence-free and $H(\mathrm{div})$-conforming. This HDG method can be proven to be mass conserving, momentum conserving and energy stable. Furthermore, I will show that the approximate velocity field, when used as flow field, is compatible with discontinuous Galerkin discretizations of transport equations. I will end this talk by verifying our theoretical results by numerical examples in two- and three-dimensions and for different orders of polynomial approximation.

This is joint work with Garth Wells at the University of Cambridge.

Compressible Flows with Pressure-Dependent Viscosity and Slip Through Local Constrictions

Katrin Rohlf

Ryerson University

Understanding the properties of flows through local constrictions can have significant impact in assessing the potential for vessel rupture in blood flow through constricted, or stenosed, arteries, or in assessing the flow properties in nanochannels just to name a few examples. The relatively recent use of particle-based methods for flow applications, especially for flows through constricted cylinders, have shown that their built-in compressibility may be significant in such geometries. In order to quantify this effect, an approximate analytical velocity profile, as well as the centerline pressure/density curves, have been derived from the compressible Navier-Stokes equation. The Karman-Pohlhausen approximation technique leads to an ODE for the pressure gradient that is solved numerically with Maple/Matlab to obtain the theoretical predictions.

This talk will provide velocity/pressure/density curves for flows through local constrictions. The analytical predictions will be used to demonstrate changes as a result of compressibility, slip and pressure-dependent viscosity parameter, and then compared to the velocity/pressure/density curves from particle-based flow simulations through the same geometries

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Unconditional Stability for Multistep Imex Schemes

David Shirokoff

New Jersey Institute of Technology

In this talk we introduce a new class of linear multistep ImEx schemes that have very good unconditional stability properties. Unconditional stability is a desirable property of a time stepping scheme, as it allows the choice of time step solely based on accuracy considerations. Of particular interest are problems for which both the implicit and explicit parts of the ImEx splitting are stiff. Such splittings can arise, for example, in variable-coefficient problems, or the incompressible Navier-Stokes equations. To characterize the new ImEx schemes, we introduce an unconditional stability region, which plays a role analogous to that of the stability region in conventional multistep methods. Moreover, we will show how the new diagrams explain the fundamental stability restrictions of the well-known semi-implicit backward differentiation formulas (SBDF). We further show that the new ImEx coefficients can overcome the limitations of SBDF, and highlight their utility with several examples arising from partial differential equations: such as variable diffusion, advection diffusion and, time permitting a time dependent Stokes equation.

Rapid Algorithms for the Conversion Between Bandlimited Spherical Harmonic Expansions and their Bivariate Fourier Series

Richard Mikael Slevinsky

University of Manitoba

A rapid transformation is derived between spherical harmonic expansions and their analogues in a bivariate Fourier series. The change of basis is described in two steps: firstly, expansions in normalized associated Legendre functions of all orders are converted to those of order zero and one; then, these intermediate expressions are re-expanded in trigonometric form. The first step proceeds with a butterfly factorization of the well-conditioned matrices of connection coefficients. The second step proceeds with fast orthogonal polynomial transforms via hierarchically off-diagonal low-rank matrix decompositions. Total pre-computation requires $\mathcal{O}(n^3)$ flops; and, asymptotically optimal execution time of $\mathcal{O}(n^2 \log n)$ is rigorously proved via connection to Fourier integral operators.

A Literate Approach for Improving the Verifiability, Reusability and Reproducibility of Scientific Computing Software

Spencer Smith

McMaster University

This talk describes the vision for Drasil, a framework for documenting and developing Scientific Computing Software (SCS). Drasil uses a literate approach, where the scientific and computational knowledge necessary for a particular problem are first recorded as a set of 'chunks.' From the knowledge chunks, all of the required software artifacts are generated using 'recipes,' which provide instructions for transforming the knowledge into the required artifacts. Potential generated artifacts include requirements specification, design documentation, code, test reports and build instructions. Although creating the knowledge base requires significant effort, the proposed Drasil framework provides benefits that make this effort worthwhile. For instance, Drasil improves software verifiability, since it facilities the creation of documentation that shows how the appropriate assumptions and definitions can be used to transform the original abstract theory to the final concrete code. The generative approach eliminates inconsistencies because the knowledge is not duplicated; it is captured once and transformed as needed. The generative approach further facilitates verification by providing traceability between assumptions, theory, definitions, equations, equation derivations, software modules and code. Effort invested into building the Drasil knowledge base improves reusability, since later projects can reuse the knowledge from earlier projects. Reproducibility is improved because all artifacts can be reproduced from the original knowledge chunks, as desired. Recipes that intermingle documentation, code and program output, can potentially be used to explain the complete traceability between idea and implementation. The current status of the Drasil framework will be illustrated via the example of software to simulate the temperature in a solar water heating tank.

Toward Real-time Heart Simulation

Ray Spiteri

University of Saskatchewan

Heart disease is the leading cause of death worldwide. Mathematical modelling and computer simulation can help with diagnosing heart disease, discovering new and personalized medicines, and planning surgical procedures. But in order for this to happen, the simulations must provide clinically relevant data on a clinically relevant time scale.

In 2012, a team from IBM and Lawrence Livermore National Laboratory was able to simulate one second of heart activity in about seven seconds using their highly scalable Cardioid software running on the fastest computer in the world at the time. This is a formidable accomplishment, but we still a ways to go from your cardiologist being able to do perform realistic simulations on their iPad while sitting with you in their office.

In this presentation, I relate a few of the tales from numerical analysis, scientific computing, and high-performance computing that we hope will push us over the top and achieve real-time cardiac simulation.

Extending BACOLI to Simulate Multi-Scale Models

Raymond Spiteri

University of Saskatchewan

BACOLI is a numerical software package for solving systems of parabolic partial differential equations (PDEs) in one spatial dimension. BACOLI features adaptive error control in the temporal and spatial domains. It uses a B-spline collocation method for the spatial discretization to yield a set of ordinary differential equations (ODEs), which together with the boundary conditions, form a system of differential-algebraic equations (DAEs). These DAEs are then solved using DASSL.

Multi-scale models are commonly used to mathematically describe the evolution of many interesting and important systems. They attempt to capture dynamics on multiple scales and integrate them into a common framework. One way to do this is via PDEs that do not depend on spatial derivatives to represent dynamics on small scales. Upon spatial discretization, these PDEs reduce to sets of ODEs at each discrete spatial point.

In this talk, we describe a software package that extends BACOLI to solve multi-scale models consisting of parabolic PDEs coupled with PDEs that do not depend on spatial derivatives. We demonstrate this applicability and efficiency of this extended software package on a number of examples, including the monodomain model of cardiac electrophysiology.

Regularity of Time-Fractional Reaction-Diffusion Problems and their Solution by a Graded-Mesh Finite Difference Method

Martin Stynes

Beijing Computational Science Research Center

A reaction-diffusion problem with a Caputo time derivative of order $\delta \in (0, 1)$ is considered. The solution of such a problem is shown in general to have a weak singularity near the initial time $t = 0$, and sharp pointwise bounds on certain derivatives of this solution are derived. A new analysis of a standard finite difference method for the problem is given, taking into account this initial singularity. This analysis encompasses both uniform meshes and meshes that are graded in time, and includes new stability and consistency bounds. The final convergence result shows clearly how the regularity of the solution and the grading of the mesh affect the order of convergence of the difference scheme, so one can choose an optimal mesh grading. Numerical results are presented that confirm the sharpness of the error analysis.

Preconditioning of Spectral Methods

Manfred R. Trummer and Conor McCoid

Simon Fraser University

We will present methods and results for solving two-point boundary value problems with spectral methods. A focus of the presentation is the well-known fact that spectral differentiation matrices are notoriously ill-conditioned, and how this ill-conditioning affects the robustness of the numerical methods being investigated. We then present a preconditioner based on Birkhoff interpolation. We compare its effectiveness to methods using rectangular differentiation matrices, as well as solutions obtained by the *Chebfun* software package, followed by a brief discussion of the influence of round-off error.

Fitting a Stochastic Model to Eye Movement Time Series in a Categorization Task

Paul Tupper

Simon Fraser University

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Our goal is to develop an efficient framework for fitting stochastic continuous-time models to experimental data in cognitive psychology. As a simple test problem, we consider data from an eye-tracking study of attention in learning. For each subject, the data for each trial consists of the sequence of stimulus features that the subject fixates on, together with the duration of each fixation. We fit a stochastic differential equation model to this data, using the Approximate Bayesian Computation framework. For an individual subject we infer posterior distributions for the unknown parameters in the model.

This is joint work with Thuan Pham Nguyen, Yunlong Nie, Jiguo Cao, Liangliang Wang.

The Sensitivity of Mean Quantities to Discretization Techniques

Lennaert van Veen[1] and Kazumasa Takeuchi[2]

[1]University of Ontario Institute of Technology; [2]Tokyo Institute of Technology

In various branches of physics the attention is focused on mean quantities. In turbulence, for instance, energy spectra and structure functions are used to characterize flows. Such mean quantities often exhibit universal properties that cannot be detected in individual realizations of the flow. The two main sources of error in the numerical computation of mean quantities are the error of simulating the system and the statistical error due to the finite sample size. While the statistical error is predictable, the influence of truncation and round-off errors in simulations is not. In fact, it is often quietly assumed that these errors will "cancel out" in the averaging process. We consider a model for the growth of a one-dimensional interface as an example. Various authors reported a scaling of the interface thickness in the KPZ universality class when using finite-difference space discretization and low-order time stepping. In our experiments, using pseudo-spectral methods, this scaling is not present. We investigate the possibility that the use of discretization methods with a low order of accuracy introduces noise into the system with a nett effect on the mean quantities.

Approximating Highly Anisotropic Functions with Optimally Transported Meshes

Emily Walsh

University of the West of England

The Parabolic Monge-Ampere Moving Mesh Method combines equidistribution with optimal transport. This method can produce an anisotropic mesh along a given feature by equidistributing a suitably chosen scalar monitor function. Furthermore, the general metric M, in physical space, that a mesh generated by this method aligns to, is closely related to an optimal mesh, which minimises interpolation error. Numerical examples will demonstrate the meshes generated using optimal transport methods are suitable for interpolating highly anisotropic functions or solving PDEs for which a highly anisotropic function is a solution. Furthermore, analysis of the error estimates and a comparison with those obtained for the optimal anisotropic mesh, will be presented.

Conservative Methods and Applications to Dynamical Systems

Andy Wan
McGill University

Conservative methods are numerical schemes which preserve first integrals or invariants of differential equations. While projection methods are in general conservative, they may not possess long-term stability properties as other conservative methods. Specifically, the projection step can project the numerical solution onto a different connected component of the level set of the invariants, leading to instability in long-term integration of dynamical systems. We introduce, a new class of conservative method, called the multiplier method, and show that conservative schemes can be systematically derived for general dynamical systems with arbitrary forms of first integrals. In particular, the multiplier method can be applied to non-Hamiltonian systems and without additional reformulation or transformation of variables. We demonstrate the multiplier method on a variety of dynamical systems.

This is joint work with Alexander Bihlo at Memorial University of Newfoundland and Jean-Christophe Nave at McGill University.

Unsupervised Cell Image Segmentation via RPCA and Spectral Clustering

Justin Wan
University of Waterloo

Segmentation of cells in time-lapse bright-field microscopic images is crucial in understanding cell behaviors for medical research. However, the complex nature of the cells, together with poor contrast, broken cell boundaries and the halo artifact, pose nontrivial challenges to this problem. In this talk, we present two robust mathematical models to segment bright-field cells automatically. These models treat cell image segmentation as a background subtraction problem, which can be formulated as a Principal Component Pursuit (PCP) problem. Our first segmentation model is formulated as a PCP with nonnegative constraints. In this approach, we exploit the sparse component of the PCP solution for identifying the cell pixels. However, the sparse component and the nonzero entries can scatter all over the image, resulting in a noisy segmentation. The second model is an improvement of the first model by combining PCP with spectral clustering. Seemingly unrelated approaches, we combine the two techniques by incorporating normalized-cut in the PCP as a measure for the quality of the segmentation. Experimental results demonstrate that the proposed models are effective in segmenting cells obtained from bright-field images.

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