Southern Ontario Numerical Analysis Day 2010

9:00am - 9:20am: Alireza Mohammadi (UWO)

Title: Spectrally-Accurate Method for Flows in Grooved Channels

Abstract: A grid-less, spectrally-accurate algorithm for analysis of laminar flows in channels with grooved walls is developed. The algorithm is based on the Immersed Boundary Conditions (IBC) concept, where the boundary conditions are submerged inside the computational domain and are treated as internal constraints. The flow has two-dimensional form when the grooves are aligned with the direction of the flow. The flow becomes three-dimensional when the grooves rotate away from this reference direction. The solution of the governing equations is carried out in a rotated reference system whose one axis is aligned with the direction of the grooves. It is shown that the use of such a system results in the decoupling of the field equations; one needs to solve a 4th-order equation describing a two-dimensional flow across the grooves followed by solution of a 2nd-order equation describing a flow in the direction along to the grooves, rather than a general 6th-order equation describing general three-dimensional motions. Fourier expansions are used for discretization in the direction transverse to the grooves, and Chebyshev expansions are used to discretize modal equations. Efficient solvers that take advantage of the structure of the coefficient matrices have been developed. Various tests have been conducted in order to illustrate the performance and the accuracy of the algorithm.

9:20am - 9:40am: Swathi Amarala (UW)

Title: A New Multigrid Time Stepping Scheme for Euler Equations

Abstract: The traditional way of performing multigrid methods for Euler equations has been to use fully weighted restriction and linear interpolation which delay the convergence due to numerical oscillations. In this talk, I would like to present a new multigrid approach for obtaining the steady state solution of Euler equations. The idea behind adopting multigrid approach for hyperbolic equations is to accelerate the wave propagation on multiple grids using larger time steps in coarser grids without violating the CFL condition. It was proved by Wan, Jameson [2006] that schemes with monotonicity preserving and total variation diminishing properties produce efficient multigrid methods. Upwind biased residual restriction and interpolation based on the characteristics of linear wave equation satisfy these properties. This approach is extended to nonlinear Euler equations by transforming the equations into canonical form and performing nonlinear restriction and interpolation based on local Riemann solutions. The local Riemann solution is obtained by looking at the direction of local wind flow for each of the decoupled scalar equation. We obtained results with optimal speedups. When compared with other multigrid results, our approach gives far better speedups and also permits the use of much coarser grids.

9:40am - 10:00am: Mohammad Farazmand (McMaster)

Title: Controlling the Dual Cascade of Two-dimensional Turbulence

Abstract: The Kraichnan–Leith-Batchelor (KLB) theory of statistically stationary forced homogeneous isotropic 2-D turbulence predicts the existence of two inertial ranges: an energy inertial range with an energy spectrum scaling of $k^{-5/3}$, and an enstrophy inertial range with an energy

spectrum scaling of k^{-3}. However, unlike the analogous Kolmogorov theory for 3-D turbulence, the KLB scaling laws for energy and enstrophy have not been observed *simultaneously* in any experiment or numerical simulation. For example, the high resolution (up to 16384^2) direct numerical simulations of Boffetta [J. Fluid Mech. (2007), vol. 589, pp. 253-260] have a $k^{-3.8}$ energy spectrum over the enstrophy inertial range. The present paper uses a novel optimal control theory approach to find a forcing that does produce the dual scaling ranges. This is the first time a dual cascade which follows the KLB scaling laws has been observed using a band-limited forcing. A careful analysis of the resulting forcing suggests that it belongs to a sparse subset of the square integrable (in time and space) functions. This suggests that it is unlikely to be realized in nature, or by a simple numerical model. Our results also suggest that the phase structure of the forcing (which is assumed as random in most numerical simulations and mathematical analysis) can modify the dynamics of a turbulent flow and, in particular, the scaling of its energy spectrum. By:M. M. Farazmand, N. Kevlahan and B. Protas

10:30am - 10:50am: Kante Easley (UT)

Title: Energy-based Error Control Strategies Suitable for Molecular Dynamics Simulation

Abstract: When evaluating integration schemes used in molecular dynamics (MD) simulations, energy conservation is often cited as the primary criterion by which the integrators should be compared. As a result variable stepsize Runge-Kutta methods are often ruled out of consideration due to their characteristic energy drift.

We have shown that by appropriately modifying the stepsize selection strategy in a variable-stepsize RK method it is possible for the MD practitioner to obtain substantial control over the energy drift during the course of a simulation. This ability has been previously unreported in the literature, and we present numerical examples to illustrate that it can be achieved without sacrificing computational efficiency under currently obtainable timescales.

10:50am - 11:10am: Jonathan Gustafsson (McMaster)

Title: Computation of Steady Incompressible Flows in Unbounded Domain

Abstract: The objective of this research is to study steady exterior flows in 2D unbounded domains, such as the flow around a infinite cylinder. More specifically, our goal is to classify solutions to the steady Navier–Stokes equations based upon the rate at which the velocity fields tend towards their asymptotic values. The second objective is to identify the family of Euler solutions which corresponds to the limit of the flow around a cylinder when the Reynolds number goes towards infinity. Because of our focus on the asymptotic behavior of the solution at infinity, it is not possible to use domain truncation typically employed in such problems. Instead, an approach based on the rational Chebyshev functions is proposed. These functions are defined on semi-infinite intervals and are useful for approximating functions that tend towards their asymptotic values very slowly. Our method is being implemented in two steps: the first step is an algebraic mapping from a semi-infinite interval to the interval [-1,1], in the second step, Chebyshev polynomials are used on the mapped domain. Another element of our approach is the tau-collocation method. It is closely related to the tau method, but is implemented as a collocation technique, rather than the Galerkin technique. This method is needed in order to implement the extra boundary conditions required for the stream function. Using a combination of these methods we aim to compute solutions to the steady-state Navier-Stokes characterized by distinct behavior at infinity. Some preliminary calculations will be presented featuring flows with and without recirculation regions.

11:10am - 11:30am: Michael Lam (UW)

Title: Biologically Inspired Neural-Network Model of the Visual System

Abstract: Humans have an astounding ability to understand the world through sight. The visual system alone is one of the most complicated and intriguing areas of the brain, comprising a large percent it. Recently our understanding of this complex system has been significantly broadened.B However one question remains largely untouched: How does the mammalian visual system initially configure itself to do powerful low-level tasks such as edge detection?

In the past decade researchers have been endeavouring to use neural networks to mimic visual learning. Some of these approaches employ sparsity or topology, with a focus more on image reproduction rather than biological feasibility. I will discuss and illustrate a novel variation of a statistical model for neural learning in the visual cortex. This biologically inspired model, based on Deep Belief Networks, can be used to produce neural responses similar to those observed by neurological probing of monkey and cat visual systems. Hopefully with such a model we can further understand deeper, more obscure areas of the visual system, or possibly gain more insight into how the brain works in general.

11:30am - 12:15pm: Prof. Hongmei Zhu (York), keynote speaker

Title: Channelized Instantaneous Frequency, Local Group Delay and Their Applications

Abstract: Most signals in real life contain multiple frequency components whose frequency characteristics vary over time. Channelized instantaneous frequency and local group delay, mathematically dual concepts, are defined as functions of both time and frequency. While channelized instantaneous frequency characterize behaviors of local frequencies simultaneously occurred within a local time frame, local group delay defines the average local time arrival for these frequencies. These two measures can be estimated from their time-frequency distributions of a signal and are very important in various applications such as speech phonation analysis and sound tracking. In this talk, we will first present an overview of these two concepts and then discuss their numerical implementations and applications.

1:40pm - 2:00pm: Alexander Dubitski (UOIT)

Title: Numerical Continuation of Parameter Dependent Solutions to Nonlinear Problems

Abstract: Our problem is a nonlinear problem of the form f(x,λ)=0 where x is a vector with n components and λ is a parameter. We know the solution at λ=0 and want to know it at λ=λ_GOAL. To compute it at λ=λ_GOAL we use a continuation algorithm to find a solution curve(x(s),λ(s)).

1.increment (x,λ) by ds*T, where T is the unit tangent to the solution curve.
2.solve f(x,λ) by Newton iterations
3.recompute T
4.adjust ds
repeat 1-4 until λ=λ_GOAL

The expensive part of the computation is the Newton iteration, because for each iteration we need to solve an nxn matrix-vector problem. Consequently, we want to take as a few continuation steps as possible, which means taking ds as large as possible. However, if we choose ds too large, the Newton iterations diverge and a lot of computational time is wasted. Therefore, what we want to do is to attempt several steps with different step sizes ds in parallel. We keep track of the convergence (i.e. the residue of the Newton iterations) and accept the step with the largest ds that converges in reasonable time.

2:00pm - 2:20pm: Yiqing Huang (UW)

Title: A Penalty Method for Pricing Guaranteed Minimum Withdrawal Benefits (GMWB)

Abstract: The no arbitrage pricing of Guaranteed Minimum Withdrawal Benefits (GMWB) contracts results in a singular stochastic control problem which can be formulated as a Hamilton Jacobi Bellman (HJB) Variational Inequality (VI). Recently, a penalty method has been suggested for solution of this HJB variational inequality. This method is very simple to implement. We present a rigorous proof of convergence of the penalty method to the viscosity solution of the HJB VI. Numerical tests of the penalty method are presented which show the experimental rates of convergence, and a discussion of the choice of the penalty parameter is also included.

2:20pm - 2:40pm: Vladislav Bukshtynov (McMaster)

Title: Reconstruction of Solution-Dependent Parameters in Constitutive Relations

Abstract: This research is motivated by the need to reconstruct temperature–dependent material properties in complex multiphysics systems. As a first step, we consider a simple model problem based on the steady–state heat conduction equation $-\boldsymbol{\nabla} \cdot [k(T)\boldsymbol{\nabla} T(\mathbf{x})] = g(\mathbf{x})$, where $\mathbf{x} \in \Omega$, $\Omega \in \mathbb{R}^n$, $n = 1, 2, 3$. Assuming that some pointwise observations $\{\tilde{T}_i\}_{i=1}^M$ of the actual solution $T : \Omega \to \mathbb{R}$ are available, an inverse problem is formulated to recover the thermal diffusivity $k = k(T)$ in the form of an infinite–dimensional PDE–constrained optimization problem. This problem is solved using a gradient descent method in which cost functional gradients are obtained from solutions of the adjoint equations. Computational results will be presented to validate the proposed approach. Next we extend the approach to more complicated problems involving systems of coupled PDEs depending on time and defined on domains with higher dimensions. We will consider a problem in which the constitutive relation appearing in one equation depends on the state variable governed by a different equation, e.g., reconstruction of the temperature dependence of the viscosity coefficient in the momentum equation where the temperature is governed by a separate energy equation.

2:40pm - 3:00pm: Duy Minh Dang (UT)

Title: Pricing of Cross-Currency Interest Rate Derivatives on Graphics Processing Units

Abstract: We present a Graphics Processing Unit (GPU) parallelization of the computation of the price of exotic cross-currency interest rate derivatives via a Partial Differential Equation (PDE) approach. In particular, we focus on the GPU-based parallel pricing of long-dated foreign exchange (FX) interest rate hybrids, namely Power Reverse Dual Currency (PRDC) swaps with Bermudan cancelable features. We consider a three-factor pricing model with FX volatility skew which results in a time-dependent parabolic PDE in three spatial dimensions. Finite difference methods on uniform grids are used for the spatial discretization of the PDE, and the Alternating Direction Implicit (ADI) technique is employed for the time discretization. We then exploit the parallel architectural features of GPUs together with the Compute Unified Device Architecture (CUDA) framework to design and implement an efficient parallel algorithm for pricing PRDC swaps. Over each period of the tenor structure, we divide the pricing of a Bermudan cancelable PRDC swap into two independent pricing subproblems, each of which can efficiently be solved on a GPU via a parallelization of the ADI timestepping technique. Numerical results indicate that GPUs can provide significant increase in performance over CPUs when pricing PRDC swaps.

3:30pm - 3:50pm: Xuan Vinh Doan (UW)

Title: A Robust Algorithm for Semidefinite Optimization Problem

Abstract: We derive and test a numerically stable primal-dual interior-point methods, p-d i-p, for semidefinite programming. We realize a distinct improvement in accuracy relative to current public domain programs. This is for random problems as well as for problems of special structure. The algorithm is based on a Gauss-Newton approach with a preconditioned iterative method for finding the search direction. Preliminary numerical results are shown for the well-known Lovasz theta function problem. This is joint work with Serge Kruk and Henry Wolkowicz.

3:50pm - 4:10pm: Anis Sardar Haque (UWO)

Title: Cache Friendly Sparse Matrix-vector Multiplication

Abstract: We revisit ordering techniques as a preprocessing step for improving the performance of sparse matrix-vector multiplication (SpMXV) on modern hierarchical memory computers. In computing SpMXV the main purpose of ordering of columns (or rows) is to improve the performance by enhancing data reuse. In this work, we present a new column ordering algorithm based on the binary reflected gray codes that runs in linear time with the number of nonzeros. We analyze the cache complexity of SpMXV when the sparse matrix is ordered by our technique. The results from numerical experiments with very large test matrices clearly demonstrates the performance gains rendered by our proposed technique.

4:10pm - 4:30pm: Diego Ayala (McMaster)

Title: Maximum Enstrophy Growth in Burgers Equation

Abstract: It is well known that the regularity of solutions to Navier-Stokes equation is controlled by the boundedness in time of the enstrophy. However, there is no proof of the existence of such bound. In fact, standard estimates for the instantaneous rate of growth of the enstrophy lead to finite time blow up, when straightforward time integration of the estimate is used. Moreover, there is recent numerical evidence to support the sharpness of these instantaneous estimates for any given instant of time. The central question is therefore, how to extend these instantaneous estimates to a finite time interval $(0, T]$ in such a way that the dynamic imposed by the PDE is taken into account.

We state the problem of saturation of finite time estimates for enstrophy growth as an optimization problem, where the cost functional is the total change of enstrophy in a given time interval. We provide an iterative algorithm to solve the optimization problem using Viscous Burgers Equation (VBE) as a “toy” version of Navier-Stokes equation. We give numerical evidence that analytic finite time estimates for enstrophy growth in VBE are conservative, in the sense that they are not saturated.

4:30pm - 4:50pm: Stephen (Shu Tong) Tse

Title: A Very Efficient and Almost Exact Simulation of the Cox-Ingersoll-Ross(CIR) Process

Abstract: The CIR process has been widely used in computational finance to model short term interest rate or stochastic volatility. Fast and efficient simulation of the CIR process is an essential ingredient for pricing exotic derivatives under such models. Surprisingly, despite the use of the CIR process for decades, satisfactory simulation schemes have not been developed until recent years. Broadie and Kaya achieved a breakthrough in 2004 by showing that the CIR process can be simulated exactly. Their method is not very useful in practice, however, because of the heavy computational cost involved. Since then, a lot of researchers have developed approximations to the exact schemes which sacrifice a small amount of accuracy for a big boost in performance. In this presentation, a very efficient and accurate approximation to the most time-consuming and complicated step in the exact scheme is proposed.