

The 36th Southern Ontario Numerical Analysis Day

Friday, May 4, 2018

Sandford Fleming Building, room SF 1105, University of Toronto,
10 King's College Rd, Toronto, Ontario M5S3A4, Canada

organized by

**The Department of Computer Science
University of Toronto**

9:30	Registration
9:45	Opening remarks
9:50	Robert Corless (invited lecture), Western University Optimal Backward Error and the Leaky Bucket
10:35	Eunice Chan, Western University Algebraic Linearizations of Matrix Polynomial
10:50	Leili Rafiee Sevyeri, Western University The Runge Example for Interpolation and Wilkinson's Examples for Rootfinding
11:05	Break
11:25	Reza Zolfaghari, McMaster University An Hermite-Obreschkoff Method for Stiff High-Index DAEs
11:40	Jienan Yao, University of Toronto Numerical PDE methods for a discontinuous diffusion problem with application to brain cancer growth
11:55	Shashwat Sharma, University of Toronto An accelerated solver for Maxwell's equations in integral form with application to integrated circuit design
12:10	Lunch - on your own
13:40	Justin Wan (invited lecture), University of Waterloo Multigrid Methods for Solving Cooperative, Non-cooperative and Mean Field Games arising from Economics
14:25	Michael Chiu, University of Toronto Backward Simulation of Poisson Processes
14:40	Edward Cheung, University of Waterloo Nonsmooth Frank-Wolfe with Uniform Affine Approximations
14:55	Break
15:15	Pritpal Matharu, McMaster University Determination of Optimal Closures for Hydrodynamic Models
15:30	Vishal Siewnarine, York University High Order Pole Conditions for the Solution of the Poisson Equation
15:45	Dongfang Yun, McMaster University On Maximum Enstrophy Growth and Extreme Vortex States in Three-dimensional Incompressible Flows
16:00	Giselle Sosa Jones, University of Waterloo Hybridizable Discontinuous Galerkin Method for Linear Free Surface Problems
16:15	Break
16:30	Paulo Zúñiga, University of Concepcion and University of Waterloo A high order mixed-FEM for the Poisson problem on curved domains
16:45	Xiulei Cao, York University Electro-Neutral Models for Dynamic Poisson-Nernst-Planck System
17:00	Keegan Kirk, University of Waterloo Error Analysis of a Space-Time Hybridizable Discontinuous Galerkin Method for the Advection-Diffusion Equation
17:15	Sujanthan Sriskandarajah, York University Identification of the dielectric parameters of a tissue using optimization subject to Maxwell's Equations

INVITED LECTURES

Robert Corless

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Department of Applied Mathematics

Optimal Backward Error and the Leaky Bucket

Abstract: This talk is based on my 2016 SIREV (Education) paper with Julia Jankowski, “Variations on a Theme of Euler”. In that paper, we looked at very simple methods for solving $\dot{y} = -\sqrt{y}, y(0) = 1$ (and other models of a leaky bucket, in follow-on work). The perspective of backward error for Initial-Value Problems for ODE is something I acquired from Wayne Enright, quite a few years ago now. I’m still a fan of the idea, as you will see in the talk. Although the talk will contain some ideas and techniques that might be new to you, they are suitable to be taught to undergraduates (hence the SIREV article).

Justin Wan

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Department of Computer Science

Multigrid Methods for Solving Cooperative, Non-cooperative and Mean Field Games arising from Economics

Abstract: Dynamic Bertrand oligopolies are competitive markets in which a small number of firms producing similar goods use price as their strategic variable. In particular, each firm wants to determine the optimal price that maximizes its expected discounted lifetime profit. In a two person cooperative game, it can be modeled as a zero-sum game which can be formulated as an Hamilton-Jacobi-Bellman (HJB) PDE. If they compete non-cooperatively, it will then give rise to a nonzero-sum game, which leads to a system of HJB equations. For multi-person competition, they are often formulated as mean field games where each firm competes with the rest as a group. In this talk, we will present numerical methods for solving the corresponding model equations. In particular, we will propose finite difference discretization schemes that are convergent to the viscosity solution and efficient multigrid methods for solving the discrete nonlinear equations. Finally, we will present numerical results for a number of application problems.

CONTRIBUTED TALKS

Eunice Chan

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Algebraic Linearizations of Matrix Polynomials

Abstract: We show how to construct linearizations of matrix polynomials $z\mathbf{a}(z)\mathbf{d}_0 + \mathbf{c}_0$, $\mathbf{a}(z)\mathbf{b}(z)$, $\mathbf{a}(z) + \mathbf{b}(z)$ (when $\deg(\mathbf{b}(z)) < \deg(\mathbf{a}(z))$), and $z\mathbf{a}(z)\mathbf{d}_0\mathbf{b}(z) + \mathbf{c}_0$ from linearizations of the component parts, $\mathbf{a}(z)$ and $\mathbf{b}(z)$. This allows the extension to matrix polynomials of a new companion matrix construction.

Joint work with Robert Corless, Western University.

Leli Rafiee Sevyeri

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Applied Mathematics

The Runge Example for Interpolation and Wilkinson's Examples for Rootfinding

Abstract: We look at two classical examples in the theory of numerical analysis, namely the Runge example for interpolation and Wilkinson's example (actually two examples) for rootfinding. We use the modern theory of backward error analysis and conditioning, as instigated and popularized by Wilkinson, but refined by Farouki and Rajan. By this means, we arrive at a satisfactory explanation of the puzzling phenomena encountered by students when they try to fit polynomials to numerical data, or when they try to use numerical rootfinding to find polynomial zeros. Computer algebra, with its controlled, arbitrary precision, plays an important didactic role.

Joint work with Robert Corless, Western University.

Reza Zolfaghari

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Computational Science and Engineering

An Hermite-Obreschkoff Method for Stiff High-Index DAEs

Abstract: We are interested in solving high-index differential-algebraic equations (DAEs). The DAETS solver by Nedialkov and Pryce can integrate numerically high-index, arbitrary order DAE systems. Based on explicit Taylor series, this solver is efficient on non-stiff to mildly stiff problems, but due to stability restrictions, it takes very small steps on highly stiff problems.

Hermite-Obreschkoff (HO) methods can be viewed as a generalization of Taylor series methods. The former have smaller truncation error than the latter, and have excellent stability properties: an implicit HO method can be A- or L-stable. Implicit HO methods are challenging to implement due to the required higher-order derivatives and Jacobians.

We develop such a method for numerical solution of stiff high-index DAEs. As in DAETS, our method employs Pryce's structural analysis to determine the constraints of the problem and to organize the computations of higher-order derivatives for the solution, which are obtained through automatic differentiation. We discuss the overall integration scheme: finding a consistent initial point, computing an initial guess for Newton's method, automatic differentiation for constructing the needed Jacobians in it, and stepsize control. We report numerical results on several stiff DAE and ODE systems illustrating the performance of this method, and in particular its ability to take large steps on stiff problems.

Joint work with Ned Nedialkov, McMaster University.

Jienan Yao

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Computer Science, Numerical Analysis

**Numerical PDE methods for a discontinuous diffusion problem
with application to brain cancer growth**

Abstract: Error analysis and convergence results for standard Partial Differential Equation (PDE) discretization methods normally assume that the coefficient functions are continuous. However, when the discretization methods are applied to PDEs (Boundary Value Problems - BVPs or Initial Value Problems - IVPs) with discontinuous coefficients, they may not exhibit the standard rate of convergence, and, even more, convergence is not guaranteed. In this research, we study a mathematical model simulating the invasion of brain cancer (glioma) which involves a PDE with discontinuous diffusion coefficient due to the heterogeneous nature of the brain, consisting of white and grey matter. The discontinuity of the diffusion coefficient results in continuity for the solution function, and a certain type of discontinuity of its spatial derivative, across the interface between the white and grey matters. We propose two approaches to adjust the standard Finite Difference methods, so that the numerical solution satisfies the continuity and discontinuity constraints. One technique treats the PDE as multi-domain problem with (interior) interface conditions, and the other relates the limits of the functional and forcing terms from both sides of the interface point. Numerical results will be provided to assess and compare the performance of the proposed methods.

Joint work with Christina Christara, University of Toronto.

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**An accelerated solver for Maxwell's equations in integral form
with application to integrated circuit design**

Abstract: Electromagnetic interference and cross-talk is a growing concern in the design of integrated circuits, due to the increase in operating speed, complexity and miniaturization. Microelectronic companies rely heavily on numerical solvers to predict and minimize unwanted electromagnetic phenomena in the intricate network of wires that distribute signals and power across an integrated circuit. This task requires the numerical solution of Maxwell's equations in a very complex geometry. In this work, a surface integral formulation is proposed for efficient, robust and accurate analysis of these large-scale electromagnetic problems. A special treatment of interior and exterior regions of electrical conductors is leveraged to avoid the need for an extremely fine mesh, without sacrificing accuracy. The computation is accelerated with fast Fourier transforms (FFTs), by projecting weakly-contributing mesh elements on to a regular grid. Additionally, the formulation is integrated with an advanced multilayer Green's function to allow for modelling realistic structures embedded in stratified media. The performance of the proposed solver is validated against a commercial finite element tool, and demonstrated on a wide range of structure sizes and operating frequencies.

Joint work with Piero Triverio, University of Toronto.

Michael Chiu

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Computer Science, Numerical Analysis

Backward Simulation of Poisson Processes

Abstract: Poisson processes have many important applications in Insurance, Finance, and many other areas of Applied Probability. We discuss the Backward Simulation (BS) approach to modelling Poisson processes and analyze the connection to the Extreme Measures describing the joint distribution of the processes at the end of the time horizon. We also discuss the extension of this technique to a broader class of processes such as the Multivariate Mixed Poisson processes. The BS approach relies on the conditional uniformity of the arrival times, given the number of events and allows for the linear correlation coefficient between Poisson processes to take extreme values. In an earlier work, the forward continuation of the BS was introduced for Poisson processes in order to achieve richer correlation profiles. It was also shown that the forward continuation of the BS is asymptotically stationary. Along with the extension of the BS to multivariate mixed Poisson processes, we investigate the forward continuation of the BS approach for multivariate mixed Poisson processes.

Joint work with Ken Jackson, University of Toronto.

Edward Cheung

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Computer Science, Scientific Computing

Nonsmooth Frank-Wolfe with Uniform Affine Approximations

Abstract: Frank-Wolfe methods (FW) have gained significant interest in the machine learning community due to its ability to efficiently solve large problems that admit a sparse structure (e.g. sparse vectors and low-rank matrices). However the performance of the existing FW method hinges on the quality of the linear approximation. This typically restricts FW to smooth functions for which the approximation quality, indicated by a global curvature measure, is reasonably good.

In this paper, we propose a modified FW algorithm amenable to nonsmooth functions by optimizing for approximation quality over all affine functions given a neighborhood of interest. We analyze theoretical properties of the proposed algorithm and demonstrate that it overcomes many issues associated with existing methods in the context of nonsmooth low-rank matrix estimation.

Joint work with Yuying Li, University of Waterloo.

Pritpal Matharu

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Department of Mathematics and Statistics

Determination of Optimal Closures for Hydrodynamic Models

Abstract: This investigation is motivated by the question about performance limitations characterizing certain common closure models for nonlinear models of fluid flow. The need for closures arises when for computational reasons first-principles models, such as the Navier-Stokes equations, are replaced with their simplified (filtered) versions such as the Large-Eddy Simulation (LES). In the present investigation, we focus on a simple model problem based on the 1D Kuramoto-Sivashinsky equation with a Smagorinsky-type eddy-viscosity closure model. The eddy viscosity is assumed to be a function of the state (flow) variable whose optimal functional form is determined in a very general (continuous) setting using a suitable adjoint-based variational data-assimilation approach. In the presentation, we will review details of the formulation of the computational approach and will discuss some computational results.

Joint work with Bartosz Protas, McMaster University.

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Mathematics and Statistics

High Order Pole Conditions for the Solution of the Poisson Equation

Abstract: A tricky problem that arises in computing numerical solutions of the Poisson equation in cylindrical coordinates is the treatment of the solution at $r = 0$, where some conditions must be specified, in addition to those known on the exterior boundary of the computational domain. These so-called pole conditions effectively determine the solution value at $r = 0$ in terms of data at surrounding points. Typical approaches to handling this problem are accurate only to first or second order in the spatial step size. Our approach to the problem, which we outline in this talk, is fourth order in the spatial step size, and is easily generalized to higher order. Further, the method is readily applied to the solution of the Poisson problem, in other coordinate systems, including spherical and toroidal coordinates.

Joint work with Michael Haslam, York University.

Dongfang Yun

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Department of Mathematics and Statistics

**On Maximum Enstrophy Growth and Extreme Vortex States
in Three-dimensional Incompressible Flows**

Abstract: Enstrophy is a key quantity in determining finite-time singularities formation to solutions of Navier-Stokes equations. In this study, we investigate extreme vortex states defined as incompressible velocity fields which lead to the maximum possible enstrophy growth $\mathcal{E}(t)$ in three-dimensional incompressible flows on a periodic domain. For finite time windows and values of enstrophy, the problem of maximizing enstrophy growth can be stated as a constrained variational optimization problem, which is solved numerically by Adjoint-based Gradient Method. In the limit of small time window, maximizing vortex states are chosen to be maximizers of the instantaneous rate of growth of enstrophy. For larger time windows, a family of maximizing vortex states can be constructed in combination with the continuous technique. Numerical results indicate that using vortex states, which achieve maximum instantaneous growth rate of enstrophy growth as initial condition, does not guarantee maximum enstrophy growth in finite-time scale. Regarding values of enstrophy increase, it is found that enstrophy has a longer increasing period and a larger relative increase. The structure of optimal vortex states is visualized and compared.

Keywords: Enstrophy growth, Constrained maximization, Gradient method, Adjoint problem

Joint work with Bartosz Protas, McMaster University.

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Applied Mathematics

Hybridizable Discontinuous Galerkin Method for Linear Free Surface Problems

Abstract: In this talk, we present the discretization of the free surface problem for irrotational flows with linearized boundary conditions using the Local Hybridizable Discontinuous Galerkin (L-HDG) method and the Interior Penalty Discontinuous Galerkin (IP-DG) method. The IP-DG case follows the work done by van der Vegt et al. in 2005. For the time discretization, we employ a BDF scheme. Through static condensation, the linear system to be solved on each time step in the HDG method is in general smaller than the one obtained with DG. Moreover, in L-HDG the gradient of the scalar variable converges with optimal rate, in contrast to IP-DG where the gradient converges sub-optimally. L-HDG also allows superconvergence of the scalar variable through local postprocessing. We show two different numerical tests, one where the analytical solution is known, and another one where we simulate waves generated by a wave maker. For the first case, we show the rates of convergence of both methods when using linear, quadratic and cubic polynomials.

Joint work with Sander Rhebergen, University of Waterloo.

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A high order mixed-FEM for the Poisson problem on curved domains

Abstract: In this talk, we propose and analyze a high order mixed finite element method for the Poisson problem with Dirichlet boundary condition on curved domains O . The method is based on approximating O by a polygonal/polyhedral subdomain D , where a high order Galerkin method approximates the solution. To approximate the Dirichlet boundary data on the boundary of D , a transferring technique, based on integrating the extrapolated discrete gradient, is employed. Considering generic finite dimensional subspaces, we prove that the resulting Galerkin scheme, which is $H(\text{div}; D)$ -conforming, becomes well-posed provided suitable hypotheses on the aforementioned subspaces. A feasible choice of discrete spaces is given by Raviart-Thomas elements of order $k \geq 0$ for the vectorial variable and discontinuous polynomials of degree k for the scalar variable, yielding optimal convergence whenever the distance between the computational and the curved boundaries is of order of the mesh-size h . We also provide an approximation of the solution in the relative complement of D with respect to O . Finally, we provide numerical experiments illustrating the optimal performance of the scheme and confirming the theoretical rates of convergence.

Joint work with Ricardo Oyarzúa, University of Bío-Bío, Chile, and Manuel Solano, University of Concepcion, Chile.

Visiting student supervisor: Sander Rhebergen, University of Waterloo.

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Mathematics and Statistics

Electro-Neutral Models for Dynamic Poisson-Nernst-Planck System

Abstract: The Poisson-Nernst-Planck (PNP) system is a standard model for describing ion transport. In many applications, e.g., ions in biological tissues, the presence of thin boundary layers poses both modelling and computational challenges. We derive simplified electro-neutral (EN) models where the thin boundary layers are replaced by effective boundary conditions. There are two major advantages of EN models. First of all, it is much cheaper to solve them numerically. Secondly, EN models are easier to deal with compared with the original PNP, therefore it is also easier to derive macroscopic models for cellular structures using EN models.

Keegan Kirk

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Applied Mathematics

Error Analysis of a Space-Time Hybridizable Discontinuous Galerkin Method for the Advection-Diffusion Equation

Abstract: Many important applications of fluid mechanics require the solution of time-dependent partial differential equations on evolving and deforming domains. Notable examples include the simulation of rotating wind turbines in strong air flow, wave impact on offshore structures, and arterial blood flow in the human body.

A viable candidate for such problems is the space-time discontinuous Galerkin (DG) method. The problem is fully discretized in space and time instead of the typical method of lines treatment of time-dependent problems on fixed domains. The resulting scheme is well suited to handle moving and deforming domains, but at a significant increase in computational cost in comparison to traditional time-stepping methods. Attempts to rectify this situation have led to the pairing of space-time DG with the hybridizable DG (HDG) method, which was developed solely to reduce the expense of DG. The combination of the two methods results in a scheme that retains the high-order accuracy and geometric flexibility of space-time DG without the associated computational burden.

We perform an a priori analysis of a space-time HDG method for the non-stationary advection-diffusion problem posed on a time-dependent domain. We discuss anisotropic trace and inverse inequalities valid for moving meshes, which are essential for our analysis. Stability of the scheme is proven through the satisfaction of an inf-sup condition. Finally, we derive theoretical rates of convergence.

Supervisor: Sander Rhebergen

Joint work with Tamas Horvath, Sander Rhebergen, and Aycil Cesmelioglu.

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Identification of the dielectric parameters of a tissue using optimization subject to Maxwell's Equations

Abstract: Eddy currents are induced by rapidly switching currents of the gradient coils in a MRI scanner. Several finite difference time domain (FDTD) based numerical schemes have been proposed to solve Maxwell's equations, however many of them have a stability condition. Another numerical scheme, namely, the energy conserved splitting FDTD (EC-S-FDTD) scheme was introduced to solve Maxwell's equations. It has unconditional numerical stability and conserves the energy property of Maxwell's equations. It has been implemented in the Cartesian co-ordinates for other electromagnetic applications. The method provides an accuracy of second order in both time and space. Typical MRI scanners are cylindrical in shape, hence the use of cylindrical co-ordinates is more numerically efficient. A specific electromagnetic scattering occurs when an electric field propagates through non homogenous regions. An inverse problem can be formulated where the dielectric properties of a tissue is approximated based on how close it's electromagnetic scattering matches the experimental values. In this talk, we propose an inverse problem where the differential evolution genetic algorithm would be used to compute the optimal dielectric parameter value of the non-homogenous regions. The objection function will solve Maxwell's equations based on estimated parameters, and compute how close it resembles the experimental values. This method will be extended into testing the ability of eddy currents to distinguish tissues with varying parameters, and its results will be discussed.

Joint work with Dong Liang and Hongmei Zhu, York University.