New geometric and numeric tools for the analysis of differential equations

Aug 13 - Aug 15, 2010

Programme

Eating

Coffee Breaks (included in the workshop): As per daily schedule, 2nd floor lounge, Corbett Hall

Meals (included in the workshop): Vistas main dining room, 4-th floor Sally Borden Building (breakfast buffet: 7:00-9:30am; lunch buffet: 11:30am-1:30pm; dinner buffer: 5:30-7:30pm).

Other (user pays) food venues: At the Banff Centre these include: Gooseberry's Deli, located in the Sally Borden Building; the Maclab Bistro, located on the first floor of the Kinnear Centre. There are also plenty of restaurants and cafes in the town of Banff, a 10-15 minute walk from Corbett Hall.

Meeting Rooms

All lectures are held in Max Bell 159. LCD projector, overhead projectors and blackboards are available for presentations

Note that the meeting space designated for BIRS is the lower level of Max Bell, Rooms 155-159. Please respect that all other space has been contracted to other Banff Centre guests, including any Food and Beverage in those areas.

** 2-day workshops are welcome to use BIRS facilities (2nd Floor Lounge, Max Bell Meeting Rooms, Reading Room) until 15:00 on Sunday, although participants are still required to checkout of the guest rooms by 12 noon. There is no coffee break service on Sunday afternoon, but self-serve coffee and tea are always available in the 2nd floor lounge of Corbett Hall. **

Changes (August 9, 2010)

Slight changes in the user pays venues; Schedule (Zeng and Hauenstein's talk times have been swapped); JF Williams abstract is added; Poster titles and book display titles have been added.

A final printed version of the programme will be available at the conference on Friday, August 13.

Changes (August 13, 2010)

Posters by Wenui Hao (Notre Dame) and Benson Muite (University of Michigan) added.

Friday

4:00 pm	Check-in begins (Front Desk - Professional Development Centre - open 24 hours) Lecture rooms are available after 4:00 pm
5:30 - 7:30 pm	**Dinner in Vistas main dining room, 4-th floor Sally Borden Building**
7:30 pm	Informal Reception in 2nd floor lounge, Corbett Hall (snacks provided)

Saturday **Schedule**

7:00-8:30 am	**Breakfast in Vistas main dining room, 4-th floor Sally Borden Building**
8:25-8:30	Opening Remarks: Greg Reid
8:30-9:00	Brynjulf Owren: Integral preserving numerical integrators for PDEs
9:00-9:30	Peter Hydon: Tools for preserving conservation laws
9:30-10:00	Jukka Tuomela: Numerical solution of overdetermined PDEs
10:00-10:30	**Coffee Break**, 2nd floor lounge, Corbett Hall
10:30-11:00	Melvin Leok: Discrete Hamiltonian variational integrators & discrete Hamilton-Jacobi theory
11:00-11:30	**Poster Session I (outside Max Bell 159)**
11:30-12:00	Elena Celledoni : Energy preserving integrators
12:00-1:30	**Lunch in Vistas main dining room**
1:30-2:00	JF Williams: Scale-invariant adaptivity for PDEs with finite time blow up
2:00-2:30	Silvana Ilie: Adaptivity for one-step numerical methods for differential equations
2:30-3:00	**Coffee Break**, 2nd floor lounge, Corbett Hall
3:00-3:30	Theodore Kolokolnikov: Solving singular boundary value problems with very thin layers
3:30-4:00	**Poster Session II (outside Max Bell 159)**
4:00-4:30	Olivier Verdier: Reduction procedures for constrained linear PDEs
5:30 - 7:30 pm	**Dinner in Vistas main dining room**

Sunday **Schedule**

7:00-9:00 am	**Breakfast in Vistas main dining room**
8:30-9:00	Jonathan Hauenstein: Regeneration and differential equations
9:00-9:30	Charles Wampler: Mechanism mobility and a local dimension test
9:30-10:00	Zhonggang Zeng: Subspace Strategy for Solving Polynomial Problems
10:00-10:30	**Coffee Break**, 2nd floor lounge, Corbett Hall
10:30-11:00	Greg Reid: The numerical geometry of differential equations and applications
11:00-11:30	Andrew Sommese: Zebra Fish, Tumor Growth, and Numerical Algebraic Geometry **Checkout by 12 noon**
12:00-1:30	**Lunch in Vistas main dining room**

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Abstracts
(in alphabetical order by speaker surname)

Speaker: **Elena Celledoni** (Department of Mathematical Sciences, Norwegian University of Science and Technology)
Title: *Energy preserving integrators*
Abstract: Geometric integration of differential equations has received a lot of interest over the past decade. This talk will be concerned with numerical integrators that preserve first integrals of differential equations exactly, in particular energy-preserving integrators. The preferred method to preserve first integrals of differential equations is the Discrete Gradient Method. This method relies on the construction of a so-called discrete gradient of the first integral, and requires the user to know and input the first integral to be preserved. The average vector field method is an integration method which belongs to this class but also to the class of so-called B-series methods. These are methods which have an associated Lie algebra of energy-preserving linear combinations of elementary differentials, much like symplectic B-series methods have an associated Lie algebra of Hamiltonian linear combinations of elementary differentials. We have characterized the linear subspaces of energy-preserving (EP) and Hamiltonian modified vector fields which admit a B-series, their finite-dimensional truncations, and their annihilators. We have also studied the manifolds of B-series conjugate to Hamiltonian and conjugate to energy-preserving.

Speaker: **Jonathan Hauenstein** (Department of Mathematics, Texas A&M University)
Title: *Regeneration and differential equations*
Abstract: One way to study biological models is to discretize the system of differential equations and solve the resulting polynomial system. These large-scaled polynomial systems may have fewer solutions than their total degree root, but are often too large to use traditional polytope methods. Regeneration can solve such large-scale polynomial systems by algorithmically revealing the underlying structure of the polynomial system during the equation-by-equation solving process. After describing regeneration, we will apply it to polynomial systems arising from biological applications.

Speaker: **Peter Hydon** (Department of Mathematics, University of Surrey)
Title: *Tools for preserving conservation laws*
Abstract: Although conservation laws of partial differential equations (PDEs) have a cohomological origin, there is a well-established procedure for determining them without reference to cohomology. The key is to find inequivalent characteristics of conservation laws by solving a linear PDE. This method relies on two fundamental aspects of differentiation, namely the product and chain rules.

Suppose that one wishes to construct a finite difference approximation that preserves several conservation laws of a given PDE. (Preserving only one is too easy!) The most obvious approach is to try to preserve characteristics. But this leads to an apparent impasse: difference (and shift) operators obey neither the product rule nor the chain rule. So is it possible to characterize (uniquely) a conservation law of a difference equation? If so, does such a characterization enable one to preserve multiple conservation laws of the original PDE?

Speaker: **Silvana Ilie** (Department of Mathematics, Ryerson University)
Title: *Adaptivity for one-step numerical methods for differential equations*
Abstract: We consider the problem of adaptivity for one-step numerical methods for differential equations,

with a view to constructing meshes of minimal computational cost. We describe a recent realistic computational complexity model for numerical differential equation solving. The focus is on the numerical solution of IVP and BVP for ordinary differential equations with local error control, as well as on the numerical solution of IVP for differential algebraic equations with defect control. In the new setting, we compare the cost of adaptive meshes with the cost of using non-adaptive meshes and show that the efficiency gain due to adaptivity may be arbitrarily high. Future research directions will also be discussed.

This is joint work with Gustaf Söderlind, Rob Corless and Greg Reid.

Speaker: **Theodore Kolokolnikov** (Department of Mathematics and Statistics, Dalhousie University)
Title: *Solving singular boundary value problems with very thin layers*
Abstract: A singular boundary value problem is an ODE that depends on a small parameter epsilon which premultiplies the highest derivative. Such problems typically contain thin boundary layers that are diffucult to resolve numerically for small values of epsison. Usually, a straighforward formulation using the standard collocation code with adaptive gridding – such as Maple's dsolve – is able to resolve the layer for (say) $\varepsilon = 0.01$. However, a standard formulation becomes hopless for (say) $\varepsilon = 10^{-5}$, because the number of meshpoints becomes huge. In this talk, I present several test problems of this type. I then show how I was able to obtain a numerical solution even with $\varepsilon = 10^{-6}$, using only 50 meshpoints.

Speaker: **Melvin Leok** (Department of Mathematics, University of California, San Diego)
Title: *Discrete Hamiltonian Variational Integrators and Discrete Hamilton-Jacobi Theory*
Abstract: We consider the continuous and discrete-time Hamilton's variational principle on phase space, and characterize the exact discrete Hamiltonian which provides an exact correspondence between discrete and continuous Hamiltonian mechanics. This approach also yields a discrete Hamilton-Jacobi theory, which may provide an alternative characterization of discrete integrable systems.

The variational characterization of the exact discrete Hamiltonian naturally leads to a class of generalized Galerkin Hamiltonian variational integrators, which include the symplectic partitioned Runge-Kutta methods. This generalization allows for the construction of Galerkin variational integrators even when the Hamiltonian is degenerate, and there is no corresponding Lagrangian formulation of the dynamical system. The appropriate notion of group invariance for discrete Hamiltonians is introduced, and this leads to a discrete Noether's theorem.

Speaker: **Brynjulf Owren** (Department of Mathematical Sciences, Norwegian University of Science and Technology)
Title: *Integral preserving numerical integrators for PDEs*
Abstract: We consider partial differential equations that can be written in the form

$$u_t = \mathcal{D}\frac{\delta\mathcal{H}}{\delta u} \tag{1}$$

where $\mathcal{H}[u]$ is a first integral for example a Hamiltonian functional, and $\mathcal{D}$ is a skew-adjoint operator which may depend on u, but not necessarily define a Poisson bracket. A fundamental type of numerical time integrator for (1) is one that preserves $\mathcal{H}$ exactly for all times, and its construction is well-known. These type of scheme is usually implicit, and a consequence of this is that one needs to solve an algebraic system exactly (or the machine precision) in every time step in order to maintain the preservation of $\mathcal{H}$. For this reason, we shall here propose a procedure which will, in the case that $\mathcal{H}$ is an integral of a polynomial function in u, result in a scheme that is only linearly implicit. This means that the solution of one linear system in each time step succes to obtain a conservative scheme.The procedure is based on a polarization technique, in which $\mathcal{H}$ is replaced by a multivariate function $\mathcal{H}$ such that $\mathcal{H}[u] = H[u;\ldots;u]$. We investigate how the invariance of $\mathcal{H}$ under the cyclic group of permutations, not only ensures that the resulting integrator is conservative, but also that its formal order of consistency is at least two.

Finally we shall comment on the spatial discretization of the PDE and consider the discrete Euler-Lagrange operator for the new procedure and its properties.

Speaker: **Greg Reid** (Applied Mathematics Department, University of Western Ontario)
Title: *The numerical geometry of differential equations and applications*
Abstract: This talk is about stable numeric-geometric methods for general systems of differential equations with constraints (so-called differential-algebraic equations or DAE, or more generally partial differential algebraic equations or PDAE).

There are software packages that support high-level physics-based modeling and simulation. One of the latest is MapleSim based on the mathematical manipulation language Maple which allows you to build component diagrams that represent physical systems in a graphical form. Models are automatically generated by dragging and dropping components from menus. In particular this software automatically generates model differential equations with constraints (so-called differential-algebraic equations or DAE on manifolds) . The simulations include striking 3 D videos of mechanisms arising in electro-mechanical modeling. Unlike other approaches MapleSim enables the equations to be treated in analytical form.

Determination of constraints for DAE and PDAE is needed for the determination of consistent initial conditions and the numerical solution of such systems. This talk will concentrate on introduction of concepts from the (Jet) geometry of differential equations, illustrated by visualizations and simple examples.

This talk will be an introduction to stable numerical methods for such general systems. The corresponding problem for the non-differential case, that of approximate polynomial systems, has only recently been given a solution, through the works of Sommese, Wampler and others. The new area called numerical algebraic geometry, will also be described. Key data structures are certain witness points on jet manifolds of solutions, computed by stable homotopy continuation methods.

Speaker: **Andrew Sommese** (Department of Mathematics, University of Notre Dame)
Title: *Zebra Fish, Tumor Growth, and Numerical Algebraic Geometry*
Abstract: Problems of central importance in engineering and science often lead to systems of partial differential equations, for which the only hope of solution is to compute numerical solutions. Often the systems are intrinsically nonlinear with several solutions corresponding to the same set of physical conditions. Discretizations of such systems of differential equations often lead to large systems of polynomial equations whose solutions correspond to potential solutions of the system of differential equations. These naturally arising polynomial systems are well beyond the pale of systems previously investigated in numerical algebraic geometry.

This talk will describe some of the recent work of Wenrui Hao, Jonathan Hauenstein, Bei Hu, Yuan Liu, Timothy McCoy, Yong-Tao Zhang, and myself in successfully solving such systems.

Following an overview of homotopy continuation methods and what they allow us to compute, I will discuss two applications to numerical solution of partial differential equations.

The first is our work on finding steady state solutions of a reaction-diffusion model on zebrafish dorsal-ventral patterning. Here, using a new approach we found seven solutions with the boundary conditions, of which three are stable: only stable solutions have meaning in the physical world.

The second is our work on the solution of several models for tumor growth. Here the boundary of the tumor is the most important part of the solution: the goal is to solve this free boundary problem as mu, a parameter of the model called the "tumor aggressiveness factor," varies. There is a family of easily computed radially symmetric solutions, which, for certain discrete values of mu, meets branches of solutions that are not radially symmetric away from the point where the branches meet. The problem is to compute the solutions on the nonradial branch. There are no standard ways of solving this sort of free boundary problem for any but very small distances from the radial solutions. Our successful solution of this problem required a new approach that came to grips with some of the numerical algebraic geometry underlying systems of several thousand polynomials in a like number of variables.

Finally, I will also discuss the direction this research is going.

Speaker: **Jukka Tuomela** (Department of Physics and Mathematics, University of Eastern Finland)
Title: *Numerical solution of overdetermined PDEs*
Abstract: The standard numerical software for the solution of differential equations is designed for the

case where there are as many equations as unknowns (square systems). In the overdetermined case (when the system has constraints) many different approaches have been proposed for various models. Here I will present a new framework which can be useful in many different situations. The idea is to use the compatiblity operator associated to the given overdetermined system. This permits the return to square systems and then the standard finite elements can again be used, and at the same time the relevant constraints are taken into account. The approach is fairly constructive, although it seems that several questions related to the computation of the compatibility operator (and more generally to compatibility complex) are quite open. I will illustrate the approach with the Stokes problem and a microfluidic system.

Speaker: **Olivier Verdier** (Department of Mathematical Sciences, Norwegian University of Science and Technology)
Title: *Reduction procedures for constrained linear PDEs*
Abstract: In order to solve a saddle point problem, like the Stokes equation, one has to make sure that the chosen functional spaces fulfill a condition called the "inf-sup" condition. I will show how this may be generalized to arbitrary constrained linear PDEs, like elastodynamics, and some "mixed" formulations of the Poisson problem. The essential idea is that one may progressively remove the constraints, each such step being called a reduction. Reductions occur in two flavors: "observation" and "control" type. In order for each reduced system to be equivalent to the original system, some compatibility conditions must be fulfilled. In the saddle point problem case, two reductions are necessary, and the compatibility conditions exactly reduce to the standard inf-sup condition. I will also discuss how Galerkin methods may be applied to solve such general constrained problems.

Speaker: **Charles Wampler** (General Motors Research and Development Center, Warren, MI and Department of Mathematics, University of Notre Dame)
Title: *Mechanism mobility and a local dimension test*
Abstract: The mobility of a mechanism is the number of degrees of freedom (DOF) with which it may move. This notion is mathematically equivalent to the dimension of the solution set of the kinematic loop equations for the mechanism. It is well known that the classical Gruebler-Kutzbach formulas for mobility can be wrong for special classes of mechanisms, and even more refined treatments based on displacement groups fail to correctly predict the mobility of so-called "paradoxical" mechanisms. This article discusses how recent results from numerical algebraic geometry can be applied to the question of mechanism mobility. In particular, given an assembly configuration of a mechanism and its loop equations, a local dimension test places bounds on the mobility of the associated assembly mode. This is joint work with Jon Hauenstein and Andrew Sommese.

Speaker: **JF Williams** (Department of Mathematics, Simon Fraser University)
Title: *Scale-invariant adaptivity for PDEs with finite time blow up*
Abstract: This talk will describe scale-invariant adaptive strategies in both time and space for the reliable resolution of finite-time singularities arising in evolutionary PDE. Both strategies are based on preserving the underlying symmetries of the physical PDE. Examples in one, two and three dimensions of both exact and asymptotic similarity will be presented as well as a difficult case where nothing seems to work. This is joint work with CJ Budd.

Speaker: **Zhonggang Zeng** (Department of Mathematics, Northeastern Illinois University)
Title: *Subspace Strategy for Solving Polynomial Problems*
Abstract: Matrix computation is essential in numerical solution of many polynomial problem such as computing GCD, factorization and dual spaces. When the number of indeterminates of the multivariate polynomials increases, the computational difficulty can escalate to a prohibitive level due to huge dimensions of the underlying vector spaces. In this talk, we elaborate the subspace strategies for reducing the matrix sizes in large scale problems, particularly the fewnomial subspace strategy for GCD finding and the closedness subspace technique for computing dual spaces. The algorithms incorporating such strategies can improve computing efficiency hundreds of times.

Posters
(in alphabetical order by surname; presenter's are asterisked with a *)

Philippe Gaudreau*, Richard M. Slevinskyz and Hassan Safouhiz, (Mathematics, University of Alberta)
Computation of Tail Probability Distributions via Extrapolation Methods

Wenrui Hao*, (Mathematics Department, University of Notre Dame)
A free boundary problem modeling tumor growth

C. Klein, B.K. Muite*, K. Roidot, (Mathematics Department, University of Michigan)
Numerical Study of the Davey Stewartson System

Austin Roche*, (Maplesoft)
A New Method for Functional Decomposition of Rational Invariants, and the Solution of Abel's Differential Equation via the Equivalence Method

Richard M. Slevinskyz* and Hassan Safouhiz, (Mathematics, University of Alberta)
New formulae for higher order derivatives and applications

Paranai Vasudev* and Hassan Safouhiz, (Mathematics, University of Alberta)
Nuclear Magnetic Resonance Parameters for Molecules

Carl Wulfman*, (Physics, University of the Pacific)
Recently Recognized Physical Consequences of The SO(4,2) invariance of Maxwell's Equations

Yang Zhang*, (Mathematics, University of Manitoba)
Computing normal forms of quaternion matrices

Book Display
(in alphabetical order by surname; presenter's are asterisked with a *)

George Bluman* (Mathematics, University of British Columbia), **Alexei Cheviakov** (Mathematics, University of Saskatchewan) and **Stephen Anco*** (Mathematics, Brock University)
Applications of Symmetry Methods to Partial Differential Equations

Peter Hydon* (Mathematics, University of Surrey)
Symmetry Methods for Differential Equations

Elizabeth Mansfield (Mathematics and Statistics, University of Kent)
A Practical Guide to the Invariant Calculus

Andrew Sommese* (Mathematics, Notre Dame) and **Charles Wampler*** (Notre Dame and General Motors)
The numerical solution of systems of polynomials arising in engineering and science

Carl Wulfman* (Physics, University of the Pacific)
Dynamical Symmetry