New geometric and numeric tools for the analysis of differential equations

Elizabeth Mansfield (Kent at Canterbury), Greg Reid (Western Ontario),
Andrew Sommese (Notre Dame), Jukka Tuomela (Eastern Finland)

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1 Summary

This meeting focused on geometrical approximation techniques and symbolic algorithms for differential equations with a particular focus on symbolic invariant calculus and discrete invariant calculus. A key goal of the meeting was to bring together researchers working at the intersection of the above areas; and highlight open problems in the development of these areas.

Remarkably for a 2 day workshop, the meeting attracted a very large number (32) of participants: 18 from Canada, 9 from the US and 5 from Europe. We had 3 undergraduates attend who gave well received posters. In an email after the meeting one told us that they had decided to continue to graduate research based on their experience. Another 4 in attendance were either PhD students or Postdoctoral fellows.

We mention some highlights of the presentations. Brynjulf Owren's (Trondheim) talk focused on a general framework for geometrical integrators for PDE. Most existing work has focused on ODE. Jonathan Hauenstein's (Field's PDF) presentation gave the first extensions of numerical algebraic geometry, an exciting emerging area, to the computation of non-unique equilibrium solutions for certain reaction diffusion systems. Conventional BVP techniques require initial guesses close to solutions - the new homotopy methods stably find all such solutions. Peter Hydon's (Surrey) talk gave algorithms for the computation of conservation laws for difference equations, essential for applications to numerics. Melvin Leok (UCSD) characterized the exact discrete Hamiltonian which provides an exact correspondence between discrete and continuous Hamiltonian mechanics, yielding a discrete Hamilton-Jacobi theory providing a new approach for discrete integrable systems. Olivier Verdier (PDF, Trondheim) described reduction procedures for arbitrary constrained linear PDE through generalizing a function space approach fulfilling an *inf-sup* condition to the constrained case. His examples included elastodynamics, and some "mixed" formulations of the Poisson problem, together with subsequent application of Galerkin methods. Greg Reid described new developments in numerical Jet geometry, where jet manifolds of constrained differential systems are efficiently represented using witness points computed using numerical algebraic geometric techniques.

Despite a fairly dense schedule the talks were well attended and energetic discussion generated. A poster session was also well subscribed; as well as a book display. We, the organizers felt that the schedule was too dense, and that a 5 day format would have been more appropriate. Feedback from participants was very positive, especially from an enthusiastic group of undergraduates from Alberta. Strong participation from industry included Elena Shmoylova (Maplesoft) and Charles Wampler (General Motors) who spoke on a numerical local dimension test to compute the mobility of mechanisms.

In conclusion the meeting was very successful, driven partly by the rapid developments, and the enthusiastic response from participants.

2 Overview and Recent Developments in the Field

Our workshop proposal was prompted by remarkable recent progress in three areas in the geometric analysis of differential equations:

1. Geometrical Approximation Techniques
2. Symbolic Invariant Calculus
3. Discrete Variational Calculus

These topics are united under the umbrella of effective algorithmic algebraic-geometric approaches. Geometry, viewed as the study of group actions and their invariants, pervades all three. The aim of the workshop is to promote interaction between researchers from these areas, and to make progress on the many open problems that lie at their intersections. Computer implementation of methods is an important sub-theme of the workshop.

The basic idea behind these approaches is that geometric objects characterize various properties of differential equations. However, to study these properties in a constructive way we must first formulate the problem in algebraic terms and then try to solve the corresponding algebraic problem. In non-trivial situations this in turn requires the use of intensive symbolic and numeric computation.

3 Recent Developments and Open Problems

This new approach leads for example to applications of Lie group integrators for numerical schemes that guarantee the solution remains on the manifold of the Lie group. This is vital for geometric integrators such as those used in computer graphics where the animation needs to emulate the correct physics in order to be convincing. This would significantly extend the existing work on geometric integration pioneered by Iserles, Budd, Hairer and others (e.g. see [1]).

The deep connections between symmetries and conservation laws constitute the relationship between symbolic invariant calculus and variational calculus. The importance of variational principles in finite element techniques has prompted the recent development of discrete variational and discrete exterior calculus, and its related homological constructions. Our focus on unification of geometric and numeric methods means that variational calculus and its discrete formulations are of particular interest to us, and another of the three main areas of the workshop. There are several related major advances here. One is the seminal work of Douglas Arnold and his collaborators, in the construction of numerically stable "compatible discretisations" for the finite element method. Finally there are several important recent applications of the discrete variational formulations, such as Leok's application of such methods to the Schrödinger Equation.

While algebraic methods are powerful and provide an algorithmic foundation for manipulations on the underlying manifolds, in each of the areas and applications above, they are not stable when applied to the approximate data that usually accompany real applications. Thus the other ingredient of our workshop, which addresses this issue, will be the new area of Numerical Algebraic Geometry. In this area solution sets of polynomial systems are represented stably by certain approximate (witness) points, which are efficiently computed by homotopy continuation methods. This topic was pioneered by Sommese, Verschelde and Wampler (with the first book on the subject by Sommese and Wampler [2]. Their work builds on previous work on homotopy methods and the computation of isolated solutions of polynomial systems by Allgower, Georg, Li, Morgan, Shub, Smale and others. Numerical algebraic geometry provides the first stable approximate version of algebraic geometry that deals with positive dimensional solution sets. Previous unsuccessful attempts had been more or less literal translations of exact approaches resulting in seriously unstable computations.

Objectives

The aim of the workshop is to foster interaction between mathematicians, engineers, and scientists working with algorithmic geometrical methods for differential equations at the intersection of the three areas: geometrical approximation techniques; symbolic invariant calculus; discrete variational and discrete exterior calculus. A key motivation underlying the objectives of the workshop is that problems from applications are now big enough and the inputs have enough numerical error that methods are needed that take full advantage of the geometry with the numerics always in sight. Symbolic tools should be used to the extent they can be, but in the end we need to develop tools that address problems that actually arise.

The expected outcomes include significant progress on creation and development of new algorithmic tools for the geometric analysis of differential equations and their approximations. Specific goals of the workshop include sharing progress made, open problems, and technical set-ups, with a view to developing or applying tools that utilize the best ideas in the three areas. In particular the specialists of each subtopic will learn of the techniques and software being developed in other areas which will help them to tackle overlapping facets of the common problems.

The relevant technical background comes from numerical algebraic geometry, algorithmic algebraic geometry, differential algebra, symbolic invariant calculus, moving frames, and invariantization methods. The growing common realization that nontrivial computational advances in the above sub-areas, requires a combination of geometrical and numerical techniques, has already prompted initial contacts between people working in the above sub-areas. While many conferences and workshops have considered geometric analysis of differential equations, and discrete exterior and variational calculus, none have considered them all with an underlying theme of approximation using numerical algebraic geometry.

The unique combination of themes exposes many new open problems and has a high potential for important breakthroughs. As examples we can cite combining Lie group integrators with numerical applications of moving frames; combining discrete variational methods with discrete exterior calculus in the context of Finite Element Methods; using Numerical Algebraic Geometry to characterize singular orbits of group actions and special solutions of PDE; determining hidden constraints and compatibility conditions using numerical approaches.

4 Further presentation highlights

Andrew Sommese (Notre Dame) gave an overview of Numerical Algebraic Geometry in his talk with applications on striping for Zebra fish and tumor growth models. Existing techniques only find highly symmetric tumors while the new homotopy techniques search for all solutions. In order to do this one must be able to analyze systems of thousands of nonlinear equations in thousands of variables. This is possible using a new technique called *Regeneration*. The standard numerical software for the solution of BVP for PDE is designed for the case where there are as many equations as unknowns (square systems). Jukka Tuomela presented a new framework for over-determined BVP based on using the compatiblity operator and the compatibility complex associated to the given overdetermined system. This permits the return to square systems and then standard finite elements can again be used, and at the same time the relevant constraints are taken into account. Promising numerical results were obtained for the Stokes problem and a microfluidic system. Tuomela also described open problems related to the algebraic computation of compatibility operators. Elena Celledoni (Norwegian University of Science and Technology) presented a new class of numerical methods for Hamiltonian systems that preserve an input first integral exactly.

Young faculty members Silvana Ilie (Ryerson), JF Williams (SFU) and Theodore Kolokolnikov (Dalhousie) gave well-received talks. In particular Ilie discussed geometric adaptivity that rigorously establishes polynomial cost numerical methods for constrained differential systems and scale-invariant adaptive geometric integrators for PDE with finite time blow up. B.K. Muite from the University of Michigan presented a poster *Numerical Study of the Davey Stewartson System* using geometric integration.

We even had some undergraduates attend the meeting, and contributed posters. One of them emailed us after the meeting to let us know that the positive experience had inspired him to continue to apply to grad school. New PhD student Austin Roche (Maplesoft) presented a poster on an equivalence method for functional decomposition of invariants and the Solution of Abel's equation. PhD student Wenrui Hao (Notre Dame) presented a poster on *A free boundary problem modeling tumor growth* using Numerical Algebraic Geometry. An enthusiastic group of undergraduates Paranai Vasudev, Philippe Gaudreau and Richard Slevinskyz from the University of Alberta presented some excellent posters (see the programme). Carl Wulfman and Yang Zhang (Manitoba) presented well received posters. A lively book display was also given with most of the authors in attendance [3], [2], [4] provided some good background material for the conference.

References

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[2] A. J. Sommese and C. W. Wampler, The Numerical Solution of Systems of Polynomials Arising in Engineering and Science World Scientific (2005).

[3] G. Bluman, A. Cheviakov and S. Anco, Applications of Symmetry Methods to Partial Differential Equations, *Springer*, (2010).

[4] E. Mansfield, A Practical Guide to the Invariant Calculus, CUP (2010).