Timetable

The pattern of the symposium was Short Courses in the morning, with the Specialist and Main Speakers in the afternoon. The courses were divided into three general subject areas,

- geometric numerical methods
- symplectic methods
- integrable, symmetry methods

for the purpose of balancing the programme. A course from each of the three series ran every day.

	Fri 14	Sat 15	Sun 16	Mon 17	Wed 19	Thurs 20	Fri 21	Sat 22	Sun 23
09:20-10:05	Budd	Budd	Budd	McLachlan	McLachlan	McLachlan	Hairer	Hairer	Owren
10:15-11:00	Olver	Olver	Olver	Hydon	Hydon	Hairer	King	King	King
				Morning	**Tea**				
11:20-12:05	Leimkuhler	Leimkuhler	Hydon	Lewis	Lewis	Lewis	Zanna	Zanna	Zanna
12:15-1:00	Clarkson	Clarkson	Leimkuhler	Clarkson	Lubich/Iserles	Kozlov/Roubtsov	Reich	Reich	Reich
				Lunch					
3:20-3:40	Karasozen	Wensch	Marletta	Murua	Bila	*********	Iserles	Munthe-Kaas	
3:45-4:30	Van Vleck	Huang	Roulstone	Ablowitz	Quispel	**Afternoon**	Chu	Reid	
				Afternoon	**Tea**	*********			
5:00-5:20	Engo	Cano	Kuznetsov	Titi	Mansfield	**Excursion**	Celledoni	Hauser	
5:25-6:10		West/Athorne	Cullen/Dorodnitsyn	Wolf/Udriste	Stoffer/Janezic	*********	Blanes/Casas	Bloch/Pekarsky	

LONDON MATHEMATICAL SOCIETY
DURHAM SYMPOSIUM

GEOMETRIC INTEGRATION

13th–23rd July 2000

University of Durham

ABSTRACTS FOR SPECIALIST TALKS

Chaotic dynamics of modulational instability in water waves

MARK ABLOWITZ

Modulational instability in water waves is a well known phenomena, having been discovered by Benjamin and Feir over 30 years ago. Recent experiments and analytical and computational results have demonstrated that in certain parameter regimes the experiments are not reproducible and the dynamics are temporally irregular/chaotic. This phenomena is similar to that found in computational chaos and is expected to arise in other physical problems; e.g nonlinear optics.

Symmetry Reductions for the Monge–Ampère–Tzitzeica Equations

NICOLETA BÎLĂ, C. Udrişte

We apply the classical Lie method of infinitesimal transformations and the nonclassical method to the Monge–Ampére–Tzitzeica equations. One makes the connection with the direct method for several results. One finds again the symmetry groups of the homogeneous Monge–Ampèr–Tzitzeica equations, the Tzitzeica surfaces equation, the elliptic Monge–Ampère–Tzitzeica equation and hyperbolic Monge–Ampère–Tzitzeica equation. In order to apply the classical method, some of these results are verified by using the LIE Program for analysis of partial differential equations in IBM type PCs. We shall restrict ourselves to determining nonclassical symmetries, which arise from the vector field $X = \partial_x + \eta\partial_y + \phi(\eta)\partial_u$, where the component $\eta = \eta(x, y)$ is a solution of the Monge equation. This allows us to write certain solutions of particular Monge–Ampère–Tzitzeica PDEs as solutions of a first order PDEs system. We find again the general solution of the homogeneous Monge–Ampère–Tzitzeica PDE, given by Fairlie and Lznov and a new class of solutions for the hyperbolic Tzitzeica PDE. One constructs a class of Monge-Ampère-Tzitzeica PDE which is invariant under the considered nonclassical symmetries.

Optimising geometric integrators for time-dependent linear differential equations

SERGIO BLANES, F. Casas and J. Ros

Some *Geometric Integrators* for time-dependent linear differential equations are considered: Magnus, Fer, Cayley and splitting technique. The efficiency of each method will depend on the problem as well as on its implementation. In order to build competitive methods it is important to optimise the number of evaluations of the time-dependent part as well as to simplify the method in terms of matrix operations (for reducing CPU time). These tasks can be done separately for each method. However, considering that the Magnus series has been widely studied and optimised as a numerical method, we will see how all other methods can be easily optimised simply by considering their relation with Magnus. This procedure can be used for optimising other methods and also for solving time-dependent non-linear differential equations. Some numerical examples showing the performance of these algorithms will be presented.

The Symplectic Structure and Integration of the Symmetric Rigid Body Equations.

ANTHONY BLOCH

In this talk I will various aspects of the geometry and dynamics of the smooth and discrete symmetric rigid body equations. The symmetric rigid body equations are a form of the rigid body equations on the cross of orthogonal groups. I will discuss the symplectic structure on this space and relationship of this system with the standard generalized rigid body systems. In addition I will discuss a discretization of the equations and its relationship with the Moser-Veselov equations. I will also discuss integrability. This is joint work with P. Crouch, J. Marsden and T. Ratiu.

Geometric Integrators with Processing

FERNANDO CASAS, Sergio Blanes and José Ros

In this communication we analyze the processing technique in the context of geometric integration of ordinary differential equations. More specifically, we consider numerical methods defined by $e^P e^{hK} e^{-P}$ in which the kernel e^{hK} and the processor e^P are both compositions of basic first or second order geometric integrators. Conditions for achieving effective order up to 12 are explicitly obtained when the basic method is self-adjoint. In addition, it is shown that the minimum truncation error attained by processing is determined uniquely by the kernel.

Several situations are considered: (i) when the vector field associated with the ordinary differential equation can be split into two parts, $X = A + B$, whre the vector fields A and B can be integrated exactly; (ii) when the splitting satisfies an RKN-type condition, and (iii) in a near-integrable case, i.e., when $X = A + \epsilon B$ and $\epsilon \ll 1$. The resulting high-order geometric integrators with processing are found to be more efficient than other non-processed composition schemes of the same order. This gain in efficiency is mainly due to the important reduction in the number of function evaluations required by the algorithms.

Numerical integration of odes on the Stiefel and Grassman manifolds

ELENA CELLEDONI and Brynjulf Owren

The problem of computing the numerical solution of ODEs on Stiefel and Grassmann manifolds arises in a variety of applications. The Stiefel manifold for example is a homogeneous space whose elements can be represented by $n \times p$ matrices with orthogonal columns. The naive application of a Lie group integrator to ODEs on the Stiefel manifold gives rise to computations of order n^3 complexity, that by careful implementation might be reduced to n^2p. Even lower complexity can be however achieved using projection methods, in which the orthogonality if not preserved is in any case recovered. In this talk we will address the problem of constructing intrinsic numerical integrators preserving orthogonality with complexity of order np^2. The case of more general homogeneous spaces is also considered.

Evolution of Lax Dynamics and Its Applications

MOODY CHU

The notion of differential geometry is known to have played a fundamental role in unifying aspects of the physics of particles and fields, and have completely transformed the study of classical mechanics. Later on it is found to play an even larger role in control theory, robotics and computer vision. Recently an exciting connection between dynamical systems on manifolds and numerical algorithms has also been unveiled. Some major catalysts of the latest development include the classical work of Symes showing that there is a close link between the QR algorithm and the Toda lattice flow, the geometric setting by Bayer and Lagarias describing the interior point methods for linear programming and Karmarkar's algorithm in the context of smooth dynamical systems, and the seminal work by Brockett relating a number of finite automata to a smooth flow defined by the so called double bracket equation. Many of these differential system can be expressed in the so called Lax form. It has been observed that in some cases, there are remarkable connections between smooth flows and discrete numerical algorithms. In other cases, the flow approach seems advantageous in itself for tackling very difficult problems.

In this expository talk the emphasis is on using differential equation techniques as a special continuous realization process for linear algebra problems. The matrix differential equations are cast in fairly general frameworks of which special cases correspond to important and practical iterative schemes. The main thrust then should be to study the dynamics of various flows and to propose effective numerical implementation. This approach has potential applications ranging from new development of numerical algorithms to theoretical solution of open problems. Various applications using this evolution idea will be discussed in this presentation.

Applications of geometric integration techniques to meteorological problems.

MIKE CULLEN

A theoretical analysis is given of both the 3d Euler equations, which describe the small scale strucyure of the atmosphere, and the 3d semi-geostrophic equations, which describe the large scale structure. The analysis identifies key conservation properties, which geometric integration can exploit. Evidence of deficiencies of current methods are shown. An example of benefit is given for an idealised problem.

Invariant difference model for nonlinear Schrödinger equation with conservation of Lagrangian structure.

VLADIMIR DORODNITSYN

We consider symmetry preserving difference schemes for the nonlinear Schrödinger equation

$$i\frac{\partial u}{\partial t}+\frac{\partial^2 u}{\partial r^2}+\frac{n-1}{r}\frac{\partial u}{\partial r}+u|\ u\ |^2=0,$$

where n is the number of space dimensions.

This equation describes one dimensional evolution in n space dimensions in many physical situations, including phenomena in plasma physics and nonlinear optics. We consider nonintegrable case $n \geq 2$, and construct schemes that have the same Lie group properties and Lagrangian structure, as its continuous counterpart.

Our approach is to start with Lie symmetries of a differential equation and to introduce a difference equation together with a symmetry adapted mesh by means of difference invariants in such a way that all the symmetries and Lagrangian structure of the original differential equation are preserved .

The research reported here was performed in collaboration with C.Budd.

Using the Singular Value Decomposition for the Computation of Lyapunov Exponents

RAPHAEL HAUSER

An alternative to the classical QR method for the computation of Lyapunov exponents is to use the singular value decomposition. This is interesting for example in applications where finite-time information about the blow-up behaviour of perturbations in the initial conditions of ODEs are important. Computing the SVD is more delicate than computing the QR decomposition, due to problems that arise when singular values coalesce. In this talk we are going to compare the finite-time truncation errors of both the QR and the SVD method for the computation of Lyapunov exponents, and we are going to address how the difficulties associated with the coalescence of singular values can be overcome.

Global error and highly-oscillatory ODEs: classical and Lie-group methods

ARIEH ISERLES

In this talk we revisit, re-proof and generalise a global-error formula, originally due to Peter Henrici, and demonstrate that, properly interpreted, it allows to estimate the global error of time-stepping algorithms from the knowledge of asymptotics of the exact solution and the variational equation. We apply this technique to equations of the form $y'' + g(t)y = 0$, where $g(t)$ is large and the solution oscillates very fast, to obtain very precise estimates of the envelope of the error for both classical and Lie-group solvers. We also introduce an enhancement of the Magnus expansion which is even better suited to the integration of highly-oscillating ODEs.

¿From ART to the science of Lie-group expansions

ARIEH ISERLES

The has been recently a great deal of interest in the Algebra of Rooted Trees: from "Butcher trees" in the expansion of Runge–Kutta methods, to the Sanz-Serna–Murua work on splittings, to Magnus and Cayley expansions in Lie groups, all the way to recent work of Brouder and Connes, applying this set of ideas to Hopf algebras and quantum field theory. In this talk, concerning work in progress, we present a unified framework for expansions in Lie groups (Magnus, various generalizations thereof, cayley, BCH, ...) using free graded algebras of rooted trees.

On elementary Bäcklund transformations

VADIM KUZNETSOV

We will give a general setup for constructing one- and two-point Bäcklund transformations for integrable Hamiltonian problems having 2x2 Lax matrices. Important features of the constructed maps are: (i) they are time-discretizations of some continuous flows, (ii) they are symplectic maps, (iii) they are exact discretizations, in the sense that they preserve integrals of motion of the continuous flow, (iv) they are parametrized by one or two points on the spectral curve; (v) they have the spectrality property. Because of the above properties, these maps are suitable as symplectic geometric integrators of integrable flows. Examples will include Heisenberg and Gaudin magnets, Lagrange top and Toda lattice.

On geometric integration and multiple time scales

CHRISTIAN LUBICH

A major expectation from geometric integrators is that they show better long-time behaviour than standard integrators. Backward error analysis indeed gives a sound mathematical justification to such expectations. However, it applies only when the product of the time step with the highest frequency (the CFL number) is very small, a situation that is often not met in practical computations.

Do geometric properties such as symplecticity or symmetry of the numerical scheme still yield improved behaviour for larger time steps where the CFL number is bounded away from zero?

This question is studied for a class of highly oscillatory Hamiltonian systems which includes the Fermi-Pasta-Ulam chain of alternating stiff linear and soft nonlinear springs as a prominent example. The results show, surprisingly, that

- symplecticity is unrelated to long-time near-conservation of the total energy and of adiabatic invariants;
- symplecticity is incompatible with giving the correct slow energy exchange between stiff components.

On the other hand, symmetry of the scheme is still essential and further conditions of an apparently non-geometric nature come into play.
The talk is based on recent joint work with Ernst Hairer.

Variational methods for difference equations

ELIZABETH MANSFIELD and Peter Hydon

The variational complex encodes the answers to classical questions such as, when is an equation an Euler-Lagrange equation for some Lagrangian, or when is a conservation law trivial? In this talk we show that a completely analogous complex can be constructed for difference equations and systems. A discrete Noether's theorem connecting variational symmetries and conservation laws is also presented.

Second and fourth order split integration symplectic method for Hamiltonian systems

DUŠANKA JANEŽIČ

There is growing recognition in the last few years that the symplectic integration methods are often the right way of integrating the equations of motion. Recent advances in development of the second and the fourth order split integration symplectic method (SISM) for numerical solution of the Hamiltonian system based on a factorization of the Liouville propagator are presented.

The technique, derived in terms of the Lie algebraic language, is based on the splitting of the total Hamiltonian of the system into two pieces, each of which can either be solved exactly or more conveniently than by using standard methods. The individual solutions are then combined in such a way as to approximate the evolution of the original equation for a time step, and to minimize errors.

The SISM uses an anlytical treatment of high frequency motions within a second order generalized leap-frog scheme and within a fourth order scheme. The computation cost per integration step of SISM is approximately the same as that of commonly used algorithms, and it allows an integration time step up to an order of magnitude larger than can be used by other methods of the same order and complexity. The second and the fourth order SISM have been tested on a variety of examples. In all cases the SISM posses long term stability and the ability to take larger time steps. The results also show that the fourth order SISM benefits for accuracy for small step sizes, only.

The approach developed here is general, but illustrated at present by application to the harmonic oscillator, the pendulum and the Hénon-Heiles Hamiltonians.

Cosymmetric ODEs and numerical discretization

V. Govorukhin, BULENT KARAZÖZEN and V. Tsybulin

A continuous symmetry group or a sequence of cosymmetries may be the reason for the existence of a one-paramter family of equilibria in a system of ordinary differential equations. Simple two-dimensional conservative and non-conservative model systems are integrated with several explicit and implicit Runge-Kutta methods. The preservation of symmetry and cosymmetry, the stability of equilibria, spurious cycles, basin of equilibria, stable and unstable manifolds, transition to chaos are investigated by presenting analytical and numerical results.

Conservation laws of semidiscrete Hamiltonian equations

ROMAN KOZLOV

Many evolution partial differential equations can be cast into Hamiltonian form. Conservation laws of these equations are related to one–parameter Hamiltonian symmetries admitted by the PDEs. We consider symmetries and the Noether's theorem for semidiscrete Hamiltonian equations which are obtained by space discretization of Hamiltonian PDEs. Using symmetries one can find conservation laws of these equations. Several applications are presented. They include a transfer equation and Korteweg-de Vries equation.

High Order Variational Integrators, Runge-Kutta methods, and Finite Elements

MATTHEW WEST

Variational integrators are constructed using a discrete version of Hamilton's principle of extreme action, and are automatically symplectic and momentum preserving. In this talk we explore the relationship between a continuous-time system and its variational discretizations, and we see how this leads to a very natural class of high order variational integrators.

Furthermore, using the discrete Legendre transform allows us to realize these integrators as maps on the cotangent bundle, and in this form they are a particular case of symplectic partitioned Runge-Kutta methods. From the original derivation, it is clear that such schemes can also be regarded as polynomial finite element methods in time, thus providing a link between several familiar areas.

Finally, we show that variational discretizations can be extended in a very natural way to include external forces and constrained systems. The high order integrators arising in these contexts can once again be interpreted as either constrained symplectic partitioned Runge-Kutta methods, or as constrained finite element schemes. The variational methodology provides an integrated framework for understanding and extending these integrators.

The integration of systems of linear PDEs using conservation laws of their syzygies

THOMAS WOLF

The method of computing a differential Groebner basis to bring a system of linear PDEs into a consistent form provides as a by-product identities called syzygies between the PDEs of the resulting basis. These syzygies come for free when computing the differential Groebner Basis. If either the syzygies themselves have the form of conservation laws, or if conservation laws can be computed for a system of syzygies then there is a method that uses this information to integrate PDEs in the differential Groebner basis. Apart from being completely algorithmic this method has a number of other computational advantages compared with conventional integration techniques used in computer algebra packages so far.

Special integrators in spectral theory

MARCO MARLETTA

This talk will discuss the need for special integrators in the numerical investigation of spectral properties of systems of differential equations.

We will review some of the spectral theory of selfadjoint problems, including counting functions and related differential equations on unitary groups. We will also discuss non-selfadjoint problems and explain ways in which special integrators may be used to avoid the need for Riccati systems and/or compound matrices when solving these problems. If time permits we shall also explain how singularities may cause problems for geometric integrators which they sometimes do not cause for more traditional methods.

Geometric aspects of RK methods applied to semi-explicit index-2 DAEs.

ANDER MURUA URIA

A geometric approach to the understanding of the application of implicit RK methods to index-2 DAEs in Hessenberg form is presented. We focus our attention to methods with invertible RK matrix that are not stiffly accurate, so that the numerical solution does not satisfy exactly the algebraic constraints. An invariant manifold result is presented and aspects of backward error analysis are outlined. Special attention is paid to Gauss collocation methods, which may be of special interest when some symmetry of the DAE is to be preserved.

A Lie algebraic approach to analysing the error in splitting methods

BRYNJULF OWREN

This work is motivated by observations made from numerical tests indicating that the splitting method proposed by Strang may suffer from order reduction when one of the splitting terms is a stiff vector field. Earlier work by Kozlov and Owren explains this behaviour for linear differential equations, using eigenvalue analysis. In this talk we will present a nonlinear analysis, based on calculation with Lie series and using the Lie Poisson bracket of vector fields on a manifold. We distinguish between two important cases, when the two vector fields of the splitting belong to a finite or infinite dimensional Lie algebra. The former case can be handled in a similar way as the linear case. The infinite dimensional case is both more common in applications and more challenging, but we shall see through examples that it is possible to extract useful information in many cases by use of the presented approach. In particular we will look closely at the stiff van der Pol equation.
Joint work with Roman Kozlov, NTNU

Symmetry Reduction of Discrete Lagrangian Mechanics on Lie groups

SERGEY PEKARSKY

We show that when a discrete Lagrangian $L : G \times G \to \mathbb{R}$ is G-invariant, a Poisson structure on (a subset) of one copy of the Lie group G can be defined by means of reduction under the symmetry group G of the canonical discrete Lagrange 2-form ω_L on $G \times G$. Alternatively, for the corresponding reduced discrete mechanical system on a Lie group G determined by the (reduced) Lagrangian ℓ we can define a Poisson structure via the pull-back of the Lie-Poisson structure on the Lie algebra g^* by the corresponding Legendre transform. Our main result shows that these two structures coincide and govern the corresponding discrete reduced dynamics. In particular, the symplectic leaves of this structure become dynamically invariant manifolds which are manifestly preserved under the structure preserving discrete Euler-Poincaré algorithm.

Applications of symmetric spaces and Lie triple systems in numerical analysis

REINOUT QUISPEL

Symmetric spaces can be regarded as generalizations of groups, and continuous symmetric spaces can be regarded as generalizations of Lie groups. I will start with ageneral introduction to symmetric spaces and their linearizations called Lie Triple Systems (LTS).The rest of the talk will be devoted to applications of finite-dimensional and infinite-dimensional symmetric spaces and LTS in dynamical systems and in numerical analysis. This work was done in collaboration with Antonella Zanna and Hans Munthe-Kaas.

New Differential Elimination Algorithms for Differential Systems

GREGORY REID

Differential elimination algorithms, by a finite number of differentiations, in analogy to Groebner Basis and Gauss algorithms for algebraic systems, manipulate systems of non-linear differential equations into forms with desirable properties.

A symbolic differential elimination algorithm implemented in C, which runs at speeds several orders of magnitude faster than our implementation in a general Computer Algebra System is described. It is applied to obtain new results, and critical dimension behavoir for large classes of Nonlinear Schroedinger equations. A hybrid symbolic-numeric differential elimination algorithm, using techniques from Numerical Linear Algebra, is also discussed.

Rigorous proof of chaotic behaviour in a dumbbell satellite model

DANIEL STOFFER, Urs Kirchgraber, Ulrich Manz

We consider a satellite with the shape of a dumbbell. It is composed of two equal point masses connected by a rigid massless bar. It is assumed that the motion takes place in a plane and that the size of the satellite is small compared to the distance of the satellite to (the center of) the central body. In the limit the satellite moves on a Keplerian ellipse. The orientation of the dumbbell satellite is then described by a second order time periodic differential equation. We apply a computer assisted method developed earlier to rigorously establish the existence of chaotic behaviour in the dumbbell satellite model.

Postprocessing Galerkin Methods

EDRISS TITI

In this talk we will present a postprocessing procedure for the Galerkin method which involves the use of an approximate inertial manifold to model the high wavenumbers component of the solution in terms of the low wavenumbers. This *postprocessed Galerkin method*, which is much cheaper to implement computationally than the Nonlinear Galerkin (NLG) Method, possess the same rate of convergence (accuracy) as the simplest version of the NLG, which is more accurate than the standard Galerkin method. Our results valid in the context of spectral and finite element Galerkin methods and for many nonlinear parabolic equations including the Navier-Stokes equations. We will also present some computational study to support our analytical results.
This talk is based on joint works with Bosco Garcia-Archilla and Julia Novo.

Lagrangians of First Order Produced by PDEs and Metrics

CONSTANTIN UDRŞTE, Nicoleta Bîlă

Using parametrized curves or parametrized sheets, and suitable metrics, we treat the jet bundle of order one as a semi-Riemann manifold. This point of view allows the description of solutions of DEs as pregeodesics and the solutions of PDEs as potential maps via Lagrangians of order one or via generalized Lorentz world-force laws. Implicitly, we solved a problem rised first by Poincaré: find a suitable geometric structure that converts the trajectories of a given vector field into geodesics. Further, we realize the passage from the Lagrangian dynamics to the covariant Hamilton equations.

Extrapolation methods in Lie groups

JOERG WENSCH

Considered are differential equations on Lie groups given by $y' = v(t,y)|_{y(t)}$. Here $y : \mathbb{R} \to G$ is a curve on a Lie group and and v is a map into the corresponding Lie algebra. This Lie algebra is to be interpreted as the set of right invariant vector fields. The generalisation of Runge-Kutta methods of order 3 and higher on this class of problems makes the introduction of correction functions neccessary. Here we consider the application of extrapolation methods on this class of problems. An asymptotic expansion of the global error in quadratic terms for symmetric methods is proved. The explicit midpoint rule is used as the basic method for an extrapolation algorithm. The new methods of order 4 and 6 are compared with standard extrapolation procedures of the same order.