ICMS Workshop: The future of structure-preserving algorithms.

Organisers: Franco Brezzi, Elena Celledoni, G. Reinout W. Quispel, Chus Sanz-Serna
International Centre for Mathematical Sciences, 47 Potterrow Edinburgh, EH8 9BT

	Mon	**Tue**	**Wed**	**Thur**	**Fri**
9:00	Registration Opening(9:30)	Elliott	Quispel	Iserles	Schratz
9:40	Marini	Styles	Owren	Casas	Niesen
10:20	**Coffee**	**Coffee**	**Coffee**	**Coffee**	**Coffee**
10:40	Brezzi	Budd	Riis	Kropielnicka	Offen
11:20	Licht	Awanou	Leok	Singh	Celledoni
12:00	**Lunch**	**Lunch**	**Lunch**	**Lunch**	**Lunch**
13:40	Malham	Kovács		Leimkuhler	
14:20	Blanes	Düring		Wiese	
15:00	**Coffee**	**Coffee**		**Coffee**	
15:20	Stern	Frasca-Caccia		Zygalakis	
16:00	Faou				
16:45	Wine reception				
19:00				Workshop dinner	

- The workshop dinner will take place at the Blonde Restaurant, 71-75 St Leonards Street, Edinburgh, EH8 9QR.

Book of abstracts

Gerard Awanou

Title: The second boundary value problem for a discrete Monge-Ampère equation with symmetrization

Abstract: We propose a natural discretization of the second boundary condition for the Monge-Ampère equation of geometric optics and optimal transport. For the discretization of the differential operator, we use a recently proposed scheme which is based on a partial discrete analogue of a symmetrization of the subdifferential. Existence, unicity and stability of the solutions to the discrete problem are established. Convergence results to the continuous problem are given.

Sergio Blanes

Title: On the construction of symmetric second order methods for ODEs

Abstract: I will consider the construction of explicit symmetric second order methods for solving ordinary differential equations. The proposed schemes are obtained by using simple splitting methods on an extended phase space. By construction, the schemes are symmetric and of second order allowing to recover most well known and frequently used schemes from the literature. These schemes can be used to get higher order methods by extrapolation or composition. We show how to obtain them in the general case as well as how to get Nyström methods, methods for stiff problems, Lie group integrators or symplectic integrators, but the technique can also be used to build explicit and implicit methods for many other problems.

Franco Brezzi

Title: Virtual Element Methods in domains with curved boundaries

Abstract: After a brief recall of the basic ideas of Virtual Element Methods, the case of "polygons with curved boundaries" will be treated, with some numerical examples and some discussions on pros and cons of different choices.

Bertram Düring

Title: A Lagrangian scheme for the solution of nonlinear diffusion equations

Abstract: Nonlinear diffusion equations whose dynamics are driven by internal energies and given external potentials, e.g., the porous medium equation and the fast diffusion equation, have received a lot of interest in mathematical research and practical applications alike in recent years. Many of them have been interpreted as gradient flows with respect to some metric structure. When it comes to solving partial differential equations of gradient flow type numerically, it is natural to ask for appropriate schemes that preserve the equations' special structure at the discrete level.

In this talk we present a Lagrangian numerical scheme for solving nonlinear degenerate diffusion equations in multiple space dimensions. The key ingredient in our approach is the gradient flow structure of the dynamics. For discretization of the Lagrangian map, we use a finite subspace of linear maps in space and a variational form of the implicit Euler method in time. Thanks to that time discretisation, the fully discrete solution inherits energy estimates from the original gradient flow, and these lead to weak compactness of the trajectories in the continuous limit. We discuss the consistency of the scheme in two space dimensions and present numerical experiments for the porous medium equation.

Chris Budd

Title: The Moving Mesh SISL method

Abstract: Semi-Implicit Semi-Lagrangian (SISL) discretisations are a natural way of numerically solving PDEs with advection. They have the merit over other comparable methods of not having a CFL restriction, and are widely used in numerical weather prediction. In the backwards trajectory version, as used e.g. in the Met Office's dynamical core, the trajectories for the SISL method are calculated to arrive at a given mesh, then the fields are interpolated at their departure points to solve at the new time level. Unfortunately this procedure introduces both diffusive and dispersive errors, which can increase as the computational time-step is reduced. In the first part of this talk we shall use backward error analysis to analyse the structure of the diffusive and dispersive errors ,which are present in a Semi-Lagrangian discretisation of both Burgers' equation and also the shallow water equation. By doing this, we will show that the diffusive errors are smallest when the CFL number is an integer, and the dispersive errors when it is a half integer.

Fernando Casas

Title: Composition methods for the time integration of kinetic equations

Abstract: Splitting and composition methods are by now standard numerical procedures to integrate differential equations in the realm of Geometric Numerical Integration, where preserving whatever invariants the systems has is of paramount importance. This class of schemes has also been used for the time integration of Vlasov equations appearing in the simulation of plasma physics problems. For the particular case of the Vlasov–Maxwell equation describing the time evolution of an ensemble of charged particles in a plasma together with the electric and magnetic fields generated by the particles, we propose new composition methods taking advantage of the separation of the problem into three solvable parts. The resulting schemes are fourth order accurate in time and preserve the Gauss condition exactly. In this talk we detail the construction strategy and illustrate the new schemes on some numerical examples.

Elena Celledoni

Title: Deep learning as optimal control problems: models and numerical methods

Abstract: We consider recent work where deep learning neural networks have been interpreted as discretisations of an optimal control problem subject to an ordinary differential equation constraint. We review the first order conditions for optimality, and the conditions ensuring optimality after discretisation. This leads to a class of algorithms for solving the discrete optimal control problem which guarantee that the corresponding discrete necessary conditions for optimality are fulfilled. The differential equation setting lends itself to learning additional parameters such as the time discretisation. We explore this extension alongside natural constraints (e.g. time steps lie in a simplex). We compare these deep learning algorithms numerically in terms of induced flow and generalisation ability.

Charles Elliott

Title: Evolving finite element spaces

Abstract: Time dependent finite element spaces are useful for discretising PDEs on moving meshes. Here we define an abstract concept and realisations for evolving triangulations of bulk and surface domains. The finite element spaces are constructed using isoparametic Lagrange elements. Motivation arises from PDEs on evolving domains, ALE methods and geometric equations. This is joint work with Tom Ranner.

Erwan Faou

Title: Long time behavior of small solutions to the nonlinear wave equation in arbitrary dimension, and application to numerical schemes.

Abstract: I will present some recent results obtained in collaboration with J. Bernier (Toulouse) and B. Grébert (Nantes). We consider nonlinear wave equations on a d-dimensional torus with small initial data in Sobolev space. We prove that the solution remains small and smooth over very long times. The method is to decompose the solution into low and high frequencies and use normal form analysis. The difficulty with the dimension $d > 1$ comes with the fact that the equation is more resonant than in dimension $d = 1$, and some diophantine estimates are degenerating. We will apply these technics to show that geometric numerical schemes reproduce this behaviour also beyond the usual CFL regime for generic time step.

Gianluca Frasca-Caccia

Title: Bespoke preservation of local conservation laws.

Abstract: Preserving a local conservation law of a PDE gives, in general, a stricter constraint than preserving the corresponding global invariant. Schemes able to preserve it keep this property regardless of the type of boundary conditions assigned to the problem. A new symbolic-numeric approach to develop bespoke finite difference schemes that preserve multiple local conservation laws of a PDE has been recently introduced in [1,2]. However, the effectiveness of this approach has been limited by the complexity of the symbolic computations. Some key simplifications that made the approach practical and efficient for PDEs with polynomial nonlinearity have been introduced in [3,4,5]. Alternatively the symbolic-numeric strategy above can be efficiently applied for obtaining a semidiscretization of the PDE having semidiscrete conservation laws. The integration in time can be done through a suitable ODEs integrator that preserves the fully discrete local conservation laws.

[1] T. J. Grant. LMS J. Comput. Math. 2015.

[2] T. J. Grant, P. E. Hydon. Found. Comput. Math. 2013.

[3] G. Frasca-Caccia, P. E. Hydon. IMA J. Numer. Anal. (in press).

[4] G. Frasca-Caccia, P. E. Hydon. J. Comput. Dyn. (accepted).

Arieh Iserles

Title: Exponentials of differentiation matrices

Abstract: The subject matter of this talk is fast approximation of an exponential of a skew-symmetric tridiagonal matrix and of its square. Such matrices occur naturally once a combination of spectral and splitting methods is applied to dispersive PDEs and the goal is to compute such $N \times N$ matrix in $O(N \log_2 N)$ operations. We describe a general approach to this problem, based on the divide-and-conquer technique.

This is joint work with Elena Celledoni.

Balázs Kovács

Title: A convergent algorithm for mean curvature flow without and with forcing

Abstract: We will sketch a proof of convergence is for semi- and full discretizations of mean curvature flow of closed two-dimensional surfaces. The proposed and studied numerical method combines evolving surface finite elements, whose nodes determine the discrete surface like in Dziuk's algorithm proposed in 1990, and linearly implicit backward difference formulae for time integration. The proposed method differs from Dziuk's approach in that it discretizes Huisken's evolution equations (from [Huisken (1984)]) for the normal vector and mean curvature and uses these evolving geometric quantities in the velocity law projected to the finite element space. This numerical method admits a convergence analysis, which combines stability estimates and consistency estimates to yield optimal-order H^1-norm error bounds for the computed surface position, velocity, normal vector and mean curvature. The stability analysis is based on the matrix–vector formulation of the finite element method and does not use geometric arguments. The geometry enters only into the consistency estimates. We will also present various numerical experiments to illustrate and complement the theoretical results. Furthermore, we will give an outlook towards problems coupling mean curvature forced by a surface PDE. The talk is based on joint work with Biyang Li (Hong Kong) and Christian Lubich (Tübingen).

Karolina Kropielnicka

Title: Efficient splittings for Magnus expansions

Abstract: Linear systems of ordinary differential equations with time dependent matrix $\mathbf{u}'(t) = A(t)\mathbf{u}(t)$ can be solved analytically via Magnus or Ferr expansions. For the sake of stability and/or computational cost one would often use the first and present the solution as $\mathbf{u}(t) = \exp[\Theta(t)]\mathbf{u}_0$, where $\Theta(t)$ is an infinite series of nested integrals of nested commutators. The higher the desired precision of numerical approximation, the more Magnus terms are required and the cost increases rapidly. In this talk, we will present and effective approach based on splitting and Magnus expansions and present some examples originating in Schrödinger and Klein-Gordon equations.

Benedict Leimkuhler

Title: Geodesic integrators for molecular modelling and data science

Abstract: TBA

Melvin Leok

Title: The Connections Between Discrete Geometric Mechanics, Information Geometry and Machine Learning

Abstract: Geometric mechanics describes Lagrangian and Hamiltonian mechanics geometrically, and information geometry formulates statistical estimation, inference, and machine learning in terms of geometry. A divergence function is an asymmetric distance between two probability densities that induces differential geometric structures and yields efficient machine learning algorithms that minimize the duality gap. The connection between information geometry and geometric mechanics will yield a unified treatment of machine learning and structure-preserving discretizations. In particular, the divergence function of information geometry can be viewed as a discrete Lagrangian, which is a generating function of a symplectic map, that arise in discrete variational mechanics. This identification allows the methods of backward error analysis to be applied, and the symplectic map generated by a divergence function can be associated with the exact time-h flow map of a Hamiltonian system on the space of probability distributions.

Martin Licht

Title: Experiences implementing finite element differential forms in C++

Abstract: This talk outlines some experiences in implementing finite element differential forms in C++ and solving the Hodge Laplace equations. We discuss the implementation of Whitney forms of arbitrary order and polynomial degree over simplicial complexes of arbitrary dimension. A simple straightforward implementation operates with symmetric singular matrices. Their defect spaces are either artifacts of the discretization or correspond to intrinsic qualities of the partial differential equations that should be preserved on the discrete level. We discuss some consequences to numerical linear algebra.

Simon Malham

Title: Nonlinear systems, coagulation-fragmentation and Fredholm Grassmannians

Abstract: We will present an approach, using Fredholm Grassmann manifolds, to linearise large classes of systems with nonlocal nonlinearities, including in particular Smoluchowski coagulation-fragmentation models. At the same time we will explore: (i) The connection of our approach to the solution of classical nonlinear PDEs; (ii) Coalescent and branching processes; and (iii) A plethora of applications.

Donatella Marini

Title: Lowest order Virtual Element approximation of magnetostatic problems

Abstract: We present a lowest order Serendipity Virtual Element method, and show its use for the numerical solution of linear magneto-static problems in three dimensions. The method can be applied to very general decompositions of the computational domain (as is natural for Virtual Element Methods) and uses as unknowns the (constant) tangential component of the magnetic field H on each edge, and the vertex values of the Lagrange multiplier p (used to enforce the solenoidality of the magnetic induction B). In this respect the method can be seen as the natural generalization of the lowest order Edge Finite Element Method (the so-called "first kind Nedelec" elements) to polyhedra of almost arbitrary shape, and as we show on some numerical examples it exhibits very good accuracy (for being a lowest order element) and excellent robustness with respect to distortions.

Jitse Niesen

Title: Solving differential equations with Fourier extension

Abstract: Spectral methods for solving differential equations are wonderful, as long as the domain is nice, for instance a rectangle. Fourier extension allows us to approximate functions on arbitrary domains, by embedding the domain in a rectangle and approximating the function by a two-dimensional Fourier series on the rectangle. The talk will discuss the use of Fourier extension to solve boundary value problems and (briefly) evolutionary PDEs.

Christian Offen

Title: Bifurcations in Variational Differential Equations

Abstract: Catastrophe theory has been attracting researcher for more than half a century. Nowadays a highly-developed framework is available to describe singularities and bifurcations. In my talk I will show that bifurcations of solutions to Hamiltonian boundary value problems fit into this setting and that using a symplectic integrator is essential to preserve generic bifurcations.

Brynjulf Owren

Title: Searching for preserved measures and integrals for the Kahan map by aromatic series

Abstract: The numerical integrator of Kahan is used for vector fields where the components are multivariate quadratic polynomials. It is known that the method of Kahan leads to a birational map with many interesting geometric properties, such as the preservation of modified measures and first integrals, and ultimately, its integrability for certain vector fields. The map is also known under the name Hirota-Kimura and these two were the first ones to discover some of its remarkable properties. Later, Petrera, Suris and coworkers have unveiled many more examples of integrability properties of this map. Celledoni et al. have also made contributions to this area. In 2007, two seemingly unrelated papers (Chartier and Murua, Iserles and Quispel and Tse) appeared on a certain type of generalised B-series, now called aromatic series. In this talk we are studying the preservation properties of Kahan's method in the context of such aromatic series. We show that one can in many cases obtain elegant results where e.g. preserved measure can be represented in a unified way for a large class of vector fields.

Reinout Quispel

Title: The future of discrete Darboux polynomials

Abstract: Very recently it has been discovered that modified first and second integrals and preserved measures of discretizations of Ordinary Differential Equations can be found using a novel theory of Darboux polynomials for discrete systems. In this talk we will introduce some of these new ideas and results and apply them to discretizations obtained using Kahan's method or Hone's method. This work was done in collaboration with Celledoni, Evripidou, Hone, McLaren, Offen, Owren, Tapley, and Van der Kamp.

Erlend Skaldehaug Riis

Title: A Geometric Integration Approach to Nonsmooth, Nonconvex Optimization

Abstract: Discrete gradient methods are well-known numerical methods from geometric integration for solving systems of ODEs. They are known for preserving structures of the continuous system, e.g. energy dissipation, making them interesting for optimisation problems. We consider a derivative-free discrete gradient applied to dissipative ODEs such as gradient flow, thereby obtaining optimisation schemes that are implementable in a black-box setting and retain favourable properties of gradient flow. We give a theoretical analysis in the nonsmooth, nonconvex setting, and conclude with numerical results.

Katharina Schratz

Title: Nonlinear Fourier integrators for dispersive equations

Abstract: A large toolbox of numerical schemes for nonlinear dispersive equations has been established, based on different discretization techniques such as discretizing the variation-of-constants formula (e.g., exponential integrators) or splitting the full equation into a series of simpler subproblems (e.g., splitting methods). In many situations these classical schemes allow a precise and efficient approximation. This, however, drastically changes whenever non-smooth phenomena enter the scene since the underlying PDEs have very complicated solutions exhibiting high oscillations and loss of regularity. This leads to huge errors, massive computational costs and ultimately provokes the failure of classical schemes. Nevertheless, non-smooth phenomena play a fundamental role in modern physical modeling (e.g., blow-up phenomena, turbulences, high frequencies, low dispersion limits, etc.) which makes it an essential task to develop suitable numerical schemes.

Pranav Singh

Title: Convergence of Magnus based methods for Schrödinger equations

Abstract: Magnus expansion based methods are an efficient class of Lie group methods whose behaviour is well understood for ODEs. However, it was not till the work of Hochbruck and Lubich in 2003 that a rigorous analysis justifying the application to PDEs with unbounded operators, such as the Schrödinger equation, was presented.

In this talk I will present an extension of this analysis to the semiclassical regime, where the highly oscillatory solution conventionally suggests large errors and a requirement for extremely small time steps. Crucial to this extension is the conservation of certain quantities, which allows us to find uniform in time bounds for the oscillatory behaviour of the solution.

Ari Stern

Title: Constraint-preserving hybrid finite element methods for Maxwell's equations

Abstract: Maxwell's equations describe the evolution of electromagnetic fields, together with constraints on the divergence of the magnetic and electric flux densities. These constraints correspond to fundamental physical laws: the nonexistence of magnetic monopoles and the conservation of charge, respectively. However, one or both of these constraints may be violated when one applies a finite element method to discretize in space. This is a well-known and longstanding problem in computational electromagnetics.

We use domain decomposition to construct a family of primal hybrid finite element methods for Maxwell's equations, where the Lagrange multipliers are shown to correspond to a numerical trace of the magnetic field and a numerical flux of the electric flux density. Expressing the charge-conservation constraint in terms of this numerical flux, we show that both constraints are strongly preserved. As a special case, these methods include a hybridized version of Nédélec's method, implying that it preserves the constraints more strongly than previously recognized. These constraint-preserving properties are illustrated using numerical experiments in both the time domain and frequency domain. Additionally, we observe a superconvergence phenomenon, where hybrid post-processing yields an improved estimate of the magnetic field.

Vanessa Styles

Title: Numerical approximations of a tractable mathematical model for tumour growth

Abstract: We consider a free boundary problem representing one of the simplest mathematical descriptions of the growth and death of a tumour. The mathematical model takes the form of a closed interface evolving via forced mean curvature flow where the forcing depends on the solution of a PDE that holds in the domain enclosed by the interface. We derive sharp interface and diffuse interface finite element approximations of this model and present some numerical results.

Anke Wiese

Title: The Exponential Lie Series for Itô Integrals

Abstract: We consider stochastic differential systems driven by a multi-dimensional Wiener process (or more generally by continuous semimartingales) and governed by non-commuting vector fields. The flow map describes the transport of the initial condition to the solution of the differential equation at a future time. We prove that the logarithm of the flow map is a Lie series. We will discuss this important property for the development of strong Lie group integration schemes that ensure approximate solutions themselves lie in any homogeneous manifold on which the solution evolves.

Konstantinos Zygalakis

Title: Explicit stabilised Runge-Kutta methods and their application to Bayesian inverse problems

Abstract: The concept of Bayesian inverse problems provides a coherent mathematical and algorithmic framework that enables researchers to combine mathematical models with data. The ability to solve such inverse problems depends crucially on the efficient calculation of quantities relating to the posterior distribution, giving rise to computationally challenging high dimensional optimization and sampling problems. In this talk, we will connect the corresponding optimization and sampling problems to the large time behaviour of solutions to differential equations. Establishing such a connection allows utilising existing knowledge from the field of numerical analysis of differential equations. In particular, we will show that numerical stability is key for a good performing algorithm, and hence we will explore the applicability of explicit stabilised Runge-Kutta methods for optimization and sampling problems. These methods are optimal in terms of their stability properties within the class of explicit integrators and we will show that when used as optimization methods they match the optimal convergence rate of the conjugate gradient method for quadratic optimization problems, with the behaviour remaining the same for nonlinear problems. In the case of sampling, we will investigate their applicability to Bayesian inverse problems arising in computational imaging and show that explicit stabilised methods deliver much better MCMC samples than the current state of the art algorithms.

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