Advances and Applications in Geometric and Structure-Preserving Discretizations
Avancées et applications dans le domaine des discrétisations géométriques et préservant la structure
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JOERN BEHRENS, Universitaet Hamburg, Dept. Mathematics, Germany
Multiple Scales and Structure Preservation for Conservation Laws in Geophysical Applications

Transport oriented processes in atmosphere and ocean can often be described by mathematical conservation equations of mixed hyperbolic and parabolic type. Very subtle balances from equilibrium states play an important role as main driving forces in these geophysical applications. In order to simulate atmosphere or ocean circulation, tracer transport or wave dispersion, these balances and corresponding conservation principles need to be preserved in numerical discretization schemes.

As an additional difficulty, most of the important processes in the atmosphere or oceans interact in a multitude of scales. Representing the smallest influential spatial or time scales in a global domain poses severe demands on computational resources as well as mathematical tools for accurate representation.

In this presentation, we will introduce a few examples of such multi-scale conservation laws, derived from applications such as volcano ash transport or tsunami wave dispersion. We will list requirements to discretization schemes for accurate representation of the underlying conservation principles, and give alternative structure-preserving discretizations, solving the above mentioned problems. With such carefully designed mathematical methods implemented in modern algorithms scientific computing - as a sub-branch of mathematical sciences - can help prepare for and mitigate natural disaster.

ONNO BOKHOVE, University of Leeds
Variational time integrators for water-wave, wave-structure and internal-wave dynamics

Novel and existing variational and Hamiltonian integrators will be (re)derived using a discontinuous Galerkin finite-element framework in time. These can, geometrically, be interpreted as limits of continuous Galerkin finite-element integrators on a non-uniform mesh with a subset of (odd-numbered) elements shrinking to zero in size. The integrators will be and have been applied in simulations of nonlinear water-wave dynamics, (linear and constrained) water-wave-structure interactions, and (linear) internal gravity and inertial waves in asymmetric domains permitting wave attractors. Some simulations will be discussed, possibly including our latest results on a new wave-energy device, which conservative limit satisfies one grand variational principle of coupled wave dynamics, buoy motion and magnetically-induced electrical power.

JOHN BOWMAN, University of Alberta
A New Technique for Constructing Exponential Integrators

A new method is proposed for deriving exponential integrators for stiff ordinary differential equations. Exponential integrators are explicit discretizations that solve the linear part exactly. An important property of exponential integrators is that they reduce to classical discretizations in the limit of vanishing linearity. We review the history and current status of exponential integrators, which have been rediscovered many times since Certaine first used an exponential method in 1960.

While first- and second-order exponential integrators are well understood, higher-order methods are difficult to construct. We demonstrate a technique that can circumvent this problem, converting classical integration methods into corresponding exponential discretizations.

Stiff-order conditions for exponential integrators were developed in a Banach space framework by Hochbruck and Ostermann [2005]. They showed that in the worst case, the well-known ETDRK4 integrator of Cox and Matthews can exhibit an order reduction from four to two. Although they speculated that a four-stage exponential integrator with stiff-order four does not exist, we have nevertheless succeeded in constructing a four-stage exponential version of the classical RK4 integrator with stiff-order four. Our ERK4 integrator performs well in numerical tests and generalizes to the case where the dependent variable is a vector and the linear operator is a diagonal matrix. We plan to extend our construction to the case where the linear operator is a general square matrix. We also wish to derive embedded exponential Runge-Kutta pairs that efficiently generate both a high- and low-order estimate, allowing dynamic adjustment of the time step to achieve a specified accuracy.

RUDIGER BRECHT, Memorial University of Newfoundland
a geometric variational discretization of compressible fluids: the rotating shallow water equations on the sphere

We develop a variational integrator for the shallow-water equations on a rotating sphere. The variational integrator is built around a discretization of the continuous Euler–Poincaré reduction framework for Eulerian hydrodynamics. We describe the discretization of the continuous Euler–Poincaré equations on arbitrary simplicial meshes. Standard numerical tests are carried out to verify the accuracy and the excellent conservational properties of the discrete variational integrator.

ELSA CARDOSO-BIHLO, Memorial University of Newfoundland
Invariant high-order parameterization schemes

Numerical weather prediction relies on the process of averaging systems of nonlinear differential equations which leads to a closure problem: unresolved subgrid-scale terms have to be replaced by functions of the explicitly resolved variables. This process is called parameterization. In this talk we tackle the problem of finding invariant parameterization schemes for geostrophic eddies in a barotropic ocean model. As a model we consider the system of incompressible inviscid two-dimensional Euler equations on the beta plane. The parameterization used for the eddy vorticity flux and eddy energy flux are of one-and-a-half order type, as we also consider the equation for turbulent kinetic energy in the closure schemes. By preserving the infinite dimensional maximal Lie invariance group of our model we construct invariant higher-order closure schemes. We carry out numerical experiments to assess the performance of the invariant scheme versus that of the non-invariant scheme.

ANDREA DZIUBEK, SUNY Poly, Utica, NY
Literature Review of Structure Preserving Discretizations for Shell Models

With their interconnection of differential geometry and continuum mechanics, shell models are a natural place to study covariant discretization methods of metric dependent operators. Research in the area of exterior calculus based computational methods for elasticity is currently very active and recent progress has been made on the discrete counterparts of a connection, the covariant derivative, and the stress-tensor (a co-vector-valued two-form), which are essential operators in elasticity. However, a covariant discretization of shells is not yet formulated. A starting point is to formulate shell equations in the language of exterior calculus (differential forms).

We will review shell models and discuss some of the issues of structure-preserving discretizations of shell equations.

TAGIR FARKHUTDINOV, University of Alberta
Variational Methods in the Dynamics of Porous Media

We use the variational approach to derive the equations of motion of compressible homogeneous elastic porous media filled with an incompressible non-viscous fluid. The total energy density equation is computed in the form of conservation law. The linearization of the system of equations is found and investigated to confirm the stability of wave propagation. Phase and group velocities of $s-$ and $p-$ waves and corresponding attenuation coefficients are computed numerically for a number of non-dimensional parameter sets. We compared our linearized system with the equations of porous mechanics from Biot's 1962 paper and found a partial correspondence of our parameters with Biot's phenomenological coefficients.

FRANCOIS GAY-BALMAZ, CNRS - Ecole Normale Supérieure
Towards a geometric variational discretization of compressible fluid dynamics

We present a geometric variational discretization of compressible fluid dynamics. The numerical scheme is obtained by discretizing, in a structure preserving way, the Lie group formulation of fluid dynamics on diffeomorphism groups and the associated variational principles. Our framework applies to irregular mesh discretizations in 2D and 3D. It systematically extends work previously made for incompressible fluids to the compressible case. We consider in detail the numerical scheme on 2D irregular simplicial meshes and evaluate the behavior of the scheme for the rotating shallow water equations. While our focus is fluid mechanics, our approach is potentially useful for discretizing problems involving evolution equations on diffeomorphism groups.

ANDREW GILLETTE, University of Arizona
Structure Preservation in (Trimmed) Serendipity Finite Element Methods

Serendipity finite element methods present a promising computational advantage over traditional tensor product finite elements: a significant reduction in degrees of freedom without sacrificing the order of accuracy in the computed solution. The theory of serendipity methods dates back to the 1970s but has seen a resurgence of interest in recent years within the context of finite element exterior calculus and the Periodic Table of the Finite Elements. In this talk, I will focus on the structure preserving properties of serendipity elements and how these properties led us to discover an accompanying space of "trimmed serendipity" elements that are even more computationally efficient. This is based on joint work with Snorre Christiansen and Tyler Kloefkorn.

YOUSAF HABIB, COMSATS University Islamabad, Lahore Campus
Effective order methods for separable differential equations

The idea of effective order was pioneered by J. C. Butcher to construct Runge-Kutta methods of order five with just five stages. For separable differential equations such as separable Hamiltonian systems, one can solve some components of its unknown dependent variable by one Runge–Kutta method and solve the remaining components with another Runge–Kutta method. The scheme is termed as Partitioned Runge-Kutta (PRK) methods. We have extended the idea of effective order to construct efficient symplectic PRK methods for separable differential equations which can preserve some of the underlying geometric properties as well.

PHILIP MORRISON, University of Texas at Austin
Simulated Annealing for the Calculation of Steady States

Two simulated annealing approaches based on geometric/Hamiltonian structure will be described. The first [G. Flierl et al., "Jovian Vortices and Jets," arXiv:1809.08671] uses a combination Dirac constraint theory and double brackets, while the second [C. Bressan et al., "Relaxation to Magnetohydrodynamics Equilibria via Collision Brackets", arXiv:1809.03949] uses metriplectic dynamics. The methods along with various fluid and plasma steady states, steady states of physical relevance, will be described.

ANDREA NATALE, INRIA
An optimal transport Lagrangian approach for the Camassa-Holm variational model

In this talk I will consider a multi-dimensional generalization of the Camassa-Holm variational fluid model, describing geodesics on the group of diffeomorphisms with respect to the $H(div)$ metric. Such a model has been recently reformulated as a geodesic equation for the L^2 metric on a subgroup of the diffeomorphism group of the cone over the domain. This point of view is fruitful for several reasons. On one hand, it allows one to give a precise definition to solutions of the relative boundary value problem (in which the final configuration of fluid particles is provided instead of their initial velocity). On the other hand, it can be used to generate a simple Hamiltonian particle-based discretization of the initial value problem using semi-discrete unbalanced optimal transport. This approach further develops a similar one proposed for the incompressible Euler equations, by including compressibility effects. I will present our methodology together with some numerical results illustrating the behaviour of the scheme.

ALEXANDER OSTERMANN, University of Innsbruck
Low regularity Fourier integrators

Nonlinear Schrödinger equations are usually solved by pseudo-spectral methods, where the time integration is performed by splitting schemes or exponential integrators. Notwithstanding the benefits of this approach, its successful application requires additional regularity of the solution. For instance, second-order Strang splitting requires four additional derivatives for the solution of the cubic nonlinear Schrödinger equation.

In this talk, we introduce as an alternative low regularity Fourier integrators. They are obtained from Duhamel's formula in the following way: first, a Lawson-type transformation eliminates the leading linear term and second, the dominant nonlinear terms are integrated exactly in Fourier space. For nonlinear Schrödinger equations, first order convergence of such methods only requires the boundedness of one additional derivative of the solution, and second-order convergence the boundedness of two derivatives. This allows us to impose lower regularity assumptions on the data. Numerical experiments underline the favorable error behavior of the newly introduced integrators for low regularity solutions compared to classical splitting and exponential integration schemes.

This is joint work with Marvin Knöller and Katharina Schratz (KIT, Karlsruhe).

ARTUR PALHA, Delft University of Technology
Algebraic dual polynomials for mimetic spectral element methods

In this work the High Order Mimetic Discretization Framework will be presented together with a construction of algebraic dual polynomials.

The degrees of freedom are associated to geometric objects, and a relation to differential forms will be remarked. We show how to construct discrete polynomial function spaces of arbitrary degree associated to these geometric degrees of freedom, constituting a discrete de Rham complex:

$$\mathbb{R} \longrightarrow V_h^0 \subseteq H(\nabla,\Omega) \xrightarrow{\nabla} V_h^1 \subseteq H(\nabla\times,\Omega) \xrightarrow{\nabla\times} V_h^2 \subseteq H(\nabla\cdot,\Omega) \xrightarrow{\nabla\cdot} V_h^3 \subseteq L^2(\Omega) \longrightarrow 0\,.$$

In this way it is possible to exactly discretize topological equations even on highly deformed meshes.

An important aspect in the numerical solution of partial differential equations is the efficient construction of the system matrix and its subsequent solution. Given a polynomial basis Ψ_i which spans the polynomial vector space $\mathcal{P}$, this work addresses the construction and use of the algebraic dual space $\mathcal{P}'$ and its canonical basis. It will be shown that a primal-dual formulation using these algebraic dual basis results in a very sparse system matrix where two of the sub-matrices consist of only incidence matrices. The method will be applied to a Dirichlet and Neumann problem and it is shown that the finite dimensional approximations satisfy $\phi^h = \nabla \cdot \boldsymbol{q}^h$ on any grid. The dual method is also applied to a constrained minimization problem, which leads to a mixed finite element formulation. The discretization of the constraint and the Lagrange multiplier will be independent of the grid size, grid shape and the polynomial degree of the basis functions.

KATHARINA SCHRATZ, Karlsruhe Institute of Technology
Low-regularity exponential-type integrators for the KdV equation

Meanwhile, a large toolbox of numerical schemes for evolution equations was 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 such as for problems at low-regularity and high oscillations. Classical schemes fail to capture the oscillatory parts within the solution which leads to severe instabilities and loss of convergence. In this talk I present a new class of low-regularity exponential-type integrators for the Korteweg-de Vries (KdV) equation. The key idea in the construction of the new schemes is to tackle and hardwire the underlying structure of resonances into the numerical discretization. This allows for a robust and stable approximation overcoming any CFL-type condition.