Structure-Preserving Discretizations and their Applications

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Structure Preserving Discretizations for Magnetohydrodynamics

In this talk, we consider different models for magnetohydrodynamics (MHD) that incorporate linear (resistive MHD) or nonlinear (Hall MHD) Ohm's laws. We discuss finite difference and finite element methods for these models that preserve at the discrete level important continuum properties, such as the divergence free nature of magnetic and velocity fields. These are important structure preserving properties required in MHD simulations to avoid spurious or non-physical numerical solutions. We discuss recent computational techniques for MHD kinematics as well as full MHD simulations in two spatial dimensions that are based on the framework of the Virtual Element Method which is a generalization of the finite element method to general polygonal and polyhedral meshes.

JOHN BOWMAN, University of Alberta

Conservative, Symplectic, and Exponential Integrators

Novel integration algorithms for initial value problems can be formed by applying conventional explicit discretizations in a transformed space. One can devise integration methods that respect desired properties of ordinary differential equations such as first integrals, positivity, or unitary structure. For example, traditional numerical integration algorithms, which are polynomials in the time step, typically lead to systematic drifts of nonlinear first integrals. For a 4-body classical mechanics problem, we compare conservative integration with conventional symplectic discretization, which conserves only an approximate Hamiltonian.

One can also develop new numerical integration methods that preserve analytical structure by discretizing perturbations of exactly solvable differential equations. For example, exponential integrators are ideal for solving linearly stiff first-order ordinary differential equations, where the nonlinearity varies slowly on the time scale of the linearized equations.

We use the stiff-order criteria of Hochbruck and Ostermann [2005] to derive efficient embedded exponential pairs of high- and low-order estimates to support dynamic time-step adjustment. A key requirement is that the pair be robust: if the nonlinear source function has a nonzero total time derivative, the order of the low-order estimate should never exceed its design value. Robust exponential Runge–Kutta (3,2) and (4,3) embedded pairs that are well-suited to initial value problems with a dominant linearity are constructed.

CHUNYI GAI, University of Northern British Columbia

Pattern Formation and Spike Dynamics in the Presence of Noise

Noise plays a crucial role in the formation and evolution of spatial patterns in various reaction-diffusion systems in mathematical biology and ecology. In this talk, I give two examples where noise significantly influences spatial patterning. The first example describes how patterned states can provide a refuge and prevent extinction under stressed conditions. It also illustrates the importance of not only the absolute level of climate change, but also the speed with which it occurs. The second example studies the effect of noise on dynamics of a single spike pattern for the classical Gierer-Meinhardt model on a finite interval.

NILIMA NIGAM, Simon Fraser University

Structure-preservation and the Steklov eigenfunctions

Spectral methods for elliptic and time-dependent PDE - in which the approximation space consists of eigenfunctions of the underlying operator - exhibit excellent accuracy properties and are naturally structure-preserving. Most spectral methods in practice use either Dirichlet or Neumann eigenfunctions for this purpose.

In this talk I'll motivate and describe the use of Steklov eigenfunctions as a spectral basis, particularly when solving boundary value problems with mixed data. This is joint work with K. Imeri.

YUZHE QIN, The University of British Columbia
A second-order accurate numerical scheme for the Poisson-Nernst-Planck-Navier-Stokes (PNPNS) system

In this talk, I will present a second order accurate (in both time and space) numerical scheme for the Poisson-Nernst-Planck-Navier-Stokes system, which describes the ion electro-diffusion in fluids. In particular, the Poisson-Nernst-Planck equation is reformulated as a non-constant mobility gradient flow in the Energetic Variational Approach. The marker and cell finite difference method is chosen as the spatial discretization, which facilitates the analysis for the fluid part. In the temporal discretization, the mobility function is computed by a second order extrapolation formula for the sake of unique solvability analysis, while a modified Crank-Nicolson approximation is applied to the singular logarithmic nonlinear term. Nonlinear artificial regularization terms are added in the chemical potential part, so that the positivity-preserving property could be theoretically proved. Meanwhile, a second order accurate, semi-implicit approximation is applied to the convective term in the PNP evolutionary equation, and the fluid momentum equation is similarly computed. In addition, an optimal rate convergence analysis is provided, based on the higher order asymptotic expansion for the numerical solution, the rough and refined error estimate techniques. The following combined theoretical properties have been established for the second order accurate numerical method: (i) second order accuracy, (ii) unique solvability and positivity, (iii) total energy stability, and (iv) optimal rate convergence. A few numerical results are displayed to validate the theoretical analysis.

SETH TAYLOR, McGill University
A functional discretization of the coadjoint action on the diffeomorphism group

The coadjoint orbits of a Lie group play a fundamental role in the geometry underlying many continuum mechanical systems. In this talk, we will present a geometric integrator designed to preserve this infinite-dimensional geometric structure under discretization without using a finite-dimensional analogue. The key idea behind the construction is the use of a functional discretization of the coadjoint action which avoids truncating the solution in the dual of the Lie algebra. We will present an analysis and numerical results of the application of this integrator, illustrating its unique resolution properties for invariant Hamiltonian systems on the space of diffeomorphisms of a compact manifold. The talk is based on joint work with Jean-Christophe Nave and Xi-Yuan Yin.

MAYYA TOKMAN, University of California, Merced
Exponential integration and applications

In this talk we will discuss several ways in which the ideas of exponential integration can be used to construct accurate and efficient schemes for stiff systems of differential equations. We will present a new framework to develop and to analyze new class of schemes we call stiffness resilient methods. Previously proposed exponential integrators are typically derived using either classical or stiff order conditions. These order conditions are complex and difficult to solve to construct high order schemes. Classically derived methods can also suffer from the order reduction phenomenon. The new φ-order conditions we propose allow greatly simplified construction of exponential methods with favorable properties. The structure of the error of these methods is designed to prevent order reduction for many important stiff problems. At the same time stiffness resilient schemes are easy to derive using our proposed approach. In addition, we will discuss new exponential schemes for simulating particle dynamics in the presence of electromagnetic fields. We will show that these methods are highly competitive compared to the state-of-the-art integrators, such as Boris algorithm, which have been used extensively in particle-in-cell (PIC) plasma simulations.

DANIEL VENN, Simon Fraser University
Meshfree Integration Techniques for Scattered Data on Curves and Surfaces

We present high-order, meshfree methods for integration on curves and surfaces. Accurately integrating functions defined on surfaces is a challenging task, particularly for implicitly-defined surfaces and those without a readily-available mesh. Our approach is quite general and works as long as scattered points can be generated on the curve or surface of interest. We examine the methods for a variety of surfaces, including those with and without boundary and those defined by level sets. Also of note for our approach is that integration weights can be generated for any point arrangement; this is useful in the case that function data is only given on a specific sample of points. Analytical convergence results are also presented. Lastly, we use the generated integration weights to impose constraints on partial differential equations on curves or surfaces.

ANDY WAN, University of California, Merced
Minimal ℓ^2 Norm Discrete Multiplier Method

Many dynamical systems possess multiple conserved quantities and preserving such quantities are fundamental for accurate long-term simulations. Well-known examples include energy and momentum for physical systems, but time-dependent conserved quantities may also exist for dissipative systems. Unfortunately, traditional integrators do not in general preserve such quantities, leading to recent developments on general conservative integrators, such as Discrete Gradient Method or Discrete Multiplier Method (DMM). While both approaches can lead to systematic derivation of conservative integrators, they can be difficult to apply in practice for large systems with multiple conserved quantities.

To alleviate such practical difficulty, we introduce the Minimal ℓ^2 Norm Discrete Multiplier Method (MN-DMM) to extend the practical applicability of DMM, where conservative schemes are constructed procedurally. In essence, MN-DMM utilizes a Moore-Penrose pseudoinverse of the discrete multiplier matrix leading to a unique consistent conservative scheme with the minimal ℓ^2 norm via a suitable fixed point iteration. We show the wide applicability of MN-DMM and its relative ease of implementation on various examples.

This is joint work with Erick Schulz (Plexim GmbH).

SIQI WEI, Kwantlen Polytechnic University
Operator-splitting methods for qualitative property preservation of production-destruction systems

When solving a production-destruction system, the numerical solution should respect certain qualitative properties that reflect the physical reality of the system. The SIR model is an example of a production-destruction system. Based on suitable assumption, the solution of the SIR model should preserve the positivity of all variables, conserve the total population, and preserve the monotonicity of the S and R variables. When using operator-splitting methods, three aspects affect the quality of the numerical solution: the splitting strategy of the system, the splitting scheme used for time integration, and the choice of the sub-integration methods. In this talk, we will use the SIR model to discuss how these aspects affect the desired qualitative properties.