天元數學國際交流中心

Tianyuan Mathematics Research Center

Frontiers in the Theory and Application of Structure-Preserving Algorithms



Sept. 7-13, 2025

Kunming, CHINA

Organizing Committee

Yushun Wang, Nanjing Normal University, China

Yajuan Sun, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, China

Chaolong Jiang, Yunnan University of Finance and Economics, China

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Workshop Schedule

September 7, Sunday: Registration and Arrival
September 13, Saturday: Departure

DATE / TIME	Sept. 8 (Monday)	Sept.9 (Tuesday)	Sept.10 (Wednesday	Sept.11 (Thursday)	Sept.12 (Friday)
08:20-08:50	**Opening Ceremony**				
Chair	**Alexander Ostermann**	**Donghua Shi**	**Yingzhe Li**	**Yushun Wang**	**Yushun Wang**
08:50-09:35	Jie Shen	Chuchu Chen	Yong Zhang	Yifei Wu	Xiaoping Wang
09:35-10:20	Yajuan Sun	Xiaojie Wang	Hanquan Wang	Wenjun Cai	Xiaofei Zhao
10:20-10:40	Tea Break	Tea Break	Tea Break	Tea Break	Tea Break
Chair	**Jie Shen**	**Chuchu Chen**	**Chaolong Jiang**	**Yifei Wu**	**Wenjun Cai**
10:40-11:25	Alexander Ostermann	Jian Liu	Dongling Wang	Yushun Wang	Nan Lu
11:25-12:10	Jianbo Cui	Benedikt Brantner	Gengen Zhang	Yuezheng Gong	Chaolong Jiang
12:10-14:30	**Lunch**	**Lunch**	**Lunch**	**Lunch**	**Lunch**
Chair	**Yajuan Sun**	**Jian Liu**	**Free Discussion**	**Free Discussion**	**Free Discussion**
14:30-15:15	Donghua Shi	Bin Wang			
15:15-16:00	Chunmei Su	Yingzhe Li			
16:00-16:20	Tea Break	Tea Break			
16:20-17:05	Liying Sun	Tianai Yin			
18:00-20:00	**Dinner**	**Dinner**	**Dinner**	**Dinner**	**Dinner**

Titles & Abstracts

08:50-09:35, September 8, Monday

Structure preserving schemes using the Lagrange multiplier approach

Jie Shen

Eastern Institute of Technology, Ningbo, China

Abstract:I will present a Lagrange multiplier approach to construct highly efficient and accurate structure preserving schemes for a class of complex nonlinear systems with global (e.g., energy dissipation) and/or local (e.g. positivity or length preserving) constraints. I shall also present some recent advances on the error analysis of this approach in some special cases.

09:35-10:20, September 8, Monday

Variational principle and numericalmethods

Yajuan Sun

Academy of Mathematics and Systems Science, Chinese Academy of Sciences, China

Abstract: The framework of variational principles is a powerful mathematical tool that provides a unified approach for formulating and analyzing dynamical systems. Its discrete formulation naturally leads to structure-preserving numerical algorithms, which exhibit excellent stability and accuracy in long-term simulations.In this talk, we offer a brief introduction to classical and generalized variational principles, witha focus on Herglotz's variational principle. Thisvariational Principle can incorporate non-conservative and dissipative effects. We also discuss potential applications of variational integrators in engineering, especially for solving multiphysics coupling problems involving strongly interacting electromagnetic, mechanical, and thermal fields.

10:40-11:25, September 8, Monday

A conservative dynamical low-rank algorithm

Alexander Ostermann

University of Innsbruck, Austria

Abstract: Kinetic equations present computational challenges due to their (up to) six-dimensional phase space dependence, resulting in high memory requirements and high computational cost. Traditional particle methods alleviate this burden, but generally suffer from noise. Dynamical low-rank approximation is a novel approach that significantly reduces the computational burden, but often fails to preserve physical invariants such as mass, momentum, and energy. This destroys the inherent physical structure of the problem. In this talk, we present a modified low-rank algorithm that conserves mass and momentum while improving energy conservation. The resulting method is applied to the Vlasov-Poisson equations, though the same strategy can be applied to other kinetic equations. Numerical results for phenomena such as Landau damping and two-stream instability demonstrate the effectiveness of the new method.

11:25-12:10, September 8, Monday

Wasserstein Hamiltonian flow and its structure preserving numerical scheme

Jianbo Cui

The Hong Kong Polytechnic University, China

Abstract: We study discretizations of Hamiltonian systems on the probability density manifold equipped with the L2-Wasserstein metric. For low dimensional problems, based on discrete optimal transport theory, several Wasserstein Hamiltonian flows (WHFs) on graph are derived. They can be viewed as spatial discretizations to the original systems. By regularizing the system using Fisher information, we propose a novel regularized symplectic scheme which could preserve several desirable

longtime behaviors. Furthermore, we use the coupling idea and WHF to propose a supervised learning scheme for some high-dimensional problem. If time permits, we will talk about more details on solving high-dimensional Hamilton-Jacobi equation via the density coupling and supervised learning.

14:30-15:15, September 8, Monday

Recent progress on Hamel's formalism for classical field theory and its applications

Donghua Shi

Beijing Institute of Technology, China

Abstract: To meet the demand for fast and qualitatively accurate algorithms in the dynamics computation and control of swarms and multi-field coupling systems, Hamel's formalism is derived within the framework of classical field theory, employing the moving frame method and exterior calculus. This formalism comprises the Hamel field equations characterized the dynamics, and geometric compatibility conditions, facilitating symmetry reduction and obviate the need to solve high-complexity mixed-type equations.

Building upon this formulation, several Hamel field integrators on fiber bundles are introduced for infinite-dimensional constrained and stochastic systems. The efficacy of the proposed algorithms is demonstrated through numerical simulations of geometrically exact beams/shells, among others. In terms of control, a unified framework for flexible swarm formations is established. A discrete maximum principle for optimal control of nonholonomic systems is also provided. Furthermore, an infinite-dimensional controlled Lagrangian method is proposed, with applications shown in the stabilization of flexible inverted pendulums.

15:15-16:00, September 8, Monday

Temporal high-order structure-preserving parametric finite element methods for curvature flows

Chunmei Su

Tsinghua University, China

Abstract: The quality of the mesh is crucial for simulating curvature flows, as standard approaches may fail due to mesh distortion. We first present a series of high-order parametric finite element methods based on the BGN formulation for solving various types of flows involving curves and surfaces. Extensive numerical experiments demonstrate the anticipated high-order accuracy while maintaining favorable mesh quality throughout the evolution process. Secondly, for flows involving multiple geometric structures, such as surface diffusion—which reduces area while preserving volume—we propose a type of structure-preserving method that incorporates two scalar Lagrange multipliers along with two evolution equations related to area and volume, respectively. These schemes effectively preserve the geometric structure at a fully discrete level. Comprehensive numerical experiments illustrate that our methods achieve the desired temporal accuracy, while simultaneously preserving the geometric structure of the surface diffusion.

16:20-17:05, September 8, Monday

Energy-preserving numerical scheme for stochastic nonlinear wave equation

Liying Sun

Capital Normal University

Abstract: In this talk, we propose and analyze energy-preserving numerical schemes for the stochastic nonlinear wave equation. These numerical schemes, called stochastic scalar auxiliary variable (SAV) schemes, are constructed by transforming the considered equation into a

higher dimensional stochastic system with a stochastic SAV. We prove that they can be solved explicitly, and preserve the modified energy evolution law and the regularity structure of the original system. These structure-preserving properties are the keys to overcoming the mutual effect of noise and nonlinearity. By providing new regularity estimates of the introduced SAV, we obtain the strong convergence rate of stochastic SAV schemes under Lipschitz conditions. Furthermore, based on the modified energy evolution laws, we derive the exponential moment bounds and sharp strong convergence rate of the proposed schemes for equation with a non-globally Lipschitz nonlinearity in the additive noise case.

08:30-09:15, September 9, Tuesday

Stochastic modified equations for symplectic methods applied to rough Hamiltonian systems

Chuchu Chen

Academy of Mathematics and Systems Science, Chinese Academy of Sciences, China

Abstract: Stochastic Hamiltonian systems play a central role in various disciplines. A defining characteristic of such systems is the preservation of the stochastic symplectic structure by the phase flow. When numerically approximating these systems, it is natural to seek methods that inherit this structure, which has driven the development of stochastic symplectic methods. These methods have shown clear advantages over non-symplectic schemes, particularly in long-time simulations, as confirmed by numerous numerical experiments. In this talk, we investigate stochastic modified equations to reveal the mathematical mechanisms behind the effectiveness of stochastic symplectic methods. In particular, for stochastic symplectic methods, the associated stochastic modified equations are proved to have Hamiltonian formulations. And the pathwise error between the numerical solution and the modified equation can be made exponentially small with respect to the time step size.

09:15-10:00, September 9, Tuesday

High-dimensional sampling algorithms based on time discretizations of SDEs

Xiaojie Wang

Central South University, China

Abstract: Generating samples from a high dimensional probability distribution is a fundamental task with wide-ranging applications in the area of scientific computing, statistics and machine learning. This talk will focus on non-asymptotic error bounds for high dimensional sampling algorithms based on time discretizations of stochastic differential equations (SDEs). New error bounds will be then provided for the considered sampling algorithms without log-concavity, where the convergence rate and the dimension dependence are explicitly revealed. Numerical experiments will be finally presented to corroborate the theoretical findings.

10:20-11:05, September 9, Tuesday

Research on simulating particle dynamics of plasmas using machine learning mechods

Jian Liu

Shandong University, China

Abstract: Particle simulations play key roles in plasma physics research. The application of machine learning methods in plasma particle simulation in an interesting topic. Structure preserving algorithms have achieved fruitful results in plasma particle simulations. We hope to replace or improve traditional methods using machine learning methods.

11:05-11:50, September 9, Tuesday

Structure-preserving neural networks for geometric machine learning

Benedikt Brantner

Max Planck Institute for Plasma Physics, Germany

Abstract: In recent years, neural networks have emerged as a potent tool for data-driven tasks in geometric integration and reduced order modeling. By designing architectures that respect the underlying physics, we can create models with improved long-term stability. These structure-preserving neural networks share properties analogous to methods in e.g. geometric numerical integration, ensuring the conservation of inherent structure by construction.

This talk provides an overview of several architectures. We mention networks that learn a system's governing function, such as Hamiltonian Neural Networks (HNNs) and Lagrangian Neural Networks (LNNs), networks that learn the system's flow directly, like Symplectic Neural Networks (SympNets), or identify structure-preserving low-dimensional embeddings, such as Symplectic Autoencoders (SAEs).

We will discuss implementation details, also with a view towards our library `GeometricMachineLearning.jl`, a Julia package for developing and deploying these models and point out difficulties associated with training specialized neural networks as well as how to mitigate them.

14:30-15:15, September 9, Tuesday

Fourth-order uniformly accurate integrators for the nonlinear Dirac equation in the nonrelativistic regime

Bin Wang

Xi'an Jiaotong University, China

Abstract: In this talk, we propose two novel fourth-order integrators that exhibit uniformly high accuracy and long-term near conservations for

solving the nonlinear Dirac equation (NLDE) in the nonrelativistic regime. In this regime, the solution of the NLDE exhibits highly oscillatory behavior in time. To ensure uniform temporal accuracy, we employ a two-scale approach in conjunction with exponential integrators, utilizing operator decomposition techniques for the NLDE. The proposed methods are proved to achieve fourth-order uniform accuracy in time and long-term near conservation properties.

15:15-16:00, September 9, Tuesday

Geometric structures and numerical methods for the plasma hybrid model with kinetic ions and massless electrons

Yingzhe Li

Max Planck Institute for Plasma Physics, Germany

Abstract: In this talk, we will discuss the Hamiltonian formulations and structure-preserving methods for a plasma hybrid model with kinetic ions and massless fluid electrons. We present a direct proof of the Jacobi identity for the associated Poisson brackets. On the numerical side, we focus on semi-Lagrangian methods that conserve mass, momentum, and energy. These conservation properties are ensured by a specially designed mean velocity, a modified midpoint rule for time discretization, and the intrinsic conservation features of spline-based semi-Lagrangian schemes. The methods are computationally efficient, since nonlinear iterations are required only for the fields, while the Vlasov equation is solved explicitly. Moreover, thanks to the use of exact splitting, solving the Vlasov equation requires only one-dimensional translations. We will also discuss the implementation in the code packages Gysela and GEMPICX, and conclude with numerical validations and applications.

16:20-17:05, September 9, Tuesday

Research on structure-preserving numerical schemes for the Boltzmann equation

TianaiYin

Eastern Institute of Technology, Ningbo, China

Abstract: This work presents a series of structure-preserving numerical schemes for the spatially homogeneous Boltzmann equation, developed using the Lagrange Multiplier Approach. A key element is the introduction of a scaling factor η for the collision term, enforced via a nonlinear algebraic equation, to guarantee entropy dissipation. The approach is extended to second-order Crank-Nicolson and high-order BDF$_k$ schemes, both of which preserve entropy dissipation under the standard definition. Furthermore, a fully structure-preserving method with multiple Lagrange multipliers is proposed to simultaneously enforce entropy dissipation, positivity, and conservation laws. The resulting nonlinear system is efficiently solved using a semi-smooth Newton method. Numerical results confirm the accuracy, efficiency, and robustness of the proposed schemes, demonstrating their potential for advanced structure-preserving simulations of kinetic equations.

08:30-09:15, September 10, Wednesday

Exponential supplementary variable methods for complex-valued Hamiltonian PDEs with applications to rotating Gross-Pitaevskii equation

Yong Zhang

Tianjin University, China

Abstract: In this talk, we propose an exponential supplementary variable method, ingeniously merging the supplementary variable method initially conceived for gradient flows [20, 25] with the Lawson transform

methodology [24], to preserve multiple conserved quantities for complex-valued Hamiltonian partial differential equations. We first reformulate the original system by introducing several supplementary scalar variables, which are equal to zero on the analytical level, to enforce the multiple conservation laws. Then, leveraging the Lawson transform framework, we develop a novel class of highly efficient high-order exponential integrators utilizing prediction and correction Lawson Runge-Kutta schemes. The multiple conservation laws are preserved on the discrete level by solving a set of scalar algebraic equations, which can be efficiently computed via iterative methods. The proposed methods manifest a better numerical performance in terms of accuracy, efficiency and long-term simulation. To substantiate their precision, effectiveness, and overarching excellence, we apply these methods to the Gross-Pitaevskii equation, multi-component Gross-Pitaevskii equations and Schrodinger-Poisson equation, showcasing their prowess in simulating intricate dynamics such as the evolution of a quantized vortex lattice within a rotating Bose-Einstein condensate.

09:15-10:00, September 10, Wednesday

Sobolev gradient flows for computing ground state of ultracold dipolar fermi gas

Hanquan Wang

Yunnan University of Finance and Economics, China

Abstract: We first provide an overview of gradient flow for functional minimization problem. Then we extend the recent work on Sobolev gradient flows (SGFs) for the functional minimization problem in Bose-Einstein condensation, and proposed some SGFs for computing the DFT-based ground state solution of ultracold dipolar fermi gas. We prove that the SGFs have the properties of orthonormal preserving and energy diminishing, which is desirable for the computation of the ground state solution. We give a convergence proof of the SGFs. We propose an

efficient and accurate numerical scheme — semi-implicit Euler method in time and Fourier spectral method in space for discretizing these SGFs and use them to find the ground states of the fermi gas numerically. Extensive numerical examples in three dimensions for ground states are reported to demonstrate the power of the numerical methods.

10:20-11:05, September 10, Wednesday

Average block nonlinear Kaczmarz method with adaptive momentum for nonlinear system

Dongling Wang

Xiangtan University, China

Abstract: The Kaczmarz method has received significant attention as an efficient iterative algorithm for solving large-scale linear systems due to its simplicity and low memory requirements. However, progress in developing nonlinear Kaczmarz variants for solving nonlinear systems of substantial scale remains limited. This paper presents a novel class of momentum-accelerated averaging block nonlinear Kaczmarz methods designed to address large-scale nonlinear systems and ill-posed problems. Our main contribution is twofold: (1) We develop an adaptive parameter selection mechanism for step sizes and momentum coefficients, culminating in the proposed Average Block Nonlinear Kaczmarz Method with Adaptive Momentum (ABNKAm); The algorithm achieves exceptional computational efficiency requiring only minimal vector inner-product computations per iteration, resulting in dramatically reduced arithmetic complexity and memory footprint; (2) We provide rigorous theoretical convergence guarantees under standard assumptions and obtain an exponential convergence rate.

Meanwhile, under appropriate assumptions, we show that the convergence factor of the algorithm with momentum is strictly smaller than that of the algorithm without momentum, thereby theoretically confirming the acceleration effect of the momentum term.

Comprehensive numerical experiments demonstrate that ABNKAm outperforms existing nonlinear Kaczmarz variants in both the number of iterations and computation time, particularly excelling in large-scale problems where it achieves significantly better performance.

11:05-11:50, September 10, Wednesday

Mass- and energy-preserving exponential wave integral pseudo-spectral method for quantum Zakharov equation

Gengen Zhang

Yunnan University, China

Abstract: This work constructs and analyzes an exponential wave integrator Fourier pseudo-spectral (EWI-FP) method for the quantum Zakharov system (QZS). The method combines exponential wave integration in time with Fourier pseudo-spectral discretization in space, preserving discrete mass and energy invariants--a property we rigorously prove. Through error analysis, we establish a uniform consistency error bound of $O(h^{m_0}+ \tau^2)$, where h and τ denote spatial and temporal step sizes respectively, with m_0 dependent on solution regularity. Numerical experiments validate the theory and simulate QZS dynamics, including soliton collisions, pattern formation, and singular point phenomena.

08:30-09:15, September 11, Thursday

The construction of energy-preserving algorithm using the auxiliary variable method

Yushun Wang

Nanjing Normal University, China

Abstract: This report takes the Camassa–Holm equation as an example and presents a class of arbitrarily high-order Runge–Kutta methods capable of preserving the original energy of the system. Subsequently, the auxiliary variable approach for constructing structure-preserving algorithms for general gradient flow systems is discussed, and the structural properties of the extended system are investigated.The report examines the mechanism of the energy quadratization method from the perspective of structure-preserving algorithms, analyzes the reasons why it can only preserve modified energy, and attempts to construct algorithms that preserve the original energy by leveraging the structure of the extended system.

09:15-10:00, September 11, Thursday

Low regularity Fourier integrators for some nonlinear dispersive equations

Yifei Wu

Nanjing Normal University, China

Abstract: In recent years, driven by practical considerations in modeling complex physical systems characterized by rough initial data and non-smooth potentials,there has been growing interest in developing numerical methods capable of handling low regularity scenarios. In this talk, some Fourier integrators are proposed for solving the KdV equation and the nonlinear Schrodinger equation, including the rough initial data

and non-smooth potentials. The designation of the scheme is based on the exponential-type integration, Splitting methods andthe Phase-Space analysis of the nonlinear dynamics.

10:20-11:05, September 11, Thursday

Explicit and CPU/GPU parallel energy-preserving schemes for the Klein-Gordon-Schrödinger equations

Wenjun Cai

Nanjing Normal University, China

Abstract: A highly efficient energy-preserving scheme for univariate conservative or dissipative systems was recently proposed in [Comput. Methods Appl. Mech. Engrg. 425 (2024) 116938]. This scheme is based on a grid-point partitioned averaged vector field (AVF) method, allowing for pointwise decoupling and easy implementation of CPU parallel computing. In this talk, we further extend this idea to multivariable coupled systems and propose a dual-partition AVF method that employs a dual partitioning strategy based on both variables and grid points. The resulting scheme is decoupled, energy-preserving, and exhibits greater flexibility. For the Klein-Gordon-Schr\"odinger equations, we apply the dual-partition AVF method and construct fully explicit energy-preserving schemes with pointwise decoupling, where the computational complexity per time step is $\mathcal{O}(N^d)$, with d representing the problem dimension and N representing the number of grid points in each direction. These schemes not only enable CPU parallelism but also support parallel computing on GPUs by adopting an update strategy based on a checkerboard grid pattern, significantly improving the efficiency of solving high-dimensional problems.

11:05-11:50, September 11, Thursday

Original-energy-dissipation-preserving methods for the incom-pressible Navier-Stokes equations

Yuezheng Gong

Nanjing University of Aeronautics and Astronautics, China

Abstract: This talk introduces a robust reformulation of the incompressible Navier-Stokes equations, establishing a foundational framework for designing efficient, structure-preserving algorithms that strictly conserve the original energy dissipation law. By leveraging Crank-Nicolson schemes and backward differentiation formulas, we develop four first- and second-order time-discrete schemes. These schemes exactly preserve the original energy dissipation law at each time step, requiring only the solutions of three linear Stokes systems and one 2×2 system of linear equations. Furthermore, the finite difference approximation on a staggered grid is employed for these time-discrete systems to derive fully discrete structure-preserving schemes. We rigorously prove that all proposed fully discrete methods both maintain the original energy dissipation law and admit unique solutions. Moreover, we present their efficient implementation. Extensive numerical experiments are carried out to verify the accuracy, efficacy, and advantageous performance of our newly developed methods.

08:30-09:15, September 12, Friday

A novel fully-decoupled energy stable scheme for the multiphase flow with variable density

Xiaoping Wang

The Chinese University of Hong Kong, Shenzhen, China

Abstract: We design an efficient and unconditionally energy stable method for simulating the dynamics of the multi-phase flow based on the Cahn-Hilliard-Navier-Stokes phase field model with variable density and

viscosity. An improved SAV type scheme is developed. We introduce some nonlocal auxiliary variables and associated ordinary differential equations to decouple the nonlinear terms. The resulting scheme is completely decoupled and unconditionally energy stable. The accuracy and stability of the algorithm are verified by extensive numerical simulation.

09:15-10:00, September 12, Friday

Some computations towards tokamak: multiscale methods and AI tools

Xiaofei Zhao

Wuhan University, China

Abstract:This talk presents my past and recent research works on simulations of tokamak. The multiscale methods to overcome the strong magnetic field will be presented firstly. Then, the prediction of tearing instabilities based on AI tools will discussed.

10:20-11:05, September 12, Friday

Decoupled and energy stable schemes for phase-field surfactant model based on mobility operator splitting technique

Nan Lu

Southern University of Science and Technology, China

Abstract: In this paper, we investigate numerical methods for the phase-field surfactant (PFS) model, which is a gradient flow system consisting of two nonlinearly coupled Cahn-Hilliard type equations. The main challenge in developing high-order efficient energy stable methods for this system results from the nonlinearity and the strong coupling in the two variables in the free energy functional. We propose two fully decoupled, linear and energy stable schemes based on a linear

stabilization approach and an operator splitting technique. We rigorously prove that both schemes can preserve the original energy dissipation law. The techniques employed in these schemes are then summarized into an innovative approach, which we call the mobility operator splitting (MOS), to design high-order decoupled energy stable schemes for a wide class of gradient flow systems. As a particular case, MOS allows different time steps for updating respective variables, leading to a multiple time-stepping strategy for fast-slow dynamics and thus serious improvement of computational efficiency. Various numerical experiments are presented to validate the accuracy, efficiency and other desired properties of the proposed schemes. In particular, detailed phenomena in thin-film pinch-off dynamics can be clearly captured by using the proposed schemes.

11:05-11:50, September 12, Friday

High-order mass- and energy-preserving methods for the Schrödinger-Poisson equation

Chaolong Jiang

Yunnan University of Finance and Economics, China

Abstract: In this talk, we first present a new arbitrarily high-order mass- and energy-conserving RK scheme in time for the Schrödinger-Poisson system. More specifically, by taking the partial differential derivative of the Poisson equation with respect to the time variable, we firstly reformulate the original system into an equivalent system. Then, the symplectic Runge-Kutta (RK) method is then employed to the new system in time. The resulting scheme is satisfies discrete versions of the mass and original energy of the system, and can achieve arbitrarily high-order accurate in time. Moreover, the classical Crank-Nicolson scheme method can be obtained as a special case of the proposed scheme. Subsequently, based on the exponential supplementary variable method, a novel mass- and energy-presenting integrating factor Runge-Kutta

method is presented. The proposed method only requires solving a constant-coefficient linear systems plus three algebraic equations efficiently solved by using the Newton iteration at every time step. Finally, various numerical results are addressed to verify the efficiency, accuracy and energy-preserving properties.

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