Day1: 2026 年 2 月 2 日 星期一

Recent Advances on Structure Preserving Schemes Using the Lagrange Multiplier Approach

沈捷
宁波东方理工大学

I will present some recent advances on the construction and analysis of Lagrange multiplier approach of efficient and accurate structure preserving schemes for a class of complex nonlinear systems with global (e.g., energy dissipation, norm conservation, etc.) constraints.

An Efficient Discontinuous Galerkin Framework with Exponential Bases for All-Electron Kohn-Sham Equation

徐岩
中国科学技术大学

With the growing interest in simulating phenomena such as Auger effects, all-electron density functional theory faces increasing computational challenges.In this paper, we propose a discontinuous Galerkin framework for both finite and periodic systems, in which the space is partitioned into atom-centered spheres and interstitial regions, with the wavefunctions described by polynomial and exponential radial basis with spherical harmonics and by plane waves, respectively. Towards reducing the computational complexity in discretization theoretically, several techniques have been designed.It is worth mentioning that the two issues from the LAPW methods, i.e. energy-parameter selection and continuity constraints can be overcame by our framework, which makes it more robust and systematically convergent. Compared with existing frameworks based on finite element methods, numerical experiments demonstrate a significant reduction in degrees of freedom alongside improved accuracy, making the method a competitive one in the market.

四阶问题的混合有限元方法

胡俊
北京大学

本报告围绕四阶偏微分方程的混合有限元方法展开，介绍基于 H(divdiv) 且 H(div) 协调对称张量有限元的构造、数值实现及其应用。在单纯形网格与长方体网格上系统构造了具有 H(divdiv) 且 H(div) 协调性的对称张量有限元空间，其基函数容易构造，且易于程序实现。

DUE: Deep Uknown Equations

吴开亮
南方科技大学

This talk introduces a deep learning framework and library called "DUE" for modeling unknown differential equations, along with the neural flow map methods for learning time-dependent differential equations from measurement data. We will present a range of data-driven modeling strategies using deep neural networks. In particular, we will show that residual networks are especially well-suited for unknown flow map learning, as they can serve as exact time integrators for numerical prediction. Furthermore, we will discuss deep learning approaches for identifying unknown partial differential equations in both modal and nodal spaces, as well as recent advances in structure-preserving learning techniques for unknown equations and Position-induced Transformer (PiT) for operator learning.

Machine-Learning Interatomic Potentials for Long-Range Systems

徐振礼
上海交通大学

Machine-learning interatomic potentials have emerged as a revolutionary class of force-field models in molecular simulations, delivering quantum-mechanical accuracy at a fraction of the computational cost and enabling the simulation of large-scale systems over extended timescales. However, they often focus on modeling local environments, neglecting crucial long-range interactions. We propose a Sum-of-Gaussians Neural Network (SOG-Net), a lightweight and versatile framework for integrating long-range interactions into machine learning force field. The SOG-Net employs a latent-variable learning network that seamlessly bridges short-range and long-range components, coupled with an efficient Fourier convolution layer that incorporates long-range effects. By learning sum-of-Gaussians multipliers across different convolution layers, the SOG-Net adaptively captures diverse long-range decay behaviors while maintaining close-to-linear computational complexity during training and simulation via non-uniform fast Fourier transforms. The method is demonstrated effective for a broad range of long-range systems.

爆轰问题的状态方程建模和保结构数值方法

赵伟峰
北京科技大学

气体爆轰是一类重要的流体力学问题，在国防和航空航天领域具有广泛应用。反应欧拉方程是描述爆轰问题的经典模型，属于典型的一阶双曲型偏微分方程，本报告将从偏微分方程适定性角度讨论爆轰问题的状态方程，提出一类新的非理想气体状态方程，证明在该状态方程下模型的适定性，并通过数值算例验证其有效性。进一步，基于适定性分析，构造了反应欧拉方程的熵稳定格式，该格式不仅对数学熵和热力学熵都满足熵稳定，并且保密度、压力和质量分数为正，数值算例表明格式对间断问题也有很好效果。

辐射输运方程的渐近保持显隐格式

付津雪
天津工业大学

辐射输运方程在大气物理、武器物理和惯性约束聚变中扮演着重要角色。然而，该方程因其高维度、多尺度、非线性和强刚性等特性，其数值求解面临着严峻的挑战。本报告主要介绍基于球谐函数方法框架的辐射输运方程的渐近保持显隐格式，格式的渐近保持性质及一系列的基准算例的数值结果。

一种用于模拟惯性约束聚变中 α 粒子输运的机器学习增强混合方法

刘畅
北京应用物理与计算数学研究所

α 粒子输运导致的等离子体加热是惯性约束聚变（ICF）中的主要自加热机制，它决定着靶丸内爆的性能。由于 α 粒子能量很高，同时 ICF 靶丸热点温度也很高，体系中存在显著的非平衡效应，连续介质力学在此情形下失效。为了在数值模拟中准确描述内爆过程及带电粒子输运，必须求解 Boltzmann 方程以捕捉动力学效应。然而，七维 Boltzmann 方程、高频库仑碰撞以及多重积分形式的阻止本领公式，严重限制了计算效率并对计算能力提出了巨大挑战。为克服高频库仑碰撞所带来的高计算代价，我们提出了一种混合碰撞模型，将碰撞划分为低频的大角度碰撞和高频的小角度擦碰。大角度碰撞过程基于库仑截面进行精确求解；而对于高频小角度擦碰，则构建了一种具有时间二阶精度的统计模型。该混合碰撞模型使散射计算的代价降低了两个数量级。针对多重积分形式的阻止本领计算，我们引入神经网络以提升计算效率。基于所提出的算法，我们开发了一维至三维的模块化程序，能够直接求解 α 粒子输运的 Boltzmann 方程。该 α 输运模块进一步集成至多物理量 LARED-S 程序中。所开发的 MC 版本 ICF 软件已通过对 N210207 和 N191110 实验的模拟研究得到验证。

Uniform Accuracy of Implicit-Explicit Methods for Linear Hyperbolic Relaxation Systems

马志婷
北京雁栖湖应用数学研究院

This work is concerned with the uniform accuracy of implicit-explicit methods for general linear hyperbolic relaxation systems satisfying the structural stability condition . We prove the uniform stability and accuracy of a class of implicit-explicit backward differentiation formulas (IMEX-BDF) and implicit-explicit Runge-Kutta (IMEX-RK) schemes discretized spatially by a Fourier spectral method. The result reveals that the accuracy of the fully discretized schemes is independent of the relaxation time in all regimes. It is verified by numerical experiments on several applications to traffic flows, rarefied gas dynamics and kinetic theory.

Day2: 2026 年 2 月 3 日 星期二

刚性神经元动力学方程的多尺度建模与快速数值模拟

周栋焯
上海交通大学

随着神经科学实验技术的进步，神经元活动数据的积累使得基于生物约束的大尺度神经网络建模成为可能。这类模型通常以描述神经元膜电位与离子通道动力学的非线性方程为核心，系统具有显著的刚性与多尺度特征。当进一步考虑树突的空间结构时，模型可自然扩展为时间刚性的非线性偏微分方程组，从而在时间步进稳定性与空间分辨率上带来严峻挑战。本报告从偏微分方程数值计算的角度出发，介绍针对神经元系统的多尺度建模框架与高效数值算法设计。通过在不同时间与空间尺度上的分离与近似，可显著提升大尺度网络的模拟效率，使基于实验数据约束的脑区级数值计算成为可能。该研究为刚性非线性系统的高效计算提供了新的思路，并为理解神经系统的动力学机制奠定了数学与计算基础。

The Jump Filter in the Discontinuous Galerkin Method for Hyperbolic Conservation Laws

夏银华
中国科学技术大学

When simulating hyperbolic conservation laws with discontinuous solutions, high-order linear numerical schemes often produce undesirable spurious oscillations. In this talk, we present the jump filter within the discontinuous Galerkin (DG) method to mitigate these oscillations. This filter operates locally based on jump information at cell interfaces, targeting high-order polynomial modes within each cell. Besides its localized nature, our proposed filter preserves key attributes of the DG method, including conservation, L2 stability, and high-order accuracy. We also explore its compatibility with other damping techniques, and demonstrate its seamless integration into a hybrid limiter. In scenarios featuring strong shock waves, this hybrid approach, incorporating this jump filter as the low-order limiter, effectively suppresses numerical oscillations while exhibiting low numerical dissipation. Special attention will also be given to steady-state simulations of the Euler equations, where conventional limiters may leave small post-shock oscillations that hinder residual convergence. By introducing transition zones between smooth regions and shock waves through moment-wise damping, the jump filter enables the residual to decrease to levels indistinguishable from machine zero. We also extend the discussion to unstructured meshes, where the jump filter is formulated using Dubiner polynomial bases associated with Sturm–Liouville operators.

高阶保正守恒重映方法与 ALE 计算

成娟
首都师范大学

任意拉格朗日 - 欧拉（ALE）方法在多介质流数值模拟中有着广泛的应用，设计高精度且保物理特性的 ALE 方法是计算流体力学中具有挑战性的重要课题。间接 ALE 方法包括三个步骤：拉格朗日步、网格重分步和物理量重映步。本报告中，我们将介绍有限体积和间断有限元框架下的高阶保正守恒重映方法的研究进展。进一步结合保持界面的网格重分策略与高精度保正拉格朗日格式，构建了高阶保正守恒 ALE 方法。数值算例验证了上述方法的有效性。

Energy-Stable Accelerated Optimization using Scalar Auxiliary Variables

毛志平
宁波东方理工大学

We propose a family of novel optimization algorithms by using the Scalar/Vector Auxiliary Variable (SAV) method. By reformulating the optimization process as ordinary differential equations, we construct Lyapunov energy functions that enables systematic incorporation of the SAV/VAV framework, leading to energy-stable discrete schemes. We also develop the adaptive extensions. Additionallyto enhance global exploration in highly nonconvex landscapes, we design a stochastic variant, combining ideas from Langevin dynamics and simulated annealing. The energy stability is guaranteed for all proposed methods.Extensive experiments on benchmark functions and deep learning tasks show that, overall, our methods outperform state-of-the-art optimizers in convergence speed, accuracy, and stability.

GPU-Centered Singular Value Decomposition and Eigen Decomposition

李会元
中国科学院软件研究所

Singular value decomposition (SVD) and generalized eigendecomposition (GED) fundamental tools in scientific and engineering compution, machine learning and data science. However, traditional SVD and GED computations are hindered by slow panel factorization, frequent CPU-GPU data transfers, inefficient memory access and workload imbalance on GPUs, despite advancements in GPU computational capabilities. In this talk we first introduce a GPU-centered SVD algorithm, incorporating a novel GPU-based bidiagonal divide-and-conquer (BDC) method. We reformulate the algorithm and data layout of different steps for SVD computation, performing all panel level computations and trailing matrix updates entirely on GPU to eliminate CPU-GPU data transfers. We further integrate related computations to optimize BLAS utilization, thereby increasing arithmetic intensity and fully leveraging the computational capabilities of GPUs. Additionally, we introduce a newly developed GPU-based BDC algorithm that restructures the workflow to eliminate matrix-level CPU-GPU data transfers and enable asynchronous execution between the CPU and GPU. At the same time, we discuss similar optimization techniques for the generalized eigendecomposition of dense symmetric-definite matrices. Particular focuses are set on Cholesky decomposition and SYR2K, multi-level pre-aggregation strategy for symmetric matrix-vector multiplication (SYMV) and general matrix-vector multiplication (GEMV). Experimental results on AMD MI210 and NVIDIA V100 GPUs demonstrate that our proposed method achieves speedups of up to 1293.64x/7.47x and 14.10x/12.38x compared to rocSOLVER/cuSOLVER and MAGMA, respectively. While experiments on AMD MI60 GPUs show that our optimized eigensolver outperforms the previous state-of-the-art with roughly 1.8x-3.8x speedups.

辐射输运流体系统跨尺度算法

唐敏
上海交通大学

辐射输运流体系统具有高维度、非线性、多尺度的特点。其中辐射输运方程包含 7 个维度；多尺度主要来源于光速和流体速度的尺度差异、介质对不同能级光子的散射吸收系数可以差 5 个以上数量级；非线性除了流体系统中的非线性，能量的普朗克分布和散射吸收系数中都包含关于温度的 3 或者 4 次方，甚至更强的非线性。为了解决模拟惯性约束核聚变数值模拟中耗时最多的高维辐射输运流体系统带来的挑战，报告介绍宏观微观分解的思路，并将这种思路一步步从能量变量处于平衡普朗克分布的黑体辐射输运方程推广到辐射输运和磁流体耦合系统、能量变量处于非平衡态的频率依赖辐射输运方程，讨论这些越来越复杂、越来越接近实际应用的高维系统中的大时空步长、低计算复杂度算法。

A Generalized SAV Approach for Nonlinear Dissipative Systems

黄富铿
宁波东方理工大学

In this talk, I will present the generalized SAV approach, which possessed the following attractive properties:1)It yields a long time uniform upper bound for the numerical solutions unconditionally; 2) It is applicable to general dissipative systems, not limited to gradient flow systems; 3)It enables the construction of arbitrarily high-order schemes with low computational cost. As an application, we construct the longtime stable schemes for the forced Navier-Stokes equations. Numerical examples will be presented to demonstrate the advantages of our approach. This talk is based on the joint works with Jie Shen, Xiaoming Wang, Ke Wu and Zhiguo Yang.

基于多项式混沌展开的不确定性量化数据驱动嵌套求积方法

周元诚
上海师范大学

针对随机输入信息有限且计算成本高昂的不确定性量化问题，我们提出了一种数据驱动的嵌套求积与多项式混沌方法。该方法结合任意多项式混沌构造和嵌套求积优化算法，能够处理

连续和离散概率测度，并利用稀疏网格实现高维计算。基于此理论，我们开发了一个模块化、可扩展的软件框架，能够在有限数据条件下高效完成随机 ODE 与 PDE 的不确定性量化分析，为工程和科学计算提供高效、可复用的数值工具。

A lattice Boltzmann Method with a Novel Conservative Boundary Scheme for Viscoelastic Fluid Flows

余愿
湘潭大学

The high Weissenberg number problem has been a persistent challenge in the numerical simulation of viscoelastic fluid flows. This paper presents an improved lattice Boltzmann method for solving viscoelastic flow problems at high Weissenberg numbers. The proposed approach employs two independent two-relaxation-time regularized lattice Boltzmann models to solve the hydrodynamic field and conformation tensor field of viscoelastic fluid flows, respectively. The viscoelastic stress computed from the conformation tensor is directly embedded into the hydrodynamic field using a newly proposed local velocity discretization scheme, thereby avoiding spatial gradient calculations. The constitutive equations are treated as convection-diffusion equations and solved using an improved convection-diffusion model specifically designed for this purpose, incorporating a novel auxiliary source term that eliminates the need for spatial and temporal derivative computations. Additionally, a conservative non-equilibrium bounce-back (CNEBB) scheme is proposed for implementing solid wall boundary conditions in the constitutive equations. The robustness of the present algorithm is validated through a series of benchmark problems. The simplified four-roll mill problem demonstrates that the method effectively improves numerical accuracy and stability in bulk regions containing stress singularities. The Poiseuille flow problem validates the accuracy of the current algorithm with the CNEBB boundary scheme at extremely high Weissenberg numbers (tested up to $\mathrm{Wi} = 10000$). The flow past a circular cylinder problem confirms the superior stability and applicability of the scheme for complex curved boundary problems compared to other existing common schemes.

Day3: 2026 年 2 月 4 日 星期三

Heterogeneous Multiscale Methods for Multiscale PDEs: Conception, Algorithm and Beyond

明平兵
中国科学院数学与系统科学研究院

We shall discuss the methodology of heterpgeneous multiscale metod (HMM) applying to multiscale partial differential equations, which is a framework for constructing and analyzing multiscale method. The focus is to design an efficient method to achieve high accuracy, which is based on an online-offline strategy. Arbitrary high accuracy may be achieved for deriving the macroscopic information. We shall also discuss HMM for the strain gradient elasticity model for heterogeneous media, which is a representative for the higher order elliptic system. This is a joint work with Yulei Liao (National University of Singapore) and Si Qi Song (AMSS).

Modeling Effects of Randomness in High Entropy Alloys

项阳
香港科技大学

High entropy alloys (HEAs) are single phase crystals that consist of random solid solutions of multiple elements in approximately equal proportions. This class of novel materials have exhibited superb mechanical properties, such as high strength which is associated with the motion of dislocations. We obtain a stochastic continuum model based on the Peierls-Nabarro framework for dislocations in an HEA from an atomistic model that incorporates the atomic level randomness and short-range order. This approach provides a fundamental explanation to the origin of the high strength of HEAs based on the stochastic effects on the intrinsic strength. We also develop a machine learning framework to unravel the complex relationship between chemical composition and materials properties in HEAs.

A Cartesian Grid-based Boundary Integral Method for Acoustic Scattering

应文俊
上海交通大学

We present a Cartesian grid method for homogeneous and inhomogeous scattering problems on complex domains. The method is a generalization of the traditional boundary integral method. It solves the scattering problem in the framework of boundary integral method but avoids direct evaluation of boundary and volume integrals. The evaluation is done by indirectly solving equivalent interface problems on Cartesian grids with fast solvers. For (exterior) problems on unbounded domains, we introduce an artificial circle or sphere to accelerate the solution of interface problems, while preserving accuracy. In the talk, we shall also present numerical examples to demonstrate the method.

张量神经网络及其应用

谢和虎
中国科学院数学与系统科学研究院

本报告介绍我们设计的张量型的神经网络结构，这种神经网络最重要的一个特点是可以将高维神经网络函数的积分转化成一维函数的积分，进而可以设计出高精度的高维积分方法，并且计算量是维数的多项式量级。接下来，我们利用张量神经网络可进行高精度高维积分的特点设计了求解高维问题的高精度机器学习算法，并将之应用于一些高维偏微分方程的求解。这里将关注高维的边值问题和特征值问题。报告的目的是想表明 Monte-Carlo 采样并不是机器学习求解高维问题的唯一途径，为大家带来更多的视角。

Day4: 2026 年 2 月 5 日 星期四

科学软件与人才培养

汤涛
广州南方学院

TBA

Temporal High-Order Parametric Finite Element Methods for Geometric Flows

苏春梅
清华大学

We propose a series of temporal high-order parametric finite element methods to simulate geometric flows. Particularly, for those flows with multiple geometric structures, e.g., surface diffusion which decreases the area and preserves the volume, we propose a type of structure-preserving methods by incorporating two scalar Lagrange multipliers and two evolution equations involving the area and volume, respectively. These schemes can effectively preserve the structure at a fully discrete level. Extensive numerical experiments demonstrate that our methods achieve the desired temporal accuracy, while simultaneously preserving the geometric structure of the surface diffusion.

Stability and Error Analysis of Fully Discrete Original Energy-Dissipative and Length-Preserving Scheme for the Landau-Lifshitz-Gilbert Equation

李晓丽
山东大学

In this talk, we first construct a linear and fully discrete finite difference numerical scheme, based on the projection method for the LLG equation, which is capable of simultaneously preserving the non-convex manifold constraint and an unconditional original energy dissipation. In the error analysis, the classical theoretical technique becomes ineffective, due to the presence of the nonlinear Laplacian term, which in turn poses a significant challenge. To overcome this subtle difficulty, we carefully rewrite the numerical method in an equivalent weak form, in which a point-wise length preserving feature of the numerical solution plays an essential role. Based on such a reformulation, a nonlinear Laplacian estimate is avoided, and the rest nonlinear error bounds could be derived with the help of discrete Sobolev interpolation, as well as a Law-of-Cosine style estimate of the numerical errors at the renormalization stage. As a result of these estimates in the reformulated weak form, an optimal convergence rate could be theoretically established. Some numerical experiments are presented to verify the theoretical findings and illustrate the robustness and effectiveness of the proposed method.

面向材料断裂模拟的新型有限元算法及其高性能计算

张继伟
武汉大学

非局部模型是基于非局部效应建立起来的数学物理模型，其中一个典型的范例是近场动力学，一直是计算数学领域研究的重要研究方向。全三维非局部模型的有限元实现涉及高维积分、巨大的计算量和存储量，因此在算法设计、网格生成、数据结构优化、面向 CPU 和 GPU 并行平台的算法架构等诸多方面都提出了巨大的计算挑战。本报告将简单介绍我们在近场动力学的基于切球策略的有限元高精度算法及其高性能实现等方面所做的努力和尝试，并将这些高性能有限元算法应用到基于近场动力学的材料断裂模拟。

北太天元科学计算与系统仿真软件介绍

刘浩洋
北京大学

北太天元科学计算与系统仿真软件是在北京大学数学科学学院、北京大学大数据分析与应用技术国家工程实验室、北京大学重庆大数据研究院的指导和支持下，由北京大学重庆大数据研究院基础软件科学研究中心自主研发的国内首款具有完全自主知识产权的科学计算平台。该软件聚焦科学计算领域“卡脖子”问题的解决，实现了科学计算领域根技术的突破。其具备强大的底层数学函数库，可提供科学计算、可视化、交互式程序设计功能，支持数值计算、数据分析、数据可视化、数据优化、算法开发等场景，并通过 SDK 与 API 接口，扩展支持各类学科与行业应用。目前软件已发布 2025 版本，已有 300 多所高校开展试用，提供 6 次学会大型赛事支持，获得中央电视台、重庆新闻联播等媒体宣传报道。本次报告将介绍其核心算法、技术与功能，并探讨未来可能的发展方向。

量子科学计算平台 UnitaryLab

胡俊鹏
上海酉术量子科技有限责任公司

UnitaryLab 是首个系统性集成偏微分方程求解等量子算法的量子科学计算平台，目标是开发面向科学与工程应用的量子算法，涵盖偏微分 / 常微分方程求解、数值线性代数、优化、机器学习、统计计算等领域，并通过量子算法突破经典计算的算力瓶颈，赋能科学与工程问题的高效求解。UnitaryLab 1.0 专注于解决科学与工程领域中广泛存在的偏微分方程量子计算难题。其基于上海交通大学量子科学计算团队原创的“薛定谔化”等系列算法，成功突破了传统求解方法的效率瓶颈，实现了“数学模型 → 量子算法 → 量子线路模拟”的全链路覆盖，为偏微分方程的量子计算提供了从开发工具到实际应用的全流程支持。

Traceability of Water Pollution: An Inversion Scheme Via Dynamic Complex Geometrical Optics Solutions

蔚辉
湘潭大学

We investigate the identification of the time-dependent source term in the diffusion equation using boundary measurements. This facilitates tracing back the origins of environmental pollutants. Employing the concept of dynamic complex geometrical optics (CGO) solutions, a variational formulation of the inverse source problem is analyzed, leading to a proof of uniqueness result. Our proposed two-step reconstruction algorithm first determines the point source locations and subsequently reconstructs the Fourier components of the emission concentration functions. Numerical experiments on simulated data are conducted. The results demonstrate that the proposed two-step reconstruction algorithm can reliably reconstruct multiple point sources and accurately reconstruct the emission concentration functions. Additionally, by partitioning the algorithm into online and offline computations, and concentrating computational demand offline, real-time pollutant traceability becomes feasible. This method, applicable in various fields - especially those related to water pollution, can identify the source of a contaminant in the environment, thus serving as a valuable tool in environmental protection.

Research on Structure-Preserving Numerical Methods for the Boltzmann Equation

尹天爱
宁波东方理工大学

We propose two classes of structure-preserving numerical schemes for the spatially homogeneous Boltzmann equation based on a Lagrange multiplier approach. In the first class, we develop partially structure-preserving schemes by introducing two Lagrange multipliers, each tailored to enforce positivity and entropy dissipation, respectively. Specifically, the multiplier $\lambda(t, \boldsymbol{v})$ is solved pointwise to guarantee positivity, while $\eta(t)$ is obtained from a nonlinear algebraic equation to ensure entropy dissipation. In the second class, we design a fully structure-preserving Lagrange multiplier method that simultaneously enforces entropy dissipation, positivity, and the exact conservation of mass, momentum, and energy within a unified framework. This approach requires solving a nonlinear algebraic system for the Lagrange multipliers, which is efficiently handled by a semi-smooth Newton method, rendering the additional computational cost of structure preservation negligible. Numerical experiments demonstrate the accuracy, stability, and structure-preserving properties of the proposed schemes, highlighting their effectiveness for kinetic simulations.

Day5: 2026 年 2 月 6 日 星期五

Adaptive Feature Capture Method for Solving Partial Differential Equations with near Singular Solutions

王筱平
香港中文大学（深圳）

We propose the Adaptive Feature Capture Method (AFCM), a novel machine learning framework that adaptively redistributes neurons and collocation points in high-gradient regions to enhance local expressive power. Inspired by adaptive moving mesh techniques, AFCM employs the gradient norm of an approximate solution as a monitor function to guide the reinitialization of feature function parameters. This ensures that partition hyperplanes and collocation points cluster where they are most needed, achieving higher resolution without increasing computational over- head. The AFCM extends the capabilities of RFM to handle PDEs with near-singular solutions while preserving its mesh-free efficiency. Numerical experiments demonstrate the method’s effectiveness in accurately resolving near-singular problems, even in complex geometries. By bridging the gap between adaptive mesh refinement and randomized neural networks, AFCM offers a robust and scalable approach for solving challenging PDEs in scientific and engineering applications.

AMG 解法器：从大规模到智能化

徐小文
北京应用物理与计算数学研究所

经过 40 多年的发展，代数多重网格（AMG）解法器已在科学工程计算与工业仿真领域得到广泛应用，在实际应用中取得了很大的成功。随着应用场景越来越丰富、计算规模越来越大，实际应用特征的复杂性和多样性越来越凸显，且伴随着动态演化特征，如何设计具有自动调优能力的智能 AMG 解法器是实际应用中非常关注的重要问题，其核心是自动地实现矩阵特征空间与 AMG 算法空间的最优映射。本报告介绍在智能 AMG 解法器方面的探索与实践。

偏微分方程通用数值库 AFEPack 及应用

胡光辉
澳门大学

报告将简要介绍偏微分方程通用型数值库 AFEPack 及相关应用，包括数值库的设计理念、数据结构及算法、网格自适应算法实现等等。应用部分，将针对计算流体、电子结构计算中前沿问题介绍 AFEPack 的使用情况。最后将介绍一个强化学习与 AFEPack 耦合使用的例子，展示 AFEPack 在人工智能时代的作用。

High-Dimensional Density Estimation

熊云丰
北京师范大学

Density estimation is one of the fundamental problems in statistics, the target of which is to learn the underlying density from the observed data in R^d. When d is low, it is easy to approximate the density by either the histogram and the kernel density estimation. However, these approaches might not be scaled easily to large d (e.g., d = 10, 20, 100) because of the well-known curse of dimensionality. In this talk, we would like to discuss a recently developed tree-based density estimation via controlling the discrepancy. This method uses several number-theoretic measures of the uniformity (or irregularity) of a sequence, including the star discrepancy, the mixed discrepancy or the moment estimation, to guide the tree-based partition and adaptive clustering of particles. The efficiency of such method for d = 2 to 30 is presented, which may give us some insight on the power of combinatorial techniques in boosting the statistical learning. Our motivation to study the adaptive density estimation comes from numerical resolution of high-dimensional PDEs. We will start from the negative particle method for solving PDEs in finance and quantum mechanics and point out that the density estimation is indispensable mainly for two reasons: First, the density estimation helps reconstruct the solution from the point clouds. Second, the density estimation can be used to cancel out the positive and negative particles and consequently alleviate the exponential growth of stochastic variances.

北京雁栖湖应用数学研究院
Beijing Institute of Mathematical Sciences and Applications

Zhiting Ma
Assistant Professor
Beijing Institute of Mathematical Sciences and Applications (BIMSA)
Email: mazt@bimsa.cn

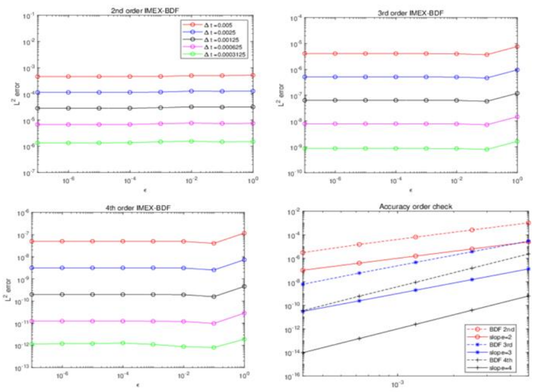
Research Interests

- Uniform accuracy of numerical schemes for multiscale hyperbolic systems
- Stability and compatibility analysis of hyperbolic relaxation equation
- Thermodynamics-based modeling of complex flows
- Physically constrained machine learning for PDE discovery

Representative Work

Uniform Accuracy of IMEX Schemes for Hyperbolic Relaxation Systems

Hyperbolic relaxation systems contain stiff source terms governed by small relaxation parameters, leading to severe accuracy degradation for standard time discretizations. We establish **the uniform stability and accuracy of a class of IMEX-BDF and IMEX-RK schemes** for general linear hyperbolic relaxation systems.



- Valid across non-stiff, stiff, and transitional regimes
- Theoretical proofs supported by numerical experiments

Academic Profile

- **Ph.D.** in Mathematics, Tsinghua University.
- Postdoctoral Researcher, Peking University
- Assistant Professor, BIMSA

Selected Publications

Uniformly Accurate IMEX Methods

1. **Z. Ma**, J. Huang, W.-A. Yong, *Uniform accuracy of implicit-explicit backward differentiation formulas (IMEX-BDF) for linear hyperbolic relaxation systems*, **Math. Comp**, 2025.
2. **Z. Ma**, J. Huang, *Uniform accuracy of IMEX Runge–Kutta methods for linear hyperbolic relaxation systems*, **J. Sci. Comput,** 2025.

Relaxation Limits and Multiscale Analysis

3. **Z. Ma**, W.-A. Yong, Y. Zhu, A thermodynamics-based turbulence model for isothermal compressible flows. 2025, arXiv:2504.18755.
4. **Z. Ma**, W. Zhao, *Validity of relaxation models arising from numerical schemes for hyperbolic-parabolic systems*. arXiv:2510.22923, 2025.
5. **Z. Ma**, W.-A. Yong, *Nonrelativistic limit of the Euler-HMP_N approximation models arising in radiation hydrodynamics*, **Math. Methods Appl. Sci.** 2023.
6. **Z. Ma**, *Navier-Stokes limit of globally hyperbolic moment equations*, **Kinet. Relat. Models**,2021.

Machine Learning for PDEs

7. J. Zhao, W. Zhao, **Z. Ma**, W.-A. Yong, B. Dong, *Finding models of heat conduction via machine learning*, **Int. J. Heat. Mass. Transf.** 2022.
8. J. Huang, **Z. Ma**, Y. Zhou, W.-A. Yong, *Learning thermodynamically stable and Galilean invariant partial differential equations for non-equilibrium flows*, **J. Non-Equilib. Thermodyn.** 2021.

Current & Ongoing Projects

- Uniform accuracy for nonlinear relaxation systems with high-order spatial discretizations
- Multiscale numerical methods for hyperbolic–parabolic coupling problems
- Thermodynamically consistent turbulence modeling
- Physically constrained machine learning for reduced-order PDE model

北京计算科学研究中心
BEIJING COMPUTATIONAL SCIENCE RESEARCH CENTER

Division of Mechanics

Yanli Wang's Group

Lab Members

Yanli Wang Principle Investigator
Report to duty: Aug. 2019
Ph.D in Mathematics, PKU, 2014

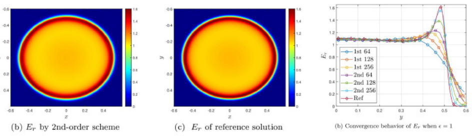
Yanli Wang's Group contains five postgraduate students in CSRC and three postgraduate (Ph.D candidate) students from SMS, PKU (Yixiao Lu, Shengtong Liang, Jie Wu)

Projects (2024-2025)

Interest: Model reduction in kinetic theory

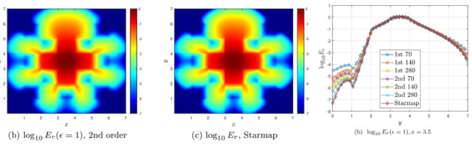
An AP IMEX PN method for the gray model of the radiative transfer equation

An asymptotic-preserving (AP) implicit-explicit PN numerical scheme is proposed for the gray model of the radiative transfer equation, where the first- and second-order numerical schemes are discussed for both the linear and nonlinear models.

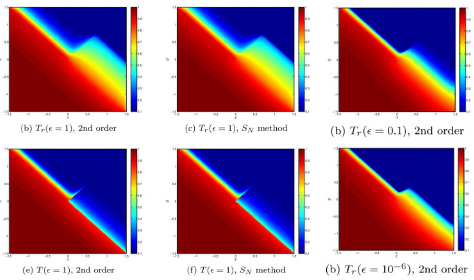


Line source problem

The AP property of this numerical scheme is proved theoretically and numerically, while the numerical stability of the linear model is verified by Fourier analysis. Several classical benchmark examples are studied to validate the efficiency of this numerical scheme.



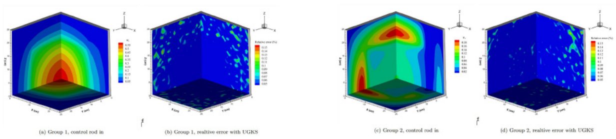
Lattice problem



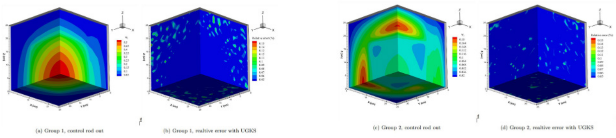
2D Riemann problem with different regimes

The unified gas kinetic wave-particle method for the neutron transport equation

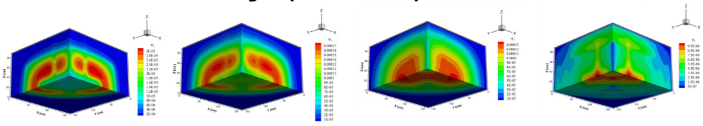
We present a unified gas-kinetic wave-particle (UGKWP) method for solving the neutron transport equation, addressing the inherent multiscale nature of neutron propagation in both optically thin and thick regimes. The UGKWP method couples macroscopic and microscopic transport processes within a unified time-dependent framework, where the microsopic transport particles are split into the collision and free-streaming part to further reduce the computational cost. Several numerical examples are studied to validate this method.



The KUCA core two-group benchmark problem (control rod in).



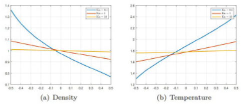
The KUCA core two-group benchmark problem (control rod out).



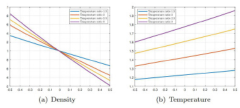
Four-group axially heterogeneous FBR

A fast Fourier spectral method for the linearized Boltzmann collision operator

We introduce a fast Fourier spectral method to compute linearized collision operators of the Boltzmann equation for variable hard-sphere gases. While the state-of-the-art method provides a computational cost O(MN4log N), with N being the number of modes in each direction and M being the number of quadrature points on a hemisphere, our method reduces the cost to O(N4log N), removing the factor M, which could be large in our numerical tests.



Fourier flow with different Kn



Fourier flow with different T ratio

Table 6: Numbers of Newton iterations for Fourier flows

	$\theta_R = 1.5$	$\theta_R = 2$	$\theta_R = 2.5$	$\theta_R = 3$
$Kn = 0.1$	3	4	4	5
$Kn = 1$	3	3	4	4
$Kn = 10$	2	2	3	3

different velocity

Papers (2024-2025)

1) R. Li, Y.X. Lu and **Y.L. Wang***. A highly efficient asymptotic preserving IMEX method for the quantum BGK model. Journal of Computational Physics,522(1): 113619, 2025.
2) J.X. Fu, J. Cheng, W.M. Li, T. Xiong and **Y.L. Wang***. An asymptotic-preserving IMEX PN method for the gray model of the radiative transfer equation. Journal of Scientific Computing, 103:71, 2025
3) J.T. Jiang, **Y.L. Wang**, Y.F. Wang, and H.H. Xie. FieldTNN-based machine learning method for Maxwell eigenvalue problems. Submitted, 2024 [arXiv:2411.15828].
4) G.W. Liu, L. Liu and Y.L. Wang. A bi-fidelity method for the uncertain Vlasov-Poisson system near quasineutrality in an asymptotic-preserving PIC framework. Submitted, 2024 [arXiv:2412.05663].
5) R. Li, W.M. Li, S.T. Liang, Y.H. Shao, M. Tang and **Y.L. Wang***. An asymptotic-preserving method for the three temperature radiative transfer equation. Submitted, 2024 [arXiv:2402.19191].
6) Z.N. Cai, R. Li, Y.X. Lu and **Y.L. Wang***. A Framework of Model Reduction with Arbitrary Orders of Accuracy for the Boltzmann Equation. Submitted, 2025 [arXiv:2505.11184].
7) T.A. Yin Z.N. Cai, and **Y.L. Wang***. A fast Fourier spectral method for the linearized Boltzmann collision operator. Submitted, 2025 [arXiv:2503.09580].

Funding

PI: Numeircal Simulation for Radiative Transfer Equation and Application in ICF，Foundation of Present of CAEP, ￥1200000, 01/2023-12/2025.
PI: Model Reduction and Numerical Simulation for Boltzmann Equation with Quadratic Collision Term，NSFC (Genergal Program), ￥580000, 01/2022-12/2025.
Co-PI: Numerical Methods and Analysis for Multiscale Kinetic Equations with Uncertainties, NSFC (Key Program, Joint with Prof. Shi Jin)，￥2490000, 01/2021-12/2025.

北京计算科学研究中心
BEIJING COMPUTATIONAL SCIENCE RESEARCH CENTER

A highly efficient asymptotic preserving IMEX method for the quantum BGK equation

R. Li, Y.X. Li, and **Y.L. Wang*** (ylwang@csrc.ac.cn)

Abstract

This paper presents an asymptotic preserving (AP) implicit-explicit (IMEX) scheme for solving the quantum BGK equation using the Hermite spectral method. The distribution function is expanded in a series of Hermite polynomials, with the Gaussian function serving as the weight function.
The main challenge in this numerical scheme lies in efficiently expanding the quantum Maxwellian with the Hermite basis functions. To overcome this, we simplify the problem to the calculation of polylogarithms and propose an efficient algorithm to handle it, utilizing the Gauss-Hermite quadrature. Several numerical simulations, including a spatially 2D lid-driven cavity flow, demon- strate the AP property and remarkable efficiency of this method.

Quantum Boltzmann equation

The quantum Boltzmann equation governs the time evolution of the phase-space density $f(t,\boldsymbol{x},\boldsymbol{v})$, representing the probability of finding a quantum particle at time $t \geqslant 0$ in the phase-space volume $\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{v}$. It has the form

$$\frac{\partial f}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} f = \frac{1}{\epsilon}\mathcal{Q}_{\mathrm{qBGK}}[f](\boldsymbol{v}), \quad t \geqslant 0, \quad \boldsymbol{x}\in\Omega\subset\mathbb{R}^D, \quad \boldsymbol{v}\in\mathbb{R}^D,$$

where ϵ is the Knudsen number, and D is the dimension. $\mathcal{Q}_{\mathrm{qBGK}}[f]$ is the quantum BGK model as

$$\mathcal{Q}_{\mathrm{qBGK}}[f](\boldsymbol{v}) = \mathcal{M}_q - f,$$

$\mathcal{M}_q$ represents the local equilibrium, also known as the quantum Maxwellian:

$$\mathcal{M}_q(t,\boldsymbol{x},\boldsymbol{v}) = \triangleq \frac{1}{|\theta_0|}\frac{1}{(z|\theta_0|)^{-1}\exp\left(\frac{(\boldsymbol{v}-\boldsymbol{u})^2}{2T}\right)+\mathrm{sign}(\theta_0)}$$
$$= \frac{1}{z^{-1}\exp\left(\frac{(\boldsymbol{v}-\boldsymbol{u})^2}{2T}\right)+\theta_0},$$

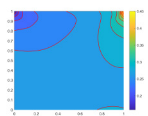
where $z|\theta_0| > 0$ represents the fugacity, and $T > 0$ is the temperature. $\mathcal{M}_q$ also satisfies $\mathcal{Q}_q[\mathcal{M}_q] = 0$. when $z\theta_0 = -1$, Bose-Einstein condensation occurs, and it has the form,

$$\widetilde{\mathcal{M}}_q(t,\boldsymbol{x},\boldsymbol{v}) = m_0\delta(\boldsymbol{v}-\boldsymbol{u}) + \frac{1}{|\theta_0|}\frac{1}{\exp\left(\frac{(\boldsymbol{v}-\boldsymbol{u})^2}{2T}\right)-1},$$

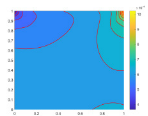
where m_0 is the critical mass, and $\delta(\cdot)$ is the Dirac delta function. For the Fermi gas ($\theta_0 > 0$), no additional constraint on z is required to obtain a quantum Maxwellian $\mathcal{M}_q$. If $\theta_0 = 0$, $\mathcal{M}_q$ reduces to the classical Maxwellian with macroscopic velocity $\boldsymbol{u}$ and temperature T:

$$\mathcal{M}_c^{\boldsymbol{u},T}(\boldsymbol{v}) = \frac{\rho}{(2\pi T)^{D/2}}\exp\left(-\frac{|\boldsymbol{v}-\boldsymbol{u}|^2}{2T}\right).$$

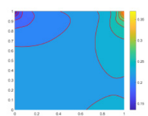
2D lid-driven cavity flow



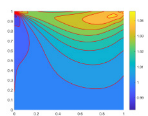
fugacity $z|\theta_0|$, $\theta_0 = 4$



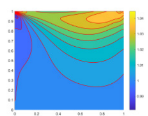
fugacity $z|\theta_0|$, $\theta_0 = 0.01$



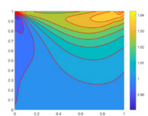
fugacity $z|\theta_0|$, $\theta_0 = 0.01$



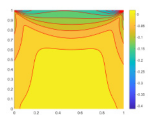
Temperature T, $\theta_0 = 4$



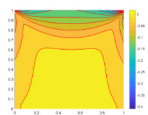
Temperature T, $\theta_0 = 0.01$



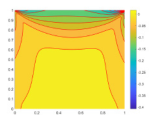
Temperature T, $\theta_0 = 0.01$



shear stress p_{12}, $\theta_0 = 4$



shear stress p_{12}, $\theta_0 = 0.01$



shear stress p_{12}, $\theta_0 = 0.01$

Hermite spectral method

The distribution function f is expanded as

$$f(t,\boldsymbol{x},\boldsymbol{v}) \approx \sum_{|\alpha|\leqslant M} f_\alpha(t,\boldsymbol{x})\mathcal{H}_\alpha^{\overline{\boldsymbol{u}},\overline{T}}(\boldsymbol{v}),$$

where $\mathcal{H}_\alpha^{\overline{\boldsymbol{u}},\overline{T}}(\boldsymbol{v}) = H_\alpha^{\overline{\boldsymbol{u}},\overline{T}}(\boldsymbol{v})\mathcal{M}_c^{\overline{\boldsymbol{u}},\overline{T}}(\boldsymbol{v})$ are the Hermite basis functions. The quantum Maxwellian is approximated as

$$\mathcal{M}_q(t,\boldsymbol{x},\boldsymbol{v}) \approx \sum_{|\alpha|\leqslant M}\mathcal{M}_{q,\alpha}(t,\boldsymbol{x})\mathcal{H}_\alpha^{\overline{\boldsymbol{u}},\overline{T}}(\boldsymbol{v}).$$

where M is the expansion order.

Expansion of the quantum Maxwellian

To obtain the expansion coefficients $\mathcal{M}_{q,\alpha}$, we only need to compute the coefficients

$$\mathcal{M}_\alpha = \int_{\mathbb{R}^D}\mathcal{M}_q(\boldsymbol{v})\boldsymbol{v}^\alpha\mathrm{d}\boldsymbol{v}, \qquad \boldsymbol{v}^\alpha = \prod_{d=1}^{D} v_d^{\alpha_d}, \qquad |\alpha| \leqslant M.$$

Then $\mathcal{M}_{q,\alpha}$ is calculated as

$$\mathcal{M}_{q,\alpha} = \sum_{\beta\in\mathbb{N}^D:\ \beta_i\leqslant\alpha_i} \mathcal{C}^{[\overline{\boldsymbol{u}},\overline{T}]}(\alpha,\beta)\mathcal{M}_\beta, \qquad |\alpha| \leqslant M.$$

When all entries of α are even, the expression of $\mathcal{M}_\alpha$ is given by

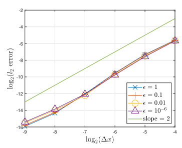
$$\mathcal{M}_\alpha = \int_{\mathbb{R}^D} z\exp\left(-\frac{\boldsymbol{v}^2}{2T}\right)\frac{\boldsymbol{v}^\alpha}{1+z\theta_0\exp\left(-\frac{\boldsymbol{v}^2}{2T}\right)}\mathrm{d}\boldsymbol{v}.$$

When $|z\theta_0| < 1$ and $\theta_0 \neq 0$, the expression of $\mathcal{M}_\alpha$ becomes

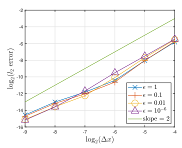
$$\mathcal{M}_\alpha = -\frac{\overline{\Gamma}\left(\frac{\alpha+1}{2}\right)}{\theta_0}(2T)^S\sum_{n=1}^{+\infty}\frac{(-z\theta_0)^n}{n^S}, \qquad S = \frac{|\alpha|+D}{2},$$

where $\overline{\Gamma}\left(\frac{\alpha+1}{2}\right) = \prod_{l=1}^{D}\Gamma\left(\frac{\alpha_l+1}{2}\right)$ and $\Gamma(\cdot)$ denotes the Gamma function.

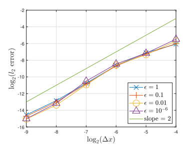
Numerical example: AP test



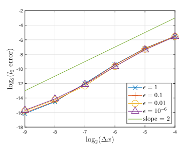
density ρ, $\theta_0 = 9$



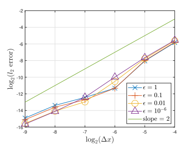
temperature T, $\theta_0 = 9$



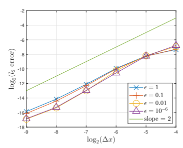
fugacity $z|\theta_0|$, $\theta_0 = 9$



density ρ, $\theta_0 = -9$



temperature T, $\theta_0 = -9$



fugacity $z|\theta_0|$, $\theta_0 = -9$

Reference: 1. R. Li, Y. Lu, Y. Wang. J. Comput. Phys. 2025.

北太天元

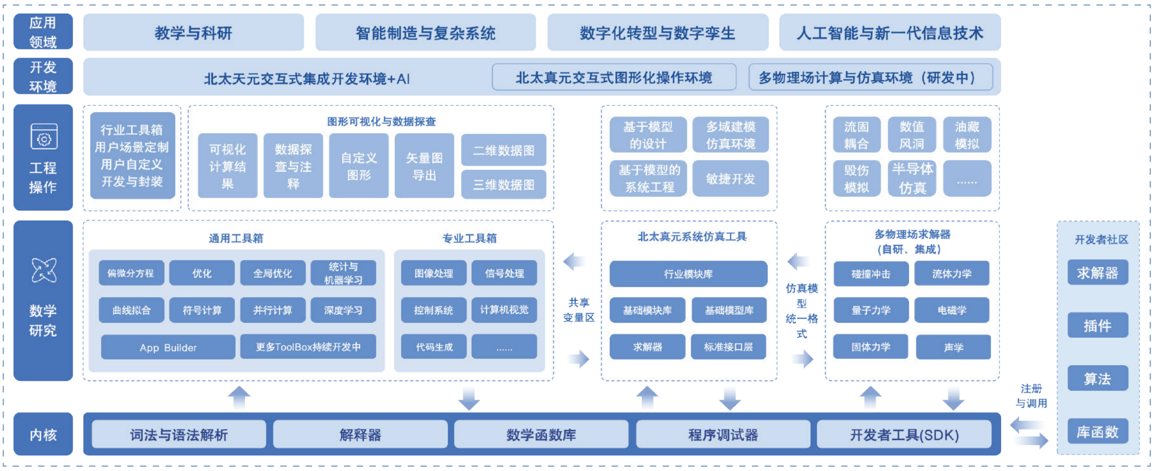
北太天元科学计算与系统仿真软件

北太振寰（重庆）科技有限公司（简称“北太振寰”）成立于2022年6月，是北京大学重庆大数据研究院基础软件科学研究中心孵化的科技型企业，总部位于重庆，在北京、成都设有全资子公司。

北太振寰致力于打造国产通用型科学计算与系统仿真软件，融合数学、物理、计算机、工业工程等多种学科的理论知识与实践经验，围绕国产自主知识产权的科学计算软件底层根技术，推动国内数学软件、工业软件、专业软件等核心关键软件的发展，积极构建以应用数学为基础的技术、应用与产业生态。

北太振寰已完成A轮融资，投后估值数亿元。

产品架构



产品竞争力

北太天元在国产通用型科学计算软件领域取得了核心技术突破，内核根技术完全自主可控，为国产科学计算软件发展提供了根本保障。

全面兼容MATLAB语法
全面兼容MATLAB语法，用户迁移“零成本”，交互体验无区别

数学函数库自主化
数学函数库自主化率已超过80%，确保了技术的安全可控

支持高性能科学计算任务
自研矩阵计算引擎与高性能数学库，支持多线程与GPU计算，全面覆盖科学计算场景底层需求

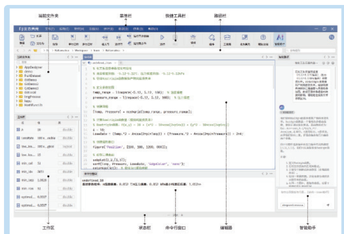
国产操作系统与硬件环境适配
支持麒麟、统信、龙芯、飞腾、摩尔线程等主流国产操作系统与硬件环境，支撑信创教育与工业的可持续发展

- 内核自主可控
- 自主科学计算解释型高级编程语言
- 科学计算能力
- 系统仿真能力
- 人工智能基础
- IDE交互
- 计算性能
- 兼容性

核心技术优势

● 软件界面

北太天元



北太真元