深圳北理莫斯科大学
УНИВЕРСИТЕТ МГУ–ППИ В ШЭНЬЧЖЭНЕ
SHENZHEN MSU–BIT UNIVERSITY

# 2024 深北莫偏微分方程数值算法研讨会

会议时间:2024 年 6 月 14-16 日

地点：深圳北理莫斯科大学主楼 336

主办单位：
深圳北理莫斯科大学计算数学与控制系；
莫大-北理-深北莫应用数学联合研究中心

# 日程安排

## June 14

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| 9:00-18:00 | Registration & discussion |
| 18:00-19:30 | Dinner |

## June 15

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| around 8:40 | Bus from hotel |
| Host：Ye Zhang<br>Opening remarks | |
| 09:00-09:30 | Kewei Liang, ZJU<br>深度学习在接触问题求解中的一些应用 |
| 09:30-10:00 | Xiaozhe Hu, Tufts University【Online】<br>Robust preconditioners for multi-physics problems |
| 10:00-10:30 | Fei Wang, XJTU<br>Local Randomized Neural Networks Methods for Interface Problems |
| 10:30-11:00 | Zhengfang Zhang, HDU<br>Multi-artificial neural network method for inverse eigenvalue problem of weighted Helmholtz equation |
| 11:00-11:15 | Coffee break |
| Host：Kewei Liang | |
| 11:15-11:45 | Shenggao Zhou, SJTU<br>Thermal Electrokinetics in Charging and Discharging Processes of Supercapacitors：Modeling and Computation |
| 11:45-12:15 | Daming Yuan, JXNU<br>S2 synthetic acceleration and positivity-preserving schemes for solving the neutron transport |
| 12:15-14:00 | Lunch |
| Host：Qinghua Ran | |
| 14:00-14:30 | Lele Yuan, LCU<br>Solving Inverse Problem of Distributed-Order Time-Fractional Diffusion Equations Using Boundary Observations and L^2 Regularization |
| 14:30-15:00 | Xing Shen, NetEase<br>Preconditioned Nonlinear Conjugate Gradient Method for Real-time Interior-point Hyperelasticity |
| 15:00-15:30 | Hailing Xuan, ZAFU<br>Error estimates and numerical simulations of a thermoviscoelastic contact problem with damage and long memory |
| 15:30-16:00 | Coffee break |
| Host：Ye Zhang | |

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| 16:00-16:30 | Xilu Wang, AHU<br>两类用变分-半变分不等式描述的弹性-刚性障碍模型 |
| 16:30-17:00 | Rongfang Gong, NUAA<br>Determining Sources in the Bioluminescence Tomography Problem |
| 17:00-17:30 | Prof. Xiaoliang Cheng, ZJU<br>回望四十年<br>Group photo |
| 18:00-19:30 | Dinner |

## June 16

| Host：Ye Zhang | |
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| 09:00-09:30 | Wensi Wang, ZJU<br>On a Navier-Stokes hemivariational inequality for incompressible fluid flows with damping |
| 09:30-10:00 | Ying-ao Wang, BIT<br>On a class of linear regression methods |
| 10:00-10:30 | You Sun, BIT<br>A concentration preserving discontinuous Galerkin method for nonlinear multi-component chromatography models |
| 10:30-12:00 | Discussion |

# 学术报告和摘要

（按报告顺序排序）

**深度学习在接触问题求解中的一些应用**

***Kewei Liang, ZJU***

聚焦于深度学习技术在求解接触问题中的应用，内容涵盖了从接触问题的正向求解，到接触反问题的求解。报告首先介绍深度学习在接触问题求解中的基本方法，然后探讨如何利用深度学习技术解决接触反问题。

**Robust preconditioners for multi-physics problems**

***Xiaozhe Hu, Tufts University***

We are interested in reliable simulations of some biophysical processes in the brain, such as blood flow and metabolic waste clearance. Modeling those processes results in interface-driven multi-physics problems that can be coupled across dimensions. However, the complexity of the interface coupling often deteriorates the performance of standard methods in finding the numerical solution. Therefore, based on the physics-based operator preconditioning framework, we design parameter-robust preconditioners that specifically target such multi-physics problems. Different techniques, such as rational approximations for fractional operators and specially tailored algebraic multigrid method that preserves the coupling information, are developed to handle the coupling that enforces interface constraints. We theoretically prove the parameter-robustness of the proposed preconditioners. We also present several numerical examples of realistic geometries, such as the viscous-porous flow coupling of the cerebrospinal fluid or the mixed-dimensional model of flow in vascularized brain tissue, to demonstrate their effectiveness and scalability in practical applications.

**Local Randomized Neural Networks Methods for Interface Problems**

***Fei Wang, XJTU***

Accurate modeling of complex physical problems, such as fluid-structure interaction, requires multiphysics coupling across the interface, which often has intricate geometry and dynamic boundaries. Conventional numerical methods face challenges in handling interface conditions. Deep neural networks offer a mesh-free and flexible alternative, but they suffer from drawbacks such as time-consuming optimization and local optima. In this talk, we introduce a mesh-free approach based on Randomized Neural Networks (RNNs), which avoid optimization solvers during training, making them more efficient than traditional deep neural networks. Our approach, called Local Randomized Neural Networks (LRNNs), uses different RNNs to approximate solutions in different subdomains. We discretize the interface problem into a linear system at randomly sampled points across the domain, boundary, and interface using a finite difference scheme, and then solve it by a least-square method.

For time-dependent interface problems, we use a space-time approach based on LRNNs. We show the effectiveness and robustness of the LRNNs methods through numerical examples of elliptic and parabolic interface problems. We also demonstrate that our approach can handle high-dimension interface problems. Compared to conventional numerical methods, our approach achieves higher accuracy with fewer degrees of freedom, eliminates the need for complex interface meshing and fitting, and significantly reduces training time, outperforming deep neural networks.

### *Multi-artificial neural network method for inverse eigenvalue problem of weighted Helmholtz equation*

***Zhengfang Zhang, HDU***

The inverse eigenvalue problem for a weighted Helmholtz equations is investigated. The density function is recovered from the observation of the limited spectral data. The inverse eigenvalue problem is reformulated as an optimization problem, and a multi-objective loss function is defined accordingly. A multi-artificial neural network (multi-ANN) algorithm is proposed. The properties of the existence and stability of the solution to the optimization problem and the convergence of the multi-ANN solution to the solution to the optimization problem are proved. The numerical results of one-dimensional and two-dimensional inverse eigenvalue problems of the weighted Helmholtz equation are given. Compared with the traditional finite element method, the robustness and effectiveness of the proposed multi-ANN method are illustrated.

### **Thermal Electrokinetics in Charging and Discharging Processes of Supercapacitors：Modeling and Computation**

***Shenggao Zhou, SJTU***

This work proposes a new variational, thermodynamically consistent model to predict thermal electrokinetics in supercapacitors by using an energetic variational approach. The least action principle and maximum dissipation principle from the non-equilibrium thermodynamics are employed to develop modified Nernst-Planck equations for non-isothermal ion transport with temperature inhomogeneity. Laws of thermodynamics are employed to derive a temperature evolution equation with heat sources due to thermal pressure and electrostatic interactions. Property-preserving numerical schemes are discussed as well. Numerical simulations successfully predict temperature oscillation in the charging-discharging processes of supercapacitors, indicating that the developed model is able to capture reversible and irreversible heat generations. The impact of ionic sizes and scan rate of surface potential on ion transport, heat generation, and charge current is systematically assessed in cyclic voltammetry simulations. It is found that the thermal electrokinetics in supercapacitors cannot follow the surface potential with fast scan rates, showing delayed dynamics with hysteresis diagrams. Our work thus provides a useful tool for physics-based prediction of thermal electrokinetics in EDLCs. This is a joint work with Xiang Ji, Jie Ding, Pei Liu, and Chun Liu.

**S2 synthetic acceleration and positivity-preserving schemes for solving the neutron transport equation**

***Daming Yuan, JXNU***

For the numerical solution of neutron transport equations, both the positivitypreserving property and speeding up the iterative convergence are important and challenging issues. In this work, the combination of the S2 synthetic acceleration method and a positivity-preserving scheme are derived and analyzed. For the neutron transport and the S2 equations, we discretize them by the linear discontinuous differencing scheme and apply linear scaling limiter to obtain the non-negative solution. The limiter is simple to implement. Numerical results for solving optically thick problems verify the efficiency of the proposed schemes.

**Solving Inverse Problem of Distributed-Order Time-Fractional Diffusion Equations Using Boundary Observations and L^2 Regularization**

***Lele Yuan, LCU***

This article investigates the inverse problem of estimating the weight function using boundary observations in a distributed-order time-fractional diffusion equation. We propose a method based on L^2 regularization to convert the inverse problem into a regularized minimization problem, and we solve it using the conjugate gradient algorithm. The minimization functional only needs the weight to have L^2 regularity. We prove the weak closedness of the inverse operator, which ensures the existence, stability, and convergence of the regularized solution for the weight in L^2 (0, 1). We propose a weak source condition for the weight in C[0, 1] and, based on this, we prove the convergence rate for the regularized solution. In the conjugate gradient algorithm, we derive the gradient of the objective functional through the adjoint technique. The effectiveness of the proposed method and the convergence rate are demonstrated by two numerical examples in two dimensions.

**Preconditioned Nonlinear Conjugate Gradient Method for Real-time Interior-point Hyperelasticity**

***Xing Shen, NetEase***

In the field of computer graphics, the Incremental Potential Contact (IPC) method has emerged as a powerful tool utilizing the barrier function from interior-point methods for robust, accurate, and differentiable simulations in elastodynamics and contact scenarios.This method has the capability to consistently produce high-quality results for codimensional solids across a wide range of scenarios, ensuring interpenetration-free simulations. This method has been successfully applied in various areas. We will provide a overview of IPC from the perspective of numerical solutions of partial differential equations. Additionally, we introduce our preconditioned nonlinear conjugate gradient method, which further enhances the capabilities of IPC. Our method can accurately simulate objects comprising over 100,000 elements in complex self-collision scenarios at real-time speeds.

## Error estimates and numerical simulations of a thermoviscoelastic contact problem with damage and long memory

***Hailing Xuan, ZAFU***

This report aims to investigate a thermal frictional contact model with damage and long memory effects. We consider a deformable body made of viscoelastic material and assume the process to be dynamic.

The material is expected to adhere to the Kelvin-Voigt constitutive law, with damage and thermal effects incorporated. The variational formulation of the model results in a coupled system comprising a history-dependent hemivariational inequality governing the displacement field, a parabolic variational inequality describing the damage field and an evolution equation for the temperature field. In the analysis of this system, we initially introduce a fully discrete scheme, and then concentrate on deriving error estimates of numerical solutions. An optimal order error estimate is attained under some appropriate solution regularity assumptions. Numerical simulations are provided for the contact problem to validate the theoretical results.

## 两类用变分-半变分不等式描述的弹性-刚性障碍模型

***Xilu Wang, AHU***

论文《Numerical analysis for a new kind of obstacle problem》中提出一类新的弹性-刚性障碍模型，推导出模型的变分不等式并进行了理论分析与数值求解。

基于上述论文模型，当障碍对弹性膜的反作用力与弹性膜向弹性-刚性障碍渗入的距离呈不单调多值关系时，只能在半变分不等式框架下进行研究。

本次报告聚焦半变分不等式在障碍问题中的应用，分别给出椭圆型和抛物型障碍模型对应的变分-半变分不等式的理论分析与数值求解。此时，反映不单调多值关系的 Clarke 次微分项处于整个区域，而非常见的区域边界。

## Determining Sources in the Bioluminescence Tomography Problem

***Rongfang Gong, NUAA***

In this talk, we revisit the bioluminescence tomography (BLT) problem, where one seeks to reconstruct bioluminescence signals (an internal light source) from external measurements of the Cauchy data. As one kind of optical imaging, the BLT has many merits such as high signal-to-noise ratio, non-destructivity and cost-effectiveness etc., and has potential applications such as cancer diagnosis, drug discovery and development as well as gene therapies and so on. In the literature, BLT is extensively studied based on diffusion approximation equation, where the distribution of peak sources is to be reconstructed and no solution uniqueness is guaranteed without adequate a priori information. Motivated by the solution uniqueness issue, several theoretical results are explored. The major contributions in this talk that are new to the literature are two-fold: first, we show the theoretical uniqueness of the BLT problem where the light sources are in the shape of

$C^2$ domains or polyhedral- or corona-shaped; second, we support our results with plenty of problem-orientated numerical experiments.

**On a Navier-Stokes hemivariational inequality for incompressible fluid flows with damping**

***Wensi Wang, ZJU***

In this paper, a Navier-Stokes hemivariational inequality is studied for incompressible fluid flows with the damping effect. The hemivariational inequality feature is caused by the presence of a nonsmooth slip boundary condition of friction type. Well- posedness of the Navier-Stokes hemivariational inequality is established through the consideration of a minimization problem. Mixed finite element methods are introduced to solve the Navier-Stokes hemivariational inequality and error estimates are derived for the mixed finite element solutions. The error estimates are of optimal order for low-order mixed element pairs under suitable solution regularity assumptions. Efficient solution algorithms are introduced to solve the mixed finite element system. Numerical results are reported on the performance of the algorithms.

**On a class of linear regression methods**

***Ying-ao Wang, BIT***

This presentation introduces a new class of linear regression methods defined by a generator function, offering improved accuracy over traditional approaches. The proposed methods, including Landweber, Showalter, Heavy Ball with Friction, and Second Order Asymptotic regression, exhibit strong consistency and reduced mean squared error. Numerical experiments on both uniformly distributed synthetic data and the Cancer Cell Line Encyclopedia (CCLE) dataset demonstrate the efficacy of these methods in prediction tasks, though at a higher computational cost. Future work aims to extend these methods to infinite-dimensional cases and debiased regression.

**A concentration preserving discontinuous Galerkinmethod for nonlinear multi-component chromatography models**

***You Sun, BIT***

The mass balance equations for liquid chromatography consist of nonlinear convection dominated partial differential equations. This talk includes designing, analyzing and numerically validating a concentrations preserving discontinuous Galerkin method for solving various multi-component chromatographic models. The semi-discrete formulation is shown to preserve the concentrations of all components in both mobile and stationary phase. The numerical experiments demonstrate optimal rates of convergence. In this talk, it also shows that the shape of the solution, after long time simulation, is well preserved due to the invariant preserving property.