



# 14th SIAM Student Chapter Symposium at NUS

**Date:** April 24, 2025

Venue: S17-04-04, Department of Mathematics, NUS

**Organizer: SIAM Student Chapter at NUS** 

Homepage: https://siamnus.github.io/website/

## **Organizing Committee:**

Prof. Bao Weizhu (<u>matbaowz@nus.edu.sq</u>, Faculty Advisor)

• Mr. Liu Shuigen (<a href="mailto:shuigen@u.nus.edu">shuigen@u.nus.edu</a>, President)

• Ms. Liu Shuya (e0675581@u.nus.edu, Vice President)

• Mr. Hou Di (dihou@u.nus.edu, Secretary)



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### **Plenary Speaker:**

- Prof. Ren Weiging, Department of Mathematics
- Prof. Cai Zhenning, Department of Mathematics

## **Student Speaker:**

- Mr. Cheng Jingpu, Department of Mathematics
- Dr. Lin Xiaotong, Department of Statistics and Data Science
- Mr. Chen Junyu, Department of Mathematics
- Dr. Wang Shiwei, Institute of Operational Research and Analytics
- Ms. Sun Yixiao, Department of Mathematics
- Mr. Zhang Yulin, Department of Mathematics (SJTU)
- Mr. Zhou Tao, Department of Mathematics
- Mr. Lyu Runcao, Department of Mathematics

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# **Program:**

14th SIAM Student Chapter Symposium at NUS			
April 24, 2025 (S17-04-04)			
Time	Title	Name	
8:55–9:00 AM	Opening Remarks		
Chair: Liu Shuigen			
9:00–9:45 AM	Plenary Talk: On the Holway-Weiss debate on smooth shock profiles in Grad's moment method	Cai Zhenning	
9:45–10:15 AM	Universal Approximation in Deep Neural Networks: A Controllability Approach	Cheng Jingpu	
10:15–10:45 AM	Hypothesis Testing in Gaussian Graphical Models: Novel Goodness-of-Fit Tests and Conditional Randomization Tests	Lin Xiaotong	
10:45–11:00 AM	Coffee Break		
Chair: Hou Di			
11:00–11:30 AM	Semidefinite Relaxations of the Gromov-Wasserstein Distance	Chen Junyu	
11:30–12:00 PM	A Minimization Approach for Minimax Optimization with Coupled Constraints	Wang Shiwei	
12:00–2:00 PM	Lunch Break		
Chair: Liu Shuya			
2:00–2:45 PM	Plenary Talk: Modelling rare events in complex systems	Ren Weiqing	
2:45–3:15 PM	Tensor Train Representation of the Bath Influence Functional for Inchworm Simulation of Open Quantum Systems	Sun Yixiao	







3:15–3:45 PM	A generalized structure-preserving parametric finite element method for anisotropic curvature flows on closed curves	Zhang Yulin	
3:45–4:00 PM	Coffee Break		
Chair: Cheng Jingpu			
4:00–4:30 PM	Nonradial stability of self-similar blowup to Keller-Segel equation in three dimensions	Zhou Tao	
4:30–5:00 PM	Graphical solutions to fractional Laplacian free boundary problems	Lyu Runcao	







### **Abstracts**

# On the Holway-Weiss debate on smooth shock profiles in Grad's moment method

### **Prof. Cai Zhenning**

Department of Mathematics, NUS

Grad's moment method is a classical modeling technique to approximate the Boltzmann equation in the gas kinetic theory. Despite its simplicity and flexibility, the method is known to suffer from several shortcomings, including the loss of hyperbolicity and the prediction of unphysical subshocks in shock profiles. These issues are well known and broadly acknowledged. However, there is another possible issue that spurred some arguments in the history of moment methods. In a seminal 1965 paper, Holway argued that there is an upper bound on the Mach number beyond which smooth shock profiles do not exist for all Grad's moment equations. However, more than three decades later, Weiss challenged this claim, arguing that this restriction does not exist. In this talk, we will revisit the debate, discuss their findings, and explain that both arguments have a correct and an incorrect part. Inspired by the debate, we will present a new strategy to improve Grad's moment method.

# Modelling rare events in complex systems Prof. Ren Weiging

Department of Mathematics, NUS

Many problems in applied sciences can be abstractly formulated as systems navigating over complex energy landscapes. Well-known examples include conformational changes of biomolecules, chemical reactions, nucleation events during phase transitions, and extreme events in some cases that lead to material or system failure, etc. These events happen infrequently relative to the relaxation timescale of the system, but when they do happen, they usually happen rather







quickly and have important consequences. In this talk, I will discuss numerical methods for the study of such rare events, including the string method and the recently developed machine learning techniques.

# Universal Approximation in Deep Neural Networks: A Controllability Approach

### Mr. Cheng Jingpu

Department of Mathematics, NUS

This talk explores the expressive power of deep ResNets and transformers through the lens of control theory. By idealizing deep ResNets as continuous-time control systems, we reformulate interpolation and approximation as controllability problems, establishing general universal approximation results that hold independent of specific architectural choices. Extending this approach to transformers, we derive a general and verifiable condition for their universal approximation capability, applicable to a range of practical architectures and useful for guiding the design of new architectures.

## Hypothesis Testing in Gaussian Graphical Models: Novel Goodness-of-Fit Tests and Conditional Randomization Tests

## Dr. Lin Xiaotong

Department of Statistics and Data Science, NUS

We introduce novel hypothesis testing methods for Gaussian graphical models, whose foundation is an innovative algorithm that generates exchangeable copies from these models. We utilize the exchangeable copies to formulate a goodness-of-fit test, which is valid in both low and high-dimensional settings and flexible in choosing the test statistic. This test exhibits superior power performance, especially in scenarios where the true precision matrix violates the null hypothesis with many small entries. Furthermore, we adapt the sampling algorithm for constructing a new conditional randomization test for the conditional independence between a response Y and a vector







of covariates X given some other variables Z. Thanks to the model-X framework, this test does not require any modeling assumption about Y and can utilize test statistics from advanced models. It also relaxes the assumptions of conditional randomization tests by allowing the number of unknown parameters of the distribution of X to be much larger than the sample size. For both of our testing procedures, we propose several test statistics and conduct comprehensive simulation studies to demonstrate their superior performance in controlling the Type-I error and achieving high power. The usefulness of our methods is further demonstrated through real-world applications.

# Semidefinite Relaxations of the Gromov-Wasserstein Distance Mr. Chen Junyu

#### Department of Mathematics, NUS

The Gromov-Wasserstein (GW) distance is an extension of the optimal transport problem that allows one to match objects between incomparable spaces. At its core, the GW distance is specified as the solution of a non-convex quadratic program and is not known to be tractable to solve. In particular, existing solvers for the GW distance are only able to find locally optimal solutions. In this work, we propose a semi-definite programming (SDP) relaxation of the GW distance. The relaxation can be viewed as the Lagrangian dual of the GW distance augmented with constraints that relate to the linear and quadratic terms of transportation plans. In particular, our relaxation provides a tractable (polynomial-time) algorithm to compute globally optimal transportation plans (in some instances) together with an accompanying proof of global optimality. Our numerical experiments suggest that the proposed relaxation is strong in that it frequently computes the globally optimal solution. Our Python implementation is available at <a href="https://github.com/tbng/gwsdp">https://github.com/tbng/gwsdp</a>.







# A Minimization Approach for Minimax Optimization with Coupled Constraints

#### Dr. WANG Shiwei

#### Institute of Operational Research and Analytics, NUS

In this talk, we focus on the nonconvex-strongly-concave minimax optimization problem (MCC), where the inner maximization subproblem contains constraints that couple the primal variable of the outer minimization problem. Based on the nondegeneracy of the coupled constraints, we prove that by introducing the dual variable of the inner maximization subproblem, (MCC) has the same first-order minimax points as a nonconvex-strongly-concave minimax optimization problem without coupled constraints (MOL). We then extend our focus to a class of nonconvex-strongly-concave minimax optimization problems (MM) that generalize (MOL). By performing the partial forward-backward envelope to the primal variable of the inner maximization subproblem, we propose a minimization problem (MMPen), where its objective function is explicitly formulated. We prove that the first-order stationary points of (MMPen) coincide with the first-order minimax points of (MM). Therefore, various efficient minimization methods and their convergence guarantees can be directly employed to solve (MM), hence solving (MCC) through (MOL). Preliminary numerical experiments demonstrate the great potential of our proposed approach.

# Tensor Train Representation of the Bath Influence Functional for Inchworm Simulation of Open Quantum Systems

#### Ms. Sun Yixiao

#### Department of Mathematics, NUS

We propose a method for simulating non-Markovian open quantum systems by combining the inchworm framework with deterministic numerical quadrature and tensor train (TT) approximation.

The inchworm algorithm enables efficient real-time propagation by recursively constructing short-time propagators. To evaluate the resulting high-dimensional integrals, we represent the integrand—including the costly bath influence functional (BIF), which can be expressed as a sum of products of two-point correlation (TPC) functions—in TT format and contract the TT cores





sequentially. This TT-based structure avoids the curse of dimensionality and allows the method to scale efficiently with the integral dimension. The precomputed BIF-TT can also be reused for different system Hamiltonians. Numerical results confirm the accuracy and efficiency of the approach.

# A generalized structure-preserving parametric finite element method for anisotropic curvature flows on closed curves

### Mr. Zhang Yulin

Department of Mathematics, SJTU

In this talk, we propose and analyze a structure-preserving parametric finite element method (SP-PFEM) for the evolution of a closed curve under anisotropic curvature flow with surface energy density  $\gamma(\theta)$ . The proposed method introduces a surface energy matrix  $G_k^{\alpha}(\theta)$  with a parameter  $\alpha$  and a stabilizing function  $k(\theta)$ , which leads to a conservative weak formulation. By selecting different values of  $\alpha$ , we obtain weak forms that degenerate into various formulations proposed in previous research. The full discretization via SP-PFEM of the conservative weak form rigorously preserves the conservation of enclosed area. We provide a detailed analysis of the unconditional energy stability of SP-PFEM with respect to different values of the parameter  $\alpha$ .

# Nonradial stability of self-similar blowup to Keller-Segel equation in three dimensions

### Mr. Zhou Tao

#### Department of Mathematics, NUS

In three dimensions, the parabolic-elliptic Keller-Segel system exhibits a rich variety of singularity formations. Notably, it admits an explicit self-similar blow-up solution whose radial stability, conjectured more than two decades ago in [Brenner-Constantin-Kadanoff-Schenkel-Venkataramani, 1999], was recently confirmed by [Glogić-Schörkhuber, 2024]. This paper aims to extend the radial stability to the nonradial setting, building on the finite-codimensional stability







analysis in our previous work [Li-Zhou, 2024]. The main input is the mode stability of the linearized operator, whose nonlocal nature presents challenges for the spectral analysis. Besides a quantitative perturbative analysis for the high spherical classes, we adapted in the first spherical class the wave operator method of [Li-Wei-Zhang, 2020] for the fluid stability to localize the operator and remove the known unstable mode simultaneously. Our method provides localization beyond the partial mass variable and is independent of the explicit formula of the profile, so it potentially sheds light on other linear nonlocal problems. This talk is based on the joint work with Zexing Li.

# Graphical solutions to fractional Laplacian free boundary problems Mr. Lyu Runcao

Department of Mathematics, NUS

TBD.