## SIAM Student Chapter @NUS

## 9<sup>th</sup> Symposium on Applied and Computational Mathematics

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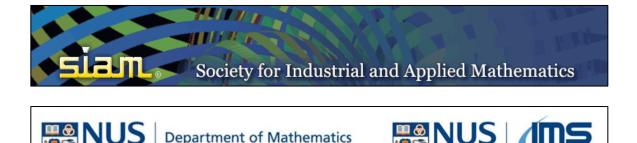
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**Faculty of Science** 



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Mathematical Sciences

### Date & Venue

- 17 June 2020, Wednesday
- Zoom
   Join Zoom Meeting:
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   <u>sg.zoom.com.cn/j/6683843602?pwd=cnJFOXFCTU1PU2NGa</u>
   <u>VFRZk0vY1FOUT09</u>
   Meeting ID: 668 384 3602 Password: NUS0617

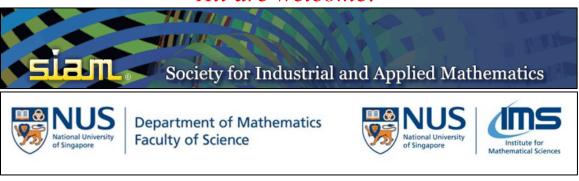
### Sponsors

- Society of Industrial and Applied Mathematics (SIAM)
- National University of Singapore (NUS)

### Guest Speakers

- Prof. Christine A. Shoemaker, Department of Industrial Systems Engineering & Management and Department of Civil and Environmental Engineering
- Prof. Xinliang An, Department of Mathematics
- Dr. Simon Etter, Department of Mathematics
- Dr. Quan Zhao, Department of Mathematics
- Dr. Yang Kuang, Department of Mathematics
- Mr. Weixi Wang, Department of Mathematics
- Mr. Shuaijie Qian, Department of Mathematics
- Ms. Xizhi Su, Department of Mathematics

# All are welcome!



# Programme

Time	Guest Speaker	Talk Title/Topic Series
08:50-09:00	Opening Remarks	
09:00-10:00	Prof. Christine A. Shoemaker	Using Mathematics, Computers and Data to An- alyze Societal Problems and How I Got There after My B.S. in Mathematics • Optimization
10:00-10:10		Break
10:10-11:10	Prof. Xinliang An	<ul> <li>Polynomial Blow-up Upper Bounds for the Einstein-scalar Field System under Spherical Symmetry</li> <li>Partial Differential Equation, General Relativity</li> </ul>
11:10-11:50	Dr. Simon Etter	Rational Matrix Functions for Electronic Struc- ture Theory • Computational Physics
11:50-13:30		Lunch & Noon Break
13:30-14:10	Dr. Quan Zhao	An Energy-stable Finite Element Method for the Simulation of Moving Contact Lines in Two-phase Flows • Computational Physics
14:10-14:50	Dr. Yang Kuang	Numerical Investigations of Complex Langevin Dynamics • Computational Physics
14:50-15:30	Mr. Weixi Wang	Some Theoretical Results of Kernel Recovery in Blind Deconvolution • Image Processing
15:30-15:40	Break	
15:40-16:20	Mr. Shuaijie Qian	Non-concave Portfolio Optimization without the Concavification Principle • Mathematical Finance
16:20-17:00	Ms. Xizhi Su	<ul><li>Portfolio Selection Under Partial Information and Relative Performance Concerns</li><li>Mathematical Finance</li></ul>

### Using Mathematics, Computers and Data to Analyze Societal Problems and How I Got There after My B.S. in Mathematics

#### Christine A. Shoemaker

#### Abstract

During my undergraduate and PHD years as a mathematics student, I wondered if my choice of mathematics as a major truly fit my interests. I loved mathematics, but also wanted to do something that would contribute to society. I will discuss the evolution of my career and the steps in the decision process that lead eventually to professorships in US and Singapore where my research focuses on application of optimization and computational mathematics to societal problems including environmental protection and efficient solutions to engineering problems. (Talk about 15 minutes)

I will describe my group's current research focuses on computational methods for optimization of "black box" computer simulation models using surrogate global optimization algorithms my research group has developed that is in our software toolbox pySOT (88,000 downloads in Github). Being able to solve such optimization problems has societal importance because many real systems are described by complex, multimodal, computationally expensive computer models for which no neat analytical equation exists and derivatives are perhaps not continuous. We want for example a simulation model to be able to make accurate predictions (by optimally calibrating the model parameter against data) and help us make optimal management decisions. We approach this problem by contributing to the field of surrogate global optimization, whereby the optimization search selects points at which the (objective) simulation model is calculated and this search is guided by a continually updated approximation (surrogate) of the true objective function based on previously evaluated objective function values. This approach greatly improves the optimization results when relatively few evaluations of the simulation model can be made because of computational expense. I will show applications of these methods to improve simulation models that assess environmental health of Singapore lakes (using supercomputers) and machine learning for flood control. Mathematical proofs of convergence support this analysis. Other practical applications not discussed include financial engineering and manufacturing. (Talk about 35 minutes)

### Polynomial Blow-up Upper Bounds for the Einstein-scalar Field System under Spherical Symmetry

#### Xinliang An

#### Abstract

In the gravitational collapse of the Einstein-scalar field system, with the focusing initial data, a black hole region could form. Within the black hole region, singularities at \$r=0\$ could arise. It is quite mysterious how strong these singularities could be. In this talk, I will present two new results in this direction within spherical symmetry. i) With Ruixiang Zhang we show that even in the most singular scenario, along the singular boundary r=0, the curvature (Kretschmann scalar) would obey polynomial blow-up upper bounds  $O(1/r^N)$ . This improves previously best-known double-exponential upper bounds  $O(\exp(1/r))$ . Our result is sharp in the sense that there are known examples showing that no sub-polynomial upper bound could hold. ii) With Dejan Gajic, we extend the aforementioned result to a global one and calculate the precise polynomial rate-\$N\$. We find that, when it is close to the timelike infinity, the blow-up rates of Kretschmann scalar could be different from the Schwarzschild value. In particular, the blow-up rates are not limited to discrete finite choices and they are related to the Price's law along the event horizon. This indicates a new blow-up phenomenon, driven by a PDE mechanism, rather than an ODE mechanism.

## Rational Matrix Functions for Electronic Structure Theory

#### Simon Etter

#### Abstract

Density Functional Theory (DFT) and related electronic structure models are some of the largest consumers of computing power in supercomputing centres worldwide, and the bulk of this time is spent on evaluating functions of large, sparse matrices. Traditionally, such matrix functions have been computed using eigenvalue decompositions, but the cubic scaling of eigensolvers with respect to the matrix size renders this ansatz prohibitively expensive in many applications. Eigendecompositions can be avoided if we replace generic matrix functions with rational approximations since these can be evaluating using only matrix sums, products and inverses, but doing so requires effective rational approximation schemes and fast algorithms for evaluating inverses of sparse matrices. This talk will provide a gentle introduction to both of these topics.

### An Energy-stable Finite Element Method for the simulation of Moving Contact Lines in Two-phase Flows

#### Quan Zhao

#### Abstract

The moving contact line model we consider is a sharp-interface model consisting of the two-phase incompressible Navier-Stokes/Stokes equations with the classic interface conditions, the Navier boundary condition for the slip velocity along the wall, and a contact line condition which relates the contact angle to the contact line velocity. We propose an efficient method for the model. The method combines a finite element method for the Naiver-Stokes/Stokes equations on the bulk mesh with a parametric finite element method for the dynamics of the fluid interface.

In this method, the contact line condition is formulated as a time-dependent Robin-type boundary condition for the interface so it is naturally imposed in the weak form of the model. The numerical schemes enjoy a similar energy law as in the continuum model. Numerical examples are presented to demonstrate the convergence and accuracy of the numerical method.

### Numerical Investigations of Complex Langevin Dynamics

#### Yang Kuang

#### Abstract

The complex Langevin (CL) method can solve the sign problem appearing in numerical simulations of lattice field theories with a complex action. However, it sometimes fails to converge or even converges to a wrong result. In this work, we are trying to describe the behavior of the method by investigating some special cases. The local support of the probability distribution is studied by solving the Fokker-Planck equation. Specifically, we focus on the critical point where the support of the distribution is about to disappear and we then explain that the complex Langevin method may lead to a wrong result when the support disappears from both analytical and numerical aspects.

### Some Theoretical Results of Kernel Recovery in Blind Deconvolution

#### Weixi Wang

#### Abstract

Blind deconvolution aims to recover an unknown kernel and activation signal from their convolution. Unfortunately, it is an ill-posed problem in general. To mitigate the ill-posedness, we focus on the short and sparse (SaS) blind deconvolution. We introduce some theoretical results of kernel recovery in the SaS deconvolution. The discussion is based on two models: deterministic model and probabilistic model. In deterministic model we analysis the relation between the ground truth kernel and optimal solution. In probabilistic model we introduce a regional analysis given by John Wright et al.

### Non-concave Portfolio Optimization without the Concavification Principle

#### Shuaijie Qian

#### Abstract

The problems of non-concave utility maximization appear in many areas of finance and economics, such as in behavior economics, incentive schemes, aspiration utility, and goal-reaching problems. Existing literature solves these problems using the concavification principle. We provide a framework for solving non-concave utility maximization problems, where the concavification principle may not hold and the utility functions can be discontinuous. In particular, we find that adding bounded portfolio constraints, which makes the concavification principle invalid, can significantly affect economic insights in the existing literature. Theoretically, we give a new definition of viscosity solution and show that a monotone, stable, and consistent finite difference scheme converges to the solution of the utility maximization problem. This work is jointly with Min Dai, Steven Kou, and Xiangwei Wan.

### Portfolio Selection Under Partial Information and Relative Performance Concerns

#### Xizhi Su

#### Abstract

We establish a Nash equilibrium in a market with N agents with CARA utility and the relative performance criteria when the market return is unobservable. Each investor has a Gaussian prior belief on the return rate of the risky asset. The investors can be heterogeneous in both the mean and variance of the normal random variable. By a separation result and a martingale argument, we show that the optimal investment strategy under a stochastic return rate model can be characterized by a fully-coupled FBSDE with linear coefficients. Two sets of deep neural networks are used for the numerical computation to first find each investor's estimate of the mean return rate and then solve the FBSDEs. We are the first to establish the uniqueness result for the class of FBSDEs with stochastic coefficients. The deep learning scheme for solving the game under partial information is also novel. We demonstrate the efficiency and accuracy by comparing with the numerical solution from PDE for the linear filter case and apply the algorithm to the general case of nonlinear hidden variable process. Simulations of investment strategies demonstrate a herd effect that investors trade more aggressively under relative performance. Partial information mitigated the herd effect, and the investor with the most accurate initial estimate is likely to be the leader.