

## Speakers

- 1 Hui Ji
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# Abstracts

Workshop 3 on Scientific computing and applications

(1 March 2023)

## 1 Hui Ji

*National University of Singapore, Singapore*

[Data-free Deep learning for solving Inverse Imaging problems](#)

### Abstract

Deep learning has emerged as a powerful tool for solving many challenging problems, including inverse imaging problems. Most existing deep learning methods rely on supervised learning, which requires many labeled data for training a deep neural network (DNN). Such a prerequisite on training datasets limits their practical applicability in the domains such as medicine and science. This talk will discuss a series of works on self-supervised learning for solving inverse imaging problems, which teaches a DNN to predict images from their noisy and partial measurements without using any training data. The main ingredient in these works is the neutralization of Bayesian inference with DNN-based over-parametrization of images. Coming as a surprise to most, without given any training data, the proposed data-free deep learning method can compete well against supervised learning methods in some real-world imaging tasks.

## 2 Yifei Li

*National University of Singapore, Singapore*

[A symmetrized parametric finite element method for anisotropic surface diffusion](#)

Abstract

In this talk, we deal with a long-standing problem about how to design an energy-stable numerical scheme for solving the motion of a closed curve under anisotropic surface diffusion with a general anisotropic surface energy  $\gamma(\mathbf{n})$  in two dimensions. By introducing a novel symmetric surface energy matrix  $Z_k(\mathbf{n})$ , we derive a new symmetrized variational formulation for anisotropic surface diffusion. The variational formulation is further discretized in time by an implicit structure-preserving scheme (SP-PFEM) which can rigorously preserve the enclosed area at the fully-discrete level. Furthermore, we prove that the SP-PFEM is unconditionally energy-stable for almost any anisotropic surface energy  $\gamma(\mathbf{n})$  under a simple and mild condition on  $\gamma(\mathbf{n})$ . And we construct  $Z_k(\mathbf{n})$  explicitly for several commonly used anisotropic surface energies.

## 3 Christian Lubich

*University of Tübingen, Germany*

[Convergent evolving surface finite element algorithms for geometric evolution equations](#)

Abstract

Geometric flows of closed surfaces are important in a variety of applications, ranging from the diffusion-driven motion of the surface of a crystal to models for biomembranes and tumor growth. Basic geometric flows are mean curvature flow (described by a spatially second-order evolution equation) and Willmore flow and the closely related surface diffusion flow (described by spatially fourth-order evolution equations).

Devising provably convergent surface finite element algorithms for such geometric flows of closed two-dimensional surfaces has long remained an open problem, going back to pioneering work by Dziuk in 1988. Recently, Balázs Kovács, Buyang Li and I arrived at a solution to this problem for various

geometric flows including those mentioned above. The proposed algorithms discretize nonlinear parabolic evolution equations for geometric quantities along the flow, in our cases for the normal vector and mean curvature, and use these evolving geometric quantities in the velocity law interpolated to the finite element space. This numerical approach admits a stability and convergence analysis with optimal rates of convergence for finite elements of polynomial degree at least two.

## 4 Zuowei Shen

*National University of Singapore, Singapore*  
[Deep Approximation via Deep Learning](#)

Abstract

The primary task of many applications is approximating/estimating a function through samples drawn from a probability distribution on the input space. The deep approximation is to approximate a function by compositions of many layers of simple functions, that can be viewed as a series of nested feature extractors. The key idea of deep learning network is to convert layers of compositions to layers of tuneable parameters that can be adjusted through a learning process, so that it achieves a good approximation with respect to the input data. In this talk, we shall discuss mathematical theory behind this new approach and approximation rate of deep network; we will also show how this new approach differs from the classic approximation theory, and how this new theory can be used to understand and design deep learning networks.

## 5 Xin Tong

*National University of Singapore, Singapore*  
[Sampling with constraints using variational methods](#)

Abstract

Sampling-based inference and learning techniques, especially Bayesian inference, provide an essential approach to handling uncertainty in machine learning (ML). As these techniques are increasingly used in daily life, it

becomes essential to safeguard the ML systems with various trustworthy-related constraints, such as fairness, safety, interpretability. We propose a family of constrained sampling algorithms which generalize Langevin Dynamics (LD) and Stein Variational Gradient Descent (SVGD) to incorporate a moment constraint or a level set specified by a general nonlinear function. By exploiting the gradient flow structure of LD and SVGD, we derive algorithms for handling constraints, including a primal-dual gradient approach and the constraint controlled gradient descent approach. We investigate the continuous-time mean-field limit of these algorithms and show that they have  $O(1/t)$  convergence under mild conditions.

## 6 Chushan Wang

*National University of Singapore, Singapore*

[Error estimates of numerical methods for the nonlinear Schrödinger equation with low regularity potential and nonlinearity](#)

Abstract

We establish optimal error bounds of time-splitting methods and the exponential wave integrator for the nonlinear Schrödinger equation (NLSE) with low regularity potential and nonlinearity, including purely bounded potential and locally Lipschitz continuous nonlinearity. In certain physical applications, low regularity potential and nonlinearity are introduced into the NLSE such as some discontinuous potential widely used in the physics literature or the non-integer power nonlinearity in the Lee-Huang-Yang correction which is adopted in modelling and simulation of quantum droplets. Most of the classical numerical methods can be directly extended to solve the NLSE with the aforementioned potential and nonlinearity, however, the performance of these methods becomes very different from the smooth case and the error estimates of them are subtle and challenging.