Workshop on Scientific Computing and Optimization

Conference Brochure

Hong Kong, China

Dec 12-13, 2020

Department of Mathematics,

Institute of Mathematical Research,

Research Division of Mathematical and Statistical Science.

The University of Hong Kong

1. Conference Schedule

Online Venue:

ZOOM Meeting ID: 395 997 5372

Password: 20201213

Dec 12, 2020 (Saturday)		
9:00--9:30	JIN Bangti	Numerical analysis of diffusion coefficient identification in elliptic and parabolic problems
9:30--10:00	ZHOU Tao	Time fractional phase field equations: energy stability and adaptive time-stepping
10:00--10:10	Tea Break	
10:10--10:40	ZHANG Wenlong	The applications of group sparse method in inverse problems
10:40--11:10	CHAI Lihui	Seismic tomography -- Frozen Gaussian approximation and stochastic gradient reconstruction
11:10--11:40	LI Lei	Using random batches to speed up molecular dynamics simulations
11:40--14:00	Lunch & Break	
14:00--14:30	SHI Zuoqiang	Point integral method for elliptic equation on point cloud
14:30--15:00	CHANG Haibin	Deep-Learning based Inverse Modeling Approaches
15:00--15:10	Tea Break	
15:10--15:40	JIAO Yuling	Deep Representation Learning

15:40--16:10	CHEN Jingrun	MIM: A deep mixed residual method for solving high-order partial differential equations
16:10--16:40	ZHOU Zhennan	Fokker-Planck equations of neuron networks: rigorous justification and numerical simulation

Dec 13, 2020 (Sunday)		
9:00--9:30	ZHANG Lei	Adaptive QM/MM coupling
9:30--10:00	CUI Tiangang	Tensorised Rosenblatt Transport for High-Dimensional Stochastic Computation
10:00--10:10	Tea Break	
10:10--10:40	LIAO Qifeng	A flow-based domain-decomposed approach for uncertainty analysis
10:40--11:10	YANG Yanfang	A two-grid preconditioner with an adaptive coarse space for flow simulations in highly heterogeneous media
11:10--11:40	HUANG De	Potential Singularity Formation of the 3D Euler Equations and Related Models
11:40--14:00	Lunch	
14:00--14:30	JIANG Lijian	Data-driven model reduction for nonlinear dynamic multiscale problems
14:30--15:00	ZHANG Xiaoqun	Stochastic primal dual splitting algorithms for convex composite optimization in imaging
15:00--15:10	Tea Break	

15:10--15:40	TIAN Wenyi	An ADMM-Newton-CNN Numerical Approach to a TV Model for Identifying Diffusion Coefficients in Elliptic Equations with Gradient Observations
15:40--16:10	ZHANG Jin	Bi-Level Programming in meta Learning and hyper-parameter optimization
16:10--16:40	YUAN Rui	Sketched Newton-Raphson Method

2. Title & Abstracts

Online Venue: ZOOM ID 395 997 5372

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Numerical analysis of diffusion coefficient identification in elliptic and parabolic problems

JIN Bangti

University College London

In this talk, I will discuss numerical identification of the diffusion coefficient in elliptic and parabolic type problems from distributed pointwise observations. The numerical recovery is based on the standard Galerkin finite element discretization of the regularized problem with an H^1 penalty, and the time stepping is based on backward Euler method. We derive error estimates on the numerical approximation in terms of mesh size, noise level and regularization parameter. The results are illustrated with numerical experiments.

Time fractional phase field equations: energy stability and adaptive time-stepping

ZHOU Tao

Chinese Academy of Sciences

We discuss in this talk two essential topics related to the time fractional phase field equations: the energy stability and adaptive time-stepping schemes. We shall also introduce some open questions.

The applications of group sparse method in inverse problems

ZHANG Wenlong

Southern University of Science and Technology

In this talk, we present novel reconstruction methods for multifrequency electrical impedance tomography and multi wavelength diffuse optical spectroscopic imaging. They are based on linearization and group sparsity. We consider an isotropic conductivity and diffusion distributions with a finite number of unknown inclusions. We also discuss the reconstruction for an imperfectly known boundary and show that, with multi-frequency or wavelength data, the method can reduce the influence of modelling errors and still recover the PDE coefficients. Extensive numerical experiments are presented to support our analysis.

Seismic tomography -- Frozen Gaussian approximation and stochastic gradient reconstruction

CHAI Lihui

Sun Yat-sen University

In this talk, we present some recent developments of using Frozen Gaussian approximation (FGA) in seismic tomography. The FGA is rigorously derived for scalar/elastic wave equation with analysis of its accuracy determined by the ratio of short wavelength over large domain size. We develop the FGA as an efficient parallel asymptotic solver for high-frequency seismic wave propagation and apply it in seismic inversion. In order to overcome the computational difficulty in summing up a large number of Gaussians targeted at a 3-D mesh, we use stochastic sampling techniques to reduce the number of Gaussians and reconstruct ``low-resolution" wavefieds, but the resulted ``stochastic gradient" still preserves necessary information and leads the iteration process converge to the correct velocity model. This is the joint work with James Hateley (Vanderbilt U), Yixiao Hu (Tsinghua), Zhongyi Huang (Tsinghua), Ping Tong (NTU), Xu Yang (UCSB).

Using random batches to speed up molecular dynamics simulations

LI Lei

Shanghai Jiao Tong University

We focus on the simulations for many body systems in canonical ensembles. We will introduce both an MC and an MD algorithm that we propose recently in which we use random batch ideas to speed up the computation. In the Random Batch Monte Carlo method, a singular potential is split into a smooth long range part and a singular short range part. We use the smooth part with random batch strategy to generate a proposal sample and use the singular part to do rejection. This reduces the computational cost for sampling from O(N) to O(1) in one iteration. In the random batch Ewald method, we apply the random batch idea in frequency part, and results in efficient molecular dynamics method. The random mini-batch idea is famous for its application in SGD and also has been used by Jin et al to interacting particle systems.

Point integral method for elliptic equation on point cloud

SHI Zuoqiang

Tsinghua University

In this talk we will introduce a novel numerical approach for elliptic equation on point cloud. The main idea is to approximate the elliptic operator by an integral operator with properly designed kernel functions. Then the integral equation is easy to discretized on point cloud. The convergence is proved and numerical results will be shown to demonstrate the performance of the proposed methods.

Deep Representation Learning

Jiao Yuling

Wuhan University

It is widely believed that Deep learning is actually deep representation learning, i.e., the success of deep learning depends on its automatic data representation abilities". In this talk, we present a mathematical framework with theoretical guarantee to achieve a good data representation that enjoys information preservation, low dimensionality and disentanglement. First, we formulate the ideal representation learning task as finding a nonlinear representation map that minimizes the sum of losses characterizing conditional independence and disentanglement. Then, we estimate the target map with samples nonparametrically with deep neural networks. We derive a bound on the excess risk of the deep nonparametric estimator. Finally, the proposed method is validated via regression and classification with the learned representation. The resulting prediction accuracies are at least comparable with fine-tuned deep models.

MIM: A deep mixed residual method for solving high-order partial differential equations

CHEN Jingrun

Soochow University

In this work, we propose a deep mixed residual method (MIM) to solve PDEs. In MIM, we first rewrite a high-order PDE into a first-order system, very much in the same spirit as local discontinuous Galerkin method and mixed finite element method in classical numerical methods for PDEs. We then use the residual of first-order system in the least-squares sense as the loss function, which is in close connection with least-squares finite element method. For aforementioned classical numerical methods, the choice of trail and test functions is important for stability and accuracy issues in many cases. MIM shares this property when DNNs are employed to approximate unknowns functions in the first-order system. In one case, we use nearly

the same DNN to approximate all unknown functions and in the other case, we use totally different DNNs for different unknown functions. Numerious numerical results are provided to show the advantages of MIM.

Fokker-Planck equations of neuron networks: rigorous justification and numerical simulation

ZHOU Zhennan

Peking University

In this talk, we are concerned with the Fokker-Planck equations associated with the Nonlinear Noisy Leaky Integrate-and-Fire model for neuron networks. Due to the jump mechanism at the microscopic level, such Fokker-Planck equations are endowed with an unconventional structure: transporting the boundary flux to a specific interior point. In the first part of the talk, we present an alternative way to derive such Fokker-Planck equations from the microscopic model based on a novel iterative expansion. With this formulation, we prove that the probability density function of the "leaky integrate-and-fire" type stochastic process is a classical solution to the Fokker-Planck equation. Secondly, we propose a conservative and positivity preserving scheme for these Fokker-Planck equations, and we show that in the linear case, the semi-discrete scheme satisfies the discrete relative entropy estimate, which essentially matches the only known long time asymptotic solution property. We also provide extensive numerical tests to verify the scheme properties, and carry out several sets of numerical experiments, including finite-time blowup, convergence to equilibrium and capturing time-period solutions of the variant models.

Deep-Learning based Inverse Modeling Approaches

CHANG Haibin

Peking University

In this talk, two categories of deep-learning based inverse modeling methods are presented. The first category is deep-learning surrogate-based inversion methods, in which the Theory-guided Neural Network (TgNN) is constructed as a deep-learning surrogate for problems with uncertain model parameters. By incorporating physical laws and other constraints, the TgNN surrogate can be constructed with limited simulation runs and accelerate the inversion process significantly. Three TgNN surrogate-based inversion methods are proposed, including the gradient method, the iterative ensemble smoother (IES), and the training method. The second category is direct-deep-learning-inversion methods, in which TgNN constrained with geostatistical information, named TgNN-geo, is proposed as the deep-learning framework for direct inverse modeling. Since the prior geostatistical information can be incorporated, the direct-inversion method based on TgNN-geo works well, even in cases with sparse spatial measurements or imprecise prior statistics. The proposed methods are tested with several subsurface flow problems.

Adaptive QM/MM coupling

ZHANG Lei

Shanghai Jiao Tong University

Hybrid quantum/molecular mechanics models (QM/MM methods) are widely used in material and molecular simulations when MM models do not provide sufficient accuracy but pure QM models are computationally prohibitive. Adaptive QM/MM coupling methods feature on-the-fly classification of atoms during the simulation, allowing the QM and MM subsystems to be updated as needed. In this work, we propose such an adaptive QM/MM method for material defect simulations based on a new residual based a posteriori error estimator, which provides both lower and upper bounds for the true error. We validate the analysis and illustrate the effectiveness of the new scheme on numerical simulations for material defects.

Tensorised Rosenblatt Transport for High-Dimensional Stochastic Computation

CUI Tiangang

Monash University

Characterising intractable high-dimensional random variables is one of the fundamental challenges in stochastic computation. It has broad applications in statistical physics, machine learning, uncertainty quantification, econometrics, and beyond. The recent surge of transport maps offers a mathematical foundation and new insights for tackling this challenge.

In this talk, we present a functional tensor-train (FTT) based monotonicity-preserving construction of inverse Rosenblatt transport in high dimensions. It characterises intractable random variables via couplings with tractable reference random variables. By integrating our FTT-based approach into a nested approximation framework inspired by deep neural networks, we are able to significantly expand its capability to random variables with complicated nonlinear interactions and concentrated density functions. We demonstrate the efficacy of the FTT-based inverse Rosenblatt transport on a range of applications in statistical learning and uncertainty quantification, including parameter estimation for dynamical systems, PDE-constrained inverse problems, and Bayesian filtering. This is joint work with Dr. Sergey Dolgov (Bath) and Mr. Yiran Zhao (Monash)

A flow-based domain-decomposed approach for uncertainty analysis

LIAO Qifeng

ShanghaiTech University

The domain decomposition uncertainty quantification method (DDUQ) (SIAM J. SCI. COMPUT (37) pp. A103-A133) provides a decomposed strategy to conduct uncertainty analysis for complex engineering systems governed by PDEs. In DDUQ, uncertainty analysis on each local component is independently conducted in an ``offline" phase, and global uncertainty analysis results are assembled using precomputed local information in an ``online" phase through importance sampling. The performance of DDUQ relies on the coupling surrogates and probability density estimation during the importance sampling procedure. Since coupling surrogates can give high-dimensional interface parameters, we in this work develop a dynamic flow model based interface coupling strategy, which dramatically improve the efficiency of DDUQ.

A two-grid preconditioner with an adaptive coarse space for flow simulations in highly heterogeneous media

YANG Yanfang

Guangzhou University

In this talk, a two-grid preconditioner with an adaptive coarse space for flow simulations is introduced. We consider flow simulation in highly heterogeneous media that has many practical applications in industry. To enhance mass conservation, we write the elliptic problem in a mixed formulation and introduce a robust two-grid preconditioner to seek the solution. We first need to transform the indefinite saddle problem to a positive definite problem by preprocessing steps. The preconditioner consists of a local smoother and a coarse preconditioner. For the coarse preconditioner, we design an adaptive spectral coarse space motivated by the GMsFEM (Generalized Multiscale Finite Element Method). We test our preconditioner for both Darcy flow and two phase flow and transport simulation in highly heterogeneous porous media. Numerical results show that the proposed preconditioner is highly robust and efficient.

Potential Singularity Formation of the 3D Euler Equations and Related Models

HUANG De

California Institute of Technology

Whether the 3D incompressible Euler equations can develop a singularity in finite time from smooth initial data is one of the most challenging problems in mathematical fluid dynamics. We first review the numerical evidence of finite time singularity for 3D axisymmetric Euler equations by Luo and Hou. The singularity is a ring like singularity that occurs at a stagnation point in the symmetry plane located at the boundary of the cylinder. We then present a novel method of analysis and prove that the 1D HL model and the original De Gregorio model develop finite time self-similar singularity. We will also report some recent progress from our research group in analyzing the finite time singularity of the axisymmetric 3D Euler equations with initial data considered by Luo and Hou. Finally, we present some recent numerical results on singularity formation of the 3D axisymmetric Euler equation along the symmetry axis.

Data-driven model reduction for nonlinear dynamic multiscale problems

JIANG Lijian

Tongji University

In this talk, I present a data-driven model reduction method for nonlinear dynamic multiscale problems. The proposed method combines Constraint Energy Minimizing Generalized Multiscale Finite Element Method (CEM-GMsFEM) and Dynamic Mode Decomposition (DMD) to significantly reduce the computational complexity. Although CEM-GMsFEM can give an accurate coarse model, it involves calculating the residual and the Jacobian on a fine grid for nonlinear problems. DMD method is a data-driven method and used to estimate nonlinear terms and decomposes the nonlinear dynamic system into spatio-temporal coherent structures for short-term future state prediction. The proposed approach avoids the repeated evaluation of the nonlinear terms in an online stage. In order to achieve a full coarse model for the nonlinear dynamic problem, we utilize a coarse-scale observation in DMD. When the nonlinear dynamic multiscale problem is unknown, we use Koopman operator and deep learning to predict the solution by observation data.

Stochastic primal dual splitting algorithms for convex composite optimization in imaging

ZHANG Xiaoqun

Shanghai Jiao Tong University

Primal dual splitting algorithms are largely adopted for composited optimization problems arising in imaging. In this talk, I will present stochastic extensions of some popular composite optimization algorithms in convex settings and their applications to image restoration and statistical learning problems. The algorithms are designed for convex linearly composite problems by combining stochastic gradient with the so-called primal dual fixed point method (PDFP). As a natural generalization of

proximal stochastic gradient types methods, we proposed stochastic PDFP (SPDFP) and its variance reduced version SVRG-PDFP which do not require subproblem solving. The convergence and convergence orders are established for the proposed algorithms based on some standard assumptions. The numerical examples on graphic Lasso, graphics logistic regressions and image reconstruction are provided to demonstrate the effectiveness of the proposed algorithm. In particular, we observe that for large scale image reconstruction problems, SVRG-PDFP exhibits some advantages in terms of accuracy and computation speed, especially in the case of relatively limited high performance computing resource.

An ADMM-Newton-CNN Numerical Approach to a TV Model for Identifying Diffusion Coefficients in Elliptic Equations with Gradient Observations

TIAN Wenyi

Tianjin University

Identifying the discontinuous diffusion coefficient in an elliptic equation with observation data of the gradient of the solution is a nonlinear and ill-posed inverse problem. Models with total variational (TV) regularization have been widely studied for this problem, while the theoretically required nonsmoothness property of the TV regularization and the hidden convexity of the models are usually sacrificed when numerical schemes are considered in the literature. In this work, we show that the favorable nonsmoothness and convexity properties can be entirely kept if the well-known alternating direction method of multipliers (ADMM) is applied to the TV-regularized models. The ADMM subproblems can be well solved by the active-set Newton method along with the Schur complement reduction and the CNN, respectively. The resulting ADMM-Newton-CNN approach is demonstrated to be easily implementable and very efficient even for higher-dimensional spaces with fine mesh discretization.

Bi-Level Programming in meta Learning and hyper-parameter optimization

ZHANG Jin

Southern University of Science and Technology

In this talk, we will discuss some recent advances in the applications of Bi-Level Programming Problem (BLPP). We study a gradient-based bi-level optimization method for learning tasks. In particular, by formulating bi-level models from the optimistic viewpoint and aggregating hierarchical objective information, we establish Bi-level Descent Aggregation (BDA), a flexible and modularized algorithmic framework for bi-level programming. Theoretically, we derive a new methodology to prove the convergence of BDA. Extensive experiments justify our theoretical results and demonstrate the superiority of the proposed BDA for different tasks, including hyper-parameter optimization and meta learning. This is a joint work with R.S. Liu, P. Mu, X.M. Yuan and S.Z. Zeng.

Sketched Newton-Raphson Method

YUAN Rui

Facebook AI Research and Télécom Paris

We propose a new globally convergent stochastic second order method. Our starting point is the development of a new Sketched Newton-Raphson (SNR) method for solving large scale nonlinear equations of the form F(x) = 0. We then show how to design several stochastic second order optimization methods by re-writing the optimization problem of interest as a system of nonlinear equations and applying SNR. For instance, by applying SNR to find a stationary point of a generalized linear model (GLM), we derive completely new and scalable stochastic second order methods. We show that the resulting method is very competitive as compared to state-of-the-art variance reduced methods. Using a variable splitting trick, we also show that the Stochastic Newton method (SNM) is a special case of SNR, and use this connection to establish the first global convergence theory of SNM. Indeed, by showing that SNR can be interpreted as a variant of the stochastic gradient descent (SGD) method, we are able to leverage proof techniques of SGD and establish a global convergence theory and rates of convergence for SNR. As a special case, our theory also provides a new global convergence theory for the original Newton-Raphson method under strictly weaker assumptions as compared to what is commonly used for global convergence.

3. Information for Participants

1. Date December 12-13, 2020

2. Venue: ZOOM ID: 395 997 5372 Password: 20201213

3. Organizing Committee

Dr. Guanglian Li

Dr. Zheng Qu

Dr. Zhiwen Zhang

4. Scientific Committee

Prof. Wai-Ki Ching

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Prof. Michael Ng

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