2023 年科学与工程计算青年研讨会报告题目和摘要

Robust AI-aided Imaging Models without Labeled Samples

包承龙
(清华大学)

摘要：The observations in practical imaging systems always contain complex noise such that classical approaches are difficult to obtain satisfactory results. In recent years, deep neural networks directly learned a map between the noisy and clean images based on the training on paired data. Despite its promising results in various tasks, collecting the training data is difficult and time-consuming in practice. In this talk, in the unpaired data regime, we will discuss our recent progress for building AI-aided robust models and their applications in image processing. Leveraging the Bayesian inference framework, our model combines classical mathematical modeling and deep neural networks to improve interpretability. Experimental results on various real datasets validate the advantages of the proposed methods. Finally, I will report the recent progresses on solving the preferred orientation problems in cyroEM using the developed tools.

Diffeomorphic Optimal Transportation and Its Applications in Imaging Science

陈冲
(中国科学院数学与系统科学研究院)

摘要：Motivated by the image reconstruction in spatiotemporal imaging, we introduce a concept called diffeomorphic optimal transportation (DOT), which combines the Wasserstein distance with Benamou--Brenier formula in optimal transportation and the flow of diffeomorphisms in large deformation diffeomorphic metric mapping. Using DOT, we propose a new variational model for joint image reconstruction and motion estimation, which is suitable for spatiotemporal imaging involving mass-preserving large diffeomorphic deformations. The proposed model is easy-to-implement and solved by an alternating gradient descent algorithm, which is compared against existing alternatives theoretically and numerically. Moreover, we present more extensions with applications to image registration based on DOT. Under appropriate conditions, the proposed algorithm can be adapted as a new algorithm to solve the models using quadratic Wasserstein distance. The performance is validated by several numerical experiments in spatiotemporal tomography, where the projection data is time-dependent sparse and/or high-noise.

Time Discretizations of Wasserstein-Hamiltonian Flows

崔建波

(香港理工大学)

摘要： We study discretizations of Hamiltonian systems on the probability density manifold equipped with the L2-Wasserstein metric. Based on discrete optimal transport theory, several Hamiltonian systems on a graph (lattice) with different weights are derived, which can be viewed as spatial discretizations of the original Hamiltonian systems. We prove consistency of these discretizations. Furthermore, by regularizing the system using the Fisher information, we deduce an explicit lower bound for the density function, which guarantees that symplectic schemes can be used to discretize in time. Moreover, we show desirable long time behavior of these symplectic schemes, and demonstrate their performance on several numerical examples. Finally, we compare the present approach with the standard viscosity methodology

Deep Learning Methods for Parameter Identification in Elliptic Equations: Model and Error Analysis

焦雨领

(武汉大学)

摘要： In this presentation, we introduce a deep learning method for parameter identification in elliptic equations. We begin by establishing novel stability estimates that serve as the guiding principle for proposing appropriate loss functions. We propose a model that leverage Tikhonov regularization and physics-informed neural networks (PINNs). Furthermore, we conduct a rigorous analysis for convergence rates of reconstructions which provide valuable a priori insights for the choice of regularization parameters, as well as the size of the neural networks. Finally, we demonstrate the remarkable stability of the method with respect to the data noise through various numerical experiments.

Using Random Batches to Speed Up Molecular Simulations

李磊

(上海交通大学)

摘要： I will introduce both a Monte Carlo method and a molecular dynamics algorithm in which we have used 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.

Efficient and Parallel Solution of High-order Continuous Time Galerkin for Dissipative and Wave Propagation Problems

刘勇

(中国科学院数学与系统科学研究院)

摘要：In this talk, we propose efficient and parallel algorithms for the implementation of the high-order continuous time Galerkin method for dissipative and wave propagation problems. By using Legendre polynomials as shape functions, we obtain a special structure of the stiffness matrix that allows us to extend the diagonal Padé approximation to solve ordinary differential equations with source terms. The unconditional stability, *hp* error estimates, and *hp* superconvergence at the nodes of the continuous time Galerkin method are proved. Numerical examples confirm our theoretical results. This work is joint with Prof. Zhiming Chen.

Numerical Ergodicity of Monotone SDEs Driven by Multiplicative Noise

刘智慧

(南方科技大学)

摘要： We consider the ergodicity of Markov Chains constructed by the backward Euler scheme for monotone SODEs and Galerkin-based backward Euler schemes of monotone SPDEs with polynomial growth coefficients (including the stochastic Allen--Cahn equation) driven by multiplicative trace-class noise.

A Linear Monolithic Finite Element Method for Fluid-shell Interaction: Stability and Error Estimates

佘邦伟

(首都师范大学)

摘 要： We propose a linear monolithic scheme for the approximation of a fluid-structure interaction problem, that is a deformable plate interacting with a viscous incompressible fluid. We take the backward Euler method for the time discretization, and use P1-bubble/P1/P1 elements for the approximation of the fluid velocity, pressure, and the structure displacement. We use the arbitrary-Lagrange-Euler method and work on the reference domain, meaning that re-meshing is not needed during the time evolution. We prove the stability of the numerical solution as well as the linear convergence rate with respect to the size of the time step Δt and mesh h. Finally, we present the numerical experiments to illustrate the theoretical results.

Solving Large-Scale Optimization Problems via Learning-Based Algorithms

王阿康
(深圳市大数据研究院)

摘 要： Recently, machine learning has been utilized to expedite optimization algorithms. In this talk, we will discuss two learning-based methods. The first one is a "predict-and-search" algorithm for addressing mixed-integer linear programs, while the second one is an "approximate-and-optimize" method for solving stochastic nonlinear programs. We conduct computational results and demonstrate the effectiveness of our proposed approaches.

拓扑优化问题的迭代卷积阈值算法

王东（香港中文大学（深圳））

摘要：在本次报告中，我们讲主要介绍针对一般性拓扑优化问题的鲁棒且无条件稳定的迭代卷积阈值算法。该算法主要基于区域特征函数的自由界面表示方式及相应近似以及预估校正思想，实现了针对一般性拓扑优化问题的保证目标泛函下降的迭代格式。

Certifying Ground-state Properties of Quantum Many-body Systems

王杰
(中国科学院数学与系统科学研究院)

摘要： A ubiquitous problem in quantum physics is to understand the ground-state properties of many-body systems. Confronted with the fact that exact diagonalisation quickly becomes impossible when increasing the system size, variational approaches are typically employed as a scalable alternative: energy is minimised over a subset of all possible states and then different physical quantities are computed over the solution state. Despite remarkable success, rigorously speaking, all what variational methods offer are upper bounds on the ground-state energy. On the other hand, so-called relaxations of the ground-state problem based on semidefinite programming represent a complementary approach, providing lower bounds to the ground-state energy. However, in their current implementation, neither variational nor relaxation methods offer provable bound on other observables in the ground state beyond the energy. In this work, we show that the combination of the two classes of approaches can be used to derive certifiable bounds on the value of any observable in the ground state, such as correlation functions of arbitrary order, structure factors, or order parameters. We illustrate the power of this approach in paradigmatic examples of 1D and 2D spin-one-half Heisenberg models. To improve the scalability of the method, we exploit the symmetries and sparsity of the considered systems to reach sizes of hundreds of particles at much higher precision than previous works. Our analysis therefore shows how to obtain certifiable bounds on many-body ground-state properties beyond energy in a scalable way.

Advanced Learning Rate Schedules for SGD

王小玉
(香港科技大学)

摘要：Stochastic Gradient Descent (SGD) is a commonly used optimization algorithm for training machine learning models. The learning rate (step-size), as a crucial hyperparameter in SGD, directly affects the magnitude of parameter updates. To improve the convergence speed and performance of models, researchers have proposed a variety of advanced learning rate scheduling methods. The objective of this talk is to review advanced learning rate schedules for SGD including step-decay, cyclical step-size, and adaptive learning rate. By comprehensively comparing these advanced learning rate scheduling methods, we can observe their respective advantages and applicability on different problems and datasets. Choosing an appropriate learning rate schedule is a crucial step in optimizing the model training process, leading to improved performance and convergence speed.

Structure Preserving Primal Dual Methods for Gradient Flows with Respect to Transport Distances

魏朝祯
(电子科技大学)

摘要：I will present a novel structure-preserving numerical method for gradient flows w.r.t Wasserstein-like transport distances induced by concentration-dependent mobilities, which arise widely in materials science and biology. Based upon the minimizing movement scheme and modern operator-splitting schemes, our method has built-in positivity or boundedness preserving, mass conservation, and energy-dissipative structures. I will show the flexibility and performance of our methods through simulation examples including porous medium equations, nonlocal aggregation diffusion equations and Cahn-Hilliard equations with degenerate mobility and wetting boundary conditions.

Physics-data Combined Machine Learning Method for ROM and AI Based Non-linear ROM

肖敦辉
(同济大学)

摘要： Reduced-order modelling (ROM) provides an economical way to construct low-dimensional parametric surrogates for rapid predictions of high-dimensional physical fields. This talk will present basic idea of non-intrusive reduced order model and a non-linear non-intrusive ROM based on Auto-encoder and self-attention is also presented.In addition, a physics-data combined machine learning (PDCML) method for non-intrusive ROM in small-data regimes will also be presented. To overcome labelled data scarcity, the physics-data combined ROM framework is developed to jointly integrate the physical principle and the small labelled data into feedforward neural networks (FNN) via a step-by-step training scheme. This new PDCML method is tested on a series of nonlinear problems with different numbers of physical variables, and it is also compared with the data-driven ROM and the physics-guided ROM. The results demonstrate that the proposed method provides a cost-effective way for non-intrusive parametric ROM via machine learning, and it possesses good characteristics of high prediction accuracy, strong generalization and extrapolation capability, and small data requirement.

神经网络求解高维 ODE

许志钦
(上海交通大学)

摘要：在这个报告中，我将讨论用神经网络算法求解高维 ODE，主要应用在加速模拟燃烧化学反应模型的相关工作。燃烧模拟有两个重要的难点，一是化学组分多，二是刚性强。这两个难点使得化学反应的模拟占据了大部分燃烧模拟的计算量。我们首先是发展基于深度学习的模型简化方法，其次是发展基于深度学习的替代模型。这些方法在保持精度的同时，显著提升了燃烧的模拟效率。

Unbiased Compression Saves Communication in Distributed Optimization: When and How Much?

袁坤
(北京大学)

摘要: Communication compression is a common technique in distributed optimization that can alleviate communication overhead by transmitting compressed gradients and model parameters. However, compression can introduce information distortion, which slows down convergence and incurs more communication rounds to achieve desired solutions. Given the trade-off between lower per-round communication costs and additional rounds of communication, it is unclear whether communication compression reduces the total communication cost. This paper explores the conditions under which unbiased compression, a widely used form of compression, can reduce the total communication cost, as well as the extent to which it can do so. To this end, we present the first theoretical formulation for characterizing the total communication cost in distributed optimization with communication compression. We demonstrate that unbiased compression alone does not necessarily save the total communication cost, but this outcome can be achieved if the compressors used by all workers are further assumed independent. We establish lower bounds on the communication rounds required by algorithms using independent unbiased compressors to minimize smooth convex functions, and show that these lower bounds are tight by refining the analysis for ADIANA. Our results reveal that using independent unbiased compression can reduce the total communication cost. These theoretical findings are supported by experimental results.

Inverse Scattering with Phaseless Data

张海文
(中国科学院数学与系统科学研究院)

摘要：Inverse scattering with phased data (i.e., data with phase information) has been widely studied mathematically and numerically over the past decades due to its significant applications in such diverse scientific areas as radar and sonar detection, remote sensing, geophysics, medical imaging, and nondestructive testing. However, in many practical applications, it is much harder to obtain data with accurate phase information compared with only measuring the modulus or intensity of the data. Therefore, it is often desirable to study inverse scattering problems with phaseless data (i.e., data without phase information). In this talk, we will introduce our recent work on the numerical algorithms for inverse scattering problems with phaseless data.

Structure-preserving Front-tracking Methods for Two-phase Flow

赵泉

(中国科学技术大学)

摘要：In this talk, I will consider the structure-preserving front-tracking methods fora sharp-interface model of two-phase flow in both the unfitted and fitted mesh approaches, meaning that the volume preservation and energy decay are satisfied on the discrete level. In the unfitted approach, the constructed method is based on an Eulerian weak formulation, while in the fitted approach, the method is devised in the arbitrary Lagrangian-Eulerian (ALE) framework. We compare the numerical results of the two approaches by using the example of a rising bubble.