第三届“偏微分方程数值方法与理论暑期学校”

前沿学术研讨会日程

2019 年 8 月 10 日（星期六）

前沿学术报告

主持人：冯民富 **研究生院一区 104**

09:00—09:30	**Direct and inverse time-harmonic wave scattering problems** 胡广辉（北京计算科学研究中心）
09:30—10:00	**Direct discretization method for the Cahn-Hilliard equation on surfaces** 李义宝（西安交通大学）
10:00—10:20	**茶歇**

主持人：贺巧琳 **研究生院一区 104**

10:20—10:50	**A convergent evolving finite element algorithm for mean curvature flow of closed surfaces** 李步扬（香港理工大学）
10:50—11:20	**Solution of parametric electromagnetic radiation problems using a residual-based POD reduced order method** 李　良（电子科技大学）
11:20—11:50	**Numerical methods for scattering problems in unbounded domain** 吕俊良（吉林大学）

主持人：王　皓　　**研究生院一区 104**

14:30—15:00	**An efficient numerical method to compute the ground state of rotating dipolar Bose-Einstein Condensates** 唐庆猕（四川大学）
15:00—15:30	**Variational approach for learning Markov processes from time series data** 吴　昊（同济大学）
15:30—16:00	**茶歇**

主持人：马　强　　**研究生院一区 104**

16:00—16:30	**Computing convolutions, the story so far** 徐　宽（中国科学技术大学）
16:30—17:00	**GePUP: A Fourth-order Projection Method for Solving the Incompressible Navier-Stokes Equations** 张庆海（浙江大学）
17:00—17:30	**Towards a mathematical understanding of surface hopping methods** 周珍楠（北京国际数学研究中心）

2019 年 8 月 11 日（星期日）

暑期学校闭幕式

主持人：胡　兵　　**研究生院一区 104**

08:30—10:00	暑期学校闭幕式（含优秀学员颁奖）

前沿学术报告题目及摘要

胡广辉（北京计算科学研究中心，hu@csrc.ac.cn）

题目: Direct and inverse time-harmonic wave scattering problems

摘要： Wave scattering phenomena and theory have attracted many physicists and mathematicians since more than one hundred years and have played a central role in twentieth century mathematical physics. When the (acoustic, elastic or electromagnetic) wave fields encounter an obstacle (cracks, voids, inclusions or unbounded interfaces), reflected waves will be scattered back because of the discontinuity in media. In the case that no scattered wave is incited, the underlying scatterer is 'unseen' by detectors and hence must have been cloaked. Suppose that a time-harmonic plane or point source wave is incident onto a bounded obstacle. The direct (forward) problem is to compute the scattering effect caused by the obstacle, whereas the inverse problem consists in determining the location, shape and physical properties of the obstacle from measured scattered fields. In this talk I will introduce basic concepts and fundamental questions in direct and inverse scattering problems. For shape identification problems, a data-driven imaging scheme will be reported based on rigorous mathematical theory. Such an inversion scheme makes use of a priori far-field data of known obstacles (e.g. sound-soft disks and spheres with different radius and centers) and requires only a single far-field pattern corresponding to the unknown scatterer.

李义宝（西安交通大学数学与统计学院，yibaoli@xjtu.edu.cn）

题目： Direct discretization method for the Cahn-Hilliard equation on surfaces

摘要： In this talk, we will introduce simple and efficient direct discretization methods for solving the Cahn–Hilliard (CH) equation on the fix and evolving surfaces. By using a conservation law and transport formulae, we derive the CH equation on evolving surfaces. An evolving surface is discretized using an unstructured triangular mesh. The discrete CH equation is defined on the surface mesh and its dual surface polygonal tessellation. The evolving

triangular surfaces are then realized by moving the surface nodes according to a given velocity field. The proposed scheme is based on the Crank–Nicolson scheme and a linearly stabilized splitting scheme. The scheme is second-order accurate, with respect to both space and time. The resulting system of discrete equations is easy to implement, and is solved by using an efficient biconjugate gradient stabilized method. Several numerical experiments are presented to demonstrate the performance and effectiveness of the proposed numerical scheme. The joint work with Junseok Kim (Korea University).

李步扬（香港理工大学应用数学系，buyang.li@polyu.edu.hk）

题目：A convergent evolving finite element algorithm for mean curvature flow of closed surfaces

摘要：A proof of convergence is given for semi- and full discretizations of mean curvature flow of closed two-dimensional surfaces. The numerical method proposed and studied here combines evolving finite elements, whose nodes determine the discrete surface like in Dziuk's method, and linearly implicit backward difference formulae for time integration. The proposed method differs from Dziuk's approach in that it discretizes Huisken's evolution equations for the normal vector and mean curvature and uses these evolving geometric quantities in the velocity law projected to the finite element space. This numerical method admits a convergence analysis in the case of finite elements of polynomial degree at least two and backward difference formulae of orders two to five. The error analysis combines stability estimates and consistency estimates to yield optimal-order H^1-norm error bounds for the computed surface position, velocity, normal vector and mean curvature. The stability analysis is based on the matrix-vector formulation of the finite element method and does not use geometric arguments. The geometry enters only into the consistency estimates. Numerical experiments illustrate and complement the theoretical results.

李　良（电子科技大学数学科学学院，plum.liliang@gmail.com）

题目：Solution of parametric electromagnetic radiation problems using a residual-based POD reduced order method

摘要： In this work we present a parametric reduced order model (ROM) based on the proper orthogonal decomposition (POD) method combined with Galerkin projection for the solution of the system of time-domain Maxwell’s equations. The ROM with a significantly smaller dimension is constructed by creating a reduced subspace composed of a set of time- and parameter-independent POD basis vectors, which are generated by the snapshots extracted from the discontinuous Galerkin time-domain (DGTD) solutions. Then we seek the approximate solutions within this reduced subspace via Galerkin projection. In particular, a greedy offline algorithm for the snapshot selection in the parameter space is developed to obtain an efficient ROM. Moreover, we introduce a residual-based estimation of the error associated with the ROM. The performance of the parametric POD-Galerkin ROM is demonstrated by considering the scattering of a plane wave by a dielectric cylinder and a multi-layer heterogeneous medium.

吕俊良（吉林大学数学学院，lvjl@jlu.edu.cn)

题目：Numerical methods for scattering problems in unbounded domain

摘要： In this talk, I will give some recent work on scattering problems, including acoustic scattering by obstacles, electromagnetic scattering by grating structures, and elastic scattering by periodic materials. One of main difficulties for solving these problems with finite element methods is the unboundedness of physical domains. Two effective strategies to truncate these unbounded domains into bounded computable domains are introduced. One is the transparent boundary condition (TBC) approach, the other is the perfectly matched layer (PML) technique. Moreover, Adaptive mesh refinement methods based on the a posteriori estimates are considered to deal with complex problem geometries and potential discontinuous material parameters. Some numerical results will be presented to illustrate the competitive behavior of the proposed method.

唐庆猕（四川大学数学学院，qinglin_tang@163.com)

题目：An efficient numerical method to compute the ground state of rotating dipolar Bose-Einstein Condensates

摘要： In this talk, we will present an efficient numerical method for computing the ground state of the rotating dipolar Bose-Einstein Condensates (BEC). The method consists two main merits: (i) efficient and accurate numerical methods will be proposed to evaluate the nonlocal dipole-dipole interaction. (ii). a nonlinear conjugate gradient method, accelerated by some well-adapted preconditioners, will be developed to compute the ground states. This work is realized in collaboration with Xavier ANTOINE (IECL, Lorraine, France), Antoine LEVITT (Inria, Paris, France) and Yong ZHANG (Tianjin University, Tianjin, China).

吴　昊（同济大学数学科学学院，hwu@tongji.edu.cn）

题目：Variational approach for learning Markov processes from time series data

摘要： Inference, prediction and control of complex dynamical systems from time series is important in many areas, including financial markets, power grid management, climate and weather modeling, or molecular dynamics. The analysis of such highly nonlinear dynamical systems is facilitated by the fact that we can often find a (generally nonlinear) transformation of the system coordinates to features in which the dynamics can be excellently approximated by a linear Markovian model. Moreover, the large number of system variables often change collectively on large time- and length-scales, facilitating a low-dimensional analysis in feature space. In this paper, we introduce a variational approach for Markov processes (VAMP) that allows us to find optimal feature mappings and optimal Markovian models of the dynamics from given time series data. The key insight is that the best linear model can be obtained from the top singular components of the Koopman operator. This leads to the definition of a family of score functions called VAMP-r which can be calculated from data, and can be employed to optimize a Markovian model. In addition, based on the relationship between the variational scores and approximation errors of Koopman operators, we propose a new VAMP-E score, which can be applied to cross-validation for hyper-parameter optimization and model selection in VAMP. VAMP is valid for both reversible and nonreversible processes and for stationary and non-stationary processes or realizations.

徐　宽（中国科学技术大学数学科学学院，kuanxu@ustc.edu.cn）

题目：Computing convolutions, the story so far

摘要： Convolution is found ubiquitously dense in mathematics and engineering. In this talk, we'll review classic results in literature on convolution quadrature before moving on to the most recent development of powerful numerical methods for computing convolution integrals. Based on the spectral approximation of convolution operators via classic orthogonal polynomials or Fourier extensions, we'll arrive at fast and spectrally-accurate algorithms which make the calculation of convolution integrals possible in the sense of "computing with functions" and these new methods are believed to lay the very foundation of the first spectral methods for convolution integral equations.

张庆海（浙江大学数学科学学院，qinghai@zju.edu.cn）

题 目： GePUP: A Fourth-order Projection Method for Solving the Incompressible Navier-Stokes Equations

摘要： A generic projection maps one vector to another such that their difference is a gradient field and the projected vector does not have to be solenoidal. By studying the commutator of Laplacian and the generic projection, the incompressible Navier-Stokes equations with no-slip conditions are reformulated as the sole evolution of a divergent velocity with the incompressibility constraint enforced by a pressure Poisson equation. This GePUP formulation yields numerical methods with distinguishing features as follows. (1) The velocity divergence is governed by a heat equation, and thus bounded by the maximum principle. (2) The method is fourth-order accurate both in time and in space, and both for the velocity and for the pressure. (3) The linear systems are solved with geometric multigrid, yielding optimal complexity. (4) The time integrator is treated as a black box in the framework of method-of-lines (MOL) so that changing from explicit time integration to implicit-explicit time integration is trivial, making the formulation applicable to flows with both low and high Reynolds numbers. This finite-volume solver is further augmented with parallel computing and adaptive mesh refinement. We have generalized the solver to domains with irregular boundaries and are working on domains with moving boundaries.

周珍楠（北京国际数学研究中心，zhennan@bicmr.pku.edu.cn)

题目：Towards a mathematical understanding of surface hopping methods

摘要： We develop a surface hopping algorithm based on frozen Gaussian approximation for semiclassical matrix Schrödinger equations, in the spirit of Tully' s fewest switches surface hopping method. The algorithm is asymptotically derived from the Schrödinger equation with rigorous approximation error analysis. The resulting algorithm can be viewed as a path integral stochastic representation of the semiclassical matrix Schrödinger equations. Our results provide mathematical understanding to and shed new light on the important class of surface hopping methods in theoretical and computational chemistry.