Plenary Talks

Approximation of nonlinear hyperbolic problems and the property of conservation

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Abstract. In this talk, I am interested in problems of the type

$$\frac{\partial u}{\partial t} + \text{ div } f(u) = 0 \tag{1}$$

written on Ω an open subset of $\mathbb{R}^d$. The solution u belongs to $D \subset \mathbb{R}^p$, and the flux is $f = (f_1, \ldots, f_d)$ where the f_i are smooth functions defined on D with values in $\mathbb{R}^p$. This problem is equipped with initial conditions and boundary conditions, and is assumed to be hyperbolic, i.e., for any $\mathbf{n} = (n_1, \ldots, n_d)$, the matrix

$$\sum_{i=1}^{d} \frac{\partial f_i}{\partial x_i} n_i$$

is diagonalisable on $\mathbb{R}$. The typical example is that of the Euler equations.

Since the celebrated theorem by Lax and Wendroff who showed that a numerical scheme for (1) written in conservation form, if it is stable, will converge to a weak solution of the approximated hyperbolic problem, most of the work in this area of Research has been focussed on schemes that can be written, in a way or another, with flux. This is obviously true for finite volume schemes, whatever the order of accuracy, this is also true for a class of scheme using the discontinuous Galerkin paradigm: they use a discretised version of the weak form, and numerical flux.

However, there exist many schemes that seems no to be in a flux form. An example is the streamline diffusion method, and more generally continuous stabilized finite element methods. And it is also known they work very well!

In this talk, I show that all the known schemes, except maybe one (the so-called Active Flux scheme by Roe and co-authors), can be reformulated in flux form thanks to a reformulation of the conservation property. I will show how to exploit this reformulation to construct schemes compatible with other conservation constraints, such as the entropy inequality, and more generally speaking thermodynamical compatibility, or schemes on staggered grids.

Some new directions in computational inverse problems

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Abstract. Inverse problems are concerned with determining model parameters from the observed data, which have played an important role in diverse application area. A well-known representative inverse problem is electrical impedance tomography (EIT), also known as Calderón's problem, which involves determining the electrical conductivity from the voltage to current map on the boundary. The EIT problem arises in many practical applications, such as medical imaging and nondestructive testing. However, the problem is known to be severely ill-posed, in particular, small perturbations in the measured data may lead to large errors in the reconstructions. Stable numerical solution of the EIT problem remains a big challenge in computational inverse problems.

In this talk, the speaker will discuss some new directions for solving inverse problems. Of particular interest are recursive linearization methods based on multiple frequency data; deep learning methods, and optimal transportation approaches. These methods are suitable for solving severely ill-posed problems. Numerical results will be presented to validate the effectiveness and feasibility of the methods. The talk is based on the recent joint work with Yixuan Zhang.

Structure-preserving parametric finite element methods (PFEM) for geometric PDEs and applications

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Abstract. In this talk, I begin with a review of different geometric flows (PDEs) including mean curvature (curve shortening) flow, surface diffusion flow, Willmore flow, etc., which arise from materials science, interface dynamics in multi-phase flows, biology membrane, computer graphics, geometry, etc. Different mathematical formulations and numerical methods for mean curvature flow are then discussed. In particular, an energy-stable linearly implicit parametric finite element method (PFEM) is presented in details. Then the PFEM is extended to surface diffusion flow and anisotropic surface diffusion flow, and a structure-preserving implicit PFEM is proposed. Finally, sharp interface models and their PFEM approximations are presented for solid-state dewetting. This talk is based on joint works with Harald Garcke, Wei Jiang, Yifei Li, Robert Nuernberg, Yan Wang and Quan Zhao.

Deep neural network algorithms for oscillatory flows, causality operators, and high dimensional Fokker-Planck equations

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Abstract. In this talk, we will present results on new types of deep neural networks (DNNs) in the following areas: (a) a multi-scale DNN method for solving highly oscillatory Navier-Stokes flows in complex domains, and rigorous mathematical analysis will also be given explaining the improved performance of the multi-scale DNN; (b) a causality DNN learning algorithm for operators in highly oscillatory function spaces encountered in seismic wave responses and other evolution PDEs systems with causalities; (c) a DNN based on forward and backward stochastic differential equations (FBSDEs) for high dimensional PDEs such as Fokker-Planck equations arising from statistical descriptions of biochemical systems.

Nonlocal models with local boundary conditions

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Abstract. We consider nonlocal integro-differential equations on bounded domains with finite-range nonlocal interactions that are localized at the boundary. Through a careful study of boundary localized convolutions, we are able to establish a nonlocal Green's identity, which leads to the well-posedness of these nonlocal problems with various types of classical local boundary conditions. We investigate the regularity properties of the nonlocal problems with rough data and examine the convergence of solutions of these nonlocal boundary-value problems with their classical local counterparts in the local limit.

Emergent dynamics of Kuramoto oscillators

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Abstract. We present the state-of-the-art results on the emergent behaviors of the Kuramoto oscillators. In particular, we discuss relations between the finiteness of collisions and phase-locking of the Kuramoto model. When there is no inertial effect, it is well known that the finiteness of collisions is equivalent to the emergence of phase-locking. Thus, when a Kuramoto ensemble is under the effect of inertia, whether the same equivalence relation hold or not is an intricate question. In this talk, we show that in a small inertia regime, the aforementioned equivalence still holds, whereas in a large inertia regime, we show that a homogeneous Kuramoto ensemble with the same natural frequencies can exhibit phase-locking, while there are countable number of collisions between Kuramoto oscillators. This is a contrasted effect of a large inertia in phase-locking process. This is a joint work with Hangjun Cho (SNU) and Jiu-Gang Dong (Dalian Univ. of Technology).

Structure-preserving model order reduction

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Abstract. The development of reduced order models for complex applications promises rapid and accurate evaluation of the output of complex models under parameterized variation with applications to problems which require many evaluations, such as in optimization, control, uncertainty quantification and applications where near real-time response is needed. However, many challenges remain to secure the flexibility, robustness, and efficiency needed for general large scale applications, in particular for nonlinear and/or time-dependent problems.

We discuss the recent developments of projection-based model order reduction (MOR) techniques targeting Hamiltonian problems. Hamilton's principle completely characterizes many high-dimensional models in mathematical physics, resulting in rich geometric structures, with examples in fluid dynamics, quantum mechanics, optical systems, and epidemiological models. MOR reduces the computational burden associated with the approximation of complex systems but classic reduction approaches do not guarantee conservation of the delicate dynamics of Hamiltonian problems, resulting in reduced models plagued by instability or accuracy loss.

By approaching the reduction process from the geometric perspective of symplectic manifolds, the resulting reduced models inherit stability and conservation properties of the high-dimensional formulations. We first introduce the general principles of symplectic geometry, including symplectic vector spaces and Darboux' theorem. This setting is used

as a starting point for the development of different structure-preserving reduced basis (RB) algorithms. We also briefly discuss extensions to problems posed on noncanonical Hamiltonian form.

We conclude by discussing the extension of structure preserving models within a framework of nonlinear reduced order models in which a local basis allows to maintain a small basis even for problems with a slowly decaying Kolmogorov n-width such a transport dominated problems. We demonstrate the efficiency of such techniques for nonlinear transport dominated problems, including for the Poisson-Vlasov problem of kinetic plasma physics.

This work is done in collaboration with B. Maboudi (DTU), C. Pagliantini (TU/e), N. Ripamonti (EPFL).

Quantum computation of partial differential equations

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Abstract. Quantum computers have the potential to gain algebraic and even up to exponential speed up compared with its classical counterparts, and can lead to technology revolution in the 21st century. Since quantum computers are designed based on quantum mechanics principle, they are most suitable to solve the Schödinger equation, and linear PDEs (and ODEs) evolved by unitary operators. The most efficient quantum PDE solver is quantum simulation based on solving the Schrödinger equation. It became challenging for general PDEs, more so for nonlinear ones. Our talk will cover three topics:

1) We introduce the "warped phase transform" to map general linear PDEs and ODEs to Schrödinger equation or with unitary evolution operators in higher dimension so they are suitable for quantum simulation; 2) For (nonlinear) Hamilton-Jacobi equation and scalar nonlinear hyperbolic equations we use the level set method to map them—exactly—to phase space linear PDEs so they can be implemented with quantum algorithms and we gain quantum advantages for various physical and numerical parameters. 3) For PDEs with uncertain coefficients, we introduce a transformation so the uncertainty only appears in the initial data, allowing us to compute ensemble averages with multiple initial data with just one run, instead of multiple runs as in Monte-Carlo or stochastic collocation type sampling algorithms.

Solving elliptic interface problems by neural networks

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Abstract. In this talk, we shall introduce a machine learning methodology based on neural networks to solve PDEs. First, I would like to discuss why and how the artificial neural network can be used to solve PDEs in different types. Then I will talk about our recent works on solving elliptic interface problems by neural network methods. There are three novel features in our present network; namely, (i) jump discontinuities are accurately captured, (ii) it is completely shallow, comprising only one hidden layer, (iii) it is completely mesh-free so the problems in irregular domains with irregular interfaces can be handled easily. Numerical results show better accuracy and easier implementation than the traditional finite difference methods.

Liouville type theorems and *a priori* estimates

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Abstract. In this lecture, we present some of our work on the study of regularity, *a priori* estimates, and Liouville type theorems. Our presentation is focused on problems related to fractional Laplacian and problems arising from the study of the incompressible Navier-Stokes and Euler equations. Most of the results presented here are the joint work with Chenkai Liu, Yingshu Lv, Chunjing Xie, Shaodong Wang and Ran Zhuo.

Actor-critic method for solving high dimensional Hamilton-Jacobi-Bellman type PDEs

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Abstract. In this talk, we will discuss numerical approach to solve high dimensional Hamilton-Jacobi-Bellman (HJB) type partial differential equations (PDEs). The HJB PDEs, reformulated as optimal control problems, are tackled by the actor-critic framework inspired by reinforcement learning, based on neural network parametrization of the value and control functions. Within the actor-critic framework, we employ a policy gradient approach to improve the control, while for the value function, we derive a variance reduced least-squares temporal difference method using stochastic calculus. We will also discuss convergence analysis for the actor-critic method, in particular the policy gradient method for solving stochastic optimal control. Joint work with Jiequn Han (Flatiron Institute) and Mo Zhou (Duke University).

Generalized SAV approach for general dissipative nonlinear systems with particular application to Navier-Stokes equations

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Abstract. I will present some recent advances on using the generalized scalar auxiliary variable (GSAV) approach to develop highly efficient and accurate schemes for a large class of dissipative nonlinear systems. These schemes are easy to implement, can be high-order in time, and lead to a uniformly bound for the numerical solution in a suitable norm that plays an essential role in corresponding error analysis. It can also be positivity/bound preserving through a function transform.

We combine this GSAV approach with a new consistent splitting scheme for the Navier-Stokes equations, and obtain, for the first time, a strongly unconditional stable, decoupled schemes with uniform second-order accuracy for the velocity and pressure.

Deep approximation via deep learning

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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.

Multiscale modeling for non-equilibrium transport

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Abstract. In this talk, we will introduce the direct modelling for the development of numerical algorithms for multiscale transport. This framework is about to model the physical laws directly in a discretized space, where the transport dynamics depends on the cell resolution, such as the so-called cell's Knudsen number. With the variation of local cell's Knudsen number, multiscale transport can be obtained automatically, such as the capturing of particle free transport and continuum wave propagation at the same time in different numerical cells according to the local cell's Knudsen number. The multiscale algorithms, such as the unified gas-kinetic scheme (UKGS) and unified gas-kinetic wave-particle (UGKWP) method, have been successfully used in rarefied gas dynamics, radiative and neutron transfer, plasma physics, and gas-solid particle multiphase flow.

Two problems on the Boltzmann equation with boundary effect

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Abstract. Two problems on the Boltzmann equation with boundary effect will be discussed. The first one is about the 1D steady Boltzmann flow in a channel. The walls of the channel are assumed to be steady with different temperatures. This problem was studied by Esposito et al. for which they showed that the solution tends to a local Maxwellian with parameters satisfying the compressible Navier-Stokes equation with no-slip boundary condition. However, a lot of numerical experiments reveal that the fluid layer does not entirely stick to the boundary. In the regime where the Knudsen number is reasonably small, the slip phenomenon is significant near the boundary. Thus, we revisit this problem by taking into account the slip boundary conditions. Following the previous study by Coron, we will first give a formal asymptotic analysis to show that the flow governed by the Boltzmann equation is accurately approximated by a superposition of a steady CNS equation with a temperature jump condition and two Knudsen layers located at end points. Then we establish a uniform estimate on the remainder and derive the slip boundary condition for compressible Navier-Stokes equations rigorously. The second problem is about the plane Couette flow of a rarefied gas between two parallel infinite plates moving relatively to each. In case of the Maxwell molecule collision, we establish the existence of spatially inhomogeneous non-equilibrium stationary solutions to the steady problem for any small relative shear velocities via an elaborate perturbation approach using Caflisch's decomposition together with Guo's L-infinity-L2 theory. In addition, the large time asymptotic stability of the stationary solution with an exponential convergence is obtained so that the nonnegativity of the steady profile is justified. The talk is based on recent joint work with Renjun Duan and Shuangqian Liu and Zhu Zhang.

Deep learning of multiscale dynamical systems

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Abstract. Advances in deep learning have made constructing, training and deploying deep neural networks more accessible than ever before. Due to their flexibility and predictive accuracy, neural networks have ushered in a new wave of data-driven as well as data-free modeling of physical phenomena. With several key research breakthroughs, modern deep learning architectures are now more accurate and generalizable facilitating improved physics-informed models. This presentation briefly explores the use of several different deep learning approaches for learning physical dynamics including Bayesian neural networks, generative models, physics-constrained learning, graph neural networks, and self-attention. By leveraging these recent deep neural network advancements and probabilistic frameworks, powerful multiscale deep learning approaches that incorporate known physical constraints as prior knowledge can be used for predictive modeling of complex dynamics. We will highlight such techniques with various applications including flows in complex heterogeneous media, turbulent flows as well as molecular modeling and design.

On the one time-varying component regularity criteria for 3-D Navier-Stokes equations

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Abstract. In this paper, we consider the one time-varying component regularity criteria for local strong solution of 3-D Navier-Stokes equations. Precisely, if $\beta(t)$ is a piecewise H^1 unit vector from $[0,T]$ to $\mathbb{S}^2$ with finitely many jump discontinuities, we prove that if $\int_0^T \|u(t)\cdot\beta(t)\|^2_{\dot{H}^{\frac{3}{2}}(\mathbb{R}^3)}\,dt<\infty$, then the solution u can be extended beyond the time T. Compared with the previous results [CZ5,CZZ,LeiZhao] concerning one-component regularity criteria, here the unit vector $\beta(t)$ varies with time variable.

Invited Talks

Orthogonality preserving schemes for electronic structure calculations

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Abstract. To obtain convergent numerical approximations without orthogonalization operations is of great importance in electronic structure calculations. In this talk, we will introduce an extended gradient flow based Kohn-Sham DFT model, for which we prove the flow is orthogonality preserving and the solution evolves to the ground state. With the help of the gradient flow based Kohn-Sham DFT model, we propose and analyze a class of iteration schemes for the discretized Kohn-Sham model, which preserves the orthogonality of the Kohn-Sham orbitals automatically. With our schemes, the iterative approximations are guaranteed to converge to the Kohn-Sham orbitals without any orthogonalization operations when the initial orbitals are orthogonal. We prove the convergence and get the local convergence rate of the numerical approximations under some reasonable assumptions. This is a joint work with Qiao Wang, Liwei Zhang and Aihui Zhou.

Spectral gap formation to kinetic equations in soft potentials

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Abstract. In the talk I will consider the spectral gap for the linearized Boltzmann or Landau equation with soft potentials. It is known that the corresponding collision operators admit only the degenerated spectral gap. We rather prove the formation of spectral gap in the spatially inhomogeneous setting where the space domain is bounded with an inflow boundary condition. The key strategy is to introduce a new Hilbert space with an exponential weight function that involves the inner product of space and velocity variables. The action of the transport operator on such space-velocity dependent weight function induces an extra non-degenerate relaxation dissipation in large velocity that can be employed to compensate the degenerate spectral gap. Joint work with Dingqun Deng (Tsinghua University).

Difference finite element method for 3D incompressible N-S and MHD equations

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Abstract. In this work, a difference finite element (DFE) method is presented for 3D incompressible Navier-Stokes (N-S) and MHD equations. This new method consists of transmitting the FE solution of 3D steady N-S (MHD) equations into a series of the FE solution of 2D steady Oseen iterative equations, which are solved by using the FE pair (P1b,P1b,P1)×P1 satisfying the discrete LBB condition in 2D domain. Moreover, we use FE pair ((P1b,P1b,P1)×P1)×(P1×P0) to solve 3D Oseen iterative equations, where the pair satisfies the discrete LBB condition in 3D domain. Next, we provide the existence and uniqueness of the DFE solutions of 3D Oseen iterative equations and deduce the first order convergence of the DFE solutions to the exact solution of 3D problems. Finally, numerical examples are presented to show the accuracy and effectiveness. This work was jointly completed with Prof. He and Dr. Lu from Xi'an Jiaotong University.

New optimized Robin-Robin domain decomposition methods using Krylov solvers for the Stokes-Darcy system

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Abstract. In this presentation, we design optimized Schwarz domain decomposition algorithms to accelerate the Krylov type solution for the Stokes-Darcy system. We use particular solutions of this system on a circular geometry to analyze the iteration operator mode by mode. We introduce a new optimization strategy of the so-called Robin parameters based on a specific linear relation between these parameters, using the min-max and the expectation minimization approaches. Moreover, we use a Krylov solver to deal with the iteration operator and accelerate this new optimized domain decomposition algorithm. Several numerical experiments are provided to validate the effectiveness of this new method.

Efficient numerical methods for density functional theory and a software AFEABIC

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Abstract. Density functional theory is one of the most successful approximate models for the Schrödinger equation. In this talk, our efforts on developing efficient numerical methods for solving Kohn-Sham and time-dependent Kohn-Sham equations will be introduced in detail, including a quality construction of the approximation space for the numerical solutions, fast calculations for the electrostatic field, fast solvers for the system of linear equations and eigenvalue problems, as well as acceleration techniques based on multiple precisions, parallel computing, etc. Then a software, entitled AFEABIC, will be introduced for its data structure, realization of each competent. Numerical experiments will be provided to show the efficiency of our methods, and effectiveness of our software.

Incompressible limit of compressible dissipative elastodynamics with vanishing shear viscosity in dimension two

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Abstract. We will discuss the incompressible limit of compressible dissipative elastodynamics when the shear viscosity converges to zero in dimension two. The incompressible limit is characterised by the large value of the volume viscosity. In the limit, the dispersive effect of pressure waves disappears and the global convergence to the limit system around an equilibrium is justified with the help of vector fields and the ghost weight method. This is a joint work with Xiufang Cui.

Some high order methods for delay differential equations

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Abstract. In this talk, we first introduce delay differential equation widely used in science and engineering. For partial differential equations with constant delay, discontinuous Galerkin and ETD-Pade approximations are used in time and continuous finite element method in space respectively, and the numerical stability and error estimation of spatio-temporal fully discrete scheme are given. Numerical experiments are presented to verify the proposed methods.

Overcoming the curse of dimensionality: from nonlinear Monte Carlo to the training of neural networks

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Abstract. Partial differential equations (PDEs) are among the most universal tools used in modelling problems in nature and man-made complex systems. Nearly all traditional approximation algorithms for PDEs in the literature suffer from the so-called "curse of dimensionality" in the sense that the number of required computational operations of the approximation algorithm to achieve a given approximation accuracy grows exponentially in the dimension of the considered PDE. With such algorithms it is impossible to approximately compute solutions of high-dimensional PDEs even when the fastest currently available computers are used. In the case of linear parabolic PDEs and approximations at a fixed space-time point, the curse of dimensionality can be overcome by means of Monte Carlo approximation algorithms and the Feynman-Kac formula. In this talk we present deep learning based methods which seem to be able to solve also nonlinear PDEs in very high dimensions. In addition, we prove that deep neural network approximations overcome the curse of dimensionality in the case of a general class of semilinear parabolic PDEs. Finally, we also specify concrete examples of smooth functions which can not be approximated by shallow neural networks without the curse of dimensionality but which can be approximated by deep neural networks without the curse of dimensionality.

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Conductivity imaging using deep neural networks

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Abstract. Conductivity imaging from various observational data represents one fundamental task in medical imaging. In this talk, we discuss numerical methods for identifying the conductivity parameters in elliptic PDEs. Commonly, a regularized formulation consists of a data fidelity and a regularizer is employed, and then it is discretized using finite difference method, finite element methods or deep neural networks in practical computation. One key issue is to establish *a priori* error estimates for the recovered conductivity distribution. In this talk, we discuss our recent findings on using deep neural networks for this class of problems, by effectively utilizing relevant stability results.

Low regularity integrators for semilinear parabolic equations with maximum bound principles

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Abstract. This work is concerned with structure-preserving, low regularity time integration methods for a class of semilinear parabolic equations of Allen-Cahn type. Important properties of such equations include maximum bound principle (MBP) and energy dissipation law; for the former, that means the absolute value of the solution is pointwisely bounded for all the time by some constant imposed by appropriate initial and boundary conditions. The model equation is first discretized in space by the central finite difference, then by iteratively using Duhamel's formula, first and second-order low regularity integrators (LRIs) are constructed for time discretization of the semi-discrete system. The proposed LRI schemes are proved to preserve the MBP and the energy stability in the discrete sense. Furthermore, some semi-discrete and fully-discrete error estimates are also successfully derived under the low regularity requirement that the corresponding exact solution is only assumed to be continuous in time. Numerical results show that the proposed LRI schemes can be more accurate and achieve better convergence than classic exponential time differencing schemes, especially when the interfacial parameter approaches zero.

Energy transfer and generalized Fermi's golden rule in Hamiltonian nonlinear Klein-Gordon equations

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Abstract. More than 20 years ago, Soffer-Weinstein considered a class of nonlinear Klein-Gordon equations with nice potentials. For the first time they proved that spatially localized and time-periodic solutions of the linear problem are destroyed by generic nonlinear Hamiltonian perturbations via slow radiation of energy to infinity, via energy transfer from the discrete to continuum modes, under the condition that the discrete modes are close to the continuous spectral modes. Since then, a long-standing open question is to study the corresponding problem with small eigenvalues, which was also raised in the paper of Soffer-Weinstein 1999. In this talk, we will report our recent result on this problem which settles the above open question. This is a joint work with my students Jie Liu and Zhaojie Yang.

On OP-Mapped WENO schemes

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Abstract. The WENO scheme is one of the most welcomed numerical schemes for conservation laws by its virtues that high order accuracy is achieved while numerical oscillations are prevented. For very long time numerical simulations, it seems a much more difficult to keep the same numerical effect. This difficulty has been concerned in a lot of papers in the last decade. One of the major developments is the schemes referred as mapped WENO schemes. In our recent works, we pointed out that the mappings in the mapped WENO schemes often change the order of the nonlinear weights, which maybe the key to resolve the problem. This finding guided us to propose a class of OP-Mapped WENO schemes, which remarkably improve the numerical performances.

Analytic regularization effect for the non-cutoff Boltzmann equation

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Abstract. We verify that the spatially inhomogeneous Boltzmann equation with strong angular singularity admits the analytic smoothing effect, just like its diffusive models such as the Landau and Fokker-Planck equations. To overcome the degeneracy in the spatial variable, a family of well-chosen vector fields with time-dependent coefficients will play a crucial role, and the analytic regularization effect of weak solutions relies on a quantitative estimate on directional derivatives in these vector fields.

Solving PDEs on rough surfaces

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Abstract. We are interested in simulating patterns on rough surfaces. First, we consider periodic rough surfaces with analytic parametric equations, which are defined by some superposition of wave functions with random frequencies and angles of propagation. The amplitude of such surfaces is also an important variable in the provided eigenvalue analysis for the Laplace-Beltrami operator and in our numerical studies. Simulations show that the patterns become irregular as the amplitude and frequency of the rough surface increase. Next, for the sake of easy generalization to closed manifolds, we propose another construction method of rough surfaces by using random nodal values and discretized heat filters. We provide numerical evidence that both surface constructions yield comparable patterns to those found in real-life animals.

Inverse problems for mean field games

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Abstract. In this talk, I shall discuss our recent study on several inverse problems associated with mean field games, and the mathematical methods we developed. Our aim is to establish a comprehensive mathematical theory for this emerging field of research.

Constraint dissolving approaches for a class of Riemannian optimization problems

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Abstract. We propose constraint dissolving approaches for optimization problems over a class of Riemannian manifolds. In these proposed approaches, solving a Riemannian optimization problem is transferred into the unconstrained minimization of a constraint dissolving function named CDF. Different from existing exact penalty functions, the exact gradient and Hessian of CDF are easy to compute. We study the theoretical properties of CDF and prove that the original problem and CDF have the same first-order and second-order stationary points, local minimizers, and Łojasiewicz exponents in a neighborhood of the feasible region. Remarkably, the convergence properties of our proposed constraint dissolving approaches can be directly inherited from the existing rich results in unconstrained optimization. Therefore, the proposed constraint dissolving approaches build up short cuts from unconstrained optimization to Riemannian optimization. Several illustrative examples further demonstrate the potential of the proposed approaches.

From single to collective cell migration: A robust and efficient adaptive multigrid method for geometric surface PDEs

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Abstract. In this talk, I want to present an image-based modelling approach for single and collective cell migration that is based on geometric surface PDEs. The idea is to propose and investigate a novel solution strategy to efficiently and accurately compute approximate solutions to semi-linear optimal control problems, focusing on the optimal control of phase field formulations of geometric evolution laws with applications to cell migration. The optimal control of geometric evolution laws arises in a number of applications in fields including material science, image processing, tumour growth and cell motility. Despite this, many open problems remain in the analysis and approximation of such problems. In the current work I focus on a phase field formulation of the optimal control problem, hence exploiting the well-developed mathematical theory for the optimal control of semi-linear parabolic partial differential equations. Approximation of the resulting optimal control problem is computationally challenging, requiring massive amounts of computational time and memory storage. The main focus of this work is to propose, derive, implement and test an efficient solution method for such problems. The solver for the discretised partial differential equations is based upon a geometric multigrid method incorporating advanced techniques to deal with the nonlinearities in the problem and utilising adaptive mesh refinement. An in-house two-grid solution strategy for the forward and adjoint problems, that significantly reduces memory requirements and CPU time, is proposed and investigated computationally. Furthermore, parallelisation as well as an adaptive step gradient update for the control are employed to further improve efficiency. Along with a detailed description of the proposed solution method together with its implementation I will present a number of computational results that demonstrate and evaluate the algorithms with respect to accuracy and efficiency. A highlight of the present work is simulation results on the optimal control of phase field formulations of geometric evolution laws in 3-D which would be computationally infeasible without the solution strategies proposed in the present work.

This work was jointly carried out with Dr Feng Wei Yung (Warwick University), Dr Chandrasekhar Venkataraman (University of Sussex) and Professor Vanessa Styles (University of Sussex).

Well-posedness of nonlocal and local quasilinear evolution equations in fluids and geometry

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Abstract. In this talk, I will present some recent results on local and global well-posedness and regularity for the Muskat problem, the 2d/3d Peskin problem, the mean curvature flow, the surface diffusion flow, the Willmore flow of entire graphs.

Diffuse-interface approach to competition between viscous flow and diffusion in pinch-off dynamics

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Abstract. For decades there have been numerous works dedicated to the study of pinch-off dynamics. However, most of the existing works were performed in the regime where the interfacial motion is driven by mass flow. Therefore, the role of diffusive transport in the pinch-off of liquid threads largely remains to be explored and studied. The aqueous two-phase systems inject new ingredients into the classical problem of pinch-off dynamics because of the enhanced diffusion and the weakened capillary flow close to the critical point. It has been experimentally observed that when the interfacial tension is lower than normal liquids by two to three orders, the pinch-off dynamics is dominated by bulk diffusion [PRL 123, 134501 (2019)], showing a scaling behavior distinct from that dominated by the Stokes flow.

In this work, we employ the Cahn-Hilliard-Navier-Stokes model to investigate the pinch-off dynamics of a liquid thread surrounded by a viscous external fluid. A characteristic length scale is introduced to measure the competition between diffusion and viscous flow in interfacial motion. This length scale is adjustable in the model and can approach micrometer scale for aqueous two-phase systems close to the critical point. In a cylindrical domain with axisymmetry, ample numerical examples are presented to show the pinch-off processes in the Stokes regime and the diffusion-dominated regime respectively. In particular, the crossover between these two regimes is investigated numerically and analytically to reveal how the scaling behaviors of similarity solutions are to be qualitatively changed as the characteristic length scale is accessed by the pinching neck of the interface.

This is a joint work with Weizhu Bao and Fukeng Huang of National University of Singapore. T. Qian was supported by the Hong Kong RGC.

Decoupled, linear, and unconditionally energy-stable SPH methods for single-phase and two-phase flows

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Abstract. Due to the advantage of the Lagrangian treatment of convection, Smoothed particle hydrodynamics (SPH) has become a popular mesh-free method for solving complex fluid flows. In this work, a novel Smoothed Particle Hydrodynamics (SPH) method is proposed and implemented for incompressible single-phase fluid flow and two-phase fluid flow. The new SPH method is decoupled, linear, and unconditionally energy-stable. For single-phase flow modeled by the Navier-Stokes equation, we apply operator splitting to break the momentum equation into equations involving the non-pressure term and pressure term separately. The idea behind the splitting is to simplify the calculation into a few linear steps while still maintaining unconditional energy stability. With the projection procedure to decouple the momentum and continuity equations, the numerical scheme meets the divergence-free condition. For two-phase flow

modeled by the Navier-Stokes–Cahn–Hilliard (NSCH) equation system, we propose a pioneering energy-stable operator splitting strategy to design an efficient Smoothed particle hydrodynamics discretization of the Navier-Stokes-Cahn-Hilliard model, which is again unconditionally energy-stable and includes only linear sub-steps.

For both the single-phase flow and two-phase flow, we prove that our SPH method inherits mass and momentum conservation and the energy dissipation properties from the PDE level to the ODE level, and then to the fully discrete level. Consequently and desirably, it also helps increase the stability of the numerical method. Due to its conditional stability, the time step size can be much larger than that of the traditional ISPH methods. This energy-stable SPH method also alleviates the tensile instability without using any particle-shifting strategies, which may destroy the rigorous mathematical proof. Numerical experiments are carried out to show the performance of the proposed energy-stable SPH method for both single-phase and two-phase flows. The inheritance of mass and momentum conservation and the energy dissipation properties are verified numerically. For single-phase flow, numerical examples are presented and compared to the analytical solutions, suggesting that the proposed method has improved accuracy and stability. For two-phase flow, the numerical results also demonstrate that our method captures the interface behavior and the energy variation process well. This presentation is based on our joint work with Xiaoyu Feng (KAUST), Jisheng Kou (Shaoxing University), Zhonghua Qiao (HK PolyU), and Xingyu Zhu (KAUST).

A positivity preserving, energy stable finite difference scheme for the Flory-Huggins-Cahn-Hilliard-Navier-Stokes system

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Abstract. A finite difference numerical scheme is proposed and analyzed for the Cahn-Hilliard-Navier-Stokes system, with logarithmic Flory-Huggins energy potential. In the numerical approximation to the singular chemical potential, the logarithmic term and the surface diffusion term are implicitly updated, while an explicit computation is applied to the concave expansive term. Moreover, the convective term in the phase field evolutionary equation is approximated in a semi-implicit manner. Similarly, the fluid momentum equation is computed by a semi-implicit algorithm: implicit treatment for the kinematic diffusion term, explicit update for the pressure gradient, combined with semi-implicit approximations to the fluid convection and the phase field coupled term, respectively. Such a semi-implicit method gives an intermediate velocity field. Subsequently, a Helmholtz projection into the divergence-free vector field yields the velocity vector and the pressure variable at the next time step. This approach decouples the Stokes solver, which in turn drastically improves the numerical efficiency. The positivity-preserving property and the unique solvability of the proposed numerical scheme is theoretically justified, i.e., the phase variable is always between -1 and 1, following the singular nature of the logarithmic term as the phase variable approaches the singular limit values. In addition, an iteration construction technique is applied in the positivity-preserving and unique solvability analysis, motivated by the non-symmetric nature of the fluid convection term. The energy stability of the proposed numerical scheme could be derived by a careful estimate. A few numerical results are presented to validate the robustness of the proposed numerical scheme.

Euler equations and transonic flows

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Abstract. In this talk, we will consider the Euler equations of gas dynamics and applications in transonic flows. First the basic theory of Euler equations will be reviewed. Then we will present the results on the transonic flows past obstacles, transonic flows in the fluid dynamic formulation of isometric embeddings, and the transonic flows in nozzles. We will discuss global solutions and stability obtained through various techniques and approaches.

An efficient unconditionally stable method for computing Dirichlet partitions in arbitrary domains

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A Dirichlet k-partition of a domain is a collection of k pairwise disjoint open subsets such that the sum of their first Laplace–Dirichlet eigenvalues is minimal. In this talk, we propose a new relaxation of the problem by introducing auxiliary indicator functions of domains and develop a simple and efficient diffusion generated method to compute Dirichlet k-partitions for arbitrary domains. The method only alternates three steps: 1. convolution, 2. thresholding, and 3. projection. The method is simple, easy to implement, insensitive to initial guesses and can be effectively applied to arbitrary domains without any special discretization. At each iteration, the computational complexity is linear in the discretization of the computational domain. Moreover, we theoretically prove the energy decaying property of the method. Experiments are performed to show the accuracy of approximation, efficiency and unconditional stability of the algorithm. We apply the proposed algorithms on both 2- and 3-dimensional flat tori, triangle, square, pentagon, hexagon, disk, three-fold star, five-fold star, cube, ball, and tetrahedron domains to compute Dirichlet k-partitions for different k to show the effectiveness of the proposed method. Compared to previous work with reported computational time, the proposed method achieves hundreds of times acceleration.

Free boundary problems in compressible ideal MHD

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Abstract. We present the joint works with Professor Yuri Trakhinin on the local well-posedness of free boundary problems in ideal compressible magnetohydrodynamics with or without surface tension.

Global solvability and stability of a three-species food chain model with prey-taxis and alarm-taxis

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Abstract. In this talk, we shall first introduce a three-species food chain model with prey-taxis and discuss its global solvability and stability. Then we include an alarm-taxis as an anti-predation strategy into the model and discuss its global solvability and stability. Compared to the two-species food chain model (i.e. predator-prey model) with prey-taxis, the three-species food chain model with prey-taxis has some essential differences in model structures and some new ideas are needed to establish the global well-posedness of the model.

Convexity, uniqueness, and stability of the regular shock reflection-diffraction problem

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Abstract. We will talk about our recent results on the convexity, uniqueness, and stability of regular reflection solutions for the potential flow equation in a natural class of self-similar solutions. The approach is based on a nonlinear version of the method of continuity.

Deep Operator-Splitting Network for Solving PDEs

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Abstract. Deep neural networks (DNNs) recently emerged as a promising tool for analyzing and solving complex differential equations arising in science and engineering applications. Alternative to traditional numerical schemes, learning based solvers utilize the representation power of DNNs to approximate the input-output relations in an automated manner. However, the lack of physics-in-the-loop often makes it difficult to construct a neural network solver that simultaneously achieves high accuracy, low computational burden, and interpretability. In this work, focusing on a class of evolutionary PDEs characterized by decomposable operators, we show that the classical "operator splitting" technique can be adapted to design neural network architectures. This gives rise to a learning-based PDE solver, which we name Deep Operator-Splitting Network (DOSnet). Such non-black-box network design is constructed from the physical rules and operators governing the underlying dynamics, and is more efficient and flexible than the classical numerical schemes and standard DNNs. To demonstrate the advantages of our new AI-enhanced PDE solver, we train and validate it on several types of operator-decomposable differential equations. We also apply DOSnet to nonlinear Schrodinger equations which have important applications in the signal processing for modern optical fiber transmission systems, and experimental results show that our model has better accuracy and lower computational complexity than numerical schemes and the baseline DNNs.

Regularized boundary integral equation methods solving scattering wave problems

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Abstract. In this talk, we propose high-order accurate regularized boundary integral equation methods for dynamic poro-elastic problems and acoustic layered-medium problems. For both problems, new regularized formulations of the strongly-singular and hyper-singular boundary integral operators are derived. Regarding to the poro-elastic scattering problem, a novel low-GMRES-iteration regularized boundary integral equation based on an analytical preconditioner is presented. As for the acoustic layered-medium scattering problems, the original scattering problem is truncated onto a bounded domain by the PML. We derive BIEs on local defects only in terms of using PML-transformed free-space Green's function, and the four standard integral operators. Numerical results will be given indicating the accuracy and efficiency of the proposed methods.

Port-Hamiltonian formulations of the incompressible Euler equations with a free surface

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Abstract. In this paper, we present the port-Hamiltonian formulations of incompressible Euler equations in three sets of variables: velocity, solenoidal velocity and vorticity. We start by extending the classical Hamiltonian system with free surface into generalized Hamiltonian system in terms of three sets of variables by using the language of exterior calculus. Then we will provide the corresponding port-Hamiltonian formulations with inhomogeneous boundary conditions. The novelty of our work is to consider the nonhomogeneous surface that is composed of free surface and permeable fixed surface. The key point of constructing a port-Hamiltonian system is the definition of Stokes-Dirac structure. Based on the theory of the generalized Hamiltonian system, we can define the boundary ports in the Stokes-Dirac structure.

Structure-preserving particle-in-cell methods for plasma simulations

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Abstract. We introduce two energy-conserving particle-in-cell (PIC) algorithms for plasma simulations. This first algorithm is based on the asymptotic-preserving scheme for the Vlasov-Maxwell system at the quasi-neutral limit characterized by the Debye length, where the electric field is calculated through a generalized Ohm law. The Boris correlation and an additional Lagrange multiplier are introduced to achieve both the Gauss-law satisfying and the energy conservation. In the second method, we construct curl-free basis functions for the Vlasov-Ampère equations which is equivalent to the Vlasov-Poisson equations. The scheme with energy conservation is designed, together with an asymptotic-preserving preconditioner such that the scheme can simulate systems at the quasi-neutral limit. Classical benchmarks including the Landau damping, two-streaming instability and bump-on-tail instability are present to show the necessity of energy conservation and the attractive performance of the new algorithms.

Energy dissipation of time-fractional phase-field equations: analysis and numerical methods

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Abstract. There exists a well-defined energy dissipation law for classical phase-field gradient flows, i.e., the free energy is non-increasing with respect to time. However, it is not clear how to extend the energy definition to time-fractional phase-field equations so that the corresponding dissipation law is still satisfied. In this talk, we will try to partly settle this problem for phase-field equations with Caputo time-fractional derivative, by defining a nonlocal energy as an averaging of the classical energy with a time-dependent weight function. To deal with this, we propose a new technique on judging the positive definiteness of a symmetric function, that is derived from a special Cholesky decomposition. Then, the nonlocal energy is proved to be dissipative under a simple restriction of the weight function. Moreover, the time fractional derivative of classical energy for time-fractional phase-field models can be proved to be always nonpositive. At the discrete level, a fast L2-1_σ method on general nonuniform meshes is employed. The global-in-time H^1-stability is established via the same framework.

Weak Galerkin finite element scheme and its applications

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Abstract. The weak Galerkin (WG) finite element method is a newly developed and efficient numerical technique for solving partial differential equations (PDEs). It was first introduced and analyzed for second order elliptic equations and further applied to several other model equations, such as the Brinkman equations, the eigenvalue problem of PDEs to demonstrate its power and efficiency as an emerging new numerical method. This talk introduces some progress on the WG scheme.

Stability threshold of the Couette flow at high Reynolds number

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Abstract. Since Reynolds' experiment in 1883, the hydrodynamic stability has been an active field in fluid mechanics and mathematics. This field is mainly concerned with how laminar flow becomes unstable and transit to turbulence. In order to understand the transition mechanism of laminar flow, Trefethen et al (Science 1993) proposed the transition threshold problem "how much disturbance will lead to the instability of the flow and the dependence of disturbance on the Reynolds number". In this talk, I will introduce some recent progress on the stability threshold of the Couette flow.

Dispersive limit of kinetic models for collisional plasma

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Abstract. The motion of charged particles can be described by the Vlasov-Poisson-Boltzmann (VPB) system. Compared to the classical Boltzmann equation for dilute gases, solutions to VPB are expected to have dispersive behaviour because of the dispersion mechanism on the dynamics of plasma in different scales of physical interest. By a formal spectrum analysis, we can observe asymptotic relations between VPB and some limiting dispersive equations in a suitable regime. Then we justify that the propagation of non-linear ions-acoustic waves are governed by the KdV equation. This is a joint work with T. Yang.

Green's function and pointwise behaviors of the 1-D Vlasov-Maxwell-Boltzmann system

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Abstract. In this talk, we study the pointwise space-time behavior of the Green's function of the one-dimensional Vlasov-Maxwell-Boltzmann (VMB) system. It is shown that the Green's function consists of the macroscopic diffusive waves and Huygens waves with the speed $\pm\sqrt{\frac{5}{3}}$ at low-frequency, the hyperbolic waves with the speed ± 1 at high-frequency, the singular kinetic and leading short waves, and the remaining term decaying exponentially in space and time. Note that these high-frequency hyperbolic waves are completely new and can not be observed for the Boltzmann equation and the Vlasov-Poisson-Boltzmann system. In addition, we establish the pointwise space-time estimate of the global solution to the nonlinear VMB system based on the Green's function. Compared to the Boltzmann equation and the Vlasov-Poisson-Boltzmann system, some new ideas are introduced to overcome the difficulties caused by the coupling effects of the transport of particles and the rotating of electro-magnetic fields, and investigate the new hyperbolic waves and singular leading short waves.

Deep adaptive sampling for numerical PDEs

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Abstract. Adaptive computation is of great importance in numerical simulations. The ideas for adaptive computations can be dated back to adaptive finite element methods in 1970s. In this talk, we shall propose a deep adaptive sampling method for solving PDEs where deep neural networks are utilized to approximate the solutions. In particular, we propose the failure informed PINNs (FI-PINNs), which can adaptively refine the training set with the goal of reducing the failure probability. Compared to the neural network approximation obtained with uniformly distributed collocation points, the developed algorithms can significantly improve the accuracy, especially for low regularity and high-dimensional problems.