

**Workshop and Summer School on Kinetic
Theory and Related Applications**

06/28-07/01 Online

Title and Abstracts

Data-driven epidemic models with social structure

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We introduce a mathematical description of the impact of sociality in the spread of infectious diseases by integrating epidemiological dynamics with a kinetic modeling of population-based contacts. The kinetic description leads to study the evolution over time of Boltzmann-type equations describing the number densities of social contacts of susceptible, infected and recovered individuals, whose proportions are driven by a classical SIR-type compartmental model in epidemiology. Explicit calculations show that the spread of the disease is closely related to moments of the contact distribution. Furthermore, the kinetic model allows to clarify how a selective control can be assumed to achieve a minimal lockdown strategy by only reducing individuals undergoing a very large number of daily contacts. In a second part, using a detailed dataset furnished by Italian National Health Authorities, we propose to determine the essential features of the ongoing COVID-19 pandemic in terms of contact dynamics. This combines the mathematical description of the spread of an infectious disease with a detailed analysis of the dataset of all traced infected individuals in an Italian Province. These information are used to develop a data-driven model in which calibration and feeding of the model are extensively used. The results obtained permit, thanks to an uncertainty quantification approach and in the short time horizon, forecasting the average number and the confidence bands of expected hospitalized patients classified by age and to test different options for an effective vaccination campaign with age-decreasing priority.

Kinetic and moment-driven methods for optimal control in collective behavior

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Mathematical description of collective behavior has been studied in a wide spectrum of applications such as animal behavior, cellular aggregation, opinion dynamics, and human crowd motion. Our research addresses the design of external control actions able to influence a large system of interacting agents towards prescribed stable patterns. We address this challenge by means of optimal control techniques, thus minimizing an energy measure of both the control and the state of the system. In order to circumvent the solution of such large scale non-linear optimization problem we introduce mean-field optimal control problems, where the microscopic dynamics is approximated by the evolution of a nonlocal PDE model.

For the numerical realization of these problems, we will propose different strategies. First, we will introduce a class of asymptotic stochastic methods based on the statistical description of constrained binary interactions via Boltzmann-type equation. This approach allows generating a hierarchy of feedback controls for the mean-field dynamics reducing the overall computational cost associated with the original problem. Second, under limited access to measurements of the dynamics, we propose moment-driven methods. These approaches are based on a dynamic linearization of the optimal control problem via Riccati-type equations and estimates on moment decay of the mean-field density.

The efficiency and robustness of these methods is validated with several numerical examples for the control of flocking and swarming behaviors.

The Landau equation: Particle Methods & Gradient Flow Structure

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The Landau equation introduced by Landau in the 1930's is an important partial differential equation in kinetic theory. It gives a description of colliding particles in plasma physics, and it can be formally derived as a limit of the Boltzmann equation where grazing collisions are dominant. The purpose of this talk is to propose a new perspective inspired from gradient flows for weak solutions of the Landau equation, which is in analogy with the relationship of the heat equation and the 2-Wasserstein metric gradient flow of the Boltzmann entropy. Moreover, we aim at using this interpretation to derive a deterministic particle method to solve efficiently the Landau equation. Our deterministic particle scheme preserves all the conserved quantities at the semidiscrete level for the regularized Landau equation and that is entropy decreasing. We will illustrate the performance of these schemes with efficient computations using treecode approaches borrowed from multipole expansion methods for the 3D relevant Coulomb case. From the theoretical viewpoint, we use the theory of metric measure spaces for the Landau equation by introducing a bespoke Landau distance d_L . Moreover, we show for a regularized version of the Landau equation that we can construct gradient flow solutions, curves of maximal slope, via the corresponding variational scheme. The main result obtained for the Landau equation shows that the chain rule can be rigorously proved for the grazing continuity equation, this implies that H-solutions with certain apriori estimates on moments and entropy dissipation are equivalent to gradient flow solutions of the Landau equation. We crucially make use of estimates on Fisher information-like quantities in terms of the Landau entropy dissipation developed by Desvillettes.

On conservative Fourier-Galerkin spectral methods for kinetic equations

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In this talk we will review some recent results on the development of Fourier-Galerkin spectral methods for kinetic equations that preserve the main relevant physical properties of the kinetic model, namely the conservation of moments and equilibrium states. In particular, we will show how these properties can be recovered without sacrificing spectral accuracy. Applications to the challenging case of the Boltzmann equation will also be presented.

On the stability of conservative discontinuous Galerkin/Hermite spectral methods for the Vlasov- Poisson system

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We propose a class of conservative discontinuous Galerkin methods for the Vlasov-Poisson system written as an hyperbolic system using Hermite polynomials in the velocity variable. These schemes are designed to be systematically as accurate as one wants with provable conservation of mass and possibly total energy. Such properties in general are hard to achieve within other numerical method frameworks for simulating the Vlasov-Poisson system. The proposed scheme employs discontinuous Galerkin discretization for both the Vlasov and the Poisson equations, resulting in a consistent description of the distribution function and electric field. Numerical simulations are performed to verify the order of accuracy and conservation properties. Finally, we propose a new stability analysis in a weighted L^2 space.

Application Of The Moment Method In The Slip And Transition Regime

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A state of a gas can be described either from a macroscopic or microscopic view. It is adequate to use traditional thermo-hydrodynamic variables such as the gas density, temperature and velocity and their governing equations to describe the dynamics of the flow fields when the state of the gas is close to the equilibrium. However, it is a great challenge to predict the flow behaviour accurately and efficiently with traditional thermo-hydrodynamic variables when the gas is away from the equilibrium, e.g. if it is rarefied or in a microsystem. From a microscopic point of view, the molecular distribution governed by the Boltzmann equation can predict rarefied gas dynamics accurately. However, tremendous effort is required to solve the Boltzmann equation for practical applications because of its high dimensionality and the complexity of the collision term, particularly in the slip and early transition regime.

By combining the moment method of Grad and the Chapman-Enskog expansion, the regularized moment equations can be derived from the Boltzmann equation to describe rarefied gas flows at different levels of rarefaction. With an extra number of macroscopic variables and a relatively small amount of increased computational requirements, in comparison to traditional computational fluid dynamics, the moment equations are accurate enough to capture non-equilibrium phenomena in the slip and early transition regime.

In the present talk, using the 26-moment system as an example, the procedure to obtain the regularized moment equations will be introduced, along with the wall boundary conditions. To extend the range of the applications, a hybrid algorithm of coupling the moment equations and the Boltzmann equation will be presented.

Canonical non-equilibrium problems are analyzed to validate the macroscopic equations of different orders. In comparison with data from kinetic theory, it is found that the R26 moment equations provide an excellent qualitative description of the hydrodynamic and thermal Knudsen layer in terms of the velocity and temperature defect. An existence criterion, which identifies the limits for the presence of vortices, is discovered for flow past a stationary cylindrical cylinder in the transition regime.

Geometric Particle-In-Cell methods for the Vlasov-Maxwell equations

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The Vlasov-Maxwell equations can be derived from a variational principle or a non-canonical hamiltonian structure. This leads to a certain number of invariants, like mass, momentum, energy and the conservation of the Gauss laws.

In this talk we shall show how these structures can be kept at the discrete level by using a particle-in-cell method for the Vlasov equations and Finite Element Exterior Calculus for Maxwell's equations involving a discrete de Rham complex and an appropriate Finite Element approximation of each field.

This leads to a Finite Dimensional Hamiltonian system, which then can be discretised in time with geometric integrators like hamiltonian splitting or exact energy preserving discrete gradient methods.

Finite Element Discretizations for Moment Equations in Kinetic Gas Theory

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It is generally accepted that kinetic theory and the Boltzmann equation based on a statistical description of the gas provides a valid framework to describe processes in a rarefied regime or at small scales. However, in many applications this detailed statistical approach yields a far too complex description of the gas. It turns out to be desirable to have a continuum model based on partial differential equations for the fluid mechanical field variables, like density, velocity and temperature. This model should accurately approximate the multi-scale phenomena present in kinetic gas theory in a stable and compact system of field equations.

For small Knudsen numbers the classical laws of Navier-Stokes and Fourier are very successfully applied. In the transition regime at intermediate Knudsen numbers up to $\text{Kn} < 1$, a fluid description is still possible, although a larger set of field variables or higher derivatives may be needed. The Regularized-13-Moment equations (R13) is a stable and accurate moment model which has been successfully used in recent years to predict rarefied and micro-flows of gases.

This talk discusses the discretization of the linear R13 equations using the finite element approach. Fundamental for this is the derivation of a weak form or variational formulation which can be derived and comes as generalization of the weak form of a standard Stokes problem. Using this result it is straight forward to implement R13 in finite element libraries, like FEniCS, and we will show convergence studies and realistic simulation results.

Fast Converging and Asymptotic Preserving Method for Multiscale Rarefied Gas Flows

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The macroscopic length and time characterizing the gas flows found in various engineering applications usually vary by several orders of magnitude. The macroscopic transport equations such as the Navier-Stokes-Fourier, Burnett, and 13 moments equations, are only valid when the Knudsen number, i.e., the ratio between the mean free path (mean collision time) of gas molecules and a characteristic flow length (time) is small. For multiscale flows of general values of Knudsen number, the kinetic equation that describes the microscopic behavior of gases from a statistical viewpoint should be adopted.

When solving the gas kinetic equation, an iterative solver is usually required as the integral nature of the collision operator makes the discretized equation not invertible. It is well known that the conventional iterative scheme (CIS) is efficient when the Knudsen number is around one and larger; however, for multiscale flows with small-Knudsen-number regions involving, it converges extremely slow, and the solution is vulnerable to large numerical dissipation when the spatial cell size is not refined enough.

To overcome the shortcomings of the CIS, we have introduced the general synthetic iterative scheme (GSIS). The key ingredient of the GSIS is that during each iteration, the kinetic equation is simultaneously solved with its macroscopic moment equations, where the latter ones provide the macroscopic quantities appearing in the collision operator and guide the inefficient evolution of the velocity distribution function.

The constitutive relations for stress (heat flux) and strain (temperature gradient) in the macroscopic equations are strictly derived from the kinetic equation, in which the high-order terms beyond the Newtonian and Fourier's laws are directly evaluated from the velocity distribution function, thus guaranteeing accuracy over all flow regimes. Rigorous

s Fourier stability analysis and Chapman-Enskog expansion show that the GSIS can converge within dozens of iterations at arbitrary Knudsen numbers and asymptotically preserve the Navier-Stokes-Fourier limit over a coarse spatial mesh. Therefore, the scheme can achieve accurate and efficient simulations for multiscale rarefied gas flows.

The GSIS has been applied to various problems, such as shear/thermal driven flows in microscopic devices, pressure driven flows through porous media, and high-speed flows around objectives. Compared to the CIS, the saving of computational resources in the GSIS is significant. The methodology to design the scheme is not restricted to any specific form of a kinetic equation. The GSIS has been used to solving the Boltzmann equation and kinetic models for linear/nonlinear steady flows of monatomic gases as well as kinetic models for linear polyatomic gaseous flows. Recently, it has been successfully extended to unsteady problems. The idea will also be applicable for more complicated flows, such as multicomponent flows, chemical reactive flows and dense gas flows.

Highly-oscillatory evolution equations: averaging and numerics

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Usual numerical methods become inefficient when they are applied to highly oscillatory evolution problems (order reduction or complete loss of accuracy). This is due to the non-uniform boundeness of the time-space derivatives of the solution with respect to the oscillation frequency. The numerical parameters of these schemes must then be adapted to the high frequencies that come into play in order to correctly capture the desired information, and in general this induces a prohibitive computational cost. Furthermore, the numerical resolution of averaged models, even with high order asymptotics, is not sufficient to capture low frequencies and intermediate regimes. We present two strategies allowing to remove this obstacle for a large class of evolution problems, by introducing new suitable formulations of the problem: a 2-scale formulation and a micro/macro decomposition. We consider both the constant frequency case and varying - possibly vanishing - frequency framework and show that the hierarchy of averaged models in the vanishing case is more complex than in the constant frequency case since stationary-phase effects must be taken into account. A main consequence of these strategies is the fact that usual numerical schemes of arbitrary order automatically work on the new formulations and their order of accuracy no longer depends on the frequency of oscillation. One then speaks of uniform accuracy (UA) for these schemes. Finally, a new technique for systematizing the implementation of the two methods will be presented. Its purpose is to reduce the number of inputs that the user must provide to apply the method in practice. In other words, only the values of the field defining the evolution equation (and not its derivatives) are used. These methods have been successfully applied to solve some well-known evolution models: non-linear Schrödinger and Klein-Gordon equations, Vlasov-Poisson kinetic equation with strong magnetic field, quantum transport in graphene.

A bi-fidelity method for different kinetic models with uncertain parameters

Liu Liu

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In this talk, we first introduce the bi-fidelity stochastic collocation method in uncertainty quantification, then adopt it to solve a class of kinetic models with random parameters and multiple scalings. We use the Boltzmann, the linear transport and kinetic epidemic models as examples to illustrate our idea, with different motivations of choosing the low-fidelity models in the bi-fidelity approximation. A formal uniform-in-Knudsen number error estimate, practical error bound and numerical experiments will be presented to demonstrate the accuracy and efficiency of our proposed method. This is a joint work with Xueyu Zhu and Lorenzo Pareschi.