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Abstracts

Workshop on Modelling and Numerical Simulation
of Non-Equilibrium Processes Part 1

27 September–1 October 2021

1 Michael R. A. Abdelmalik

Eindhoven University of Technology, Netherlands
Entropy-based Ansatz for the Boltzmann equation

Abstract

In this talk we develop an entropy-stable finite-element-moment method for the Boltzmann equation with binary collisions. The proposed method engenders a discontinuous-Galerkin method in position and temporal dependence, and a moment-method in velocity dependence. We base our moment-method on a converging sequence of approximations to the binary collision operator $C(f)$, denoted by $C_N(f)$. We associate with each member of the sequence a φ-divergence-based renormalization-map and entropy. We show that each $C_N(f)$ inherits salient properties from $C(f)$, such as the preservation of the collision invariants, Galilean invariance, and that the linearization of $C_N(f)$ coincides with the linearization of $C(f)$. We show that our proposed finite-element- moment method is entropy-stable for each member of the sequence of approximations to $C_N(f)$. Finally, we apply our finite-element-moment method to the Boltzmann equation with collision operator $C(f)$ and demonstrate the corresponding approximation properties, using benchmark test cases, in comparison to Direct Simulation Monte Carlo.

This is joint work with Torsten Kessler and Sergej Rjasanow from the Saarland University, and Irene Gamba from UT Austin.

2 Alejandro Alvarez-Laguna

Laboratoire de Physique des Plasmas, École Polytechnique, France
A Grad's moment closure for multi-component reacting low-temperature plasmas

Abstract

Low-temperature plasmas are difficult to model because of the strong non-equilibrium conditions and the complex interplay with the electromagnetic field. Standalone fluid-based models usually fail to fully represent the physics in weakly-collisional regimes. In this talk, we will derive a velocity-moment plasma model from the kinetic equation by means of Grad's method that accounts for a multi-component reacting mixture in chemical and thermal non-equilibrium with the effect of an electromagnetic field. The model considers the evolution of mass, momentum, energy, heat flux vector, and the contracted fourth moment balance. By doing this, the excess kurtosis of the electron population at high energies, typical in low-temperature plasmas, is self-consistently captured by the model. We will explain the derivation of the collisional terms for both elastic and inelastic collisions by using the full Boltzmann operator as opposed to a simplified BGK operator. Different asymptotic limits of these equations with respect to the collisionality, quasi-neutrality, and electron inertia will be discussed. We will discuss the discretization of the system of equations with asymptotic-preserving schemes in order to avoid severe time-step restrictions due to the resolution of the small scales. Comparison of the plasma moment model with kinetic simulations and experimental results will be also discussed in this seminar.

3 Rodney Fox

Iowa State University, USA
Hyperbolic quadrature method of moments for the kinetic equation

Abstract

For applications such as rarefied gas dynamics or spray flows, there is an interest in developing moment methods from a kinetic description of the gas or the spray since such methods can be computationally efficient. In this context, a solution is proposed to a longstanding open problem in kinetic

theory, namely, given any set of realizable velocity moments up to order 2n, a closure for the moment of order 2n+1 is constructed for which the moment system found from the free-transport term in the one-dimensional (1-D) kinetic equation is globally hyperbolic and in conservative form. This is a reformulation and generalization of the hyperbolic quadrature method of moments (HyQMOM) introduced in our prior work.

The HyQMOM closure is defined based on the properties of the monic orthogonal polynomials Qn that are uniquely defined by the velocity moments up to order 2n 1. Thus, HyQMOM is strictly a moment closure and does not rely on the reconstruction of a velocity distribution function with the same moments. Moreover, one can show the hyperbolicity of the corresponding system, at least for n <= 11, and the good behavior of the eigenvalues of the problem when the moment vector tends to the boundary of the moment space, a property that can be important for applications such as sprays. An efficient algorithm for computing the moment of order 2n + 1 from the moments up to order 2n is developed, based on the Chebyshev algorithm. The analytical solution to a 1-D Riemann problem is used to demonstrate convergence of the HyQMOM closure with increasing n. As time allows a possible extension to 2-D and 3-D kinetic equations will be discussed.

4 Hossein Gorji

Empa - Swiss Federal Laboratories for Materials Science and Technology, Switzerland

Fokker-Planck kinetics, data-driven coupling and beyond

Abstract

Kinetic interactions comprise challenging problems across different fronts of modelling, computation and analysis. While the Boltzmann equation provides a formal and neat starting point, the high dimensionality and stiffness of the collisions render it intractable in many practical settings. Yet by interpreting discrete collisions as continuous random forces, we can expand the applicability of the kinetic framework and provide an efficient remedy to the overwhelming collision operations. In this talk, I address such continuous stochastic models governed by the Fokker-Planck equation. I present a rather detailed recipe to construct such models, where physical constraints including conservation and entropy laws are met, and furthermore significant compu-

tational gains are obtained in the near continuum and transitional regimes. Next, to integrate the kinetic models in a hybrid framework, I review the upscaling by means of data-driven closures. By leveraging the Gaussian-Process regression, a computationally efficient Maximum-Entropy-Distribution suitable for coupling kinetic and continuum simulators is obtained. I conclude the talk by offering a more general overview of Fokker-Planck equations, Maximum-Entropy-Distributions, and their connections to the Schrödinger bridge: presenting possible generalisation of the devised methodology beyond kinetic problems.

5 Clinton Groth

University of Toronto, Canada

Maximum-entropy-inspired interpolative-based moment closures for predicting nonequilibrium radiative heat transfer in non-gray participating media

Abstract

Maximum-entropy-inspired interpolative-based moment closure methods are considered for the prediction of nonequilibrium radiative transfer in non-gray participating media. In particular, interpolative-based versions of both the first- and second-order maximum entropy closures, M_1 and M_2, respectively, are described and examined. The interpolative-based closures are constructed so as to duplicate many of the desirable mathematical properties of maximum-entropy closure techniques, including positivity and moment realizablility of the distribution of radiative energy and hyperbolicity of the resulting moment equations while offering significant computational savings compared approaches that involve the direct numerical solution of the optimization problem for entropy maximization. Theoretical details of the proposed interpolative-based moment closures, along with a description of an efficient Godunov-type finite-volume scheme that has been developed for the numerical solution of the moment equations on multi-block body-fitted quadrilateral meshes with anisotropic adaptive mesh refinement (AMR) are described. The predictive capabilities of the proposed non-gray interpolative-based M_1 and M_2 closures are assessed by considering their application to a number of canonical radiative transfer problems involving transport through real gases with a strong spectral dependence of the absorption coefficient. The latter is evaluated using a statistical narrow-band correlated-k model.

The assessment includes comparisons to the predictions of the more commonly adopted first-order, P_1, and third-order, P_3, spherical harmonic moment closures, as well as the popular discrete ordinates method (DOM). The numerical results demonstrate the potential of the maximum-entropy-inspired closures. In particular, the non-gray interpolative-based M_1 and M_2 closures are shown to provide improved predictions compared to the P_1 closure and are of comparable or improved accuracy compared to the P_3 closure, while providing additional computational robustness relative to the spherical harmonic closures.

6 Xiao-Jun Gu

Science and Technology Facilities Council, UK

Modelling non-equilibrium gas flows by coupling kinetic and extended thermodynamic methods

Abstract

It is a great challenge to predict the flow behaviour accurately and efficiently with traditional thermo-hydrodynamic variables and their governing equations when the gas is away from the equilibrium, such as it is rarefied or in a microsystem. Although the molecular distribution function governed by the Boltzmann equation can predict the rarefied gas dynamics accurately, tremendous efforts are 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.

With the extra number of macroscopic variables, i.e. the higher moments of the molecular distribution function and a relatively small amount of increasing the computational requirements in comparison to the traditional computational fluid dynamics, the method of moments provides an alternative proximate solution procedure to the Boltzmann equation for the non-equilibrium gas flow in the slip and early transition regime. However, the method of moments, as an extended thermodynamic approach, is less accurate close to the wall where non-equilibrium effects are strong. Therefore, a hybrid algorithm is proposed that combines the discrete velocity method with the method of moments to accurately simulate rarefied gas flows in the transition regime. A discrete velocity approach for the kinetic equation, combined with Maxwell's wall boundary condition, is employed in the near-wall

region and the moment equations are used to describe the bulk flow field.

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 equations will be presented.

7 Vinay Kumar Gupta

Indian Institute of Technology Indore, India

Modelling dilute granular gases via Grad's moment method

Abstract

A collection of macroscopic solid particles characterized by dissipative (or inelastic) collisions is referred to as a granular material. Granular materials are ubiquitously present in nature, e.g. in the form of sand, debris, avalanches, dust storms, asteroid belt, planetary rings, etc., and are also encountered in our day-to-day life, e.g. in the form of food grains, coffee beans, cereals, nuts, etc. They are also an integral part of several industries, such as pharmaceutical, fertilizers, cement, coal, etc. Owing to dissipative collisions, granular materials are inherently in non-equilibrium and exhibit several intriguing phenomena, such as standing wave patterns, shear banding, clustering, mixing and segregation, jamming, etc. While some of the phenomena pertaining to granular materials can be explained theoretically using the granular Navier–Stokes equations, the others are still poorly understood due to the unavailability of sophisticated mathematical models and efficient numerical frameworks.

Depending on the energy input, granular materials can exist in the solid, liquid or gaseous state or can coexist in these states. In this talk, the focus will be on the gaseous state of granular materials, for which—similarly to molecular gases—mathematical tools can be developed within the framework of kinetic theory. The talk will be based on my two recent papers [1, 2] and will present the development of Grad moment equations for a dilute granular gas composed of (inelastic) (i) hard spheres and (ii) Maxwell molecules. Furthermore, it will be shown that the considered Grad moment equations lead to more accurate transport coefficients. As an application, the

homogeneous cooling state and its stability against the small perturbations will also be demonstrated.

Acknowledgements: The author gratefully acknowledges the financial support through the "MATRICS" project MTR/2017/000693 funded by the SERB India.

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8 Weiming Li

Institute of Applied Physics and Computational Mathematics, China

Direct flux gradient approximation to moment closure of kinetic equations

Abstract

To close the moment model deduced from kinetic equations, the canonical approach is to provide an approximation to the flux function not able to be depicted by the moments in the reduced model. In this talk, we propose a new closure approach. Instead of approximating the flux function, the new approach close the moment model by approximating the flux gradient. Precisely, we approximate the space derivative of the distribution function by an ansatz which is a weighted polynomial, and the derivative of the closing flux is computed by taking the moments of the ansatz. Consequently, the method provides us an improved framework to derive globally hyperbolic moment models, which preserve all those conservative variables in the low order moments. It is shown that the linearized system at the weight function, which is often the local equilibrium, of the moment model deduced by our new approach coincides with the system deduced from the classical perturbation theory. This is a property which can not be satisfied by previous hyperbolic regularization framework. Taking the Boltzmann equation as example, the linearlization of the moment model gives the correct Navier-Stokes-Fourier

law same as that the Chapman-Enskog expansion gives. Most existing globally hyperbolic moment models are re-produced by our new approach, and several new models are proposed based on this framework.

9 Duncan Lockerby

University of Warwick, UK
Simulation of micro-scale particulate motion in gases

Abstract

Low-speed gas flow around micro-scale particles (e.g. soot and other pollutants), and through suspensions of particles, are surprisingly rich in physics and challenging to simulate. The hydrodynamic reach of a single particle is extremely wide, preventing application of straightforward numerical-simulation approaches (e.g. finite-volume CFD). Furthermore, their scale renders the conventional Navier-Stokes equations, and associated boundary conditions, inaccurate, unable to capture rarefied effects such as thermophoresis and velocity slip. The problems are especially challenging in the transitional Knudsen regime for non-canonical geometries.

In this talk we report recent developments in simulating micro-scale particulate flows using the Method of Fundamental Solutions applied to the linearised Grad's 13 moment equations, which provides a convenient and numerically efficient alternative to solving the full Boltzmann equation. We look at a range of particulate geometry, including agglomerates, and describe how particle conductivity can be coupled with the external gas flowfield to provide accurate predictions of thermophoretic response.

The talk describes research funded in the UK by the EPSRC (EP/N016602/1).

10 James McDonald

University of Ottawa, Canada
Extended Gaussian moment methods for polydisperse multiphase flow with evaporation and turbulence

Abstract

This talk demonstrates the extension of the classical Gaussian, ten-moment closure of gas dynamics for the treatment of polydisperse multiphase flows.

By extending the distribution function and kinetic equation into an arbitrary number of independent variables that differentiate the individual particles (size, temperature, etc.), an expanded moment method that offers predictions for the mean value as well as variance and covariance of all variables is produced. The resulting closures are all robustly hyperbolic and have a relatively simple eigenstructure, thus facilitating reliable numerical solution.

As examples, two different closures for polydisperse flow are presented. Particle drag, evaporation, and the effects of an under-resolved turbulent background flow are considered. As example applications, atmospheric dispersion, fuel sprays, and biological droplets from coughs or sneezes are examined.

11 Anirudh Singh Rana

Birla Institute of Technology and Science, Pilani, India

Simulation of evaporation and condensation processes in nanodevices using mesh-free methods

Abstract

The generation of localized heat loads in high power electrical components, such as in modern information communication technologies, poses significant thermal management challenges in defence, space and commercial sectors. The key to further advancement of such state-of-the-art technologies lies in developing disruptive innovations to device cooling, moving from a solid-state heat sink to an active cooling technology.

Two of the main challenges in the modelling of phase-change processes in micro/nanoscale thermal–fluidic transport systems are: (i) the classical continuum theories based upon the Navier-Stokes-Fourier equations fail to accurately capture the vapor flow characteristics as the representative physical length scale of the flow becomes comparable to the mean free path in the vapor, i.e., the Knudsen number 1. (ii) 3D simulations describing such processes are computationally very expensive/intractable.

In my talk, I present a robust, scalable and computationally efficient numerical framework using truly mesh-free methods (method of fundamental solutions) for the coupled constitutive relations (CCR), with an emphasis on evaporation/condensation from nano-structures.

12 James Rossmanith

Iowa State University, USA
Spectral element moment-closures for kinetic models

Abstract

In many applications, the dynamics of gas and plasma can be accurately modeled using kinetic Boltzmann equations. These equations are integrodifferential systems posed in high-dimensional phase space. If the system is sufficiently collisional, the kinetic equations may be replaced by a fluid approximation. In general, finding a suitable robust moment-closure is still an open problem. In this work, we consider spectral element moment-closures, in which we first divide the velocity space into a discrete mesh, and then introduce moments that are local only to each velocity space element. In standard moment-closures the only mechanism to improve the approximation is to add more global moments; in the spectral element approach, one can either vary the number of moments in each velocity element, vary the number of velocity elements, or both. An important advantage of this approach is that we are able to utilize in each velocity element a simple linear moment-closure that is provably symmetric hyperbolic, rather than a nonlinear closure that may be only conditionally hyperbolic. We develop for this closure a high-order discontinuous Galerkin scheme and test apply to various test problems. This is joint work with Christine Vaughan and Alberto Passalacqua.

13 Neeraj Sarna

Max Planck Institute for Dynamics of Complex Technical Systems Magdeburg, Germany
Convergence and stability properties of Grad's Hermite approximation

Abstract

We consider Grad's Hermite approximation for a linearised Boltzmann equation arising from rarefied gas dynamics. In both spatially continuous and spatially discrete setting, we present boundary conditions that ensure the L2-stability of the Hermite approximation. Furthermore, we discuss the importance of stability in deriving convergent error bounds. We analyse the

different sources of sub-optimality in our error bound and attempt to recover a fast converging Hermite expansion.

14 Henning Struchtrup

University of Victoria, Canada
26 moment equations for liquid-vapor interfaces

Abstract

The Enkog-Vlasov equation is an extension of the Boltzmann equation that accounts for large densities through the Enskog collision term, and for long-range particle interaction through the Vlasov term [1, 2, 3]. The equation describes states from compressed liquid to non-ideal, or ideal, gas vapor, including diffusive phase interfaces. Thus, it provides an excellent tool for modelling of processes with liquid-vapor interfaces and adjacent Knudsen layers, and allows us to look at slip, jump and evaporation coefficients from a different perspective.

A set of 26 moment equations is derived from the Enskog-Vlasov equation by means of the Grad moment method [4]. The equations provide a meaningful approximation to the underlying kinetic equation, and include the description of compressible liquid and non-ideal gas behavior as well as fully resolved liquid-vapor interfaces. Moreover, the equations include rarefaction effects such as Knudsen layers, transpiration flow, thermal stresses or heat transfer without temperature gradients. This contribution focusses on numerical results for simple flow problems (Couette flow, heat transfer, forced evaporation) that highlight the richness of the equations. Results are discussed with emphasis on the behavior at interfaces, where the equations resolve temperature jumps, velocity slip, and evaporation processes, which appear not as jumps, but as steep changes. Comparison with classical sharp interface models gives insight into values for jump, slip and evaporation coefficients.

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15 Yanli Wang

Beijing Computational Science Research Center, China

Regularized 13-moment equations for inverse power law models

Abstract

We propose a systematic methodology to derive the regularized thirteen-moment equations in the rarefied gas dynamics for a general class of linearized collision models. Detailed expressions of the moment equations are written down for all inverse power law models as well as the hard-sphere model. By linear analysis, we show that the equations are stable near the equilibrium. The models are tested for shock structure problems to show its capability to capture the correct flow structure in strong nonequilibirum.

16 Wen-an Yong

Tsinghua University, China

Learning Galilean invariant and thermodynamically stable PDES for non-equilibrium flows

Abstract

In this talk, I will present a method for learning thermodynamically stable and Galilean invariant PDEs. As governing equations for non-equilibrium flows in one dimension, the learned PDEs are parameterized by fully-connected neural networks and satisfies a certain thermodynamical stability criterion automatically. In particular, they are hyperbolic balance laws and Galilean invariant. The training data are generated from a kinetic model with smooth initial data. Numerical results indicate that the learned PDEs can achieve

good accuracy in a wide range of Knudsen numbers. Remarkably, the learned dynamics can give satisfactory results with randomly sampled discontinuous initial data and Sod's shock tube problem although it is trained only with smooth initial data.