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Abstracts

Workshop on Modelling and Numerical Simulation
of Non-Equilibrium Processes Part 2

24–28 January 2022

1 Walter Boscheri

University of Ferrara, Italy

High order finite volume (FV) and discontinuous Galerkin (DG) schemes with IMEX time stepping for the Boltzmann model on unstructured meshes

Abstract

In this work, we present a family of time and space high order finite volume and discontinuous Galerkin schemes for the solution of the full Boltzmann equation. The velocity space is approximated by using a discrete ordinate approach while the collisional integral is approximated by spectral methods. The space reconstruction is implemented by integrating the distribution function, which describes the state of the system, over arbitrarily shaped and closed control volumes using a Central Weighted ENO (CWENO) technique. Compared to other reconstruction methods, this approach permits to keep compact stencil sizes which is a remarkable property in the context of kinetic equations due to the considerable demand of computational resources. The full discretization is then obtained by combining the previous phase-space approximation with high order Implicit–Explicit Runge–Kutta schemes (DG-IMEX-RK) and Implicit–Explicit Linear Multistep Methods based on Backward-Finite-Differences (DG-IMEX-BDF) for solving the Boltzmann model on multidimensional unstructured meshes. These methods guarantee stability, accuracy and preservation of the asymptotic state. Comparisons of the Boltzmann model with simpler relaxation type kinetic models (like BGK) are proposed showing the capability of the Boltzmann equation to capture

different physical solutions. The theoretical order of convergence is numerically measured in different regimes and the methods are tested on several standard two-dimensional benchmark problems in comparison with Direct Simulation Monte Carlo results. The talk ends with a prototype engineering problem consisting of a subsonic and a supersonic flow around a NACA 0012 airfoil. All test cases are run with MPI parallelization on several cores, thus making the proposed methods suitable for parallel distributed memory supercomputers.

2 Stéphane Brull

Université de Bordeaux, France
Approximation of the bi-temperature Euler system in 2 space dimensions

Abstract

This lecture is devoted to the numerical approximation of the bi-dimensional bi-temperature Euler system. This model is a non-conservative hyperbolic system describing an out of equilibrium plasma in a quasi-neutral regime. This system is a non-conservative hyperbolic system, because it contains products of the velocity with a pressure gradient. This cannot be transformed into a divergence form for non regular solutions.

We develop a second order numerical scheme by using a discrete BGK model. The second order extension is based on a subdivision of each cartesian cell into four triangles to perform affine reconstructions of the solution. Such ideas have been developed before in the literature for systems of conservation laws. We show in in the present case how they can be used in our non-conservative setting.

In the last part, we will present test cases to validate the method.

3 Nicolas Crouseilles

National Institute for Research in Digital Science and Technology (INRIA), France
High order numerical methods for a hybrid kinetic/fluid plasma model

Abstract

In this talk, we focus on the numerical approximation of a hybrid fluid-kinetic plasma model for electrons, in which energetic electrons are described by a Vlasov kinetic model whereas a fluid model is used for the cold population of electrons. First, we study the validity of this hybrid model in a two dimensional context (one dimension in space and one dimension in velocity) against the full (stiff) Vlasov kinetic model and second, a four dimensional configuration is considered (one dimension in space and three dimensions in velocity). To do so, we consider two numerical Eulerian methods. The first one is based on the Hamil- tonian structure of the hybrid system and the second approach, which is based on exponential integrators, enables to derive high order integrator and remove the CFL condition induced by the linear part. The efficiency of these methods, which are combined with an adaptive time stepping strategy, are discussed in the different configurations and in the linear and nonlinear regimes.

4 Martin Frank

Karlsruhe Institute of Technology, Germany
Structure-preserving artificial neural networks for moment closures

Abstract

We present how artificial neural networks can be used to substitute an otherwise costly moment closure. Specifically, we study entropy closures which have many desirable properties (among them guaranteed hyperbolicity, positivity and entropy decay). We will need to construct very specific artificial neural networks that are guaranteed to preserve these advantages. Furthermore, we address the question of data sampling. Several numerical results are shown.

5 Chang Liu

Institute of Applied Physics and Computational Mathematics, China
Multiscale numerical methods for kinetic equations and the applications in transport problems

Abstract

Constructing efficient and accurate multiscale numerical schemes for the simulation of particle transport problems has kept drawing researchers' attention for the past decades. The two major topics in multiscale modeling are the asymptotic-preserving (AP) property and the regime-adaptive property. The AP property measures the numerical scheme's capability to preserve the asymptotic property of the kinetic equations on a finite scale of cell size and time step, which can be much larger than the kinetic scale. The regime-adaptive property means that the degree of freedom of the numerical scheme reduces as the Knudsen number decreases. More specifically, the high dimensional (7D) equations are solved in the rarefied regime, and low dimensional (4D) equations are solved in the continuum regime.

The unified gas kinetic scheme (UGKS) is developed to achieve a second-order AP scheme, which preserves the NS level asymptotic behavior on the $\sqrt{Kn}$ scale. Based on the unified gas kinetic scheme, we propose the unified gas kinetic wave-particle method, which has the properties of second-order AP and regime adaptive. Both schemes have been applied in multiscale gas transport, photon transport, and plasma transport problems and show advantages in accuracy and efficiency.

This talk will introduce the construction and numerical properties of the UGKS and UGKWP schemes and the applications of the two methods in the multiscale transport problems.

6 Raphaël Loubère

Université de Bordeaux, France

Efficient deterministic numerical scheme to solve BGK and Boltzmann equation in 7D

Abstract

In this talk we will present an overview of our effort of research made towards improving the simulation of kinetic models (BGK and Boltzmann) in 3 dimension in space and velocity. The curse of high-dimensionality enforces us to find clever and cheap numerical methods, to exploit the resources efficiently, obviously relying on parallelism.

We will present our numerical method based on Discrete velocity Model, a spliting between transport and collision stages and a Fast Spectral Scheme to solve the expensive Boltzmann collision operator.

A large validation campaign will be presented to assess the good properties of this numerical method in 3Dx3Dx1D in parallel with or without embedded objects in the computational domain.

7 Ryan McClarren

University of Notre Dame, USA
Low-rank method for radiation transport calculations

Abstract

The numerical solution of the radiation transport equation (RTE) is challenging due to the high computational costs and the large memory requirements caused by the high-dimensional phase space. Here we detail an attempt to reduce the memory required, and computational cost of solving RTE by applying the dynamical low-rank (DLR) method, where a memory savings of about an order of magnitude without sacrificing accuracy is observed. The DLR approximation is an efficient technique to approximate the solution to time-dependent matrix differential equations. The desired approximation has three components similar to factors in singular value decomposition (SVD), and each of them is solved by integrating the matrix differential equation projected onto the tangent space of the low-rank manifold. This talk presents our recent work that builds on the established DLR method and aims to enable low-rank schemes for practical radiation transport applications. We propose a high-order/low-order (HOLO) algorithm to overcome the conservation issues in the low-rank scheme by solving a low-order equation with closure terms computed via a high-order solution calculated using DLR. With the properly chosen rank, the high-order solution well approximates the closure term, and the low-order solution can be used to correct the conservation bias in the DLR evolution. This improvement goes a long way to making the method robust enough for a variety of physics applications. We also introduce a low-rank scheme with discrete ordinates discretization in angle (SN method). This low-rank-SN system allows for an efficient algorithm called "transport sweep," which is highly desirable in computation. The derived low-rank SN equations can be cast into a triangular form in the same way as standard iteration techniques.

8 Luc Mieussens

Université de Bordeaux, France

Mesoscopic Boltzmann model equations for thermally perfect gases

Abstract

We propose a way to derive Bhatnagar-Gross-Krook and Fokker-Planck models of the Boltz- mann equation for rarefied flows of thermally perfect gases. These models can allow for various internal energies (rotation, vibration, electronic), which is required for high temperature flows, like in atmospheric reentry problems. However, our models do not contain any internal degrees of freedom: instead, they are accounted for by a mesoscopic approach. The molecular velocity is the only kinetic variable in the models, that makes their computational complexity similar to that of simple monoatomic gases. Moreover, we prove that these models satisfy conservation and entropy properties (H-theorem), and we derive their corresponding compressible Euler and Navier-Stokes asymptotics.
(joint work with Julien Mathiaud, Centre Lasers Intenses et Applications, Université de Bordeaux-CNRS-CEA UMR 5107)

9 Zhichao Peng

Michigan State University, USA

Asymptotic numerical scheme and reduced order model for the radiative transfer equation

Abstract

As the Knudsen number goes to zero, the radiative transfer equation (RTE) asymptotically converges to its diffusion limit. On one hand, it is a challenge to design efficient numerical schemes preserving the underlying physical limit. On the other hand, this limit also suggests the existence of a low-rank structure in the angular space which can be utilized to design reduced order models (ROMs). In the first part of this talk, we present an asymptotic preserving method solving time-dependent RTE based on the micro-macro decomposition and Schur complement. The proposed method is unconditionally stable in the diffusive regime and has standard CFL conditions in the transport regime. In the second part of the talk, we present a reduced basis method to build an angular-space ROM for the steady state RTE.

10 Teddy Pichard

École Polytechnique, France
Construction and analysis of the projective closures

Abstract

In this talk, I will describe the construction of a closure for systems of moments extracted from a generic kinetic equation. This closure is based on the decomposition of the representing distribution into two part: 1-a regular part representing an equilibrium, commonly a Maxwellian or a distribution minimizing an entropy, and 2-a singular part composed of a sum of Diracs. Such a decomposition was originally interpreted using a projection of a realizable moment vector on the boundary of the moment set.
From its construction, this closure is able to capture exactly both equilibrium and purely anisotropic regimes. It possesses therefore features from both entropy minimizing models (Levermore's or M_N) and quadrature models (QMOM). I will analyze and compare the hyperbolicity and entropy decay through the projective model with those models.

11 Kunlun Qi

The Chinese University of Hong Kong, China
A fast Fourier spectral method for the non-cutoff Boltzmann equation

Abstract

Numerical approximation of the Boltzmann equation is a challenging problem due to its high-dimensional, nonlocal, and nonlinear collision integral. In this talk, we will introduce a fast Fourier spectral method for the spatially homogeneous Boltzmann equation with non-cutoff collision kernels. Such kernels contain non-integrable singularity in the deviation angle which arise in a wide range of interaction potentials. Albeit more physical, the non-cutoff kernels bring a lot of difficulties in both analysis and numerics, hence are often cut off in most studies (the well-known Grad's angular cutoff assumption). We demonstrate that the general framework of the fast Fourier spectral method developed for cutoff collision kernels can be extended to handle the non-cutoff case as well, achieving the accuracy/efficiency comparable to the cutoff case. We also show through several numerical examples that the solution to the

non-cutoff Boltzmann equation enjoys the smoothing effect, a striking property absent in the cutoff case. This talk is based on joint work with Jingwei Hu (UW).

12 Jingmei Qiu

University of Delaware, USA

A conservative adaptive low rank high order tensor approach for nonlinear Vlasov equations

Abstract

We propose a conservative adaptive low-rank tensor approach to approximate nonlinear Vlasov solutions. The approach takes advantage of the fact that the differential operators in the Vlasov equation is tensor friendly, based on which we propose to dynamically and adaptively build up low-rank solution basis by adding new basis functions from discretization of the PDE, and removing basis from an SVD-type truncation procedure. For the discretization, we adopt a high order finite difference spatial discretization and a second order strong stability preserving multi-step time discretization.

While the SVD truncation will destroy the conservation properties of the full rank conservative scheme, we further develop low rank schemes with local mass, momentum and energy conservation for the corresponding macroscopic equations. The mass and momentum conservation are achieved by a conservative SVD truncation, while the energy conservation is achieved by replacing the energy component of the kinetic solution by the ones obtained from conservative schemes for macroscopic energy equation. Hierarchical Tucker decomposition is adopted for high dimensional problems, overcoming the curse of dimensionality. An extensive set of linear and nonlinear Vlasov examples are performed to show the high order spatial and temporal convergence of the algorithm, the significant CPU and storage savings of the proposed low-rank approach especially for high dimensional problems, as the local conservation of macroscopic mass, momentum and energy.

(Joint work with Wei Guo from Texas Tech University)

13 Thomas Rey

Université de Lille, France

On projective integration scheme for single and multiple species gases

Abstract

Projective integration has been recently proposed as a viable alternative to fully implicit and micro-macro methods for providing light, nonintrusive and almost AP integrators for collisional kinetic equations. We shall present in this talk fully explicit projective integration and telescopic projective integration schemes for the multispecies Boltzmann and BGK equations. The methods employ a sequence of small forward-Euler steps, intercalated with large extrapolation steps. The telescopic approach repeats said extrapolations as the basis for an even larger step. This hierarchy renders the computational complexity of the method essentially independent of the stiffness of the problem, which permits the efficient solution of equations in the hyperbolic scaling with very small Knudsen numbers. We validate the schemes on a range of scenarios, demonstrating its prowess in dealing with extreme mass ratios, fluid instabilities, and other complex phenomena.

14 Manuel Torrilhon

RWTH Aachen University, Germany

Finite element discretizations for moment equations in kinetic gas theory

Abstract

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 succesfully applied. In the transition regime at intermediate Knudsen numbers up to 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.

15 Lei Wu

Southern University of Science and Technology, China

GSIS: a fast-converging and asymptotic-preserving numerical scheme for the non-equilibrium gas dynamics

Abstract

One of the central problems in the study of rarefied gas dynamics is to find the solution of the Boltzmann equation quickly. When the Knudsen number is large, the conventional iterative scheme can find the steady-state solution within a few iterations. However, when the Knudsen number is small, hundreds of thousands iterations are needed, and yet the "converged" solutions are prone to be contaminated by large numerical dissipation.

We first put forward a general synthetic iterative scheme (GSIS) to find the steady-state solutions of rarefied gas flows within dozens of iterations at any Knudsen number. The key ingredient of our scheme is that the macroscopic equations, which are solved together with the Boltzmann equation and help to adjust the velocity distribution function, not only asymptotically preserve the Navier-Stokes limit in the framework of Chapman-Enskog expansion, but also contain the Newton's law for stress and the Fourier's law for heat conduction explicitly. As a result, the constraint that the spatial cell size should be smaller than the mean free path of gas molecules is removed. The fast convergence and asymptotic preserving of GSIS are rigorously proven by the Fourier stability analysis. What's more, the method of construction is universal as the GSIS does not rely on the specific collision operator.

We then extend the GSIS to time-dependent systems, to push the multiscale

simulation of unsteady rarefied gas flows to a new boundary, that is, the numerical solution not only converges within dozens of iterations in each time step, but also asymptotic preserves the Navier-Stokes-Fourier limit in the continuum flow regime, when the spatial grid is coarse, and the time step is large (e.g., in the extreme slow decay of two-dimensional Taylor vortex, the time step is even at the order of vortex decay time).
Finally, we will show that the GSIS can be extended to non-equilibrium phonon dynamics described by the Callaway model. The coupling of GSIS with DSMC will also be discussed.