1st Kinetic Theory Workshop in the Netherlands KINED

2 Feb 2024, University of Groningen

Kinetic theory covers many applications ranging from rarefied gases (hypersonic flows, atmospheric entry, microchip manufacturing) and plasma flows (nuclear fusion, jet engines, lasers) via agent-based models (opinion dynamics, swarming models, financial markets) to geophysical flows (free surface flows, rivers, flooding, tsunami waves). The purpose of this workshop is to bring Dutch scientific experts and industry representatives from different applications together to exchange about the state-of-the-art in the respective fields. International experts are invited to contribute new ideas to the growing Dutch community of young and established researchers on kinetic theory. We hope that this workshop will be the start of a closer collaboration of the different groups working on related topics and that this also leads to a closer link with the Dutch high-tech industry.

We thank 4TU.AMI and NWO for supporting this workshop.

Organization committee: Julian Koellermeier, University of Groningen
Harald van Brummelen, TU Eindhoven
Michael Abdelmalik, TU Eindhoven
Mathias Schlottbom, U Twente

Program outline

9:30 – 10:00	Registration and arrival
10:00 – 10:15	Welcome by the organizers
10:15 – 10:45	**Manuel Torrilhon**, RWTH Aachen University Regularized 13-Moment-Equations: Mathematical Modelling and Simulation for Rarefied Gases
10:45 – 11:15	**Tomasz Tyranowski**, U Twente Stochastic variational principles for the collisional Vlasov–Maxwell and Vlasov–Poisson equations
11:15 – 11:45	Coffee break
11:45 – 12:15	**Erik Arlemark**, ASML Impact of Rarefied Gas Flows in EUV Lithography and Simulation Needs
12:15 – 12:45	**Josefine Proll**, TU Eindhoven (Gyro)kinetic theory – tools for understanding turbulence in nuclear fusion
12:45 – 14:00	Lunch break
14:00 – 14:30	**Giovanni Samaey**, KU Leuven Multilevel kinetic-diffusion schemes for high-collisional linear kinetic equations for plasma edge simulations in fusion energy
14:30 – 15:00	**Julian Koellermeier**, RU Groningen Model order reduction and moment models: on finding intrinsic variables
15:00 – 15:30	Coffee break
15:30 – 16:00	**Torsten Kessler**, TU Eindhoven Towards High Performance Solvers for Kinetic Equations
16:00 – 16:30	**Federico Toschi**, TU Eindhoven TBA
16:30 – 17:00	Closing and farewell

Abstracts of invited speakers:

Erik Arlemark, ASML
Title: Impact of Rarefied Gas Flows in EUV Lithography and Simulation Needs
Abstract: ASML is the only provider of EUV lithography, needed to produce the most powerful computer chips as off today. For a sufficient amount of EUV light to be transmitted through our system a low pressure gas environment of hydrogen needs to be maintained. As the high energetic EUV light interacts with the hydrogen buffer gas a plasma is generated creating electrical forces, new gas species and surface reactions. As even the smallest amounts of molecular or particulate contamination can harm our machine or product, gas purging is introduced on sensitive parts. Also the requirement of thermal stability needs to be correct within milli-Kelvin as thermal expansion could be comparable to our nanometer scale design patterns. To categorize the level of present rarefaction and hence need of simulation approaches one can consider that the EUV lithography machine has gas flow domain sizes ranging from millimeter to meter and pressures within medium vacuum category, so the rarefaction regime goes between continuum and Free-Molecular. Finally, as the EUV lithography machine is very expensive it is important that trustworthy simulation tools are used in the design such that a machine can be built on a “first time right principle”.

Torsten Kessler, TU Eindhoven
Title: Towards High Performance Solvers for Kinetic Equations
Abstract: Modern technology crucially depends on our understand of the dynamics of fluids. Kinetic theory offers models that are valid in the full range of modern applications in science and industry, from gas flows near vacuum to high Mach number flows. However, the numerical solution of these models requires the discretization of the six-dimensional phase space, the product of position and velocity space. This has limited the use of higher order discretization in applications, particularly for domains with complicated geometry. In this talk, we describe the challenges on the way to high performance solver for kinetic equations. We show how to exploit their special structure to drastically reduce memory and computational complexity. We argue that the most challenging part of kinetic equations is not the collision mechanism but boundary conditions as they couple space and velocity in a nonseparable way. We close with numerical applications of the new framework to the method of moments.

Julian Koellermeier, RU Groningen
Title: Model order reduction and moment models: on finding intrinsic variables
Abstract: The numerical simulation of kinetic equations still poses challenges due to the large number of variables necessary to resolve the high-dimensional phase space. Moment models are one way to choose a small number of variables representative for the full dynamics. This results in physically interpretable and analytical equations that are feasible to simulate efficiently. However, it is not a-priori clear how many and which moments to include in a simulation. In this presentation we show how data-driven approaches like neural networks can be employed to identify the intrinsic variables of the kinetic equation. This paves the way for future, more efficient moment models.

Josefine Proll, TU Eindhoven
Title: (Gyro)kinetic theory – tools for understanding turbulence in nuclear fusion experiments
Abstract: The loss of heat and particles through turbulence is one of the main bottle necks for building economically viable fusion reactors. Gyrokinetic theory – kinetic theory where the fast gyromotion of the particles around the magnetic field lines has been averaged out – has been found to be a powerful tool to study turbulence both with analytic theory and linear and nonlinear simulations.

In this talk, I will discuss the reasoning behind gyrokinetics and how it is commonly used with simulations. I will then discuss two techniques that have only recently emerged in fusion kinetics: that of using moment models while retaining hyperbolicity, and that of available energy as a turbulence measure.

Giovanni Samaey, KU Leuven
Title: Multilevel kinetic-diffusion schemes for high-collisional linear kinetic equations for plasma edge simulations in fusion energy
Abstract: In this talk, we discuss a hybrid kinetic-diffusion particle method for the Monte Carlo simulation of linear kinetic equations. In the low-collisional regime, the method reverts to the standard velocity-jump process. In the high-collisional regime, the method collapses to a standard random walk process. We analyze the error of the presented scheme in the low-collisional regime for which we obtain the order of convergence in the time step size. We furthermore provide an analysis in the high-collisional regime that demonstrates the asymptotic-preserving property. To eliminate the bias introduced by this scheme, we incorporate it in a multilevel Monte Carlo hierarchy.

Manuel Torrilhon, RWTH Aachen University
Title: Regularized 13-Moment-Equations: Mathematical Modelling and Simulation for Rarefied Gases
Abstract: Computational fluid dynamics is widely successful to predict flow processes in many different scenarios. However, rarefied gas flow often shows thermal non-equilibrium due to lack of particle collisions, that is, the Knudsen number - the ratio between the mean free path and a macroscopic length - becomes significantly large. The traditional equations of fluid dynamics with the constitutive laws of Navier-Stokes and Fourier for stress tensor and heat flux are known to lose their validity in these situations. Instead, the non-equilibrium regime requires modeling based on the statistical description of kinetic gas theory. Using moment equations extend the classical fluid dynamic equations for processes with moderate Knudsen numbers.
We will present non-equilibrium models within the framework of moment approximations in kinetic theory. In particular, the regularized 13-moment-equations (R13) offer a compromise between stability and robustness, simplicity and physical accuracy. We will discuss the mathematical structure and physical predictions of the R13 system in detail. Combined with kinetic boundary conditions the R13 equations allow to derive a weak formulation to be used in numerical simulations based finite-element-discretizations. We will present simulation results based on an implementation which is based on the FEM library FEniCS and is openly available. Moment approximations also provide a hierarchy of models in a cascading nature such that a lower level set of equations is contained in a higher level. The talk will discuss how the moment hierarchy can be used to estimate model errors. In the future it will be possible to perform model-adaptive simulations.

Federico Toschi, TU Eindhoven
Title: TBA
Abstract: TBA

Tomasz Tyranowski, U Twente
Title: Stochastic variational principles for the collisional Vlasov–Maxwell and Vlasov–Poisson equations
Abstract: In this talk I will recast the collisional Vlasov-Maxwell and Vlasov-Poisson equations as systems of coupled stochastic and partial differential equations, and I will derive stochastic variational principles which underlie such reformulations. I will also propose a stochastic particle method for the collisional Vlasov-Maxwell equations and provide a variational characterization of it, which can be used as a basis for a further development of stochastic structure-preserving particle-in-cell integrators.