Tensorial turbulent viscosity model for LES: properties and applications

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In the Large Eddy Simulation approach to the numerical solution of the equations for a turbulent flow, a low-pass filter in space is applied to the Navier-Stokes equations, removing eddies smaller than the filter size. The sub-grid scale (SGS) stress tensor, deriving from the filtering of the nonlinear term, accounts for the effect of the small unresolved scales on the resolved motion, and it must be modeled. The filter should operate in the inertial range, where a scale similarity law is assumed, and the SGS stresses must represent adequately the energy transfer between resolved and unresolved scales. Moreover the turbulent flows of practical interest are generally inhomogeneous and anisotropic, also at the small scales of motion. So a good SGS models should take in account this anisotropic character of unresolved structures of turbulence. An anisotropic tensorial turbulent viscosity model has been developed in the research team of Prof. Cercignani [1] to take into account all these aspects. The turbulent viscosity is represented by a fourth order tensor. To reduce the number of unknown parameters this tensor is projected in a local reference frame leading to six independent coefficients wich are determined using the Germano dynamic procedure [2]. Several a priori tests have been performed to analyse the energetic and structural properties of this SGS model. Moreover Large Eddy Simulations of many different turbulent flows confirmed the capability of the anisotropic model to well represent the contribution of unresolved scales.

This presentation will start illustrating the formulation of the original anisotropic eddy viscosity model [1], its peculiarities with particular attention to the statistical correlation and alignment properties derived by a priori tests. An overview of the performance of the model will be completed by the results obtained by its application to the simulations of different types of turbulence (homogeneous isotropic turbulence, boundary layers, rotating flows, thermal convection, jets). Then the extension of the model to compressible flows [3] and its application to numerical simulation of variable density currents using a Discontinuous Galerkin finite element method [4] will be presented A recent version of the anisotropic eddy viscosity model based on an unconventional SGS stresses decomposition [5] will complete the presentation.

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Model Boltzmann equations for a polyatomic gas and applications

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Kinetic theory of polyatomic gases is becoming increasingly important because their non-equilibrium flows are encountered in many applications. Since the Boltzmann equation for a polyatomic gas is too complex, model Boltzmann equations are often used in practical applications. In the present talk, we will focus on one of such models, that is, the ellipsoidal statistical (ES) model for a polyatomic gas that was proposed by Andries et al. and explain the form and basic properties of the model. This model is for an ideal polyatomic gas with constant specific heats (thermally perfect gas). We will also extend the ES model to a polyatomic ideal gas with temperature-dependent specific heats (calorically perfect gas). Then, these models are applied to investigating the problem of gas flows with slow relaxation of internal modes, such as the shock structure for carbon dioxide gas.

The Fermi-Pasta-Ulam problem and its underlying integrable dynamics

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In 1954 Fermi, Pasta and Ulam for the first time used a computer to study the ergodic behavior of a system with many degrees of freedom, aiming to investigate the foundations of Statistical Mechanics. Several branches of physical and mathematical investigations started from that paper. The aim of the talk is to revisit, in the light of some recent numerical results, one of the leading ideas, namely that the model should be understood as a perturbation of the Toda model, well known in Statistical Mechanics, which is nonlinear but integrable. The behavior at the thermodynamic limit turns out to be particularly delicate.

Half-space problems for multi-component mixtures

Niclas Bernhoff
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Half-space problems in the kinetic theory of gases are of great importance in the study of the asymptotic behavior of solutions of boundary value problems for the Boltzmann equation for small Knudsen numbers. They provide the boundary conditions for the fluid-dynamic-type equations and Knudsen-layer corrections to the solution of the fluid-dynamic-type equations in a neighborhood of the boundary. These problems are well-studied for single species, including some important contributions by Carlo Cercignani, and it is well-known that the number of additional conditions needed to be imposed depends on different regimes for the Mach number (corresponding to subsonic/supersonic evaporation/condensation). However, the case of mixtures is not as well studied in the literature.

In this talk, we will discuss some extensions of the results for half-space problems for single species to the case of multi-component mixtures.

Data-driven and equation informed tools to model and reconstruct turbulent flows.

Luca Biferale
Università di Roma Tor Vergata, Italy

We discuss the applicability of artificial intelligence tools to data assimilation (DA) and inpainting in fluid dynamics. We explore the capability of a couple of Context Econders based on Generative Adversarial Network (GAN) to produce an optimal guess for missing data in turbulent configurations. In particular, we investigate on a quantitative basis, their use in reconstructing 2d damaged snapshots extracted from a large database of numerical configurations of 3d turbulence in the presence of rotation, a case with multi-scale random features where both large-scale organized structures and small-scale highly intermittent and non-Gaussian fluctuations are present. If time allows, we will also compare the DA methods with equation-informed tools, based on Nudging [1,2,3,4,5,6].

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Scale-free evolution in random and periodic systems

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We review the mechanisms at the basis of the intermittent response typical of random ferromagnets (Barkhausen noise) and crystal plasticity (strain avalanches at the microand nanoscale). The comparison between numerical experiments and laboratory experiments evidences good agreement and allows to extract microscopic information from the macroscopic response.

A general internal states framework for kinetic modelling of polyatomic gases

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We propose a kinetic Boltzmann model for polyatomic gases, where the internal structure of a molecule is described by a single internal state parameter, belonging to a suitable space. Proper options for such a space of internal states and for the measure defined on it allow to recover some models commonly used in kinetic theory for polyatomic particles: the description based on a set of discrete internal energy levels [1,2], and the one involving a continuous internal energy variable [3]. Moreover, within this general framework it is possible to build up a new model, highly desirable for physical applications, where the internal energy is separated into two different components, the rotational and the vibrational ones, the former approximated by means of a continuous variable, keeping the latter discrete. We investigate collision invariants, equilibrium distributions and the number of degrees of freedom corresponding to each option. We prove that all models that fit our framework fulfil Boltzmann H-theorem. Possible generalizations of our formulation to gas mixtures of polyatomic and monoatomic constituents, even in presence of chemical reactions, are also discussed.

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On self-similar solutions of the Boltzmann equation

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We consider the nonlinear Boltzmann equation and discuss various classes of its self-similar solutions. Some of them were investigated in joint works of the author with Carlo Cercignani (and also with Irene Gamba) in 2000s. This work can be considered as a development of some ideas of that time. In particular, we consider the class of so-called homoenergetic flows and their generalizations. For the case of pseudo-Maxwell molecules we give a constructive proof of existence and uniqueness of selfsimilar solutions and show that these solutions are attractors for certain classes of initial conditions. The possible power-like tails of solutions are briefly discussed. Some results of the talk are obtained jointly with Alessia Nota and Juan Velazquez [1].

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Some new ideas about Cercignani's conjecture

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We propose a proof for new versions of Cercignani's conjecture for the Landau equation with general potentials (including Coulomb potential). This conjecture relates the entropy dissipation and the relative entropy of a velocity distribution. An intermediate quantity which plays a central role is a weighted (and in some sense anisotropic) variant of the Fisher information.

Wealth distribution under the spread of infectious diseases

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We develop a mathematical framework to study the economic impact of infectious diseases by integrating epidemiological dynamics with a kinetic model of wealth exchange. The multi-agent description leads to study the evolution over time of a system of kinetic equations for the wealth densities of susceptible, infectious and recovered individuals, whose proportions are driven by a classical compartmental model in epidemiology. Explicit calculations show that the spread of the disease seriously affects the distribution of wealth, which, unlike the situation in the absence of epidemics, can converge towards a stationary state with a bimodal form. Furthermore, simulations confirm the ability of the model to describe different phenomena characteristics of economic trends in situations compromised by the rapid spread of an epidemic, such as the unequal impact on the various wealth classes and the risk of a shrinking middle class.

Kinetic Theory Approach to Non-equilibrium Two-phase Flows

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In two-phase systems, in which liquid and vapor/gas regions are coexisting, deviations from hydrodynamic description occur next to interfaces. In the past, a large number of studies has addressed the description of the Knudsen layers formed at the vapor-liquid boundary as a results of evaporation or condensation processes. Although the structure and role of kinetic layers in connecting hydrodynamic regions on the two sides of the interface can be considered as clear, the adequacy of the quite phenomenological kinetic boundary conditions is still under investigation. Moreover, recent results indicate that non-equilibrium effects and deviations from hydrodynamic behavior persist in dense vapor flow, which are not well described by the Boltzmann equation. The presentation aims at reviewing available results, highlighting the contributions of Carlo Cercignani to the subject and to present the problems still awaiting a solution.

The Einstein classical program in the Cercignani's sense of the "shortcut". A review of some results

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It is well known that Einstein explicitly formulated the program of recovering quantum theory (undoubtedly the "good" theory), in some "realistic" frame. In his novel "la creazione secondo Michele", Carlo Cercignani summarizes such a program as "the shortcut" (la scorciatoia), in the extreme sense that Quantum Mechanics may be proved as a kind of theorem within purely classical "physics". We illustrate here some progress along such lines. A key point is that one should make use of the completion of classical electrodynamics obtained by Dirac (1938) and Wheeler-Feynman (1945). This allows one to prove that, according to classical physics, electrons don't fall on nuclei and ions don't come to rest within matter in bulk, notwithstanding their accelerated motions. Two examples are illustrated here, namely: 1) a remarkably good reproduction of the infrared spectra of ionic crystals in terms of the ionic Newtonian trajectories; and 2) the existence of the chemical bond in the simplest case involving just one electron (i.e., the ion of the H_2 molecule) in a purely classical three-body Coulomb model. The case of ionic motions in ionic crystals will be further illustrated in the talk by F. Gangemi, and the application of the Wheeler-Feynman theory to the "optical thickness" of plasmas will be illustrated in the talk by M. Zuin.

The Boltzmann Equation modeling Mixtures and Polyatomic Gases

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We considered well posedness problem for the system Boltzmann flow for mixtures with disparate masses and the scalar flow for Polyatomic gases, as well as functional properties involving the propagation in $L^p_k(\mathbb{R}^d)$ theory and Sobolev spaces. These models are presented in a unified framework from a functional viewpoint that identifies the role of the differential cross section, with integrable angular forms, into getting a priori moment estimates that generate coercivity and uniform bound, so a common functional framework applied. We have established existence and uniqueness theory in the space in $L^1_k(\mathbb{R}^d)$, for well prepared weights depending on such collisional cross section forms, as well as control of exponential moments that control the high energy tail decay, explicitly characterized by the coercive and upper bounds, much in the classical theory of PDE in Sobolev spaces. From there, it follows the propagation of $L^p(\mathbb{R}^d)$, for $1 < p \leq \infty$, polynomially and exponentially weighted, as well as higher Sobolev regularity theory. Their bounds can be traced back to the coercive constants and a priori moments upper bounds estimates. A functional ODE in Banach spaces ties up the existence, uniqueness as well as stability results. One interesting point associated to the polyatomic gas collisional model is that the additional interchange of internal energy variables interplays with possible differential cross sections depending on the integrability of partition functions of kinetic and internal energies. One of these differential cross sections enables a fully consistent derivation of the extended thermodynamics moments equation for approximating Polyatomic gas models. This is work with Milana Pavic-Colic and Erica de la Canal.

The Cercignani conjecture about a classical zero-point energy. Preliminary results

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A characteristic feature of Quantum Mechanics is that it predicts zero-point motions, i.e., the existence of states with a nonvanishing kinetic energy at zero temperature. This is a fact that is experimentally verified and is considered to be ununderstandable in a classical frame. In the year 1972 Carlo Cercignani advanced the idea that classical zero-point motions may be conceived, if one understands them as characterized by the qualitative property of being ordered rather than chaotic. Here we report preliminary results on such a line, concerning the ionic trajectories in ionic crystal models, which are already known to reproduce in a remarkably good way the experimental infrared spectra.

Taking the heritage: recent developments in the anisotropic eddy viscosity

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In the poliedric activity of Carlo Cercignani, from rarefied gasdynamics to turbulence in continuum flows, the study of subgrid models based on anisotropic eddy viscosities represents a singular and particular chapter. In this contribution devoted to the memory of his premature death, the origin and the development of this topic with his stricter collaborators is traced, and new recent results are illustrated, in the ideal continuity of a common and cooperative research.

Half-space problems for the Boltzmann equation with phase transition at the boundary

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In the early 1980s, C. Cercignani conjectured the number of compatibility conditions to be imposed to the boundary data of a half-space problem for the linearized Boltzmann equation in order for the solution to vanish at infinity. His conjecture involved the signature of the Hessian of the entropy flux at the linearization Maxwellian, viewed as a quadratic form restricted to the space of collision invariants. Cercignani's conjecture is in complete agreement with the theory of boundary data for the acoustic system. Slightly later, Y. Sone, K. Aoki and their collaborators investigated systematically a nonlinear variant of Cercignani's problem by careful numerical simulations. Consider the half-space problem for the (nonlinear) Boltzmann equation, assuming that the distribution function of particles entering the half-space is the centered Maxwellian with saturating vapor pressure corresponding to the temperature of the gas at the boundary. Y. Sone, K. Aoki and their collaborators proposed a complete classification of the Maxwellians state at infinity for solutions of the half-space problem for the Boltzmann with such boundary conditions. Their theory involves a number of compatibility conditions on the pressures and temperatures at the boundary and at infinity, and on the Mach number at infinity which coincides with C. Cercignani's conjecture in the linearized case. This problem has been studied systematically by T.-P. Liu and S.-H. Yu by a time marching strategy involving their theory of Green functions for the linearized Boltzmann equation. The purpose of this talk is to offer an alternative approach to treat the transition between evaporation and condensation at the boundary which is based on the standard energy method, and on Nicolaenko's theory of generalized eigenfunctions for the linearized collision integral. (Work in collaboration with N. Bernhoff.)

Simulation of the gas mixture behaviors using Hard Sphere and Ab Initio potentials

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In a such case the temperature and pressure of a vapor are supposed to be equal to those of a solid. When the gas becomes more rarefied the equilibrium at gas-solid interface is disturbed and the kinetic methods or Navier-Stokes equation with jump boundary conditions should be applied for the accurate description of the interface. The development and implementation of a such kind of approaches are in a focus of interests of the present work. Let us consider a mixture of the monatomic gases, Helium and Argon, confined between two parallel infinite solid layers of Argon, with colder surface at y=-0.5 and hotter at y=0.5. One component of this mixture, Helium, can just reflect from the solid surface, while another component of the mixture, Argon, represents the gaseous fraction of the solid phase and so can sublimate or deposit (de-sublimate). The Boltzmann type kinetic equation is used to simulate the gas sublimation in the gas mixture flow for arbitrary gas rarefaction. Here the McCormack model [1] is used for the simulation of the collision term. Since only small temperature and pressure difference are considered the distribution function of each species is linearized. This procedure leads to the system of two linearized kinetic type equations. The Discrete Velocity Method (DVM) is used to solve this system. The spatial derivatives are approximated by the second-order accurate TVD type numerical scheme [2]. The Gauss-Hermit polynomials are used for the discretization in the molecular velocity space. The specific temperature range was chosen, where He cannot be in a solid state while Ar can sublimate and deposit. Two values of the reference temperature, T0=50K and 70K, are chosen based on the sublimation curve of Argon provided in Ref. [3]. Two type of potential are used in the simulations: the classical Hard Sphere (HS) potential [4] and ab initio (AI) potential [5]. The values of the molecular diameter ratio are needed to the implementation of the HS model, which was calculated from Ref. [4]. The profiles of the macroscopic parameters, pressure and temperature of the mixture are shown on Figs. 1 and 2, respectively for the initial concentration of He equal to 50near to the colder solid surface. This phenomenon, called also “negative temperature gradient” was also found in the numerical simulations of the evaporation and concentration [6]. As it is clear from these Figures the results obtained by two potentials are very close.

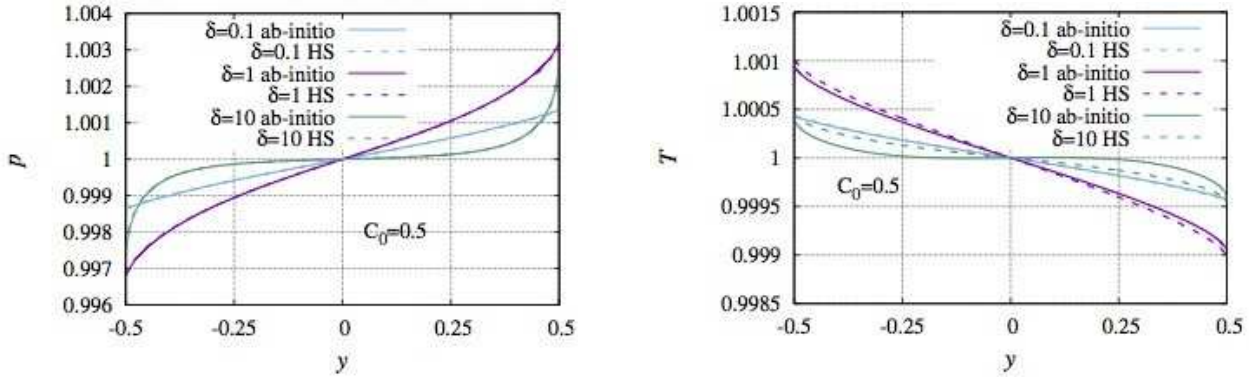

Figure 1: Pressure (a) and temperature (b) of gas mixture

Acknowledgements The work of A. Polikarpov was financially supported by RFBR grant 18-31-00194. I. Graur would like to acknowledge the financial support provided by the European Union network program

H2020, MIGRATE project under Grant Agreement No.643095.

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Consistent BGK models for gas mixtures and applications

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Relaxation time approximations of BGK type constitute one of the most popular and flexible simplified kinetic models of the true integrodifferential Boltzmann equation in Rarefied Gas Dynamics, retaining the most significant mathematical and physical features of the actual Boltzmann equation. Their extension to more complex physical scenarios, like multicomponent flows, is not trivial since some inconsistencies can arise, like breakdown of positivity of densities and temperature fields and of the indifferentiability principle. In this talk, some consistent relaxation time-approximation models of BGK-type for inert gas mixtures are presented and their main properties are discussed. Consistency is based on three basic properties: correct reproduction of conservation laws, H-theorem and uniqueness of equilibrium solution.

The main peculiarities of the presented BGK models will be highlighted with reference to their continuum limits obtained by Chapman-Enskog expansions. In particular, we will focus on a recent BGK model, reproducing the structure of the Boltzmann collision operator for mixtures and well suited to deal with various intermolecular collisional potentials, and on its Navier Stokes asymptotics in different collision dominated regimes. Finally, some applications to evaporation-condensation problems and shock wave structure will be presented.

Random walk in a one-dimensional Lévy random medium

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One speaks of anomalous diffusion when a process (e.g., a mechanical system of particles or a stochastic process) diffuses through space with a different law than that of the Brownian motion. These types of systems are observed both in physics (rarefied gases, certain glassy materials) and in other sciences (e.g., ethology, social sciences, financial mathematics). The most realistic models of anomalous diffusion are those where the anomalous behavior is caused by particular properties of the media the process lives in. The mathematical literature on such systems is rather scant. We present a continuous-time random walk in random medium which generalizes a system known in the physical literature as Lévy-Lorentz Gas: a particle travels at constant speed between target points that are randomly placed on the real line with fat-tailed interdistances. Depending on the decay of the tail of the distribution, this process may exhibit different types of anomalous diffusion.

Variational solutions of the linearized Boltzmann equation for hard-sphere molecules and Cercignani-Lampis boundary conditions

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In this work, a variational approach has been used to obtain asymptotic near-continuum solutions of the linearized Boltzmann equation for hard-sphere molecules, in order to provide analytical expressions for the thermal slip coefficients needed to extend the validity of the Navier-Stokes equations into the transition regime. The Cercignani-Lampis boundary conditions have been considered in order to take into account the influence of the tangential momentum and the normal energy accommodation coefficients on the slip parameters. The theoretical results have been compared with the experimental data for five different noble gases (helium, neon, argon, krypton and xenon) and, for each of them, the accommodation coefficients have been extracted. Then, these values have been used to evaluate the temperature-driven mass flow rate and the thermal molecular pressure exponent by means of our variational technique. A comparison with the experimental measurements reveals a fairly good agreement within the range of validity of the proposed second-order slip model.

Nonlocal kinetic models for cell-cell adhesion

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In this talk we present a nonlocal kinetic model for cell-cell adhesion, i.e. the tendency of cells to form junctions between their membranes. We will deal with a transport equation with a nonlocal quadratic interacting operator which implements a velocity-jump process, that is the typical microscopic stochastic dynamics that describes cell motion. Moreover, we have nonlocality because we suppose that cells sense the environment by extending their protrusions up to a maximum sensing radius. Furthermore, the model can be enriched with the volume filling effect also introducing physical limits of migration, that is when cells cannot move because of overcrowding. In order to obtain physical results, the sensing radius determining the nonlocality depends on time, position and direction of sensing. A linear stability analysis in the one dimensional case will be performed. We analyse how the actual possible sensing of the environment influences the dynamics by recovering the appropriate macroscopic limits and by integrating numerically the kinetic transport equation.

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The key role of the functions of the Mittag-Leffler type in eternal solutions of the Boltzmann equation

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In 2002 Bobylev and Cercignani published two papers in Journal of Statistical Physics where they considered two classes of solutions of the Boltzmann equation with infinite energy. The corresponding solutions turn out to be self-similar and eternal (using their language) and it is suitable to revisit them in a more general framework, also considering plots not present in their papers. As a matter of fact, these solutions are indeed expressed in terms of special functions of the Mittag-Leffler type, that in those times were practically unknown to most applied mathematicians and physicists. In this presentation we recall the main properties of these functions that are known to play fundamental roles in differential equations of fractional order; as a consequence, this could presage a possible use of the fractional calculus in dealing with some aspects related to the Boltzmann equation.

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Propagation of two-dimensional localized vibroacoustic disturbances in a rarefied gas

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We study the effect of gas rarefaction on the propagation of pressure disturbances in a two-dimensional setup of a gas confined by an infinite plane undergoing non-uniform small-amplitude vibrations. Focusing on harmonic oscillations that are applied to only part of the surface, the problem is analyzed in the entire range of gas rarefaction rates, governed by the ratio between the gas mean free path and wavelength of imposed wall perturbations. Analytical solutions are obtained in the free-molecular and continuum limits, and are supplemented by direct simulation Monte Carlo calculations. The primary effect of gas rarefaction in increasing the decay rate of acoustic perturbations is discussed and rationalized.

Charge transport in graphene nanoribbons

Giovanni Nastasi
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Charge transport in graphene nanoribbons is investigated by solving the Boltzmann equation with a discontinuous Galerkin method. All the electron-phonon phonon scattering mechanisms are taken into account. As energy bands we adopt those proposed by M. Bresciani et al. (Solid-State Electronics, 54, 1015-2021, 2010) while according to V.K. Dugaev and M.I. Katsnelson (Physical Review B, 88, 235432, 2013) the edge effects are included as an additional scattering obtained from the Berry-Mondragon model which is valid for moderate edge disorder. With this approach a 1D transport problem has been solved. A degradation of the electron velocity, and consequently of the current, is found by reducing the nanoribbons width.

BGK models for gas mixtures, polyatomic molecules and gases with chemical reactions: Modeling and theory

Marlies Pirner
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A kinetic description for evolving gases with a simplification of the collision operator is given by the BGK model. I will present such models for gas mixtures, polyatomic molecules and gases with chemical reactions. They are multi-species models, for which we can show conservation properties, H-Theorem, existence of solutions, results on the large-time behavior and macroscopic limits.

In this talk I will present recent theoretical results on these models concerning existence of solutions, large-time behavior and the non-linear limit to reaction diffusion equations.

This is joint work with Christian Klingenberg, Gabriella Puppo, Christian Schmeiser and Gianluca Favre.

On the size of backward clusters in a low-density regime for hard-sphere systems

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Consider a system of N hard spheres of diameter ε in the three dimensional torus. For a given particle, fixed a time $t > 0$, let us introduce its backward cluster, namely the subset of particles which really influence the motion of this particle up to the time t. This notion, interesting in itself, has been introduced in [1]. Now we are interested in estimating the mean size (with respect to a given probability measure) of a backward cluster. This problem has been approached in [1] in the Boltzmann-Grad limit, namely when $N \to \infty$, $\varepsilon \to 0$ and $\varepsilon N = 1$. Then we can use the Boltzmann equation and the mean size can be estimated almost explicitly by means of the Wild sum. However, before the limit, the control of the mean size of the backward cluster is straightforward only for a short time interval, while this is an open difficult problem in general, like as the global validity problem for the Boltzmann equation. Here I present an estimate global in time, uniform in ε, N for $\varepsilon N = 1$, when the averages are computed by means of an equilibrium measure at a given temperature. This is a result obtained in collaboration with S.Simonella [2].

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A Gas-Kinetic Scheme for Turbulent Flow

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Gas-Kinetic Schemes (GKS) of various orders can be derived for the Navier-Stokes equations [5] for the finite volume and finite element discretizations; they often require a greater computational effort but offer a number of advantages in terms of accuracy. They may serve as a starting point to develop "unified" schemes able to seamless model the numerical fluxes of the Navier-Stokes equations over a range of Knudsen number [6]. GKS may also be used with closures for the RANS, LES and hybrid RANS-LES techniques. Remarkably, this particular aspect couples the two main areas of research led by Prof. Cercignani.

It was indeed his suggestion who prompted me to implement one of these schemes into a finite-volume solver, following one of Xu's earlier paper [7]. Little time later, I quit academia for industry and came back in 2009. It was then a few years later that I came to realize the potential of GKS to improve the accuracy of turbulence modelling; this paper summarizes the study I led between 2012 and 2016 [4,2,3] and offers a few considerations in the light of newly available investigation techniques.

GKS model the numerical fluxes on the basis of the Boltzmann equation instead of the Navier-Stokes equations as is conventionally done. In practical terms, these schemes provide a higher accuracy and, more importantly, they come with an in-built "multiscalar" mechanism, i.e. the ability to somehow adjust themselves to the size of unresolved scales of motion. The paper by Chen is remarkably clear [1].

This property makes them suitable for particular classes of flows, for instance shock-capturing and rarefied flow. Gas-Kinetic Scheme may be coupled to conventional RANS turbulence models; it is shown in this paper that the turbulent stress tensor is naturally adjusted as a function of the unresolved-to-resolved scales ratios and achieves a higher physical consistency than conventional schemes.

A rationale for this higher accuracy is presented: large unresolved scales of motion may invalidate the splitting, on mathematical and numerical level, of advective and diffusive fluxes. This is indeed well accepted when dealing with rarefied flow. However the same principle is not followed when modelling turbulence. Historically, modelling the unresolved turbulent scales of motion was inspired by the diffusion process which models thermal fluctuations in the continuum approach to fluid mechanics. However, unlike thermal fluctuations, unresolved turbulent fluctuations are spread over a wide range of frequencies; a clear separation from the resolved scales of motion may not exist. In turbulent simulations, one might want to introduce the measure of a "virtual degree of rarefaction" given by the ratio of unresolved turbulent scales of motion to a reference resolved scale. In the RANS approach, the effect of large and small turbulent scales of motion are accounted for by a modelled stress tensor. The (turbulent) unresolved-to-resolved scales ratio assumes large values in some flow regions in the presence of turbulence production mechanisms. In this paper, this ratio is assessed in a few test cases and shown to reach peak values of several hundredths or even a few tenths; i.e. well beyond the virtual threshold of rarefaction.

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Mathematical issues in charge transport in graphene

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The last years have witnessed a great interest for 2D-materials due to their promising applications. The most investigated one is graphene which is considered as a potential new material to exploit in nano-electronic and optoelectronic devices. Charge transport in graphene can be described with several degrees of physical complexity. At quantum level an accurate model is represented by the Wigner equation but in several cases its semiclassical limit, the Boltzmann equation, constitutes a fully acceptable model. However, the numerical difficulties encountered in the direct solution of both the Wigner and the semiclassical Boltzmann equation has prompted the development of hydrodynamical, energy transport and drift diffusion models, in view of the design of a future generation of electron devices where graphene replaces standard semiconductors like silicon and gallium arsenide. Moreover, thermal effects in low dimensional structures play a relevant role and, therefore, also phonon transport must be included. Interesting new mathematical issues related to the peculiar features of graphene arise. The main aspects will be discussed and recent results [1-10] illustrated in the perspective of future developments, in particular the optimization of graphene field effect transistors.

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Kinetic Theory and Extended Thermodynamics of Polyatomic Gas incorporating Molecular Rotation and Vibration

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In many physical systems, one encounters situations where phenomena occur at different scales. An example is the modeling of a rarefied gas at varying Knudsen number (Kn). Large Kn is where Boltzmann equation is the most appropriate model while, for small Kn, one can obtain Euler or the Navier-Stokes-Fourier system. At intermediate regimes, using the mathematical methods of Rational Extended Thermodynamics (RET), one can obtain the closure of moments system associated with the Boltzmann equation considering a distribution function depending on an extra variable that takes into account the internal motion of polyatomic gas (rotation and vibration). In this talk, we consider a more refined version of Kinetic Theory and RET in which molecular rotational and vibrational relaxation processes are treated individually. In this case, we need a triple hierarchy of the moment system and the system of balance equations is closed via the maximum entropy principle. Three different types of production terms in the system, which are suggested by a generalized BGK-type collision term in the Boltzmann equation, are adopted. In particular, the rational extended thermodynamic theory with seven independent fields is analyzed in detail and the dispersion relation of ultrasonic wave is confirmed by the experimental data for several gases. Finally is presented a possible simple approach of dense gases.

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Evolution of Mutually Gravitating Particles System with Possible Collisions

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We consider the gravitating particles that can collide. Collisions can be described in various ways. We can use the theory of inelastic interaction of solids with Newton's recovery coefficient for the relative velocity of colliding particles. In numerical implementation, the main difficulty of this approach is to track and refine a huge number of time moments of particle collisions. Another approach is to add to the gravitational potential the potential of repulsive forces, similar to the intermolecular Lennard-Jones forces. Numerical experiments show that when the Jacobi stability condition is satisfied, both models lead to a qualitatively identical character of evolution with the possible formation of stable configurations. As it is known, when pair collisions of an infinitely large number of gravitating particles are taken into account, the probability density function evolves in accordance with the Vlasov-Boltzmann-Poisson system of equations. We suggest a research method using the Vlasov equation with the Lennard-Jones type potential. This allows to take into account the size of the interacting particles, and also take into account not only paired, but also triple or more collisions of the particles. For this dynamical system the existence of a large class of nonlinearly stable equilibrium solutions is proved by the Energy-Casimir method.

Cercignani-Lampis scattering kernel and its applications to rarefied gas flows

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The paper by Cercignani and Lampis about a kinetic model for gas-surface interaction [1] was published in 1971. At the moment, it is the most cited paper written by Cercignani and his coauthors that shows a high relevance of the result reported in this work. The proposed kernel for gassurface interaction is completely different from the well known diffuse-specular model. The main difference is that the Cercignami-Lampis (CL) kernel contains two accommodation coefficients, while the diffuse-specular model has just one parameter. Over the past decades, the CL model has been widely used as a boundary condition to solve the kinetic Boltzmann equation (or its model), see e.g. Refs.[2-4]. The model was also implemented into the direct simulation Monte Carlo method [5]. An application of this model allowed to explain experimental results on thermo-molecular pressure difference [6]. The accommodation coefficients of the CL kernel were extracted from experimental data on various flows of rarefied gases [7]. It was shown that the energy accommodation coefficient for helium can be extremely small [8], while the tangential momentum accommodation coefficient only slightly differs from unity. The aim of this presentation is to compile theoretical works based on the CL kernel, to analyze its advantages and shortcomings. Finally, experimental values of the accommodation coefficients of the CL kernel are analyzed and their recommended values are provided for several pairs gas-surface.

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Kinetic theory and Direct Simulation Monte Carlo method – basic relations

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The basic ideas underlying the Direct Simulation Monte Carlo (DSMC) method will be discussed and a novel non-homogeneous N-particle kinetic equation describing the randomized mathematical model of DSMC will be presented. It will be shown that different collision-partner selection schemes, including No-Time-Counter (NTC) and Bernoulli-trials schemes, are approximations of the general transition operator of the randomized model. The popular collision-partner selection schemes, represented by the standard NTC and Bernoulli-trials approximations of the general transition operator, represented by Simplified Bernoulli-trials (SBT) and Generalized Bernoulli-trials (GBT) schemes, are tested on the one-dimensional rarefied gas heat transfer problem against conditions of two approximation limits: first, leading to the Boltzmann equation and second, leading to the novel N-particle kinetic one. From viewpoint of above considerations a new application strategy of the DSMC method will be commented.

Kinetic theory of soft flowing matter

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In the last decades kinetic theory has developed into a very elegant and effective framework to handle a broad spectrum of problems involving complex states of flowing matter, far beyond the original realm of rarefied gas dynamics. In this paper, we present recent applications of the lattice Boltzmann method to the computational design of soft mesoscale materials, including soft flowing crystals, dense multicore emulsions, as well as Petascale simulations of deep-sea glassy sponges. This talk is a tribute to the groundbreaking work of Carlo Cercignani and his undiminished impact on modern non-equilibrium statistical physics.

Half-range moment method for rarefied gas flows driven by harmonically oscillating boundaries

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The approximation of the Boltzmann or kinetic model equations using moment equations remains an active topic of research and has received considerable attention over the last decades. The moment equations are constructed by successively applying integral operators to the Boltzmann or kinetic equations and closing the deduced system with certain assumed expressions. Several approaches have been reported in the literature. One of the most promising approaches is the construction of moment equations using half-range orthogonal polynomials, which are discontinuous in the velocity space. The main advantage of this approach is the derivation of the boundary conditions in a systematic manner directly from the kinetic ones and the inherent treatment of the discontinuities of the distribution function in the domain including the boundaries. Moment methods, obtained using half-range orthogonal polynomials, have been successfully applied to study stationary boundary and pressure driven low-speed rarefied gas flows. In the present work, the formulation of the half-range moment method for oscillatory flows, where the quantities of interest are complex functions, is presented and its range of applicability in terms of the gas rarefaction and the oscillation frequency is examined. More specifically the Stokes second problem and the oscillatory planar Couette flow are considered. It is demonstrated that the half-range moment method provides accurate results in a wide range of gas rarefaction, and for oscillation frequency of the same or lower order than the collision frequency. In higher oscillation frequencies spurious oscillations in the macroscopic quantities arise. To treat these spurious oscillations, a distribution function splitting scheme is introduced to the kinetic equation leading to a homogeneous equation that is analytically solved and to a non-homogeneous one that is numerically solved using the half-range moment method. This approach increases the range of validity of the half-range moment method in terms of the oscillation parameter.

Human behavior and lognormal distribution. A kinetic description.

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In recent years it has been increasing evidence that lognormal distributions are widespread in physical and biological sciences, as well as in various phenomena of economics and social sciences. In social sciences, the appearance of lognormal distribution has been noticed, among others, when looking at body weight, and at women's age at first marriage. Likewise, in economics, lognormal distribution appears when looking at consumption in a western society, at call-center service times and others. The common feature of these situations, which describe the distribution of a certain attribute of agents, is the presence of a desired target to be reached by repeated choices. In this talk, we discuss a possible explanation of lognormal distribution forming in human activities, by resorting to classical methods of statistical mechanics of multi-agent systems [1, 2, 3].

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Non-conservative viral load-based kinetic description of epidemic spread on networks

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We present a Boltzmann-type kinetic approach to the spread of an infectious disease on a network which describes the links (migration paths) among countries, cities or districts depending on the spatial scale of interest. We model the disease transmission in terms of exchange of microscopic viral load mediated by social contacts among the individuals within the nodes of the network. We study in particular the hydrodynamic limit of the model, which ultimately provides a viral load-based macroscopic description of the spread of the disease on the network. This is an ongoing research in collaboration with Nadia Loy and Rossella Della Marca [1,2,3].

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Oscillatory rarefied gas flows in long capillaries

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Time-dependent rarefied gas flows driven by oscillating boundaries or pressure gradients have great theoretical interest and technological impact. The former ones have been extensively investigated in a variety of systems in order to control and optimize the resolution and sensitivity of the signal. Combined vibro- and thermo-acoustic effects to enhance or reduce acoustic transduction through single gases and gas mixtures have been also considered. On the contrary, the corresponding work in pressure-driven oscillatory and pulsatile rarefied gas flows is rather limited. Here, some recent work concerning oscillatory pressure-driven flow of rarefied single gases and binary gas mixtures through long capillaries of various cross sections is presented in the whole range of gas rarefaction and for arbitrary frequency. Modeling is based on the linearized BGK and McCormack kinetic models. The output quantities include the amplitude and phase of all macroscopic quantities of practical interest (velocity, shear stress, flow rate, viscous and inertia forces, pumping power). At moderate and high frequencies the flow consists of the inviscid piston flow in the core and the oscillating Stokes layer at the wall with the velocity overshooting, but as the gas rarefaction increases higher oscillation frequencies are needed to trigger these phenomena. Always, as the oscillation frequency increases the amplitude of the macroscopic quantities decreases and their phase lag with respect to the pressure gradient increases. In binary gas mixture flow the effect of the molar fraction and the molecular mass ratio of the species is investigated. Due to inertia forces, the heavier species are affected more drastically than the lighter ones, resulting to large differences between the flow rate amplitudes, which are unexpectedly increased as the flow becomes less rarefied, provided that the oscillation frequency is adequately high. Also, the mixture flow rate amplitude is larger, while its phase angle is smaller than the corresponding ones of the single gas and they both vary non-monotonically with the molar fraction. Furthermore, some remarks on the equivalence between half-space boundary and pressure driven oscillatory flows are stated. The present work may be useful in the design of micro devices, based on oscillatory configurations, operating at moderate and high frequencies in rarefied and dense atmospheres.

Computing accurate approximations of kinetic systems at diffusive regime

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This presentation deals with the numerical discretization of kinetic models, motivated by wide-range applications. We will focus our attention on the preservation of stationary solutions to build so-called well-balanced schemes in different regimes of parameters. In particular, we will require that the schemes do not deteriorate at the diffusive regime. Our well-balanced method relies on a decomposition of stationary solutions of kinetic systems in normal modes, see for instance [1, 2, 3]. It leads to time-marching schemes involving a "scattering S-matrix" [4]. At diffusive regime, one common feature shared by several kinetics models is the type of diffusive approximation: their macroscopic densities solve drift-diffusion systems, for which a distinguished numerical scheme is Il'in/Scharfetter-Gum mel's "exponential fitting" discretization. To deal with small parameters, a decomposition of the S-matrix for a very simple two-stream kinetic models has been proposed in [5]. Then, we prove in [6] that the well-balanced schemes for more general kinetic systems relax in parabolic scaling towards the Il'in exponential-fitting discretization by means of an appropriate decomposition of the S-matrix. This is the so-called asymptotic preserving (or uniformly accurate) property.

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Numerical schemes for a multi-species BGK model with velocity-dependent collision frequency

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We consider a kinetic model of a gas mixture. Each gas species is described by a BGK model, where for N species we have N BGK terms for each species, describing the pairwise interaction of each species with every other. The special feature of our model is that the collision frequency may vary not only in time and space but also with the microscopic velocity. In that model the Maxwellians are replaced by a generalization of such Maxwellians whose existence is proven by using a variational procedure. That procedure inspired us in this project to design an analogous numerical method. In our IMEX scheme the essential step is to minimize a certain potential function mimicking the Lagrange functional in theory. The theoretical properties like conservation of mass, total momentum and total energy, entropy dissipation, as well as positivity of the distribution functions are preserved. Here this will be presented and its usefulness and effectiveness illustrated in numerical examples.

Kinetic models for epidemic dynamics

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We introduce a mathematical description of the impact of sociality in the spread of infectious diseases by integrating an 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 classical compartmental models in epidemiology. Explicit calculations show that the spread of the disease is closely related to moments of the contact distribution. Motivated by the COVID-19 pandemic, part of the talk will be dedicated to the calibration of the proposed model based on data of the Province of Pavia thanks to an ongoing collaboration with ATS. We conduct numerical experiments which confirm the ability of the model to describe different phenomena characteristic of the rapid spread of an epidemic.

Loss of magnetic confinement above a critical density in a microscopic model of magnetized plasma

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Magnetic confinement of a plasma relies on the ordered gyrational motions of charged particles transverse to the field. Here we study a model, which shows that ordered motions can exist only if particle density is below a threshold, which is proportional to the square of the magnetic field. We consider a microscopic model of a plasma, conceived as a system of point electrons obeying Newton equations, immersed in a constant magnetic field within a neutralizing background. In the model, both the retarded electromagnetic interactions among all particles equally spaced along a magnetic field line and the radiation reaction force are taken into account, the magnetic field due to electron motion being neglected, and for the electric field the well-known expression for a dipole is considered. The stability properties of the system are studied, by computing the normal modes and determining the values of particle density for which some frequencies become complex. The observed instability involves normal modes with wavelengths of the order of the mean electron distance, so that such phenomenon is lost in a continuum approximation, i.e., it is a characteristic feature of the discrete structure of matter. Thus, through this extremely simplified model of a magnetized plasma, based on first principles, the existence is proven of a density limit, beyond which the system becomes unstable so that magnetization is lost. The predictions of the model are compared to the experimental data from several magnetized plasmas. Considering typical values of the applied magnetic field, the density limit deduced from the model turns out to be well in the range of the working densities reached in the present devices for thermonuclear fusion research. The instability here described could thus play a relevant role in determining the confinement properties of these devices. Analogous results are obtained also in a 3-dimensional model.