KTE2018

Kinetic and Transport Equations: Mathematical Advances and Applications

Parma, 10-12 October 2018

BOOK OF ABSTRACTS

Shock wave structure for a polyatomic gas with large bulk viscosity

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The structure of a standing plane shock wave in a polyatomic gas is investigated on the basis of kinetic theory, with special interest in gases with large bulk viscosities, such as the CO2 gas. The ellipsoidal statistical (ES) model for a polyatomic gas (polytropic gas) is employed, and the shock structure is obtained numerically for different upstream Mach numbers and for different (large) values of the ratio of the bulk viscosity to the shear viscosity. The double-layer structure consisting of a thin upstream layer with a steep change and a much thicker downstream layer with a mild change is obtained. An analytical solution, consisting of a jump condition and a slowly varying solution, that can approximate the double-layer structure well is also presented. Some results based on an ES model for a non-polytropic gas are also presented. [Joint work with Shingo Kosuge (Kyoto University)]

Simulations of nonequilibrium flows of gas mixtures with chemical reactions in a problem with "membrane-like" boundary conditions

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New problems for kinetic equations are formulated and solved keeping in mind to describe nonequilibrium open systems. The nonequilibrium (in a general case) boundary conditions are accepted. Nonclassical stress and heat transfer has been found in these flows. Different kinetic equations including the Boltzmann equation with a full collision integral and the model equations by Spiga, Groppi, Bisi et al. for mixtures with chemical reactions are used. The boundary problem with the so-called membrane-like boundary conditions is studied, for these boundaries molecules outcoming the region under consideration do not interact with particles entering this region. Some zones with the anomalous transport are observed in numerical simulations. Under these conditions the generalization for the gas mixtures with chemical reactions are discussed. Application of more complex boundary conditions implies the constructions of more complex nonequilibrium open systems. One of the

main issue is a search of possible entire systems (or although a part of the system) which could possess anomalous transport properties.

Asymptotic analysis of kinetic equations – a journey from transport theory through population dynamics to evolution on networks

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Asymptotic analysis is a way to aggregate complex systems by deriving simpler ones with approximately the same dynamics. This, for instance, can be achieved when the evolution of the original system is driven by processes with widely different typical time scales. Then we can consider a quasi-steady state approximation by assuming that fast processes have already reached their equilibrium states.
The methods of asymptotic analysis are universal but they can lead to unexpected approximations in different models. We shall discuss such limits for classical linear Boltzmann type equations, a structured population model and network transport – all representing various faces of kinetic models.

Discrete velocity models for polyatomic molecules for multicomponent mixtures and shock profiles

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We discuss a general discrete Boltzmann equation (DBE) for a multicomponent mixture where each species might have a finite number of different internal energies. In a natural way, the equation can be extended to bimolecular chemical reactions.
The DVMs are constructed in such a way that we for the shock-wave problem obtain similar structures as for the DBE for one species, and therefore will be able to apply previously obtained results. In fact the DBE becomes a system of ordinary differential equations (dynamical system) and the shock profiles can be seen as heteroclinic orbits connecting two singular points (Maxwellians). We obtain existence of shock profiles for shock speeds close to a typical speed, corresponding to the sound speed in the continuous case.

On some properties of Vlasov-Poisson-Landau kinetic equations

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We consider some properties of the Vlasov-Poisson-Landau kinetic equations for the case when the typical length is the mean free path, not the Debye redius. What are the limiting equations in that case? Are they well posed? How to describe the corresponding necessary conditions of transition to the limit? These and similar questions are the main subject of the talk. All our formal considerations for the non-linear case are supported by more serious analysis of the linearized equations and their exact solutions.

A kinetic approach of the bitemperature Euler system

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This talk is devoted to the numerical approximation of the bitemperature Euler system that has been derived from an underlying kinetic model by performing an hydrodynamic limit. This fluid model describes a plasma in an out of equilibrium situation. This system enters into the framework of the non conservative hyperbolic systems, whose theory is up to now not well understood. In the situation of shocks the numerical solutions of such systems show plateaux depending on the viscosity of the schemes. In the present work, we propose a discretisation of the kinetic model which is conservative in order to select the non regular solutions of the system.

Glioma invasion and its interplay with the nervous tissue: a multiscale model

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The invasion of tumor cells into healthy tissue is a highly complex process involving several scales, from the microscopic to the macroscopic level. Furthermore, most of the events taking place on the various scales are still not completely understood.

In this work we focus on glioma, a particular invasive brain tumor, that, owing to the peculiarities of the underlying nervous tissue geometry, shows highly anisotropic diffusion and heterogeneous patterns.
We formulate a multiscale model for the glioma cell migration and proliferation, taking also into account a possible therapeutic approach, in the line of well-established approaches in this field [1, 2]. Starting with the description of the subcellular level, we formulate the equation for the mesoscopic level and we derive the macroscopic partial differential for the glioma density function.
After the model set up, we focus on the study of coefficient functions involved in the equations that highlight the role of the fibers in the tumor dynamics [3]. In particular, we consider the fiber density function, with the aim of comparing different possible choices in order to understand which approach could better describe the actual fiber density and orientation. We ultimate the study with some numerical simulations, based on real data, that show the role of each modelled process in the evolution of the solution. [Joint work with M. Groppi (University of Parma), L. Preziosi (Politecnico di Torino) and L. Gerardo-Giorda (BCAM)]

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A reaction-diffusion-drift equation in the Continuum Physics of scintillating crystals

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Keywords: Reaction-Diffusion-Drift equations, Asymptotic Convergence, Scintillators.

A scintillating crystal is a wavelength shifter, namely a material which converts γ- or X-ray energy into visible light. The scintillation process is a microscopic one: the incoming energy creates a population of excitation carriers (charged particles) which recombine in a dissipative and non linear manner to yield photons in the visible range [1]. We represent the excitation carrier at a mesoscopic scale with an *m*-dimensional vector *n* and we assume that the crystal can be represented as a

continuum with microstructure, to arrive at a system which describes the excitation carriers generation and recombination process [2]:

$$\mathrm{div}(D\nabla n + MN(n)q \otimes \nabla\varphi) + r(n) = \dot{n}$$

$$-\varepsilon_0 \Delta\varphi = q \cdot n\,,$$

where, *M* and *D* are the temperature dependent *Mobility* and *Diffusivity* $m \times m$ matrices, $q \in Z^m$ is the charge number vector, *r(n)* is the non-linear temperature dependent *Recombination term* and $N(n) = diag(n_1, n_2, \dots n_m)$. This Reaction-Diffusion-Drift system generalizes the phenomenological model of [3] and is the same as the semiconductors equations obtained, by starting from a totally different approach, into [4].

We obtained results about the solution global existence in time, and its asymptotic behavior by following the techniques used into [5] and [6]: these results give, for the first time in terms of the equation physical parameters, an explicit representation of the scintillator *Decay time* which is a measure of the scintillating crystal resolution [7].

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Multi species Boltzmann equations for reactive monoatomic and polyatomic gases: modeling and mathematical analysis

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In this talk, based on a paper in preparation with Yemin Chen and Lingbing He, we present the latest developments concerning a model for mixtures of complex reactive rarefied gases first introduced in a paper in collaboration with R. Monaco and F. Salvarani almost fifteen years ago.
In particular we explain how some key elements of the mathematical theory of the monoatomic Boltzmann equation can be extended in complex situations when there are more than one species involved in the mixture, when some of those species may be polyatomic, and when at least one binary chemical reaction is considered. We especially focus on renormalized solutions.

Kinetic theory problems in two-phase flows

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In a countless number of applications or experimental investigations fluids are present both in their liquid and vapor/gas phases. Although the bulk of liquid and vapor/gas regions are well described by hydrodynamic equations, liquid-vapor “interfaces” (in an extended sense) require particular attention and the adoption of a variety of theoretical and numerical tools. Out of thermo-mechanical equilibrium, liquid and vapor/gas hydrodynamic regions are separated by layers consisting in the vapor-liquid interface and a Knudsen (kinetic) layer. The latter has to be described by kinetic equations, supplemented with kinetic boundary conditions. A vast literature has been devoted to the kinetic treatment of evaporation/condensation flows, mainly when a one-dimensional steady approximation is valid. The latter is reasonable when the Knudsen layer thickness is much smaller than the interface curvature and many flow problems can be described on ground of jump formulas. Problems in which the extent of the kinetic flow region is larger have attracted less attention, their treatment being limited to simple geometries. The talk will describe and discuss the structure and applications of a few theoretical/numerical tools allowing a more flexible description of liquid-vapor flows. Such goal can be achieved either by a single mathematical model, capable of describing both phases (Diffuse Interface Models, Enskog-Vlasov kinetic model), or by a hybrid model, based on the

direct coupling of the Navier-Stokes-Fourier description of the liquid phase with the Boltzmann equation describing the vapor/gas.

A mathematical realization of entropy through neutron slowing down

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Neutron slowing down in an infinite homogeneous medium is a classic problem of neutron transport theory. Neutrons (test particles) collide elastically with nuclei (field particles) and thereby lose energy to recoil. Thus, we have a common collisional process as described by a balance in energy phase space between the neutron source and the neutrons scattering into and out of an infinitesimal energy increment. By limiting our investigation to a non-absorbing infinite medium, spatial and directional variations have naturally been eliminated. One can analytically solve the resulting equation for the neutron collision density distribution as it tends toward energy equilibrium. Interestingly, while the slowing down equation is deterministic, it nevertheless, describes the statistical scattering process as illuminated by the associated mathematics.

Linear Boltzmann equation and fractional diffusion

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Consider the linear Boltzmann equation of radiative transfer in a half-space, with constant scattering coefficient σ. Assume that, on the boundary of the half-space, the radiation intensity satisfies the Lambert (i.e. diffuse) reflection law with albedo coefficient α. Moreover, assume that there is a temperature gradient on the boundary of the half-space, which radiates energy in the half-space according to the Stefan-Boltzmann law. In the asymptotic regime where $\sigma \to +\infty$ and $1 - \alpha \sim C/\sigma$, we prove that the radiation pressure exerted on the boundary of the half-space is

governed by a fractional diffusion equation. This result provides an example of fractional diffusion asymptotic limit of a kinetic model which is based on the harmonic extension definition of $\sqrt{-\Delta}$. This fractional diffusion limit therefore differs from most of other such limits for kinetic models reported in the literature, which are based on specific properties of the equilibrium distributions ("heavy tails") or of the scattering coefficient as in [U. Frisch-H. Frisch: Mon. Not. R. Astr. Not. 181 (1977), 273-280]. [Work in collaboration with C. Bardos and I. Moyano]

Vlasov-Poisson system tackeled by particle simulation utilizing Boundary Element Methods

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In this talk, we present a grid-free method for the numerical treatment of the three-dimensional Vlasov-Poisson system. After the discretisation of the density function with a standard particle method, the solution of the Poisson equation is split into two parts: a particle-particle part and a solution of a Laplace problem. Solving the later with the Boundary Element Method (BEM) leads to a (volume) grid-free method.

The BEM makes use of an equivalent boundary integral formulation of the Laplace problem, which is discretised on a boundary mesh. This reduces the three-dimensional volume problem to a two-dimensional problem on the boundary. Consequently, the number of degrees of freedom of the BEM is typically much smaller than the number of particles.

The electric field is approximated by hierarchical matrices which are computed on the fly. The computational complexity for their evaluation is linear in the number of particles and nearly linear in the number of degrees of freedom of the BEM. The numerical experiments confirm the theoretical complexity estimates.

Some mathematical models and numerical simulations describing the decoherence phenomenon

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The aim of this talk will be to give an overview over some different mathematical models (based on the Schrödinger equation) describing the decoherence phenomenon and also to discuss the related theoretical and numerical difficulties.
Decoherence is a purely quantum mechanical effect without analogue in classical physics. In more details, quantum decoherence occurs due to the interaction of a quantum system with the environment, fact which leads to the suppression of interference patterns in the quantum system, patterns which are typical quantum mechanical features. This suppression phenomenon is the so-called “quantum decoherence” and is nowadays considered as the key concept in the description of the transition from the quantum to the classical world. The interest in the study of the decoherence effect appeared not only with the research in fundamental quantum mechanics, but also in applied physics. For example, in quantum computation (QC), electron spin resonance (ESR), and nuclear magnetic resonance (NMR) it is of paramount importance to preserve the quantum behaviour, so decoherence is not desired and efforts are made in order to avoid it. On the other hand, in quantum interference effect transistors (QuIET) decoherence is exploited to control the quantum current flow. In such devices, decoherence acts like a switch to modulate the current flow, the device being switched ``off'' in the completely coherent state and ``on'' when interference disappears.

Kinetic theories of inert and reactive mixtures

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I will consider mathematical and physical problems for various kinetic models of inert and reactive mixtures. In contrast to the line-of-center kinetic models of reactive mixtures, the kinetic models presented in the talk have built-in the microscopic reversibility (detailed balance), and thus, all mathematical aspects of the reactive models can be fully justified.
I will also consider stochastic variants for both reactive and inert mixtures. This extends the work previously developed for liquid-state kinetic theory with interaction potentials that are continuously varying (such as Lennard-Jones particles and inverse-power-law potentials), rather than discontinuous (such as the hard-sphere or square-well potentials).

Recent developments in the application of the backward Master equation to stochastic particle populations

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The generalization of transport theory to describe strongly stochastic neutron populations, typically associated with weak source driven supercritical systems, has been elegantly articulated in the classic works of Pal and Bell and rigorously grounded in the theory of branching Markov processes of discrete particles distributed on a continuous phase space. The mathematical formulation yields the well known backward Master equation for the neutron number probability distribution, or its more familiar form in terms of the probability generating function. The approach has been widely used to obtain statistical moments of the neutron number, extinction and divergent probabilities of neutron chains, and, in the point kinetic or lumped framework, closed form expressions of the neutron probability distribution function. These simplified formulations have facilitated the analysis and understanding of supercritical excursions associated with criticality accidents and fast burst or pulsed reactors, and enabled prediction of neutron-gamma multiplicity distributions, as well as mass and composition of special nuclear material, in nuclear safeguards applications.

In this presentation we describe two recent developments relating to the application of the backward Master equation to stochastic particle populations. First we present a generalization of the Master equation to account for the cumulative number of fissions and the cumulative energy deposited in fissions, which evolve stochastically with the neutron number. The distribution of deposited energy is equally important in characterizing dynamic stochastic phenomena as the neutron number but exhibits unique stochastic behavior. Second, we derive a novel nonlinear transport equation in which the neutron number appears as a continuous independent variable, for which existing deterministic numerical solution methods can be adapted and offers an alternate approach to computationally demanding Monte Carlo simulation for constructing neutron number distributions. Random internal sources are readily accommodated and the formalism can be generalized to also describe the fission number and deposited energy. We present some preliminary numerical results to demonstrate the computational utility of this deterministic formulation.

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 [1-9] illustrated in the perspective of future developments, in particular the optimization of graphene field effect transistors.

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Multiscale phenomena in Continuum Mechanics: mesoscopic justification of Rational Extended Thermodynamics of gases with internal structure

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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 of an extra variable that take into account the internal motion of polyatomic gas (rotation and vibration). In this talk we consider a more refined version or 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 the 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. Finally, the dispersion relation of ultrasonic wave is confirmed by the experimental data for several gases.

Heat equation and viscoelasticity

Giuseppe Saccomandi
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The equations of nonlinear Kelvin-Voigt viscoelasticity, in a suitable asymptotic limit, reduces to a nonlinear heat equation. The aim of the talk it is to show that this relationship is twinned with the global existence problem for viscoelastic waves.

Oscillations in reaction-diffusion systems with linear and nonlinear cross-diffusion

Marco Sammartino
University of Palermo, Italy

In this talk we shall discuss two mechanisms leading to oscillatory behaviors in reaction diffusion equations. The first, which is well known, involves the interaction between Turing and Hopf instabilities. We shall see this mechanism in the Schnakenberg system with linear cross-diffusion. In the neighborhood of the codimension-two bifurcation point we shall perform a normal form reduction and the corresponding bifurcation diagram will be compared with the bifurcation diagram of the full system.
The second mechanism, which is relatively new, is due to resonance between a Turing mode and its subharmonic. We shall show this mechanism in a predator-prey system with nonlinear cross-diffusion. We stress that this oscillatory behaviors occurs in absence of any Hopf instability of the kinetics and it has to be ascribed to a complex interaction between the nonlinear diffusion and the kinetics. We shall also describe a sequence of bifurcations leading to spatiotemporal chaos.
Well-posedness of the discussed systems will also be addressed.

Finding friends in scientific cooperation

Ferdinand Schuerrer
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Entropy growth within the shock wave in binary multi-temperature mixture

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Entropy and entropy production rate are analyzed in stationary shock waves in the multi-temperature model of binary mixture of gases. The model is developed within the framework of extended thermodynamics which leads to a proper definition of the non-equilibrium entropy, as well as the entropy production rate. The entropy profiles are analyzed for the whole mixture and for the constituents. The analysis of entropy growth rate distinguished the contributions of diffusion (momentum exchange) and internal energy exchange between the constituents.

On the Maxwell-Stefan diffusion limit for a mixture of reacting gases

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We consider a chemically reactive mixture described in the frame of the Boltzmann equation and study the reaction-diffusion limit of the kinetic system of equations.
Under certain assumptions, we formally derive a reaction-diffusion system of Maxwell-Stefan type, extending previous approaches for non-reactive multicomponent mixtures.
The emphasis is on the contributions resulting from the chemical reaction and the case of a reactive mixture of polyatomic gases is also analysed.

Cross-diffusion predator-prey models arising by time-scale arguments

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Laurent Desvillettes
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Starting from microscopic models incorporating the dynamics of handling and searching predators, or active and hidden prey, we obtain reaction cross-diffusion systems of predator-prey type involving classical functional responses, by the exploitation of different time-scales. We also provide a study of the Turing instability domain of the obtained equations and (in the case of the Beddington-DeAngelis functional response) compare it to the same instability domain when the cross-diffusion is replaced by a standard diffusion.

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Acknowledgements:
FCT-Fundação para a Ciência e Tecnologia (project UID/MAT/04561/2013), French-Italian program Galileo (project G14-34), and INdAM-GNFM.
French "ANR blanche" Project Kibord: ANR-13-BS01-0004, and Universitè Sorbonne Paris Citè, in the framework of the "Investissements d'Avenir", convention ANR-11-IDEX-0005.

Kinetic modelling of soft flowing crystals

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We present the main ideas behind the kinetic modelling of soft-flowing crystals, with special attention to the microfluidic design of novel mesoscale porous materials for biomedical engineering applications.

Human behavior and lognormal distribution

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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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Kinetic insights into the rise and fall of popularity on social media

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We will introduce a novel kinetic model of opinion formation on social networks, which takes into account a realistic statistical description of the background connectivity of the users of the social media. The model is then coupled with a kinetic-type description of the spreading of the popularity of an online content (such as e.g., an advertisement, a message, a video and the like) based on the interactions of such a content with the evolving opinions of the users of the social network. Analytical investigations and numerical experiments show that the model is able to explain the emergence of time trends such as the rise and fall of popularity of hashtags empirically observed in some recent social media campaigns. The model also provides preliminary hints on communication strategies which may foster the permeation of a content in the society.
The talk is based on the contents of the work: G. Toscani, A. Tosin, M. Zanella, "Opinion modeling on social media and marketing aspects", submitted, 2018 (preprint: arXiv:1805.01892). [Work in collaboration with Giuseppe Toscani and Mattia Zanella].

Exact solutions of integrable nonlinear evolution equations

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In this talk we present a unified approach by means of matrix triplets to derive in closed form the multi-soliton solutions of various continuous-time nonlinear evolution equations. These solutions are obtained by applying the inverse scattering transform, where the inverse scattering step is implemented by solving the Marchenko integral equation by separation of variables. In particular, we present the multi-soliton solutions of the NLS, Hirota, and sine-Gordon equations and the Heisenberg ferromagnetic equation.

Control strategies for road risk mitigation in kinetic and hydrodynamic traffic modelling

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We present a Boltzmann-type kinetic approach to the modelling of road traffic dynamics, which includes control strategies at the level of microscopic binary interactions aimed at the mitigation of speed-dependent road risk factors. Such a description is meant to mimic a system of driver-assist vehicles, which by responding locally to the actions of their drivers can impact on the large-scale traffic dynamics, including those related to the collective road risk and safety.
Furthermore, we present the derivation of the corresponding kinetic-controlled hydrodynamic equations for the evolution of macroscopic quantities. The derived control term results embedded in the definition of a constrained flux function. First and second order fluid equations are obtained with appropriate closure methods. Suitable numerical methods are necessary to observe the described hierarchy of scales.

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