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Mini-Workshop: Innovative Trends in the Numerical Analysis and Simulation of Kinetic Equations

Organised by
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Abstract. In multiscale modeling hierarchy, kinetic theory plays a vital role in connecting microscopic Newtonian mechanics and macroscopic continuum mechanics. As computing power grows, numerical simulation of kinetic equations has become possible and undergone rapid development over the past decade. Yet the unique challenges arising in these equations, such as high-dimensionality, multiple scales, random inputs, positivity, entropy dissipation, etc., call for new advances of numerical methods. This mini-workshop brought together both senior and junior researchers working on various fast-paced growing numerical aspects of kinetic equations. The topics include, but were not limited to, uncertainty quantification, structure-preserving methods, phase transitions, asymptotic-preserving schemes, and fast methods for kinetic equations.

Mathematics Subject Classification (2010): 82B40, 82C05, 35Q20, 65R10.

Introduction by the Organisers

The mini-workshop *Innovative Trends in the Numerical Analysis and Simulation of Kinetic Equations* was devoted to the numerical novel aspects of kinetic modelling. Kinetic modelling has become one of the most powerful tools in applied mathematics to bridge microscopic and macroscopic descriptions of many body systems during the last 30 years, see [12] for a review. The flexibility of the methods stemming from kinetic and large deviation theories have had numerous applications in physical, biological and technological problems. They typically involve a huge number of individuals, showing some sort of "collective behaviour", from

which we want to extract average or macroscopic information, see [5, 10, 12, 7, 2] and the references therein. Some classical and modern instances of applications are: molecules in gases, electron transport in semiconductor materials, ions and electrons in plasmas, grains or beads in granular gases, stars or galaxies in astrophysics, endothelial cells in chemotactic movement for angiogenesis, neurons spike dynamics in neuroscience, fuel droplets in Diesel engines, dust particles in atmospheric pollution, animals in a swarm, agents in an economic market, pedestrians strolling around complex building geometries...

This diversity of applications should not hide the common underlying methods, models and structural equations derived in all of these problems. Not only the beauty of applications but also the inherent mathematical difficulty of these models have attracted the attention of leading mathematicians from the modelling, analysis and numerical viewpoints as international scientific databases demonstrate. In all of these models, a fine study of the stability properties, the long-time asymptotics [12], the numerical methods and their simulation in the applications are relevant questions [7].

The individual behaviour of the "particles" is typically modelled via stochastic or deterministic ODEs from which one obtains mesoscopic descriptions based on kinetic type PDEs, while the average dynamics is usually described via continuum mechanics systems of hyperbolic, diffusive, or hydrodynamic type. The interplay between the long- and short-range interactions, transport and diffusion, and their nonlocal and nonlinear features are the main mathematical difficulties in understanding equilibrium states, their stability and asymptotic analysis.

On the other hand, the relation between kinetic equations and nonlinear nonlocal aggregation diffusion equations appears at the level of homogeneous kinetic models and Fokker-Planck type equations in which the exchange of different methods and techniques has recently provided important advances [8, 1, 4]. Hydrodynamic models are usually derived from kinetic equations via moment closures or via asymptotic limits. Nevertheless, plenty of challenging related questions remain at the hydrodynamic and kinetic description levels.

Finally, the development of numerical schemes for both the microscopic and the kinetic level descriptions [7] faces the curse of the high dimensionality of the problems, not to mention the intricate structure of the convolution-like operators involved. The connection to macroscopic problems is then obtained through asymptotic limits, sometimes performed even at the level of the numerical schemes. These asymptotic preserving schemes are certainly a strategy to attack the reduction of computational cost at the kinetic level while keeping track of the microscopic dynamics if needed. On the other hand, numerical discretisations of macroscopic equations should reflect their structural properties. Therefore, one natural idea is to take advantage of the gradient flow structure in the macroscopic equations to construct numerical schemes based on calculus of variations or optimal transport viewpoint.

The mini-workshop *Innovative Trends in the Numerical Analysis and Simulation of Kinetic Equations*, organized by Jose A. Carrillo (London), Martin Frank

(Karlsruhe), Jingwei Hu (West Lafayette), and Lorenzo Pareschi (Ferrara) was well attended by 17 participants, including both junior and senior researchers and 3 females. We brought researchers working on various numerical aspects of kinetic modelling, their numerical analysis and their applications to exchange ideas and promote collaborations. Every participant contributed a talk which makes a total of 17 talks. In particular, there was a joint session on Thursday that gathered all the participants from the three mini-workshops held concurrently in the same week (all focused on numerics). Antoine Cerfon from our workshop gave a talk on kinetic simulation of plasmas in the joint session.

Several topics on various numerical aspects of kinetic equations were addressed in the mini-workshop. Here is a brief summary.

Uncertainty quantification (UQ) for kinetic equations. The kinetic equations often contain uncertainties in their collision kernels or scattering coefficients, initial or boundary data, forcing terms, geometry, etc. Quantifying the uncertainties in kinetic models have important engineering and industrial applications. There was a big emphasis in the mini-workshop on this topic. Specifically, the opening talk by Shi Jin conducted the sensitivity analysis for kinetic equations and used it to prove the spectral convergence of the stochastic Galerkin (sG) method. The talks by Giacomo Dimarco and Lorenzo Pareschi focused on the Monte Carlo (MC) method, where a control variate approach was introduced to reduce the variance of standard MC techniques. Finally, the talk by Mattia Zanella considered the UQ for kinetic equations arising in collective dynamics and a hybrid sG-MC method was presented.

Structure-preserving methods for kinetic equations. Kinetic equations model the time evolution of the probability density function (PDF) and is usually endowed with an entropy functional. As such, the numerical methods that can preserve the properties of the solution, e.g., positivity, conservation, entropy-decay, are highly-desirable. Furthermore, the kinetic equations are connected to macroscopic fluid equations as the Knudsen number (ratio of the mean free path and typical length scale) goes to zero. A numerical scheme that can capture the fluid limit without resolving the small scale, i.e., asymptotic-preserving (AP), is also attractive, especially for handling multiscale problems. Several talks in the mini-workshop focused on the design of structure-preserving methods for kinetic equations. Jingwei Hu introduced a time discretization method for a class of stiff kinetic equations that is both positivity-preserving and AP. Thomas Rey proposed a finite volume scheme for the linear kinetic equation that is able to capture the solution in long time and diffusive limit. Both Li Wang and Jose A. Carrillo studied a general nonlinear nonlocal Fokker-Planck type equation with a gradient flow structure: Li presented an optimization method based on Wasserstein metric and Jose presented a finite volume method. Both approaches are able to preserve the positivity and energy decay of the solution. Finally Giovanni Russo introduced a high-order semi-Lagrangian method for the BGK and Vlasov-Poisson equation whose key property is the conservation of mass.

Fast deterministic methods for kinetic equations. A prominent feature of many kinetic equations, for instance, the Boltzmann equation, is a nonlinear, nonlocal, high-dimensional collision operator. Numerically approximating these operators has been a big challenge in science and engineering for decades, and the Monte Carlo based stochastic method has been historically popular due its low complexity and simplicity. In recent years, the deterministic numerical methods (e.g., spectral method, discontinuous Galerkin (DG) method) have seen their revival as the computing power grows. We have two talks in our mini-workshop addressing the deterministic approximation of the Boltzmann type equations. The talk by Ralf Hiptmair reported the recent progress of constructing finite element approximation of the Boltzmann equation. The talk by Zheng Ma introduced a fast Fourier spectral method for the inelastic Boltzmann collision operator.

Numerical methods in plasma physics. Kinetic description plays an important role in plasma physics where the underlying equation is the Vlasov-Poisson (or Maxwell) equations. If the collision is desired (for example, in hot plasmas), a term such as the Fokker-Planck or Landau operator would be added as well. This mini-workshop gathered both mathematicians and plasma physicists to discuss many challenging problems in plasma simulations. The talk by Francis Filbet addressed the asymptotics of the Vlasov equation in a strong magnetic field. The talk by Luis Chacon focused on the collisional plasmas. The talk by Antoine Cerfon introduced a sparse grid technique to speed up large scale computations.

Other topics. A few other topics were also presented. Axel Klar's talk was on the derivation of coupling conditions in a domain decomposition method in networks. Qin Li's talk focused on the inverse problem aspect of kinetic equations. Martin Frank's talk proposed a new moment closure method to reduce the dimension of kinetic equations.

Summary. The aims of the conference were all achieved, new collaborations were established between different groups present in the workshop, and the results will be seen in the next following years in terms of common publications in this thriving area of research in Numerical Analysis of PDEs.

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Mini-Workshop: Innovative Trends in the Numerical Analysis and Simulation of Kinetic Equations

Table of Contents

Abstracts

Hypocoercivity based sensitivity analysis for multiscale kinetic equations with uncertainties

Shi Jin

In this talk we will study the generalized polynomial chaos-stochastic Galerkin (gPC-SG) approach to kinetic equations with uncertain coefficients/inputs, and multiple time or space scales, and show that they can be made asymptotic-preserving, in the sense that the gPC-SG scheme preserves various asymptotic limits in the discrete space. This allows the implementation of the gPC methods for these problems without numerically resolving (spatially, temporally or by gPC modes) the small scales. Rigorous analysis, based on hypocoercivity of the collision operator, will be provided for general kinetic equations to prove uniform convergence toward the local or global equilibrium, and the spectral convergence of the gPC-SG method.

Kinetic layers and coupling conditions for hyperbolic PDEs on networks

Axel Klar
(joint work with Raul Borsche)

Networks of hyperbolic PDEs arise in different applications, e.g. modeling water- or gas-networks, road traffic or the human circulatory system. In this talk a new approach for deriving coupling conditions based on an underlying kinetic description is discussed. Starting from the kinetic equation on the network we derive coupling conditions for the macroscopic limit equations via an analysis of kinetic half space problems

$$v\partial_x\varphi = Q(f) \ , \quad x \in [0,\infty] \ .$$

Combining such half-space problems for all edges α connected to a node, leads to a fix-point problem at each node involving the Albedo operator A. This operator gives the outgoing solution of a half-space problem depending on the ingoing solution b^α. The fix point problem reads for outward oriented edges α

$$b^\alpha(v) = \sum_{\alpha'} c_{\alpha\alpha'} A[b^{\alpha'}](-v), \ v > 0.$$

Solving this problem approximately and determining, in particular, the values at ∞ yields finally the coupling conditions for the corresponding macroscopic equations. We consider linearized BGK equations and simple hyperbolic relaxation models and their limit equations, i.e. the wave equation and the nonlinear Burgers' problem on networks and discuss more complicated nonlinear hyperbolic relaxation systems. Numerical comparisons between the solutions of the macroscopic

equation and the kinetic solution show the properties of the different coupling conditions.

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Asymptotics of the three dimensional Vlasov equation in the large magnetic field limit

Francis Filbet

(joint work with Luis Miguel Rodrigues and Hamed Zakerzadeh)

Since fusion configurations involve very hot plasmas, they typically require a careful design to maintain fast moving particles inside the core of the device on sufficiently long times. In the magnetic confinement approach [1, 7, 11], in particular in tokamak plasmas, a strong external field is applied to enforce the oscillatory nature of the fast motions.

Various models are in use to describe such phenomena. In the kinetic modeling, the unknowns are the number densities of particles, $f \equiv f(t, \mathbf{x}, \mathbf{v})$ depending on time $t \geq 0$, position $\mathbf{x} \in \Omega \subset \mathbf{R}^3$ and velocity $\mathbf{v} \in \mathbf{R}^3$. Such kinetic models provide an appropriate description of turbulent transport in a fairly general context, but in fusion configurations their numerical simulations require to solve a stiff six-dimensional problem, leading to a huge computational cost. To bypass this obstacle, it is classical — see for instance [8] — to use reduced asymptotic models that describe only the slowest part of the plasma dynamics hence effectively reducing both the stiffness of the problem and the number of variables (since fastest variables are omitted). Over the years, due to its rich and fundamental nature, the physically-based derivation of such models has grown as a — still very active — field of its own, often referred to as gyrokinetics. Besides the already mentioned general monographs [1, 7, 11, 16, 17], the reader may consult [12, 3] and references therein as more specialized entering gates to the field.

Despite considerable efforts in recent years, concerning mathematically rigorous derivations from collisionless kinetic equations, unfortunately the state of art is such that one must choose between linear models that neglect couplings due to self-consistent fields or nonlinear ones set in a deceptively simple geometry. See for instance the introductions and bibliographies of [10] for relatively recent panoramas on the question. For instance, for the kind of problem considered here, on the nonlinear side of the literature the most significant mathematical result — which

requires a careful analysis — is restricted to a two-dimensional setting with a constant magnetic field and interactions described through the Poisson equation, and yet validates only half of the slow dynamics; see [19], building on [9] and recently revisited in [15].

We consider here a plasma confined by a strong unsteady inhomogeneous magnetic field without any a priori geometric constraint but, in order to allow for such a generality, we do neglect effects of self-consistent fields. The plasma is thus entirely modeled with a scalar linear kinetic equation, where the unknown is one of the number densities of particles. The approach that we follow focuses on the characteristic equations associated with the kinetic conservation law. By itself the study of those equations may follow the classical roadmap of the averaging of ordinary differential equations, as expounded in [20]. Yet, here, beyond the body of work already required to follow this road in usual ODE problems, a careful track of the dependence of averaging estimates on initial data, living here in an unbounded phase space, is necessary so as to derive asymptotics for the solutions of the original partial differential equations problem.

To be more specific, the Lorentz force term in our original nondimensionalized kinetic equation is scaled by a large parameter, $1/\varepsilon$, where ε stands for the typical cyclotron period, *i.e.* the typical rotation period of particles about a magnetic field line (or Larmor rotation). The dynamical time scales we focus on are in any case much larger than the cyclotron period and we establish asymptotic descriptions in the limit $\varepsilon \to 0$. As is classical in the field, we distinguish between short-time scales that are $\mathcal{O}(1)$ with respect to ε, and long time scales that are $\sim 1/\varepsilon$ in the limit $\varepsilon \to 0$. Correspondingly, slow dynamics refer to dynamics where typical time derivatives are at most of order $\mathcal{O}(1)$ on short-time scales, and at most of order $\mathcal{O}(\varepsilon)$ on long-time scales so that on long time scales two kinds of fast dynamics may co-exist, principal ones at typical speed of order $1/\varepsilon$ and subprincipal ones at typical speed of order 1; see for instance [4] for a description of those various oscillations in a specific class of axi-symmetric geometries, without electric field and with a magnetic field nowhere toroidal and whose angle to the toroidal direction is also independent of the poloidal angle. With this terminology in hands, our results may be roughly stated as the identification and mathematical proofs of

(1) a second-order — that is, up to $\mathcal{O}(\varepsilon^2)$ — description of the slow dynamics on short time scales but in arbitrary geometry;
(2) a first-order description of the slow dynamics on long time scales but in an axi-symmetric geometry with a magnetic field everywhere poloidal and an electric field everywhere orthogonal to the magnetic field.

The geometry of the latter is very specific and the proof of such a description is mostly carried out here to illustrate that the short-time second-order description contains all the ingredients to analyze long-time dynamics at first-order. Note that in any case, on long-time scales some restrictions are indeed necessary to ensure that sub-principally fast dynamics do not prevent long-time confinement

and are of oscillatory type so that the issue of the identification of a long-time slow dynamics becomes meaningful.

A key feature of our analysis that underpins a treatment of essentially arbitrary fields is that we make no explicit use of any geometric structure, neither Hamiltonian (see for instance [14, 2]) nor Lagrangian (see [18]). The main role of these structures in the averaging process is to ease the identification of terms that are asymptotically irrevelant as time-derivatives of small terms. Instead, in the present contribution this explicit identification hinges heavily on the linearity of principal oscillations. As an upset, besides generality, we gain the freedom to use change of variables that are also arbitrary and to focus on slow variables instead of carrying geometric constraints all along.

A key motivation for our methodology is that in the design of well-adapted numerical schemes, that capture the slow part of the dynamics even with discretization meshes too rough to compute stiff scales, one might correspondingly aim at large classes of schemes of arbitrary order; see for instance [13, 5, 6].

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Polar Spectral Polynomial Schemes for Boltzmann Evolutions

Ralf Hiptmair
(joint work with Philipp Grohs and Simon Pintarelli)

Boltzmann evolution. We consider the spatially inhomogeneous transient Boltzmann equation ($k_n > 0$ the Knudsen number)

$$\partial_t f + \boldsymbol{v} \cdot \boldsymbol{\nabla}_{\boldsymbol{x}} f = \frac{1}{k_n} Q(f,f) \quad \text{on} \quad [0,T] \times \Omega \,, \tag{1}$$

for a time-dependent distribution function $f = f(t, \boldsymbol{x}, \boldsymbol{v})$ defined on 2-dimensional phase space $\Omega := D \times \mathbb{R}^d$, $D \subset \mathbb{R}^d$ a bounded "physical domain". The bilinear *collision operator* Q is of the usual form with a collision kernel satisfying Grad's cut-off assumption so that it can be split into a gain and loss term. We remind that the collision operator $Q(f,f)$

(Q1) involves integration over $\mathbb{R}^d \times \mathbb{S}^{d-1}$, $\mathbb{S}^{d-1}$ the sphere in $\mathbb{R}^d$,
(Q2) does neither depend on the spatial variable $\boldsymbol{x}$ nor on time t,
(Q3) and commutes with translations and rotations in velocity direction $\boldsymbol{v}$.

The partial differential equation (1) has to be supplemented with boundary conditions on the inflow boundary $\Gamma^- := \{(\boldsymbol{x},\boldsymbol{v}) \in \partial D \times \mathbb{R}^d,\, \boldsymbol{v} \cdot \boldsymbol{n}(\boldsymbol{x}) < 0\}$, $\boldsymbol{n}$ the exterior normal at ∂D. Direct inflow conditions, and specular or diffusive reflection are commonly employed.

Tensor-product Galerkin discretization. An approximation of the distribution function is sought in a finite-dimensional tensor-product space $V_x \times V_v$ with $V_x \subset L^2(D)$ and V_v contained in the Schwarz space $\mathcal{S}(\mathbb{R}^d)$ of smooth rapidly decaying functions. For fixed $\boldsymbol{v}$, (1) represents a pure linear transport equation and stabilization is required for any piecewise polynomial finite element discretization in physical space.

In [3] we opted for least-squares stabilization of the transport operator combined with split-step timestepping. Let $\mathcal{M}$ be a finite-element mesh of D. The distribution function is approximated in $V_\Omega := \mathcal{P}_n^0(\mathcal{M}) \times V_v$ with $\mathcal{P}_n^0(\mathcal{M})$ the space of *continuous* $\mathcal{M}$-piecewise polynomials of total degree n. Then a single timestep

$f_h^{(n-1)} \to f_h^{(n)}$ of size $\tau > 0$ amounts to solving [7, Ch. 3]

$$
\begin{aligned}
&\text{(I):} \quad f_h^* = \operatorname*{argmin}_{f_h \in V_\Omega} \left\| \frac{1}{\tau}(f_h - f_h^{(n-1)}) + \boldsymbol{v} \cdot \boldsymbol{\nabla}_{\boldsymbol{x}} f_h \right\|^2_{L^2(D\times\mathbb{R}^d)} , \\
&\text{(II)} \quad \int_D \int_{\mathbb{R}^d} \frac{f_h^{(n)} - f_h^*}{\tau} \, \Phi \, \mathrm{d}\boldsymbol{v}\mathrm{d}\boldsymbol{x} = \int_D \int_{\mathbb{R}^d} Q(f_h^*, f_h^*) \, \Phi \mathrm{d}\boldsymbol{v}\mathrm{d}\boldsymbol{x} \quad \forall \Phi \in V_\Omega \, .
\end{aligned} \tag{2}
$$

The second step is purely local in space und involves decoupled updates for individual basis functions of $\mathcal{P}_n^0(\mathcal{M})$.

In [5, 6] the authors propose spatial semi-discretization by means of an *upwind discontinuous Galerkin method* Based on a mesh $\mathcal{M}$ of D, they choose $V_x = \mathcal{P}_n^{-1}(\mathcal{M})$, the space of discontinuous $\mathcal{M}$-piecewise polynomials of total degree n and arrive at the semi-discrete variational formulation: seek $f_h \in \mathcal{P}_n(\mathcal{M}) \times V_v$ such that [5, Sect. 3]

$$
\begin{aligned}
&\sum\nolimits_{K\in\mathcal{M}} \int_K \int_{\mathbb{R}^d} \partial_t f_h \, \Phi - f_h \boldsymbol{\nabla}_{\boldsymbol{x}} \Phi \, \mathrm{d}\boldsymbol{v}\mathrm{d}\boldsymbol{x} + \int_{\partial K} \int_{\mathbb{R}^d} \widehat{F}(\boldsymbol{x}, \boldsymbol{v}) \Phi \, \mathrm{d}\boldsymbol{v}\mathrm{d}S(\boldsymbol{x}) \\
&\qquad = \int_D \int_{\mathbb{R}^d} Q(f_h, f_h) \Phi \, \mathrm{d}\boldsymbol{v}\mathrm{d}\boldsymbol{x} \quad \forall \Phi \in \mathcal{P}_k(\mathcal{M}) \times \widetilde{V}_v \, ,
\end{aligned} \tag{3}
$$

where $\widetilde{V}_v$ is the trial space in velocity direction, and $\widehat{F}$ is the *upwind numerical flux*: for $\boldsymbol{x} \in \partial K \cap \partial K'$, K, K' cells of the mesh, $\widehat{F}(\boldsymbol{x}, \boldsymbol{v})$ agrees with $f_h(\boldsymbol{x}, \boldsymbol{v})\boldsymbol{n}(\boldsymbol{x}) \cdot \boldsymbol{v}$ where f_h is take from that cell, for which $\boldsymbol{v}$ points in the direction of the outward normal $\boldsymbol{n}$. On ∂D the boundary conditions enter $\widehat{F}$. Temporal discretization of (3) can rely on explicit Runge-Kutta methods.

Approximation in velocity. Based on [1, Sect. 4], in [3, Sect. 3] the choice for V_v was Gaussian-modulated polynomials of fixed total degree

$$
\begin{aligned}
V_v &:= \{\boldsymbol{v} \mapsto \exp(-\tfrac{1}{2} \|\boldsymbol{v}\|^2) p(\boldsymbol{v}), \; p \in \mathcal{P}_n(\mathbb{R}^2)\} \, , \\
\dim V_v &= \binom{n+d}{d} = O(n^d) \, .
\end{aligned} \tag{4}
$$

The same space is used as trial space in (2). The work [2] also relies on the trial space from (4), but, in the spirit of Petrov-Galerkin approaches, uses plain polynomials as test functions: $\widetilde{V}_v = \mathcal{P}_n(\mathbb{R}^d)$. A standard polynomial test space is also embraced in [6]. In this work, in the context of (3) and breaking the simple tensor-product structure, the velocity trial spaces are chosen differently for each mesh cell $K \in \mathcal{M}$ as Maxwellian-modulated polynomials:

$$
V_k(K) := \{\boldsymbol{v} \mapsto \exp\Big(-\tfrac{1}{2}\big(\frac{\boldsymbol{v} - \overline{\boldsymbol{v}}_K}{T_K}\big)\Big) \cdot p(\boldsymbol{v}), \; p \in \mathcal{P}_n(\mathbb{R}^d)\} \, , \tag{5}
$$

where $\overline{\boldsymbol{v}}_K$ and T_K are *cell-local* approximations of momentum density and temperature that are dynamically adjusted during timestepping.

Remark. Using a polynomial test spaces in velocity of degree ≥ 2 ensures the conservation of collision invariants in semi-discrete spatially homogeneous Boltzmann evolutions [2, Sect. 3.1.3].

Basis functions for V_v. Assuming exact arithmetic the choice of basis functions for V_v does not affect the solution. Yet, it makes a huge difference for numerical stability and computational efficiency. We discuss the approach of [3] in two dimensions ($d = 2$). For V_v as in (4) we use the $L^2(\mathbb{R}^d)$-orthogonal *polar Laguerre basis*, here written in 2D polar coordinates, [3, Sect. 3]

$$V_v = \operatorname{span}\left\{ (r,\varphi) \mapsto \Psi^a_{k,j}(r,\varphi), \quad \begin{array}{l} k = 0,\dots,n\ , \\ j = 0,\dots \lfloor k/2 \rfloor\ , \\ a \in \{\sin,\cos\}\ , \end{array} \right\} \tag{6a}$$

$$\Psi^a_{k,j}(r,\varphi) := e^{-\frac{1}{2}r^2} r^{2j} \cdot \begin{cases} L^{(2j)}_{k/2-j}(r^2) a(2j\varphi) & \text{for even } k\ , \\ r L^{(2j+1)}_{(k-1)/2-j}(r^2) a((2j+1)) & \text{for odd } k\ , \end{cases} \tag{6b}$$

where $L^{(\alpha)}_\ell$ are the associated Laguerre polynomials. Beside orthogonality the big benefit of this basis is that the bulk of the $O(n^6)$ entries of the third-order tensor

$$\mathbf{Q} := \left[\int_{\mathbb{R}^2} Q(b_j, b_k)(\boldsymbol{v}) b_i(\boldsymbol{v}) \,\mathrm{d}\boldsymbol{v} \right]_{j,k,i=1}^{N} \tag{7}$$

will vanish: only $O(n^5)$ are non-zero [3, Sect. 4.3]. This also determines the asymptotic effort for the evaluation of the discrete collision operator.

Remark. Thanks to (Q2) the same precomputed tensor $\mathbf{Q}$ can be used everywhere in space and for all timesteps.

The number of basis functions needed for the accurate evaluation of the collision tensor can be reduced substantially by *recentering* the local velocity approximation to momentum = 0. This shift in velocity space entails transforming the basis expansion coefficients. This can be done efficiently with an asymptotic effort of $O(n^3)$ via representations through tensor products of Hermite polynomials [7, Sect. 2.1].

Conclusion. Gaussian/Maxwellian-modulated polynomial spectral approximation schemes of distribution functions in velocity usually offers exponential convergence in the polynomial degree. Their computational cost scales worse than that for steady state preserving Fourier spectral methods with FFT-boosted fast approximate evaluations. Yet, for spatially inhomogeneous Boltzmann evolutions modulation with spatially varying local Maxwellians [4, Sect. 4.4] may pave the way for extremely efficient approximation in $\boldsymbol{v}$-direction, which promises to offset the higher effort needed for the evaluation of the discrete collision operator [6].

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Optical tomography and the Calderéon problem

Qin Li
(joint work with Ke Chen, Ru-Yu Lai, Andrew Stuart, Gunther Uhlmann, Li Wang)

It is a summary talk on a number of works in the same direction. Optical tomography and the Calderéon problem are medical and mathematical terms for the same problem: photons (high/low energy) are sent into biological tissues and measurements are taken at the surface, and with the incoming and outgoing light intensity data, one can reconstruct optical properties of the bio-tissue. However, it has been longly known that high energy photons give sharp reconstruction while low energy photons give blurred image. We address the reason in this talk. The forward model for photon propagation is the radiative transfer equation, and in small Knudsen number (Kn) regime, photon particles scatter frequently, and mathematically, the radiative transfer equation (RTE) is asymptotically equivalent to the diffusion equation (DE). Correspondingly, the albedo operator that maps incoming to outgoing data for RTE converges to the Dirichlet-to-Neumann (DtN) map for DE. Generally speaking, the inverse problem for the radiative transfer equation is well-posed and well-conditioned, while the inverse problem for the limiting diffusion equation (the Calderéon problem) is severely ill. We try to understand the connection. In the linearized setting (work with Chen and Wang): we study the conditioning of the linearized albedo operator, and it can be proved that the conditioning of the operator blows up algebraically in Kn; In the non linear setting (work with Lai and Uhlmann): we separate singularities of the albedo operator and compare it with X- ray transform, upon which uniqueness is shown. We also show that the difference between the albedo operator and the X-ray solution enlarges exponentially fast in the small Kn regime, which leads to exponential instability. Numerically, both Bayesian formulation and PDE-constraint minimization are applied. Bayesian formulation studies the posterior distribution of the to-be-reconstructed parameter given the collected data and the visualization is done through Markov-chain Monte Carlo (in the work with Newton and Stuart), and the PDE-constraint minimization looks for the smallest mismatch upon Tikhonov regularization (work with Chen).

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Multiscale, Conservative, Implicit Algorithms for the Multispecies Vlasov-Fokker-Planck-Landau Equation

Luis Chacón
(joint work with W. Taitano, A. Simakov)

Kinetic physics in semi-collisional plasmas is governed by the multispecies Vlasov-Fokker-Planck-Landau equation, which is a high-dimensional (three physical+three velocity+time), multiscale set of equations supporting very disparate time and length scales. The Fokker-Planck-Landau [1, 2] collision operator is nonlinear and nonlocal, and features strict conservation invariants in the continuum (mass, momentum, and energy) that must be enforced numerically for asymptotic well-posedness and long-term accuracy. While this equation system has attracted a lot of attention in the literature over the years (see e.g. [3]), a conservative multiscale algorithm capable of spanning temporal and spatial scales has not been available.

We introduce a fully conservative, adaptive, fully implicit algorithm for the multispecies Vlasov-Rosenbluth-Fokker-Planck equation in 1D-2V. The approach achieves exact numerical conservation by nonlinearly enforcing the collision operator symmetries and by enslaving numerical truncation errors in the Vlasov equation [4, 5, 6, 7]. Positivity is enforced by taking advantage of the advection-diffusion structure of the Fokker-Planck collision operator, and by careful advection of the Vlasov equation. The approach features a moving mesh in physical space [7], and an adaptive scheme in velocity space [5, 7] that optimally resolves the distribution function locally regardless of temperature and bulk flow spatio-temporal disparities. Solver-wise, the code relies on optimal multigrid-preconditioned Jacobian-free Newton-Krylov strategies [8], which we have generalized to deal with multiple ion species [4].

Our proposed algorithm has been specifically designed to deal with challenges present in Inertial Confinement Fusion (ICF) capsule simulations. It treats ions kinetically as described above, and electrons as a quasineutral, ambipolar fluid. We will provide a number of numerical examples demonstrating the accuracy and efficiency of the scheme, and we will use it to provide first insights into the importance of kinetic physics in the fusion reactivity of ICF capsules [9].

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A second-order asymptotic-preserving and positivity-preserving exponential Runge-Kutta method for a class of stiff kinetic equations

Jingwei Hu

(joint work with Ruiwen Shu)

We consider the kinetic equations of the form

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon}\mathcal{Q}(f), \quad t \geq 0, \quad x \in \Omega \subset \mathbb{R}^d, \quad v \in \mathbb{R}^d, \tag{1}$$

where $f = f(t, x, v)$ is the one-particle probability density function (PDF) of time t, position x, and particle velocity v. $\mathcal{Q}$ is the collision operator which acts only in the velocity space and models the interactions between particles. Examples of $\mathcal{Q}$ include: the Boltzmann collision operator (a nonlinear integral operator), the BGK operator (a relaxation type operator), the kinetic Fokker-Planck operator (a diffusion type operator), among others. ε is the Knudsen number defined as the ratio of the mean free path and typical length scale. The magnitude of ε indicates the degree of rarefaction of the system. When ε is small, collisions happen very frequently so that the system is close to the fluid regime. In fact, one can derive the compressible Euler equations from (1) as the leading-order asymptotics by sending $\varepsilon \to 0$.

In this work, we introduce a second order time discretization method for the equation (1). The method is asymptotic-preserving (AP) – can capture the Euler limit without numerically resolving the small Knudsen number; and positivity-preserving – can preserve the non-negativity of the solution which is a PDF for arbitrary Knudsen numbers. The method can be applied to a large class of stiff kinetic equations including the collision operators mentioned above. Furthermore, we show that when coupled with suitable spatial discretizations the fully discrete scheme satisfies an entropy-decay property.

The AP schemes have undergone rapid development over the past decades (see [1, 2] for an overview). To handle the kinetic equations of the form (1), essentially one needs some implicit treatment of the stiff collision term. This is possible under the general framework of IMEX schemes [3] or exponential integrators [4].

However, the task becomes highly non-trivial if the positivity is also required even for the second order scheme. In an earlier work [5], we developed an IMEX scheme that is both AP and positivity-preserving. Yet, it relies on a correction step which applies only to the BGK operator. The method developed in this work is more general and is based on a new formulation of the exponential Runge-Kutta method. In a nutshell, it can be viewed as a delicate splitting between the convection and collision steps. Since the scheme is unconventional, it does not fit into any existing category of the AP schemes. Hence an interesting problem is to seek some high order extension of the method.

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Multi-scale control variate methods for uncertainty quantification in kinetic equations

Giacomo Dimarco

(joint work with Lorenzo Pareschi)

Kinetic equations play a major rule in modeling large systems of interacting particles. Uncertainties may be due to various reasons, like lack of knowledge on the microscopic interaction details or incomplete informations at the boundaries. These uncertainties, however, contribute to the curse of dimensionality and the development of efficient numerical methods is a challenge. In this talk, we consider the construction of novel multi-scale methods for such problems which, thanks to a control variate approach, are capable to reduce the variance of standard Monte Carlo techniques.

We consider kinetic equations of the general form

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon} Q(f, f), \tag{1}$$

where $f = f(z, x, v, t)$, $t \geq 0$, $x \in \mathcal{D} \subseteq \mathbb{R}^{d_x}$, $v \in \mathbb{R}^{d_v}$, $d_x, d_v \geq 1$, and $z \in \Omega \subseteq \mathbb{R}^{d_z}$, $d_z \geq 1$, is a random variable. The parameter $\varepsilon > 0$ is the Knudsen number and the particular structure of the interaction term $Q(f, f)$ depends on the kinetic model considered. If $z \in \Omega$ is distributed as $p(z)$ we denote the expected value by

$$\mathbb{E}[f](x, v, t) = \int_\Omega f(z, x, v, t) p(z)\, dz. \tag{2}$$

The standard Monte Carlo estimator, given M independent identically distributed (i.i.d.) samples $f^k(x,v,t)$, $k=1,\dots,M$ of the solution to the Boltzmann equation, reads

$$E_M[f] = \frac{1}{M}\sum_{k=1}^{M} f^k(x,v,t). \tag{3}$$

where a standard estimation, in a suitable norm, is

$$\|\mathbb{E}[f] - E_M[f]\| \leq C\sigma_f M^{-1/2}, \tag{4}$$

with σ_f is the norm of the variance. A variance reduction strategy can be obtained by modifying the Monte Carlo estimator via the following control variate estimator

$$\tilde{E}^{\lambda}_M[f](x,v,t) = \frac{1}{M}\sum_{k=1}^{M} f^k(x,v,t) - \lambda\left(\frac{1}{M}\sum_{k=1}^{M}\tilde{f}^k(x,v,t) - \tilde{\mathbf{f}}(x,v,t)\right). \tag{5}$$

where $\tilde{f}(z,x,v,t)$ is the solution of a simplified model, whose evaluation is significantly cheaper than computing $f(z,x,v,t)$ and where $\tilde{\mathbf{f}}(x,v,t) = \mathbb{E}[f(\cdot,x,v,t)]$ or an opportune accurate approximation of the same quantity. Finally, $\tilde{f}^k(x,v,t)$, $k=1,\dots,M$ are independent identically distributed samples. For example, $\tilde{f}(z,x,v,t)$ can be the solution of the BGK approximation

$$\frac{\partial \tilde{f}}{\partial t} + v\cdot\nabla_x f = \nu(\tilde{f}^{\infty} - \tilde{f}) \tag{6}$$

with ν a relaxation frequency and $\tilde{f}^{\infty}$ the local equilibrium state. For this simplified model, we can assume that the expected value of the control variate $\mathbb{E}[\tilde{f}](v,t)$ can be computed with much higher accuracy at a comparable cost.

Thus, if we now use the estimator

$$\mathbb{E}[f] \approx \mathbb{E}[\tilde{f}] + E_M[f-\tilde{f}] \tag{7}$$

we have an error like

$$\|\mathbb{E}[f](\cdot,x,v,t) - \mathbb{E}[\tilde{f}](\cdot,x,v,t) - E_M[f-\tilde{f}](\cdot,x,v,t)\| \simeq \sigma_{f-\tilde{f}} M^{-1/2},$$

where one can show that $\sigma_{f-\tilde{f}} \ll \sigma_f$ in many situations.

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Primal dual methods for Wasserstein gradient flows

Li Wang
(joint work with Jose Carrillo, Katy Craig, Chaozhen Wei)

We develop a variational method for nonlinear equations with a gradient ow structure. Such equations arise in applications of a wide range, such as porous median flows, material science, animal swarms, and chemotaxis. Our method builds on the JKO framework [1], which evolves the equation as a gradient ow with respect to the Wasserstein metric. We further reformulate the Wasserstein distance into a convex optimization subject to a linear PDE constraint. As a result, we end up with one nested structure of optimization problem with two time scales: one accounts for the inner time scale in the dynamic formulation of Wasserstein distance, and the other is the outer time step used in the JKO scheme. We adopt a recent primal dual three operator splitting scheme [2] with provable convergence to solve the

nal optimization problem. Thanks to the variational structure, our method has a built-in positivity preserving, entropy decreasing properties, and overcomes stability issue due to the strong nonlinearity and degeneracy. Furthermore, our method is massively parallelizable, and thus extremely efficient in high dimensions. Upon discretization of the PDE constraint, we also prove the Γ-convergence of the fully discrete optimization towards the continuum JKO scheme.

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Hypocoercivity and diffusion limit of a finite volume scheme for linear kinetic equation

Thomas Rey
(joint work with Marianne Bessemoulin-Chatard, Maxime Herda)

In this work, we are interested in the asymptotic analysis (large time/small ε) of a finite volume scheme for approximating the solutions to the following scaled, one dimensional linear kinetic equation

$$\begin{cases} \varepsilon \dfrac{\partial f^\varepsilon}{\partial t} + v \dfrac{\partial f^\varepsilon}{\partial x} = \dfrac{1}{\varepsilon} \mathcal{Q}(f^\varepsilon), \\ \\ f^\varepsilon(0,x,v) = f_0(x,v) \geq 0\,, \quad x \in \mathbb{T}, v \in \mathbb{R}, \end{cases} \tag{1}$$

with either Fokker-Planck

$$\mathcal{Q}_{FP}(f)(v) = \partial_v \left(\partial_v f + v f \right),$$

or linearized BGK collision operators

$$\mathcal{Q}_{BGK}(f)(v) = \rho M(v) - f(v), \qquad \rho = \int_{\mathbb{R}} f(v)\,\mathrm{d}v\,.$$

Both collision operators admit a gaussian equilibrium $M(v)$.

When $\varepsilon \to 0$, the first moment in velocity ρ^ε of the solutions to this type of equation converges toward a solution ρ to the classical heat equation

$$\frac{\partial \rho}{\partial t} - \partial_x(D\partial_x \rho) \,=\, 0\,, \quad x \in \mathbb{T}.$$

Moreover, it is known that these models exhibit an *hypocoercive* behavior, namely that there are constants $\kappa > 0$ and $C \geq 1$ such that the solution satisfies

$$\|f^\varepsilon(t) - m_f M\|_{\mathcal{X}} \leq C\|f_0 - m_f M\|_{\mathcal{X}} e^{-\kappa t},$$

where

$$m_f = \iint_{\mathbb{R}\times\mathbb{R}} f_0\,\mathrm{d}x\,\mathrm{d}v\,,$$

and $\mathcal{X}$ is some appropriate functional space. The constants C and κ can sometimes be chosen so that the estimate holds uniformly for small ε.

In the work [1], we propose Finite Volume schemes for solving numerically (1) for both the BGK and Fokker-Planck cases. Thanks to appropriate uniform estimates valid in the fully discrete setting, we establish that the proposed schemes are Asymptotic-Preserving [3]: in the diffusive limit $\varepsilon \to 0$, the kinetic scheme provides a convergent numerical scheme for the limit macroscopic heat equation. Moreover, we adapt to the discrete framework the hypocoercivity method proposed by J. Dolbeault, C. Mouhot and C. Schmeiser in [2] to prove the exponential return to equilibrium of the approximate solution. We obtain decay estimates that can be proved to be uniform in the diffusive limit. In these two aspect, we prove that our numerical schemes mimick the asymptotic properties of the continuous kinetic equation. Finally, we present an efficient implementation of the proposed numerical schemes, and perform numerous numerical simulations assessing their accuracy and efficiency in capturing the correct asymptotic behaviors of the models, as shown in Figures 1 and 2.

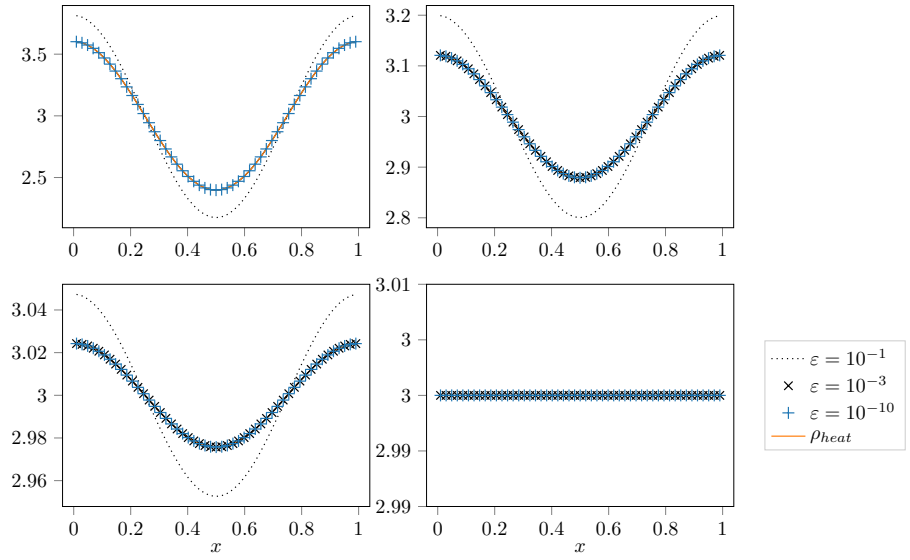

FIGURE 1. Comparison of the approximate solution to the heat equation (solid line) with the approximate densities obtained with the kinetic scheme for different ε, at times $t = 0.1$, 0.2, 0.3 and 10, in the BGK case.

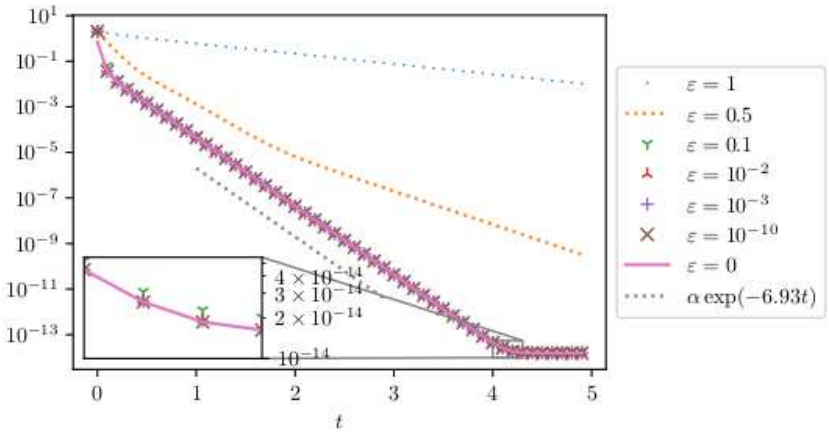

FIGURE 2. Comparison of the rate of convergence of $\|f - m_f\mathcal{M}\|_{L^2(M^{-1})}$ for different values of ε, in the **Fokker-Planck** case, with f_0 uniformly distributed in the $(x, v)-$phase-plane.

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Hierarchical multi-scale control variates methods for kinetic equations with uncertainties

Lorenzo Pareschi
(joint work with Giacomo Dimarco)

Hyperbolic and kinetic equations with random inputs have attracted a lot of attention in the recent years. Most of the literature on kinetic equations is based on the use of Stochastic-Galerkin methods based on on generalized Polynomial Chaos and only recently these problems have been analyzed in the framework of statistical sampling methods based on Monte Carlo (MC) techniques. We refer to [1, 5, 8, 9] for recent results and surveys on numerical methods for kinetic equations and uncertianty quantification.

From a mathematical viewpoint, we consider kinetic equations of the form

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon} Q(f, f),$$

where $f = f(z, x, v, t)$, $t \geq 0$, $x \in \mathcal{D} \subseteq \mathbb{R}^{d_x}$, $v \in \mathbb{R}^{d_v}$, $d_x, d_v \geq 1$, and $z \in \Omega \subseteq \mathbb{R}^{d_z}$, $d_z \geq 1$, is a random variable. The parameter $\varepsilon > 0$ is the Knudsen number and the structure of the interaction term $Q(f, f)$ depends on the kinetic model considered.

Recently in [2, 3] we introduced a control variate technique which takes advantage of the multi-scale nature of the kinetic equation which is capable to strongly accelerate the slow convergence of MC methods. In this talk we consider this class of methods in the case of multiple-control variates. More precisely, first we introduce a standard multiple control variate approach and then consider the construction of recursive multiple control variate methods based on a hierarchical structure. A particular attention is devoted to the case of two control variates. Relations with multi-level Monte Carlo methods [4, 6] and multi-fidelity methods [7] are also discussed.

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Uncertainty Quantification for Kinetic Equations of Collective Behavior

Mattia Zanella

Kinetic equations play a leading role in the modelling of large systems of interacting particles/agents with a proved effectiveness in describing real world phenomena ranging from plasma physics to socioeconomic dynamics. Their formulation has often to deal with physical, or even *social*, forces deduced empirically and of which we have at most statistical information. Hence, to produce realistic descriptions of the underlying phenomena it is of paramount importance to consider the presence of random inputs in the form of uncertain parameters as a structural feature of the kinetic models and to develop suitable numerical methods to capture admissible states of the systems [2, 3, 4].

In this talk we concentrate on stochastic Galerkin methods for the uncertainty quantification in aggregation-diffusion equations with nonlocal flux describing the evolution of the density $f = f(\theta, x, v, t)$, $\theta \in I_\Theta \subseteq \mathbb{R}^{d_\theta}$, $x \in \mathbb{R}^{d_x}$, $v \in \mathbb{R}^{d_v}$, $t \geq 0$, solution of

$$\begin{aligned}\partial_t f(\theta, x, v, t) + v \cdot \nabla_v f(\theta, x, v, t) = \\ \nabla_v \cdot \left[\mathcal{B}[f](\theta, x, v, t) f(\theta, x, v, t) + \nabla_v (D(v) f(\theta, x, v, t))\right],\end{aligned}$$

where

$$\mathcal{B}[f](\theta, x, v, t) = \int_{\mathbb{R}^{d_x}} \int_{\mathbb{R}^{d_v}} P(\theta, x, x_*, v, v_*)(v - v_*) f(\theta, x_*, v_*) dv_* dx_*,$$

$D \geq 0$ is a local diffusion function, and θ takes into account uncertainties in interactions. We develop methods that preserve structural properties of the introduced kinetic model and that are spectrally accurate in the random space [1, 2]. Through a micro-macro decomposition we are able to capture the long time behavior of the solution [2]. Furthermore, we introduce novel Monte Carlo generalized polynomial chaos (MCgPC) methods for which we develop fast algorithms for the evaluations of interactions. In contrast to a direct application of classical uncertainty quantification methods, which typically lead to the loss of positivity, the proposed schemes are capable to achieve high accuracy in the random space without losing nonnegativity of the expected solution. Applications of the developed methods are presented in the context of social and swarming dynamics.

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Fighting the curse of dimensionality in kinetic simulations of plasmas

Antoine Cerfon
(joint work with M. Landreman, L. Ricketson, T. Sánchez-Vizuet, J. Wilkening)

Background - Motivation

The dynamics of hot diffuse plasmas is given by the Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\nabla f + \frac{q}{m}\left(\mathbf{E}+\mathbf{v}\times\mathbf{B}\right)\cdot\nabla_{\mathbf{v}} f = \left(\frac{\partial f}{\partial t}\right)_{\text{coll}} \tag{1}$$

where $f(\mathbf{x},\mathbf{v},t)$ is the phase space distribution function of the plasma at time t, $\mathbf{x}$ is the three-dimensional vector for the position in configuration space, $\mathbf{v}$ is the three-dimensional vector for the position in velocity space, $\mathbf{E}(\mathbf{x})$ and $\mathbf{B}(\mathbf{x})$ are the long range electric and magnetic fields, and $(\partial f/\partial t)_{\text{coll}}$ is a quadratic parabolic collision operator representing binary grazing collisions between charged particles, usually called the Landau-Fokker-Planck collision operator [1]. The long range $\mathbf{E}$ and $\mathbf{B}$ fields are given by Maxwell's equations, in which the charge density $q\int_{\mathbb{R}^3} f d\mathbf{v}$ and current density $q\int_{\mathbb{R}^3}\mathbf{v} f d\mathbf{v}$ of the plasma are sources (often in addition to external sources). Here, we have considered for simplicity a plasma composed of a single species, with particles with charge q and mass m. Solving Eq.(1) numerically is challenging, because 1) the equation is nonlinear; 2) f is a function of seven variables; 3) one is often interested in physical phenomena spanning a wide range of spatial and temporal scales. Even a modest grid resolution for each of the six phase space dimensions pushes the limits of today's largest supercomputers. Properly resolving the dynamics spanning well separated spatial and temporal scales requires simulations whose run times are measured in tens of millions of CPU-hours, which means weeks on the largest supercomputers [2].

The curse of dimensionality, i.e. the fact that the computational complexity of grid based algorithms scales exponentially with the number of dimensions, is a chief reason for the large run times mentioned above. It spurred the development of particle based algorithms, such as the Particle-in-Cell (PIC) scheme, the most popular particle scheme in plasma physics [3]. In standard particle algorithms, the distribution function f is represented in terms of a finite number of discrete macro-particles whose trajectories are given by Newton's laws computed for self-consistent electromagnetic fields. Different particle schemes rely on different methods for computing these fields. In PIC, the charge density and current density are interpolated from the particle positions to a fixed Eulerian grid, where they are used to solve Maxwell's equations. Once the fields are known on the Eulerian grid, they are interpolated back to the particle positions. The advantage of PIC compared to a full grid based solver is that the Eulerian grid in PIC is only

three-dimensional. However, the probabilistic nature of PIC schemes introduces a statistical noise, which slowly decays as the inverse of the square root of the number of simulated particles per cell. In the end, although the curse of dimensionality is reduced, the additional statistical error in PIC leads to a computational complexity which may be worse than for fully grid based solvers [4].

In this presentation, we talked about two recent methods for accelerating the simulations of plasmas described by Eq.(1). For PIC schemes, we studied the benefits of using the sparse grids combination technique [5] to reduce the grid based error *as well as* the statistical noise. For grid based solvers, we proposed efficient representations velocity space in simulations of magnetized confined plasmas, giving high accuracy with few grid points, and thereby alleviating the curse of dimensionality.

Noise reduction in PIC simulations via sparse grids

The sparse grids combination technique [5] was invented to reduce the dependence of computational complexity of PDE solvers on the dimension of the problem. It is clear that it can be applied in PIC codes to reduce the grid based error associated with interpolation as well as the calculation of the electromagnetic fields. Remarkably, we recently showed that the sparse grids combination technique also eliminated the curse of dimensionality for the particle sampling error. Intuitively, this can be understood as follows. The combination technique relies on a hierarchy of grids which each have larger cells than in a regular PIC solver. As a result, for a given number of macro-particles, each sparse grids computation has more particles per cell than a standard PIC simulation, resulting in lower overall noise.

We ran numerical tests for standard problems in plasma physics, which confirmed the significant noise reduction as compared to a standard PIC scheme. This often translated to a smaller computation time for a target accuracy, as well as much smaller memory requirements, since fewer particles had to be tracked. However, for some of the problems we considered, the noise reduction was not sufficient for the sparse PIC algorithm to perform better than standard PIC. That is because the sparse grids combination technique only works effectively for functions with special properties, such as alignment with the axes [7]. When the plasma developed small scale structures which did not align well with our computational grid, the grid based error in sparse PIC led to performance which could be worse than in standard PIC. We are currently exploring adaptive mesh refinement strategies as well as clever mesh constructions which could address this limitation.

Efficient discretizations for the velocity variablesin grid based solvers

The high dependence of the computational complexity of grid based solvers on dimension implies that one should seek the most efficient discretization for each dimension. Accurate solutions of Eq.(1) require an accurate method for the evaluation of velocity integrals, in order to accurately compute the sources for Maxwell's equations, and an accurate method for the computation of velocity

space derivatives, since $(\partial f/\partial t)_{\text{coll}}$ involves second derivatives in velocity space. In that context, pseudo-spectral collocation methods are appealing.

For optimal efficiency, the choice of collocation points may be guided by physics considerations. In magnetically confined plasmas, two elements suggest optimal choices. First, the presence of a strong magnetic field leads to a strong anisotropy in the dynamics, and a convenient coordinate system for the velocity variables is therefore the cylindrical coordinate system $(v_\perp, \varphi, v_\parallel)$, where $v_\parallel$ is the velocity parallel to the magnetic field. Second, even if the collision term $(\partial f/\partial t)_{\text{coll}}$ does not dominate the dynamics in Eq.(1), rare collisions are sufficient to drive a *well confined* plasma to a Maxwell-Boltzmann distribution at the lowest order [1]. Hermite polynomials provide efficient collocation points for integration and differentiation of distribution functions close to Maxwell-Boltzmann distributions for the $v_\parallel$ variable [8], which can be understood from the fact that these polynomials are orthogonal with respect to the weight function $e^{-v_\parallel^2}$ on $\mathbb{R}$. The perpendicular velocity $v_\perp$ is defined on the interval $[0, +\infty)$. Requiring that the polynomials for $\mathbf{v}_\perp$ be orthogonal with respect to the weight function $e^{-v_\perp^2}$ on $\mathbb{R}^+$ leads to the construction of a non-standard family of orthogonal polynomials called Maxwell polynomials [9, 10, 11]. Pseudo-spectral collocation schemes based on these little known Maxwell polynomials were recently implemented for time-independent [12] and time-dependent [13] kinetic equations for confined plasmas with collisions, leading to much improved accuracy as compared to more standard discretization schemes. The schemes have not yet been applied to the general form of Eq.(1), but are used in reduced variants of it [14] (for Maxwell polynomials defined on a finite interval for that particular case). Their merits compared to other methods remain to be tested in the general Boltzmann setting.

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A regularized entropy-based moment method for kinetic equations

Martin Frank
(joint work with Graham W. Alldredge, Cory D. Hauck)

This abstract is based on the paper [5], and most material has been taken from that paper.

Kinetic equations model systems consisting of a large number of particles that interact with each other or with a background medium. These equations evolve the *kinetic density function* $f\colon [0,\infty)\times X\times V\to[0,\infty)$ according to

$$\partial_t f(t,x,v)+v\cdot\nabla_x f(t,x,v)=\mathcal{C}(f(t,x,\cdot))(v). \tag{1}$$

The function f depends on time $t\in[0,\infty)$, position $x\in X\subseteq\mathbf{R}^d$, and a velocity variable $v\in V\subseteq\mathbf{R}^d$. The operator $\mathcal{C}$ introduces the effects of particle collisions; at each x and t, it is an integral operator in v.

The structure of the kinetic equation (1) plays a definitive role in the design of numerical methods. This structure is induced by properties of the collision operator $\mathcal{C}$ and the advection operator $\mathcal{A}=\partial_t+v\cdot\nabla_x$. Key properties are e.g. summarized in [5] and include invariant range of f, conservation, collision invariants, hyperbolicity, entropy dissipation, an H-Theorem, and Galilean invariance.

Moment methods encapsulate the velocity-dependence of f in a vector-valued function

$$u(t,x)=(u_0(t,x),u_1(t,x),\dots,u_{n-1}(t,x))) \tag{2}$$

that approximates the velocity averages of f with respect to the vector of basis functions

$$m(v)=(m_0(v),m_1(v),\dots,m_{n-1}(v))); \tag{3}$$

that is, $u_i(t,x)\simeq\langle m_i f(t,x,\cdot)\rangle$ for all $i\in\{0,1,\dots n-1\}$, where we have introduced the shorthand notation $\langle\cdot\rangle=\int_V\cdot\,dv$ for the velocity integration. The entropy-based moment method is a nonlinear Galerkin discretization in the velocity variable. Th principle underlying this method has been first proposed by Jaynes [1] as a method to select the most likely state of a thermodynamical system having only incomplete information. It has subsequently been developed in [2] and other papers, and has become the main concept of rational extended thermodynamics [3].

The entropy closure has the form

$$\partial_t\langle mF_u\rangle+\nabla_x\cdot\langle vmF_u)\rangle=\langle m\mathcal{C}(F_u)\rangle\,, \tag{4}$$

where $F_u=F_{u(t,x)}(v)$ is an ansatz that approximates the distribution function f and is consistent with the moment vector u. Unlike the trial function in a

traditional (linear) Galerkin method, F_u is not assumed to be a linear combination of the basis functions in m. Instead, in an entropy-based moment method, the ansatz is given by the solution of a constrained optimization problem whose objective function is defined via the kinetic entropy density η. Let

$$\mathcal{H}(g) := \langle \eta(g) \rangle . \tag{5}$$

Then the defining optimization problem is

$$\min_{g \in F(V)} \mathcal{H}(g) \qquad s.t.\ \langle mg \rangle = u, \tag{6}$$

where $u \in \mathbf{R}^n$ and

$$F(V) = \{ g \in L^1(V) : \text{Range}(g) \subseteq D \}. \tag{7}$$

The appeal of the entropy-based approach to closure is that (4) inherits many of the structural properties of the kinetic equation (1). These include conservation, collision invariants, hyperbolicity, entropy dissipation, an H-Theorem, and Galilean invariance. The invariant range of f can be obtained by a suitable choice of the entropy.

Although several algorithms to numerically compute the entropy closure have been designed, each has significant limitations. They require limiters not rigorously shown to preserve accuracy [4], require spatial reconstructions for every node of the quadrature in the v variable, rely on an expensive approximate descriptions of the invariant set (whose concrete description in general remains an open problem), and all second- or higher-order methods so far have been limited to explicit time integration.

We present a new entropy-based moment method for the velocity discretization of kinetic equations. This method is based on a regularization of the optimization problem defining the original entropy-based moment method, and this gives the new method the advantage that the moment vectors of the solution do not have to take on realizable values. We show that this equation still retains many of the properties of the original equations, including hyperbolicity, an entropy-dissipation law, and rotational invariance. The cost of the regularization is mismatch between the moment vector of the solution and that of the ansatz returned by the regularized optimization problem. However, we show how to control this error using the parameter defining the regularization. This suggests that with proper choice of the regularization parameter, the new method can be used to generate accurate solutions of the original entropy-based moment method, and we confirm this with numerical simulations.

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A Fast Spectral Method for the Inelastic Boltzmann Collision Operator

Zheng Ma
(joint work with Jingwei Hu)

In this talk, we present a simple fast Fourier spectral method for the inelastic Boltzmann collision operator, with its application to one of the widely used models of granular gases [1], the inelastic Boltzmann equation with a heating source. Compared to the direct Fourier spectral method [2], our fast algorithm reduces the computational complexity from $O\left(N^6\right)$ to $O\left(MN^4 \log N\right)$ per evaluation of the collision operator in three dimensions, where N is the number of discretization points in each velocity dimension and $M \ll N^2$ is the number of quadrature points used on the unit sphere. We test the numerical accuracy and efficiency of the proposed method in both two dimensional and three dimensional examples, where in the latter case the famous Haff's cooling law for granular flows is successfully recovered.

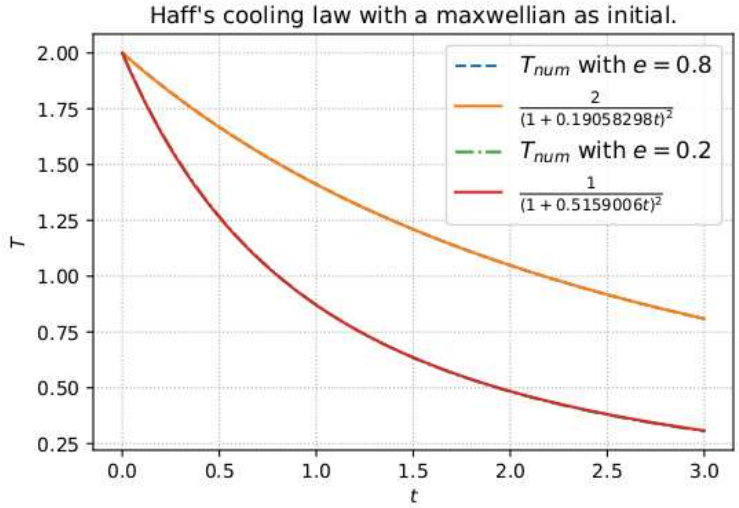

Figure 1. Haff's cooling law by our fast spectral method.

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Phase transitions & fully discrete energy decaying schemes for nonlinear Fokker-Planck equations

José Antonio Carrillo

Phase transitions driven by noise are important to understand the robustness of asymptotic properties for particular solutions of kinetic equations. They encounter applications in many instances of mathematical physics and they have lately received lots of attention due to their importance in mathematical descriptions of large interacting particle systems in life and social sciences. The mean-field limit of these interacting systems leads to kinetic equations with non standard nonlinear nonlocal friction terms such as the Cucker-Smale model or the Vicsek-Fokker-Planck equation in swarming models, see [6, 10] and the references therein for details. Phase transitions driven by noise were obtained in the Vicsek model in [8]. The kinetic locallzed Cucker-Smale model for the evolution of the probability of particles in phase space $f(t, x, v)$ is given by

$$\partial_t f + v\nabla_x f = \nabla_v \cdot \left(\alpha(|v|^2 - 1)vf + (v - u_f)f + D\nabla_v f\right) .$$

where

$$u_f(t, x) = \frac{\int v f(t, x, v)\, dv}{\int f(t, x, v)\, dv}.$$

Here α and D are respectively the self-propulsion force and noise intensities. We have chosen scales such that the alignment force, modelled by the term $(v - u_f)f$, has intensity equal to 1. This model was shown to converge in [4] towards the Vicsek-Fokker-Planck equation on the sphere when the friction term diverges $\alpha \to \infty$. Therefore, one could expect phase transitions driven by noise for the model above. This was already proven in one dimension in [12]. We showed that this is the case in any dimension fo the model above in [2]. More precisely, we proved in the homogeneous setting that for small values of the noise D there are more solutions that the trivial one, while for large values of the noise the trivial symmetric in velocity solution is the unique steady state. In short the bifurcation diagram for velocity of the homogeneous in space stationary state versus noise looks like in the figure above. Phase transitions appear ubiquitously in different models of synchronization and consensus in physics, life and social sciences, see , see [9, 3, 7, 5] and the references therein. Due to the complicated structure of the possible bifurcations for the solutions, it is desirable to have a numerical scheme capable to keep the main properties of the solutions. Structure preserving methods have also been introduced in [5, 11] able to cope with phase transitions in the

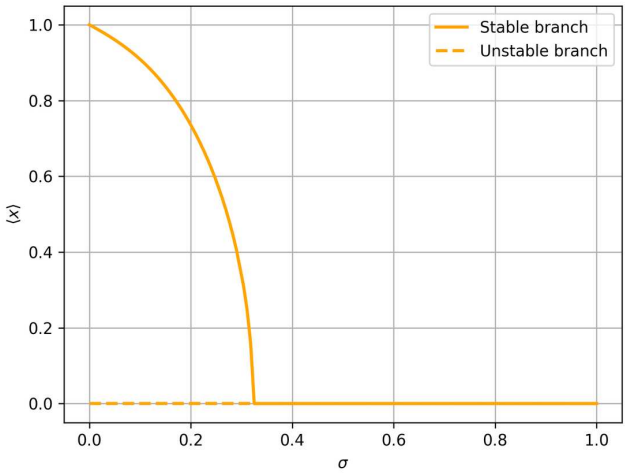

FIGURE 1. Stationary states and phase transition for $\alpha = 1$ in 2D.

Kuramoto models. We presente a new fully discrete scheme positivity preserving and energy decaying for general nonlinear Fokker-Planck equations recently proposed in [1]. In particular, it is applicable to the model introduced above. The scheme is based on a implicit discretization of the diffusion and a suitable treatment of the nonlocality leading to a fully discrete energy decaying property unconditional with respect to the discretization parameters. We also show unconditional positivity of the scheme. These two properties are essential to show that the scheme is well-balanced and that you converge at the discrete level towards discrete stationary states satisfying a discretization of the continuum steady state condition and therefore asymptotically consistent. The new scheme allows to deal with complicated asymptotic phenomena such as metastability and to compute accurately the phase transitions for linear and nonlinear diffusions. Figure above is obtained using this new developed scheme in [1].

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High order conservative Semi-Lagrangian schemes for kinetic equations

Giovanni Russo
(joint work with S. Boscarino, S.B.Yun, S. Cho, J. Qiu, T. Xiong)

The purpose of the talk is to present some techniques for the construction of conservative semi-Lagrangian schemes for the BGK model of the Boltzmann equation and for the Vlasov-Poisson system.

The semi-Lagrangian approach seems natural for the numerical solution of kinetic equations, since the treatment of the transport term along the characteristics allows good accuracy, low numerical diffusion, and avoids the CFL type restriction on the time step typical of hyperbolic systems.

Let us consider the BGK model first. It its simplest form the BGK model can be written as

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\kappa}(M[f] - f)$$

where $f(t, x, v)$ denotes the unknown distribution function in phase space, and, for any distribution f, $M[f]$ denotes the corresponding Maxwellian, which shares with f the the first three moments (i.e. mass, momentum and energy density). Here κ denotes the Knudsen number.

An implicit treatment of the collision term allows handling arbitrarily small Knudsen numbers, with no necessity to resolve small time scales.

Once che equation is discretised on a grid in phase space: $(t = n\Delta t, x_i = i\Delta x, v_j = j\Delta v)$, the simplest first order semi-Lagrangian scheme is obtaiened by integrating the BGK equation along the characteristics, and can be written as

$$f_{ij}^{n+1} = \tilde{f}_{ij} + \frac{\Delta t}{\kappa}(M[f]_{ij}^{n+1} - f_{ij}^{n+1})$$

Here $\tilde{f}_{ij}$ denotes some reconstruction of the distribution function at time t^n, at space location $\tilde{x}_{ij} = x_i - v_j\Delta t$.

The implicit scheme can be explicitly solved, thanks to the conservation properties of the collision operator.

Indeed, the moments of the Maxwellian can be explicitly computed by multyplying the above equation by 1, v_j, and v_j^2, and summing over j: the right hand side vanishes and the moments of f^{n+1} (and therefore the Maxwellian M^{n+1}) can be explicitly computed.

High order accuracy in space is obtained by adopting high order accurate reconstruction of the distribution function at the foot of the characteristics. Such reconstructions may be obtained, for example, by high order essentially non oscillatory (ENO) or Weighted ENO reconstructions. In addition to providing high order accuracy, such reconstructions prevent the formation of spurious oscillations.

High order in time may be obtained by using Runge-Kutta of BDF schemes [1]. Convergence proofs of the schemes have also been obtained both for the standard BGK model [2], and for the elliptical BGK model [3].

Numerical experiments show that such SL schemes have good conservation properties when the solutions are smooth and enough grid-points in velocity are adopted.

With few grid points in velocity space conservation is not guaranteed. The reason for the lack of conservation is identified in the use of continuous Maxwellian in a discrete scheme: the moments of a continuous Maxwellian are obtained from the function f by integration over velocity, while in the method they are computed by approximating the integral by a sum. This lack of conservation can be cured by adopting the discrete Maxwellian introduced by Mieussens [4] in place of the continuous Maxwellian.

It is shown that high order SL schemes based discrete Maxwellian and high order piecewise polynomial reconstructions (with linear weights) are indeed conservative, however they do not prevent formation of spurious oscillations in case of discontinuous solutions. On the other hand, non-linear high order reconstruction such as WENO destroy translation invariance and cause loss of strict conservation. This results in an error in the shock propagation speed for very small Knudsen number, error than does not vanish with grid refinement.

In order to overcome such a problem, a conservative reconstruction is proposed. The reconstruction is based on the computation of a *non-conservative prediction*, obtained by some previously developed SL scheme, followed by a *conservative correction*.

The predicted values are used to compute the flux at cell center, which are then reconstructed at cell edges. Such reconstructed values are adopted to compute the flux at cell edges. Once the fluxes are known, a conservative solution is then computed from them. This approach has already been adopted in the context hyperbolic systems for the construction of conservative schemes in which most of the computation is performed by non-conservative schemes [5]. The conservation property of the scheme is trivially proven, and numerically verified on smooth solutions and moving shocks within machine precision. Conservation is important for the construction of a scheme which is Asymptotic Preserving with respect to the underlying Euler equations as the Knudsen number vanishes.

At variance with standard non conservative SL scheme, the conservative correction is only conditionally stable. The stability of the method is explored in [6]. We have to keep in mind that even if classical SL scheme are unconditionally stable for the treatment of the transport term, a practical stability condition arises for small Knudsen number, since the time step is limited by the CFL condition induced by the underlying Euler limit.

In order to overcome such stability restriction, a second technique is proposed, which is based on a conservative reconstruction, which can be easily constructed once a piecewise essentially non oscillatory polynomial is computed in each cell. Making use of discrete Maxwellians, the technique allows the construction of a very effective conservative SL scheme with no stability restriction (except, of course, the gas dynamic CFL restrictions imposed by the Euler limit).

The conservative reconstruction technique is applied to the Vlasov-Poisson system

$$\frac{\partial f}{\partial t} + v \cdot \nabla f + \frac{e}{m} E \cdot \nabla f = 0,$$

where $f = f(t, x, v)$ is the particle distribution function in phase space, and E is the electric field, self-consistently related to the charge density $\rho = \int f(t, x, v)\, dv - 1$ by the Poisson equation

$$E = -\nabla \Phi, \quad -\nabla^2 \Phi = \rho.$$

The non-conservative predictor is based on the semilagrangian technique developed in [7]: the equation is discretised on a grid in phase space, and the characteristis are integrated *backward* in time from each grid node (x_i, v_j). The corrector is obtained in a conservative finite-difference framework, by reconstructing the fluxes at each cell edge using 1D reconstructions performed dimension-by-dimension.

Because of the presence of the self-consistent electric field, the conservative method is not designed to be rigorously conservative in any of the conserved quantities (such as, for example, mass or energy). However, the conservative scheme obtained in this way presents better conservation properties than previous SL scheme [6].

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