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Classical and Quantum Mechanical Models of Many-Particle Systems

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Abstract. This meeting was focused on recent results on the mathematical analysis of many-particle systems, both classical and quantum-mechanical in scaling regimes such that the methods of kinetic theory can be expected to apply. Thus, the Boltzmann equation is in many ways the central equation investigated in much of the research presented and discussed at this meeting, but the range of topics naturally extended from this center to include other non-linear partial differential and integro-differential equations, especially macroscopic/fluid-dynamical limits of kinetic equations modeling the dynamics of many-particle systems. A significant subset of the talks focused on propagation of chaos, and the validation and derivation of kinetic equations from underlying stochastic particle models in which there has been much progress and activity. Models were discussed with applications not only in physics, but also engineering, and mathematical biology. While there were a number of new participants, especially younger researchers, an interesting aspect of the conference was the number of talks presenting progress that had its origins in the previous meeting in this series held in 2010.

Introduction by the Organisers

The workshop *Classical and Quantum Mechanical models of Many-Particle Systems*, organized by Anton Arnold (Vienna), Eric Carlen (New Brunswick) and Laurent Desvillettes (Cachan) was well attended with 54 participants with broad geographic representation, and a significant number of women (10) and young researchers. We remark that most of the participation slots were actually filled in the first round of invitations. So there were very few replacements (due to a pregnancy, e.g.) or cancellations (due to a recent car accident, e.g.). Two of the

participating post-docs were supported be the NSF-grant for "junior Oberwolfach fellows", and four PhD-students were funded as "Oberwolfach Leibniz graduate students".

32 participants gave a lecture; these mostly were either 30 or 45 minute talks, though on the first days we had two longer survey talks to familiarize young researchers especially with the range of topics that would be covered.

A number of the talks presented progress on issues concerning *propagation of chaos*, a subject that was introduced by Mark Kac in the 1950's, but which has become very active in the last few years, with much significant progress, especially concerning stronger notions of chaos, such as entropic chaos, and our meeting certainly reflected this.

Four talks dealt with this topic. The talk by Einav dealt with the construction of chaotic initial data by novel probabilistic methods. The talk of Hauray dealt with propagation of chaos for Vlasov equations and obtained strong new results for potentials with singularities approaching Coulomb singularities and with propagation of entropic chaos. Mischler, whose recent work with Mouhot has sparked much of the recent activity in the field, gave a talk on propagation of chaos for the two dimension viscous vortex model, again obtaining results concerning entropic chaos. Finally, the talk by Pezzotti concerned propagation of chaos for a quantum kinetic system. Since chaos is an "asymptotic independence" property of a multiparticle system, and since fermions are necessarily correlated due to the Pauli exclusion principle, this is a topic in which there are interesting conceptual issues as well as technical mathematical problems. The report on this work was discussed by a number of participants of the meeting, and future progress will likely come from this. In fact, the meeting was the setting for a number of lively discussion on propagation of chaos, and these discussions will certainly lead to future progress.

The perspective of kinetic theory, and kinetic methods such as entropy-entropy dissipation relations has continued to be useful in the study of a number of evolution equations that do not come from kinetic theory *per se*, but nonetheless have certain structural similarities to kinetic equations. Two example that were the focus of talks at the meeting are the Cahn-Hilliard equation and the Keller-Segel equation. The Cahn-Hilliard equation describes phase segregation in a non-equilibrium statistical mechanical system, and describes the evolution of the *order parameter* as the system organizes itself into a regular free-energy minimizing pattern of regions of low and high values of the order parameter. The talk of Felix Otto presented a significant advance in this direction. This concerned joint work with Maria Westdickenberg in which is was shown for the first time that certain steady state free-energy minimizing transition profiles, describing the phase boundary, are not only non-linearly stable under small perturbation, but also under large perturbations. The methodology is very novel, and will lead to much further progress.

The theme of hypocoercivity was further studied and the concept of degenerate hypocoercivity was discussed in the talk of Salvarani.

Several talks concerned the Keller-Segel equation which describes chemotaxis in a bacteria population. Jean Dolbeault presented remarkable recent work on the sub-critical Keller-Segel model, in which diffusion overwhelms the effects of the chemical attractant, and showed how a sub-critical log-Hardy-Littlewood-Sobolev inequality (and a dual Onofri type inequality) could be used to obtain sharp control of the evolutions. This line of investigation continues to produce interesting new inequalities, as well as new applications. His talk discussed application to crowd behavior and herding.

Another interesting talk on chemotaxis, but this time concerning a linear equation instead of the Keller-Segel equation was presented by Schmeiser. The equation he studied, in joint with Calvez and Raoul, bears a resemblance to the linearized Boltzmann equation. These authors prove the existence of non-trivial steady states, describe them qualitatively, and prove exponential relaxation to them using a novel mixture of *microscopic coercivity* and *macroscopic coercivity*.

There were several other talks on population biological problems in which kinetic theory provided the strategy for the solution, but through a wide range of methods. The talks of Barbaro, Carrillo, Degond, Frouvelle and Motsch all added to the lively development of this theme at the meeting. The talk of Alonso also concerned a biological-like application, but at the cellular level rather than the population level.

The quantum mechanical side of the topic was represented by a number of talks besides that of Pezzotti that has been mentioned above. The talks of Jin, Carles, Lasser and Negulescu all presented results on problems in which quantum mechanics played a central role. It is important to note that these topics were well integrated into the rest of the discussions, and indeed, most of these speakers have also worked on classical kinetic problems, or had collaborated with others at the meeting who presented work on classical kinetic theory. For example, the work presented by Negulescu is joint work with Adami and Hauray, whose work on propagation of chaos was discussed above.

We also wish to mention the talks on topics which have been developed all along the series of Oberwolfach meetings devoted to kinetic equations: the numerical approximation of Boltzmann or Vlasov equation, with a new approach by Bobylev and a talk by Sonnendrücker devoted to realistic plasmas; the variants of Vlasov-Poisson equation, with a talk by Bardos; the qualitative properties of the standard or inelastic Boltzmann equation, represented by Gamba, Kim, Lods, Matthes; the coagulation/fragmentation problems, with a talk by Canizo.

The talk by Fellner illustrated the usefulness of the Oberwolfach meetings devoted to kinetic theory: he indeed presented a result (on reaction-diffusion PDEs) which is a direct application of discussions with Otto in the previous meeting of the series.

New applications of kinetic theory were investigated, as shown by the talk of Lorz on computations of the flows in the human lung in presence of a spray, and by the talk of Moussa on theoretical aspects of the same subject.

Finally, the talks by Brenier, Marahrens and Yu were devoted to PDEs of different types (MHD, elliptic, hyperbolic), in which the mathematical treatment involved methods which have common points with those used in kinetic theory.

Workshop: Classical and Quantum Mechanical Models of Many-Particle Systems

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Abstracts

Viscoelastic fiber networks: Particle model, applications and mechanical properties.

Ricardo Alonso
(joint work with Jennifer Young, Yingda Cheng)

Dynamic, cross-linked, biological fiber networks play major roles in cell and tissue function. They are challenging structures to model due to the vast number of components and the complexity of the interactions within the structure. We present here a particle-based model for fiber networks inspired from flocking theory, where fibers are modeled as point particles and cross-link interactions are modeled via distance-based potential functions. The frictional potential in flocking models takes on the form of a function that decays with increasing inter-particle distance, with the specific form of this function fit for a particular model. The basic flocking model is also modified to include an elastic potential as well as drag from the surrounding fluid. Conceptually, the proposed model can be understood as a distributed *Kelvin-Voigt* particle model. The model is able to simulate behaviors such as strain hardening, viscoelastic creep, stress relaxation, network rupture, and network reformation, which are common characteristics of biological fiber networks. The benefits of this particle model over polymer-based models are that they are computationally simple to implement and can be easily connected to kinetic and continuum-level models.

1. Mathematical Model

Our model consists of a cross-linked system of n fibers evolving in the plane $\mathbb{R}^2$. Each fiber is assigned a length L and mass m, (lumped into two masses $(m/2)$ at its two end points). Each fiber i, $1 \leq i \leq n$, is described by its center of mass position vector $\mathbf{x}_i = \langle x_1, x_2 \rangle \in \mathbb{R}^2$ and center of mass velocity vector $\mathbf{v} = \langle v_1, v_2 \rangle \in \mathbb{R}^2$. Fibers also have an orientation angle denoted by $\theta_i \in [-\pi/2, \pi/2)$ with associated angular velocity $\omega_i \in \mathbb{R}$. In the case of fibers moving in the plane, θ_i is simply the angle between the filament and the horizontal axis.

In principle, free moving fibers follow simple physical laws of fluid dynamics, however, what make them special is their interaction with close neighbors via cross-links. We propose here a modified Cucker-Smale model [2] for the description of the evolution of the fiber network. The equations for the evolution of the center

of mass position $\mathbf{x}_i$ and velocity $\mathbf{v}_i$ for the i^{th}-fiber, $1 \leq i \leq n$ are:

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i \tag{1a}$$

$$m\,\frac{d\mathbf{v}_i}{dt} = -\beta_1\mathbf{v}_i - \frac{\lambda_1}{n}\sum_{j=1}^{n} U_{fr}(r_{ij})(\mathbf{v}_i - \mathbf{v}_j) - \frac{\lambda_2}{n}\sum_{j=1}^{n} U_e'(r_{ij})\frac{\mathbf{x}_i - \mathbf{x}_j}{r_{ij}} + \mathbf{F}(t, \mathbf{x}_i). \tag{1b}$$

The term $\beta_1\mathbf{v}_i$ represents drag forces from an interstitial fluid (for example, cytosol within the cell) on the fiber where β_1 is the drag coefficient, computed using slender body theory. The quantities $U_{fr}(r_{ij})$ and $U_e(r_{ij})$ are the friction and elastic potentials, that are computed based on $r_{ij} := |\mathbf{x}_i - \mathbf{x}_j|$, the distance between fibers i and j. The sum with $U_{fr}(r_{ij})$ should be thought of as representing the total frictional force from the interaction between neighboring fibers that produces a tracking phenomenon. That is, the velocity $\mathbf{v}_i$ tracks a weighted average of its neighboring fibers' velocities. The parameter λ_1 is related to the friction coefficient for the fibers. Intuition tells us that the potential $U_{fr}(r_{ij})$ should be a function that decays as r_{ij} increases, likely vanishing after several fiber lengths L. We propose that $U_{fr}(r_{ij})$ takes the form of a Gaussian:

$$U_{fr}(r_{ij}) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{r_{ij}^2}{2\sigma^2}}$$

where σ is the standard deviation. It is possible to validate this choice by performing several hundred times, with different initial random networks, a fully microscopic simulation of a fiber network and performing a curve-fit through the data. By fully microscopic we mean that each fiber is modeled as a chain of masses and springs allowing fiber deformation. In general we note that σ depends on several of the parameters such as the network's density and fiber length L.

We now return to Equations (1a) and (1b) to look at the third term. The sum with $U_e(r_{ij})$ represents the total elastic force acting on fiber i based on its direct cross-link interactions with other fibers. The idea is that a virtual spring appears between two fibers i and j whenever r_{ij} is below a given threshold distance R. If r_{ij} is greater than R then fibers i and j do not directly interact elastically, and no contribution is made to the sum. This "on-off" switch behavior is reflected in the structure of the $U_e(r_{ij})$ potential function

$$U_e(r_{ij}) = \begin{cases} \frac{1}{2}k_0(r_{ij} - r_0)^2 - \frac{1}{2}k_0(R - r_0)^2 & r_{ij} < R\,, \\ 0 & r_{ij} \geq R\,, \end{cases} \tag{2}$$

where k_0 is the spring constant of a cross-link, and r_0 is the cross-link equilibrium length. This set-up of the elastic interaction model easily allows the model to capture cross-link rupture (if r_{ij} transitions from less than R to greater than R) and cross-link reformation (if r_{ij} transitions from greater than R to less than R). The cross-link interaction distance R depends in general on the geometrical properties of the network constituents such as typical fiber length, fiber orientation

and most importantly the typical biding mechanism length (actin-biding protein typical length). The parameter λ_2 (like λ_1) is an adjustable parameter relating to the elastic behavior of the network. The elastic potential (2) models repulsive, attractive and rupture zones in the cross-link behavior. In Equation (1b), the final term $\mathbf{F}(t, \mathbf{x}_i)$ represents any external forces imposed on the fiber. Conceptually, Equations (1a) and (1b) represent a *Kelvin–Voigt* model between any pair of fibers having a viscosity of value $\frac{\lambda_1}{n} U_{fr}(r_{ij})$ and elasticity of $\frac{\lambda_2}{n} U_e'(r_{ij})$. The equations for the evolution of θ_i and ω_i have a similar structure to Equations (1a) and (1b), namely

$$\frac{d\theta_i}{dt} = \omega_i, \tag{3a}$$

$$I\frac{d\omega_i}{dt} = -\beta_2\omega_i - \frac{\lambda_3}{n}\sum_{j=1}^{n} \bar{U}_{fr}(r_{ij})(\omega_i - \omega_j) + \frac{L}{2}\,\Delta\mathbf{F}(t, \mathbf{x}_i)\cdot(-\sin(\theta_i), \cos(\theta_i)). \tag{3b}$$

The potential $\bar{U}_{fr}$ models, in the same spirit explained previously, the rotational friction forces between neighboring fibers and the fibers tendency to rotate together depending on the forces exerted on them. The parameters I and λ_3 are the inertia of a rigid rod and the rotational friction coefficient respectively.

Finally, we mention that in spite of the fact that only distance based potentials have been used to define system (3), this is not a restriction of the model since more complicated ones are perfectly valid. For instance, angular dynamics of the fibers can strongly influence the translational dynamics by using anisotropic potentials $U\big(r_{ij}, \theta_{ij}\big)$, in this way it is possible to consider anisotropic shear and stronger alignment effects. Furthermore, virtually any microscopic or macroscopic quantity such as fiber velocity, local density or temperature can be included as a valid variable in the potentials. This flexibility could partially resolve local complex effects appearing in shearing like bending or bucking without including more degrees of freedom per fiber.

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Effects of contagion on flocking models

Alethea Barbaro
(joint work with Andrea Bertozzi, Jesús Rosado)

The question of how a crowd moves in emergency situations is not yet well understood. However, many models have been proposed to simulate the dynamics of socially interacting organisms. The Cucker-Smale model [3] and the model by Vicsek et al. [6] are the most well-studied, particularly in the kinetic community. In this talk, we explore how incorporating a variable representing a contagious emotion (such as fear, excitement, etc.) can affect the dynamics of flocking models.

Building from a simple model in the literature in which a particle moves away from a point with a speed proportional to its evolving fear level [5], we incorporate flocking dynamics to allow the particles to change their directional headings. To this end, we begin with a model similar to the Cucker-Smale and Vicsek models, but we also include a variable that tracks the level of emotion that a particle feels. In our model, x_i denotes the position of the ith particle, ω_i denotes its directional heading, and q_i is its emotion level:

$$\begin{cases} \dot{x_i} = q_i \omega_i, \\ \dot{\omega_i} = \nu(Id - \omega_i \otimes \omega_i) \left[\frac{1}{N} \sum_j \frac{q_j \omega_j}{(1+|x_i - x_j|^2)^\beta} \right], \\ \dot{q_i} = \frac{1}{N} \sum_j \frac{(q_j - q_i)}{(1+|x_i - x_j|^2)^\gamma}. \end{cases}$$

Note that the projection $(Id - \omega_i \otimes \omega_i)$ constrains ω_i to the unit sphere if the initial directional headings are on the unit sphere. Without the emotion variable, this would constrain the velocity to the unit sphere, as in continuous-time versions of the Vicsek model [4]. In our model, this projection ensures that the emotional level serves as the speed. In the second equation, the emotion level acts as a weight, determining how much a particle's directional heading affects the directions of those around it. The last equation models the evolution of the emotion variable. The first and third equations, taken together, should call to mind models for flocking in which a particle's speed is determined by averaging the speeds of others nearby [1].

We propose the mesoscopic limit for this system following the ideas in [2], and we offer convergence results for both the directional heading and the emotion variable under certain conditions. We also explore several possible variations on the model, including one where the emotion variable increases dependent on the surrounding particle density, and one where the particles have a cone of vision. When both of these effects are included, the model can be seen to produce a solid, liquid, and crystalline phase depending on the density of particles.

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About the Vlasov-Dirac-Benney Equation

Claude Bardos

This is a report on project initiated with Anne Nouri [2] in progress, in collaboration with Nicolas Besse [1], and also in interactions with other colleagues: Yann Brennier, Bruno Desprès and Rémi Sentis.

It concerns a version of the Vlasov equation where the self interacting Coulomb potential is replaced by a Dirac mass.

$$\begin{aligned} &\partial_t f(t,x,v) + v\partial_x f(t,x,v) - \partial_x \rho_f(t,x)\partial_v f(t,x,v) = 0\,, \\ &\rho_f(t,x) = \int_R f(t,x,v)dv\,. \end{aligned} \tag{1}$$

Hence the instabilities, when they appear, have a much more severe effect than in the classical Vlasov Poisson equation.

Emphasis is put on the relations between the linearized version, near a constant profile

$$G(v) \geq 0 \qquad \int G(v)dv = 1\,; \quad \partial_t f(t,x,v) + v\partial_x f(t,x,v) - \partial_x \rho_f(t,x)G'(v) = 0\,,$$

the full non linear problem and also on natural connections with several other equations of mathematical physics. On the linearized equation one observed that when $G(v)$ has only one maximum the problem is well posed and described by a unitary group of operators in a convenient Hilbert space.

If several maxima are present the Cauchy problem may be only well posed (locally in time) in the class of analytic initial data. It may have no solution when $G(v)$ has more than one maximum.

These results have their counterpart at the level of the non linear problem.

The extreme cases of the one maximum profile are the either when $G(v)$ is the delta distribution or when $G(v)$ has the shape of a plateau. In both cases non linear perturbation of this profile are described by classical equations of fluid mechanics. In the first case it is the equation of an isentropic fluid and in the second it is the Benney equation for water waves (Hence the name Vlasov-Dirac-Benney) and therefore the non linear problem is also (but locally in time) well posed.

Eventually any Vlasov type equation is at least formally (in the sense of Wigner transform and Wigner measure) the limit of a self consistent non linear Schrödinger equation and what is observed in the present talk is that non formal but rigorous convergence results in such limit (cf. [3] and [5]) are in full agreement with the above analysis.

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Landau equation: Monte Carlo methods and some open mathematical problems

Alexander Bobylev
(joint work with Irina Potapenko)

The talk consists of two parts. Its first part is devoted to Monte Carlo (DSMC) methods. The general DSMC method for solving Boltzmann equation for long-range potentials and Landau-Fokker-Planck equation was proposed by Bobylev and Nanbu in 2000 [1] (partly as a development of earlier approach of Nanbu [2] to Coulomb collisions). The methods of [1],[2] were later applied to various model problems of plasma physics, discussed in detail and further developed by several authors (see, for example, [3],[4] and references in [4]). However the general method of [1] was not clearly understood and therefore many authors still use a more complicated original scheme of [2] with reference to [1] just for the formal proof of consistency with the Landau-Fokker-Planck equation. The reason is that the first presentation of the method was done in [1] in too formal and general way. We present in this talk a completely different approach, which leads to basically the same general method, but makes its essence absolutely clear and transparent. The method is explained for the general case of multi-component plasma. We also present some rigorous estimates for accuracy of the method. Finally some numerical results on typical problems of physics of collisional plasma are presented and discussed. The details of the first part of the talk can be found in the recently published paper [5]. The second part of the talk is devoted to a brief discussion of some open mathematical problems for the Landau equation. In particular, these are problems related to (a) consistency of this equation with dynamics, (b) existence of the global in time solution for the spatially homogeneous case, and

(c) some asymptotic problems. It is important to stress that the discussion is related to the true Landau equation which formally corresponds to the Coulomb potential. This is because all other forms of the Landau equation (as a formal limit of the Boltzmann equation for grazing collisions) are not directly connected with physics. On the other hand, the true Landau equation is connected not only with physical systems of charged particles, but also with particles interacting via any bounded smooth potential in the weak coupling limit.

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Dissipative and Quantum incompressible MHD

Yann Brenier

A key equation in ideal incompressible MHD is the induction equation

$$\partial_t B + \nabla \cdot (B \otimes v - v \otimes B) = 0, \quad \nabla \cdot B = 0, \tag{1}$$

where $B = B_t(x) \in \mathbf{R}^d$ is the magnetic field, coupled to the divergence-free fluid velocity $v = v_t(x) \in \mathbf{R}^d$. For simplicity, we consider x in the periodic cube $\mathbf{T}^d$. When v is smooth, this equation just means that a curve $s \to \eta_0(s)$ is an integral line of B_0 [i.e. $\eta_0'(s) = B_0(\eta_0(s))$] if and only if $s \to \eta_t(s) = \xi_t(\eta_0(s))$ is an integral line of B_t [i.e. $\eta_t'(s) = B_t(\eta(s))$], where ξ_t is the diffeomorphism uniquely generated by v through $\partial_t \xi_t(x) = v_t(\xi_t(x))$, $\xi_0(x) = x$. Consequently, the topology of the integral lines of B is preserved by (1) during the evolution. In addition, we easily get by direct calculation and integration by part, for smooth (B, v),

$$\frac{d}{dt}||B_t||^2 + 2((G_t, v_t)) = 0, \quad G_t = \nabla \cdot (B_t \otimes B_t), \tag{2}$$

$||\cdot||$ and $((\cdot,\cdot))$ respectively denoting the norm and the inner product in $L^2(\mathbf{T}^d)$.

Dissipative incompressible MHD. Classical ideal incompressible MHD reads

$$\partial_t v + \nabla \cdot (v \otimes v) + \nabla p = \nabla \cdot (B \otimes B), \quad \nabla \cdot v = 0, \tag{3}$$

for some scalar field $p = p_t(x) \in \mathbf{R}$, coupled to (1). For this model, the total energy $||B_t||^2 + ||v_t||^2$ is (formally) conserved. Some authors (in particular Moffatt [6]) have suggested the following dissipative alternative to ideal MHD, typically

$$(-\triangle)^\sigma v_t = \mathbf{P}G_t, \quad G_t = \nabla \cdot (B_t \otimes B_t) \tag{4}$$

(where $\mathbf{P}$ denotes the L^2projection "Helmholtz" operator onto divergence-free zero-mean vector fields on $\mathbf{T}^d$), which could be called "Darcy" or "Stokes" MHD models as $\sigma = 0$ or $\sigma = 1$. For such models the magnetic energy dissipates according to

$$\frac{d}{dt}||B_t||^2 = -2||v_t||^2. \tag{5}$$

Equilibria, formally obtained as $t \to +\infty$ by cancelling v_∞, correspond to stationary solutions $B_\infty(x)$ to the Euler equations: $\mathbf{P}\nabla \cdot (B_\infty \otimes B_\infty) = 0$, $\nabla \cdot B_\infty = 0$. Because the topology of B_t is preserved by (1), we may hope that B_∞ inherits (at least partly) the topology of B_0. So, Darcy and Stokes MHD models open a way to solving the stationary Euler equations under topological constraints. (See [2] for such topics.) Unfortunately, the corresponding equations (4,1) are very non-linear (cubic in B) non-local degenerate parabolic equations and even the existence of local smooth solutions does not look obvious to us (see [7]). Nevertheless, a "dissipative" formulation can be obtained in the following way (essentially equivalent to the one followed by us in [3]). First, we notice that (4) can be equivalently expressed in variational form

$$2((G_t, z_t - v_t)) + ||v_t||_\sigma^2 - ||z_t||_\sigma^2 \leq 0, \ \forall \ z = z_t(x), \ \text{ smooth s.t. } \nabla \cdot z_t = 0, \tag{6}$$

where $|| \cdot ||_\sigma$ denotes the $\sigma-$ Sobolev semi-norm on $\mathbf{T}^d$. Thus, using (2), both Darcy and Stokes MHD are exactly encoded by (1) together with

$$\frac{d}{dt}||B_t||^2 \ + 2((G_t, z_t)) + ||v_t||_\sigma^2 - ||z_t||_\sigma^2 \ \leq 0, \quad \forall \ z, \ \text{ s.t. } \nabla \cdot z_t = 0. \tag{7}$$

Next, again using (2), we get, for each divergence-free test field $z = z_t(x)$,

$$2((G_t, z_t)) = -((B_t \otimes B_t, \nabla z_t + \nabla z_t^T)),$$

Let us now choose a constant r, depending on z, such that

$$rI_d - \nabla z_t(x) - \nabla z_t(x)^T \geq 0, \ \ \forall (t, x), \tag{8}$$

in the sense of symmetric matrices, where I_d denotes the identity matrix. Thus, (7) becomes

$$(\frac{d}{dt} - r)||B_t||^2 \ + \ ((B_t \otimes B_t, rI_d - \nabla z_t - \nabla z_t^T)) + ||v_t||_\sigma^2 - ||z_t||_\sigma^2 \ \leq 0 \tag{9}$$

for all smooth z and all r satisfying $\nabla \cdot z_t = 0$ and (8). Observe that this inequality only involves convex functionals of B. This leads to the following definition:

We say that $(B, v) \in (C_w^0(\mathbf{R}_+, L^2(\mathbf{T}^d)), L^2(\mathbf{R}_+ \times \mathbf{T}^d))$ is a dissipative solution to the Darcy or Stokes MHD model (with respectively $\sigma = 0$ or $\sigma = 1$), if i) the

induction equation (1) is satisfied in the sense of distributions, ii) (9) is satisfied in integral form from 0 to t for all $t \geq 0$, namely:

(10)

$$||B_t||^2 + \int_0^t [((B_s \otimes B_s, rI_d - \nabla z_s - \nabla z_s^T)) + ||v_s||_\sigma^2 - ||z_s||_\sigma^2] e^{(t-s)r} ds \ \leq ||B_0||^2 e^{tr}$$

for all smooth divergence-free and zero-mean field z and all r satisfying (8).

This definition shares some features of P.-L. Lions "dissipative solutions" to the Euler equations [4] and Ambrosio-Gigli-Savaré solutions of the linear heat equation in general metric spaces [1]. We can prove, for any given initial condition $B_0 \in L^2(\mathbf{T}^d)$, the global existence of a dissipative solution for $d = 2$ if $\sigma = 0$ and for all $d \geq 2$ is $\sigma = 1$. Concerning uniqueness, we are only able to assert that a dissipative solution is unique as long as it is Lipschitz continuous in x. Details are provided in [3].

Quantum MHD. Our proposal for a set of "quantum" incompressible MHD equations is based on Madelung's approach [5] to the Schrödinger equation. We start from Darcy MHD (1,4) as the diffusive counterpart of ideal incompressible MHD (1,3). The magnetic energy is then dissipated according to

$$-\frac{d}{dt}||B_t||^2 = 2||\mathbf{P}\nabla \cdot (B_t \otimes B_t)||^2, \tag{11}$$

where the right-hand side can be viewed as a kind of "Fisher information" for incompressible MHD. Then, our quantum incompressible MHD equations are obtained by adding this Fisher information to the action of ideal incompressible MHD. In the case $d = 3$, using suitable Lagrange multipliers (z, p, q, A), we look for saddle points of

$$\int \{||v_t||^2 - ||B_t||^2 + ((B_t \otimes B_t, \nabla z_t + \nabla z_t^T)) + ||z_t||^2\} dt$$

$$-2\int \{((z_t, \nabla q_t)) + ((v_t, \nabla p_t)) - ((B_t, \partial_t A_t)) + ((B_t \times v_t, \nabla \times A_t))\} dt.$$

Setting $D = \nabla \times A$, the resulting system of equations read

$$\partial_t B + \nabla \times (B \times v) = 0, \quad v = \nabla p + D \times B, \ \ \nabla \cdot v = 0,$$

$$\partial_t D + \nabla \times (D \times v) = \nabla \times ((I - (\nabla z + \nabla z^T))B), \ \ z = \nabla \cdot (B \otimes B) + \nabla q, \ \ \nabla \cdot z = 0.$$

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Exponential convergence to equilibrium for the Becker-Döring equations

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(joint work with Bertrand Lods)

The Becker-Döring equations are a model for the kinetics of first-order phase transitions, applicable to a wide variety of phenomena such as crystallization, vapor condensation, aggregation of lipids or phase separation in alloys. They give the time evolution of the size distribution of clusters of a certain substance through the following infinite system of ordinary differential equations:

$$\frac{\mathrm{d}}{\mathrm{d}t} c_i(t) = W_{i-1}(t) - W_i(t), \qquad i \geq 2, \tag{1a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} c_1(t) = -W_1(t) - \sum_{k=1}^{\infty} W_k(t), \tag{1b}$$

where

$$W_i(t) := a_i\, c_1(t) c_i(t) - b_{i+1}\, c_{i+1}(t) \qquad i \geq 1. \tag{2}$$

Here the unknowns are the real functions $c_i = c_i(t)$ for $i \geq 1$ an integer, and represent the density of clusters of size i at time $t \geq 0$ (this is, clusters composed of i individual particles). They give the size distribution of clusters of the phase which is assumed to have a small total concentration inside a large ambient phase — be it clusters of crystals, lipids, or droplets of water forming in vapor. The numbers a_i, b_i (for $i \geq 1$) are the *coagulation* and *fragmentation coefficients*, respectively, and we always assume them to be strictly positive.

In a recent work we have been able to show that any subcritical solution to the Becker-Döring equations (with suitable moment bounds) converges exponentially fast to the unique steady state with same mass. Our convergence result is quantitative and we show that the rate of exponential decay is governed by the spectral gap for the linearized equation, for which several bounds are provided. This improves the known convergence result by Jabin & Niethammer [6].

Our proof is based on a study of the linearization of the Becker-Döring equations around the equilibrium, for which we show the existence of a spectral gap whose size is well estimated by an explicit expression involving the coagulation and fragmentation coefficients. This implies exponential convergence to equilibrium for the linearized system, which can be extended to the nonlinear equations by means

of techniques developed in the literature on kinetic equations, and particularly on the Boltzmann equation [7, 5].

We observe that the improvement with respect to [6] comes from the use of a different method. The main tool in [6] is an inequality between the free energy (or entropy) H and its production rate D in the spirit of the ones available for the Boltzmann equation [3]. As pointed out in [6], an inequality like $H \leq CD$ for some constant $C > 0$, which would directly imply an exponential convergence to equilibrium, is roughly analogous to a functional log-Sobolev inequality, which is known *not* to hold for a measure with an exponential tail. Since this is the case for the stationary solutions of the Becker-Döring equation, it is believed (though, to our knowledge, not proved) that this inequality does not hold in general for this equation; hence, the following weaker inequality (this is, weaker for small H) is proved in [6]:

$$\frac{H}{|\log H|^2} \leq CD,$$

implying a convergence like $\exp(-Ct^{1/3})$. This obstacle has a parallel in the Boltzmann equation, for which the corresponding inequality (known as Cercignani's conjecture) has been proved not to hold in general, and can be substituted by inequalities like $H^{1+\epsilon} \leq CD$ for $\epsilon > 0$ (we refer to the recent review [3] for the history of the conjecture and a detailed bibliography). However, just as for the space homogeneous [7] and the full Boltzmann equation [5] this can be complemented by the study of the linearized equation in order to show full exponential convergence. By following a parallel reasoning for the Becker-Döring system we can upgrade the convergence rate to exponential.

Hence, our analysis is built around a study of the linearized Becker-Döring equation, which is new to our knowledge. We prove here the existence of a positive spectral gap of the linearized operator $\mathbf{L}$ around an equilibrium $(\mathcal{Q}_i)_{i\geq 1}$, in different spaces:

(1) We provide first a spectral description of $\mathbf{L}$ in a Hilbert space setting. Namely, we shall investigate the spectral properties of the operator $\mathbf{L}$ in the weighted space $\mathcal{H} = \ell^2(\mathcal{Q})$. This analysis is carried out with two (complementary) techniques: on the one hand, under reasonable conditions on the coefficients, one can show that $\mathbf{L}$ is self-adjoint in $\mathcal{H}$ and, resorting to a compactness argument, the existence of a non constructive spectral gap can be shown. On the other hand, using a discrete version of the weighted Hardy's inequality, the positivity of the spectral gap is completely characterized in terms of necessary and sufficient conditions on the coefficients. Moreover, and more importantly, quantitative estimates of this spectral gap are given.

(2) Unfortunately, as it occurs classically for kinetic models, the Hilbert space setting which provides good estimates for the linearized equation is usually not suitable for the nonlinear equation. Thus, inspired by previous results on Navier-Stokes and Boltzmann equation [4, 7], we derive the spectral properties of the linearized operator in a larger weighted ℓ^1 space. We use

for this an abstract result allowing to enlarge the functional space in which the exponential decay of a semigroup holds. This follows recent techniques developed in [5], though we give a self-contained proof simplified in our setting.

It is worth pointing out that our techniques parallel the historical development of the study of the exponential decay of the homogeneous Boltzmann equation.

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On time splitting for NLS in the semiclassical limit

Rémi Carles

Fourier time splitting methods for the nonlinear Schrödinger equation

$$i\partial_t u + \frac{1}{2}\Delta u = f\left(|u|^2\right) u, \quad t \geqslant 0,\ x \in \mathbf{R}^d, \tag{1}$$

with $u : [0,T] \times \mathbf{R}^d \to \mathbf{C}$, and $f : \mathbf{R}_+ \to \mathbf{R}$, consist in solving alternatively

$$i\partial_t u + \frac{1}{2}\Delta u = 0, \tag{2}$$

and

$$i\partial_t u = f\left(|u|^2\right) u. \tag{3}$$

Thanks to the Fourier transform, (2) is solved explicitly, and since the ordinary differential equation (3) turns out to be linear (after one has remarked that $\partial_t(|u|^2) = 0$, since f is real-valued), an explicit formula is available as well. Denoting by X^t the flow associated to (2), and by Y^t the flow associated to (3), Lie splitting method consists in considering $Z_L^{\Delta t} = Y^{\Delta t} \circ X^{\Delta t}$ or $Z_L^{\Delta t} = X^{\Delta t} \circ Y^{\Delta t}$. Higher order Fourier time splitting methods can be considered on the same basis, such as Strang splitting, $Z_S^{\Delta t} = X^{\Delta t/2} \circ Y^{\Delta t} \circ X^{\Delta t/2}$ for instance. The convergence of such methods as the time step Δt goes to zero has been established in

[2] ($d \leqslant 2$) and [6] ($d = 3$). Typically, one has the following result in the cubic defocusing case $f(|u|^2)u = |u|^2 u$. For $u_0 \in H^2(\mathbf{R}^d)$ and all $T > 0$, $\exists C, h_0$ such as if $\Delta t \in]0, h_0]$, $\forall n \in \mathbf{N}$ with $n\Delta t \in [0, T]$,

$$\left\| \left(Z_L^{\Delta t}\right)^n u_0 - u(n\Delta t) \right\|_{L^2} \leqslant C\left(m_2, T\right) \Delta t, \tag{4}$$

with $m_j = \max\limits_{0 \leqslant t \leqslant T} \|u(t)\|_{H^j(\mathbf{R}^d)}$.

In the semiclassical case

$$i\varepsilon \partial_t u^\varepsilon + \frac{\varepsilon^2}{2} \Delta u^\varepsilon = f\left(|u^\varepsilon|^2\right) u^\varepsilon, \quad \varepsilon \to 0, \tag{5}$$

considered in numerical experiments in [1], and motivated by Physics (superfluids, Bose–Einstein condensation), the above error estimate becomes irrelevant. Typically, consider WKB type initial data,

$$u^\varepsilon(0, x) = a_0(x) e^{i\phi_0(x)/\varepsilon}, \tag{6}$$

with a_0 a smooth complex-valued function, and ϕ_0 a smooth real-valued function. It is easy to see that, even in the case $\phi_0 = 0$, the scaling of (5) forces the presence of rapid oscillations in u^ε, which is ε-oscillatory. Therefore, in (4), the factor m_2 behaves like ε^{-2} as $\varepsilon \to 0$, and (4) becomes rather unsatisfactory. To overcome this issue, the idea is that the splitting scheme preserves the WKB form (6), in the following sense: at least for some time, the numerical solution, at time $t_n = n\Delta t$, is of the form

$$u_n^\varepsilon(x) = a_n^\varepsilon(x) e^{i\phi_n^\varepsilon/\varepsilon}, \tag{7}$$

where a_n^ε and ϕ_n^ε must be expected to depend on ε, but remain bounded in Sobolev spaces *uniformly in* $\varepsilon \in (0, 1]$. A similar property holds for the exact solution u^ε: seeking $u^\varepsilon = a^\varepsilon e^{i\phi^\varepsilon/\varepsilon}$, one is led to considering the system

$$\begin{cases} \partial_t \phi^\varepsilon + \dfrac{1}{2} |\nabla \phi^\varepsilon|^2 = -f\left(|a^\varepsilon|^2\right), \\ \partial_t a^\varepsilon + \nabla \phi^\varepsilon \cdot \nabla a^\varepsilon + \dfrac{1}{2} a^\varepsilon \Delta \phi^\varepsilon = i \dfrac{\varepsilon}{2} \Delta a^\varepsilon. \end{cases} \tag{8}$$

Letting $\varepsilon = 0$ in (8), and considering $(v = \nabla\phi, a)$ as a new unknown, one recovers the compressible Euler equation with pressure law related to f, in its symmetric form. For that reason, we must consider time for which the solution to

$$\begin{cases} \partial_t v + v \cdot \nabla v + \nabla f(\rho), \quad v_{|t=0} = \nabla \phi_0, \\ \partial_t \rho + \operatorname{div}(\rho v) = 0, \quad \rho_{|t=0} = |a_0|^2, \end{cases} \tag{9}$$

remains smooth. Then the time splitting scheme applied to (5) preserves the form (7), and amounts to doing time splitting on (8). Unfortunately, by this remark, we see that one has to face a loss of regularity issue, which brings us to make the following assumption:

Assumption 1. *The nonlinearity f is of the form $f(\rho) = K * \rho$, where the kernel K is such that its Fourier transform satisfies:*

- *If* $d \leqslant 2$,
$$\sup_{\xi \in \mathbf{R}^d} (1+|\xi|^2)|\widehat{K}(\xi)| < \infty.$$
- *If* $d \geqslant 3$,
$$\sup_{\xi \in \mathbf{R}^d} |\xi|^2 |\widehat{K}(\xi)| < \infty.$$

Typically, this includes the case of Schrödinger-Poisson system if $d \geqslant 3$, where $f(\rho)$ is given by the Poisson equation

$$\Delta f = \lambda \rho, \quad f, \nabla f \to 0 \text{ as } |x| \to \infty,$$

with $\lambda \in \mathbf{R}$. Our main result is he following.

Theorem 2. *Suppose that* $d \geqslant 1$*, and that* f *satisfies Assumption 1. Let* $(\phi_0, a_0) \in L^\infty(\mathbf{R}^d) \times H^s(\mathbf{R}^d)$ *with* $s > d/2+2$*, and such that* $\nabla \phi_0 \in H^{s+1}(\mathbf{R}^d)$*. Let* $T > 0$ *be such that the solution to* (9) *satisfies* $(v, \rho) \in C([0,T]; H^{s+1} \times H^s)$*. Consider* $u^\varepsilon = S_\varepsilon^t u_0^\varepsilon$ *solution to* (5) *and* u_0^ε *given by* (6)*. There exist* $\varepsilon_0 > 0$ *and* C, c_0 *independent of* $\varepsilon \in (0, \varepsilon_0]$ *such that for all* $\Delta t \in (0, c_0]$*, for all* $n \in \mathbf{N}$ *such that* $t_n = n\Delta t \in [0,T]$*, the following holds:*
1. *There exist* ϕ^ε *and* a^ε *with*

$$\sup_{t \in [0,T]} \left(\|a^\varepsilon(t)\|_{H^s(\mathbf{R}^d)} + \|\nabla \phi^\varepsilon(t)\|_{H^{s+1}(\mathbf{R}^d)} + \|\phi^\varepsilon(t)\|_{L^\infty(\mathbf{R}^d)} \right) \leqslant C, \quad \forall \varepsilon \in (0, \varepsilon_0],$$

such that $u^\varepsilon(t,x) = a^\varepsilon(t,x) e^{i\phi^\varepsilon(t,x)/\varepsilon}$ *for all* $(t,x) \in [0,T] \times \mathbf{R}^d$.
2. *There exist* ϕ_n^ε *and* a_n^ε *with*

$$\|a_n^\varepsilon\|_{H^s(\mathbf{R}^d)} + \|\nabla \phi_n^\varepsilon\|_{H^{s+1}(\mathbf{R}^d)} + \|\phi_n^\varepsilon\|_{L^\infty(\mathbf{R}^d)} \leqslant C, \quad \forall \varepsilon \in (0, \varepsilon_0],$$

such that $(Z_\varepsilon^{\Delta t})^n \left(a_0 e^{i\phi_0/\varepsilon} \right) = a_n^\varepsilon e^{i\phi_n/\varepsilon}$*, and the following error estimate holds:*

$$\|a_n^\varepsilon - a^\varepsilon(t_n)\|_{H^{s-1}} + \|\nabla \phi_n^\varepsilon - \nabla \phi^\varepsilon(t_n)\|_{H^s} + \|\phi_n^\varepsilon - \phi^\varepsilon(t_n)\|_{L^\infty} \leqslant C\Delta t.$$

Note that in the above result, the phase/amplitude representation of the exact solution u^ε and the numerical solution is not unique. This result shows in particular that the splitting solution remains bounded in L^∞, uniformly in ε, in the WKB regime. Also, this result shows that it is possible to approximate the wave function u^ε provided that $\Delta t = o(\varepsilon)$, and to approximate quadratic observables provided that $\Delta t = o(1)$: the time step can be chosen independent of $\varepsilon \in (0,1]$, which agrees with the numerical observations made in [1].

The proof of this result then relies on a general strategy used in [5], a general local error formula for Lie splitting scheme derived in [4], and on various estimates. The details are available in [3].

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Flock solutions for kinetic models: Spatial Shape and Stability

José A. Carrillo

Self-organization and pattern formation are ubiquitous in nature and science, ranging from animal aggregation and biological systems to self-assembly of nanoparticles. The intense research during the last two decades has focused on both individual-based systems and continuum equations. One of the essential features in these models is the non-zero characteristic speed of the individual agents, which has been modelled in different ways. The speed can be assumed to be constant with a direction based on the averages of the neighbours or to be driven by random noise. On the other hand, a large class of models consist of self-propelled particles powered by biological or chemical mechanisms with friction forces, resulting in a preferred characteristic speed. In general, the particles with non-zero equilibrium speed do not form any recognizable patterns, and interactions within the group have to be included to generate interesting spatial configurations. Most of these interaction forces have been taken into account in the combination of three effects: alignment, repulsion, and attraction; also called the "first principles of swarming". The basic mechanisms account for collisional avoidance and comfort regions (repulsion), grouping and socialization (attraction), and mimetic synchronization (alignment).

In the talk, we focused on the cases with velocity-independent interactions. More precisely, by introducing a pairwise symmetric interaction potential $W(x) = U(|x|)$, we consider the two-dimensional model

$$\begin{aligned} \frac{dx_i}{dt} &= v_i\,, \\ \frac{dv_i}{dt} &= \alpha v_i - \beta v_i |v_i|^2 - \sum_{j\neq i} \nabla W(x_i - x_j)\,, \end{aligned} \tag{1}$$

where $x_i, v_i \in \mathbb{R}^2, i = 1, \dots, N$ are the positions and velocities of the individual particles and α, β are effective values for self-propulsion and friction forces.

For this relatively simple system, a variety of patterns are observed, for instance coherent moving flocks and rotating mills. Delta rings, uniform distribution on a circle, were studied thoroughly for power-law like potentials, we refer to [7, 2, 3, 4, 1] for details. While the stability and bifurcation of the ring solutions can be investigated by perturbations methods because of their explicit uniform particle representations on a circle, there are few studies on the more prevalent compact steady solutions, like flocks or mills. The reason lies in the difficulties to solve some complicated integro-differential equations for most of the popular choices of the potential W at the continuum level.

A flock solution of the particle model (1) is a spatial configuration $\hat{x}$ with zero net interaction force on every particle, that translates at a uniform velocity $m_0 \in \mathbb{R}^2$ with $|m_0| = \sqrt{\frac{\alpha}{\beta}}$, hence $(x_i(t), v_i(t)) = (\hat{x_i} - tm_0, m_0)$. We note, that the spatial configuration $\hat{x}$ is a stationary state to the first-order interacting particle system

$$\frac{dx_i}{dt} = -\sum_{j \neq i} \nabla W(x_i - x_j)\,. \tag{2}$$

The continuum description level of (1) leads to a Vlasov like equation obtained as the mean field limit of the particle system (1)

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + \mathrm{div}_v[(\alpha - \beta|v|^2)vf)] - \mathrm{div}_v[(\nabla_x U * \rho)f] = 0, \tag{3}$$

where

$$\rho(t,x) = \int_{\mathbb{R}^2} f(t,x,v)\,dv\,.$$

A flock solution is a particular weak solution to (3) of the form $\bar{\rho}(x - m_0 t)\delta(v - m_0)$ with $|m_0|^2 = \frac{\alpha}{\beta}$ and $\bar{\rho}$ stationary solution of the aggregation equation, i.e., densities satisfying

$$\nabla W * \bar{\rho} = 0 \quad \text{ on the support of } \bar{\rho}\,.$$

The aggregation equation is given by the mean field limit of (2) given by

$$\begin{cases} \frac{\partial \rho}{\partial t} + \mathrm{div}\,(\rho u) = 0 \\ u = -\nabla W * \rho \end{cases}$$

The aggregation equation has a natural associated Liapunov functional defined by

$$E[\rho] = \frac{1}{2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} W(x-y)\;\rho(x)\;\rho(y)\;dx\,dy\,.$$

The first result presented in this talk concerns local minimizers of this interaction energy functional. They are the candidates to be the long time asymptotics of the aggregation equation. We showed in [3] that the dimensionality of the support of local minimizers of the interaction energy $E[\rho]$ depends on the repulsion at the origin of the potential. If the potential is essentially C^2 smooth at the origin, numerical simulations show that there is concentration on points. We show that

the dimension of the support has to be zero if of integer value for smooth potentials. For more singular potentials, we prove a bound from below on the Hausdorff dimension of the support. More precisely, if the potential behaves like the power $-|x|^b/b$ at the origin, with $2-d \leq b < 2$, $d \geq 2$, then the dimension of the support of local minimizers is larger or equal than $2-b$. Therefore, as the potential gets more and more repulsive at the origin the support of the minimizers gets larger and larger in dimension.

The second result presented in the talk is the somehow unexpected deep relation between the linear stability of the flock spatial configuration as steady state for the first-order particle swarming model (2) and the nonlinear stability of the family of associated flock solutions for the particle second-order swarming model (1). The first connection was already found in the linear stability analysis around flock solutions in [1]. There the authors showed that the linearization of (2) around the equilibrium state $\hat{x}$ has a positive eigenvalue if and only if the linearization of (1) around the steady flock solution in the co-moving frame has an eigenvalue with positive real part. Moreover, they show that if the equilibrium state $\hat{x}$ is linearly stable for (2), then the associated flock solution is always linearly unstable due to the presence of a generalized eigenvector associated to the zero eigenvalue of the linearization of the flock solution in the co-moving frame due to symmetries.

The second connection is even deeper, see [6] for details. Assume that the steady state $\hat{x}$ of (2) is linearly asymptotically stable except the obvious symmetries: translations and rotations. Then *the family of flock solutions* associated to $\hat{x}$ is *asymptotically stable* for the dynamics of (1). Here, the asymptotic stability of the family of flock solutions means that any small enough perturbation in (x, v)-space at any time t_0 will, under the dynamics of the system (1), relax towards (likely) another flock solution in the family at an exponential rate as $t \to \infty$. Let us finally emphasize that the most rigorous way of stating our main theorem uses advanced concepts of dynamical systems. Our main theorem can be rephrased as follows: the family of flock solutions to (1) associated to a linearly (except symmetries) asymptotically stable steady state of (2) forms a normally hyperbolic invariant manifold for the system (1) with an empty unstable manifold.

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Collective dynamics and self-organization

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(joint work with E. Carlen, A. Frouvelle, J. G. Liu, S. Motsch, B. Wennberg)

Collective dynamics is observed in systems of a large number of agents moving coherently and forming swarms, flocks, schools, crowds, etc. The cohesion between the agents is maintained by interactions between neighboring agents, such as attraction or alignment. The cohesive interactions are local and the group does not have a definitive leadership. In spite of the local character of the interactions, these systems often exhibit large-scale structures, with time and length scales much larger than the typical agents' interaction scales. This is 'self-organization' or 'emergence' [5].

Systems of a large number of interacting agents (or particles) can be described with various level of details. The models that provide the ultimate level of details are the 'Individual-Based Models (IBM)'. A first level of coarse-graining consists in using a statistical description of the system, *i.e.* replacing the perfect knowledge of each agent's position and state by a probabilistic description. The resulting models are termed 'Kinetic Models' (KM). They can be derived under a statistical independence assumption called 'propagation of chaos'. The ultimate level of coarse-graining is to reduce the system description to a few macroscopic quantities such as density, mean velocity, order parameter, etc, as functions of position and time. The associated models are called 'Continuum models' (CM).

The study of self-organization challenges kinetic theory in several ways. For instance, there are questions about the validity of the propagation of chaos in such systems [1, 2]. Another question is about the passage from KM to CM, which in classical physics systems relies on conservations (conservation of mass, momentum, energy etc.). Biological or social systems do not exhibit simple conservation relations. In [4], we have shown how to derive CM when conservation relations are lacking. Finally, self-organization is intimately linked to phase transitions and hysteresis. Indeed, the same system in different conditions may exhibit different states of organization. We refer the interested reader to the review [3] for a mathematical study of phase transitions in self-propelled particle systems, as well as references therein.

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Sharp asymptotics for the sub-critical Keller-Segel model

Jean Dolbeault

The Keller-Segel model describes aggregation phenomena of amoebae in biology and is used more generally for the description of collective behaviours. In the two-dimensional parabolic-elliptic case, this model has the peculiarity that a simple parameter, the mass, allows to distinguish a diffusion dominated regime from another, super-critical one in which finite time blow-up occurs. In the sub-critical regime, solutions develop a self-similar behaviour for large times which can be described accurately with an appropriate linearization of the model. Better, optimal convergence rates towards the self-similar regime can be established using a relative entropy functional, also called free energy functional.

In a series of papers written with J. Campos, sharp asymptotics for the sub-critical Keller-Segel model have been obtained, based on symmetrization techniques, a functional setting adapted to diffusions with mean field terms, the spectral analysis of the linearized problem and Duhamel type estimates. Noticeably, the linearized (non-local) operator associated with the Keller-Segel model is self-adjoint when the norm is defined by the quadratic form obtained by expanding the solution around a minimizer of the free energy, written in self-similar variables. The component along the subspace associated with the mass parameter has to be discarded by some appropriately chosen orthogonality condition. The two lowest positive eigenvalues are independent of the mass of the solution as long as they does not exceed the critical value, $8\,\pi$, when the model is properly adimensionalized. They can be interpreted in terms of invariances (translations and dilations) associated with self-similar solutions in the original variables. The underlying functional framework is dictated by a sub-critical logarithmic Hardy-Littlewood-Sobolev inequality, and has a dual counterpart, an inequality of Onofri type on the two-dimensional Euclidean space. Interesting results concerning uniqueness results for weak solutions have been recently obtained by F. Giani Egaña and S. Mischler using a technique of enlargement of the functional space for the semigroup spectral gap.

Some of these ideas have been used in a recent paper, written in collaboration with P. Markowich and G. Jankowiak, which is devoted to some crowd motion and herding models and related with models with prevention of overcrowding used for chemotaxis. In an ongoing work, G. Jankowiak is studying the stability of the self-similar solutions of the parabolic-parabolic Keller-Segel model.

Chaos and Entropic Chaos in Kac's Model Without High Moments

Amit Einav
(joint work with Kleber Carraptoso)

Kac model, proposed in 1956 by Marc Kac (see [8]), is a many body stochastic model from which, under certain conditions, a one dimensional caricature of the Boltzmann equation arises as a mean field limit.
In his model Kac considered N indistinguishable particles, with one dimensional velocities, constrained to the energy sphere $\mathbb{S}^{N-1}(\sqrt{N})$, which we will term as 'Kac's sphere'. The evolution equation (or 'master equation') describing the evolution in time of the distribution function of the ensemble is:

$$\frac{\partial}{\partial t}F_N(v_1,\dots,v_N) = -N(I-Q)F_N(v_1,\dots,v_N), \tag{1}$$

where the gain term, Q, is given by

$$QF\left(v_1,\dots,v_N\right) = \frac{\sum_{i<j}}{\pi N(N-1)}\int_0^{2\pi} F\left(v_1,\dots,v_i(\theta),\dots,v_j(\theta),\dots,v_N\right)d\theta,$$

with

$$\begin{aligned} v_i(\theta) &= v_i\cos(\theta) + v_j\sin(\theta),\\ v_j(\theta) &= -v_i\sin(\theta) + v_j\cos(\theta). \end{aligned} \tag{2}$$

Motivated by Boltzmann's 'molecular chaos' assumption, Kac defined the concept of *chaoticity*: A family of distribution functions on Kac's sphere is said to be $f-$chaotic, if there exists a probability density on $\mathbb{R}$, f, such that for any finite k the $k-$th marginal of F_N, $\Pi_k(F_N)$, satisfies

$$\lim_{N\to\infty}\Pi_k(F_N) = f^{\otimes k}, \tag{3}$$

where the limit is in the weak topology induced by bounded continuous functions.

Using a beautiful combinatorial argument, Kac showed that the property of chaoticity *propagates in time* under (1). He showed that the solution $F_N(t)$ is f_t-chaotic, and f_t satisfies the following Boltzmann-like equation:

$$\frac{\partial f}{\partial t}(v,t) = \frac{1}{\pi}\int_{\mathbb{R}}\int_0^{2\pi}\left(f\left(v(\theta)\right)f\left(v_*(\theta)\right) - f\left(v\right)f\left(v_*\right)\right)dv_*d\theta, \tag{4}$$

with initial data f_0, when $F_N(0)$ is f_0-chaotic, and $v(\theta), v_*(\theta)$ are defined as in (2).

The concept of chaoticity, and the newer and more robust one of entropic chaoticity, became a fundamental one in models of many particles. As such, identifying states that are chaotic and investigating their properties became an important part of the study of models that satisfy the propagation of chaos property. On Kac's sphere, due to the equivalence of ensembles principle, one can expect that given a distribution function f on $\mathbb{R}$, a simple way to generate a

chaotic family is to define

$$F_N(v_1,\dots,v_N) = \frac{\Pi_{i=1}^N f(v_i)}{\mathcal{Z}_N\left(f,\sqrt{N}\right)}, \tag{5}$$

where $\mathcal{Z}_N(f,\sqrt{r}) = \int_{\mathbb{S}^{N-1}(r)} \Pi_{i=1}^N f(v_i) d\sigma_r$, with $d\sigma_r$ the uniform probability measure on $\mathbb{S}^{N-1}(r)$, is the so called normalisation function. Families of the form (5) are called *conditioned tensorisation of* f, and were considered by Kac himself in his paper [8]. However, Kac imposed many restrictions on f in order to show that $\mathcal{Z}_N(f,\sqrt{r})$ is indeed concentrated around $r=\sqrt{N}$. This was extended in recent work by Carlen, Carvalho, Le Roux, Loss and Villani (see [2]). In this seminal paper, the authors proved the following:

Theorem 1. *Let f be a distribution function on $\mathbb{R}$ such that $f \in L^p(\mathbb{R})$ for some $p>1$, $\int_{\mathbb{R}} v^2 f(v)dv = 1$ and $\int_{\mathbb{R}} v^4 f(v)dv < \infty$. Then the family of conditioned tensorisation of f is $f-$chaotic.*

The key ingredient of the proof is an asymptotic approximation of $\mathcal{Z}_N(f,\sqrt{r})$, proved by using a local central limit theorem. The fourth moment of f corresponds to the deviation of the random variable V^2 from its mean, which gives rise to a Gaussian concentration of the normalisation function. However, in showing the chaoticity of conditioned tensorisation of f what matters is *not* the exponential concentration about Kac's sphere - but the fact that there is concentration about it. This leads to the current investigation of conditioned tensorisation of f, where f has moments of order 2α with $1<\alpha<2$.

The main result in the presented work, one that relies on a newly found Lévy type local central limit theorem, allowing us to find a new asymptotic expression to the normalisation function, is the following:

Theorem 2. *Let f be a distribution function such that $f \in L^p(\mathbb{R})$ for some $p>1$, $\int_{\mathbb{R}} v^2 f(v)dv = 1$ and let*

$$\nu_f(v) = \int_{-\sqrt{v}}^{\sqrt{v}} y^4 f(y)dy.$$

Then if $\nu_f(v) \underset{v\to\infty}{\sim} Cv^{2-\alpha}$ for some $C>0$ and $1<\alpha<2$ the family of conditioned tensorisation of f is $f-$chaotic.

There is much more to be said about chaoticity, entropic chaoticity, the relation between Kac's model and the trend to equilibrium in the Boltzmann equation and the importance of conditioned tensorisation in that instance. The interested reader is recommended to look at [1, 2, 3, 4, 5, 6, 7, 9] and [10].

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Entropy- and Duality Methods for Systems of Reaction-Diffusion Equations

Klemens Fellner
(joint work with Jose A. Cañizo, Laurent Desvillettes, Evangelos Latos, Stefan Rosenberger, Bao Q. Tang)

The talk presents recent advances in the existence theory (weak and classical) and the large time-behaviour of systems of nonlinear reaction-diffusion equations by applying entropy- and duality methods.

As just one application background the study of such system is motivated by models of *asymmetric stem cell division*, where particular proteins (so-called cell-fate determinants) are localised at the cell-cortex (i.e. the cell boundary) of only one of the two daughter cells during mitosis and subsequently trigger differentiation of only one daughter cell. In Drosophila, SOP stem cells provide a well-studied biological model of asymmetric stem cell division, see e.g. [2, 3, 4]. First mathematical models describing the evolution and localisation of non-phosphorylated and phosphorylated Lgl in SOP stem cells were presented in [5].

The following system (1) formulates a nonlinear mathematical core model, which strongly simplifies the biological model by focussing only on the volume-concentration $u(x,t) \geq 0$ of the phosphorylated Lgl diffusing in the cytoplasm (i.e. in the cell volume) $\Omega \subset \mathbb{R}^N$ and the surface-concentration $v(x,t) \geq 0$ of non-phosphorylated Lgl in the cell cortex diffusing on the sufficiently smooth cell-boundary of $\Gamma := \partial\Omega$ with e.g. $\Gamma \in C^3$. The interface conditions connecting these two concentrations are a nonlinear Robin-type boundary condition for $u(x,t)$ and

a matching reversible reaction source term in the equation for $v(x,t)$:

$$(1)\qquad \begin{cases} u_t - \delta_u \Delta u = 0, & x \in \Omega, t \geq 0, \\ \delta_u \frac{\partial u}{\partial \nu} = -\alpha(k_u u^\alpha - k_v v^\beta), & x \in \Gamma, t \geq 0, \\ v_t - \delta_v \Delta_\Gamma v = \beta(k_u u^\alpha - k_v v^\beta), & x \in \Gamma, t \geq 0, \\ u(0,x) = u_0(x) \geq 0, & x \in \Omega, \\ v(0,x) = v_0(x) \geq 0, & x \in \Gamma. \end{cases}$$

Here, Δ denotes the Laplace operator on Ω, Δ_Γ the Laplace-Beltrami operator on Γ, $\delta_u > 0$ and $\delta_v \geq 0$ diffusion coefficients, $\alpha, \beta \geq 1$ stoichiometric coefficients and $u_0(x) \geq 0$ and $v_0(x) \geq 0$ nonnegative initial concentrations.

The exchange of phosphorylated Lgl $u(x,t)$ and non-phosphorylated Lgl $v(x,t)$ conserves the total mass of Lgl as quantified in the following conservation law (2):

$$(2)\qquad 0 < M = \beta \int_\Omega u_0(x)dx + \alpha \int_\Gamma v_0(x)dS = \beta \int_\Omega u(t,x)dx + \alpha \int_\Gamma v(t,x)dS, \qquad \forall t \geq 0.$$

For system (1), global weak solutions (which for this system can also be bootstrapped into classical solutions by standard techniques) are shown in [6] and a so-called *entropy entropy-dissipation estimate* is derived, which entails exponential convergence to equilibrium with explicitly computable constants and rates.

The basic idea of the entropy method consists in studying the large-time asymptotics of a dissipative PDE model by looking for a nonnegative Lyapunov functional $E(f)$ and its nonnegative dissipation

$$D(f) = -\frac{d}{dt} E(f(t))$$

along the flow of the PDE model, which is well-behaved in the following sense: firstly, all states with $D(f) = 0$, which also satisfy all the involved conservation laws, identify a unique entropy-minimising equilibrium f_∞, i.e.

$$D(f) = 0 \quad \text{and} \quad \text{conservation laws} \iff f = f_\infty,$$

and secondly, there exists an *entropy entropy-dissipation estimate* of the form

$$D(f) \geq \Phi(E(f) - E(f_\infty)), \qquad \Phi(x) \geq 0, \qquad \Phi(x) = 0 \iff x = 0,$$

for some nonnegative function Φ.

In [6] an entropy entropy-dissipation estimate is derived for (1) with general stoichiometric coefficients $\alpha, \beta \geq 1$ in terms of a linear function $\Phi(x) = C(M, \Omega, \Gamma, \alpha, \beta)x$, which entails via a Gronwall argument that the relative entropy $E(u,v) - E(u_\infty, v_\infty) \geq C(\|u(t) - u_\infty\|_{L^1(\Omega)} + \|v(t) - v_\infty\|_{L^1(\Gamma)})$ decays exponentially to zero. The proof of this entropy entropy-dissipation estimate extends previous methods established in [7, 8, 9] using new ideas.

Biological realistic models certainly require larger systems compared to (1). However, the existence of global solutions for general systems of nonlinear reaction-diffusion equations poses still many open questions.

This can be illustrated by the prototypical example of four diffusing species, which react according to the mass-action kinetics $\mathcal{A}_1 + \mathcal{A}_2 \rightleftharpoons \mathcal{A}_3 + \mathcal{A}_4$, i.e.

$$\left\{\begin{array}{l} \partial_t a_1 - d_1\,\Delta_x a_1 = a_3\,a_4 - a_1\,a_2, \\ \partial_t a_2 - d_2\,\Delta_x a_2 = a_3\,a_4 - a_1\,a_2, \\ \partial_t a_3 - d_3\,\Delta_x a_3 = a_1\,a_2 - a_3\,a_4, \\ \partial_t a_4 - d_4\,\Delta_x a_4 = a_1\,a_2 - a_3\,a_4, \end{array}\right. \tag{3}$$

together with the homogeneous Neumann boundary conditions.

It was proven by Goudon and Vasseur in [10] based on an intricate use of De Giorgi's method that whenever d_1, d_2, d_3, $d_4 > 0$, there exists a global smooth solution for dimensions $N = 1, 2$, while in higher space dimensions the existence of classical solutions constitutes an open problem, where the Hausdorff dimension of possible singularities was characterised in [10]. The (technical) criticality of quadratic nonlinearities was underlined by Caputo and Vasseur in [11], where smooth solutions were shown to exist in any dimension for systems with a nonlinearity of power law type which is strictly subquadratic.

Later, in [12] a duality argument in terms of entropy variables was used to show in an elegant way the existence of global L^2-weak solutions in any space dimension also in cases where the nonnegative diffusion coefficients depend on x in such a way that their sum is bounded below by a strictly positive constant.

In [13], an improvement of this duality methods allowed to show global classical solutions in 2D of the prototypical system (3) in a quite much shorter and less technical way than via De Giorgi's method. The key lemma considers a dual problem on a bounded domain $\Omega \subset \mathbb{R}^N$ with $\partial\Omega \in C^{2+\alpha}$ for any $T > 0$,

$$\left\{\begin{array}{lll} \partial_t u - \Delta_x(M(t,x)u) = 0 & \text{on} & \Omega_T, \\ u(0,x) = u_0(x) \in L^p(\Omega) & \text{for} & x \in \Omega, \\ \nabla_x u \cdot \nu(x) = 0 & \text{on} & [0,T] \times \partial\Omega, \end{array}\right.$$

with $0 < a \le M(t,x) \le b < \infty$ for $(t,x) \in \Omega_T$.

Then, in 2D, there exists always an exponent $p' < 2$ such that any weak solution u satisfies $(1/p + 1/p' = 1)$

$$\|u\|_{L^p(\Omega_T)} \le (1 + b\,D_{a,b,p'})\,T^{1/p}\,\|u_0\|_{L^p(\Omega)}, \qquad p \in (2, +\infty),$$

for some constant $D_{a,b,p'}$.

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Local stability of Dirac masses in a kinetic model on a sphere

Amic Frouvelle
(joint work with Pierre Degond, Gaël Raoul)

We consider a kinetic version of a model of alignment of oriented particles: two particles are chosen uniformly at random and collide, their new orientation becoming their previous "mean" orientation.

More formally, for any "precollisional" orientations x_* and x'_*, we are given a jump kernel in the form of a probability measure $K(\cdot, x_*, x'_*)$ for the orientation of the particles after the collision. We suppose that the orientations are unit vectors in $\mathbb{R}^n$, so we consider probability measures in $\mathbb{S}$, the unit sphere of $\mathbb{R}^n$. The model we consider here is the midpoint model: when two colliding particles are not initially antipodal, their final orientation is the middle of the shortest geodesic (an arc of great circle) joining their initial orientations. That is to say

$$K(\cdot, x_*, x'_*) = \delta_{\frac{x_*+x'_*}{\|x_*+x'_*\|}}.$$

When these colliding particles are initially antipodal, we require the probability measure $K(\cdot, x_*, x'_*)$ to be supported in the set of possible midpoints (the corresponding "equator" $\mathbb{S} \cap {x_*}^{\perp}$).

The kinetic model describes the probability measure $\rho(t, \cdot)$ (on $\mathbb{S}$) of finding a particle with a given orientation at time t (we will write ρ instead of $\rho(t, \cdot)$ when no confusion is possible). It evolves in time according to the following partial differential equation:

$$\partial_t \rho(x) = \int_{\mathbb{S}\times\mathbb{S}} K(x, x_*, x'_*)\, d\rho(x_*)\, d\rho(x'_*) - \rho(x). \tag{1}$$

When the space variable is $\mathbb{R}^n$ instead of $\mathbb{S}$, the analogous midpoint model, given by $K(\cdot, x_*, x'_*) = \delta_{\frac{x_*+x'_*}{2}}$, is easier to study, because equation (1) conserves the mass $x_0 = \int x\, d\rho(x)$. We can then easily compute the evolution of the second moment $m_2 = \int |x - x_0|^2\, d\rho(x)$, and get $\frac{d}{dt} m_2 = -\frac{1}{2} m_2$. Therefore, since the Wasserstein distance W_2 between ρ and δ_{x_0} satisfies $W_2(\rho, \delta_{x_0})^2 = m_2$, we get that ρ converges towards a fixed Dirac mass at exponential rate $\frac{1}{4}$.

The aim of this talk is to present a method to circumvent the lack of conservation of mass when the space variable is the unit sphere $\mathbb{S}$. The main theorem is that we still get convergence to a fixed Dirac mass, with the same (optimal) exponential rate of $\frac{1}{4}$, provided the initial condition is sufficiently close to a Dirac mass (in Wasserstein distance):

Theorem 1. *There exist two positive constants C_1, η such that for any solution $\rho \in C(\mathbb{R}_+, \mathcal{P}(\mathbb{S}))$ of (1) with initial condition ρ_0 satisfying $W_2(\rho_0, \delta_{x_0}) < \eta$ for some $x_0 \in \mathbb{S}$, there exists $x_\infty \in \mathbb{S}$ such that*

$$W_2(\rho_t, \delta_{x_\infty}) \leqslant C_1 W_2(\rho_0, \delta_{x_0})\, e^{-\frac{1}{4}t}.$$

The talk will consist in presenting the main ingredients of the proof of this theorem. The first consideration is that we can define an analogous of the second moment under the form of the following energy term:

$$E(\rho) = \int_{\mathbb{S}\times\mathbb{S}} d(x,y)^2\, d\rho(x)\, d\rho(y),$$

where $d(x,y)$ is the geodesic distance on the sphere. This energy would indeed be equal to $2m_2$ if the space variable was $\mathbb{R}^n$, but its definition does not use the notion of center of mass. First of all, there is a link between this energy and the Wasserstein distance W_2 on $\mathcal{P}(\mathbb{S})$:

Lemma 2. *If $\rho \in \mathcal{P}(\mathbb{S})$, we have for any $x \in \mathbb{S}$,*

$$E(\rho) \leqslant 4\, W_2(\rho, \delta_x)^2,$$

and there exists $\bar{x} \in \mathbb{S}$ such that

$$W_2(\rho, \delta_{\bar{x}})^2 \leqslant E(\rho).$$

In that case, for any $\kappa > 0$, we have

$$\int_{\{x\in\mathbb{S};\, d(x,\bar{x})\geqslant\kappa\}} d\rho(x) \leqslant \frac{1}{\kappa^2} E(\rho), \quad \text{and} \quad \int_{\{x\in\mathbb{S};\, d(x,\bar{x})\geqslant\kappa\}} d(x,\bar{x})\, d\rho(x) \leqslant \frac{1}{\kappa} E(\rho).$$

Then we can compute the time derivative of the energy $E(\rho)$. We obtain

$$\frac{1}{2}\frac{d}{dt} E(\rho) = \int_{\mathbb{S}\times\mathbb{S}\times\mathbb{S}} \alpha(x_*, x'_*, y)\, d\rho(x_*)\, d\rho(x'_*)\, d\rho(y). \tag{2}$$

where the function α is defined by

$$\alpha(x_*, x'_*, y) = \int_{\mathbb{S}} \Big[d(x,y)^2 - \frac{d(x_*,y)^2 + d(x'_*,y)^2}{2} \Big] K(x, x_*, x'_*)\, dx.$$

The terms inside the brackets corresponds to three terms of the Apollonius formula, and would be equal to $-\frac{1}{4}d(x_*, x'_*)$ in the case of $\mathbb{R}^n$ instead of $\mathbb{S}$, when x is the midpoint of $[x_*, x'_*]$. Therefore the main ingredients of this study are two estimations of the error in Apollonius formula on the sphere (one local and one global):

Lemma 3. *For any x_*, x'_*, $y \in \mathbb{S}$, we have*

$$\alpha(x_*, x'_*, y) \leqslant -\frac{1}{4}d(x_*, x'_*)^2 + 2\, d(x_*, x'_*) \min\big(d(x_*, y),\, d(x'_*, y)\big).$$

For any $\kappa_1 < \frac{2\pi}{3}$, there exists a positive constant C_1 such that for any $\kappa \leqslant \kappa_1$, for any x_*, x'_*, $y \in \mathbb{S}$ such that $\max\big(d(x_*, y),\, d(x'_*, y),\, d(x_*, x'_*)\big) \leqslant \kappa$, we have

$$\alpha(x_*, x'_*, y) \leqslant -\frac{1}{4}d(x_*, x'_*)^2 + C_1\, \kappa^2\, d(x_*, x'_*)^2.$$

Together with a splitting of the triple integral in (2) following regions provided by Lemma 2, these two estimates allow us to obtain the local decay of the energy with exponential rate $\frac{1}{2}$, provided it is initially sufficiently small. We then control the displacement of $\bar{x}$ provided by Lemma 2 by the same kind of arguments.

A possible extension of Theorem 1 is to replace the sphere by a more general Riemannian manifold. We obtain the same result, provided we have uniform bounds on the radius of injectivity and the sectional curvature of the manifold. Indeed, these bounds allow to use a corollary of Rauch comparison theorem and we obtain the same kind of estimates in the error of Apollonius formula as we have on the unit sphere.

We are also able to study more general models where the particles do not jump exactly at the middle of the geodesic. Under a simple contraction assumption (for the mean square distance to the possible midpoints), we are able to prove the same result of convergence, at the price of a lower exponential rate.

Convergence rates for Boltzmann equation solutions for Coulombic interactions in the grazing collision limit to the Landau equation

Irene M. Gamba

(joint work with Jeffrey R. Haack and Chenglong Zhang)

The homogeneous elastic Boltzmann collision operator in the Coulombic regime is given by

$$(1)\quad Q_b(f,f)(v,t) = \int\!\!\int_{v_*\in\mathbb{R}^3\times\sigma\in S^2} (f(v'_*)f(v') - f(v_*)f(v))\,|u|^{-3} b^\delta_\varepsilon(\cos\theta) d\sigma dv_*$$

$$v' = v + \frac{1}{2}(|u|\sigma - u), \qquad v'_* = v_* - \frac{1}{2}(|u|\sigma - u), \qquad u = v - v_*$$

where $\cos\theta = \hat{u}\cdot\sigma$, $\sigma = \hat{u}'$ is the scattering direction and $b^\delta_\varepsilon(\cos\theta)$ defined below. It is known that the homogeneous Landau operator, given by

$$Q_L(f,f) = \nabla_v \cdot \left(\int_{\mathbb{R}^3} |u|^{\lambda+2} (I - \frac{u\otimes u}{|u|^2})(f(v_*)\nabla_v f(v) - f(v)(\nabla_v f)(v_*)) dv_* \right),$$

can be approximated by grazing collision ε-limit on the angular scattering cross section b^δ_ε. In this lecture we address the rate of such approximation, varying with respect to the parameter δ determining the order of an angular singularity in the scattering cross section.

We first observe that both operators can be written in Fourier space by weighted convolutions

$$\begin{aligned}\widehat{Q}(\zeta) &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \mathcal{F}\{f(v)f(v-u)\}(\zeta) G(u,\zeta) du \\ &= \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \hat{f}(\xi)\hat{f}(\xi-\zeta)\hat{G}(\xi,\zeta) du,\end{aligned}$$

where the weights for the Boltzmann and Landau operators are, respectively,

$$\begin{aligned}G_b(u,\zeta) &= |u|^\lambda \int_{S^2} b^\delta_\varepsilon(\cos\theta)\left(e^{-i\frac{\zeta}{2}\cdot(-u+|u|\sigma)} - 1\right) d\sigma \quad \text{and} \\ G_L(u,\zeta) &= |u|^\lambda \left(4i(u\cdot\zeta) - |u|^2|\zeta^\perp|^2\right) .\end{aligned}$$

Under the assumption of some regularity and decay conditions of the solution to the Boltzmann equation [2], we analytically study the ε-convergence rate of the Fourier transformed Boltzmann collision operator to the Fourier transformed Landau operator in the grazing collisions limit, for a δ-parameter family of singular angular scattering cross section models. The precise statement is as follows.

Let the angular scattering cross section $b^\delta_\varepsilon(\cos\theta)$ satisfy, for $x = \sin(\theta/2)$,

$$\begin{aligned}b^\delta_\varepsilon(\cos\theta)\sin\theta d\theta &= -\frac{1}{2\pi H_\delta(\sin(\varepsilon/2))} b^\delta(\cos\theta)\sin\theta\, 1_{\theta\geq\varepsilon}\, d\theta \\ &= -\frac{4}{2\pi H_\delta(\sin(\varepsilon/2))} \frac{H'_\delta(x)}{x^2} 1_{x\geq\sin(\varepsilon/2)}\, dx.\end{aligned}$$

where the functions $b^\delta(\cos\theta)$ are H_δ determined each other and must satisfy

$$\lim_{\varepsilon\to 0} \frac{1}{H_\delta(\sin(\varepsilon/2))} = 0 \qquad \text{and} \qquad |H_\delta(1)| \leq \infty \quad \text{with} \quad 0 \leq \delta \leq 1\,.$$

When such functions $H_\delta(x)$ take the form

$$H_0(x) = \log x\,, \quad \text{for } \delta = 0 \qquad \text{and} \qquad H_\delta(x) = -\frac{x^{-\delta}}{\delta}, \quad \text{for } 0 < \delta \leq 1\,,$$

the corresponding $b^\delta(\cos\theta)$ is then calculated to yield

$$b^0(\cos\theta) = \frac{1}{\sin^4\frac{\theta}{2}}\,, \quad \text{for } \delta = 0 \qquad \text{and} \qquad b^\delta(\cos\theta) = \frac{1}{\sin^{4+\delta}\frac{\theta}{2}} \quad \text{for} \quad 0 < \delta \leq 1\,,$$

yielding the well known scattering angular singularity of Rutherford potentials (case $\delta = 0$) and beyond.

Remark One may view these H_δ functions as primitives of the angular integration of suitable singular cross section $b^\delta(\cos\theta)$ for grazing collisions, since

$$\int_\varepsilon^\pi b^\delta(\cos\theta)\sin^2(\theta/2)\sin\theta d\theta = 4\int_{\sin(\varepsilon/2)}^1 H'_\delta(x)dx = 4(H(1) - H_\delta(\sin(\varepsilon/2)))\,.$$

With these angular δ-singularity condition, the total collision cross section $b^\delta_\varepsilon(\cos\theta)$ satisfies the *grazing collision limit condition* given by the ε-asymptotic behavior

- $\lim_{\varepsilon\to 0} 2\pi \int_0^\pi b^\delta_\varepsilon(\cos\theta)\sin^2(\theta/2)\,\sin\theta d\theta = \Lambda_0 < \infty, \qquad \Lambda_0 > 0$
- $2\pi \int_0^\pi b^\delta_\varepsilon(\cos\theta)(\sin(\theta/2))^{2+k}\,\sin\theta d\theta \to_{\varepsilon\to 0} 0 \qquad \text{for } \; k > 0\,.$
- $\forall\theta_0 > 0,\; b^\delta_\varepsilon(\cos(\theta)) \to_{\varepsilon\to 0} 0$ uniformly on $\;\theta > \theta_0.$

Under the above conditions the following theorem holds.

Theorem 1. *Assume that any solution $f^\delta_\varepsilon(v,t)$ of (1) satisfies, uniformly in time t,*

$$|\mathcal{F}\{f^\delta_\varepsilon(v) f^\delta_\varepsilon(v-u)\}(\zeta)| \le \frac{A(\zeta)}{1+|u|^{3+a}}, \quad \textit{for } a > 0 \tag{2}$$

with A uniformly bounded by $k(1+|\zeta|)^{-3}$, with k constant.

Then, the rate of convergence of the Boltzmann collision operator with grazing collisions to the Landau collision operator is given by

$$\begin{aligned}\|\frac{\partial}{\partial t}\hat{f}^\delta_\varepsilon(\zeta,t) - \widehat{Q_L}[f^\delta_\varepsilon]\|_{L^\infty} &= \|\widehat{Q_{b^\delta_\varepsilon}}[f^\delta_\varepsilon] - \widehat{Q_L}[f^\delta_\varepsilon]\|_{L^\infty} \\ &\le O\left(\frac{\left|1+(|\log(\sin(\varepsilon/2))|-1)\,1_{\{\delta=1\}}\right|}{|H_\delta(\sin(\varepsilon/2))|}\right) \to_{\varepsilon\to 0} 0\,.\end{aligned}$$

Remarks Assumption (2) relies on the existence of solutions f^δ_ε that have at least third order derivatives in v as well as strong decay in v.

Our results show that the angular singularity which corresponds to the Rutherford scattering cross section ($\delta = 0$) is *the critical singularity* for grazing collision limits for which the Boltzmann operator can approximate the Landau and that ε-convergence rate to the Landau operator is faster for any other value $0 < \delta \le 1$.

To finalize, we presented the formulation of a conservative Spectral-Lagrangian method for computation of the Boltzmann collision operator with anisotropic scattering cross-sections [2]. The method is an extension of the one developed in [3, 4], that uses the weak form of the collision operator to represent the collision operator as a weighted convolution in Fourier space. The scheme for the homogeneous variable hard potentials case is proven to converge to Maxwellians states and error estimates are provided [1]. The numerical method is tested by computing the collision operator with a Rutherford scattering cross section when $\delta = 0$ as well as for $\delta = 1$ and ε-short range cut-off Coulomb potential interaction with $\varepsilon = 10^{-4}$. Results are compared with the numerical solution of the Landau equation, which is independent of both ε and δ. As predicted by the result in the Theorem above, the case for grazing collisions with $\delta = 1$ produces a better approximation to solutions of the Landau equation with respect to $\delta = 0$ (Rutherford case) when measured in

time decay rate of the corresponding entropy functionals. However, the solutions to the Boltzmann equation Rutherford scattering exhibits much faster decay to equilibrium that the ones for the Landau equation. As a last example in collaboration with Chenglong Zhang [5], we applied the Lagrangian based conservative spectral scheme to a multi-component plasma modeled by a system of Landau equations, for a specific example of electro-neutral hydrogen system of electrons and ions for non-isotropic initial states showing their relaxation to the stationary states, conserving the total temperature of the system.

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Propagation of chaos for mean-field Vlasov equations.

Maxime Hauray
(joint work with Pierre-Emmanuel Jabin)

We study the evolution of N particles in dimension d, interacting via a interaction force K. The position and speed of the i-th particle will be denoted respectively by X_i^N and V_i^N, and we will also use the short-cut $Z_i^N = (X_i^N, V_i^N)$. The positions X_i belong to $\mathbb{T}^d$ (for simplicity, but this can be adapted to the case of $\mathbb{R}^d$) and the velocities V_i to $\mathbb{R}^d$.

The evolution of the N particles is driven by the following system of N second order ODEs

$$\forall\, i \le N, \qquad \dot{X}_i^N = V_i^N, \qquad \dot{V}_i^N = -\frac{1}{N}\sum_{j\neq i} K(X_i^N - X_j^N). \tag{1}$$

We introduce the empirical measures on the position-velocity space:

$$\mu_N(t) := \frac{1}{N}\sum_{i=1}^{N} \delta_{Z_i(t)}$$

When $K(0) = 0$, the empirical measures are exact weak solutions of the mean-field Vlasov equation:

$$\partial_t f + v \cdot \partial_x f - \partial_x E(t,x) \cdot \partial_v f = 0, \tag{2}$$
$$E(t,x) = [K * \rho(t)](x) = \int K(x-y) f(t,y,w)\, dydw.$$

It implies that the mean-field limit is equivalent to stability of measure solutions around (strong) solution of equation (2).

A simple case: attractive or repulsive Vlasov-Poisson equation in dimension one. In that case, the interaction force is (we are on the torus).

$$K(x) := -\frac{1}{2} - x \text{ if } x \in \big[-\frac{1}{2}, 0\big), \quad \frac{1}{2} - x \text{ if } x \in \big(0, \frac{1}{2}\big), \quad 0 \text{ if } x = 0, \tag{3}$$

and there is weak-strong stability principle [1]

Assume that f_t is a solution of the Vlasov Poisson equation (2) *with bounded density ρ_t for any time $t \geq 0$. Then for any global measure solution ν to the same equation with finite first order moment in v, we have the following stability estimate*

$$\forall t \in \mathbb{R}^+, \quad W_1(f_t, \nu_t) \leq e^{a(t)} W_1(f_0, \nu_0), \qquad \text{with} \quad a(t) := \sqrt{2}\, t + 8 \int_0^t \|\rho_s\|_\infty \, ds,$$

where W_1 denotes the 1 *Monge-Kantorovitch-Wasserstein distance.*

Mean-field and propagation of chaos around solutions f with bounded density, are simple consequences of that weak-strong stability principle. Propagation of entropic chaos (see [3, Definition 1.3] for a precise definition of that notion) can also be proved, using the preservation of entropy by non-degenerate transport equation.

Soft interaction in dimension three. By this, we understand a force satisfying

$$\exists \alpha < 1, \ \exists\, C > 0, \quad \forall\, x \in \mathbb{R}^d \backslash \{0\}, \quad |F(x)| \leq \frac{C}{|x|^\alpha}, \quad |\nabla F(x)| \leq \frac{C}{|x|^{\alpha+1}}. \tag{4}$$

In that case, we have the following result [2]

Theorem 1. *(Mean-field limit) Assume that* (4) *is satisfied and let $0 < \gamma < 1$. Assume that $f^0 \in L^\infty(\mathbb{R}^6)$ has compact support and total mass one, and denote by f the unique global, bounded, and compactly supported solution of the Vlasov equation* (2) *(that statement is a standard result). Assume that the initial condition $\big(Z_i^N(0)\big)_{i \leq N}$ are such that for each N, there exists a global solution to the N particle system* (1)*, and that the initial empirical distribution μ_N^0 of the particles satisfies:*

i) *For a constant C_∞ independent of N,*

$$\sup_{z \in \mathbb{R}^6} N^\gamma \mu_N^0 \Big(B_6\big(z, N^{-\frac{\gamma}{6}}\big)\Big) \leq C_\infty, \quad \text{and} \quad \|f_0\|_\infty \leq C_\infty;$$

ii) *For some $R_0 > 0$, $\forall N \in \mathbb{N}$, $\quad Supp\, \mu_N^0 \subset B_6(0, R_0)$;*

iii) *for some* $r \in (0, r^*)$ *where* $r^* := \frac{d-1}{1+\alpha}$,

$$\inf_{i \neq j} |(X_i^0, V_i^0) - (X_j^0, V_j^0)| \geq N^{-\gamma(1+r)/6}.$$

Then for any $T > 0$, *there exist constants* C_0, C_1 *such that for* $N \geq e^{C_1 T}$ *the following estimate holds*

$$\forall t \in [0,\ T], \quad W_1(\mu_N(t), f(t)) \leq e^{C_0 t}\Big(W_1(\mu_0, f_0) + 2\, N^{-\frac{\gamma}{6}}\Big). \tag{5}$$

When $\alpha < 1$, and that the initial position-velocity are i.i.d. with law f_0, it can be checked that the conditions *i*) and *iii*) are satisfied and with a probability going to one in the limit $N \to \infty$. This implies the propagation of chaos, for any finite time.

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Semiclassical Computational Methods for Quantum Dynamics with Band-crossings

Shi Jin

We develop semiclassical models and multiscale computational methods for quantum dynamics with non-adiabatic effects. Applications of such methods include surface hopping, Schrödinger equation with periodic potentials, elastic and electromagnetic waves with polarizations, and graphene. We use the Wigner transform to derive these models. The key idea is to evolve the dynamics of the entire Wigner matrices, which contain important non-adiabatic terms, not just the diagonal projections corresponding to the eigenstates of the Hamiltonians.

Regularity of the Boltzmann equation in convex domains

Chanwoo Kim
(joint work with Yan Guo, Daniela Tonon, Ariane Trescases)

The Boltzmann equation is the foundation of the kinetic theory for dilute collections of gas particles:

$$\partial_t F + v \cdot \nabla_x F = Q(F, F), \qquad (t, x, v) \in [0, T] \times \Omega \times \mathbb{R}^3. \tag{1}$$

We denote *a global Maxwellian* $\mu(v) = e^{-|v|^2/2}$, which is an equilibrium state of the Boltzmann equation.

In many physical applications, the gas particles are contained in a bounded domain Ω and the equation must be accompanied by boundary conditions. We

denote the outward normal $n(x)$. The basic types are following three boundary conditions: *On* $x \in \partial\Omega$ *and* $n(x) \cdot v < 0$

1. *Specular reflection* :
$$F(t,x,v) = F(t,x,R_x v), \qquad R_x v = v - 2(n(x)\cdot v)n(x).$$
2. *Bounce-back reflection* : $\quad F(t,x,v) = F(t,x,-v).$
3. *Diffuse reflection* :
$$F(t,x,v) = c_\mu \mu \int_{n(x)\cdot u>0} F(t,x,u)\{n(x)\cdot u\}\mathrm{d}u,$$

for some constant $c_\mu > 0$.

Assume that $\xi : \mathbb{R}^3 \to \mathbb{R}$ is smooth and convex

$$\sum_{i,j} \partial_i\partial_j \xi \eta_i \eta_j \geq C_\xi |\eta|^2, \tag{2}$$

which defines a domain as $\Omega = \{\xi(x) < 0\}$.

We introduce the *kinetic distance*, a distance toward the grazing set γ_0, as

$$\alpha(x,v) := |v\cdot\nabla\xi(x)|^2 - 2\{v\cdot\nabla^2\xi(x)\cdot v\}\xi(x). \tag{3}$$

On the other hand, we have $\partial_t\alpha + v\cdot\nabla_x\alpha \sim |v|\alpha$ unless $\nabla^3\xi \equiv 0$(e.g. Ω is a ball or ellipsoid). Such $|v|$ growth is indeed out of control in our analysis and hence we introduce a strong decay factor $e^{-L\langle v\rangle t}$ with $L \gg_\xi 1$. We are going to use $e^{-L\langle v\rangle t}\alpha$ as a weight of our norm in the main theorem.

We denote by f, $F = \mu + \sqrt{\mu} f$. We also denote $\langle v\rangle = \sqrt{1+|v|^2}$.

Theorem. *Assume* Ω *is convex,* $f_0 \in C^1$, *and the proper compatibility conditions hold. We construct weighted* C^1 *solution* f *in* $[0,T]$ *where the life span* $T = T(||e^{\zeta|v|^2} f_0||_\infty)$ *with* $\zeta > 0$ *as follows.*

1. For the specular reflection, $1 < B < \frac{3}{2}, L \gg 1$

$$||\langle v\rangle^{-1} e^{-L\langle v\rangle t}\alpha^B \partial_x f(t)||_\infty + |||v| e^{-L\langle v\rangle t}\alpha^{B-\frac{1}{2}}\partial_v f(t)||_\infty + ||\partial_t f(t)||_\infty$$
$$\leq C_t\Big\{||\alpha^{B-\frac{1}{2}}\partial_x f_0||_\infty + ||\langle v\rangle^2\alpha^{B-1}\partial_v f_0||_\infty + ||\partial_t f_0||_\infty + P(||e^{\zeta|v|^2} f_0||_\infty)\Big\}.$$

2. For the bounce-back reflection, $L \gg 1$

$$||\langle v\rangle^{-2} e^{-L\langle v\rangle t}\alpha\partial_x f(t)||_\infty + |||v|\langle v\rangle^{-2} e^{-L\langle v\rangle t}\alpha^{\frac{1}{2}}\partial_v f(t)||_\infty + ||e^{\zeta|v|^2}\partial_t f(t)||_\infty$$
$$\leq C_t\Big\{||\langle v\rangle\partial_x f_0||_\infty + ||\partial_v f_0||_\infty + P(||e^{\zeta|v|^2}\partial_t f_0||_\infty) + P(||e^{\zeta|v|^2} f_0||_\infty)\Big\}.$$

3. For the diffuse reflection, $L \gg 1$

$$||e^{-L\langle v\rangle t}\alpha^{\frac{1}{2}}\partial_{t,x,v} f(t)||_\infty \leq C_t\Big\{||\alpha^{\frac{1}{2}}\partial_{t,x,v} f_0||_\infty + P(||e^{\zeta|v|^2} f_0||_\infty)\Big\}.$$

Here P *is some polynomial.*

For the diffuse reflection, we also established $W^{1,p}$ *solution (no weight) for* $1 < p < 2$ *and* $e^{-L\langle v\rangle t}\alpha^B-$*weighted* $W^{1,p}$ *solution* $(\frac{p-2}{2p} < B < \frac{p-1}{2p}, L \gg 1)$ *for* $2 \leq p < \infty$.

Moreover we give sufficient conditions for the non-existence of second derivatives up to the boundary.

Mainly there are three crucial ingredients of the proof. We denote the backward trajectory $[X(s;t,x,v),V(s;t,x,v)]$.

1. The geometric Velocity lemma ([1, 2]):

(4)
$$e^{-C|v||s_1-s_2|}\alpha(X(s_1),V(s_1)) \le \alpha(X(s_2),V(s_2)) \le e^{C|v||s_1-s_2|}\alpha(X(s_1),V(s_1)).$$

2. We established the *dynamical non-local to local estimate*: For $\frac{1}{2} < B < \frac{3}{2}$ and $|v| \sim 1$

$$\int_0^t \int_u \frac{e^{-|V(s)-u|^2}}{|V(s)-u|} \frac{e^{-L\langle v\rangle(t-s)}}{[\alpha(X(s),u)]^B} \;\le\; O(\frac{1}{L})\frac{1}{[\alpha(x,v)]^{B-1/2}}. \tag{5}$$

3. For the specular reflection, we established the following crucial estimates:

$$\begin{aligned} &|\partial_x X(s)| \le C_\xi \frac{|v|e^{|v||t-s|}}{\sqrt{\alpha(x,v)}}, \quad |\partial_v X(s)| \le C_\xi \frac{e^{|v||t-s|}}{|v|}, \\ &|\partial_x V(s)| \le C_\xi \frac{|v|^3 e^{|v||t-s|}}{\alpha(x,v)}, \quad |\partial_x V(s)| \le C_\xi \frac{|v|e^{|v||t-s|}}{\sqrt{\alpha(x,v)}}. \end{aligned} \tag{6}$$

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Wigner type methods for molecular quantum dynamics

Caroline Lasser

(joint work with Wolfgang Gaim, Johannes Keller)

The computation of expectation values for molecular quantum dynamics is numerically challenging due to the high dimension $d \gg 1$ of the configuration space $\mathbb{R}^d$. Starting with the approach of [2], we derive a family of particle methods from the semiclassical Egorov theorem,

$$e^{iHt\varepsilon}\mathrm{op}_\varepsilon(a)e^{-iHt/\varepsilon} = \mathrm{op}_\varepsilon(a\circ\Phi^t) + O(\varepsilon^2), \qquad \varepsilon \to 0,$$

and the relation of Weyl quantized observables $\mathrm{op}_\varepsilon(a)$ to the Wigner function W_ψ,

$$\langle\psi, \mathrm{op}_\varepsilon(a)\psi\rangle_{L^2(\mathbb{R}^d)} = \int_{\mathbb{R}^{2d}} a(z)W_\psi(z)\mathrm{d}z.$$

Thereby we reformulate previous results of M. Pulvirenti [1] in terms of ordinary differential equations, which require higher order derivatives of the observable

function $a : \mathbb{R}^{2d} \to \mathbb{R}$. We discuss the asymptotic accuracy of our approximations with respect to the semiclassical parameter ε, their discretization in time and phase space $\mathbb{R}^{2d}$ and conclude by numerical experiments in up to $d = 18$ dimensions.

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Maxwellian intermediate asymptotics for visco-elastic hard spheres

Bertrand Lods

(joint work with Ricardo J. Alonso)

We are interested here in the long-time behavior of the solution to the free-cooling Boltzmann equation for hard-spheres. Namely, we consider the Cauchy problem

$$\partial_\tau f(\tau, w) = \mathcal{Q}_e(f, f)(\tau, w), \qquad f(\tau = 0, w) = f_0(w) \tag{1}$$

where the initial datum f_0 is a *nonnegative* velocity function. In such a description, the gas is described by the density of particles $f = f(\tau, w) \geq 0$ with velocity $w \in \mathbb{R}^3$ at time $\tau \geq 0$ while the collision operator $\mathcal{Q}_e$ models the interactions of particles by *inelastic binary collisions*. The inelasticity of the collision is measure by the so-called *coefficient of normal restitution* $e \in (0, 1]$. We are mostly interested in the case in which the coefficient of normal restitution is non constant and depends solely on the impact velocity between particles. More precisely, if v and $v_\star$ denote the velocities of two particles before collision, their respective velocities v' and $v'_\star$ after collision are such that

$$\big((v' - v'_\star) \cdot n\big) = -\big((v - v_\star) \cdot n\big)\, e\big(|(v - v_\star) \cdot n|\big) \tag{2}$$

where the unitary vector $n \in \mathbb{S}^2$ determines the impact direction. For the coefficient of normal restitution we shall mainly assume that

(i) The mapping $r \in \mathbb{R}^+ \mapsto e(r) \in (0, 1]$ is absolutely continuous and non-increasing.
(ii) The mapping $r \in \mathbb{R}^+ \mapsto \vartheta_e(r) := r\, e(r)$ is strictly increasing.
(iii) $\lim_{r\to\infty} e(r) = e_0 \in [0, 1)$.
(iv) There exists $\gamma > 0$ and $\mathfrak{a} > 0$ such that

$$e(r) \simeq 1 - \mathfrak{a} r^\gamma \qquad \text{as} \qquad r \simeq 0. \tag{3}$$

Such assumptions are typically met by all the existing physical models in the literature and cover in particular the relevant model of *visco-elastic hard spheres* [3]. Under such assumptions on the coefficient of normal restitution, the homogeneous Boltzmann equation for granular particles (1) is well-posed and, if the initial datum $f_0 \geq 0$ satisfies

$$\int_{\mathbb{R}^3} f_0(w)dw = 1, \quad \int_{\mathbb{R}^3} f_0(w) w dw = 0 \quad \text{and} \quad \int_{\mathbb{R}^3} f_0(w)|w|^3 dw < \infty \tag{4}$$

then existence and uniqueness of a nonnegative solution $f(\tau, w)$ to (1) has been established in [5] and the solution $f(\tau, w)$ satisfies (4) for any $\tau > 0$. The properties of this model depend heavily on the behavior at zero and infinity of the coefficient of normal restitution. Precisely, denoting by

$$\mathcal{E}(\tau) = \int_{\mathbb{R}^3} f(\tau, w)|w|^2 dw$$

the temperature of the solution $f(\tau)$ to (1), the behavior of $\mathcal{E}(\tau)$ for large time has been established rigorously in [1, 2, 5] and one has

$$\mathcal{E}(\tau) \propto (1+\tau)^{-\frac{2}{1+\gamma}} \qquad \gamma \geq 0$$

from which one deduces easily that

$$f(\tau, \cdot) \longrightarrow \delta_0(\cdot) \quad \text{ as } \tau \to \infty$$

where the converge is meant in the space of probability measures on $\mathbb{R}^3$ endowed with the weak-topology [4, 5, 1]. Therefore, it is expected that the solution $f(\tau, w)$ will converge first towards some intermediate asymptotic state $F(\tau, w)$ with $F(\tau, w) \to \delta_0$ as $\tau \to \infty$.

For constant coefficient of normal restitution $e(r) = \alpha \in (0, 1)$ such state is given by a self-similar solution

$$F_\alpha(\tau, w) = K(\tau) G_\alpha\big(V(\tau) w\big)$$

for some suitable scaling functions $K(\tau)$ and $V(\tau)$ independent of α. The profile $G_\alpha(\cdot)$ is precisely a steady state distribution of some rescaled Boltzmann equation and is known as the *homogeneous cooling state*. The existence, exponential rate of convergence towards this state, uniqueness and stability in the weakly inelastic regime can be found in [7]. Notice however that $G_\alpha(\cdot)$ *is not* a Maxwellian distribution.

In the viscoelastic case (i.e. whenever $e(\cdot)$ is non constant and satisfies the above listed properties) the solution $f(\tau, w)$ is also converging towards an intermediate asymptotic state. The difference lies in the fact that such state is *a time dependent Maxwellian distribution*. Precisely,

Theorem 1. *Assume that the coefficient of normal restitution $e(\cdot)$ satisfies the above assumptions $(i) - (iv)$ with $\gamma > 0$ (plus some additional regularity assumptions). Let $f_0 \geq 0$ satisfy the conditions given by* (4) *and*

$$f_0 \in \mathbb{H}^{m_0}_k \,, \qquad \forall\, k \geq 0$$

for some explicit $m_0 \geq 1$. Let $f(\tau, \cdot)$ denote the unique solution to (1) *and let us introduce*

$$\overline{\mathcal{M}_0}(\tau, w) = \left(\frac{1}{2\pi \mathcal{E}(\tau)}\right)^{3/2} \exp\left(-\frac{|w|^2}{2\mathcal{E}(\tau)}\right), \quad \forall \tau > 0 \,,\ w \in \mathbb{R}^3.$$

Then, for any $\tau_0 > 0$ and any $\varepsilon > 0$, there exist $A, B > 0$ such that

$$\|f(\tau, \cdot) - \overline{\mathcal{M}}_0(\tau, \cdot)\|_{L^1} \leq A\, \mathcal{E}(\tau)^{\frac{\gamma}{2(1+\epsilon)}} \leq B\, (1+\tau)^{-\frac{\gamma}{(1+\varepsilon)(1+\gamma)}} \qquad \forall \tau \geq \tau_0. \tag{5}$$

Here, $\mathbb{H}^{m_0}_k$ denotes the weighted Sobolev space defined through the norm

$$\|f\|_{\mathbb{H}^{m_0}_k} = \left(\sum_{|s|\leq m_0} \|\langle\cdot\rangle^{k/2}\partial^s f\|^2_{L^2} \right)^{1/2}$$

where $\langle v\rangle = (1+|v|^2)^{1/2}$ for any $v \in \mathbb{R}^3$.

The proof of the above result is based on the careful study of the Boltzmann equation (1) in rescaled variable. Namely, introduce the (self-similar) rescaled solution $g = g(t,v)$ by

$$f(\tau, w) = V(\tau)^3 g\big(t(\tau), V(\tau)w\big) \tag{6}$$

where $V(\tau) = \sqrt{\dfrac{\mathcal{E}(0)}{\mathcal{E}(\tau)}}$, and $t(\tau) = \int_0^\tau \dfrac{dr}{V(r)}$. Under such a scaling the rescaled solution $g(t,v)$ is such that

$$\int_{\mathbb{R}^3} g(t,v)\,|v|^2 dv = \mathcal{E}(0) \qquad \forall t > 0$$

and the rescaled solution satisfies

$$\partial_t g(t,v) + \xi(t)\nabla_v \cdot \big(v g(t,v)\big) = \mathcal{Q}_{\mathbf{e}_t}\big(g,g\big)(t,v)\,, \quad g(t=0,v) = f_0(v) \tag{7}$$

for some explicit function $\xi(t)$ and some explicit *time-dependent* coefficient of normal restitution

$$\mathbf{e}_t(r) = e(\xi(t)^{1/\gamma} r) \qquad r > 0.$$

Notice that the collision operator appearing in (7) is now depending on time. The idea of proof for Theorem 1 is surprisingly simple and it is based on the study of the *relative entropy* of $g(t,v)$ with respect to the Maxwellian $\mathcal{M}_0(v)$ with same mass momentum and energy of $g(t,v)$ (recall that $g(t,v)$ is of *constant* temperature):

$$\mathcal{H}(t) = \mathcal{H}(g(t)|\mathcal{M}_0) = \int_{\mathbb{R}^3} g(t,v)\,\log\left(\frac{g(t,v)}{\mathcal{M}_0(v)}\right) dv.$$

The convergence of $\mathcal{H}(t)$ towards zero is actually obtained from a well-known estimate between the relative entropy $\mathcal{H}(t)$ and the entropy production associated to the elastic Boltzmann operator established by C. Villani in [8, Theorem 4.1] provided $g(t,\cdot)$ is regular enough and satisfies a uniform lower bound. A particularly technical part of the work consists actually in proving such regularity and lower bound estimates.

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Kinetic models for aerosols and numerical simulations

Alexander Lorz
(joint work with Laurent Boudin, Céline Grandmont, Ayman Moussa)

This work [2] is motivated by aerosol therapies, where drugs are directly delivered to the lung via an aerosol. For these medical applications, it is important to know where aerosol particles impact in the lung

We describe a model for an aerosol, the numerical scheme which we used and the performed numerical tests. Since the aerosol is a fluid-particle mixture, we write equations for both phases first.

Fluid equations. The airflow is classically described by its velocity field $u(t,x) \in \mathbb{R}^3$ and the pressure $p(t,x) \in \mathbb{R}$, where $t \geq 0$ is the time and $x \in \mathbb{R}^3$ is the position. We assume that, in our framework, the air remains a Newtonian incompressible homogeneous fluid. Let us also denote ρ_{air} the air mass density and η the dynamic air viscosity.

In the upper airways, the airflow is governed by the incompressible Navier-Stokes equations:

$$\rho_{\text{air}}[\partial_t u + (u \cdot \nabla_x)u] = -\nabla_x p + \eta \Delta_x u + F, \qquad t \in \mathbb{R}_+, \quad x \in \Omega_t, \tag{1}$$

$$\nabla_x \cdot u = 0, \qquad t \in \mathbb{R}_+, \quad x \in \Omega_t, \tag{2}$$

where F is a vector field representing the forces acting on the fluid (gravity, aerosol retroaction). Moreover, to take into account the fact that the domain itself can move, we consider given time-indexed open sets Ω_t of $\mathbb{R}^3$.

Aerosol equation. An aerosol (or spray) is a set of particles in the airflow. When we focus on aerosols in human airways, the formalism from statistical physics and kinetic theory is especially well fitted. We assume that the aerosol particles are filled with an incompressible fluid very similar to water. The aerosol is then described by a distribution function $f : \mathbb{R}_+ \times \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}_+$. It depends not only on t and x, but also on velocity v.

This distribution function solves the Vlasov equation, i.e.

$$\partial_t f + v \cdot \nabla_x f + \nabla_v \cdot (af) = 0, \tag{3}$$

where $a(t, x, v)$ is the acceleration field acting on the aerosol.

The system (1)–(3) is supplied with suitable boundary conditions that we do not state here for the sake of simplicity.

Interaction between the fluid and the aerosol. We assume, as it is classical in fluid mechanics, that both coupling terms a and F mainly model a drag force between the fluid and the aerosol

$$a(t, x, v) = \frac{\pi r^2}{8m} \rho_{\text{air}} C_{\text{D}} |u(t, x) - v|(u(t, x) - v). \tag{4}$$

The simplest case is to use Stokes' law

$$a(t, x, v) = \frac{6\pi\eta r}{m} (u(t, x) - v),$$

but in our model a more complicated form of a was used [5]. Conversely, F is the force field exerted by the aerosol on the air, that is

$$F(t, x) = -m \int_{\mathbb{R}^3} f(t, x, v)\, a(t, x, v)\, dv, \tag{5}$$

for any t and x.

The nonlinearity in the Navier-Stokes equations and the strong coupling between Vlasov and Navier-Stokes equations are the two major difficulties in the full system (1)–(5) from both mathematical [1] and numerical viewpoints.

The aerosol is computed with a particle-in-cell (PIC) method, and the fluid using the arbitrary Lagrangian-Eulerian (ALE) form, primarily used in [3, 4] and the finite element method. The difficulty of this scheme mainly lies in the coupling between (1) and (3) through (5).

Unlike the finite element method, the particle method does not provide an approximation of f on the mesh nodes. So the distribution function is computed as a weighted sum of Dirac masses in the positions and velocities of the numerical particles.

To improve and validate the scheme as well as the C++ code we study various test cases. In a fixed domain, we compare with explicit solutions for the particle trajectories. Moreover, we check numerical stability with respect to mesh refinement, time step and we verify stability when perturbing the initial location of the particles. Furthermore, we study the influence of the mesh size on the position where the particles hit the boundary. Moreover, in a fixed domain we investigate the influence of the aerosol particles on the airflow (retroaction force). In a moving domain, we compare with non-trivial explicit solutions for the fluid.

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Regularity for elliptic equations with i. i. d. coefficients

Daniel Marahrens
(joint work with Felix Otto)

In this talk, we consider the uniformly elliptic *discrete difference* equation

$$\nabla^* a(x)\nabla u(x) = f(x) \qquad \forall x \in \mathbb{Z}^d, \tag{1}$$

where

$$\nabla u(x) = (\nabla_1 u(x), \dots \nabla_d u(x)), \qquad \nabla_i u(x) = u(x+e_i) - u(x),$$
$$\nabla^* \xi(x) = \sum_{i=1}^{d} \nabla_i^* \xi_i(x), \qquad \nabla_i^* \xi_i(x) = \xi_i(x-e_i) - \xi(x),$$

denote the gradient of $u : \mathbb{Z}^d \to \mathbb{R}$ and the (negative) divergence of $\xi : \mathbb{Z}^d \to \mathbb{R}^d$, respectively. We assume that the coefficient field $a : \mathbb{Z}^d \to \mathbb{R}^{d\times d}$ is *diagonal and uniformly elliptic* with ellipticity contrast $\lambda > 0$, i.e. $a_{ii}(x) \in [\lambda, 1]$ for $i = 1, \dots, d$. Let Ω denote the space of diagonal and uniformly elliptic coefficient fields. In this case, the well-known result due to De Giorgi on Hölder-regularity of elliptic equations yields that there exists an $\alpha_0 = \alpha_0(d, \lambda) > 0$ such that

$$\forall a \in \Omega, \ \ \forall R < \infty : \quad \sup_u \frac{\sup_{x:|x|\le R} \frac{|u(x)-u(0)|}{|x|^{\alpha_0}}}{\frac{1}{R^{\alpha_0}} \sup_{x:|x|\le R} |u(x)|} \le C(d, \lambda),$$

where the outer supremum (over u) is taken over all solutions to $\nabla^* a(x)\nabla u(x) = 0$ in the ball B_{2R} of radius $2R$, see [1, Proposition 6.2] for a discrete setting. This result cannot be improved upon in the sense that there exist counter-examples with $\alpha_0(d, \lambda) \to 0$ as $\lambda \to 0$ (at least in the continuum setting and which should in principle extend to the discrete setting).

On the other hand, in stochastic homogenization (and presumably in real-world applications), the coefficient field $a : \mathbb{Z}^d \to \mathbb{R}^{d\times d}$ is often distributed according to some *stationary* probability measure with decaying correlations, for instance *independent and identically distributed* (i. i. d.) from site to site. Stationarity here means that the coefficient fields a and $a(x + \cdot)$ have the same distribution for every $x \in \mathbb{Z}^d$ which is clearly the case for i. i. d. coefficient fields. We follow the convention in statistical physics and call the distribution of the coefficient field an *ensemble* and denote its expectation by $\langle\cdot\rangle$. Following the ideas developed by Gloria and Otto [3, 4], we quantify in [5] the decay of correlations of the coefficient

field (equivalently, the ergodicity) via the *logarithmic Sobolev inequality* (LSI): For every random variable $\zeta : \Omega \to \mathbb{R}$, we have that

$$\Big\langle \zeta^2 \log \frac{\zeta^2}{\langle \zeta^2 \rangle} \Big\rangle \leq \frac{1}{2\rho} \sum_{z \in \mathbb{Z}^d} \Big\langle \Big(\mathrm{osc}_{a(z)} \zeta \Big)^2 \Big\rangle,$$

where $\mathrm{osc}_{a(z)} \zeta$ denotes the oscillation of $\zeta = \zeta(a)$ with respect to the value of a at z, the so-called *vertical derivative*. The LSI holds for every i. i. d. coefficient field and implies that for every $p < \infty$ and $\delta > 0$, we have that

$$\langle |\zeta|^{2p} \rangle \leq C(\rho, p, \delta) \langle |\zeta| \rangle^{2p} + \delta \Big\langle \Big(\sum_{z \in \mathbb{Z}^d} \Big(\mathrm{osc}_{a(z)} \zeta \Big)^2 \Big)^p \Big\rangle, \tag{2}$$

Let $G = G(x, y)$ denote the Green function corresponding to Equation (1), i.e. the solution to

$$\nabla_x^* a(x) \nabla_x G(x, y) = \delta(x - y).$$

In [2], it was shown that, just assuming stationarity of the ensemble $\langle \cdot \rangle$, that

$$\begin{aligned} \langle |\nabla_x G(x, y)|^2 \rangle^{\frac{1}{2}} &\leq C(d, \lambda)(|x - y| + 1)^{1-d}, \\ \langle |\nabla_x \nabla_y G(x, y)| \rangle &\leq C(d, \lambda)(|x - y| + 1)^{-d}. \end{aligned}$$

In [5] and this talk, we show how to combine this estimate with (2) to obtain that all moments are bounded:

$$\begin{aligned} \langle |\nabla_x G(x, y)|^{2p} \rangle^{\frac{1}{2p}} &\leq C(d, \lambda, \rho, p)(|x - y| + 1)^{1-d}, \\ \langle |\nabla_x \nabla_y G(x, y)|^{2p} \rangle^{\frac{1}{2p}} &\leq C(d, \lambda, \rho, p)(|x - y| + 1)^{-d}, \end{aligned}$$

for all $p < \infty$. For the second mixed derivative $\nabla_x \nabla_y G(x, y)$, this is achieved by choosing $\zeta = \nabla_x \nabla_y G(x, y)$ and bounding the vertical derivatives of $\nabla \nabla G$ in terms $\nabla \nabla G$ itself. For instance, we show that

$$|\mathrm{osc}_{a(z)} \nabla_x \nabla_y G(x, y)| \leq C(d, \lambda) |\nabla_x \nabla_z G(x, z)| \, |\nabla_z \nabla_y G(z, y)|.$$

As a consequence, we obtain the following *annealed regularity result*: For all $0 \leq \alpha < 1$ and $R < \infty$, we have that

$$\left\langle \left(\sup_u \frac{\sup_{x : |x| \leq R} \frac{|u(x) - u(0)|}{|x|^\alpha}}{\frac{1}{R^\alpha} \sup_{x : |x| \leq R} |u(x)|} \right)^p \right\rangle \leq C(d, \lambda, \rho, p, \alpha),$$

where the outer supremum (over u) is taken over all solutions to $\nabla^* a(x) \nabla u(x) = 0$ in the ball B_{2R} of radius $2R$. Thus, with high probability, a-harmonic functions with, say, i. i. d. coefficient fields are almost Lipschitz-continuous, in a way that can be quantified. These results have implications in the theory of stochastic homogenization which are beyond the scope of this talk.

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Infinite energy solutions for a homogeneous inelastic Maxwell gas

Daniel Matthes

(joint work with Federico Bassetti, Lucia Ladelli)

The *spatially homogeneous Inelastic Maxwell Model* (shIMM) of collisional gas theory, see [2], is characterized by the following:

- the time-dependent velocity distribution f is independent of the position, i.e., $f(t;x,v) = f(t;v)$ satisfies the homogeneous Boltzmann equation $\partial_t f = Q[f,f]$;
- the collision rate is independent of the relative velocity of the colliding particles, i.e., the collision operator has the weak form

$$\int Q[f,f](v)\varphi(v)\,dv = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{\mathbb{S}^{d-1}} B\left(\frac{(v-v_*)\cdot n}{|v-v_*|}\right)\big(\varphi(v')-\varphi(v)\big)f(v)f(v_*)\,dv\,dv_*\,d\sigma(n),$$

  where $n\in\mathbb{S}^{d-1}$ is a unit vector, σ is the normalized measure on the unit sphere $\mathbb{S}^{d-1}$, and $B:[-1,1]\to\mathbb{R}_+$ is a given cross section,
- in each collision, the relative velocity in the direction of impact is reduced by a factor $1-2\varepsilon$, i.e., the post-collisional velocities v' and v'_* are obtained from the pre-collisional velocities v, v_* via

$$v' = v - \big[(1-\varepsilon)(v-v_*)\cdot n\big]n, \quad v'_* = v_* + \big[(1-\varepsilon)(v-v_*)\cdot n\big]n,$$

  where $\varepsilon\in(0,1/2)$ is the modulus of inelasticity.

This collision mechanism preserves the sum of the linear momenta but diminishes the sum of the kinetic energies in each collision. One easily shows that if the total kinetic energy of the gas is finite initially, then it tends to zero at the exponential rate $4\varepsilon(1-\varepsilon)$ as $t\to\infty$. The corresponding (self-similar) collapse of the velocity distribution to a Dirac delta has been exhaustively studied, see e.g. [3] and the references therein.

On the other hand, the shIMM admits *stationary* solutions of infinite kinetic energy. This has first been observed in connection with the inelastic Kac model

[6], which is a caricature of the shIMM in dimension $d = 1$. In that special case, a family of stationary states is given by α-stable laws, where the index $\alpha \in (0, 2)$ is uniquely determined by the inelasticity parameter ε. And each of these stationary solutions attracts all transient solutions that start in the respective α-stable law's normal domain of attraction (NDA), see [1].

Note that this is an analogue of Tanaka's theorem, which states that the velocity distribution in a fully elastic homogeneous Maxwell gas converges to a Gaussian (i.e., a 2-stable law) if it has finite kinetic energy (i.e., belongs to the NDA of a Gaussian) initially. In our recent article [4], we have proven a similar result for the original shIMM, in arbitrary space dimensions $d > 2$.

Theorem 1. *Let a modulus of inelasticity $\varepsilon \in (0, 1/2)$ and a cross section $B \in L^1([-1; 1])$ be given. Then, there are an index $\alpha \in (0, 2)$ and a probability measure ν on $\mathbb{R}_+$ such that the following is true.*

(1) *There is a family $(f_c)_{c>0}$ of stationary solutions f_c that are scale mixtures of radially symmetric α-stable laws. Specifically, f_c's Fourier transform is given by*

$$\hat{f}_c(\xi) = \int_0^\infty \exp\big(-cs|\xi|^\alpha\big)\, d\nu(s) \quad \text{for all } \xi \in \mathbb{R}^d.$$

(2) *Assume that $\alpha \neq 1$. If f is a transient solution with initial datum $f^0 = f(0)$ in the NDA of some (not necessarily radially symmetric) α-stable law, then f converges (weakly in the sense of probability measures) to a stationary state f_c as $t \to \infty$, where c is computable from f^0.*
(This statement is "essentially true" also for $\alpha = 1$, but the precise formulation is more intricate in that case.)

It is expected that the f_c are the *only* stationary solutions. More specifically, we conjecture that if f^0 belongs to the NDA of some α'-stable law with $\alpha' > \alpha$ instead, then the corresponding transient solution converges to a Dirac delta. And if f^0 does not belong to the NDA of any α'-stable law with $\alpha' \geq \alpha$, then the transient solution converges vaguely to zero, i.e., the kinetic energy blows up.

We remark that the family $(f_c)_{c>0}$ of stationary states f_c has already been identified in the study of radially symmetric solutions to a more general class of kinetic equations [2]. There, a part of the basin of attraction (which, however, is much smaller than the — presumably maximal — one provided by the Theorem above) has been described as well.

Our method of proof uses an extension of the *probabilistic representation* for transient solutions $f(t)$, that has originally been introduced for the Kac equation in [5]. We show the following: let V_t be a random vector in $\mathbb{R}^d$ with $\mathrm{Law}[V_t] = f(t)$, then for every $R \in \mathrm{SO}(d)$ it holds that

$$(Re_d) \cdot V_t \overset{\mathrm{Law}}{=} \sum_{k=1}^{\nu_t} (R\Lambda_{\nu_t,k} e_d) \cdot X_k,$$

where the $X_1, X_2, \ldots$ are i.i.d. random vectors in $\mathbb{R}^d$ with $\mathrm{Law}[X_j] = f^0$, the $\Lambda_{n,k}$ are random similarities in $\mathrm{GL}(n)$ whose distribution is determined by the

cross section B, and ν_t is a random natural number with Poisson distribution. Once this representation has been obtained, the proof of the Theorem reduces to a laborious application of the central limit theorem for stable laws.

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Propagation of chaos for the 2D viscous vortex model

Stéphane Mischler

(joint work with Maxime Hauray, Nicolas Fournier)

We consider a stochastic system of N particles, usually called vortices in that setting, approximating the 2D Navier-Stokes equation written in vorticity. Assuming that the initial distribution of the position and circulation of the vortices has finite (partial) entropy and a finite moment of positive order, we show that the empirical measure of the particle system converges in law to the unique solution of the 2D Navier-Stokes equation. We actually prove a slightly stronger result: the propagation of chaos of the stochastic paths towards the solution of the expected nonlinear stochastic differential equation. Moreover, the convergence holds in the stronger (entropic) sense. The result holds without restriction (but positivity) on the viscosity parameter. The main difficulty is the presence of the singular Biot-Savart kernel in the equation. To overcome this problem, we use the dissipation of entropy which provides some (uniform in N) bound on the Fisher information of the particle system, and then use extensively that bound together with classical and new properties of the Fisher information.

Let us briefly explain with a bit more details our result in the simple case when all the vortices have fixed (equal to 1) circulation.

Consider a system of N indistinguishable (exchangeable) particles, each particle being described by its position $\mathcal{X}_1^N, ..., \mathcal{X}_N^N \in \mathbb{R}^2$, which evolves according to

$$d\mathcal{X}_i = \tfrac{1}{N} \sum_{j=1}^{N} K(\mathcal{X}_i - \mathcal{X}_j)\, dt + \sqrt{2\nu} d\mathcal{B}_i \tag{1}$$

where $(\mathcal{B}_i)_{1\leq i\leq N}$ are N given independent Brownian motions, $\nu>0$ is the viscosity and $K:\mathbb{R}^2\to\mathbb{R}^2$ is the (singular) Biot-Savart kernel defined by

$$\forall\, x=(x_1,x_2)\in\mathbb{R}^2,\quad K(x)=\frac{x^\perp}{|x|^2}=\Big(-\frac{x_2}{|x|^2},\frac{x_1}{|x|^2}\Big)=\nabla^\perp\log|x|.$$

The (formal) associated mean field limit is the $2D$ Navier-Stokes equation written in vorticity formulation

$$\partial_t w_t(x)=(K\star w_t)(x)\cdot\nabla_x w_t(x)+\nu\Delta_x w_t(x), \tag{2}$$

where $w:\mathbb{R}_+\times\mathbb{R}^2\to\mathbb{R}_+$ is the vorticity function.

Roughly speaking, we may establish:
- If $\mathcal{X}_0^N$ is w_0-Kac's chaotic and "appropriately bounded" then $\mathcal{X}_t^N$ is w_t-Kac's chaotic for any time $t>0$.
- If $\mathcal{X}_0^N$ is w_0-entropy chaotic and has bounded moment of order $k\in(0,1]$ then $\mathcal{X}_t^N$ is w_t–entropy chaotic for any time $t>0$.

In the sequel we do not explain what means such a statement but we focus on a variant of such mean field convergence result for which we may write a precise statement.

In order to do so, we first introduce an intermediate problem. We say that $\mathcal{X}=(\mathcal{X}_t)_{t>0}$ a continuous stochastic process with values in $\mathbb{R}^2$ is a solution to the stochastic NS vortex equation if it satisfies the nonlinear SDE

$$d\mathcal{X}=(K*w)(\mathcal{X})dt+\sqrt{2\nu}\,d\mathcal{B}, \tag{3}$$

for some given Brownian motion $\mathcal{B}$ and where $w_t=\mathcal{L}(\mathcal{X}_t)$ is the law of $\mathcal{X}_t$. It is important to point out that (thanks to Ito formula) the law w_t of $\mathcal{X}_t$ then satisfies the NS vortex equation (2).

For a given polish space E, we also introduce the empirical probability measure one-to-one function $X\in E^N\mapsto\mu_X^N:=\frac{1}{N}\sum_{i=1}^N\delta_{x_i}\in\mathbb{P}(E)$.

We finally consider as an initial condition a function $w_0\geq 0$ such that

$$\int_{\mathbb{R}^2} w_0\,(1+|x|^k+|\log w_0|)\,dx<\infty,\quad k\in(0,1]. \tag{4}$$

Our main result reads as follows.

Theorem. *Consider a function $w_0\geq 0$ satisfying (4) and consider the vortices trajectories $\mathcal{X}^N=(\mathcal{X}_t^N)_{t\geq 0}$ associated to an i.c. $\mathcal{X}_0^N\sim w_0^{\otimes N}$ thanks to (1) and $\mathcal{X}$ the solution to the stochastic NS vortex equation associated to an i.c. $\mathcal{X}_0\sim w_0$ thanks to (3). There holds*

$$\mathcal{L}(\mu^N_{\mathcal{X}^N})\ \rightharpoonup\ \delta_{\mathcal{L}(\mathcal{X})}\quad \textit{weakly in } \mathbb{P}(\mathbb{P}(C([0,\infty);\mathbb{R}^2))\ \textit{as } N\to\infty, \tag{5}$$

$$\mathcal{L}(\mathcal{X}_1^N(t),...,\mathcal{X}_j^N(t))\to w_t^{\otimes j}\quad \textit{strongly in } L^1(\mathbb{R}^2)^j\ \textit{as } N\to\infty. \tag{6}$$

The strategy of the proof is the by-now well-known "weak stability on nonlinear martingales" approach, which goes back to Sznitmann 1984, and is based on the following steps:

• a priori estimates (on entropy, moment and Fisher information);
• tightness of the law Q^N of the empirical process $\mu^N_{\mathcal{X}^N}$ in $\mathbb{P}(\mathbb{P}(E))$;
• pass to the limit and identify the set of limit points $\mathcal{S}$ as the probability measures $q \in \mathbb{P}(E)$ associated to a process $\mathcal{X}$ which solves the (Martingale problem associated to the) stochastic NS vortex equation (3) and has finite Fisher information;
• if $q \in \mathcal{S}$ and $q = \mathcal{L}(\mathcal{X})$ then $w_t := \mathcal{L}(\mathcal{X}_t)$ is the unique solution to the NS vortex PDE (2);
• the Martingale problem associated to (3) has a unique solution $\bar{\mathcal{X}}$ and then $\mathcal{S} = \{\bar{q}\}$ where $\mathcal{L}(\bar{q}) = \bar{\mathcal{X}}$.

All together, we conclude to the Kac's chaos (5), which in turns implies (6). The proof is then quite standard except the fact that we use the Fisher information bound at each step in order to overcome the difficulties which come from the fact that the Biot-Savart kernel is singular.

Particle systems and macroscopic limits in self-organized dynamics

Sebastien Motsch

(joint work with Pierre Degond, Laurent Navoret, Jeff Haack, Irene Gamba)

Self-organized dynamics is a spectacular phenomenon to observe in nature. In a shoal of fish or in a human crowd, thousands of individuals interact and form large scale structures. To understand these complex dynamics, particle systems have been widely studied. In this talk, we are interested in the large scale behavior of these models.

We first investigate the macroscopic limit of a large class of particle systems using kinetic theory. In contrast with particle systems in physics, models of self-organized dynamics do not conserve momentum or energy. This lack of conservation requires to introduce new tools (i.e. *generalized* collisional invariants) to derive macroscopic models.

In a second part, we compare numerically the different models obtained (i.e. particle systems, kinetic equation and macroscopic limit). With this aim, we analyze the solutions of Riemann problems (e.g. shock and rarefaction waves). Since the models are non-conservative, we observe new types of solutions that remain to be understood analytically.

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A fluid/kinetic model with merging small droplets

Ayman Moussa
(joint work with Saad Benjelloun, Laurent Desvillettes)

Sprays are complex flows which are constituted of an underlying gas in which a population of droplets (or dust specks) are dispersed, cf. [8]. There are various possibilities for modeling such flows, depending in particular on the volume fraction of the liquid phase.

We focus here on the case when the volume fraction occupied by the droplets is small enough to be neglected in the equations (such sprays are called thin sprays, cf. [8]), so that the modeling of the liquid phase can be performed by the use of a pdf (*particles density function*) which solves Vlasov-Boltzmann equation (cf. [11, 1]).

Let us consider the case in which the spray is constituted of two type of particles : large particles radius 1, described by a density function f, small particles of radius ε, described by a density function h. Both density functions depends on $(t, \mathbf{x}, \boldsymbol{\xi}) \in \mathbb{R}_+ \times \mathbb{T}^3 \times \mathbb{R}^3$ where $\mathbb{T}^3$ is the three-dimensional torus. Large particles may split (with conservation of the mass) into small particles which do not split anymore. No collisions nor coalescences may occur.

If the particles are surrounded by an incompressible viscous fluid of velocity/pressure $\mathbf{u}(t, \mathbf{x})$ and $p(t, \mathbf{x})$ of constant density and viscosity, the behavior of the system may be described through the following equations (normalizing several physical constants)

$$\nabla_{\mathbf{x}} \cdot \mathbf{u} = 0, \tag{1}$$

$$\partial_t f + \boldsymbol{\xi} \cdot \nabla_{\mathbf{x}} f + \nabla_{\boldsymbol{\xi}} \cdot [f \boldsymbol{\Gamma}] = -f, \tag{2}$$

$$\partial_t h + \boldsymbol{\xi} \cdot \nabla_{\mathbf{x}} h + \nabla_{\boldsymbol{\xi}} \cdot [h \boldsymbol{\Gamma}] = \frac{1}{\varepsilon^3} h, \tag{3}$$

$$\partial_t \mathbf{u} + \nabla_{\mathbf{x}} \cdot (\mathbf{u} \otimes \mathbf{u}) + \nabla_{\mathbf{x}} p - \Delta_{\mathbf{x}} \mathbf{u} = \mathbf{F}_{\mathrm{ret}}, \tag{4}$$

where $\boldsymbol{\Gamma}$ is the drag acceleration given by the simple formula (known as "Stokes' law")

$$\boldsymbol{\Gamma}(t, \mathbf{x}, \boldsymbol{\xi}, r) = -\frac{\boldsymbol{\xi} - \mathbf{u}(t, \mathbf{x})}{r^2}, \tag{5}$$

and $\mathbf{F}_{\mathrm{ret}}$ is the retroaction of the drag force:

$$\mathbf{F}_{\mathrm{ret}}(t, \mathbf{x}) = -\int_0^{+\infty} \int_{\mathbb{R}^3} r^3 \, f \, \boldsymbol{\Gamma} \, \mathrm{d}\boldsymbol{\xi} \mathrm{d}r. \tag{6}$$

Denoting $\rho = \varepsilon^3 \displaystyle\int_{\mathbb{R}^3} h \, \mathrm{d}\boldsymbol{\xi}$, and noticing that

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\{ \int_{\mathbb{T}^3}\int_{\mathbb{R}^3} f\,\frac{|\boldsymbol{\xi}|^2}{2}\,\mathrm{d}\boldsymbol{\xi}\mathrm{d}\mathbf{x} + \int_{\mathbb{T}^3}\int_{\mathbb{R}^3} \varepsilon^3 h\,\frac{|\boldsymbol{\xi}|^2}{2}\,\mathrm{d}\boldsymbol{\xi}\mathrm{d}\mathbf{x} + \int_{\mathbb{T}^3}\frac{|\mathbf{u}|^2}{2}\,\mathrm{d}\mathbf{x}\right\}$$
$$+ \int_{\mathbb{T}^3}\int_{\mathbb{R}^3} f\,|\boldsymbol{\xi}-\mathbf{u}|^2\,\mathrm{d}\boldsymbol{\xi}\mathrm{d}\mathbf{x}$$
$$+ \frac{1}{\varepsilon^2}\int_{\mathbb{T}^3}\int_{\mathbb{R}^3} \varepsilon^3 h\,|\boldsymbol{\xi}-\mathbf{u}|^2\,\mathrm{d}\boldsymbol{\xi}\mathrm{d}\mathbf{x} + \int_{\mathbb{T}^3}|\nabla_{\mathbf{x}}\mathbf{u}|^2\,\mathrm{d}\mathbf{x} = 0,$$

we see that (at the formal level) $\varepsilon^3\, h(t,\mathbf{x},\boldsymbol{\xi}) \to \rho(t,x)\,\delta_{\boldsymbol{\xi}=\mathbf{u}(t,\mathbf{x})}$ when $\varepsilon \to 0$.

Integrating eq. (3) against $\varepsilon^3\,\mathrm{d}\boldsymbol{\xi}$, we end up with

$$\partial_t\rho + \nabla_{\mathbf{x}}\cdot[\rho\,\mathbf{u}] = \int_{\mathbb{R}^3} f\,\mathrm{d}\boldsymbol{\xi}. \tag{7}$$

Then, integrating eq. (3) against $\varepsilon^3\,\boldsymbol{\xi}\,\mathrm{d}\boldsymbol{\xi}$ and adding the result with eq. (4), we obtain

$$\partial_t((1+\rho)\,\mathbf{u}) + \nabla_{\mathbf{x}}\cdot((1+\rho)\,\mathbf{u}\otimes\mathbf{u}) + \nabla_{\mathbf{x}}p - \Delta_{\mathbf{x}}\mathbf{u} = -\int_{\mathbb{R}^3}(\mathbf{u}-\boldsymbol{\xi})\,f\,\mathrm{d}\boldsymbol{\xi} + \int_{\mathbb{R}^3} f\,\boldsymbol{\xi}\,\mathrm{d}\boldsymbol{\xi}.$$

Combining this last equation with eq. (7), we write down the system that we wish to study

$$\nabla_{\mathbf{x}}\cdot\mathbf{u} = 0, \tag{8}$$

$$\partial_t\rho + \nabla_{\mathbf{x}}\cdot[\rho\,\mathbf{u}] = \int_{\mathbb{R}^3} f\,\mathrm{d}\boldsymbol{\xi}, \tag{9}$$

$$\partial_t f + \boldsymbol{\xi}\cdot\nabla_{\mathbf{x}} f + \nabla_{\boldsymbol{\xi}}\cdot[(\mathbf{u}-\boldsymbol{\xi})\,f] = -f, \tag{10}$$

$$(1+\rho)\Big[\partial_t\mathbf{u} + \nabla_{\mathbf{x}}\cdot(\mathbf{u}\otimes\mathbf{u})\Big] + \nabla_{\mathbf{x}}p - \Delta_{\mathbf{x}}\mathbf{u} = 2\int_{\mathbb{R}^3}(\boldsymbol{\xi}-\mathbf{u})\,f\,\mathrm{d}\boldsymbol{\xi}, \tag{11}$$

where $\rho := \rho(t,\mathbf{x}) \geq 0$, $\mathbf{u} := \mathbf{u}(t,\mathbf{x}) \in \mathbb{R}^3$, $p := p(t,\mathbf{x}) \geq 0$, $f := f(t,\mathbf{x},\boldsymbol{\xi}) \geq 0$, and $t \geq 0$, $\mathbf{x} \in \mathbb{T}$, $\boldsymbol{\xi} \in \mathbb{R}^3$. Let us recall that ρ represents here the "added density" resulting from the very small particles. This is the reason why, though the fluid density was initially normalized in (4), we have in (11) the term $(1+\rho)$ in front of the convective part of the fluid equation. For a more detailed version of the previous computation, see [3].

Our goal is to study the existence theory for this limit system, completed with appropriate initial data.

Our system (8) – (11) is reminiscent of the Vlasov/incompressible Navier-Stokes equations with a variable density, see [9] for a recent study of this system (with bounded density). In fact, taking $f = 0$ in (8) – (11), leads to the usual incompressible Navier-Stokes with variable density, and it is hence natural to expect (at least) the difficulties encountered in the study of the latter system. As far as we know, in all the articles concerning the inhomogeneous Navier-Stokes, the density is always bounded (see [2, 7] or the more recent [9] for instance), but in our system the density lies in some L^p space with $p < \infty$ and the corresponding

transport equation has an unbounded right-hand side. It was suggested in [7, 5] that techniques from [5] may be adapted to treat the general case of unbounded density, and this is precisely what we have done to handle the worst non-linearities of system (8) – (11).

As for the formal limit allowing to pass from system (1) – (4) to the limit system (11) – (8), the problem seems quite hard to handle and is in fact quite close to the hydrodynamic limit studied in [6] (but with less estimates !). Compactness method seems to fail, and we do not know at the time of writing if some relative energy method may be used to justify this limit (at least locally in time, for well-prepared data).

The detailed proof of existence of global weak solutions for the limit system may be found in [4].

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Decoherence for a heavy particle interacting with a light one: new analysis and numerics

Claudia Negulescu

(joint work with R. Adami, M. Hauray)

In the present work we describe, both through a theoretical analysis and numerical simulations, the following idealized experiment: a quantum particle lies in a state given by the superposition of two localized wave functions ("bumps"),

initially separated and moving towards each other. At a certain time, the particle interacts with another particle which is considerably lighter. As a consequence, the quantum interference arising when the two bumps corresponding to the heavy particle eventually meet, is damped. The damping of the interference is called *decoherence*, and provides a description of the transition from the quantum to the classical world. Despite the conceptual relevance of decoherence in the foundations of quantum mechanics as well as in applications (e.g. in quantum computation) and, more generally, in the understanding of the classical picture of the macroscopic world, a rigorous and exhaustive description of such phenomenon is still at its beginnings.

According to the principles of quantum mechanics, the time evolution of the wave function $\psi_\epsilon(t, X, x)$ representing the two-body quantum system is given by the Schrödinger equation

$$\text{(1)} \qquad \begin{cases} i\partial_t \psi_\epsilon \;=\; -\dfrac{1}{2M}\Delta_X \psi_\epsilon - \dfrac{1}{2\varepsilon M}\Delta_x \psi_\epsilon + \dfrac{1+\varepsilon}{\varepsilon} V(x-X)\,\psi_\epsilon, \\ \psi_\epsilon(0, X, x) = \psi_\epsilon^0(X, x)\,, \end{cases}$$

where we used units in which $\hbar = 1$, M is the mass and X is the spatial coordinate of the heavy particle, while ϵM is the mass and x is the spatial coordinate of the light one. So ϵ is the ratio between the mass of the light particle and the mass of the heavy one, and we study the regime $\epsilon \ll 1$, that we call *small mass ratio* regime.

The interaction is described by the potential $\frac{1+\varepsilon}{\varepsilon}V$; the uncommon coupling constant is chosen to be of order ϵ^{-1} so that even a single collision leaves an observable mark on the heavy particle; furthermore, the factor $1+\epsilon$ hardly affects the dynamics and makes the computations less cumbersome. We shall always choose a *factorized* initial state, i.e. ψ_ϵ^0 will be the product of a function of the variable X only, and a function of the variable x only. Physically, this means that initially the two particles are uncorrelated. We shall always assume that ψ_ϵ^0, and consequently $\psi_\epsilon(t)$, is normalized in $L^2(\mathbb{R}^{2d})$.

The aim of this work is threefold: first, we rigorously derive a *collisional dynamics* for the heavy particle as an approximation of the underlying quantum evolution (1) in the limit $\epsilon \to 0$; second, we employ such a collisional dynamics in order to build up an efficient numerical scheme; third, we observe the appearance of decoherence through numerical simulation.

Concerning the analytical contribution, we show that an approximate description of the dynamics of the heavy particle can be carried out in two steps: first comes the interaction, then the free evolution. In particular, all effects of the interaction can be embodied in the action of a collision operator that acts on the initial state of the heavy particle. With respect to previous analytical results on the same topics, we turn our focus from the Møller wave operator to the full scattering operator, whose analysis proves to be simpler.

Concerning the numerical contribution, we exploit the previous analysis to construct an efficient numerical scheme that turns the original, multiscale, two-body problem in two one-body problems which can be solved separately. This leads to a considerable gain in simulation time. We present and interpret some simulations carried out on specific one-dimensional systems by using the new scheme.

Stability of kinks in Cahn-Hilliard equations—energy/energy dissipation methods

Felix Otto
(joint work with Maria Westdickenberg)

Appealing to the gradient flow structure we prove a non-perturbative non-linear stability result which gives optimal exponents in the algebraic decay. It amounts to a non-convex version of Brézis' result on convex gradient flows. As Brézis, it uses the intrinsic distance (here H^{-1}), the energy gap and the energy dissipation. It relates these three quantities, and the slow variable (=the position of the kink) by interpolation estimates and differential inequalities.

A Kac Model for Fermions

Federica Pezzotti
(joint work with M. Colangeli, M. Pulvirenti)

One of the most important and challenging mathematical problems in Kinetic Theory is the rigorous derivation of the kinetic equations from the basic mechanical laws. The first fundamental result in this direction was obtained in 1975 by O. Lanford [8], who derived the Boltzmann equation for a system of hard spheres, for short times, in the Low-Density (or Boltzmann-Grad) limit. A similar result was also obtained quite recently for particle systems interacting via a two-body short-range, smooth potential (see [6], [11] and references quoted therein).

On the other hand, a dense gas of weakly interacting particles (weak-coupling limit) is expected to be described by the Landau equation. In this case there are no rigorous results. We only mention a very preliminary consistency result [3].

Quantum systems are expected to be described by suitable Boltzmann equations in both Boltzmann-Grad and Weak-Coupling limits. In the first case the Boltzmann equation is just the classical one, with the full quantum cross-section associated with the interaction potential. In the second, more interesting, case, the Boltzmann equation (U-U equation in the sequel) differs from the classical one because it takes into account the effects of the Bose-Einstein or Fermi-Dirac statistics. It was heuristically introduced by Nordheim (1928) in [10] and Uehling and Uhlenbeck(1933) in [13].

Concerning the rigorous derivation of the U-U equation starting from an N-particle system evolving according to the Schrödinger equation, only formal or

partial results are available up to now (see [1], [2], [5] and references quoted therein).

The U-U equation reads as

$$(\partial_t + v \cdot \nabla_x)\, f = Q_\theta(f, f, f),$$

where the collision operator $Q_\theta(f, f, f)(x, v)$ is given by

$$\int dv_1 \int d\omega\, B_\theta(v - v_1; \omega)\, [f(x, v')f(x, v_1')(1 + \alpha\theta f(x, v))(1 + \alpha\theta f(x, v_1)) + \\ - f(x, v)f(x, v_1)(1 + \theta\alpha f(x, v'))(1 + \alpha\theta f(x, v_1'))]\,,$$

and $f(x, v, t)$ is the probability distribution of a test particle in the classical phase space ((x, v, t) denote position, momentum and time) describing the time evolution of the Wigner transform of a quantum state. Here $\theta = +1$ or $\theta = -1$, for the Bose-Einstein or the Fermi-Dirac statistics and $\alpha = (2\pi\hbar)^3$, where $\hbar$ is the Planck constant.

Finally $(v, v_1) \to (v', v_1')$ is the transition due to an elastic collision with scattering vector $\omega \in S^2$ and B is proportional to the symmetrized cross-section (associated with the pair interaction potential) in the Born approximation.

In 1956 M. Kac proposed a stochastic particle model yielding, in a suitable scaling limit (of Mean-Field type), the classical Boltzmann equation (see [7]). The purpose was to understand the delicate passage from an N-particle system to a one-particle kinetic description, in an easier context.

The model consists of a set of N particles with velocities $V_N = (v_1 \dots v_N)$. The positions are ignored. The original Kac Model is one dimensional (i.e., $v_i \in \mathbb{R}$, for any $i = 1, \dots, N$) and he works in the microcanonical framework, requiring the velocities to belong to the (energy) sphere $v_1^2 + \cdots + v_N^2 = N$. Here we consider a natural generalization of the original model in which velocities are three dimensional and we work in the canonical framework. The evolution is the following. At an exponential time pick a pair of particles (say i and j), select a scattering vector $\omega \in S^2$ and perform the transition $(v_i, v_j) \to (v_i', v_j')$ with the usual elastic collision rules. More precisely, if $W^N(V_N, t)$ is a probability distribution, its time evolution obeys the following Master equation

$$\partial_t W^N = \frac{1}{N} L_N^{\mathbf{K}} W^N \tag{1}$$

where

$$L_N^{\mathbf{K}} W^N(V_N) = \sum_{1 \le i < j \le N} \int_{S^2} d\omega B(v_i - v_j; \omega) \left[W^N(V_N^{i.j}) - W^N(V_N) \right] \tag{2}$$

and

$$V_N^{i.j} = \{v_1, ..., v_i', ..., v_j', ..., v_N\}.$$

It is possible to show that, in the limit $N \to \infty$, the k-particle marginals $f_k^N(V_k, t)$ of $W_N(V_N, t)$, converge to a sequence of marginals $f_k(V_k, t)$. Moreover, if initially $W^N(\cdot, 0) = f_0^{\otimes N}$, where f_0 is a one-particle distribution (namely the

particles are initially independently distributed) then $f_k(\cdot, t) = f^{\otimes k}(t)$, where $f(t)$ solves the Boltzmann equation with cross-section B.

The Kac model has been widely investigated, see the recent paper [9] and references quoted therein.

In the same spirit we modify the Kac model including an exclusion constraint mimicking the Pauli exclusion principle with the scope of deriving the U-U equation for Fermions. The exclusion principle is implemented by introducing a grid of side δ in the one-particle phase space. Then we consider only admissible configurations, namely those exhibiting at most one particle per cell. The random transition $(v_i, v_j) \to (v_i', v_j')$ takes place only if the final configuration $V_N^{i,j} = \{v_1, ..., v_i', ..., v_j', ..., v_N\}$ is still admissible. Then we perform the limit $N \to \infty$, $\delta \to 0$ with fixed $\alpha = N\delta^3$, $\alpha > 0$. In doing this we follow the Lanford strategy, namely we first derive a hierarchy of equations for the marginals $f_k^N(V_k, t)$ of the time evolution of an N-particle state. Such a derivation is straightforward, but tedious. Then we bound, locally in time, the series expansion expressing the solution of the hierarchy. We note that, due to the exclusion principle which gives us automatically a bound on the density, we can treat arbitrary times by introducing a suitable family of norms. Finally we exploit the term by term convergence by piling up a finite number of series expansions, each of them converging for a short time.

Our result is proven under suitable assumptions on the convergence of the initial data and we also provide examples of initial states fulfilling the above assumptions.

It may be worth to underline that our analysis, as well as the one suggested by the original Kac model, deals with the homogeneous U-U equation ($f(t, x, v) = f(t, v)$). Actually, the dynamics described by the Kac model is related to the interaction part of the popular numerical scheme called *Direct Simulation Method* (see e.g. [4] for a mathematical description and [12] for the convergence). Therefore the result presented in this talk could be of some interest for numerical problems associated with the simulation of the U-U equation.

We finally remark that a model similar to the one we considered can be studied for Bosons as well and it would be a very interesting issue. In this case, statistics induces particle concentration and the mathematical analysis is harder.

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On the convergence to equilibrium for degenerate kinetic equations

Francesco Salvarani
(joint work with Étienne Bernard)

We have considered some hypocoercivity properties of the degenerate linear Boltzmann equation in the torus $\mathbb{T}^d = \mathbb{R}^d/\mathbb{Z}^d$, $d \in \mathbb{N}$ with $d \geq 2$:

$$\text{(1)} \qquad \begin{cases} \partial_t f + v \cdot \nabla_x f + \sigma\,(f - Kf) = 0, & (t,x,v) \in \mathbb{R}_+ \times \mathbb{T}^d \times V \\ \\ f(0,x,v) = f^{\text{in}} \in L^1\left(\mathbb{T}^d \times V\right) & (x,v) \in \mathbb{T}^d \times V, \end{cases}$$

where either $V = \{v \in \mathbb{R}^d \,:\, 0 < v_m < v_M,\, v_m \leq |v| \leq v_M\}$ or $V = \mathbb{S}^{d-1}$ and

$$\text{(2)} \qquad Kf := \int_V k(v,w) f(t,x,w)\, dw.$$

The kernel k of the operator K is a function of class $L^\infty(V \times V)$ such that

$$\text{(3)} \qquad \int_V k(v,w)\, dw = 1 \text{ and } k(v,w) > 0 \text{ a.e. on } V \times V.$$

The measures on $\mathbb{T}^d \times V$ are normalized such that

$$\int_{\mathbb{T}^d} dx = \int_V dv = 1.$$

The function $f \equiv f(t,x,v)$ describes the density of particles that, at time $t > 0$, are located at $x \in \mathbb{T}^d$, with velocity $v \in V$, and which interact only with a fixed background (the details of the interaction being described by the cross section σ and the kernel k).

The properties of the cross section heavily influence the long-time behaviour of the Cauchy problem (1). From now on, we impose the following assumptions on

the cross sections:

$$\sigma \in L^\infty\left(\mathbb{T}^d\right), \text{ with } \sigma \geq 0 \text{ a.e. and } \int_{\mathbb{T}^d} \sigma(x)dx > 0. \tag{4}$$

It is easy to see that the only equilibria of (1) are the constants [3] and that the only candidate to be the long-time asymptotic profile is $f_\infty := \|f^{\text{in}}\|_{L^1(\mathbb{T}^d\times V)}$.

A further classification is necessary for the study of the long-time behaviour of the Cauchy problem (1) in order to take into account non-exponential convergence effects:

Definition 1. *Let σ be a cross section satisfying the requirements* (4)*. If there exists, moreover, a strictly positive constant $m > 0$ such that $\sigma \geq m$ for a.e. $x \in \mathbb{T}^d$, then the cross section is said to be non degenerate. Otherwise, it is said to be degenerate.*

In general, the exponential relaxation to equilibrium is not true for degenerate cross section. Indeed, the following theorem holds [3]:

Theorem 2. *For all $r \in (0, 1/2)$ consider the periodic open set*

$$Z_r = \{x \in \mathbb{R}^d \,:\, dist(x, \mathbb{Z}^d) > r\}$$

together with the associated fundamental domain $Y_r = Z_r/\mathbb{Z}^d$.

For all $r \in (0, 1/2)$, there exists an initial condition $f^{\text{in}} \in L^\infty(\mathbb{T}^d \times \mathbb{S}^{d-1})$ satisfying $f^{\text{in}}(x, v) \geq 0$ for a.e. $(x, v) \in \mathbb{T}^d \times \mathbb{S}^{d-1}$ and such that, for each cross section $\sigma \in L^\infty(\mathbb{T}^d)$ satisfying $\sigma(x) \geq 0$ for a.e. $x \in \mathbb{T}^d$ and $\sigma(x) = 0$ for a.e. $x \in Y_r$, the solution f of the transport problem satisfies

$$\|f - f_\infty\|_{L^2(\mathbb{T}^d\times\mathbb{S}^{d-1})} \geq \frac{C}{\sqrt{t}}$$

for each $t > r^{1-d}$, where $f_\infty = \|f^{\text{in}}(x, v)\|_{L^1(\mathbb{T}^d\times\mathbb{S}^{d-1})}|\mathbb{S}^{d-1}|$ and C is a positive constant.

The previous result has been numerically observed [6]. Positive results on the convergence speed have moreover been obtained. Historically, the first one is the following [2]:

Theorem 3. *Consider the Cauchy problem* (1)*, with a cross section $\sigma \in L^\infty(\mathbb{T}^d) \cap H^1(\mathbb{T}^d)$. Suppose that there exist $x_i \in \mathbb{T}^d$, $i = 1, \ldots, N$, $C_\sigma > 0$ and $\lambda_\sigma > 0$ such that*

$$\text{for a.e. } x \in \mathbb{T}^d, \qquad \sigma(x) \geq C_\sigma \inf_{i=1,\ldots,N} |x - x_i|^{\lambda_\sigma}.$$

and that $k \equiv 1$. If the initial condition $f^{\text{in}} \geq 0$ a.e. such that $f^{\text{in}} \in L^\infty(\mathbb{T}^d \times V)$, $\nabla_x \bar{f}^{\text{in}} \in L^2(\mathbb{T}^d)$, and $v \otimes v : \nabla_x \nabla_x f^{\text{in}} \in L^2(\mathbb{T}^d \times V)$, then there exists a unique nonnegative solution f to this system in $C(\mathbb{R}_+; L^2(\mathbb{T} \times V))$.

The solution f converges when $t \to +\infty$ to its asymptotic profile $f_\infty(x, v) = \|f^{\text{in}}\|_{L^1(\mathbb{T}^d\times V)}$ and, moreover,

$$||f(t, \cdot, \cdot) - f_\infty||^2_{L^2(\mathbb{T}\times V)} \leq C_1\, t^{-\frac{1}{1+2\,\lambda_\sigma}}.$$

The explicit constant C_1 depends on C_σ, λ_σ, $||\sigma||_{H^1(\mathbb{T}^d)\cap L^\infty(\mathbb{T}^d)}$ and f^{in}.

Even if the previous theorem is not optimal, it gives the only available quantitative result, up to now, on the convergence speed to equilibrium for the linear Boltzmann equation in the degenerate case.

An additional property on σ is necessary to guarantee an exponential convergence to equilibrium.

Definition 4. *The cross section $\sigma \equiv \sigma(x)$ verifies the geometrical condition if there exist T_0 and $C > 0$ such that*

$$\int_0^{T_0} \sigma(x - sv)ds \geq C \text{ a.e. in } (x, v) \in \mathbb{T}^d \times V. \tag{5}$$

This property is reminiscent of the Bardos-Lebeau-Rauch condition that guarantees the exponential stabilization of the wave equation [1]. The following theorem holds [4]:

Theorem 5. *Let $\sigma \in L^\infty\left(\mathbb{T}^d\right)$ be a non-negative cross section satisfying the geometrical condition* (5)*. Then there exist two constants $M > 0$ and $\alpha > 0$ such that the solution f of the Cauchy problem* (1) *satisfies the inequality*

$$\left\| f - \int_{\mathbb{T}^d \times V} f^{\text{in}}(x, v)\, dxdv \right\|_{L^1(\mathbb{T}^d \times V)} \leq Me^{-\alpha t} \left\| f^{\text{in}} \right\|_{L^1(\mathbb{T}^d \times V)} \tag{6}$$

for all $t \in \mathbb{R}_+$. Conversely, if the solution of the linear Boltzmann equation (1) *converges uniformly in L^1 to its equilibrium state at an exponential rate (i.e., it satisfies* (6)*), then σ must satisfy the geometrical condition* (5)*.*

We finally point out that it is possible to obtain an explicit and optimal exponential decay rate to equilibrium for a simplified version of the Cauchy problem (1), namely the generalized Goldstein-Taylor system:

$$\begin{cases} \dfrac{\partial u}{\partial t} + \dfrac{\partial u}{\partial x} = \sigma(x)(v - u) \\ \\ \dfrac{\partial v}{\partial t} - \dfrac{\partial v}{\partial x} = \sigma(x)(u - v), \end{cases} \qquad x \in \mathbb{T} := \mathbb{R}/\mathbb{Z},\ t \geq 0. \tag{7}$$

with non negative initial conditions

$$u(0, x) = u^{\text{in}} \in H^1(\mathbb{T}), \qquad v(0, x) = v^{\text{in}} \in H^1(\mathbb{T}). \tag{8}$$

The following result has been proved in [5]:

Theorem 6. *Let $(u^{\text{in}}, v^{\text{in}}) \in H^1(\mathbb{T}) \times H^1(\mathbb{T})$ be non negative functions and let $\sigma \in L^\infty(\mathbb{T})$ satisfy* (4)*. Denote also $u_\infty := \|u^{\text{in}} + v^{\text{in}}\|_{L^1(\mathbb{T})}$. Then, there exists a positive constant A_*, depending on $||u^{\text{in}}||_{H^1(\mathbb{T})}$, $||v^{\text{in}}||_{H^1(\mathbb{T})}$ and $||\sigma||_{L^\infty(\mathbb{T})}$, such that the solution (u, v) of the Goldstein-Taylor model* (7)-(8) *satisfies the inequality*

$$H(t) := \|u - u_\infty\|^2_{L^2(\mathbb{T})} + \|v - u_\infty\|^2_{L^2(\mathbb{T})} \leq A_* \exp(-\alpha t), \tag{9}$$

where

$$\alpha = 2\|\sigma\|_{L^1(\mathbb{T})}.$$

Moreover, the decay rate α is optimal in the following sense:

$$\alpha = \sup\left\{\beta \geq 0 \,:\, \exists A_*,\ \forall t \geq 0,\ \forall (u^{\mathrm{in}}, v^{\mathrm{in}}) \in H^1(\mathbb{T}) \times H^1(\mathbb{T}),\ H(t) \leq A_* e^{-\beta t}\right\}.$$

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Nontrivial equilibria of kinetic transport models for chemotaxis

Christian Schmeiser

(joint work with Vincent Calvez, Gaël Raoul)

Linear kinetic transport equations with velocity jumps biased towards the origin in position space are considered, as models for the chemotactic response of bacteria with run-and-tumble motility to a prescribed peaked chemoattractant concentration. For a one-dimensional model problem, the existence and dynamic stability of peaked equilibrium distributions of bacteria is shown. Exponential decay to the equilibrium is proven by hypocoercivity methods, which are related to the decay behavior of diffusive macroscopic limits taking the form of Fokker-Planck equations with confining potentials. Detailed results can be found in [1].

The linear kinetic equation for the distribution function $f(t,x,v)$, $t, x \in \mathbb{R}$, $v \in V = [-1/2, 1/2]$,

$$\partial_t f + v\,\partial_x f = Q(f) = \int_V \left(K(x,v')f(t,x,v') - K(x,v)f(t,x,v)\right) dv', \tag{1}$$

where the turning rate is increased for particles moving away from $x = 0$: $K(x,v) = 1 + \chi \mathrm{sign}(xv)$ with $0 < \chi < 1$.

Theorem 1. [1] *There exists a nontrivial steady state solution $g(x,v)$ of (1). It is positive, bounded and symmetric: $g(x,v) = g(-x,-v)$. There exists $\alpha > 0$, a positive velocity profile G, and constants $0 < c < C$ such that*

$$c\,e^{-\alpha x} G(v) \leq g(x,v) \leq C\,e^{-\alpha x} G(v), \qquad x \geq 0,\ v \in V. \tag{2}$$

Outline of the proof: The decay parameter α and the profile G solve the eigenvalue problem $-\alpha v G = Q(G)$, which determines $\alpha > 0$ uniquely and G up to a multiplicative constant. The Milne problem for $u = e^{\alpha x} g/G$ for $x > 0$ with given inflow

data $u(0,v)$, $v>0$, can be solved by standard methods, and boundedness of u in terms of the inflow data follows from the maximum principle, which eventually proves the estimate (2).

By the symmetry assumption on g the Albedo operator mapping the inflow to the outflow data can be used to formulate a fixed point problem for the determination of $u(0,v)$, $v>0$. The fixed point operator allows the application of the Krein-Rutman theorem giving the existence of a positive eigenfunction. The mass conservation property shows that the eigenvalue is equal to one.

The evolution operator $Q - v\,\partial_x$ is not coercive in the sense that the dissipation of the entropy $\|f\|^2$ (where $\|\cdot\|$ is the norm in $L^2(dv\,dx/g)$) vanishes, whenever the distribution function has the form $f(x,v)=h(x)g(x,v)$ with arbitrary $h(x)$. Our proof of *hypocoercivity,* i.e. exponential decay to the steady state, employs the approach of [2], which is based on the construction of a modified entropy functional with coercive dissipation rate. The method is based on a splitting $Q - v\,\partial_x = L - T$ of the evolution operator in a symmetric negative semidefinite operator L and a skewsymmetric operator T, such that the steady state is in the intersection of the null spaces of L and T. Since $Q(g)$ and $v\,\partial_x g$ do not vanish, the standard splitting into collision and transport operator is not suitable, but it can be modified appropriately.

Theorem 2. [1] *Let $f_I \in L^2(dv\,dx/g)$ $(\subset L^1(dv\,dx))$ and let*

$$f_\infty(x,v) := g(x,v)\int_{\mathbb{R}\times V} f_I dv\,dx \left(\int_{\mathbb{R}\times V} g\,dv\,dx\right)^{-1}.$$

Then the solution of (1) *subject to $f(t=0)=f_I$ satisfies*

$$\|f(t,\cdot,\cdot)-f_\infty\|_{L^2(dv\,dx/g)} \le Ce^{-\lambda t}\|f_I-f_\infty\|_{L^2(dv\,dx/g)}\,,$$

with positive constants C and λ, only depending on $\chi\in(0,1)$.

Main ingredients of the proof are *microscopic coercivity*, i.e. coercivity of L on the orthogonal complement of its null space, and *macroscopic coercivity*, which is equivalent to a weighted Poincaré inequality with the macroscopic density of g as weight. This also implies exponential decay to steady states for the corresponding macroscopic limit model having the form of a Fokker-Planck equation with confining potential.

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Noise reduction strategies for PIC simulations of Tokamaks and Stellarators

Eric Sonnendrücker
(joint work with Roman Hatzky, Ralf Kleiber, Abigail Wacher)

Controlled thermonuclear fusion is a potential solution for safe and sustainable energy production in the future. In order to achieve fusion conditions in a reactor deuterium and tritium atoms need to be heated to about 100 000 000 $^{\circ}C$ and confined at a high enough density for a sufficient time. This can be achieved by confining the gas of charged particles, called a plasma, with a large magnetic field. The experimental devices in which this is done are called tokamaks, when the equilibrium is axisymmetric, or stellarator, when the equilibrium plasma has a three-dimensional shape.

In order to understand energy confinement properties in these devices, turbulent transport arising due to micro-instabilities in the plasma is a key issue. This can be simulated numerically based on the so-called gyrokinetic model which is an approximation of the full kinetic Vlasov-Maxwell equations in a very large external magnetic field. The gyrokinetic model is defined in a five-dimensional phase-space, thanks to the averaging of the particle motion over the magnetic field lines which enables to remove one dimension compared to the full kinetic models. Moreover some weak collisional effects need to be taken into account to add diffusion and cut off the small scales in turbulence simulations.

Three kinds of method are generally used for such gyrokinetic simulations: fully Eulerian methods which use a grid of phase space and standard methods for transport equations like finite difference or finite volume methods with a Runge-Kutta time advance, this approach is used for example in the GENE code [4]; a second approach is the semi-Lagrangian method which is based on the method of characteristics and solves the characteristics backwards before interpolating at the grid points, this is used in the GYSELA code [3]; the third approach, which is the oldest, and that we use here is the particle in cell (PIC) method which approximates the distribution function by a set of macro-particles, see for example [5] which describes the ORB5 code. A excellent review article on the physics problems studied with such codes can be found in [2].

The PIC method we consider in this talk can be cast into a Monte Carlo setting. The quantities that need to be evaluated numerically being expected values with respect to the particle distribution function that is normalised to one and considered as being a probability density function. For this method to be competitive with the others, we need to apply noise reduction techniques to which an ample literature is devoted in the statistics community, see for example [7].

In this talk we place the gyrokinetic equation with a linear collision operator in the context of an abstract Fokker-Planck equation of the form

$$\frac{\partial f}{\partial t} + \nabla \cdot (\mathbf{A} f) - \frac{1}{2}\nu^2 \Delta_v f = 0. \tag{1}$$

The advection field $\mathbf{A}$ itself depends on the electromagnetic field. So the equation is nonlinear. But we won't discuss the computation of $\mathbf{A}$ here, as we will focus on how to reduce the noise in the evaluation of integral quantities related to the distribution function f from the particle data.

Without the collision term from which the $\Delta_v f$ stems, the equation would be a scalar transport equation that could be solved with the method of characteristics. With this term, the equation can be interpreted as a Fokker-Planck equation (or Kolmogorov backward equation) associated, using the Itô formalism, to the stochastic differential equation (SDE)

$$\mathrm{d}\mathbf{Z} = \mathbf{A}(t, \mathbf{Z})\mathrm{d}t + \nu \mathrm{d}\mathbf{W}$$

where $\mathbf{W}$ is a multidimensional Wiener process.

Now the charge and current densities which can be computed as velocity moments of the distribution functions are essential for the dynamics as they are the source terms for Maxwell's equation or their approximations that are used for the computation of the self-consistent electromagnetic field. In order to get a good accuracy in their computation, variance reduction techniques can be used. In particular for magnetic fusion applications, one can use the fact that the distribution function always stays fairly close to some analytically known equilibrium distribution. This has been used, since the 1990s in the context of the so-called δf method where the distribution function was linearised around the equilibrium distribution. This method has been later expanded to include non linear terms, but has always been expressed as a δf method. In our work, we take a different approach, where we consider a particle approximation of the full distribution function, but use the equilibrium function in order to compute the needed expected values with a considerably smaller variance. For example to compute the expected value of $\psi(\mathbb{Z})$, for some smooth function ψ, with respect to the probability density function f, we write

$$\mathbb{E}[\psi(\mathbb{Z})] = \int \psi(\mathbf{z}) f(\mathbf{z})\, \mathrm{d}\mathbf{z} = \int \psi(\mathbf{z})(f(\mathbf{z}) - f^0(\mathbf{z}))\, \mathrm{d}\mathbf{z} + \int \psi(\mathbf{z}) f^0(\mathbf{z})\, \mathrm{d}\mathbf{z}$$

where the last term can be computed analytically. Furthermore as the expected values corresponding to the first integral will be computed with the law of large number from the phase space position of marker particles representing the distribution functions $f(t, \mathbf{z})$ and $f^0(t, \mathbf{z})$, we need to represent both distribution functions with the same markers. In order to to this we need to introduce a weight for the second population of particles f^0. An equation for the evolution of the weights can be found using an extended phase space with the weight as an additional phase space variable [6, 7]. Note that it is possible, and generally done in practice, to use a third independent marker distribution g, with then two weights relating respectively f and f^0 to g.

This method works very well without collisions, and in this case the integration of the weights can be performed analytically using the characteristics. However, as shown in [6], the expected value of the weight increases as a function of time, making this control variate useless after some time.

In this talk, we perform an analysis of the problem and a solution to the weight growth problem using a splitting technique between transport and collision part and using the equilibrium function of the collision operator as the control variate f^0. Similar ideas have been used for low noise Monte Carlo simulations of the Boltzmann equations in [1].

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Wave motion

Shih-Hsien Yu

In this talk, we have presented a stable-unstable formulation to study a wave motion of linearized Burgers equation around a hyperbolic shock wave. This approach is done through a transform variable in the time domain so that the equation for the Green's function becomes an ODE. Through the ODE, the notion of stable-unstable can be used to derive an algebraic equation to describe the behavior of the wave motion crossing the shock front. Finally, those algebraic information can be transform wave propagation information in the space-time domain.

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