

A tale of two generalizations of Boltzmann equation

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Based on joint works
with Ampatzoglou and Miller

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Outline

- 1 The Boltzmann equation
- 2 Beyond binary interactions
 - Derivation of ternary Boltzmann equation
 - Derivation of the binary-ternary Boltzmann equation
- 3 Mixture of gases

The Boltzmann equation

The Boltzmann equation¹ :

$$(1.1) \quad \partial_t f + v \cdot \nabla_x f = Q_2(f, f)$$

- for the position $x \in \mathbb{R}^d$, the time $t \in \mathbb{R}^+$ and velocity $v \in \mathbb{R}^d$
- describes the evolution of the density $f(x, t, v)$ of gas particles
- where $Q_2(f, f)$ is a **quadratic integral operator that expresses the change of f due to instantaneous binary collisions of particles**. Its exact form depends on the type of interaction between particles.

¹was introduced by Maxwell and Boltzmann in late 1860's - early 1870's as a model that describes a dynamics of a dilute gas.

Who is who...

For a pair of particles let:

- $(\mathbf{v}', \mathbf{v}'_1)$ be their pre-collisional velocities, and $\mathbf{u}' = \mathbf{v}' - \mathbf{v}'_1$, $\sigma = \frac{u'}{|u'|}$.
- $(\mathbf{v}, \mathbf{v}_1)$ be their post-collisional velocities, and $\mathbf{u} = \mathbf{v} - \mathbf{v}_1$, $\hat{\mathbf{u}} = \frac{\mathbf{u}}{|\mathbf{u}|}$.

For elastic interactions, momentum and energy are conserved, i.e.

$$\begin{aligned} \mathbf{v} + \mathbf{v}_1 &= \mathbf{v}' + \mathbf{v}'_1, \\ |\mathbf{v}|^2 + |\mathbf{v}_1|^2 &= |\mathbf{v}'|^2 + |\mathbf{v}'_1|^2, \end{aligned}$$

thus,

$$\begin{aligned} \mathbf{v}' &= \frac{\mathbf{v} + \mathbf{v}_1}{2} + \frac{|\mathbf{v} - \mathbf{v}_1| \sigma}{2} \\ \mathbf{v}'_1 &= \frac{\mathbf{v} + \mathbf{v}_1}{2} - \frac{|\mathbf{v} - \mathbf{v}_1| \sigma}{2}, \quad \sigma \in S^{d-1}. \end{aligned}$$

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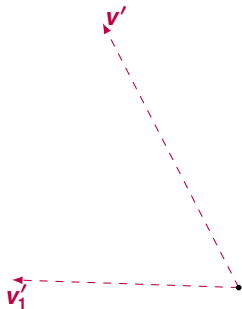
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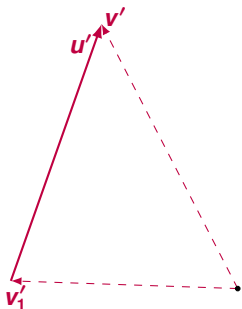
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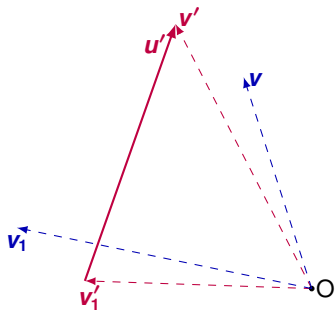
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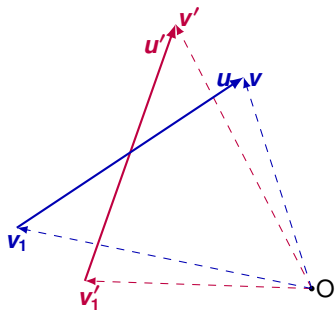
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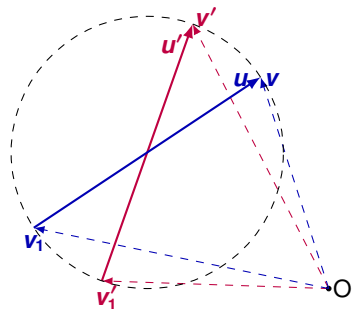
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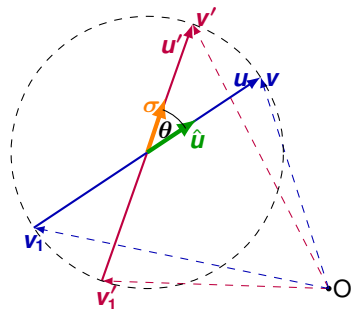
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The collisional operator

The collisional operator $Q_2(f, f)$ is defined via:

$$(1.2) \quad Q_2(f, f)(x, t, v) = \int_{\mathbb{R}^d} \int_{S^{d-1}} (f' f'_1 - f f_1) b(|u|, \hat{u} \cdot \sigma) d\sigma dv_1,$$

where

- $f' = f(x, t, v')$, $f'_1 = f(x, t, v'_1)$ etc.

The collisional kernel

In relevant physical applications, the collisional kernel $b(|u|, \hat{u} \cdot \sigma)$ is assumed to be of the form:

$$(1.3) \quad b(|u|, \hat{u} \cdot \sigma) = |u|^A \tilde{b}(\cos \theta),$$

where

- 1 $0 < A \leq 1$ corresponds to the variable hard potentials case
- 2 $A = 0$ corresponds to Maxwellian molecules
- 3 $-d < A < 0$ corresponds to the soft potentials case

First generalization of Boltzmann equation

Beyond binary interactions of particles - joint work with I. Ampatzoglou

Beyond binary interactions

- The Boltzmann equation takes into account only binary collisions of particles.
 - Ternary or higher order collisions are neglected due to lower probability of occurring compared to binary.
- However, when the gas is dense enough, higher order interactions are much more likely to happen.
 - An example of such a situation is a **colloid**, which is a homogeneous non-crystalline substance consisting of
 - ultramicroscopic particles of one substance dispersed through a second substance.
 - It was pointed out² by *Russ - Von-Günberg [2002]*, that multi interactions among particles significantly contribute to the grand potential of a colloidal gas and are modeled by a sum of higher order interaction terms.

²and further verified experimentally and numerically.

Our (long term) goal - joint work with I. Ampatzoglou

- Motivated by above, we aim to introduce and rigorously derive (from a system of classical particles) a kinetic model which goes beyond binary interactions, by incorporating a sum of higher order interaction terms in (1.1).
- Such an equation, which could serve as a toy model for a non-ideal gas, would be of the form:

$$(2.1) \quad \begin{cases} \partial_t f + v \cdot \nabla_x f = \sum_{k=2}^m Q_k(\underbrace{f, f, \dots, f}_{k\text{-times}}), & (t, x, v) \in (0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d, \\ f(0, x, v) = f_0(x, v), & (x, v) \in \mathbb{R}^d \times \mathbb{R}^d, \text{ where} \end{cases}$$

- $Q_k(\underbrace{f, f, \dots, f}_{k\text{-times}})$ is the k -th order collisional operator, and
- $m \in \mathbb{N}$ is the accuracy of the approximation.
- Equations similar to (2.1) were studied for Maxwell molecules in the works of Bobylev, Gamba and Cercignani using Fourier transform methods.

The case $m = 2$: Boltzmann equation

- The task of rigorously deriving an equation of the form (2.1) from a classical many particle system, even for the case $m = 2$, is a challenging problem³ that has been settled only in certain situations.
- For hard-sphere interactions,
 - the analysis was pioneered by *Lanford [1975]*,
 - and recently completed by *Gallagher - Saint-Raymond - Texier [2012]*.
- For short-range potentials, the analysis has been done in e.g.
 - *King [1975]*,
 - *Gallagher - Saint-Raymond - Texier [2012]*,
 - *Pulvirenti - Saffirio - Simonella [2014]*.

³Hilbert described this task, in his famous sixth problem, as one of the main challenges for mathematicians of the twentieth century.

The case $m = 3$: binary-ternary Boltzmann equation

- Up to our knowledge, the case $m = 3$ has not been studied at all.

$$\partial_t f + v \cdot \nabla_x f = Q_2(f, f) + Q_3(f, f, f), \quad (t, x, v) \in (0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d.$$

- In addition to understanding
 - binary interactions, and
 - interactions among three particles,
 - the case $m = 3$ requires careful analysis of their mutual interactions.
- We will come back to the case $m = 3$ at the end of the talk.

Derivation of ternary Boltzmann - joint work with I. Ampatzoglou

- Now we focus on rigorously deriving a purely ternary equation.

Challenge #1

How to make sense of ternary interactions so that we can detect their contributions?

Ternary interaction

- 1 In a typical dilute hard-sphere gas, the probability of a simultaneous contact of three hard-spheres is very small compared to e.g. the situation when one of the three particles is in simultaneous contact with two other particles.
- 2 In some physical situations, e.g. when one considers colloids as in *Russ - Von-Günberg [2002]* **interactions among three particles are determined by the sum of the distances of the interacting particles**, rather than by different geometric configurations.

Motivated by (1) and (2), we introduce the notion of a ternary interaction:

Definition

Let $\epsilon > 0$ and consider three particles i, j, k with positions and velocities $(x_i, v_i), (x_j, v_j), (x_k, v_k) \in \mathbb{R}^{2d}$. We say that the particles i, j, k are in $(i; j, k)$ ternary ϵ -interaction if the following geometric condition holds:

$$(2.2) \quad d^2(x_i; x_j, x_k) := |x_i - x_j|^2 + |x_i - x_k|^2 = 2\epsilon^2.$$

The parameter ϵ is called interaction zone.

Transformation of velocities at a ternary interaction

- Consider an $(i; j, k)$ ternary ϵ -interaction

$$(2.3) \quad |x_i - x_j|^2 + |x_i - x_k|^2 = 2\epsilon^2.$$

- Let v_i^*, v_j^*, v_k^* denote the velocities of the interacting particles after the interaction. Assuming the particles are of equal mass $m = 1$, we consider the interaction to be elastic i.e. the three particle momentum-energy system is satisfied:

$$(2.4) \quad v_i^* + v_j^* + v_k^* = v_i + v_j + v_k,$$

$$(2.5) \quad |v_i^*|^2 + |v_j^*|^2 + |v_k^*|^2 = |v_i|^2 + |v_j|^2 + |v_k|^2.$$

- Introducing the re-scaled vectors⁴:

$$(2.6) \quad \omega_1 := \frac{x_j(t) - x_i(t)}{\sqrt{2}\epsilon}, \quad \omega_2 := \frac{x_k(t) - x_i(t)}{\sqrt{2}\epsilon},$$

$$(2.3) \text{ is equivalent to } |\omega_1|^2 + |\omega_2|^2 = 1.$$

⁴We call the vectors ω_1, ω_2 impact directions of the interaction. 

More on transformations of velocities

- **Q:** How do we know that there is the unique solution to the system (2.4) - (2.5)?
- **A:** We impose an extra condition:
 - Since the i particle interacts with the pair of particles (j, k) , we assume that the velocities v_j, v_k transform with respect to the impact directions unit vector

$$(2.7) \quad \begin{pmatrix} v_j^* \\ v_k^* \end{pmatrix} = \begin{pmatrix} v_j \\ v_k \end{pmatrix} - c \begin{pmatrix} \omega_1 \\ \omega_2 \end{pmatrix},$$

for some $c \in \mathbb{R}$.

- Once we add condition (2.7) to the system (2.4) - (2.5), the new system has a unique solution that algebraically characterizes the conservation of momentum and energy for the type of ternary interaction defined in (2.2).
- From now on, when an $(i; j, k)$ interaction happens, we assume that velocities of the interacting particles instantaneously transform according to the collisional law

$$(2.8) \quad (v_i, v_j, v_k) \rightarrow (v_i^*, v_j^*, v_k^*).$$

The phase space

Definition

Let $d \in \mathbb{N}$, with $d \geq 2$, $N \in \mathbb{N}$ and $\epsilon > 0$. The phase space of the N -particle system of ϵ -interaction zone is defined as:

$$(2.9) \quad \mathcal{D}_{N,\epsilon} = \left\{ Z_N = (X_N, V_N) \in \mathbb{R}^{2dN} : d^2(x_i; x_j, x_k) \geq 2\epsilon^2 \quad \forall (i, j, k) \in \mathcal{I}_N \right\},$$

where

$$X_N = (x_1, \dots, x_N) \in \mathbb{R}^{dN},$$

$$V_N = (v_1, \dots, v_N) \in \mathbb{R}^{dN},$$

represent the positions and velocities of the N -particles and

$$\mathcal{I}_N = \left\{ (i, j, k) \in \{1, \dots, N\}^3 : i < j < k \right\}.$$

Evolution of the system of N particles

Consider an initial configuration $Z_N \in \mathcal{D}_{N,\epsilon}$. The motion is described as follows:

- ❶ Particles perform rectilinear motion as long as there is no interaction i.e.

$$\dot{x}_i = v_i, \quad \dot{v}_i = 0, \quad \forall i \in \{1, \dots, N\}.$$

- ❷ Assume now that

- an initial configuration $Z_N = (X_N, V_N)$ has evolved until time $t > 0$, reaching $Z_N(t) = (X_N(t), V_N(t))$, and
- there is an $(i; j, k)$ interaction at time t .

Then the velocities $v_i(t), v_j(t), v_k(t)$ instantaneously transform according to

$$(2.10) \quad (v_i(t), v_j(t), v_k(t)) \rightarrow (v_i^*(t), v_j^*(t), v_k^*(t)).$$

Challenge #2

- It is not obvious that (I)-(II) produce a well defined dynamics, since the system can possibly run into pathological configurations.
- In the case of binary interactions, *Alexander [1975]* established global well-defined dynamics, but that work does not apply to the notion of our ternary interaction.
- For ternary interactions:
 - We prove that a global in time, measure-preserving flow can be defined for almost all initial configurations.
 - In order to go from local to global in time flow we establish the following crucial fact - **if a triplet of particles was in the interaction then as the system evolves in time the subsequent interaction cannot involve the same triplet of particles.**

The Liouville equation

The global measure-preserving interaction flow yields the Liouville equation for the N -particle probability density f_N :

$$(2.11) \quad \begin{aligned} \partial_t f_N + \sum_{i=1}^N v_i \cdot \nabla_{x_i} f_N &= 0, \quad (t, Z_N) \in (0, \infty) \times \dot{\mathcal{D}}_{N,\epsilon}, \\ f_N(t, Z_N) &= f_N(t, Z_N^*), \quad \text{whenever } d^2(x_i; x_j, x_k) = 2\epsilon^2 \text{ for } (i, j, k) \in \mathcal{I}_N. \\ f_N(0, Z_N) &= f_{N,0}(Z_N), \quad Z_N \in \dot{\mathcal{D}}_{N,\epsilon}, \end{aligned}$$

where

$$\begin{aligned} Z_N^* &= (X_N, V_N^*), \\ V_N^* &= (v_1, \dots, v_{i-1}, v_i^*, v_{i+1}, \dots, v_{j-1}, v_j^*, v_{j+1}, \dots, v_{k-1}, v_k^*, v_{k+1}, \dots, v_N). \end{aligned}$$

Ternary Boltzmann equation

- Integrating by parts the Liouville equation, we derive a linear finite hierarchy of equations, referred to as BBGKY hierarchy.
- By considering the number of particles $N \rightarrow \infty$, and the interaction zone $\epsilon \rightarrow 0^+$ in the **new scaling**:

$$(2.12) \quad N\epsilon^{d-\frac{1}{2}} \simeq 1,$$

we arrive at the infinite hierarchy of equations, called Boltzmann hierarchy.

- Boltzmann hierarchy admits a special class of factorized solutions with the factor solving the new **ternary** Boltzmann equation:

$$(2.13) \quad \begin{cases} \partial_t f + v \cdot \nabla_x f = Q_3(f, f, f), & (t, x, v) \in (0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d, \\ f(0, x, v) = f_0(x, v), & (x, v) \in \mathbb{R}^d \times \mathbb{R}^d. \end{cases}$$

Ternary kernel

The expression $Q_3(f, f, f)$ is the cubic collisional kernel, given by:

$$Q_3(f, f, f) = \int_{\mathbb{S}_1^{2d-1} \times \mathbb{R}^{2d}} \frac{b_+(\omega_1, \omega_2, v_1 - v, v_2 - v)}{\sqrt{1 + \langle \omega_1, \omega_2 \rangle}} (f^* f_1^* f_2^* - f f_1 f_2) d\omega_1 d\omega_2 dv_1 dv_2,$$

where

$$b_+ = \max\{b, 0\},$$

$$b = b(\omega_1, \omega_2, v_1 - v, v_2 - v) := \langle \omega_1, v_1 - v \rangle + \langle \omega_2, v_2 - v \rangle,$$

$$f^* = f(t, x, v^*), \quad f = f(x, t, v),$$

$$f_1^* = f_1(t, x, v_1^*), \quad f_1 = f(t, x, v_1),$$

$$f_2^* = f_2(t, x, v_2^*), \quad f_2 = f(t, x, v_2),$$

Challenge #3

- Proving convergence of the BBGKY hierarchy to the (infinite particle) Boltzmann hierarchy - the heart of which lies in
 - 1 Identifying good configurations⁵ and studying their stability under adjunction of a collisional pair of particles, which turns out to be possible thanks to
 - 2 New geometric estimates
 - Spherical estimates of the intersection of \mathbb{S}_1^{2d-1} with $K_\rho^d \times \mathbb{R}^d$, where K_ρ^d is a solid cylinder in \mathbb{R}^d of radius ρ .
 - A transition map (which allows us to control post-collisional configurations using new ellipsoidal estimates)
 - Ellipsoidal estimates of the intersection of $(2d - 1)$ -dimensional ellipsoids with $K_\rho^d \times \mathbb{R}^d$.

⁵configurations that do not run into any kind of interactions under backwards time evolution.  

A remark about symmetrized equation

- The phase space (2.9) will produce the kinetic equation (2.13), in which the tracked particle is always the central particle of the interactions occurring.
- By working in the phase space

$$\tilde{D}_{N,\epsilon} = \{Z_N = (X_N, V_N) \in \mathbb{R}^{2dN} : d_l^2(x_i, x_j, x_k) \geq 2\epsilon^2, \quad \forall (i, j, k, l) \in \tilde{\mathcal{I}}_N\},$$

where

$$\tilde{\mathcal{I}}_N = \{(i, j, k, l) : (i, j, k) \in \mathcal{I}_N \text{ and } l : \{i, j, k\} \rightarrow \{i, j, k\} \text{ is a permutation}\},$$

$$d_l(x_i, x_j, x_k) = \sqrt{|x_{l_i} - x_{l_j}|^2 + |x_{l_i} - x_{l_k}|^2},$$

and using similar arguments, one can derive a symmetrized version of (2.13), in which the tracked particle can be either central or adjacent.

- It has been shown by Ampatzoglou, that the symmetrized ternary equation satisfies similar statistical and entropy production properties as the classical Boltzmann equation.

Derivation of the binary-ternary Boltzmann equation - joint work with I. Ampatzoglou

Recently we have completed the next step in our program - derivation of equation (2.1) for $m = 3$:

$$(2.14) \quad \begin{cases} \partial_t f + v \cdot \nabla_x f = Q_2(f, f) + Q_3(f, f, f), \\ f(0) = f_0, \end{cases}$$

We call this equation the **binary–ternary Boltzmann equation**.

Challenge #1 - detecting both binary and ternary interactions

The first challenge we face in deriving (2.14) is to provide a mathematical framework allowing us to detect **both**:

- binary

$$d_2(x_i, x_j) := |x_i - x_j| = \epsilon,$$

- and ternary

$$d_3(x_i; x_j, x_k) := \sqrt{|x_i - x_j|^2 + |x_i - x_k|^2} = \sqrt{2}\epsilon$$

interactions among particles.

A crucial, conceptual obstacle is the apparent incompatibility of the Boltzmann-Grad scaling dictated by binary interactions

$$(2.15) \quad N\epsilon^{d-1} = 1,$$

and the scaling of ternary interactions

$$(2.16) \quad N\epsilon^{d-1/2} = 1.$$

Addressing incompatibility of scalings

We overcome the scaling problem by assuming that

- particles are hard spheres of diameter ϵ_2 ,
- that can also interact as triplets via the interaction zone ϵ_3 , in the common scaling

$$(2.17) \quad N\epsilon_2^{d-1} = N\epsilon_3^{d-1/2} = 1.$$

- Note that (2.17) implies that $\epsilon_2 \ll \epsilon_3$.

Challenge #2 - decoupling binary and ternary interactions

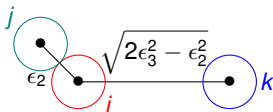
Our framework a-priori allows i.e. that particles i and j interact as hard spheres:

$$d_2(x_i, x_j) = \epsilon_2,$$

while at the same time there is another particle k such that the particle i interacts with the particles j and k :

$$d_3(x_i, x_j, x_k) = \sqrt{2}\epsilon_3,$$

as illustrated here:



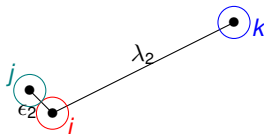
Pathological configurations, including the one above, are going to be shown to be negligible (far from trivial).

Decoupled interactions

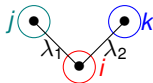
We show that as long as $0 < \epsilon_2 < \epsilon_3 < 1$, only the following two interaction scenarios are possible with non-trivial probability under time evolution:

- **Pure binary:** Two particles interact as hard-spheres while all other particles are not involved in any binary or ternary interactions at the same time.
- **Pure ternary:** Three particles interact via an interaction zone, while none of them is involved in a binary interaction with either of the other two particles of the interaction zone at the same time.

Pure binary interaction: $\epsilon_2^2 + \lambda_2^2 > 2\epsilon_3^2$, $\lambda_2 > \epsilon_2$.

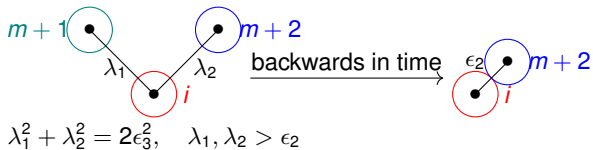


Pure ternary interaction: $\lambda_1^2 + \lambda_2^2 = 2\epsilon_3^2$, $\lambda_1, \lambda_2 > \epsilon_2$.



Challenge #3 - the stability of a good configuration

- Assume that we have a good configuration⁶ of m -particles and we add σ particles to the system, where $\sigma \in \{1, 2\}$, such that a binary or ternary interaction is formed among one of the existing particles and the σ new particles.
- Under backwards time evolution, the system could run into another binary or ternary interaction, e.g.



- This is the first time there was the need to address the possibility of a newly formed interacting configuration running into an interaction of a different type.
- We develop novel algebraic and geometric tools to show that outside of a small measure set, negligible in the limit, the newly formed configuration does not run into any additional interactions backwards in time.

⁶a configuration which does not run into any kind of interactions under backwards time evolution.

Current and future work

- Small data global well-posedness for the kinetic equation involving binary and ternary interactions (joint with Ampatzoglou, Gamba, and Tasković).
- Generation and propagation of moments for a binary-ternary Boltzmann equation (Ampatzoglou and Tasković).
- Derivation of a kinetic equation involving a linear combination of m interactions (joint work with Ampatzoglou)

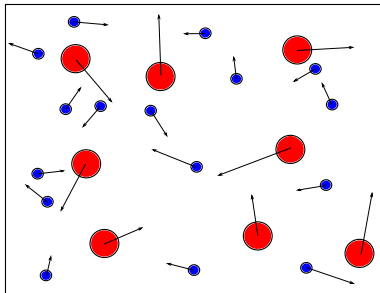
Second generalization of Boltzmann equation

Mixture of gases - joint with I. Ampatzoglou and J. Miller

Physical Motivation

Much effort has been put into studying the dynamics of a collection of interacting gases.

- Gas mixtures such as helium and xenon were studied as a possible coolant for nuclear reactors in spacecraft and thermoacoustic refrigerators.
- Sound propagation in binary mixtures and hypersonic shockwave analysis for aerospace applications have also been studied.



Boltzmann's Equation for Mixtures

Let us consider two gases, one of type A and the other of type B. If

- $g_0(x, v) : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ is an initial density distribution on phase space of the type A gas, and
- $h_0(x, v) : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ the distribution of the type B gas,

the evolution of the two gases is modeled by the Boltzmann system for mixtures:

$$(3.1) \quad \begin{cases} \partial_t g + v \cdot \nabla_x g = c_{1,1} Q_{1,1}(g, g) + c_{1,2} Q_{1,2}(g, h) \\ \partial_t h + v \cdot \nabla_x h = c_{2,2} Q_{2,2}(h, h) + c_{2,1} Q_{2,1}(h, g), \\ g(0, x, v) = g_0(x, v), \quad h(0, x, v) = h_0(x, v). \end{cases}$$

Results about (3.1) include:

- First formulations [Chapman, Cowling - 1950's], [Hamel - 1960's]
- LWP of system [Ha, Noh - 2010]
- Stability around Maxwellians [Briant, Daus - 2016]
- Propagation of moments [de la Canal, Gamba, Pavić Čolić - 2020].

Rigorous Derivation?

Despite the mathematical progress on the subject of the system (3.1), no work has been done on rigorously deriving the system from a system of particles.

A system of finitely many hard spheres

We derive the Boltzmann system (3.1) from a mixture of finitely many hard spheres. In order to do this, we consider

- N_1 hard spheres of mass M_1 and diameter ϵ_1 , mixed with
- N_2 hard spheres of mass M_2 and diameter ϵ_2 .
- For the i^{th} particle of mass M_1 , we denote its center by x_i and its velocity by v_i .
- Similarly, for the i^{th} particle of mass M_2 , we denote its center by y_i and its velocity by w_i .

For notational simplicity, we will write the vector of all positions and velocities by

$$Z_{(N_1, N_2)} = (x_1, \dots, x_{N_1}, y_1, \dots, y_{N_2}, v_1, \dots, v_{N_1}, w_1, \dots, w_{N_2}).$$

The natural phase space for this collection of particles is

$$\mathcal{D}_{(\epsilon_1, \epsilon_2)}^{(N_1, N_2)} := \left\{ Z_{(N_1, N_2)} : \begin{array}{l} \forall i \neq j, |x_i - x_j| \geq \epsilon_1, |y_i - y_j| \geq \epsilon_2, \\ \forall i, j, |x_i - y_j| \geq \frac{\epsilon_1 + \epsilon_2}{2} \end{array} \right\}.$$

Evolution of the system of $N_1 + N_2$ particles

- (i) If non-collisional, we assume that the particles perform rectilinear motion, i.e.

$$(3.2) \quad \begin{cases} \dot{x}_i = v_i, & \dot{y}_j = w_j \\ \dot{v}_i = 0, & \dot{w}_j = 0. \\ (x_i(0), v_i(0)) = (x_{i,0}, v_{i,0}), & (y_j(0), w_j(0)) = (y_{j,0}, w_{j,0}). \end{cases}$$

- (ii) For a collisional pair of particles, we assume the collision is completely elastic, i.e. energy and momentum are conserved under collisions. Consequently, we have four collisional laws, including:

- If (x_i, v_i) and (y_j, w_j) are such that $|x_i - y_j| = (\epsilon_1 + \epsilon_2)/2$, then the pre-collisional velocities (v_i, w_j) give rise to the post-collisional velocities (v_i^*, w_j^*) by

$$(3.3) \quad v_i^* = v_i - \frac{2M_2}{M_1 + M_2} \left((v_i - w_j) \cdot \frac{(x_i - y_j)}{\|x_i - y_j\|} \right) \frac{(x_i - y_j)}{\|x_i - y_j\|}$$

$$(3.4) \quad w_j^* = w_j + \frac{2M_1}{M_1 + M_2} \left((v_i - w_j) \cdot \frac{(x_i - y_j)}{\|x_i - y_j\|} \right) \frac{(x_i - y_j)}{\|x_i - y_j\|}.$$

Liouville equation

We prove that for almost every initial configuration in phase space, the flow (I)-(II) is well defined and measure preserving. Consequently, an initial density $f_{(N_1, N_2), 0}$ on the phase space $\mathcal{D}_{(\epsilon_1, \epsilon_2)}^{(N_1, N_2)}$ evolves according to the Liouville equation:

$$(3.5) \quad \begin{cases} \partial_t f_{(N_1, N_2)} + \sum_{k=1}^{N_1} \mathbf{v}_k \cdot \nabla_{x_k} f_{(N_1, N_2)} + \sum_{k=1}^{N_2} \mathbf{w}_k \cdot \nabla_{y_k} f_{(N_1, N_2)} = 0 \text{ on } \mathring{\mathcal{D}}_{(\epsilon_1, \epsilon_2)}^{(N_1, N_2)} \\ f_{(N_1, N_2)}(Z_{(N_1, N_2)}^*) = f_{(N_1, N_2)}(Z_{(N_1, N_2)}) \text{ on } \partial \mathcal{D}_{(\epsilon_1, \epsilon_2)}^{(N_1, N_2)}, \\ f_{(N_1, N_2)}(0) = f_{(N_1, N_2), 0} \end{cases}$$

where $Z_{(N_1, N_2)}^*$ is the post-collisional configuration related to the pre-collisional configuration $Z_{(N_1, N_2)}$ by the collisional laws.

Partial symmetry

In order to understand the statistical behavior of the $N_1, N_2, \epsilon_1, \epsilon_2$ particle system, we require each of the particles of the same mass to behave identically. Namely:

- $f_{(N_1, N_2)}$ is invariant under permutations of the (x_i, v_i) variables and
- $f_{(N_1, N_2)}$ is invariant under permutations of the (y_j, w_j) variables.
- Note that we do not require that $f_{(N_1, N_2)}$ is invariant under interchanging (x_i, v_i) and (y_j, w_j) variables for any i, j .

This lack of symmetry forces $f_{(N_1, N_2)}$ to take into account the behavior of each type of particles, but places the $N_1, N_2, \epsilon_1, \epsilon_2$ particle system outside of the standard framework developed for hard sphere systems of a single type.

The concept of a mixed marginal

In order to handle this partial symmetry symmetry, we introduce a mixed marginal:

Definition

For each $s \in \{1, \dots, N_1 - 1\}$ and $\ell \in \{1, \dots, N_2 - 1\}$ we define the *mixed marginal* of $f_{(N_1, N_2)}$ to be

$$f_{(N_1, N_2)}^{(s, \ell)} := \int \mathbb{1}_{\mathcal{D}_{(\epsilon_1, \epsilon_2)}^{(N_1, N_2)}} f_{(N_1, N_2)} dx_{s+1} \dots dx_{N_1} dv_{s+1} \dots dv_{N_1} dy_{\ell+1} \dots dy_{N_2} dw_{\ell+1} \dots dw_{N_2}.$$

This concept of a mixed marginal is key to our analysis and allows us to distinguish the behavior of both types of particles.

Convergence result

Theorem (Ampatzoglou, Miller, P. - 2021)

Let $N_1, N_2, \epsilon_1, \epsilon_2$ obey the mixed Boltzmann-Grad scalings. Then on certain Gaussian weighted L^∞ spaces, the following equations are locally well posed in the mild formulation:

- 1 BBGKY Hierarchy,
- 2 Boltzmann Hierarchy,
- 3 Boltzmann System for Mixtures.

Additionally, solutions of (1) converge in observables to solutions of (2) for a sequence of approximate initial data:

$$(3.6) \quad f_{N_1, N_2}^{(s, \ell)} \rightsquigarrow f^{(s, \ell)}, \quad f_{N_1, N_2, 0}^{(s, \ell)} := \mathbb{1}_{\mathcal{D}_{\epsilon_1, \epsilon_2}^{s, \ell}} f_0^{(s, \ell)}$$

Propagation of Chaos as a corollary of the convergence result

Corollary (Ampatzoglou, Miller, P. - 2021)

Let (g, h) solve the Boltzmann system (3.1) with initial data $(g_0, h_0) \in (L^\infty(\mathbb{R}^{2d}))^2$. Then solutions of the BBGKY hierarchy with initial data

$$(3.7) \quad f_{N_1, N_2, 0}^{(s, \ell)} := \mathbb{1}_{\mathcal{D}_{\epsilon_1, \epsilon_2}^{s, \ell}} g_0^{\otimes s} \otimes h_0^{\otimes \ell}$$

converge in the sense of observables

$$(3.8) \quad f_{N_1, N_2}^{(s, \ell)} \rightsquigarrow g^{\otimes s} \otimes h^{\otimes \ell}.$$

Relationship between constants

The constants $c_{1,2}$, $c_{2,1}$ are given by

$$(3.9) \quad c_{1,2} = c_2 \left(\frac{1+b}{2} \right)^{d-1}, \quad c_{2,1} = c_1 \left(\frac{1+b^{-1}}{2} \right)^{d-1},$$

where $\epsilon_1 \equiv b\epsilon_2$.

- Note that (3.9) shows that as b grows large, the constant $c_{1,2}$ grows large while the constant $c_{2,1}$ becomes small.
- This agrees with physical intuition that if one gas is comprised of larger particles than the other, it has a larger effect on the system as a whole.

Thank you!