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From the Kinetic Theory of Gases to Aerosol Flows

CMLS, Ecole polytechnique, France François Golse†

The Vlasov-Stokes and the Vlasov-Navier-Stokes systems used in the description of thin sprays or aerosol flows can be derived from the system of Boltzmann equations for binary gas mixtures. One component of this mixture is the dispersed phase (particles or droplets in the aerosol), while the other component is the propellant gas. The Vlasov-Stokes or Vlasov-Navier-Stokes systems are obtained in appropriate scaling regimes by a rather delicate asymptotic analysis.

1 Introduction

This talk reports on recent progress on the derivation of models for aerosol flows obtained in collaboration with E. Bernard, L. Desvillettes and V. Ricci [1,2].

An aerosol, or a spray, consists of a dispersed phase (solid particles or liquid droplets) moving in a surrounding gas, referred to as the propellant. A class of models for thin sprays (i.e. when the volume fraction of the dispersed phase is $\ll 0.1$) involves a noncollisional kinetic, Vlasov type equation for the dispersed phase coupled to a fluid equation for the propellant via the drag force on the particles or droplets exerted by the surrounding gas. For instance, when compressibility effects in the propellant can be neglected, one can use the Vlasov-Navier-Stokes system

$$\partial_t F + v\cdot\nabla_x F = \tfrac{\kappa}{m_p}\nabla_v\cdot((v-u)F)\,,\quad \nabla_x\cdot u = 0\,,$$
$$\partial_t u + u\cdot\nabla_x u + \tfrac{1}{\rho_g}\nabla_x p = \nu\Delta_x u + \tfrac{\kappa}{\rho_g}\int (v-u)F dv\,.$$

The unknowns in this system are the velocity distribution function $F \equiv F(t,x,v)$ of the dispersed phase, and the velocity field $u \equiv u(t,x) \in \mathbf{R}^3$ and pressure $p \equiv p(t,x)$ of the propellant. The parameters ν and κ are respectively the kinematic viscosity of the propellant and the friction coefficient, while m_p is the mass of the droplets or particles[1] and ρ_g the (constant) gas density. When the motion of the propellant is slow, the Vlasov-Stokes system can be used

$$\partial_t F + v\cdot\nabla_x F = \tfrac{\kappa}{m_p}\nabla_v\cdot((v-u)F)\,,$$
$$\nu\Delta_x u + \tfrac{\kappa}{\rho_g}\int (v-u)F dv = \tfrac{1}{\rho_g}\nabla_x p\,,\quad \nabla_x\cdot u = 0\,.$$

The purpose of this talk is to explain how these systems can be justified by means of systematic asymptotic analysis.

†E-mail: francois.golse@polytechnique.edu

[1]We assume for simplicity that the aerosol is monodisperse, i.e. all the particles or droplets in the dispersed phase are identical (with the same size and the same mass).

2 Rigorous justification of the Brinkman force

In a first series of results [3–5], one studies the quasi-static flow of the propellant around a slowly moving system of spherical particles or droplets[2] centered at N points denoted $c_1,\dots,c_N$ in a spatial domain Ω of $\mathbf{R}^3$ with smooth boundary $\partial\Omega$, moving with velocities $v_1,\dots,v_N \in \mathbf{R}^3$. Let $\Omega_r := \{x\in\Omega \text{ s.t. } |x-c_k|>r \text{ for } k=1,\dots,N\}$. The Stokes equation set in the spatial domain Ω_r is studied in the limit $r\to 0$ while $Nr=\lambda>0$:

$$\nu\Delta_x u_r = \tfrac{1}{\rho_g}\nabla_x p_r - \mathbf{f}\,,\qquad \nabla_x\cdot u_r = 0\,,\quad x\in\Omega_r\,,$$
$$u_r(x) = v_k \text{ for } |x-c_k|=r\,,\quad u_r(x)=0 \text{ for } x\in\partial\Omega\,,$$

where $\mathbf{f}$ is a square integrable, solenoidal force field. That the scaling condition $r=\lambda/N\to 0$ is natural follows from the classical formula for the drag force exerted by a slow, viscous incompressible flow on a sphere (see fla. (20.14), referred to as "Stokes' formula", in the Landau-Lifshitz treatise[6] on fluid mechanics). Roughly speaking, since the drag force on a sphere of radius r is proportional to r, one expects that the drag force exerted on a system of N spheres of radius r should be proportional to Nr, provided that these spheres are sufficiently far from each other so as to be treated independently.

Theorem 1.[4] Under the scaling condition above, assume

$$\sum_{k=1}^N |v_k|^2 \le \text{Const. } N\,,\quad \frac{1}{N}\sum_{k=1}^N \delta_{c_k,v_k} \to F(x,v)\,,$$

(where δ_{c_k,v_k} is the 6-dimensional Dirac "function" centered at c_k,v_k), and that the particle centers satisfy the separation condition

$$k\neq l \implies |c_k-c_l| > 2r^{1/3} \quad \text{and } \operatorname{dist}(c_k,\partial\Omega) > r^{1/3}\,.$$

[2]The exchange of torque between the dispersed phase and the propellant is neglected since $r\ll 1$.

Then $u_r \to u$ as $r \to 0$, where

$$\nu\Delta_x u + 6\pi\nu\lambda \int (v-u)Fdv = \tfrac{1}{\rho_g}\nabla_x p_r - \mathbf{f}\,,$$
$$\nabla_x \cdot u = 0 \ \text{ for } x \in \Omega\,, \quad u(x) = 0 \ \text{ for } x \in \partial\Omega\,.$$

The proof is based on homogenization techniques involving the notion of harmonic capacity, pioneered by V.A. Marchenko, E. Ya. Khruslov and their collaborators. The steady Navier-Stokes equation with Brinkman force can also be derived in the same way. Whether the separation condition is propagated under the dynamics of the dispersed phase remains unknown at the time of this writing, and this is why the Vlasov-Stokes or Vlasov-Navier-Stokes systems have not yet been established by this procedure. Even if this could be achieved, particle configurations satisfying the separation condition would remain of low probability in the sense of statistical mechanics, and this casts doubts on the physical interest of this approach. It should be mentioned that Hillairet [5)] has generalized the theorem above under a less stringent, and therefore more satisfying separation condition.

3 Kinetic model

Another approach to establishing the Vlasov-Navier-Stokes system uses the coupled system of Boltzmann equations for the propellant and the dispersed phase viewed as a binary gas mixture. Its unknowns are the velocity distribution functions in the dispersed phase and in the propellant, denoted respectively by $F \equiv F(t,x,v)$ and $f \equiv f(t,x,w)$. The system of Boltzmann equations governing the evolution of F and f is

$$\partial_t F + v\cdot\nabla_x F = \mathcal{B}(F,F) + \mathcal{D}(F,f)\,,$$
$$\partial_t f + w\cdot\nabla_x f = \mathcal{R}(f,F) + \mathcal{C}(f,f)\,,$$

where $\mathcal{C}(f,f)$ is the Boltzmann integral describing the instantaneous variation of f due to collisions between gas molecules. Similarly, $\mathcal{D}(F,f)$, resp. $\mathcal{R}(f,F)$ are collision integrals describing the instantaneous variation of F, resp. f, due to collisions between gas molecules and particles or droplets in the dispersed phase. Finally $\mathcal{B}(F,F)$ is the integral accounting for the effect of collisions in the dispersed phase. This model involves the following parameters:

Parameter	Definition
L	size of the container
$\mathcal{N}_p$	number of dust particles$/L^3$
$\mathcal{N}_g$	number of gas molecules$/L^3$
V_p	thermal speed of particles
V_g	thermal speed of molecules
S_{pg}	particle/gas cross-section
S_{gg}	molecular cross-section
$\eta = m_g/m_p$	mass ratio
$\epsilon = V_p/V_g$	thermal speed ratio
$\mu = m_p\mathcal{N}_p/m_g\mathcal{N}_g$	mass fraction

Introducing the dimensionless variables

$$\hat{x} = x/L\,, \quad \hat{v} = v/V_p\,, \quad \hat{w} = w/V_g\,, \quad \hat{t} = tV_p/L$$

and the dimensionless distribution functions

$$\hat{F}(\hat{t},\hat{x},\hat{v}) = \frac{V_p^3 F(t,x,v)}{\mathcal{N}_p}\,, \quad \hat{f}(\hat{t},\hat{x},\hat{w}) = \frac{V_g^3 f(t,x,w)}{\mathcal{N}_g}\,,$$

we arrive at the dimensionless form of the system of Boltzmann equations

$$\partial_{\hat{t}}\hat{F} + \hat{v}\cdot\nabla_{\hat{x}}\hat{F} = \mathcal{N}_p S_{pp} L\mathcal{B}(F,F) + \tfrac{\mathcal{N}_g S_{pg} L}{\epsilon}\mathcal{D}(F,f)$$
$$\partial_{\hat{t}}\hat{f} + \hat{w}\cdot\nabla_{\hat{x}}\hat{f} = \mathcal{N}_p S_{pg} L\mathcal{R}(f,F) + \tfrac{\mathcal{N}_g S_{gg} L}{\epsilon}\mathcal{C}(f,f)$$

Henceforth we assume that $\mathcal{N}_p S_{pp} L \ll 1$ so that the effect of collisions between solid particles or droplets in the dispersed phase can be neglected to leading order. Then we also postulate that

$$\mathcal{N}_g S_{pg} L = \epsilon/\eta\,, \quad \mathcal{N}_p S_{pg} L = (\mathcal{N}_g S_{gg} L)^{-1} = \epsilon/\mu$$

with $\eta \ll \epsilon \ll \mu$. Dropping hats on dimensionless quantities to simplify the notation, and neglecting right away the dispersed phase collision integrals, we arrive at the scaled Boltzmann system

$$\partial_t F + v\cdot\nabla_x F = \frac{1}{\eta}\mathcal{D}(F,f)\,,$$
$$\partial_t f + \frac{1}{\epsilon} w\cdot\nabla_x f = \frac{1}{\mu}\mathcal{R}(f,F) + \frac{\mu}{\epsilon^2}\mathcal{C}(f,f)\,.$$

The collision integrals $\mathcal{C}(f,f)$, $\mathcal{D}(F,f)$, and $\mathcal{R}(f,F)$ act on the velocity variables of f and F and satisfy the following identities:

$$\int \mathcal{C}(f,f)dw = \int \mathcal{R}(f,F)(w)dw = \int \mathcal{D}(F,f)dv = 0\,,$$

expressing the local conservation law of the particle number in either the dispersed phase or the propellant, together with

$$\int \mathcal{C}(f,f)wdw = 0\,,$$

expressing the local momentum conservation law in the propellant, and

$$\epsilon \int \mathcal{D}(F,f) v dv + \eta \int \mathcal{R}(f,F) w dw = 0\,,$$

expressing the momentum balance in the interaction of the dispersed phase with the propellant.

4 Dimensionless form of the collision integrals

The dimensionless form of the Boltzmann collision integral for a monatomic propellant is

$$\mathcal{C}(f,f)(t,x,w) = \iint_{|\omega|=1} (f'f'_* - ff_*) c(w-w_*,\omega) dw_* d\omega$$

where in the r.h.s. f (resp. f_*, f', f'_*) designates $f(t,x,v)$ (resp. $f(t,x,w_*)$, $f(t,x,w')$, $f(t,x,w'_*)$), while

$$c(W,\omega) = |W| \sigma_{gg}(|W|, |\cos(\widehat{W,\omega})|)\,,$$

where σ_{gg} is the differential cross-section of gas molecules. The notation w', w'_* designates

$$\begin{aligned} w' &= w'(w,w_*,\omega) = w - (w-w_*)\cdot\omega\omega\,,\\ w'_* &= w'_*(w,w_*,\omega) = w_* + (w-w_*)\cdot\omega\omega\,. \end{aligned}$$

In other words, (w', w'_*) runs through the set of all pre-collision velocity pairs leading to post-collision velocities (w, w_*) as ω runs through the unit sphere, assuming that the gas molecules are point particles and that the collisions are elastic. In particular, the Boltzmann collision integral satisfies the local conservation law of energy: for each continuous and rapidly decaying distribution function f,

$$\int \mathcal{C}(f,f) \tfrac{1}{2}|w|^2 dw = 0\,.$$

The dimensionless form of the collision integrals for the interaction between the dispersed phase and the propellant is slightly more involved. First one can assume that the solid particles or droplets in the dispersed phase are point particles, and that the collisions with the gas molecules are elastic. Denoting

$$\begin{aligned} &j(F,f)(t,x,v,w,\omega)\\ &:= F(t,x,v'')f(t,x,w'') - F(t,x,v)f(t,x,w) \end{aligned}$$

with

$$\begin{aligned} v'' &= v''(v,w,\omega) = v - \tfrac{2\eta}{1+\eta}(v - \tfrac{1}{\epsilon}w)\cdot\omega\omega\,,\\ w'' &= w''(v,w,\omega) = w - \tfrac{2}{1+\eta}(w-\epsilon v)\cdot\omega\omega\,, \end{aligned}$$

one has, in the case of elastic collisions

$$\begin{aligned} \mathcal{D}(F,f) &= \iint_{|\omega|=1} j(F,f) b(\epsilon v - w, \omega) dw d\omega\,,\\ \mathcal{R}(f,F) &= \iint_{|\omega|=1} j(F,f) b(\epsilon v - w, \omega) dv d\omega\,. \end{aligned}$$

In this case again, the collision kernel b is

$$b(U,\omega) = |U| \sigma_{pg}(|U|, |\cos(\widehat{U,\omega})|)\,,$$

where σ_{pg} is the differential cross-section of particles or droplets in the dispersed phase with the gas molecules. These collision integrals satisfy the energy balance identity

$$\epsilon^2 \int \mathcal{D}(F,f) \tfrac{1}{2}|v|^2 dv + \eta \int \mathcal{R}(F,f) \tfrac{1}{2}|v|^2 dv = 0$$

for all continuous and rapidly decaying F and f.

Another model for the collisions between the dispersed phase and the propellant is based on the idea that the droplets or solid particles in the dispersed phase are macroscopic objects, and that impinging gas molecules are diffusely reflected. In that case, the collision integrals take the form

$$\begin{aligned} &\mathcal{D}(F,f)(t,x,v)\\ &= \iint F(t,x,V) f(t,x,W) K_{pg}(v,V,W) dV dW\\ &\quad - F(t,x,v) \iint f(t,x,W) K_{pg}(\tilde{v},v,W) d\tilde{v} dW\,,\\ &\mathcal{R}(f,F)(t,x,w)\\ &= \iint F(t,x,V) f(t,x,W) K_{gp}(w,V,W) dV dW\\ &\quad - f(t,x,w) \iint F(t,x,V) K_{gp}(\tilde{w},V,w) d\tilde{w} dV\,, \end{aligned}$$

where

$$\begin{aligned} &K_{pg}(v,V,W)\\ &= \int_{|n|=1} (n\cdot(\epsilon V - W))_+ (n\cdot(\tfrac{\epsilon V+\eta W}{1+\eta} - \epsilon v))_+ dn\\ &\quad \times \tfrac{\beta^4\epsilon^3}{2\pi^2} (\tfrac{1+\eta}{\eta})^4 \exp(-\tfrac{\beta^2}{2}(\tfrac{1+\eta}{\eta})|\epsilon v - \tfrac{\epsilon V+\eta W}{1+\eta}|^2)\,,\\ &K_{gp}(w,V,W)\\ &= \int_{|n|=1} (n\cdot(\epsilon V - W))_+ (n\cdot(w - \tfrac{\epsilon V+\eta W}{1+\eta}))_+ dn\\ &\quad \times \tfrac{\beta^4}{2\pi^2} (1+\eta)^4 \exp(-\tfrac{\beta^2}{2}((1+\eta)|w - \tfrac{\epsilon V+\eta W}{1+\eta}|^2)\,. \end{aligned}$$

In these formulas, $\beta = \sqrt{\eta m_p / 2\pi k_B T_{surf}}$, where k_B is the Boltzmann constant and T_{surf} the temperature at the surface of the particles or droplets. See Ref. 7 for a thorough description of this model.

5 Main results

Assume that the collision kernels c and b satisfy Grad's "hard" angular cutoff condition:

$$\begin{aligned} 0 < c(W,\omega) &\le c_*(1+|W|)^\gamma\,,\\ 0 < b(U,\omega) &\le b_*(1+|U|)^\beta\,, \end{aligned}$$

for some $b_*, c_* > 1$ and $\beta, \gamma \in [0,1]$, while

$$\int_{|\omega|=1} c(W,\omega)d\omega \geq \frac{1}{c_*(1+|W|)}\,,$$
$$\int_{|\omega|=1} b(U,\omega)d\omega \geq \frac{1}{b_*(1+|U|)}\,.$$

Assume also that the radial function $\alpha \equiv \alpha(|w|)$ such that[3]

$$\iint_{|\omega|=1} (\alpha(|w|)w_1w_2 + \alpha(|w_*|)w_{*1}w_{*2} - \alpha(|w'|)w'_1w'_2$$
$$-\alpha(|w'_*|)w'_{*1}w'_{*2})c(|w-w_*|,\omega)M(w_*)dw_*d\omega = w_1w_2$$

is bounded, where $M(w) := (2\pi)^{-3/2}\exp(-|w|^2/2)$ is the centered, reduced Maxwellian equilibrium density (with unit pressure and temperature). For instance, if the collision kernel c is function of the form[4] $c(W,\omega) = C(|\cos(\widehat{W,\omega})|)$, the function α is a (positive) constant.

Theorem 2[1]. Assume that $\mu = 1$ and $\eta \ll \epsilon^2 \to 0$, and that $(F_{\epsilon,\eta}, f_{\epsilon,\eta})$ is a solution to the scaled Boltzmann system. Assume that

$$\sup_{\substack{t+|x|\leq R\\ v\in\mathbf{R}^3}} (1+|v|)^p|F_{\epsilon,\eta}(t,x,v) - F(t,x,v)| \to 0$$

for some $p > 3$ where F is locally bounded, while $f_{\epsilon,\eta}(t,x,w) = M(w)(1+\epsilon g_{\epsilon,\eta}(t,x,w))$ and

$$\int_0^T\iint_{|x|\leq R} |g_{\epsilon,\eta}(t,x,w) - g(t,x,w)|^2M(w)dwdxdt \to 0$$

where g is locally bounded. Then g is of the form

$$g(t,x,w) = \rho(t,x) + u(t,x)\cdot w + \theta(t,x)\tfrac{1}{2}(|w|^2-3)$$

where (F,u) is a solution of the Vlasov-Navier-Stokes system with

$$\nu = \tfrac{2}{15\sqrt{2\pi}}\int_0^\infty \alpha(r)r^6e^{-r^2/2}dr$$
$$\kappa = \tfrac{1}{3}\int |w|^2Q(|w|)M(w)dw$$

where

$$Q(|U|) = \begin{cases} 8\pi\displaystyle\int_0^1 \sigma_{pg}(|U|,\lambda)\lambda^2d\lambda & \text{(elastic case)}\\ \dfrac{\sqrt{2\pi}}{3\beta} + |U| & \text{(inelastic case)}\end{cases}$$

Theorem 3[1]. Assume that $\eta \ll \epsilon^2 \ll \mu^4 \to 0$, and that $(F_{\mu,\epsilon,\eta}, f_{\mu,\epsilon,\eta})$ is a solution to the scaled Boltzmann system. Assume that

$$\sup_{\substack{t+|x|\leq R\\ v\in\mathbf{R}^3}} (1+|v|)^p|F_{\mu,\epsilon,\eta}(t,x,v) - F(t,x,v)| \to 0$$

for some $p > 3$ where F is locally bounded, while $f_{\mu,\epsilon,\eta}(t,x,w) = M(w)(1+\epsilon g_{\mu,\epsilon,\eta}(t,x,w))$ and

$$\int_0^T\iint_{|x|\leq R} |g_{\mu,\epsilon,\eta} - g|^2(t,x,w)(1+|w|)^qM(w)dwdxdt \to 0$$

for some $q > 1$, where g is locally bounded. Then g is of the form

$$g(t,x,w) = \rho(t,x) + u(t,x)\cdot w + \theta(t,x)\tfrac{1}{2}(|w|^2-3)$$

where (F,u) is a solution of the Vlasov-Stokes system and μ and κ are given by the same formulas as in Theorem 2.

The statements of Theorems 2 and 3 include assumptions on the solutions which we do not know how to verify so far. In that sense, these theorems, although rigorous from the mathematical point of view, are "formal" justifications of the Vlasov-Stokes or Vlasov-Navier-Stokes systems in the style of Refs. 9 and 10.

A significant part of the proofs of Theorems 2 and 3 is the derivation of the Navier-Stokes equations for incompressible flows, or of the Stokes equations, from the Boltzmann equation of the kinetic theory of gases (by a joint small Mach and small Knudsen number[5] asymptotic limit). The present understanding of these fluid dynamic limits of the Boltzmann equation is very satisfying: see Refs. 9–14 and chapter 3.2 in the book [15].

The new feature in the proofs of Theorems 2 and 3 is the derivation of the drag force which couples the Vlasov equation for the dispersed phase to the motion equation (Stokes or Navier-Stokes) for the propellant. The key idea in this derivation is best explained in the case of elastic collisions between the dispersed phase and the propellant. Due to the small mass ratio η, the velocity of a particle or droplet in the dispersed phase is only slightly deflected due to collisions with a gas molecule. On the other hand, a gas molecule impinging on a heavier droplet or particle in the dispersed phase is almost specularly reflected. The integrand $j(F_{\epsilon,\eta}, f_{\epsilon,\eta})(t,x,v,w,\omega)$ is of order η and can be approximated by the first term in its Taylor expansion, because $f_{\epsilon,\eta}$ is a centered Maxwellian at leading order.

6 Conclusion

This talk discusses two strategies for deriving the Vlasov-Navier-Stokes and Vlasov-Stokes systems used in

[3] See Ref. 8 for the proof of existence and uniqueness of this function.

[4] Molecular interactions leading to such collision kernels are referred to as "(pseudo-)Maxwellian molecules".

[5] The Knudsen number is the ratio of the mean free path of gas molecules to the typical length scale in the flow of a gas described by the Boltzmann equation.

the modeling of thin sprays. The first strategy is based on complete mathematical results on the homogenization of the steady Stokes or Navier-Stokes equations, and provides a fully rigorous justification of the formula for the friction force exerted on the fluid by the dispersed phase. However, this approach put stringent conditions on the minimal distance between droplets or solid particles in the dispersed phase, whose persistence under the dynamics remains unclear at the time of this writing. This seriously complicates the task of deriving the coupled Vlasov-Stokes or Vlasov-Navier-Stokes equations by this procedure.

The second approach uses a kinetic description of the spray or aerosol viewed as a binary gas mixture, by a coupled system of Boltzmann equations. Describing the dispersed phase in terms of a Boltzmann equation is not a "first principle" model — in other words, it is not equivalent to writing Newton's second law of motion for each particle in the dispersed phase. On the other hand, this approach makes it possible to include collision effects between the particles or droplets in the dispersed phase. We have not discussed these effects in the present work for the sake of simplicity, but several physical phenomena could be taken into account with the formalism introduced in this talk (polydispersion, coagulation, fragmentation ...).

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