From the Kinetic Theory of Gases to Models for Aerosol Flows

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Works in collaboration with E. Bernard, L. Desvillettes, V. Ricci

Aerosol/Spray Flows

Aerosol/Spray=dispersed phase (solid particles, droplets) in a gas (sometimes referred to as the propellant)

A class of models for aerosols/sprays consists of

(a) a kinetic equation for the dispersed phase

(b) a fluid equation for the gas/propellant

The kinetic equation for the dispersed phase and the fluid equation for the propellant are coupled by the friction force

Aerosol/Spray flows arise in different contexts (from diesel engines to medical aerosols in the trachea and the upper part of the lungs)

Problem: How to justify these models?

In the Context of Diesel Engines...

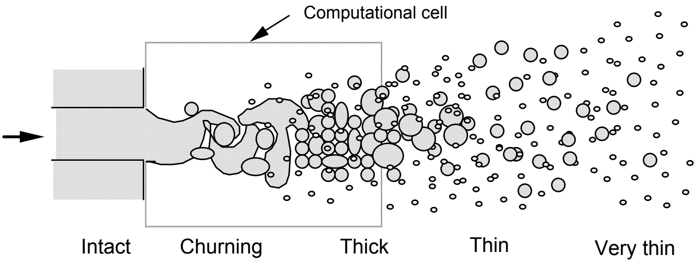


Figure: Schematic representation of spray regimes for liquid injection from a single hole nozzle [R.D. Reitz "Computer Modeling of Sprays" 1996]

Terminology taken from [P.J. O'Rourke's Ph.D. Thesis "Collective Drop Effects on Vaporizing Liquid Sprays" , Princeton University, 1981]

Thin vs. Very Thin Sprays

Local volume fraction of the dispersed phase denoted $\phi(t, x)$

•Very thin spray regime (typically $\phi(t, x) \ll 10^{-3}$)
Volume fraction of the dispersed phase negligible; particles in the dispersed phase accelerated by the friction force exerted by the propellant; no feedback from the dispersed phase on the propellant

Typical model Vlasov equation for the dispersed phase, driven by the fluid (e.g. Navier-Stokes) equation

•Thin spray regime (typically $\phi(t, x) \ll 10^{-1}$)
Same as in the very thin spray regime, except that the feedback interaction of the dispersed phase on the propellant is taken into account

Typical model Vlasov-Navier-Stokes or Vlasov-Stokes systems

Unknowns:

$F \equiv F(t,x,v)$ particle distribution function (in the dispersed phase)
$u \equiv u(t,x)$ and $p \equiv p(t,x)$ velocity and pressure fields (propellant)

Vlasov eqn for F...

$$\partial_t F + v \cdot \nabla_x F - \kappa \,\mathrm{div}_v((v-u)nF) = 0$$

... coupled to the **Navier-Stokes** eqn for (u,p) (here $\mathrm{Ma} \ll 1$)

$$\begin{cases} \mathrm{div}_x\, u = 0 \\ \partial_t u + u \cdot \nabla_x u = -\frac{1}{n}\nabla_x p + \nu \Delta_x u + \underbrace{\kappa \int (v-u) F dv}_{0 \text{ for very thin sprays}} \end{cases}$$

Parameters:

$\kappa =$ friction coefficient, $n =$ gas density, and $\nu =$ viscosity of the gas

DERIVING NAVIER-STOKES + BRINKMAN FORCE

THE HOMOGENIZATION APPROACH

L. Desvillettes, F.G., V. Ricci
J. Stat. Phys. **131** (2008), 941–967

Dispersed phase=moving system of N identical rigid spheres centered at $X_k(t) \in \mathbf{R}^3$ for $k = 1, \ldots, N$, with radius $r > 0$

Time-dependent domain filled by the propellant

$$\Omega_g(t) := \{x \in \mathbf{R}^3 \text{ s.t. } \operatorname{dist}(x, X_k(t)) > r \quad \text{for } k = 1, \ldots, N\}$$

Fluid equation for the propellant: Navier-Stokes + external force

$$\begin{cases} (\partial_t + u \cdot \nabla_x)u = -\nabla_x p + \nu\Delta_x u + \mathbf{f}\,, \quad \operatorname{div}_x u = 0\,, \quad x \in \Omega_g(t) \\ u(t, \cdot)\big|_{\partial B(X_k(t), r)} = \dot{X}_k(t)\,, \quad k = 1, \ldots, N \end{cases}$$

Solid rotation/Torque of each particle around its center neglected (one is interested in a limit where $r \to 0$)

Small parameter $0 < \tau \ll 1$; dispersed phase assumed to be slow
Slow time variable

$$\hat{t} = \tau t$$

Scaling of the particle/droplets dynamical quantities

$$X_k(t) = \hat{X}_k(\hat{t})\,, \quad \dot{X}_k(t) = \tau \hat{V}_k(\hat{t}) \quad \text{with } \hat{V}_k = \frac{d\hat{X}_k}{d\hat{t}}$$

Scaling of the fluid dynamical quantities

$$u(t,x) = \tau \hat{u}(\hat{t},x)\,, \quad p(t,x) = \tau \hat{p}(\hat{t},x)\,, \quad \mathbf{f}(t,x) = \tau \hat{\mathbf{f}}(\hat{t},x)$$

Inserting this in the Navier Stokes equation, one finds

$$\begin{cases} \tau(\partial_{\hat{t}} + \hat{u} \cdot \nabla_x)\hat{u} = -\nabla_x \hat{p} + \nu \Delta_x \hat{u} + \hat{\mathbf{f}}\,, \quad \operatorname{div}_x \hat{u} = 0 \\ \hat{u}(\hat{t},\cdot)\big|_{\partial B(\hat{X}_k(\hat{t}),r)} = \hat{V}_k(\hat{t}) \end{cases}$$

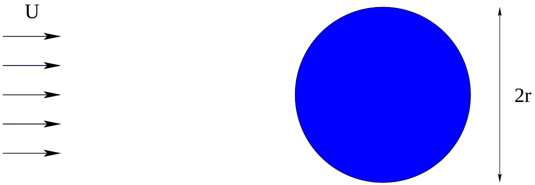
Drag Force: Stokes Formula

Stokes formula (1851) for the drag force exerted on a sphere of radius r by a viscous fluid of viscosity μ with velocity U at infinity

$$6\pi\mu rU$$

Total friction exerted by N noninteracting spheres of radius r

$$6\pi\mu NrU$$



Homogenization Assumptions

Scaling assumption on particle radius r and particle number N:

$$N \to \infty\,, \quad r \to 0\,, \quad Nr \to 1$$

Spacing condition: bounded domain $\mathcal{O}$ with smooth boundary $\partial\mathcal{O}$

$$\mathrm{dist}(X_k, X_l) > 2r^{1/3} \text{ and } \mathrm{dist}(X_k, \partial\mathcal{O}) > r^{1/3}\,, \quad 1 \le k \ne l \le N$$

Particle distribution function F continuous on $\bar{\mathcal{O}} \times \mathbf{R}^3$ s.t.

$$F_N := \frac{1}{N}\sum_{k=1}^{N} \delta_{x_k, v_k} \to F\,, \quad \sup_{N \ge 1} \iint_{\mathcal{O}\times\mathbf{R}^3} |v|^2 F_N < \infty$$

External force $\mathbf{f} \equiv \mathbf{f}(x) \in \mathbf{R}^3$ s.t.

$$\mathrm{div}_x\, \mathbf{f} = 0\,, \qquad \int_{\mathcal{O}} |\mathbf{f}(x)|^2 dx < \infty$$

Theorem 1 (Derivation of the Brinkman Force)

Let $\mathcal{O}_r := \{x \in \mathcal{O} \text{ s.t. } \operatorname{dist}(x, X_k) > r \text{ for all } 1 \leq k \leq N\}$, and for each $0 < r \ll 1$, let u_r be the solution to the Stokes equation

$$\left\{\begin{array}{ll}\nabla_x p_r = \nu\Delta_x u_r + \mathbf{f}\,, & \operatorname{div}_x u_r = 0\,, \quad x \in \mathcal{O}_r\\ u_r\big|_{\partial B(x_k,r)} = v_k\,, & u_r\big|_{\partial\mathcal{O}} = 0\end{array}\right.$$

Then, in the limit as $r \to 0$, one has

$$\int_{\mathcal{O}_r} |\nabla u_r(x) - \nabla u(x)|^2 dx$$

where u is the solution to the Stokes equation with friction force

$$\left\{\begin{array}{l}\nabla_x p = \nu\Delta_x u + \mathbf{f} + 6\pi\nu \displaystyle\int (v-u) F dv\,, \quad x \in \mathcal{O}\\ \operatorname{div}_x u = 0\,, \quad u\big|_{\partial\mathcal{O}} = 0\end{array}\right.$$

Extensions/Open Pbms

(1) Argument extends without difficulty to steady Navier-Stokes, provided that $\nu \geq \nu_0[\mathbf{f}, F, \mathcal{O}] > 0$

See also [Allaire: Arch. Rational Mech. Anal. 1990] (periodic case, based on earlier work by Cioranescu-Murat, and Khruslov's group)

(2) Recent improvement by Hillairet (arXiv:1604.04379v2 [math.AP]) relaxing the spacing condition

(3) In order to derive the coupled VNS system, one could try to propagate the spacing condition by the dynamics. Some ideas (on a different pbm) in [Jabin-Otto: Commun Math. Phys. 2004]?

(4) But even if one can propagate the spacing condition, such configurations are of negligible statistical weight...

DERIVING VLASOV-NAVIER-STOKES FROM THE KINETIC THEORY OF A BINARY GAS MIXTURE

E. Bernard, L. Desvillettes, F.G., V. Ricci
Comm. Math. Sci. **15** (2017), 1703–1741
(Kinetic and Related Models **11** (2018), 43–69)

A Multiphase Boltzmann System

Unknowns:

$F(t, x, v) =$ distribution function of dust particles/droplets
$f(t, x, w) =$ distribution function of gas molecules

Multiphase Boltzmann equation

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

Collision integrals:

•$\mathcal{D}(F, f)$ deflection of particles by collisions with gas molecules
•$\mathcal{R}(f, F)$ friction of gas molecules due to collisions with particles
•$\mathcal{C}(f)$ Boltzmann collision integral for gas molecules

Dispersed phase collisions possible, but neglected here for simplicity

Table of 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 dust particles
V_g	thermal speed of gas molecules
S_{pg}	particle/gas cross-section
S_{gg}	molecular cross-section
$\eta = m_g/m_p$	mass ratio (gas molecules/particles)
$\epsilon = V_p/V_g$	thermal speed ratio (particles/gas)

Dimensionless Quantities

Dimensionless variables

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

Dimensionless distribution functions

$$\hat{F} = V_p^3 F/\mathcal{N}_p\,, \qquad \hat{f} = V_g^3 f/\mathcal{N}_g$$

Dimensionless Boltzmann system

$$\partial_{\hat{t}}\hat{F} + \hat{v}\cdot\nabla_{\hat{x}}\hat{F} = \mathcal{N}_g S_{pg} L \frac{V_g}{V_p}\hat{\mathcal{D}}(\hat{F},\hat{f})$$

$$\partial_{\hat{t}}\hat{f} + \frac{V_g}{V_p}\hat{w}\cdot\nabla_{\hat{x}}\hat{f} = \mathcal{N}_p S_{pg} L \frac{V_g}{V_p}\hat{\mathcal{R}}(\hat{f},\hat{F}) + \mathcal{N}_g S_{gg} L \frac{V_g}{V_p}\hat{\mathcal{C}}(\hat{f})$$

Scaling assumptions

$$\begin{cases} \epsilon := V_p/V_g = \mathcal{N}_p S_{pg} L = (\mathcal{N}_g S_{gg} L)^{-1} \ll 1 \\ \\ \eta := \mathcal{N}_p/\mathcal{N}_g \ll \epsilon^2 \end{cases}$$

Scaled Boltzmann system — dropping hats on scaled quantities

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

Assumption on the **gas distribution function**

$$f(t, x, w) = M(w)(1 + \epsilon g(t, x, w)), \quad \underbrace{M(w) := \frac{1}{(2\pi)^{3/2}} e^{-|w|^2/2}}_{\text{centered Maxwellian}}$$

(Maxwell-)Boltzmann collision integral given by

$$\mathcal{C}(f)(w) = \iint_{\mathbf{R}^3\times\mathbf{S}^2} (f(w')f(w'_*) - f(w)f(w_*))c(|\tfrac{w-w_*}{|w-w_*|}\cdot\omega|)dw_*d\omega$$

where

$$\begin{cases} w' = w \ - (w - w_*)\cdot\omega\omega \\ w'_* = w_* + (w - w_*)\cdot\omega\omega \end{cases}$$

Pseudo-Maxwellian collision kernel for the gas molecules with

$$4\pi\int_0^1 c(\mu)d\mu = 1$$

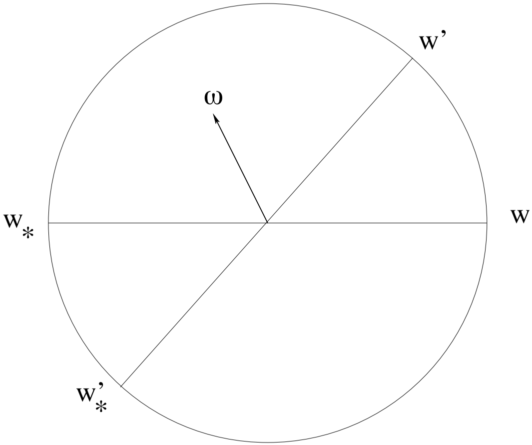


Figure: Unit vector $\omega =$ exterior angle bissector of $(w-\widehat{w_*, w'}-w'_*)$

Scaled Deflection/Friction Operators: Elastic Case

Deflection $\mathcal{D}$ and **friction** $\mathcal{R}$ integrals given by

$$\begin{cases} \mathcal{D}(F,f)(v) = \iint_{\mathbf{R}^3\times\mathbf{S}^2} (F(v'')f(w'') - F(v)f(w))b(\epsilon v - w,\omega)dwd\omega \\ \mathcal{R}(f,F)(w) = \iint_{\mathbf{R}^3\times\mathbf{S}^2} (f(w'')F(v'') - f(w)F(v))b(\epsilon v - w,\omega)dvd\omega \end{cases}$$

where

$$v'' = v - \tfrac{2\eta}{1+\eta}\left(v - \tfrac{1}{\epsilon}w\right)\cdot\omega\omega\,, \qquad w'' = w - \tfrac{2}{1+\eta}\,(w - \epsilon v)\cdot\omega\omega$$

Collision kernel of the form $b(z,\omega) = B(|z|, |\omega\cdot\frac{z}{|z|}|)$ s.t.

$$0 < b(z,\omega) \le B_*(1+|z|)\,, \quad \int_{\mathbf{S}^2} b(z,\omega)d\omega \ge \frac{1}{B_*}\frac{|z|}{1+|z|} \qquad \text{a.e.}$$

Model developed by F. Charles [PhD Thesis, ENS Cachan 2009

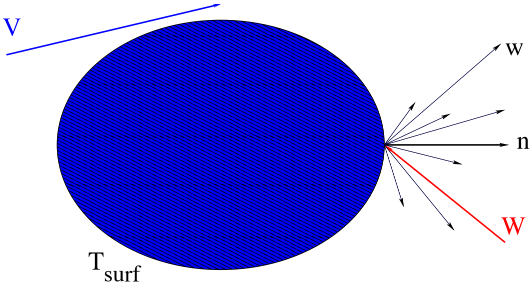


Figure: Diffuse reflection of gas molecules at the surface of a particle or of a droplet with surface temperature T_{surf}; velocity of particle/droplet denoted V; molecular velocity denoted w, W

Deflection $\mathcal{D}$ and **friction** $\mathcal{R}$ integrals given by

$$\mathcal{D}(F,f)(v)=\iint f(W)(F(V)K_{pg}(v|V,W)-F(v)K_{pg}(V|v,W))dVdW$$

$$\mathcal{R}(f,F)(w)=\iint F(V)(f(W)K_{gp}(w|V,W)-f(w)K_{pg}(W|V,w))dVdW$$

Inelastic kernels denoting $\beta := \sqrt{m_g/k_B T_{surf}}$, collision kernels are

$$K_{pg}(v|V,W) := \frac{\epsilon^3}{\pi}\int_{\mathbf{S}^2} P[\beta\tfrac{1+\eta}{\eta}](\tfrac{\epsilon V+\eta W}{1+\eta}-\epsilon v, n)((\epsilon V-W)\cdot n)_+ dn$$

$$K_{gp}(w|V,W) := \frac{1}{\pi}\int_{\mathbf{S}^2} P[\beta(1+\eta)](w-\tfrac{\epsilon V+\eta W}{1+\eta}, n)((\epsilon V-W)\cdot n)_+ dn$$

where

$$P[\lambda](\xi,n) := \frac{\lambda^4}{2\pi}\exp(-\tfrac{1}{2}\lambda^2|\xi|^2)(\xi\cdot n)_+$$

Theorem 2 (Formal VNS limit)

Let $(F_n, f_n = M(1+\epsilon_n g_n))$ be a sequence of solutions to the scaled Boltzmann system with $\eta_n \ll \epsilon_n^2$. Assume $F_n \to F$ and $g_n \to g$ with

$$(a)\ \sup_{t+|x|\leq R}\left(\sup_v |v|^7 F_n(t,x,v) + \int g_n(t,x,w)^2 M(w)dw\right) < \infty$$

$$(b)\ \int_{t+|x|<R}\left|\int (g-g_n)\phi M dv\right|^2 dxdt \to 0$$

for all $R>0$ and all continuous bounded $\phi \equiv \phi(t,x,v)$. Then

$$F \equiv F(t,x,v) \qquad \text{and} \qquad u(t,x) := \int wg(t,x,w)M(w)dw$$

satisfy the VNS system with friction rate κ defined below and

$$\frac{1}{\nu} := 6\pi \int_0^1 c(\mu)(\tfrac{5}{3}-\mu^2)\mu^2 d\mu$$

Unknowns:

$$F \equiv F(t,x,v) \geq 0, \quad u \equiv u(t,x) \in \mathbf{R}^3\,, \quad \text{and } p \equiv p(t,x) \in \mathbf{R}$$

$$\begin{cases} \partial_t F + v \cdot \nabla_x F - \kappa \operatorname{div}_v((v-u)F) = 0 \\ \partial_t u + u \cdot \nabla_x u = -\nabla_x p + \nu \Delta_x u + \kappa \displaystyle\int (v-u) F dv \\ \operatorname{div}_x u = 0 \end{cases}$$

Lemma A (Drag force)

Under the assumptions of Theorem 2

$$\frac{1}{\eta_n}\mathcal{D}(F_n, f_n)(t,x,v) \to \kappa\, \mathrm{div}_v((v-u(t,x))F(t,x,v))$$

with

$$\kappa := \begin{cases} \frac{8\pi}{3}\int |z|^2 M(z)\left(\int_0^1 B(|z|,\mu)\mu^2 d\mu\right) dz & \text{elastic} \\ \frac{1}{3}\int \left(\frac{\sqrt{2\pi}}{3\beta}+|z|\right)|z|^2 M(z) dz & \text{inelastic} \end{cases}$$

Key Idea for the Proof of Lemma A

Let $\phi \equiv \phi(v)$ be a smooth test function; collision symmetries imply

$$J := \frac{1}{\eta}\int \phi(v)\mathcal{D}(F,f)(v)dv$$

$$= \iint F(v)f(w)\left(\int \frac{1}{\eta}\underbrace{(\phi(v)-\phi(v''))}_{\text{Taylor expand at } v} b(\epsilon v - w,\omega)d\omega\right) dvdw$$

since

$$v'' = v - \tfrac{2\eta}{1+\eta}\left(v - \tfrac{1}{\epsilon}w\right)\cdot\omega\omega \quad \text{with } \eta \ll \epsilon^2 \ll 1$$

Hence

$$J \simeq -\iint F(v)f(w)\nabla\phi(v)\cdot\left(\int (v - \tfrac{1}{\epsilon}w)\cdot\omega\omega b(\epsilon v - w,\omega)d\omega\right)dvdw$$

$$\simeq -\kappa\int F(v)(v-u)\cdot\nabla\phi(v)dv \quad \text{and integrate by parts}$$

Lemma B (Brinkman (friction) force)

Under the assumptions of Theorem 2

$$\frac{1}{\epsilon_n}\int \mathcal{R}(f_n,F_n)(t,x,w)wdw \to \kappa\int (v-u(t,x))F(t,x)dv$$

Proof The integrals $\mathcal{D}(f_n,F_n)$ and $\mathcal{R}(F_n,f_n)$ satisfy the momentum balance identity

$$\epsilon_n\int \mathcal{D}(f_n,F_n)(t,x,v)vdv+\eta_n\int \mathcal{R}(F_n,f_n)(t,x,w)wdw=0$$

Multiply both sides by $1/\epsilon_n\eta_n$, apply Lemma A and integrate by parts

Fluctuation g_n of distribution function in the propellant satisfies

$$\epsilon_n \partial_t g_n + w \cdot \nabla_x g_n = M^{-1}\mathcal{R}(f_n, F_n) + M^{-1}\mathcal{C}(Mg_n) - \frac{1}{\epsilon_n} \underbrace{\mathcal{L}g_n}_{\text{lin'd coll. } \int}$$

Asymptotic fluctuation

$$\mathcal{L}g_n \to 0 \implies g(t,x,w) = \rho(t,x) + u(t,x)\cdot w + \theta(t,x)\tfrac{1}{2}(|w|^2 - 3)$$

Continuity equation

$$\epsilon_n \partial_t \int g_n M dw + \operatorname{div}_x \int w g_n M dw = 0 \implies \operatorname{div}_x u = 0$$

Momentum equation

$$\epsilon_n \partial_t \int w g_n M dw + \operatorname{div}_x \int w \otimes w g_n M dw = \int w \mathcal{R}(f_n, F_n) dw \to 0$$

$$\implies \nabla_x(\rho + \theta) = 0$$

Rescaled momentum equation, where $A(w) := w \otimes w - \frac{1}{3}|w|^2 I$

$$\underbrace{\partial_t \int w g_n M dw}_{\to u} + \operatorname{div}_x \frac{1}{\epsilon_n} \int A(w) g_n M dw + \underbrace{\nabla_x \int \frac{|w|^2}{3\epsilon_n} g_n M dw}_{\to \nabla_x \text{sthg}}$$

$$= \underbrace{\frac{1}{\epsilon_n} \int w \mathcal{R}(f_n, F_n) dw}_{\to \kappa \int (v-u) F dv}$$

Key point Observing that

$$\frac{1}{\epsilon_n} \int A(w) g_n M dw = \frac{1}{\epsilon_n} \int (\mathcal{L}^{-1} A)(w) \frac{1}{\epsilon_n} \mathcal{L} g_n M dw$$

and using the Boltzmann equation to express $\frac{1}{\epsilon_n} \mathcal{L} g_n$ shows that

$$\frac{1}{\epsilon_n} \int A(w) g_n M dw \to A(u) - \nu(\nabla_x u + (\nabla_x u)^T - \tfrac{2}{3}(\operatorname{div}_x u) I)$$

Conclusion/Extensions/Open Problems

We have presented two methods for deriving the Vlasov-Navier-Stokes system for aerosols in the thin regimes, starting either from a fluid model with immersed discrete dispersed phase, or from a kinetic model for a binary mixture

The kinetic model can be easily extended

(a) to derive the Vlasov-Stokes system

(b) to include an equation for the fluctuations of temperature

(c) to take into account compressibility in the propellant

(d) to take into account collisions in the dispersed phase

(e) to take into account polydispersion

One advantage of the kinetic model is the possibility of a description of the drag force richer than Stoke's formula
(a) inelastic collision model with temperature of the dispersed phase
(b) detailed description of rarefied flow past a sphere
[Sone-Aoki Rarefied Gas Dyn. 1977, J. Méc. Th. Appl. 1983, Sone-Aoki-Takata Phys. Fluids 1993, Taguchi J. Fluid Mech. 2015]

Formal derivations of the Navier-Stokes equation from the Boltzmann equation are well understood [Sone: Rarefied Gas Dyn. 1969, Bardos-G.-Levermore: C.R. Acad. Sci. 1988 & J. Stat. Phys. 1991]

Rigorous derivations are much more difficult, but well understood [DeMasi-Esposito-Lebowitz: Comm. on Pure Appl. Math. 1990 (local in t), Bardos-Ukai: Math. Models Meth. Appl. Sci. 1993 (small data), G.-Saint-Raymond: Invent. Math. 2004 (global in t and all data)]