Validation of spray models

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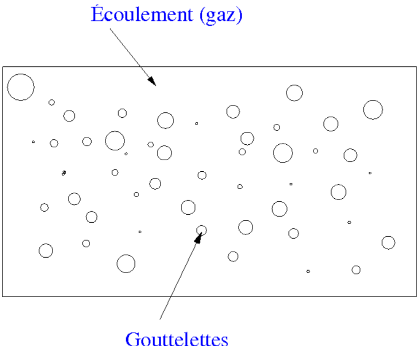
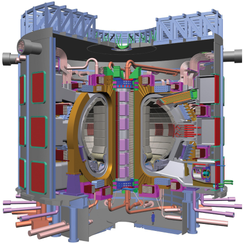
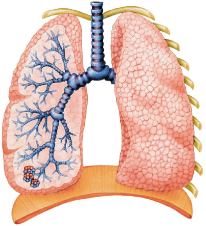
Sprays

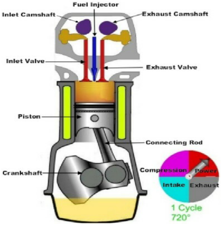
Dispersed Phase (i.-e. of small volume fraction, for example **droplets** or **dust**) in an Underlying Gas: their study is a subdomain of the study of multiphase flows



Domains of application







Multiphase flows: Microscopic modeling

We denote Ω_g the domain of the gas, Ω_p the domain of the droplets. For each phase, we write an Euler or a NS equation (for example, here, both viscous and incompressible) :

$$\partial_t u + \nabla_x \cdot (u \otimes u) + \nabla_x p = \nu_g \, \Delta_x u \quad \text{for} \quad x \in \Omega_g,$$

$$\partial_t u + \nabla_x \cdot (u \otimes u) + \nabla_x p = \nu_p \, \Delta_x u \quad \text{for} \quad x \in \Omega_p,$$

$$\nabla_x \cdot u = 0, \quad \text{for} \quad x \in \Omega_g \cup \Omega_p,$$

Boundary conditions on the free interface $\partial\Omega_g = \partial\Omega_p$.

Difficulties: useful only when the dispersed phase is not too dispersed (not too many droplets).

Multiphase flows: Macroscopic modeling (Eulerian-Eulerian methods)

Volume fraction of gas: $\alpha := \alpha(t,x) \in [0,1]$. Equations of Euler or NS type in the whole space (here both inviscid, compressible and isentropic):

$$\partial_t(\alpha\,\rho_g) + \nabla_x \cdot (\alpha\,\rho_g\,u_g) = 0,$$

$$\partial_t(\alpha\,\rho_g\,u_g) + \nabla_x \cdot (\alpha\,\rho_g\,u_g \otimes u_g) + \alpha\,\nabla_x p = D\,(u_p - u_g),$$

$$\partial_t((1-\alpha)\,\rho_p) + \nabla_x \cdot ((1-\alpha)\,\rho_p\,u_p) = 0,$$

$$\partial_t((1-\alpha)\,\rho_p\,u_p) + \nabla_x \cdot ((1-\alpha)\,\rho_p\,u_p \otimes u_p) + (1-\alpha)\nabla_x p = -D\,(u_p - u_g).$$

Pressure laws:

$$p = p_1(\rho_g) = p_2(\rho_p).$$

Traditional method of derivation: averaging of microscopic equations [uses empirical closures], Cf. Ishii. **Difficulties**: α outside of gradients, hyperbolicity not always satisfied; polydispersion badly modeled.

Modeling at the Mesoscopic Level (Eulerian-Lagrangian methods, fluid-kinetic coupling)

1. Unknowns for the gas :

$$\rho_g(t,x) \geq 0, \qquad u_g(t,x) \in \mathbb{R}^3, \qquad p(t,x) \geq 0;$$

2. Unknown for the dispersed phase :

$$f(t,x,v,r) \geq 0;$$

v : velocity of a droplet ; r: radius of a droplet

Williams 74; O'Rourke 81

The fluid-Kinetic coupling also appears in flocking issues, S.-Y. Ha

Incompressible viscous spray: Vlasov-incompressible Navier-Stokes equation (medical sprays in the upper part of the lung)

$$\partial_t u_g + (u_g \cdot \nabla_x) u_g + \nabla_x p - \Delta_x u_g = \int\int_{v,r} D(r)\,(v - u_g)\,f\,dvdr,$$

$$\nabla_x \cdot u_g = 0,$$

$$\partial_t f + v \cdot \nabla_x f + \nabla_v \cdot [-D(r)\,(v - u_g)\,f] = 0.$$

Compressible inviscid (barotropic) spray with collisions: Vlasov-Boltzmann-compressible Euler equations (diesel engine)

$$\partial_t \rho_g + \nabla_x \cdot (\rho_g \, u_g) = 0,$$

$$\partial_t(\rho_g \, u_g) + \nabla_x \cdot (\rho_g \, u_g \otimes u_g) + \nabla_x [p(\rho_g)] = \int \int_{v,r} D(r, \rho_g) \, (v - u_g) \, f \, dvdr,$$

$$\partial_t f + v \cdot \nabla_x f + \nabla_v \cdot (-D(r, \rho_g) \, (v - u_g) \, f) = Q(f).$$

Collision kernel

$$Q(f)(t,x,v,r) = \int_{v^* \in \mathbb{R}^3} \int_{r^*>0} \int_{\sigma \in S^2} \Big\{ f(t,x,v',r)\, f(t,x,v^{*'},r^*)$$

$$- f(t,x,v,r)\, f(t,x,v^*,r^*) \Big\} B\, dv^* dr^* d\sigma.$$

Cross section: $(\cos\theta = \frac{v-v^*}{|v-v_*|} \cdot \sigma)$

$$B(\theta, |v-v^*|, r, r^*) = \frac{1}{2} |v-v^*| \, (r+r^*)^2 \, \frac{\sin\theta}{2}.$$

Post collisional velocities:

$$v' = \frac{r^3\, v + r^{*3}\, v^*}{r^3 + r^{*3}} + \frac{r^{*3}}{r^3 + r^{*3}} |v - v^*| \, \sigma,$$

$$v^{*'} = \frac{r^3\, v + r^{*3}\, v^*}{r^3 + r^{*3}} - \frac{r^3}{r^3 + r^{*3}} |v - v^*| \, \sigma.$$

Models used in realistic codes

1. Internal energy for the gas and the droplets
2. Compressibility, rotation and distorsion/oscillation of droplets
3. Coagulation, inelastic collisions and breakup of droplets
4. Phase changes and chemical reactions
5. Turbulent diffusion ($k - \varepsilon$ models)

Local strong solutions to the compressible Euler-Vlasov equation (thin sprays)

Theorem (C. Baranger, LD) : We consider $\gamma > 1$, $s \in \mathbb{N}$ such that $s \geq 3$, Let $(\rho_0, \rho_0\, u_0) : \mathbb{R}^3 \to G$ relatively compact open set of $]0, +\infty[\times\mathbb{R}^3$ be functions satisfying $\rho_0 - 1 \in H^s(\mathbb{R}^3)$ and $u_0 \in H^s(\mathbb{R}^3)$. Let also $f_0 : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}_+$ be a function of $C^1_c(\mathbb{R}^3 \times \mathbb{R}^3) \cap H^s(\mathbb{R}^3 \times \mathbb{R}^3)$.
Then, one can find $T > 0$ such that there exists a unique strong solution $(\rho, \rho\, u; f)$ to the system

$$\begin{aligned}
\partial_t\, \rho + \nabla_x \cdot (\rho u) &= 0,\\
\partial_t(\rho u) + \nabla_x \cdot (\rho u \otimes u) + \nabla_x(\rho^\gamma) &= \int_{\mathbb{R}^3} f\,(\rho v - \rho u)\, dv,\\
\partial_t\, f + \nabla_x \cdot (vf) + \nabla_v \cdot (f\,(\rho u - \rho v)) &= 0,
\end{aligned}$$

$$\begin{aligned}
\forall x \in \mathbb{R}^3, &\qquad \rho(0,x) = \rho_0(x), \qquad u(0,x) = u_0(x),\\
\forall (x,v) \in \mathbb{R}^3 \times \mathbb{R}^3, &\qquad f(0,x,v) = f_0(x,v).
\end{aligned}$$

This solution belongs to $C^1([0,T]\times\mathbb{R}^3, G')\times C^1_c([0,T]\times\mathbb{R}^3\times\mathbb{R}^3,\mathbb{R}_+)$, with G' relatively compact open set of $]0,+\infty[\times\mathbb{R}^3$.
Moreover, $\rho-1,\ u\in L^\infty([0,T],H^s(\mathbb{R}^3))$; $f\in L^\infty([0,T],H^s(\mathbb{R}^3\times\mathbb{R}^3))$.

Uniqueness holds under those smoothness assumption.

Challenge : replace smooth local solutions by 1D global solutions (J. Glimm; R. DiPerna, P.-L. Lions-B. Perthame-E. Tadmor).

Extension by J. Mathiaud to the (full) compressible Euler-Vlasov-Boltzmann equation (moderately thick sprays).
The proof uses ideas from the theory of perturbative solutions of the Boltzmann equation due to Y. Guo.

Global weak solutions to the incompressible Navier-Stokes-Vlasov equation

Theorem (Laurent Boudin, L.D., Céline Grandmont, Ayman Moussa) :
Let $T > 0$. We assume that $(1 + |v|^2)\, f_0 \in L^\infty(\mathbb{T}^3 \times \mathbb{R}^3)$, $u_0 \in L^2(\mathbb{T}^3)$.
Then there exists at least one weak solution (f, u) on $[0, T]$ to

$$\partial_t u + \nabla_x (u \otimes u) + \nabla_x p - \Delta_x u = - \int_{\mathbb{R}^3} f\,(u - v)\, dv,$$
$$\partial_t f + v \cdot \nabla_x f + \nabla_v \cdot [(u - v)\, f] = 0,$$
$$\nabla_x \cdot u = 0,$$
$$f(0, x, v) = f_0(x, v),$$
$$u(0, x) = u_0(x).$$

Moreover, this solution satisfies the energy equality and the L^∞ bound

$$\|f\|_{L^\infty([0,T]\times\mathbb{T}^3\times\mathbb{R}^3)} \le e^{3T}\, \|f_0\|_{L^\infty(\mathbb{T}^3\times\mathbb{R}^3)}.$$

Principle of the proof

A priori estimates:

$$\|f\|_{L^\infty((0,T)\times\mathbb{T}^3\times\mathbb{R}^3)} \le e^{3T}\,\|f_{\rm in}\|_{L^\infty(\mathbb{T}^3\times\mathbb{R}^3)}.$$

$$||u(t,\cdot)||^2_{L^2(\mathbb{T}^3)} + \int\int_{T^3\times\mathbb{R}^3} f(t,x,v)\,|v|^2\,dvdx + \int_0^t\int_{\mathbb{T}^3} |\nabla_x u|^2 dxds \le Cst.$$

Sobolev inequality:

$$||u||_{L^2_t(L^6_x)} \le Cst\,||u||_{L^2_t(H^1_x)}.$$

Interpolation:

$$f \in L^\infty_{t,x,v};\ \int f\,(1+v^2)\,dv \in L^\infty_t(L^1_x) \qquad \Rightarrow \qquad \int f\,dv \in L^\infty_t(L^{5/3}_x).$$

Multiplication:

$$u \in L^2_t(L^6_x);\ \int f\,dv \in L^\infty_t(L^{5/3}_x) \qquad \Rightarrow \qquad u\int f\,dv \in L^2_t(L^{30/23}_x).$$

Principle of the proof

Dimension > 3:

$N = 4$: $u \int f \, dv \in L^2_t(L_x^{12/11})$;

$N > 4$: doesn't work.

Passage to the limit in the nonlinear terms : diffusive term and Aubin's lemma and/or averaging lemma.

Main difficulty: Choice of an approximating sequence.

Existence results by other teams

Stokes-Vlasov or Navier-Stokes-Vlasov equation; existence: K. Hamdache; O. Anoschenko, A. Boutet de Monvel; C. Yu; T. Goudon, P.-E. Jabin, A. Vasseur.

Stokes-Vlasov or Navier-Stokes-Vlasov equation; Blowup results and large time behavior Y.-P. Choi; Y.-P. Choi, Kwon

Compressible (barotropic) Euler/Navier-Stokes-Vlasov-Fokker-Planck equation: A. Mellet, A. Vasseur; M. Chae, K. Kang, J. Lee; T. Goudon, P.-E. Jabin, A. Vasseur; J. Carrillo, R. Duan, A. Moussa; R. Duan, S. Liu

Derivation of thin spray equations from microscopic equations

Derivation of quasistatic equations of thin sprays (f being given) when the fluid satisfies Stokes (or Navier-Stokes) equations

From the point of view of physics : mixing statistical physics and fluid mechanics

From the point of view of mathematics : homogeneisation of elliptic equations

Rigorous result

Theorem LD, F. Golse, V. Ricci: Let $\Omega \subset \mathbb{R}^3$ be a bounded domain. We consider a system of N balls $B_{x_k,\varepsilon}$ for $k = 1, \dots, N$ and $\varepsilon = 1/N$ lying in Ω and satisfying the condition $\inf_{1 \le k \neq l \le N} |x_k - x_l| > 2\,\varepsilon^{1/3}$.
We suppose that the empirical measure F_N defined by

$$F_N(x,v) = \frac{1}{N} \sum_{k=1}^{N} \delta_{x_k,v_k}(x,v)$$

has a uniformly bounded kinetic energy

$$\sup_{N \ge 1} \iint_{\Omega \times \mathbb{R}^3} \tfrac{1}{2}|v|^2 F_N(x,v)\,dx\,dv < \infty$$

and that the macroscopic density and the current converge weakly in the sense of measures when $N \to \infty$:

$$\rho_N = \int_{\mathbb{R}^3} F_N(x,v)\,dv \rightharpoonup \rho, \qquad j_N = \int_{\mathbb{R}^3} F_N(x,v)\,v\,dv \rightharpoonup j$$

with ρ and j continuous on $\bar{\Omega}$.

For each $g \in (L^2(\Omega))^3$, let u_ε be the unique weak solution in $(H^1(\Omega - \cup_k B_{x_k,\varepsilon}))^3$ of

$$\begin{cases} -\Delta u_\varepsilon + \nabla p_\varepsilon &= g, \quad \text{on} \quad \Omega - \cup_k B_{x_k,\varepsilon}, \\ \nabla \cdot u_\varepsilon &= 0, \quad \text{on} \quad \Omega - \cup_k B_{x_k,\varepsilon}, \\ u_\varepsilon|_{\partial B_{x_k,\varepsilon}} &= v_k, \quad \text{for} \quad k = 1, .., N, \\ u_\varepsilon|_{\partial\Omega} &= 0, \end{cases}$$

extended by v_k on $B_{x_k,\varepsilon}$.

Then, u_ε converges in $(L^2(\Omega))^3$ towards the solution U of

$$\begin{cases} -\Delta U + \nabla \Pi &= g + 6\,\pi\,(j - \rho\, U), \\ \nabla \cdot U &= 0, \\ U|_{\partial\Omega} &= 0. \end{cases}$$

Proof: uses an homogenisation technique close to the one due to G. Allaire, and used for more standard elliptic problems

Extension: Navier-Stokes instead of Stokes

Shortcomings: The distribution of droplets is given; Two given droplets have to remain far away from each other (Cf. M. Hillairet);

Alternative framework: starting from coupled Boltzmann equation

Density of molecules of the gas $f := f(t, x, w)$,

Density of droplets $F := F(t, x, v)$.

Relative mass: $\eta = m/M$;

Evolution of those densities due to collisions (droplets are assumed here not to collide):

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

Rescaled equations

Scaling assumptions:

$$\frac{V_p}{V_g} = 1, \qquad \frac{\mathcal{N}_g}{\mathcal{N}_p} = \frac{1}{\eta} >> 1, \qquad N_p\, S_{pg}\, L = 1, \qquad \mathcal{N}_g\, S_{gg}\, L =: \frac{1}{\delta} >> 1,$$

where $\mathcal{N}$ are typical number densities, V are typical velocities, L is a typical length and S are typical collision frequencies.

The rescaled Boltzmann system becomes

$$(\partial_t + v \cdot \nabla_x) F = \frac{1}{\eta}\, \mathcal{D}(F, f),$$

$$(\partial_t + w \cdot \nabla_x) f = \mathcal{R}(f, F) + \frac{1}{\delta}\, \mathcal{C}(f, f).$$

Collision kernels for specular reflexion

Deflection operator:

$$\mathcal{D}(F,f)(v) = \int\int_{\mathbb{R}^3\times S^2} \Big(F(v'')f(w'') - F(v)f(w) \Big) \, |(v-w)\cdot\omega| \, dwd\omega \,,$$

where

$$v'' = v \; - 2\frac{\eta}{1+\eta}\,((v - w\cdot\omega)\,\omega \,,$$
$$w'' = w \; + 2\frac{1}{1+\eta}\,((v - w\cdot\omega)\,\omega \,,$$

Friction operator:

$$\mathcal{R}(f,F)(v) = \int\int_{\mathbb{R}^3\times S^2} \Big(f(w'')F(v'') - f(w)F(v) \Big) \, |(v-w)\cdot\omega| \, dwd\omega \,.$$

Proposition (LD, F. Golse, V. Ricci): In the formal limit,

$$f_\varepsilon(t,x,w) \to \frac{n(t,x)}{(2\pi\,\theta(t,x)/m_g)^{3/2}}\,\exp\left(-\frac{m_g\,|w-u(t,x)|^2}{2\,\theta(t,x)}\right),$$

and

$$F_\varepsilon(t,x,v) \to F(t,x,v),$$

where (with $\rho = m_g\, n$)

$$\partial_t \rho + \nabla_x(\rho\, u) = 0\,,$$

$$\partial_t(\rho\, u) + \nabla_x(\rho\, u \otimes u + n\,\theta\, Id)$$

$$= \rho \int_{\mathbb{R}^3} (v_* - u)\, n\, \sqrt{\theta\, m_g}\, q(|v_* - u|/\sqrt{\theta/m_g})\, F(v_*)\, dv_*\,,$$

$$\partial_t \left(\frac{1}{2}\,\rho\,|u|^2 + \frac{3}{2}\,n\,\theta\right) + \nabla_x \cdot \left(u\,(\frac{1}{2}\,\rho\,|u|^2 + \frac{5}{2}\,n\,\theta)\right)$$

$$= \sqrt{m_g\,\theta}\,\rho \int_{\mathbb{R}^3} (v_* - u)\cdot v_*\, q(|v - u|/\sqrt{\theta/m_g})\, F(v_*)\, dv_*\,,$$

$$\partial_t F + v\cdot\nabla_x F = n\sqrt{\frac{\theta}{m_g}}\,\nabla_v \cdot \left(F(v)\,(v-u)\, q(|v-u|/\sqrt{\theta/m_g})\right).$$

where

$$q(|a|) = \frac{1}{\sqrt{2\pi}} \left\{ 2|a| I_2(|a|) + \frac{4}{3}|a|^{-1} I_4(|a|) - \frac{2}{15}|a|^{-3} I_6(|a|) \right.$$

$$\left. + \frac{8}{15}|a|^2 J_1(|a|) + \frac{8}{3} J_3(|a|) \right\},$$

and

$$I_k(x) = \int_0^x t^k \, e^{-t^2/2} \, dt, \qquad J_k(x) = \int_x^\infty t^k \, e^{-t^2/2} \, dt.$$

Extensions:

- Compressible Euler equation can be replaced by Stokes or incompressible Navier-Stokes equations by changing the scaling.
- For molecules/droplets interaction, hard spheres can be replaced by other types of collisions, including inelastic collisions (cf. F. Charles).

Challenges:

- Provide rigorous proofs for the formal asymptotics.
- Find a formal asymptotics (starting from Boltzmann-like equations) for models involving the volume fraction, and mathematical results for those models (formal passage towards macroscopic multiphase models for these models were obtained in collaboration with J. Mathiaud).