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Modélisation mathématique et étude numérique d'un
aérosol dans un gaz raréfié.
Application à la simulation du transport de particules de
poussière en cas d'accident de perte de vide dans ITER.

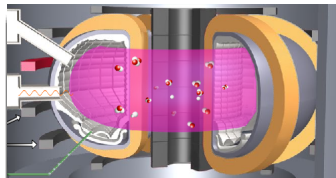
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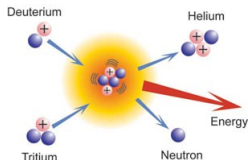
International Thermonuclear Experimental Reactor

Goals of ITER

- Prove that energy can be produced by nuclear fusion, with a rate $Q = 10$ (JET=0,65).
- Get a plasma confined during a long period of 1000 s (Toresupra : 400 s).



<http://www.itercad.org>



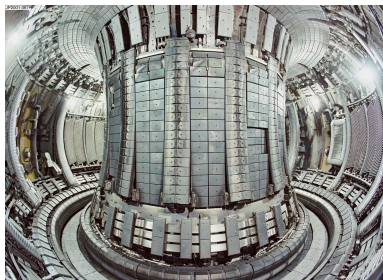
<http://www.iter.org>

About dust in ITER

Production of many non confined neutrons, and disruption of the confinement of the plasma
 \Rightarrow Abrasion of the wall
 \Rightarrow Appearance of a large amount of dust specks

- Composition : C, Be, W
- Diameter : between 10 nm and 10 μm .

Loss of Vacuum Accidents (LOVA)



- Accidental arrival of air in the vacuum inside the torus.
- Safety risk related to the dispersion of the dust specks.
- Crucial period for the study of the evolution of the dust specks : a few milliseconds after the LOVA (*Takase*¹).

¹K. Takase, *Three-dimensional numerical simulations of dust mobilization and air ingress characteristics in a fusion reactor during a lova event*, Fusion Engineering and Design, 2001.

Modeling issues

Models of sprays

- Fluid/fluid (multiphase) models : *J.R Garcia-Cascales, J. Mulas-Pérez, and H. Paillère^a*.
- Fluid/kinetic models (coupling Euler/Vlasov or NS/Vlasov by a drag force term) : code KIVA^b, *Takase, ...*

Stokes drag force :

$$F(v, r) = \frac{D_p}{m_p(r)} (\mathbf{u}_g - v).$$

- Rarefied sprays models
 - ▶ Fixed gas + linear Boltzmann for the particles (*Ferrari, Pareschi^c*).
 - ▶ Eulerian description of a Vlasov equation for the evolution of the particles (*A Frezzotti, S. Østmo, and T. Ytrehus^d*).

^aExtension of some numerical schemes to the analysis of gas and particle mixtures. *International Journal for Numerical Methods in Fluids*, 56, 845–875, 2008.

^bPJ ORourke and AA Amsden. The TAB method for numerical calculation of spray droplet breakup, In *International fuels and lubricants meeting and exposition*, 2, 1987.

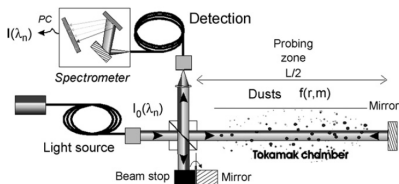
^cE. Ferrari and L. Pareschi, Modelling and numerical methods for the diffusion of impurities in a gas. *International Journal for Numerical Methods in Fluids*, 1–16, 2006.

^dKinetic theory study of steady evaporation from a spherical condensed phase containing inert solid particles. *Physics of Fluids*, 9, 211, 1997.

Objectives

First milliseconds after a LOVA in ITER

- Construction and study of a fully kinetic model for the description of the rarefied spray (few collisions).
- Numerical simulation of a "small size" (a few cm^3) of the F34 consortium experiments [results not yet available], mimicking the beginning of a LOVA.



Principle of light extinction measurements ^a

^aDust control in tokamak environment, S. Rosanvallon, C. Grisolia and Al., Fusion Engineering and Design 83, 1701-1705, 2008.

Outline

- 1 Fully kinetic modeling
 - Assumptions
 - Boltzmann-Boltzmann modeling
 - Construction of a Vlasov-Boltzmann model
- 2 Mathematical Results
 - Existence of solutions to the (space homogeneous) Boltzmann-Boltzmann system
 - Study of the convergence towards the Vlasov-Boltzmann system
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- 4 Perspectives

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Assumptions and Notations

Dust Specks

- Spheres with radiuses in $r \in [r_{min}, r_{max}]$.
- Macroscopic when compared to molecules :

$$\varrho \sim 10^{-10} \text{ m} \ll r \sim 10^{-7} \text{ m} .$$

- Rate of the number density of dust specks and the number density of molecules :

$$\alpha^\circ = \frac{n_1^\circ}{n_2^\circ} \ll 1 (\sim 10^{-6}).$$

Rate of the mass of a molecule and the mass of a dust speck

$$\forall r \in [r_{min}, r_{max}], \quad \varepsilon(r) = \frac{m_2}{m_1(r)} \ll 1 (\sim 10^{-12}).$$

We denote

$$\varepsilon_m = \varepsilon(r_{min}).$$

Construction of a Boltzmann-Boltzmann model

Number densities

$f_1(t, v, x, r)$: Number density of dust specks.

$f_2(t, v, x)$: Number density of molecules.

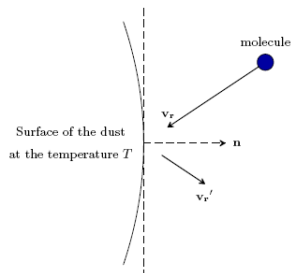
Boltzmann-Boltzmann coupling

$$(BB) \begin{cases} \frac{\partial f_1}{\partial t} + v \cdot \nabla_x f_1 = R_1(f_1, f_2), \\ \frac{\partial f_2}{\partial t} + v \cdot \nabla_x f_2 = Q(f_2, f_2) + R_2(f_1, f_2), \\ x \in \Omega, \quad v \in \mathbb{R}^3, \quad t \in \mathbb{R}^+ \end{cases}$$

+ initial and boundary conditions

Modeling of collisions

- Collisions between molecules : binary, elastic, VHS
- Collisions between dust specks : neglected ($\nu_{11} \sim 10^{-3} s^{-1}$).
- Collisions between dust specks and molecules :
 - ▶ First possibility : Elastic (Hard spheres)
→ **operators** $R_1^e(f_1, f_2)$ **and** $R_2^e(f_1, f_2)$.
 - ▶ Second possibility : Diffuse reflexion at the surface of the dust specks
→ **operators** $R_1^d(f_1, f_2)$ **and** $R_2^d(f_1, f_2)$.



Consequences :

- ▶ Kinetic energy not conserved,
- ▶ Non planar, non microreversible collisions.

Operators $R_1^d(f_1, f_2)$ and $R_2^d(f_1, f_2)$

$$R_1^d(f_1, f_2)(t, x, v_1, r) = \frac{2\beta^4}{\pi} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [n \cdot (v_1 - v_2)] [n \cdot w] \mathbb{1}_{\{n \cdot (v_1 - v_2) > 0\}} \mathbb{1}_{\{n \cdot w \geq 0\}} \\ \times (r + \varrho)^2 \left[f_1(t, x, v'_1, r) f_2(t, x, v'_2) \exp(-\beta^2 (v_1 - v_2)^2) \right. \\ \left. - f_1(t, x, v_1, r) f_2(t, x, v_2) \exp(-\beta^2 (v'_1 - v'_2)^2) \right] dndwdv_2,$$

$$R_2^d(f_1, f_2)(t, x, v_2) = \frac{2\beta^4}{\pi} \int_{r_{min}}^{r_{max}} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [n \cdot (v_1 - v_2)] [n \cdot w] \mathbb{1}_{\{n \cdot (v_1 - v_2) \geq 0\}} \mathbb{1}_{\{n \cdot w \geq 0\}} \\ \times (r + \varrho)^2 \left[f_1(t, x, v'_1, r) f_2(t, x, v'_2) \exp(-\beta^2 (v_1 - v_2)^2) \right. \\ \left. - f_1(t, x, v_1, r) f_2(t, x, v_2) \exp(-\beta^2 (v'_1 - v'_2)^2) \right] dndwdv_1 dr,$$

with $\beta = \sqrt{\frac{m_2}{2k_B T_{surf}}}$, and

$$\begin{cases} v'_1 &= \frac{1}{1 + \varepsilon(r)} (v_1 + \varepsilon(r)v_2 - \varepsilon(r)w), \\ v'_2 &= \frac{1}{1 + \varepsilon(r)} (v_1 + \varepsilon(r)v_2 + w). \end{cases}$$

Remarks

Mean frequency of collision

We consider three typical frequencies :

- molecules-molecules : ν_{22}
- dust specks-molecules (from the point of view of dust specks) : ν_{12}
- molecules-dust specks (from the point of view of molecules) : ν_{21} .

We notice that

$$\nu_{21} \sim \alpha^0 \nu_{12} \quad \text{et} \quad \nu_{22} \sim \left(\frac{\rho}{r}\right)^2 \nu_{12}.$$

Collisions between dust specks-molecules (from the point of view of dust specks)

$$v_1' - v_1 = \frac{\varepsilon(r)}{1 + \varepsilon(r)} (v_2 - w - v_1).$$

→ **Small change of velocity, analogous to grazing collisions ! ^a**

^aR. Alexandre, C. Villani, On the Landau Approximation in Plasma Physics, Annales de l'Institut Henri Poincaré/Analyse non linéaire, vol. 21, n. 1, (2004), pp. 61-95.

Non-dimensionalization

Assumptions

- Radiuses of the same order of magnitude : $r_{min} \sim r_{max}$;
- Temperatures of the same magnitude : $T_{f_1} \sim T_{f_2} \sim T^\circ$.

Velocities : Two possibilities

- (a) Starting from the thermal velocities of the dust specks and the molecules (as in Degond-Lucquin in plasma theory ^a)

$$V_1^\circ = \langle V_1 \rangle = \sqrt{\frac{8kT^\circ}{\pi m_1(r_{min})}} \quad \text{et} \quad V_2^\circ = \langle V_2 \rangle = \sqrt{\frac{8kT^\circ}{\pi m_2}}$$

$$V_1^\circ = \sqrt{\varepsilon_m} V_2^\circ.$$

- (b) Starting from the same velocity

$$V_1^\circ = V_2^\circ = V^\circ.$$

^aP. Degond, B. Lucquin, The asymptotics of collision operators for two species of particle of disparate masses. *M3AS*, 6, n° 3, 405–410, 1996.

Non-dimensionalization (sequel)

Non dimensionalization of the variables

$$\bar{t} = \frac{t}{t^\circ}, \quad \bar{r} = \frac{r}{r_{min}}, \quad \bar{x} = \frac{x}{L^\circ}, \quad \hat{v}_1 = \frac{v_1}{V_1^\circ}, \quad \check{v}_2 = \frac{v_2}{V_2^\circ},$$

$$\hat{f}_1(\bar{t}, \bar{x}, \hat{v}_1, \bar{r}) = \frac{(V_1^\circ)^3 r_{min}}{n_1} f_1(t, x, v, r), \quad \check{f}_2(\bar{t}, \bar{x}, \check{v}_2) = \frac{(V_2^\circ)^3}{n_2} f_2(t, x, v_2).$$

Expansion of $\bar{R}_1(f_1, f_2)$

For $\varphi \in \mathcal{C}_c^2(\mathbb{R}^3)$, we have (at least formally)

$$\int_{\mathbb{R}^3} \bar{R}_1(\hat{f}_1, \check{f}_2)(\hat{v}_1) \varphi(\hat{v}_1) d\hat{v}_1 = \int_{\mathbb{R}^3} \bar{\Upsilon}(\check{f}_2)(\bar{t}, \bar{x}, \hat{v}_1, \bar{r}) \cdot \nabla \varphi(\hat{v}_1) \hat{f}_1(\hat{v}_1) d\hat{v}_1 + o(1),$$

Therefore (also formally)

$$\bar{R}_1(\hat{f}_1, \check{f}_2) = -\operatorname{div}_{\hat{v}_1} \left(\bar{\Upsilon}(\check{f}_2) \hat{f}_1 \right) + o(1).$$

Vlasov-Boltzmann coupling

After re-dimensionalization, we get

$$(VB) \begin{cases} \frac{\partial f_1}{\partial t} + v_1 \cdot \nabla_x f_1 + \operatorname{div}_{v_1} (\Upsilon(f_2) f_1) = 0, \\ \frac{\partial f_2}{\partial t} + v_2 \cdot \nabla_x f_2 = Q(f_2, f_2) + R_2(f_1, f_2). \end{cases}$$

Form of $\Upsilon(f_2)$ for diffuse reflexion :

- with the non-dimensionalization (a) ($V_1^\circ = \sqrt{\varepsilon_m} V_2^\circ$) :

$$\Upsilon_a^d(f_2)(t, x, r) = \pi \varepsilon(r) r^2 \int_{\mathbb{R}^3} f_2(t, x, v_2) \left[|v_2| + \frac{\sqrt{\pi}}{3\beta} \right] v_2 dv_2,$$

- with the non-dimensionalization (b) ($V_1^\circ = V_2^\circ$) :

$$\Upsilon_b^d(f_2)(t, x, v_1, r) = \pi \varepsilon(r) r^2 \int_{\mathbb{R}^3} f_2(t, x, v_2) \left[|v_2 - v_1| + \frac{\sqrt{\pi}}{3\beta} \right] (v_2 - v_1) dv_2.$$

Vlasov-Boltzmann coupling

Drag force felt by the dust specks :

$$F_d(t, x, v, r) = m_1(r) \Upsilon(f_2)(t, x, v).$$

- No empirical coefficients.
- Model of drag force with slip flow correction (*Cunningham*^a) used in ^b :

$$F(v, r) = \frac{6\pi r \nu_a v}{1 + \frac{\lambda}{r} [1.257 + 0.4 \exp(-0.275 \frac{\lambda}{r})]}.$$

ν_a : gas viscosity,

λ : mean free path of the gas.

^aOn the velocity of steady fall of spherical particles through fluid medium. In *Proceedings of the Royal Society of London. Series A*, 357–365. The Royal Society, 1910.

^bC.M. Benson, D.A. Levin, J. Zhong, S.F. Gimelshein, and A. Montaser. Kinetic model for simulation of aerosol droplets in high-temperature environments. *Journal of Thermophysics and Heat Transfer*, **18**, n° 1, 122–134, 2004.

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We consider the spatially homogeneous system

$$(BB_h) \begin{cases} \frac{\partial f_1}{\partial t} = R_1^e(f_1, f_2), \\ \frac{\partial f_2}{\partial t} = R_2^e(f_1, f_2) + Q(f_2, f_2), \end{cases}$$

with

$$R_1^e(f_1, f_2)(t, v_1, r) = \int_{\mathbb{R}^3} \int_{S^2} [f_1(t, v'_1, r) f_2(t, v'_2) - f_1(t, v_1, r) f(t, v_2)] \\ \times (r + \varrho)^2 |(v_1 - v_2) \cdot \omega| d\omega dv_2,$$

$$R_2^e(f_1, f_2)(t, v_2) = \int_{\mathbb{R}^3} \int_{S^2} \int_{r_{min}}^{r_{max}} [f_1(t, v'_1, r) f_2(t, v'_2) - f_1(t, v_1, r) f_2(t, v_2)] \\ \times (r + \varrho)^2 |(v_1 - v_2) \cdot \omega| dr d\omega dv_1,$$

where

$$v'_1 = v_1 + \frac{2\varepsilon(r)}{1 + \varepsilon(r)} [\omega \cdot (v_2 - v_1)] \omega, \\ v'_2 = v_2 - \frac{2}{1 + \varepsilon(r)} [\omega \cdot (v_2 - v_1)] \omega,$$

$$Q(f_2, f_2)(t, v) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \left[f_2(t, v') f_2(t, v'_*) - f_2(t, v) f_2(t, v_*) \right] C_{\text{eff}} |v - v_*|^\gamma d\sigma dv_*,$$

with $v' = \frac{v + v_*}{2} + \frac{|v - v_*|}{2} \sigma$, $v'_* = \frac{v + v_*}{2} - \frac{|v - v_*|}{2} \sigma$, $C_{\text{eff}} > 0$, $\gamma \in]0, 1]$.

- Masses

$$\mu(f_1)(t, r) = \int_{\mathbb{R}^3} f_1(t, v, r) dv \quad \text{and} \quad \mu(f_2)(t) = \int_{\mathbb{R}^3} f_2(t, v) dv.$$

- Energy

$$E(f_1, f_2)(t) := \varepsilon_m \int_{\mathbb{R}^3} f_2(t, v) |v|^2 dv + \int_{\mathbb{R}^3} \int_{r_{\min}}^{r_{\max}} f_1(t, v, r) |v|^2 \left(\frac{r}{r_{\min}} \right)^3 dr dv,$$

where $\varepsilon_m = \varepsilon(r_{\min})$.

- Entropy

$$\mathcal{H}(f_1, f_2)(t) := \int_{\mathbb{R}^3} \left[f_2(t, v) \ln(f_2(t, v)) + \int_{r_{\min}}^{r_{\max}} f_1(t, v, r) \ln(f_1(t, v, r)) dr \right] dv.$$

Proposition 1

Assumptions :

$$f_{1,in} > 0, \quad f_{2,in} > 0,$$

$$\int_{r_{min}}^{r_{max}} \mu(f_{1,in})(r) dr + \mu(f_{2,in}) + E(f_{1,in}, f_{2,in}) < \infty,$$

$$\int_{\mathbb{R}^3} \int_{r_{min}}^{r_{max}} (f_{1,in} |\ln f_{1,in}|(v, r) dr + f_{2,in} |\ln f_{2,in}|(v)) dv < \infty.$$

Then, there exists (f_1, f_2) weak solution of (BB_h) such that

$$f_1 \geq 0 \quad \text{et} \quad f_2 \geq 0,$$

$$(f_1, f_2) \in \text{Lip}([0, T], L^1(\mathbb{R}^3 \times [r_{min}, r_{max}])) \times \text{Lip}([0, T], L^1(\mathbb{R}^3)),$$

$$\sup_{t \geq 0} \left[\int_{r_{min}}^{r_{max}} \mu(f_1)(t, r) dr + \mu(f_2)(t) + E(f_1, f_2)(t) \right] < \infty,$$

$$\forall t \geq 0, \quad H(f_1, f_2)(t) \leq H(f_{1,in}, f_{2,in}).$$

If moreover for $s > 1$

$$\int_{\mathbb{R}^3} \int_{r_{min}}^{r_{max}} (1 + |v|^2)^s [f_{1,in}(v, r) + f_{2,in}(v)] dr dv < +\infty,$$

then

$$\forall t \geq 0, \quad E(f_1, f_2)(t) = E(f_{1,in}, f_{2,in}).$$

Main steps of the Proof (same spirit as in Arkeryd^a)

- We introduce the approximated system

$$\begin{cases} \frac{\partial f_1^n}{\partial t} = \frac{R_1^n(f_1^n, f_2^n)}{1 + \frac{1}{n} \int \int |f_1^n| dr dv + \frac{1}{n} \int |f_2^n| dv}, \\ \frac{\partial f_2^n}{\partial t} = \frac{R_2^n(f_1^n, f_2^n) + Q^n(f_2^n, f_2^n)}{1 + \frac{1}{n} \int |f_2^n| dv + \frac{1}{n} \int \int |f_1^n| dr dv}, \end{cases} \quad (1)$$

with initial conditions $f_i^n(0, \cdot) = f_{i,in} \mathbb{1}_{\{f_{i,in} \leq n\}} + \frac{1}{n} e^{-|v|^2/2}$ for $i = 1, 2$.

- The solution (f_1^n, f_2^n) satisfies the conservation of mass and energy, and the decay of entropy
- Weak compactness : we extract a subsequence $(f_1^n, f_2^n)_{n \in \mathbb{N}}$ such that for all $\gamma < 2$

$$f_1^n \rightharpoonup f_1 \quad \text{dans} \quad L^1([0, t] \times \mathbb{R}^3 \times [r_{min}, r_{max}], |v|^\gamma dt dv dr) \quad \text{weak},$$

$$f_2^n \rightharpoonup f_2 \quad \text{dans} \quad L^1([0, t] \times \mathbb{R}^3, |v|^\gamma dt dv) \quad \text{weak}.$$

- (f_1, f_2) is Lipschitz-continuous w.r.t. time and weak solution of (BB_h) .
- Weak convergence of $(f_1^n(t, \cdot, \cdot), f_2^n(t, \cdot))_{n \in \mathbb{N}^*}$ and proof of decay of the entropy.
- Povzner's inequality and conservation of the energy.

^a L. Arkeryd, On the Boltzmann Equation, i and ii. *Arch. Rat. Mech. Anal.*, 45, 1–34, 1972.

Return to the non dimensional system

With the non-dimensionalization (a) and $t^\circ = \frac{1}{\nu_{22}} = \frac{1}{4\pi n_2^\circ \rho^2 V_2^\circ}$:

The system (BB_h) becomes :

$$(BB_{h,adim}) \begin{cases} \frac{\partial \hat{f}_1}{\partial \bar{t}} = \frac{c}{\alpha^\circ} \bar{R}_1(\hat{f}_1, \check{f}_2), \\ \frac{\partial \check{f}_2}{\partial \bar{t}} = c \bar{R}_2(\hat{f}_1, \check{f}_2) + \bar{Q}(\check{f}_2, \check{f}_2), \end{cases}$$

where

$$c := \frac{\alpha^\circ}{4\pi} \left(\frac{\eta}{\varepsilon_m} \right)^{2/3}, \quad \text{and} \quad \eta = \frac{3m_2}{4\pi\rho\varrho^3}.$$

Assumptions :

$$c \sim 1, \quad \text{et} \quad \frac{1}{\sqrt{\varepsilon_m}} \sim \frac{1}{\alpha^\circ} := p \rightarrow \infty.$$

We define

$$\xi = \frac{\alpha^\circ}{\sqrt{\varepsilon_m}}.$$

Family of solutions $(f_{1,p}, f_{2,p})_{p \geq 0}$

$$(BB_{h,p}) \begin{cases} \frac{\partial f_{1,p}}{\partial t} = p c R_1^{a,p}(f_{1,p}, f_{2,p}), \\ \frac{\partial f_{2,p}}{\partial t} = c R_2^{a,p}(f_{1,p}, f_{2,p}) + Q^a(f_{2,p}, f_{2,p}), \end{cases}$$

with initial conditions :

$$f_{1,p}(0, \cdot) = f_{1,in}, \quad f_{2,p}(0, \cdot) = f_{2,in},$$

where Q^a , $R_1^{a,p}$, $R_2^{a,p}$ are non-dimensional operators.

$$R_1^{a,p}(f_1, f_2)(v_1, r) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} [f_1(v'_{1,p}, r) f_2(v'_{2,p}) - f_1(v_1, r) f_2(v_2)] \\ \times \frac{1}{4} \left(\frac{1}{2\sqrt{\pi p c}} + r \right)^2 \left| \frac{v_1}{p} - v_2 \right| d\sigma dv_2,$$

where

$$\begin{cases} v'_{1,p} = \frac{p^2}{1 + r^3 p^2} \left[\left(v_1 r^3 + \frac{v_2}{p} \right) - \frac{1}{p} \left| v_2 - \frac{v_1}{p} \right| \sigma \right], \\ v'_{2,p} = \frac{p^2}{1 + r^3 p^2} \left[\frac{1}{p} \left(v_1 r^3 + \frac{v_2}{p} \right) + r^3 \left| v_2 - \frac{v_1}{p} \right| \sigma \right]. \end{cases}$$

Limit of the non-dimensional system

Theorem (L.D, F.C, 2009)

Assumptions : Assumptions of Proposition (1) and

$$\int_{\mathbb{R}^3} \left(\int_1^{r_0} f_{1,in}(v, r) dr + f_{2,in}(v) \right) (1 + |v|^4) dv < \infty.$$

Then for all $T > 0$

$$(f_{1,p}, f_{2,p}) \rightharpoonup (f_1, f_2) \quad \text{dans} \quad L^\infty([0, T]; M^1(\mathbb{R}^3 \times [1, r_0]) \times L^1(\mathbb{R}^3)) \quad \text{weak}^*,$$

with $(f_1, f_2) \in L^\infty([0, T]; M^1(\mathbb{R}^3 \times [1, r_0]) \times L^1(\mathbb{R}^3))$

weak solution of the system

$$\begin{cases} \frac{\partial f_1}{\partial t} + \frac{2\pi c}{r\xi} \int_{\mathbb{R}^3} |v_2| v_2 f_2(t, v_2) dv_2 \cdot \nabla_v f_1 = 0, \\ \frac{\partial f_2}{\partial t} = c \left\{ \int_{\mathbb{R}^3} \int_1^{r_0} f_{1,in}(v_1, r) r^2 dr dv_1 \right\} L(f_2) + Q^a(f_2, f_2), \end{cases}$$

where

$$L(f_2)(t, v) = \int_{\mathbb{S}^2} [f_2(t, v - 2(\omega \cdot v)\omega) - f_2(t, v)] |v \cdot \omega| d\omega.$$

Estimates of moments

Moments of order 1 and 2 :

$$\sup_{p \in \mathbb{N}^*} \sup_{t \in [0, T]} \int_{\mathbb{R}^3} (1 + |v| + |v|^2) f_{2,p}(t, v) dv < +\infty,$$

$$\sup_{p \in \mathbb{N}^*} \sup_{t \in [0, T]} \int_{\mathbb{R}^3} \int_1^{r_0} \left(1 + |v| + \frac{|v|^2}{p} \right) f_{1,p}(t, v, r) dr dv < +\infty.$$

Estimates of moments (sequel)

Moments of higher order

- Povzner-like inequality ^{a b} : for $s > 1$, one has

$$r^{3s} |v'_{1,p}|^{2s} + |v'_{2,p}|^{2s} - r^{3s} |v_1|^{2s} - |v_2|^{2s} \leq \frac{C_1}{\rho^2} (|v_1|^{2s} + |v_2|^{2s}) \\ + \frac{C_2}{\rho} [|v_1|^{2s-1} |v_2| + |v_2|^{2s-1} |v_1|] + \frac{C_3}{\rho^2} [|v_1|^{2s-2} |v_2|^2 + |v_2|^{2s-2} |v_1|^2].$$

- We deduce that

$$\sup_{t \in [0, T], \rho \in \mathbb{N}^*} \int_{\mathbb{R}^3} \int_1^{r_0} \left(\frac{1}{\rho} f_{1,\rho}(t, v, r) + f_{2,\rho}(t, v) \right) (1 + |v|^3) dr dv < +\infty.$$

^aL. Desvillettes. Some applications of the method of moments for the homogeneous Boltzmann and Kac equations. *Archive for Rational Mechanics and Analysis*, 123, n° 4, 387–404, 1993.

^bB. Wennberg. Entropy dissipation and moment production for the Boltzmann equation. *Journal of Statistical Physics*, 86, n° 5, 1053–1066, 1997.

Remark about the convergence of the sequences

- Weak compactness of $(f_{2,p})_{p \in \mathbb{N}^*}$: We can extract from $(f_{2,p})_{p \in \mathbb{N}^*}$ a subsequence which converges weakly in $L^1([0, t] \times \mathbb{R}^3)$.
- Entropy inequality :

$$\begin{aligned} & \frac{1}{\rho} \int_{\mathbb{R}^3} \int_1^{r_0} f_{1,p}(t, v, r) \ln(f_{1,p}(t, v, r)) dr dv + \int_{\mathbb{R}^3} f_{2,p}(t, v) \ln(f_{2,p}(t, v)) dv \\ & \leq \frac{1}{\rho} \int_{\mathbb{R}^3} \int_1^{r_0} f_{1,in}(v, r) \ln(f_{1,in}(v, r)) dr dv + \int_{\mathbb{R}^3} f_{2,in}(v) \ln(f_{2,in}(v)) dv, \end{aligned} \quad (2)$$

\Rightarrow No uniform equiintegrability of $(f_{1,p})_{p \in \mathbb{N}^*}$: convergence only in the sense of measures.

- But f_1 is solution of

$$\frac{\partial f_1}{\partial t} + \frac{2\pi c}{r\xi} \int_{\mathbb{R}^3} |v_2| v_2 f_2(t, v_2) dv_2 \cdot \nabla_v f_1 = 0.$$

\Rightarrow propagation of regularity of $f_{1,in}$.

- Uniqueness : The whole sequences converge.

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Simulation of the Boltzmann/Boltzmann system (*BB*)

Code

- Modification of a DSMC code developed at the CEA-Saclay for gas mixtures.
- Particle method, with Monte-Carlo simulation for the collision operators.
- Assumptions : all particles have the same radius r_p .

Principle

Splitting at each time step between the transport part

$$\frac{\partial f_i}{\partial t} + v \cdot \nabla_x f_i = 0 \quad \text{for } i = 1, 2,$$

and the collision part

$$\frac{\partial f_i}{\partial t} = R_i^d(f_1, f_2), \quad \text{for } i = 1, 2,$$

$$\frac{\partial f_2}{\partial t} = Q(f_2, f_2).$$

Particle approximation

Initialisation

For $i = 1, 2$,

$$f_{i,in}(x, v) \approx \sum_{k=1}^{N_i} \omega_i \delta(x - x_{i,in}^k) \delta(v - v_{i,in}^k)$$

- N_1, N_2 : number of numerical dust specks and numerical molecules.
- ω_1, ω_2 : representativity of numerical dust specks and numerical molecules.
Since $n_1 \ll n_2$, one has $\omega_1 \neq \omega_2$.

Solution at time t

The densities are approximated by

$$f_i(t, x, v) \approx \sum_{k=1}^{N_i} \omega_i \delta(x - x_i^k(t)) \delta(v - v_i^k(t)).$$

Transport

Modification of the positions $x_1^k(t)$ and $x_2^k(t)$ along the characteristics.

Simulation of $Q(f_2, f_2)$: Bird's method

Simulation of $R_1^d(f_1, f_2)$, in each cell (of volume V_c)

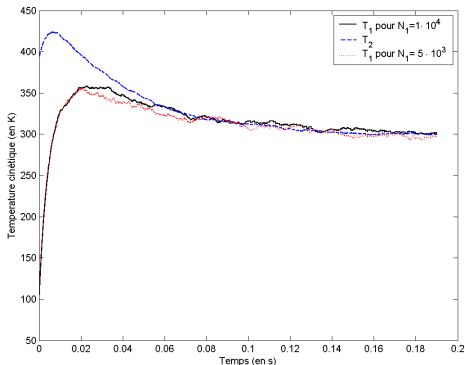
- $\omega_1 \neq \omega_2 \Rightarrow$ Nanbu's method.
- Selection of $N_{2c} N_{1c} \frac{\omega_2}{V_c} \Delta t \pi(r_p + \varrho)^2 |v_{1,2}^{rel}|_{max}$ pairs of collision.
- Each pair collides with probability $p_{k,j}^f = \frac{|v_1^k - v_2^j|}{|v_{1,2}^{rel}|_{max}}$.
- In case of collision :
 - ▶ The post-collisional relative velocity v_r' is computed according to the diffuse reflexion mechanism.
 - ▶ The velocity of a numerical dust speck is given by

$$v_1^k(t^{n+1}) = \frac{\varepsilon}{1 + \varepsilon} v_2^j(t^n) + \frac{1}{1 + \varepsilon} v_1^k(t^n) - \frac{\varepsilon}{1 + \varepsilon} v_r'$$

Thermalization of a spatially homogeneous system

$$T_{f_i}(t) = \frac{m_i}{3k_B n_{f_i}(t)} \left[\int_{\mathbb{R}^3} f_i(t, v) (v - \mathbf{u}_{f_i}(t, v))^2 dv \right].$$

- $n_2 = 10^{20} m^{-3}$, $n_1 = 5 \cdot 10^{15} m^{-3}$, $r_p = 2 \cdot 10^{-9} m$.
- Initial kinetic temperatures $T_{mol} = 400 K$, $T_{dust} = 100 K$.
- Surface temperature of the dust specks : $T_{surf} = 300 K$.



Number of collision pairs

Let $\overline{N_{coll}^{ij}}(\tau)$ be the number of numerical collisions of type (i,j) done during the time τ in the cell c . Then

$$\frac{\overline{N_{coll}^{12}}(\tau)}{\overline{N_{coll}^{21}}(\tau)} \sim \frac{N_{1c}}{N_{2c}} \frac{n_{2c}}{n_{1c}} \gg 1, \quad \text{and} \quad \frac{\overline{N_{coll}^{12}}(\tau)}{\overline{N_{coll}^{22}}(\tau)} \sim \frac{N_{1c}}{N_{2c}} \frac{1}{2\sqrt{2}} \left(\frac{r_p}{\varrho}\right)^2 \gg 1.$$

Example :

$$\left\{ \begin{array}{l} r_p = 10^{-6} \text{ m,} \\ \varrho = 2,085 \cdot 10^{-10} \text{ m,} \\ n_{1c} = 10^{14} \text{ m}^{-3}, \\ n_{2c} = 10^{21} \text{ m}^{-3}. \\ \tau = 10^{-3} \text{ s} \\ N_{1c} = 10^3 \\ N_{2c} = 10^3 \end{array} \right. \quad \begin{array}{l} \overline{N_{coll}^{12}}(\tau) \sim \mathbf{3 \cdot 10^{12}}, \\ \overline{N_{coll}^{21}}(\tau) \sim 3 \cdot 10^5, \\ \overline{N_{coll}^{22}}(\tau) \sim 4 \cdot 10^5. \end{array}$$

Solving Vlasov equation by a PIC method

- One has

$$f_1(t, x, v) \approx \sum_{k=1}^{N_1} \omega_1 \delta(x - x_1^k(t)) \delta(v - v_1^k(t)),$$

with v_1^k solution of

$$\frac{dv_1^k}{dt} = \Upsilon(f_2)(t, x_1^k, v_1^k).$$

- Explicit Euler scheme :

$$V_1^{k,n+1} = V_1^{k,n} + \Delta t \Upsilon_{b,d}^{c,n}(V_1^{k,n}),$$

where

$$\Upsilon_{b,d}^{c,n}(V_1^{k,n}) = \pi \varepsilon r_p^2 \frac{\omega_2}{V_c} \sum_{j=0}^{N_{2c}} (V_2^{j,n} - V_1^{k,n}) \left[|V_2^{j,n} - V_1^{k,n}| + \frac{\sqrt{\pi}}{3\beta} \right],$$

$V_1^{k,n}$ and $V_2^{n,j}$ are the approximations of $v_1^k(t^n)$ and $v_2^j(t^n)$.

Conditions on the time step

Numerical values for $r_p = 10^{-7}$ m, $n_1^0 = 10^{14}$ m $^{-3}$, $n_2^0 = 10^{21}$ m $^{-3}$, $\Delta x = 5 \cdot 10^{-4}$ m.

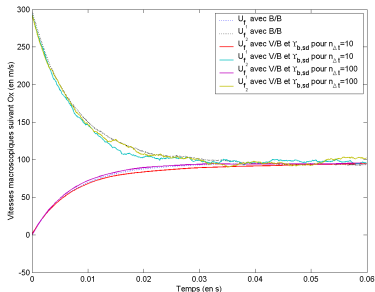
Resolution of	Condition on Δt
$\frac{\partial f_1}{\partial t} + v_1 \cdot \nabla_x f_1 = 0$	$\Delta t \leq \Delta x / \bar{v}_1 \sim 10^{-3}$ s
$\frac{\partial f_2}{\partial t} + v_2 \cdot \nabla_x f_2 = 0$	$\Delta t \leq \Delta x / \bar{v}_2 \sim 10^{-6}$ s
$\frac{\partial f_1}{\partial t} = R_1(f_1, f_2)$ (Nambu)	$\Delta t \leq 1/\nu_{12} \sim 6 \cdot 10^{-11}$ s
$\frac{\partial f_1}{\partial t} + \text{div}_{v_1}(f_1 \Upsilon(f_2)) = 0$	$\Delta t \leq 2/(\pi r_p^2 \epsilon n_2^0 \bar{v}_2) \sim 10^{-1}$ s
$\frac{\partial f_2}{\partial t} = Q(f_2, f_2)$ (Bird)	$\Delta t \leq 1/\nu_{22} \sim 2 \cdot 10^{-6}$ s
$\frac{\partial f_2}{\partial t} = R_2(f_1, f_2)$ (Nambu)	$\Delta t \leq 1/\nu_{21} \sim 6 \cdot 10^{-4}$ s

→ Introduction
of $n_{\Delta t}$

Numerical Comparison of (BB_h) and (VB_h)

Comparison of macroscopic quantities

$$\begin{cases} r_p & = 5 \cdot 10^{-9} \text{ m,} \\ n_1 & = 10^{15} \text{ m}^{-3}, \\ n_2 & = 10^{20} \text{ m}^{-3}, \\ T_{surf} & = 500 \text{ K} \end{cases}$$



CPU time

$$\begin{cases} r_p & = 2 \cdot 10^{-8} \text{ m,} \\ n_1 & = 5 \cdot 10^{13} \text{ m}^{-3}, \\ n_2 & = 10^{20} \text{ m}^{-3}, \\ \tau & = 10^{-1} \text{ s} \\ N_1 & = 10^2 \\ N_2 & = 10^4 \end{cases}$$

Model	CPU
System B/B	11410
System V/B with $\Upsilon_b^d(f_2)$ and $n_{\Delta t} = 1$	589
System V/B with $\Upsilon_b^d(f_2)$ and $n_{\Delta t} = 10$	92
System V/B with $\Upsilon_b^d(f_2)$ and $n_{\Delta t} = 100$	43

Arrival of air in a cube with absorption on one side

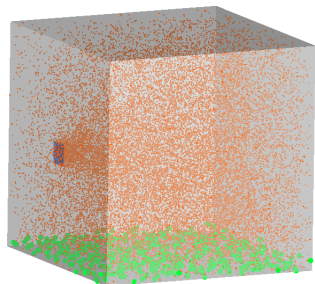
- Box of 1 cm^3 .
- Dust speck of W , $r_p = 0,5 \cdot 10^{-7} \text{ m}$, $n_1 = 10^{15} \text{ m}^{-3}$.
- Boundary conditions : absorption on the upper side, diffuse reflexion on the other sides.
- Gravity turned on.
- Arrival of air ($\mathbf{u} = (300, 0, 0) \text{ m}\cdot\text{s}^{-1}$), density $n_2 = 10^{21} \text{ m}^{-3}$.
- 64 processeurs, computation time : 24h.

- Model B/B : 45 ms of simulation.

B/B model

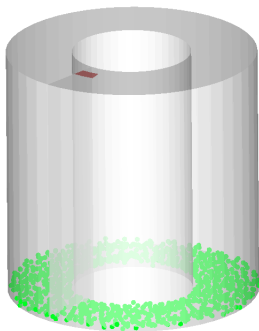
- Model V/B : 247 ms of simulation.

V/B model



Air entering in a closed cylinder

- Dimensions : $L = 10$ cm, $r_{int} = 2,5$ cm, $r_{ext} = 5$ cm.
- Dust specks (W) of radius $r_p = 0,5 \cdot 10^{-7}$ m, and density $n_1 = 10^{15} \text{ m}^{-3}$.
- Air (N_2) entering with density $n_2 = 2,45 \cdot 10^{25} \text{ m}^{-3}$.
- 480 processors, simulation time : 24h.



cylindre torique

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Perspectives

Work in Progress

Integration in the code of a module for the forces felt by the dust specks when they are at the wall.

Numerical Challenges

- Bigger boxes of simulation.
- Transition with fluid models (*P. Degond, G. Dimarco, L. Mieussens*^a).

^aOptimum Kinetic-fluid Coupling Techniques with Smooth Transitions, Preprint.

Mathematical Aspects

- Spatial inhomogeneity.
- Mathematical study of the operators $R_1^d(f_1, f_2)$ and $R_2^d(f_1, f_2)$?

Modeling

Possible improvements of the model : conservation of the energy thanks to the evolution of the surface temperature.