Mathematical and Numerical Study of a Dusty Knudsen Gas Mixture

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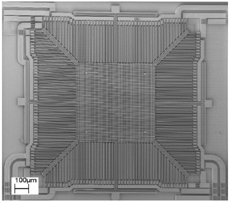
Description of the problem

Context

- Moving dust particles in a rarefied gas inside a Vessel such as in MEMs



- $\lambda_{\text{mol}} \sim 1 - 100mm \gg L \sim 100\mu m \Rightarrow$ kinetic approach
- A possibility : consider a gas-particle mixture with adapted collisional operators
- Here, we suppose that the number of dust is small and we follow them individually

Modelling

Motion of particles

- The behavior of the N_d particles is described by means of the Newton laws of classical mechanics : translation + rotation.
- No influence of the gas on dust particles.
- We denote

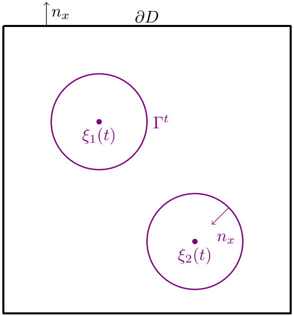
$\xi_i(t)$	Centers of particles
$B_r(\xi_i(t)) = \{x \in \mathbb{R}^\ell \; : \; \|x - \xi_i(t)\| < r\}.$	Particles
$\Gamma^t = \cup_{i=1}^{N_d} \partial B_r(\xi_i(t))$	Boundary of particles
$T_1 = \sup \Big\{ t \geq 0 : \forall s \in [0, t[, \; B_r(\xi_j(s)) \cap B_r(\xi_i(s)) = \emptyset \; \forall j, \; i = 1, \ldots, N_d, \; j \neq i \Big\}$	Maximal time of non-overlapping of particles
$c(t, x)$	Velocity at $x \in \Gamma^t$

Modelling

Description of the gas and boundaries

- Knudsen gas : no collisions between gas molecules
- Container $D \in \mathbb{R}^l$, $l = 2, 3$.
- Time T_2 which guarantee the *non-exit* of dust particles out of the domain

$$T_2 = \sup\{t \geq 0 : \forall s \in [0, t[, \inf_{x \in \partial D} \|x - \xi_i(s)\| \geq r \quad \text{for all } i = 1, \ldots, N_d\}.$$



$$\Omega^t = D \setminus \cup_{i=1}^{N_d} B_r(\xi_i(t))$$

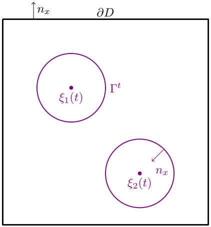
$$\partial\Omega^t = \Gamma^t \cup \partial D$$

Modelling

Boundary conditions

We suppose

- perfectly specular reflexion for the particles hitting ∂D
- diffuse reflexion conditions for the interaction between gaseous particles and dust, that is on Γ^t.
- We assume that all particles have the same temperature of surface T_p, independant of the time.



Modelling

$f(t,x,v)$: density function in gas molecules

Boundary conditions

For $x \in \partial\Omega^t$

$$f(t,x,v) = \int_{\{(w-c(t,x))\cdot n_x \geq 0\}} k(t,x,v,w) f(t,x,w) dw \, 1_{\{(v-c(t,x))\cdot n_x < 0\}},$$

- Specular reflexion and $c(t,x) = 0$ on ∂D :

$$k(t,x,v,w) = \delta(w - v + 2(v\cdot n_x)n_x), \qquad x \in \partial D,$$

that is

$$f(t,x,v) = f(t,x,v - 2(v\cdot n_x)n_x) \qquad \text{for } x \in \partial D, \quad v\cdot n_x < 0.$$

Modelling

Boundary conditions

$$f(t,x,v) = \int_{\{(w-c(t,x))\cdot n_x \geq 0\}} k(t,x,v,w) f(t,x,w) dw \, 1_{\{(v-c(t,x))\cdot n_x < 0\}},$$

- Diffuse reflexion on Γ^t :

$$k(t,x,v,w) = \sqrt{\frac{2\pi}{T_p}} M_{T_p}(v-c(t,x))(w-c(t,x)), \qquad x \in \Gamma^t$$

with

$$M_{T_p}(s) = \frac{1}{(2\pi T_p)^{\ell/2}} e^{-\frac{|s|^2}{2T_p}}, \qquad T_p > 0.$$

Modelling

Boundary conditions

$$f(t,x,v) = \int_{\{(w-c(t,x))\cdot n_x \geq 0\}} k(t,x,v,w) f(t,x,w)dw \, 1_{\{(v-c(t,x))\cdot n_x < 0\}},$$

- Flux normalization properties : $\forall x \in \partial\Omega^t$,

$$\int_{\{(v-c(t,x))\cdot n_x < 0\}} k(t,x,v,w) \frac{|(v-c(t,x))\cdot n_x|}{(w-c(t,x))\cdot n_x} dv = 1$$

and

$$\int_{\{(w-c(t,x))\cdot n_x \geq 0\}} k(t,x,v,w)\, M_{T_p}(w-c(t,x))dw = M_{T_p}(v-c(t,x))$$

Link to DG Lemma

The model

The time evolution of f is hence governed by the following PDE :

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = 0 \qquad (t, x, v) \in (0, T) \times \Omega^t \times \mathbb{R}^\ell$$

with $T = \min(T_1, T_2)$,

- with normalized non-negative initial data

$$f(0, x, v) = \begin{cases} f^{\text{in}}(x, v) & \text{if } (x, v) \in \Omega^0 \times \mathbb{R}^\ell \\ 0 & \text{otherwise} \end{cases}$$

  where $f^{\text{in}} \in L^\infty(\Omega^0 \times \mathbb{R}^\ell)$, $\|f^{\text{in}}\|_{L^1(\Omega^0 \times \mathbb{R}^\ell)} = 1$
- and boundary conditions :

$$f(t, x, v) = \int_{\{(w - c(t,x)) \cdot n_x \geq 0\}} k(t, x, v, w) f(t, x, w) dw \, 1_{\{(v - c(t,x)) \cdot n_x < 0\}},$$

Extension of Darrozes-Guiraud's Lemma

Lemma (Sonne)

For F stricly convex, f a solution of the previous system

$$-\int_{\mathbb{R}^l} [v - c(t,x)] \cdot n_x M_{T_p}(v - c(t,x)) F\left(\frac{f}{M_{T_p}(\cdot - c(t,x))}\right)(v) dv \leq 0$$

In particular for $F(s) = s^2$ we get

$$-\int_{\mathbb{R}^l} [v - c(t,x)] \cdot n_x e^{\frac{|v-c(t,x)|^2}{2T_p}} f^2(v) dv \leq 0$$

Proof

Jensen inequality and properties of the kernel k link.

Existence result

Theorem

Let $c \in L^\infty((0,T)\times\Omega)$ and let $f^{\text{in}} \geq 0$ for a.e. $(x,v) \in \Omega^0 \times \mathbb{R}^\ell$, such that $e^{\frac{|v|^2}{T_p}} f^{\text{in}} \in L^\infty(\Omega^0 \times \mathbb{R}^\ell)$. Then there exists one non-negative weak solution $f \in L^\infty((0,T)\times\Omega^t\times\mathbb{R}^\ell)$ of the initial-boundary value problem.

Backward interaction time

The *backward interaction time* $\tau_{\Omega^t}(x,v)$ for a particle starting from $x \in \Omega^t$ in the direction $v \in \mathbb{R}^l$, is defined as

$$\tau_{\Omega^t}(x,v) = \inf\{\theta > 0 \ : \ x - \theta v \in \Gamma^{t-\theta} \cup \partial D\}.$$

If the set $\Theta := \{\theta > 0 \ : \ x - \theta v \in \Gamma^{t-\theta} \cup \partial D\}$ is empty, then $\tau_{\Omega^t}(x,v) = +\infty$.

Existence result

Strategy of the proof

- Consider the auxiliary problem for the function $g : \mathbb{R}^+ \times \Omega^t \times \mathbb{R}^\ell \to \mathbb{R}$

$$\begin{cases} \dfrac{\partial g}{\partial t} + v \cdot \nabla_x g = 0, \qquad (t,x,v) \in \mathbb{R}^+ \times \Omega^t \times \mathbb{R}^\ell, \\ g(0,x,v) = f^{\text{in}}(x,v) 1_{\{\Omega^0 \times \mathbb{R}^\ell\}}(x,v) \\ g(t,x,v) = \Phi(t,x,v) \qquad \text{for a.e. } x \in \partial\Omega^t,\ (v - c(t,x)) \cdot n_x < 0 \end{cases}$$

  where $\Phi \in L^\infty((0,T) \times (\partial\Omega^t \times \mathbb{R}^l))$. The problem has a unique weak solution, given by

$$g(t,x,v) = f^{\text{in}}(x - vt, v) 1_{\{\tau_{\Omega^t}(x,v) > t\}} + \Phi(t, x^*, v) 1_{\{\tau_{\Omega^t}(x,v) < t\}},$$

  where $x^* = x - \tau_{\Omega^t}(x,v) v$, and

$$\|g\|_{L^\infty((0,T)\times\Omega^t\times\mathbb{R}^\ell)} \leq \max\{\|f^{\text{in}}\|_{L^\infty(\Omega^0\times\mathbb{R}^\ell)}, \|\Phi\|_{L^\infty((0,T)\times(\partial\Omega^t\times\mathbb{R}^l))}\}.$$

Existence result

Strategy of the proof

- We now construct a sequence $\{f_n\}_{n\in\mathbb{N}}$, such that

$$f_1(t,x,v) = 0 \text{ for a.e. } (t,x,v) \in [0,T) \times \bar{\Omega}^t \times \mathbb{R}^\ell$$

  and, for all $n \in \mathbb{N}$, $n \geq 2$, f_n is the solution of the previous problem with the boundary condition : for $x \in \partial\Omega^t$:

$$f_n(t,x,v) = \int_{\{(w-c(t,x))\cdot n_x \geq 0\}} k(t,x,v,w) f_{n-1}(t,x,w) dw \, 1_{\{(v-c(t,x))\cdot n_x < 0\}},$$

- Then we can proove that for a.e. $(t,x,v) \in (0,T) \times \Omega^t \times \mathbb{R}^l$,

$$0 \leq f_n \leq C \| f^{\text{in}} e^{\frac{|v|^2}{T_p}} \|_{L^\infty(\Omega^0 \times \mathbb{R}^l)}$$

$$h_n := f_{n+1} - f_n \geq 0 \qquad \text{for a.e. } (t,x,v) \in (0,T) \times \Omega^t \times \mathbb{R}^\ell.$$

Numerical strategy

Particle method

$f(t^n, \cdot, \cdot)$ is approached by

$$f^n_{\varepsilon, N_m}(x, v) = \sum_{k=1}^{N_m} \omega_k \, \varphi_\varepsilon(x - X^n_k) \, \varphi_\varepsilon(v - V^n_k), \qquad (1)$$

- $(X^n_k)_{1 \le k \le N_m}$ and are the positions of the "numerical molecules" at time t^n,
- $(V^n_k)_{1 \le k \le N_m}$ are their velocities
- ω_k their weight,
- φ_ε a smooth shape function.
- Initially $(X^0_k)_{1 \le k \le N_m}$ and $(V^0_k)_{1 \le k \le N_m}$ are sampled according to the initial density $f^{ini}(x, v)$.

Numerical strategy

At each time step

We compute

- the free flow of the particles in the absence of any interaction, mathematically represented by the transport operator $v \cdot \nabla$;
- the time evolution of the set of dust particles.
- the boundary conditions
  - the specular reflexion of the gas particles at the boundary ∂D ;
  - the diffuse reflexion between gas particles and spherical dust particles by computing the intersection of the trajectories of molecules and dust particles.
  - Iteration in the time $[t^n, t^n + \Delta t]$ to obtain positions and velocities of molecules at time t^{n+1}.

Numerical results

Physical quantities

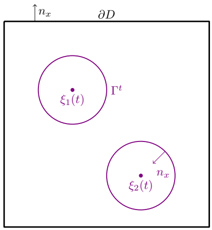
$$f^{\text{in}}(x,v) = \frac{n_0 m}{2\pi k_B T^{\text{in}}} e^{-\frac{m|v-\mathbf{u_g}|^2}{2k_B T^{\text{in}}}},$$

with $\mathbf{u_g} = (-2u_d, 0)$ or $\mathbf{u_g} = (0,0)$.

λ	K_n	T^{in}	M_a	$u_d = a\,M_a$
$2 \cdot 10^{-3}$ m	10	293 K	0.1	34.41 m/s

Particles :

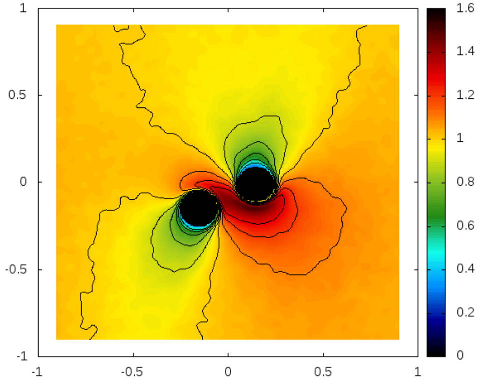
- radius $r = 10^{-5} m$
- $T_p = 500$ K.



Numerical results

Scenario 1

Evolution of a system of two particles with translational velocities $u_1 = (0, u_d)$ and $u_2 = (0, -1.5u_d)$, with $u_d = 2u^{\text{in}}$, and no rotational velocities.



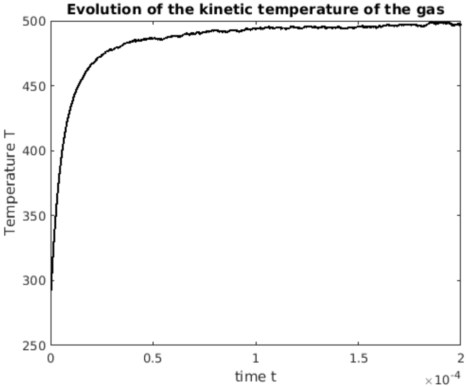
Density at time $t = 5 \cdot 10^{-7}$ (here with periodic BC)

Numerical results

Scenario 2

Time evolution of the mean temperature of the gas with a motionless particle

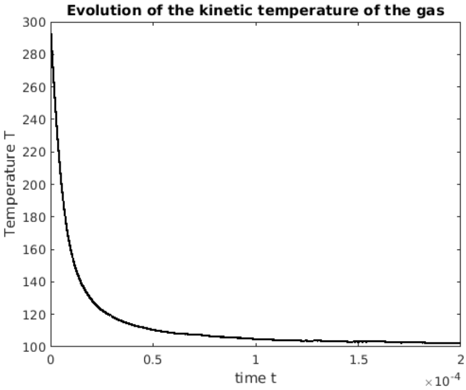
$$\langle T(t)\rangle = \int_{\Omega^t} T(t,x)dx$$



Numerical results

Scenario 3

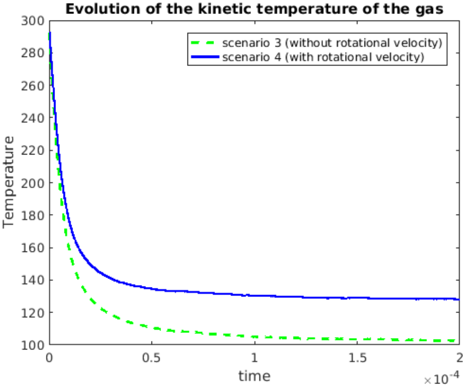
Time evolution of the mean temperature of the gas with a motionless particle at temperature $T_p = 100$ K.



Numerical results

Scenario 4

Time evolution of the mean temperature of the gas with a particle at temperature $T_p = 100$ K ; the spherical dust particle has a rotational velocity equal to $2\pi \times 10^6$ rad$\cdot$ s^{-1}.



Futur prospects

- Addition of the evolution of temperature in dust particles
- Numerical simulations with an ellipsoidal dust, with more particles...