Kinetic modelling of respiratory aerosols, numerical treatment

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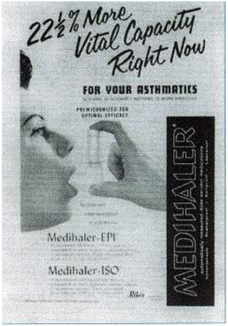
involving:
C. Grandmont, B. Grec, D. Yakoubi (2D);
C. Grandmont, A. Lorz, A. Moussa (3D);
P. Diot, S. Ehrmann, L. Vecellio (experimental comparisons).

Motivations

Studying aerosol transport in the upper part of the respiratory system (aerosoltherapy)

- Asthma, allergy, cystic fibrosis (mucoviscidosis)...
- *In vivo* observations are difficult.
- Non invasive treatments by aerosol are used for decades.
- Main issue: locating the aerosol deposition



This study can also be used for polluting particles in the atmosphere.

Outline

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Which model?

Air: viscous, Newtonian, incompressible fluid, described through its **density** ϱ, **velocity** u, and **pressure** p, depending on $t \geq 0$ and $x \in \Omega$

Aerosol:

- Differential system on a high number of aerosol particles/droplets: most commonly used, low numerical efficiency (up to 10^{10} particles)
- PDEs on **macroscopic quantities** (density, velocity...), only depending on $t \geq 0$ and $x \in \Omega$ [Wall *et al.*]
- PDE on a **distribution function** $f \geq 0$ depending on $t \geq 0$, $x \in \Omega$, $v \in \mathbb{R}^3$ and other variables describing the dynamical/thermodynamical/... state of the particles

Spray models

A generical example:

$$\begin{cases} \partial_t(\alpha\varrho) + \nabla_x \cdot (\alpha\varrho u) = 0 \\ \partial_t(\alpha\varrho u) + \nabla_x \cdot (\alpha\varrho u \otimes u) + \nabla_x p = \mathscr{F}_{\text{aero}} \\ \partial_t f + \nabla_x \cdot (f v) + \nabla_v \cdot (f a) + \partial_r(f\Phi) = Q(f,f) \end{cases}$$

- $Q(f,f)$ operator describing binary interactions between particles
- α fluid volume fraction
- $\mathscr{F}_{\text{aero}}$ action exerted by the particles on the fluid

For respiratory aerosol and airborne polluting particles: $Q(f,f) \simeq 0$; $\alpha \simeq 1$

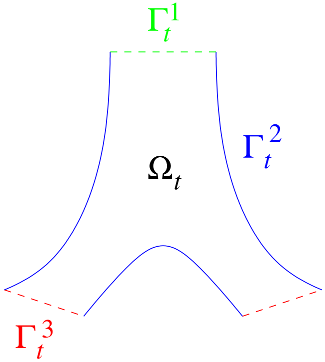
Vlasov/(incompressible) Navier-Stokes system

$$\begin{cases} \partial_t u + (u \cdot \nabla_x) u + \dfrac{1}{\varrho} \nabla_x p = \dfrac{\mu}{\varrho} \Delta_x u - \dfrac{1}{\varrho} \displaystyle\iint m \; a \; f \, \mathrm{d}v \, \mathrm{d}r \\ \nabla_x \cdot u = 0 \\ \partial_t f + \nabla_x \cdot (f v) + \nabla_v \cdot (f a) = 0 \end{cases}$$

- Particle acceleration $a = D(u - v)$
- Drag coefficient $D = \dfrac{6\pi\mu r}{m}$
- Boundary condition on f: given at the inlet

Boundary conditions for the fluid

Geometry: possibly moving domain



- Artificial boundaries Γ_t^1 and Γ_t^3: u imposed at the inlet, or difference of pressure between inlet and outlet
- Physical boundary Γ_t^2 : $u(t,x) = w(t,x)$ for $x \in \Gamma_t^2$, where w is the wall velocity

Decreasing energy

Proposition

When $\Omega_t = \Omega_0$ for any $t \geq 0$,
if $u \equiv 0$ on $\partial\Omega_0$ and if $f \equiv 0$ on $\partial\Omega_0 \times \mathbb{R}^3$ for $v \cdot n_0 < 0$, then

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{2}\iint_{\Omega_0\times\mathbb{R}^3} f(t,x,v)\,mv^2\,\mathrm{d}v\,\mathrm{d}x + \frac{1}{2}\int_{\Omega_0} \varrho u(t,x)^2 \mathrm{d}x\right) \leq 0.$$

⇒ this property should also be satisfied at the discrete level.

Existence result: LB, L. Desvillettes, C. Grandmont, A. Moussa, DIE '09
see also Anochschenko, Boutet de Monvel '97; Hamdache '98; Yu '13

Outline

Discretization (w/ C. Grandmont, A. Moussa)

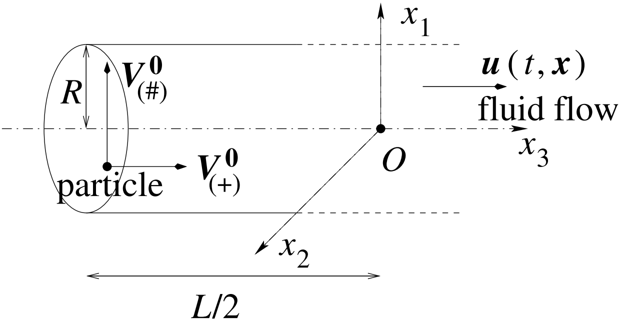
- Explicit time-advancing scheme $\Longrightarrow$ uncoupling the equations
  1. Solving the Navier-Stokes equations with the retroaction term coming from the previous time step
  2. Solving the Vlasov equation by using the fluid velocity updated at the previous stage
  3. Computing the new retroaction term to be used at the next time step (possibly with a time subcycling)

- Space discretization
  - Fluid: finite element method with an ALE approach (moving domain)
  - Aerosol: particle method with a locating algorithm

$$f(t,x,v) \simeq \sum_{p=1}^{N} \omega_p \; \delta_{x_p(t)}(x) \; \delta_{v_p(t)}(v)$$

$N \ll$ # phys. particles; ω_p representativity of particle p

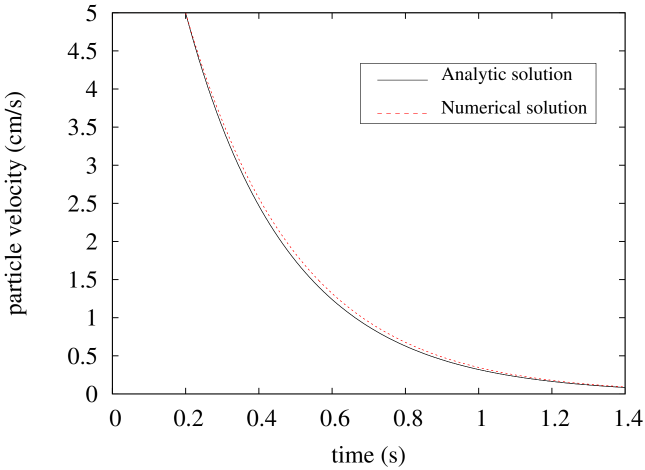
Validation frame (w/ CG, A. Lorz and AM)



- Fluid: $u(t,x) = U \times \left(1 - \frac{{x_1}^2 + {x_2}^2}{R^2}\right)$
- Particles: same size, density and initial velocity V^0

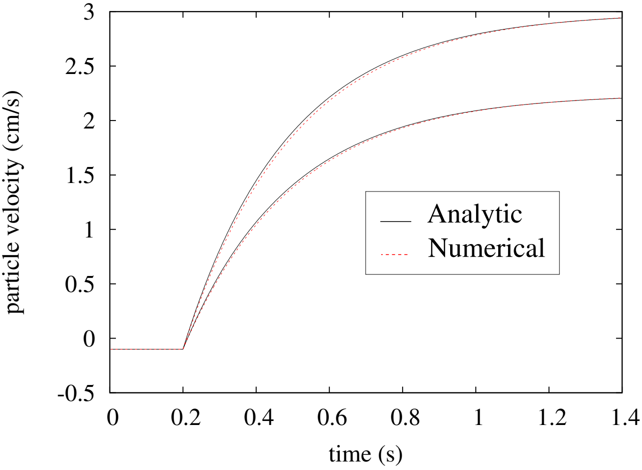
Motionless fluid in a fixed domain, w/o retroaction

One can find an analytic solution to the particles trajectories.



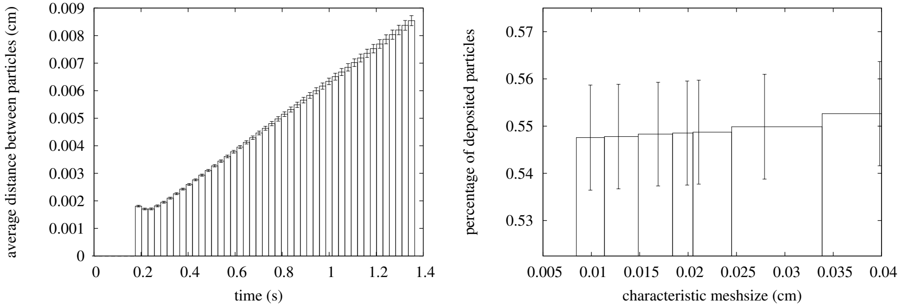
Moving fluid in a fixed domain, w/o retroaction

One can also find an analytic solution to the particles trajectories.



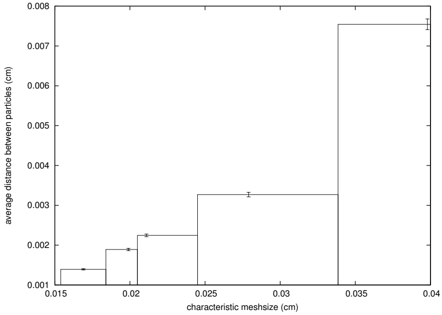
Sensitivities

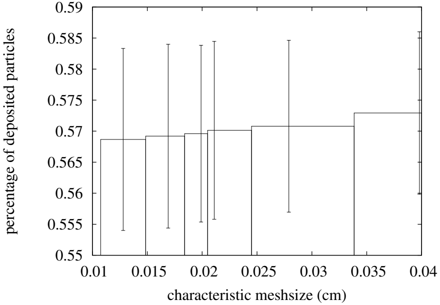
Various test-cases with varying meshes, time steps, initial data on f



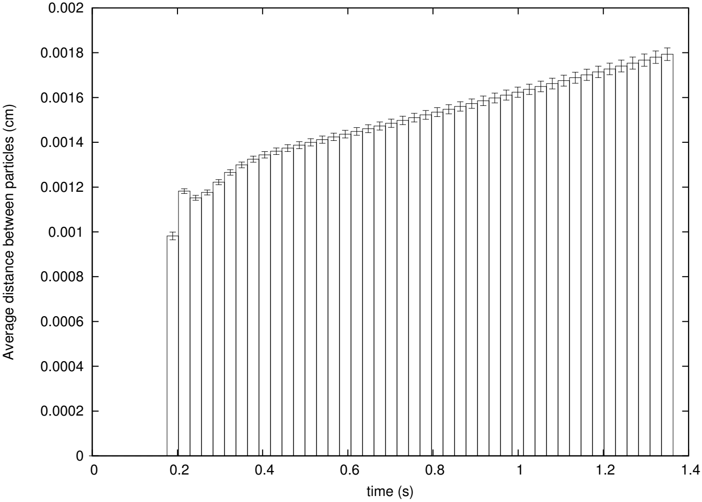
Sensitivities in a moving domain, w/o retroaction

Validation of the fluid code in a 2D moving domain thanks to an analytic solution computed in cylindrical coordinates



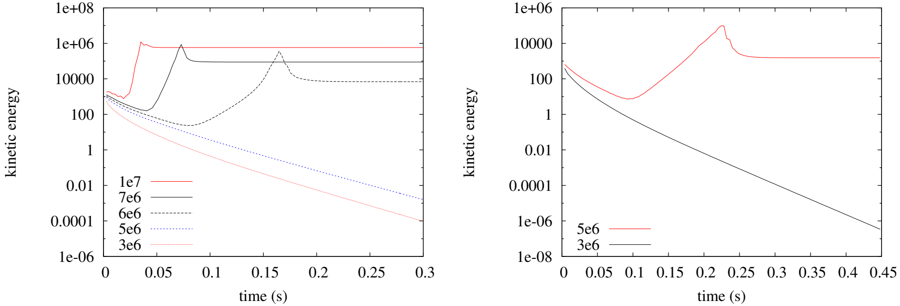


Sensitivities in a fixed domain, w/ retroaction



Representativities (1)

N constant (numerical particles)

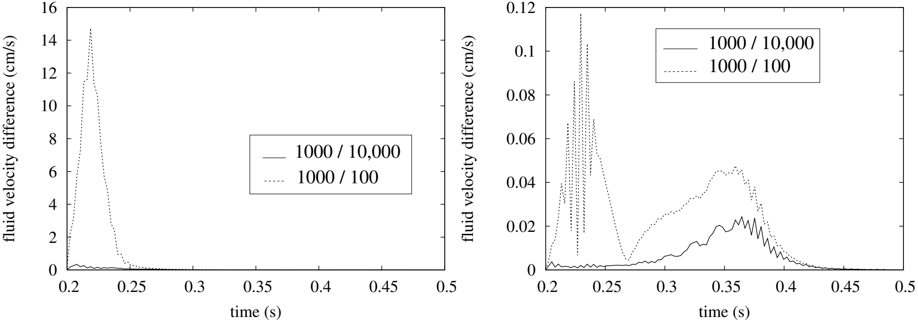


$\Rightarrow$ existence of a CFL-like condition involving, amongst others, $\omega_p \Delta t$

cf. $\mathscr{F}^n_{\text{aero}}(x) = -m \sum_{p=1}^{N} \omega_p D \left(\tilde{u}^n(x^n_p) - v^n_p \right) \delta_{x^n_p}(x)$ for $x \in \Omega_{t^n}$

Representativities (2)

$N\omega_p$ **constant** (physical particles)



Study assessment:
for particles with radius $\leq 25\ \mu$m, **retroaction can be neglected**.

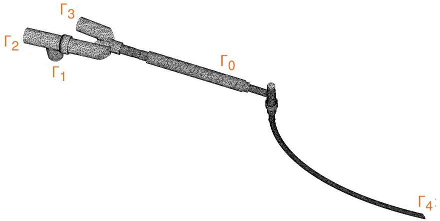
Outline

1. Fluid/kinetic models for aerosols
2. Numerical implementation and validations
3. Experimental comparisons

Joint work with Aerodrug/DTF

Goal: compare experimental and numerical results

Retroaction neglected

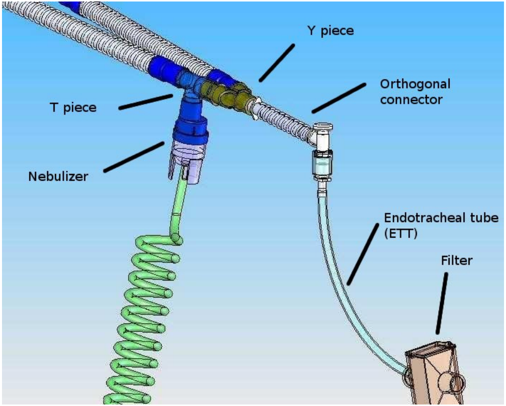


- Need an accurate location of the aerosol deposition areas

- *In vitro*: 3D imaging by scintigraphy, Gamma camera
- *In silico*: `LifeV`, finite element fluid solver in `C++`, with actual development of the particle solver

Simulation on an endotracheal tube

Filter collecting aerosol at the ETT outlet



Simulation on an endotracheal tube

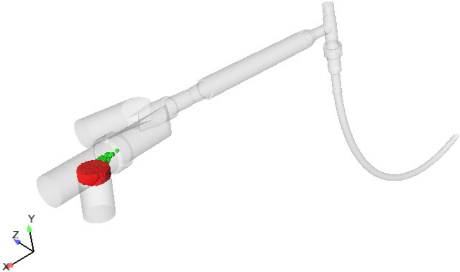
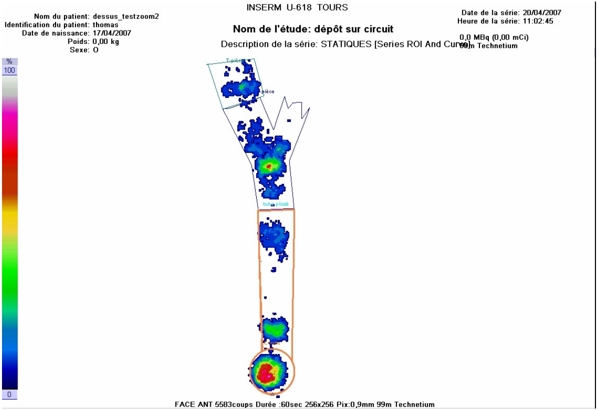
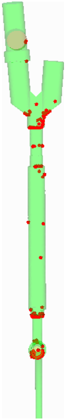


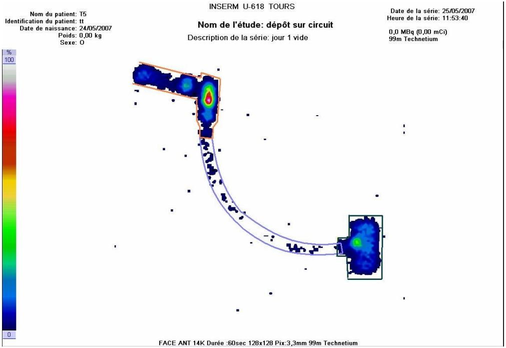
Figure: Device mesh designed by M. Grasseau.

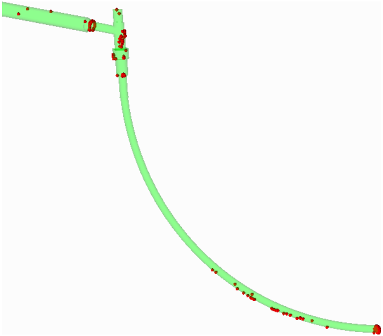
Deposition areas, view from above





Deposition areas, lateral view





Deposition rate

Experimental results

VMD/flow rate	10 L/min	20 L/min	40 L/min
5.4 μm	29%	41%	60%
14 μm	42%	73%	86%

Numerical results
(averaged on 10 random distributions of particles)

diam./flow rate	10 L/min	20 L/min	40 L/min
5.4 μm	32%	45%	72%
14 μm	41%	76%	98%

Prospects and ongoing works

- Mathematical analysis (w/ C. Grandmont and A. Moussa): existence of solutions in a moving domain
- Validation by experimental comparisons in a moving domain (in a pluridiscplinary ANR-supported team and headed by M. Filoche)
- Engeneering on aerosol nebulizers in a fixed domain (w/ Aerodrug)
- Nanometric aerosols modelling, humidity effect (w/ C. Rigault)