Fluid-Particles Interaction Models Asymptotic Models and Simulation

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in collaboration with
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(CPDE 2005) & Work in Progress

ICREA - Universitat Autònoma de Barcelona

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Outline

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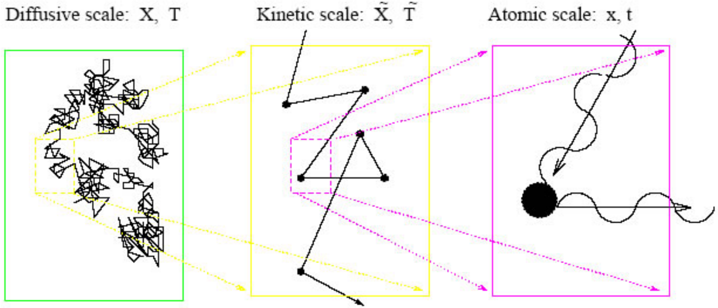
1. Motivation & Modelling
   - Kinetic Modelling
   - Fluid-Particles Interaction
2. Asymptotics
   - Dimensionless Formulation
   - Asymptotic Limits
   - Asymptotic Systems
3. Numerical Schemes & Simulation
   - Asymptotic Preserving Kinetic Schemes: Bubbling
   - Numerical Simulation
   - Conclusions & Perspectives

Atmospheric Pollution Modelling

Pollution in Los Ángeles, Madrid and Beijing.

Statistical description



- Particles Description: impossible due to their huge number.
- Kinetic Description: $f(t, x, \xi)$ represents the number density of particles at time t in position x with velocity ξ.
- Hydrodynamic Description: Continuum mechanics approach based on balance equations for density, momentum and temperature.

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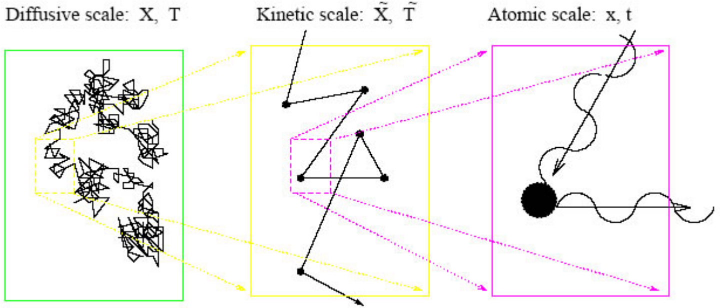

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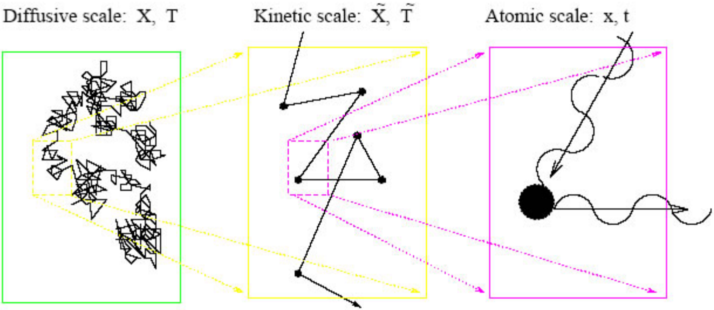

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Macroscopic Quantities: Moments

- Particle density:

$$\rho(t,x) = \int_{\mathbb{R}^3} f(t,x,\xi)\, d\xi$$

- Momentum:

$$J(t,x) = \rho U(t,x) = \int_{\mathbb{R}^3} \xi f(t,x,\xi)\, d\xi$$

- Temperature:

$$3\rho\theta(t,x) = \int_{\mathbb{R}^3} |\xi - U(t,x)|^2 f(t,x,\xi)\, d\xi$$

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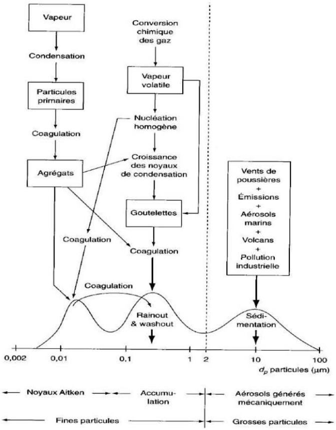
Formation of Aerosols in the atmosphere

Sources	Estimation des émissions ($10^{12} g/an$)	Catégorie de taille des particules
Sources naturelles		
Croûte terrestre et érosion éolienne	1500	grosses particules
Océans (sel)	1300	accumulation et grosses particules
Volcans	30	grosses particules
Débris biologiques	50	grosses particules
Sulphates dérivés des gaz biogéniques	130	particules très fines
Sulphates dérivés des gaz volcaniques	20	particules très fines
Matières organiques	60	particules très fines
Nitrates dérivés des NO_x	30	particules très fines
Total des sources naturelles	3100	
Sources anthropiques		
Poussières industrielles	100	particules très fines et grosses
Suie	10	particules très fines
Sulphates dérivés de SO_2	190	particules très fines
Feux	90	particules très fines
Nitrates dérivés des NO_x	50	grosses particules
Matières organiques	10	particules très fines
Total des sources anthropiques	450	
Total des deux sources	3600	



Pandis & Seinfeld (1998), Madelaine (1982)

Assumptions of the Model

Two phase flow:

- [Dense Phase] Fluid: continuum mechanics description in terms of density of the fluid $n(t,x)$ and velocity field $u(t,x)$.

  Let ρ_{F} a typical value of the fluid mass per unit volume.

  Fluid Equations: Compressible Euler.

- [Dispersed Phase] Particles: kinetic description in terms of the number density of particles $f(t,x,\xi)$ in phase space (x,ξ) to compute velocity fluctuations around the fluid velocity $u(t,x)$.

  Particles are spheres of radius $a > 0$ with mass given by $m_{\mathrm{P}} = \frac{4}{3}\rho_{\mathrm{P}}\pi a^3$, ρ_{P} being the particle mass per unit volume.

  Particles are assumed to follow a kind of Brownian motion:

$$m_{\mathrm{P}}x'' + F(t,x,x') = \Gamma(t).$$

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Forces to be considered

Forces $F(t,x,x')$:

- Friction: The fluid produces a friction force on the particles

$$6\pi\mu a\big(u(t,x)-\xi\big),$$

with $\mu>0$ being the dynamic viscosity of the fluid. Accordingly, the force exerted by the particles on the fluid is given by the sum

$$6\pi\mu a\int_{\mathbb{R}^3}(\xi-u(t,x))f\,\mathrm{d}\xi.$$

- Gravity+Buoyancy: External forces per unit volume acting on the particles $-m_{\mathrm{P}}\nabla_x\Phi$ and on the fluid $\alpha\rho_{\mathrm{F}}\nabla_x\Phi$.

  $\alpha\in\mathbb{R}$ is a dimensionless parameter which measures the ratio of the strength of the external force on each phase:

$$\Phi(x)=(1-\rho_{\mathrm{F}}/\rho_{\mathrm{P}})gx_3 \qquad \alpha=\frac{1}{1-\rho_{\mathrm{F}}/\rho_{\mathrm{P}}},$$

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Disperse Phase

Vlasov-Fokker-Planck equation:

$$\partial_t f + \xi \cdot \nabla_x f - \nabla_x \Phi \cdot \nabla_\xi f = \frac{9\mu}{2a^2 \rho_P} \operatorname{div}_\xi \left((\xi - u) f + \frac{k\theta_0}{m_P} \nabla_\xi f \right),$$

where k stands for the Boltzmann constant, and $\theta_0 > 0$ controls the noise strength.

Fokker-Planck term:

The Fokker-Planck term implies a relaxation in velocity towards equilibrium densities of the form

$$\rho(t,x)M(\xi) = \rho(t,x) \left(2\pi \frac{k\theta_0}{m_P} \right)^{-3/2} \exp\left\{ -m_P |\xi - u(t,x)|^2 / 2k\theta_0 \right\},$$

with typical Stokes relaxation time given by

$$\mathcal{T}_S = \frac{m_P}{6\pi\mu a} = \frac{2\rho_P a^2}{9\mu}.$$

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Final PDE Model

Vlasov-Euler-Fokker-Planck system:

We arrive at the system:

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$$\partial_t n + \operatorname{div}_x(nu) = 0, \qquad (2)$$

$$\rho_F \Big(\partial_t(nu) + \operatorname{Div}_x(nu \otimes u) + \alpha n \nabla_x \Phi \Big) + \nabla_x p(n) = 6\pi\mu a \int_{\mathbb{R}^3} (\xi - u) f \, d\xi. \qquad (3)$$

where k stands for the Boltzmann constant, and $\theta_0 > 0$ controls the noise strength and $p(n)$ is a general pressure law, for instance $p(n) = C_\gamma \, n^\gamma$, $\gamma \geq 1$, $C_\gamma > 0$.

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DimensionLess PDE Model

DimensionLess Vlasov-Euler-Fokker-Planck system:

$$\partial_t f + \beta\xi \cdot \nabla_x f - \eta' \nabla_x \Phi \cdot \nabla_\xi f = \frac{1}{\epsilon} \nabla_\xi \cdot \Big((\xi - \frac{1}{\beta} u) f + \nabla_\xi f \Big), \tag{4}$$

$$\partial_t n + \mathrm{div}_x(nu) = 0, \tag{5}$$

$$\partial_t(nu) + \mathrm{Div}_x(nu \otimes u) + \nabla_x p(n) + \eta\, n \nabla_x \Phi = \frac{1}{\epsilon} \frac{\rho_{\mathrm{P}}}{\rho_{\mathrm{F}}} (J - \rho u). \tag{6}$$

where

$$\rho(t,x) = \int_{\mathbb{R}^3} f(t,x,\xi)\, \mathrm{d}\xi, \qquad J(t,x) = \beta \int_{\mathbb{R}^3} \xi\, f(t,x,\xi)\, \mathrm{d}\xi.$$

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Dissipation Properties

Entropy Decay:

Assumme the scaling:

$$\frac{\rho_\mathrm{P}}{\rho_\mathrm{F}}\,\beta^2 = 1, \qquad \eta' = \varsigma\beta, \qquad \text{with } \varsigma = \pm 1.$$

Defining the free energies associated respectively to the particles and the fluid as:

$$\mathcal{F}_\mathrm{P}(t) = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \left(f\ln(f) + \frac{\xi^2}{2} f + \varsigma\Phi f \right) \mathrm{d}\xi\,\mathrm{d}x,$$

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where $\Pi : \mathbb{R}^+ \longrightarrow \mathbb{R}^+$ is defined by $s\Pi''(s) = p'(s)$. Then, we have the crucial dissipation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\mathcal{F}_\mathrm{P} + \mathcal{F}_\mathrm{F}\right) + \frac{1}{\varepsilon}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \left|(\xi - \beta^{-1}u)\sqrt{f} + 2\nabla_\xi\sqrt{f}\right|^2 \mathrm{d}\xi\,\mathrm{d}x \le 0.$$

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Dissipation Properties 2

Comments:

- Entropy Dissipation: This claim helps in understanding the asymptotic regime $\varepsilon \ll 1$: we infer that f has essentially a hydrodynamic behavior

$$f(t,x,\xi) \simeq \rho(t,x)\ (2\pi)^{-3/2}\ \exp\left(-|\xi - \beta^{-1}u(t,x)|^2/2\right) = \rho(t,x) M_{u(t,x)/\beta}(\xi).$$

Bubbling Regime

We set

$$\beta = \frac{1}{\sqrt{\varepsilon}}, \qquad |\eta'| = \frac{1}{\sqrt{\varepsilon}}, \qquad \frac{\rho_P}{\rho_F} = \varepsilon.$$

meaning that:

Stokes velocity $\simeq$ Typical velocity of the fluid $\ll$ Thermal velocity.

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Flowing Regime

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$$\beta^2 \frac{\rho_P}{\rho_F} = 1, \qquad \beta = |\eta'| \text{ a fixed positive constant}$$

meaning that

Stokes velocity $\ll$ Typical velocity of the fluid $\simeq$ Thermal velocity.

As $\varepsilon \to 0$ and β is smaller than 1, the two phases are driven by gravity, but with much more influence on the fluid.

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Diffusion Asymptotics: Bubbling Regime

DimensionLess Bubbling Regime:

$$\partial_t f + \frac{1}{\sqrt{\varepsilon}}\left(\xi \cdot \nabla_x f + \nabla_x \Phi \cdot \nabla_\xi f\right) = \frac{1}{\epsilon}\nabla_\xi \cdot \Big((\xi - \sqrt{\varepsilon}u)f + \nabla_\xi f\Big),$$

$$\partial_t n + \mathrm{div}_x(nu) = 0,$$

$$\partial_t(nu) + \mathrm{Div}_x(nu \otimes u) + \nabla_x p(n) + \eta n \nabla_x \Phi = J - \rho u.$$

where

$$\rho(t,x) = \int_{\mathbb{R}^3} f(t,x,\xi)\,\mathrm{d}\xi, \qquad J(t,x) = \frac{1}{\sqrt{\varepsilon}}\int_{\mathbb{R}^3} \xi f(t,x,\xi)\,\mathrm{d}\xi.$$

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Diffusion Asymptotics: Bubbling Regime

- As ε tends to 0, we should have that $f(t,x,\xi) \simeq \rho(t,x)M(\xi)$.
- Hilbert expansion: we plug the ansatz

$$f_\varepsilon = f^{(0)} + \sqrt{\varepsilon} f^{(1)} + \varepsilon f^{(2)} + \dots$$

into the kinetic equation.

DimensionLess Bubbling Regime:

We end up with the limiting system

$$\begin{cases} \partial_t \rho + \mathrm{div}_x\big(\rho(u + \nabla_x \Phi) - \nabla_x \rho\big) = 0, \\ \partial_t n + \mathrm{div}_x(nu) = 0, \\ \partial_t(nu) + \mathrm{Div}_x(nu \otimes u) + \nabla_x(p(n) + \rho) + (\eta n - \rho)\nabla_x \Phi = 0, \end{cases}$$

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Hydrodynamic Asymptotics: Flowing Regime

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\partial_t \rho + \mathrm{div}_x(\rho u) = 0, \\
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\partial_t\big((n+\beta^{-2}\rho)u\big) + \mathrm{Div}_x\big((n+\beta^{-2}\rho)u\otimes u\big) \\
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Outline

Bubbling Regime: Coupling of density and fluctuations

The scheme is based on the expansion

$$f_\varepsilon(t,x,\xi) = \rho_\varepsilon(t,x)M(\xi) + \sqrt{\varepsilon}r_\varepsilon(t,x,\xi)$$

with the "fluctuations" r_ε bounded in L^2 by entropy dissipation.

We rewrite the scaled kinetic equation as

$$\partial_t f_\varepsilon + \xi \cdot \nabla_x r_\varepsilon + (u_\varepsilon + \nabla_x \Phi)\nabla_\xi r_\varepsilon = \frac{1}{\varepsilon}Lf_\varepsilon + \frac{1}{\sqrt{\varepsilon}}M(\xi)S_\varepsilon(t,x,\xi),$$

where

$$S_\varepsilon(t,x,\xi) = -\xi \cdot \nabla_x \rho_\varepsilon - \xi \cdot (u_\varepsilon(t,x) + \nabla_x \Phi)\rho_\varepsilon,$$

and the evolution of the remainder obeys

$$\partial_t r_\varepsilon = \frac{1}{\varepsilon}Lr_\varepsilon - \frac{1}{\varepsilon}MS_\varepsilon - \frac{1}{\sqrt{\varepsilon}}\left[\xi \cdot \nabla_x r_\varepsilon + (u_\varepsilon + \nabla_x\Phi)\nabla_\xi r_\varepsilon - M\nabla_x \cdot \left(\int_{\mathbb{R}^3} \xi_\star r_\varepsilon \, \mathrm{d}\xi_\star\right)\right]$$

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Splitting Method 1

Given n^k, u^k, f^k, r^k, evaluation of n, u, f, r at time $k\Delta t$:

Step 0.- Solve the Euler equations for the fluid density n and velocity u.

1. Particles density is constant for this step:
$$\int_{\mathbb{R}^3} \xi r^k \,\mathrm{d}\xi - u \int_{\mathbb{R}^3} f^k \,\mathrm{d}\xi.$$
2. Numerical method: Després & Lagoutière 99'-04' which preserves with accuracy the shock structure of the hyperbolic system. This defines n^{k+1} and u^{k+1}.
3. Different stability conditions: We perform Step 0 on a time interval $(k\Delta t_h, (k+1)\Delta t_h)$, and then we make several sub-cycles (Step 1-Step 2) below on time intervals $(k'\Delta t_p, (k'+1)\Delta t_p)$, for some $\Delta t_p < \Delta t_h$. Typically, the space mesh size Δx being given, we have $\Delta t_p = \mathcal{O}(\Delta x^2)$ but $\Delta t_h = \mathcal{O}(\Delta x)$.

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Splitting Method 2

Step 1.- Solve the stiff equations

$$\partial_t f = \frac{1}{\varepsilon} Lf, \qquad \partial_t r = \frac{1}{\varepsilon} Lr + \frac{1}{\varepsilon} MS,$$

where

$$S = -\xi \cdot \nabla_x \rho + \xi \cdot (u^{k+1} + \nabla_x \Phi)\rho.$$

Note that $\rho = \int f \, d\xi$ is not modified by the first equation so that the source term in the second equation can be treated as constant in time.

Step 2.- Solve the transport part

$$\partial_t f + \xi \cdot \nabla_x r + (u^{k+1} + \nabla_x \Phi) \cdot \nabla_\xi r = 0, \qquad \partial_t r = 0$$

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Approximation of $e^{\Delta t L/\varepsilon}$

Solutions of

$$\partial_t F = \frac{1}{\varepsilon} L F + H$$

can be explicitly computed since the fundamental solution of L is given by

$$\mathcal{G}(t,\xi,\xi_\star) = D_{\gamma(t)} \exp\left(-\frac{|\xi-\gamma(t)\xi_\star|^2}{2(1-\gamma(t)^2)}\right), \qquad \gamma(t)=e^{-t}\ ,\ D_{\gamma(t)} = \frac{1}{(2\pi(1-\gamma(t)^2))^{N/2}}.$$

Duhamel formula:

$$F(t,\xi) = \int_{\mathbb{R}^3} \mathcal{G}\left(\frac{t-s}{\varepsilon},\xi,\xi_\star\right) F(s,\xi_\star)\,\mathrm{d}\xi_\star + \int_s^t \mathcal{G}\left(\frac{t-\sigma}{\varepsilon},\xi,\xi_\star\right) H(\sigma,\xi_\star)\,\mathrm{d}\xi_\star\,\mathrm{d}\sigma.$$

Since it involves the quantity $e^{-t/\varepsilon}$ with $0<\varepsilon\ll 1$, then

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We use this expansion to approximate the Duhamel formula with $H(t,x,\xi) = -\frac{1}{\varepsilon}M(\xi)S(k'\Delta t,x,\xi)$ which is not modified during the time step. Accordingly, we make appear

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Therefore, Step 1 of the method reduces to:

$$\begin{cases} f^{k'+1/2}(\xi) &= M(\xi)\left(\rho^{k'} + e^{-\Delta t/\varepsilon}\xi\int_{\mathbb{R}^N}\xi_\star f^{k'}\,\mathrm{d}\xi_\star\right), \\ r^{k'+1/2}(\xi) &= e^{-\Delta t/\varepsilon}M(\xi)\left(\xi\int_{\mathbb{R}^N}\xi_\star r^{k'}\,\mathrm{d}\xi_\star\right) + \left(1-e^{-\Delta t/\varepsilon}\right)M(\xi)S^{k'}. \end{cases}$$

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Properties Numerical Method

Remarks:

- Asymptotic Preserving: taking the completely relaxed model, i.e., $\varepsilon = 0$, yields an approximation scheme of the Smoluchowski-Euler model.
- Full discretization: A downwind discretization for $-\xi\partial_x\rho$ in Step 1 and an upwind discretization for $-\xi\partial_x r$ in Step 2. For the discretization of $(u^{k+1} - \partial_x\Phi)\partial_\xi r$ in Step 2, we choose a centered discretization in velocity.
- Boundary conditions: At the convection Step 2 specular reflections for the fluxes associated to the convection in space. At the end of Step 1, we impose a boundary condition on the fluctuations coherent with specular reflection for f.
- Well-Balanced: Equilibrium states for the kinetic equation are kept up to consistency error.

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- Full discretization: A downwind discretization for $-\xi\partial_x\rho$ in Step 1 and an upwind discretization for $-\xi\partial_x r$ in Step 2. For the discretization of $(u^{k+1} - \partial_x\Phi)\partial_\xi r$ in Step 2, we choose a centered discretization in velocity.
- Boundary conditions: At the convection Step 2 specular reflections for the fluxes associated to the convection in space. At the end of Step 1, we impose a boundary condition on the fluctuations coherent with specular reflection for f.
- Well-Balanced: Equilibrium states for the kinetic equation are kept up to consistency error.

Outline

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Conclusions & Perspectives

- Excellent Asymptotic Preserving Schemes for the simplified coupled kinetic-fluid model for atmospheric pollutants.
- Improvements of the model: coagulation in size of pollutants, different species, chemical reactions,...
- Use of these models in realistic situations: contacts underway with mechanicists in Lyon and Lille.

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