DE LA RECHERCHE À L'INDUSTRIE

Some new results on the numerical simulation of thick sprays

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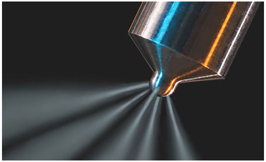
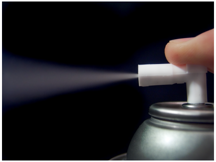
Examples : Clouds, Diesel engines, Medical sprays, Nuclear industry, Pharmaceutical industry

Thin sprays:



(a) Diesel engine fuel injector



(b) Medical spray

Thick sprays:

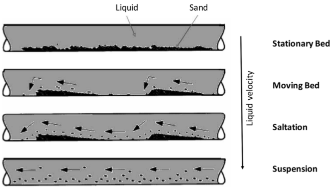
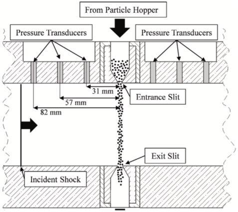


Fig. 1. Sand flow regime in horizontal pipelines.

(c) Leporini at al (2019)



(d) Daniel-Wagner (2022)

- Unknowns for the gas

$$\varrho(t, \boldsymbol{x}) \geq 0, \quad \boldsymbol{u}(t, \boldsymbol{x}) \in \mathbf{R}^3, \quad e(t, \boldsymbol{x}) \geq 0, \quad \alpha(t, \boldsymbol{x}) \in (0, 1].$$

  - Follow a hyperbolic (compressible Euler equations) or Navier-Stokes equation.
- Unknown for the dispersed phase : kinetic distribution function

$$f(t, \boldsymbol{x}, \boldsymbol{v}) \geq 0$$

  with $\boldsymbol{v}$ the velocity of the droplets.
  - Follow a Vlasov or Vlasov-Boltzmann (with collision operator) equation

  Hypothesis. The particles are monodisperse: all particle have the same radius $r_\star > 0$.

Possibility to enrich the model with various effect: internal energy of the droplets, compressibility, rotation of the droplets, inelastic collisions and breakup, chemical reactions...

A first example: Thin sprays $\alpha(t,x) \approx 1$

Euler equations coupled with a Vlasov equation through a friction force

$$\begin{cases} \partial_t \varrho + \boldsymbol{\nabla}_x \cdot (\varrho \boldsymbol{u}) = 0 \\ \partial_t (\varrho \boldsymbol{u}) + \boldsymbol{\nabla}_x \cdot (\varrho \boldsymbol{u} \otimes \boldsymbol{u}) + \boldsymbol{\nabla}_x p = D_\star \displaystyle\int_{\mathbf{R}^3} (\boldsymbol{v} - \boldsymbol{u}) f \,\mathrm{d}v \\ \partial_t f + \boldsymbol{v} \cdot \boldsymbol{\nabla}_x f + \boldsymbol{\nabla}_v \cdot (\boldsymbol{\Gamma} f) = 0 \\ m_\star \boldsymbol{\Gamma} = -D_\star (\boldsymbol{v} - \boldsymbol{u}) \end{cases}$$

with pressure $p = \varrho^\gamma$.

Compressible Vlasov-Euler equation. Coupling through a friction force and volume fraction.

$$\begin{cases} \partial_t(\alpha\varrho) + \nabla_x \cdot (\alpha\varrho\boldsymbol{u}) = 0 \\ \partial_t(\alpha\varrho\boldsymbol{u}) + \nabla_x \cdot (\alpha\varrho\boldsymbol{u}\otimes\boldsymbol{u}) + \alpha\nabla_x p = D_\star \int_{\mathbf{R}^3} (\boldsymbol{v}-\boldsymbol{u}) f \,\mathrm{d}v \\ \partial_t(\alpha\varrho e) + \nabla_x \cdot (\alpha\varrho e\boldsymbol{u}) + p(\partial_t\alpha + \nabla_x \cdot (\alpha\boldsymbol{u})) = D_\star \int_{\mathbf{R}^3} |\boldsymbol{v}-\boldsymbol{u}|^2 f \,\mathrm{d}v \\ \partial_t f + \boldsymbol{v}\cdot\nabla_x f + \nabla_v \cdot (\boldsymbol{\Gamma} f) = 0 \\ \alpha = 1 - \frac{4}{3}\pi r_\star^3 \int_{\mathbf{R}^3} f \,\mathrm{d}v \\ m_\star \boldsymbol{\Gamma} = -\frac{4}{3}\pi r_\star^3 \nabla_x p - D_\star(\boldsymbol{v}-\boldsymbol{u}) \end{cases}$$

Our interest is in all regime $0 < \alpha \leq 1$.

L. Boudin, L. Desvillettes, and R. Motte. A modeling of compressible droplets in a fluid. Commun. Math. Sci., 1(4):657-669, 2003.

- The mass of each phase is preserved

$$\partial_t(\alpha\varrho) + \nabla_x \cdot (\alpha\varrho \boldsymbol{u}) = 0, \quad \partial_t f + \nabla_x \cdot (\boldsymbol{v} f) + \nabla_v \cdot (\boldsymbol{\Gamma} f) = 0.$$

- The total momentum is preserved

$$\partial_t \left(\alpha\varrho\boldsymbol{u} + \frac{4}{3}\pi r_\star^3 \int_{\mathbf{R}^3} f \boldsymbol{v} \, \mathrm{d}v \right) + \nabla_x \cdot \left(\alpha\varrho\boldsymbol{u} \otimes \boldsymbol{u} + \frac{4}{3}\pi r_\star^3 \int_{\mathbf{R}^3} f \boldsymbol{v} \otimes \boldsymbol{v} \, \mathrm{d}v \right) + \nabla_x p = 0.$$

- The total energy is preserved

$$\partial_t \left(\alpha\varrho E + \frac{4}{3}\pi r_\star^3 \int_{\mathbf{R}^3} f \frac{|\boldsymbol{v}|^2}{2} \, \mathrm{d}v \right) + \nabla_x \cdot \Big(\alpha\varrho\boldsymbol{u}E + \frac{4}{3}\pi r_\star^3 \int_{\mathbf{R}^3} f \boldsymbol{v} \frac{|\boldsymbol{v}|^2}{2} \, \mathrm{d}v + \alpha\boldsymbol{u}p + \frac{4}{3}\pi r_\star^3 p \int_{\mathbf{R}^3} f \boldsymbol{v} \, \mathrm{d}v \Big) = 0.$$

- General thermodynamical principles are satisfied since one has

$$\partial_t(\alpha\varrho S) + \nabla_x \cdot (\alpha\varrho S \boldsymbol{u}) = \frac{D_\star}{T_\star} \int_{\mathbf{R}^3} |\boldsymbol{v} - \boldsymbol{u}|^2 f \, \mathrm{d}v \geq 0.$$

The system rewrites as a system of conservation laws.

- Models
  - in the context of combustion theory introduced in Williams [1985]
  - Classification of sprays O'Rourke [1981]
- Mathematical theory of Thin Sprays ($\alpha \approx 1$):
  - Vlasov-Euler :
    - Local-in-time well posedness for strong solution Baranger and Desvillettes [2006], Mathiaud [2010]
    - Global weak solution in 1D with finite energy Cao [2022]
  - Vlasov-Navier-Stokes :
    - Global existence of weak solution on the 3D-torus Boudin, Desvillettes, Grandmont, and Moussa [2009] and the inhomogenous case Choi and Kwon [2015]
    - Large time behavior studied in Choi [2016], Ertzbischoff, Han-Kwan, and Moussa [2021], Han-Kwan, Moussa, and Moyano [2020]
- Mathematical theory of Thick Sprays ($0 < \alpha \leq 1$) :
  - Boudin, Desvillettes, and Motte [2003].
  - Recent numerical work Benjelloun, Desvillettes, Ghidaglia, and Nielsen [2012]
  - Linear stability studied in Buet, Després, and Desvillettes [2023]
  - Local Well-posedness for regularized model Buet, Després, and F [2022]
  - Very recently, Local in time Well-posedness for the Navier Stokes (with diffusion) case and Penrose stable initial data Ertzbischoff and Han-Kwan [2023]

$$
\begin{cases}
\partial_t(\alpha\varrho) + \boldsymbol{\nabla}_x \cdot (\alpha\varrho\boldsymbol{u}) = 0 \\
\partial_t(\alpha\varrho\boldsymbol{u}) + \boldsymbol{\nabla}_x \cdot (\alpha\varrho\boldsymbol{u}\otimes\boldsymbol{u}) + \alpha\boldsymbol{\nabla}_x p = D_\star \int_{\mathbf{R}^3} (\boldsymbol{v}-\boldsymbol{u}) f \,\mathrm{d}v \\
\partial_t(\alpha\varrho e) + \boldsymbol{\nabla}_x \cdot (\alpha\varrho e\boldsymbol{u}) + p(\partial_t\alpha + \boldsymbol{\nabla}_x \cdot (\alpha\boldsymbol{u})) = D_\star \int_{\mathbf{R}^3} |\boldsymbol{v}-\boldsymbol{u}|^2 f \,\mathrm{d}v \\
\partial_t f + \boldsymbol{v}\cdot\boldsymbol{\nabla}_x f + \boldsymbol{\nabla}_v \cdot (\boldsymbol{\Gamma} f) = 0 \\
\alpha = 1 - \dfrac{4}{3}\pi r_\star^3 \int_{\mathbf{R}^3} f \,\mathrm{d}v \\
m_\star \boldsymbol{\Gamma} = -\dfrac{4}{3}\pi r_\star^3 \boldsymbol{\nabla}_x p - D_\star(\boldsymbol{v}-\boldsymbol{u})
\end{cases}
$$

- **Theory**
  - No Cauchy theory available: Loss of regularity in the equations

$$
\partial_t(\alpha\varrho) + \boldsymbol{\nabla}_x \cdot (\alpha\varrho\boldsymbol{u}) = 0 \Rightarrow \|\varrho\|_{H^k} \lesssim \|f\|_{H^{k+1}},
$$
$$
\partial_t f + \boldsymbol{v}\cdot\boldsymbol{\nabla}_x f + \boldsymbol{\nabla}_v \cdot (\boldsymbol{\Gamma} f) = 0 \Rightarrow \|f\|_{H^k} \lesssim \|\varrho\|_{H^{k+1}},
$$
$$
\Rightarrow \|\varrho\|_{H^k} \lesssim \|\varrho\|_{H^{k+2}}, \quad \|f\|_{H^k} \lesssim \|f\|_{H^{k+2}}.
$$

    Two way to overcome loss of regularity: system with diffusion $\nu\Delta u$, system with regularization: $\boldsymbol{\nabla}_x p \to \langle \boldsymbol{\nabla}_x p \rangle$.
  - No usual definition of weak solution in L^p:

$$
\boldsymbol{\nabla}_v \cdot (\boldsymbol{\Gamma} f) = -\boldsymbol{\nabla}_x p(\varrho, e)\cdot\boldsymbol{\nabla}_v f - \boldsymbol{\nabla}_v \cdot ((\boldsymbol{v}-\boldsymbol{u}) f)
$$

- **Numerics**
  - Problem of the positivity of the volume fraction

Numerics: Framework

We work on the barotropic system in 1D with periodic boundary conditions:

$$(1)\quad \begin{cases} \partial_t(\alpha\varrho) + \partial_x(\alpha\varrho u) = 0 \\ \partial_t(\alpha\varrho u) + \partial_x(\alpha\varrho u^2) + \alpha\partial_x p = \int_{\mathbf{R}} (v-u) f \,\mathrm{d}v \\ \partial_t f + v\partial_x f + \partial_v(\Gamma f) = 0 \\ \alpha = 1 - \int_{\mathbf{R}} f \,\mathrm{d}v \\ \Gamma = -\partial_x p - (v-u) \\ p(\varrho) = \varrho^\gamma, \gamma > 1. \end{cases}$$

The system (1) can be rewritten as a system of conservation laws

$$(2)\quad \begin{cases} \partial_t(\alpha\varrho) + \partial_x(\alpha\varrho u) = 0 \\ \partial_t \left(\alpha\varrho u + \int_{\mathbf{R}} fv \,\mathrm{d}v\right) + \partial_x \left(\alpha\varrho u^2 + p(\varrho) + \int_{\mathbf{R}} v^2 f \,\mathrm{d}v\right) = 0 \\ \partial_t f + v\partial_x f + \partial_v((-\partial_x p + u) f - vf) = 0 \\ p(\varrho) = \varrho^\gamma, \gamma > 1. \end{cases}$$

The fluid part of the system will be written as $\partial_t \mathbf{U} + \partial_x \mathbf{F}(\mathbf{U}, f) = 0$ with
$\mathbf{U} = \begin{pmatrix} \alpha\varrho \\ \alpha\varrho u + \int_{\mathbf{R}} fv \,\mathrm{d}v \end{pmatrix}$ and $\mathbf{F}(\mathbf{U}, f) = \begin{pmatrix} \alpha\varrho u \\ \alpha\varrho u^2 + p + \int_{\mathbf{R}} fv^2 \,\mathrm{d}v \end{pmatrix}$.

Objective: Write a conservative scheme that preserves the positivity of the volume fraction $\alpha(t,x) > 0$.

- The conservative form of the fluid part allow us to use classical hyperbolic scheme (*e.g*: Rusanov, HLL...).
- For the Vlasov equation, a possible choice is semi-Lagrangian method based on polynomial interpolation.

We use here the splitting scheme:

1. Solve $\partial_t \mathbf{U} + \partial_x \mathbf{F}(\mathbf{U}, f) = 0$
2. Solve $\partial_t f + v\partial_x f = 0$
3. Solve $\partial_t f + (u - \partial_x p)\partial_v f = 0$
4. Solve $\partial_t f - \partial_v (vf) = 0$

CFL condition. Compute the eigenvalues of the fluid part:

$$\lambda_{\pm} = u \pm \sqrt{\frac{p'(\varrho)}{\alpha}}, \quad \max(\lambda_{\pm})\frac{\Delta t}{\Delta x} \leq \frac{1}{2}.$$

Recall the formula of the volume fraction

$$\alpha(t,x) = 1 - \int_{\mathbf{R}} f(t,x,v)\,\mathrm{d}v > 0$$

Problem: Solve the free transport equation with constraint

$$\begin{cases} \partial_t f(t,x,v) + v\partial_x f(t,x,v) = 0 \\ 0 \leq \int_{\mathbf{R}} f(t,x,v)\,\mathrm{d}v < 1 \\ \iint_{\mathbf{T}\times\mathbf{R}} f(t,x,v)\,\mathrm{d}x\mathrm{d}v = \iint_{\mathbf{T}\times\mathbf{R}} f_0(x,v)\,\mathrm{d}x\mathrm{d}v \end{cases}$$

Strategy: Prediction-Correction scheme

- After a Prediction step $\tilde{f}^{n+1}(x,v) = f^n(x - \Delta t v, v)$, do **Correction** step: project on a set of admissible density $f^{n+1}(x,v) = P(\tilde{f}^{n+1}(x,v))$ in a **conservative** way
- The projection is made following ideas from the modelisation of crowd motion

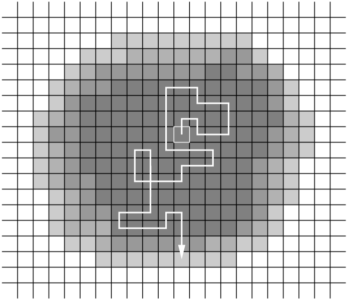


Figure: Random walk transporting the exceeding mass (Maury et al).

In a cell where the constraint is violated, do

1. Start a random walk from the cell transporting the exceeding mass
2. When the random walk encounters a cell where the density is admissible, get rid of a much mass as it can
3. Continue until the exceeding mass is zero

Bertrand Maury, Aude Roudneff-Chupin, Filippo Santambrogio, Juliette Venel. Handling congestion in crowd motion modeling. Networks and Heterogeneous Media, 2011, 6(3): 485-519. doi: 10.3934/nhm.2011.6.485

The Thick Sprays system **without** friction

$$\begin{cases} \partial_t(\alpha\varrho) + \nabla_x \cdot (\alpha\varrho\boldsymbol{u}) = 0 \\ \partial_t(\alpha\varrho\boldsymbol{u}) + \nabla_x \cdot (\alpha\varrho\boldsymbol{u} \otimes \boldsymbol{u}) + \alpha\nabla_x p = 0 \\ \partial_t f + \boldsymbol{v} \cdot \nabla_x f - \nabla_x p(\varrho) \cdot \nabla_v f = 0 \end{cases}$$

has similarity with the Vlasov-Poisson system

$$\begin{cases} \partial_t f + \boldsymbol{v} \cdot \nabla_x f - \mathbf{E} \cdot \nabla_v f = 0, \\ -\Delta\varphi = \int_{\mathbf{R}^3} f \,\mathrm{d}v - 1 \\ \mathbf{E}(t, \boldsymbol{x}) = -\nabla_x \varphi(t, \boldsymbol{x}) \end{cases}$$

- What strongly differs is the **regularity** of the pressure vs the regularity of the electric potential.
- Some techniques used for linearized Vlasov-Poisson transfer to Thick Sprays equations.

$$f_0(x, v) = (1 + \varepsilon \cos(kx))e^{-v^2/2}$$

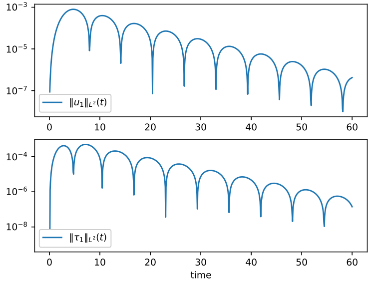


Figure: Decay of acoustic energy for Thick Sprays

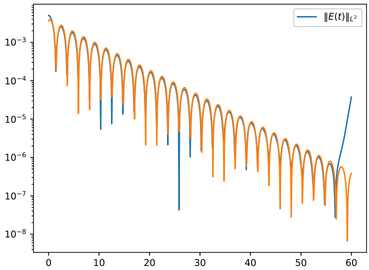


Figure: Decay of electric field for Vlasov-Poisson

Linearize the system **without friction** $D_\star = 0$ around $\varrho_0(x) = cte$, $u_0(x) = 0$, $f^0(v) = e^{-v^2/2}$

$$\begin{cases} \varrho(t,x) = \varrho_0 & +\varepsilon\varrho_1(t,x) & +O(\varepsilon^2) \\ u(t,x) = & \varepsilon u_1(t,x) & +O(\varepsilon^2) \\ \alpha(t,x) = \alpha_0 & +\varepsilon\alpha_1(t,x) & +O(\varepsilon^2) \\ f(t,x,v) = f^0 & +\varepsilon f_1(t,x,v) & +O(\varepsilon^2) \end{cases}$$

Regrouping the linearized equations for $\tau_1 = \frac{-\varrho_1}{\varrho_0^2}$, u_1 and f_1, one gets, setting the constants to one

$$\begin{cases} \partial_t \tau_1 = \partial_x u_1 + \partial_x \int_{\mathbf{R}} v f_1 \,\mathrm{d}v \\ \partial_t u_1 = \partial_x \tau_1 \\ \partial_t f_1 + v\partial_x f_1 - \partial_v f^0 \partial_x \tau_1 = 0 \end{cases}$$

For Landau damping in Vlasov-Poisson, it is well known that for a given k, the rate of decay are given by the root in the complex plane of the dispersion function

$$\mathcal{D}_{\mathrm{VP}}(\omega, k) = 1 - \frac{1}{k^2} \int_{-\infty}^{+\infty} \frac{\partial_v f^0(v)}{v - \frac{\omega}{k}} \, \mathrm{d}v$$

Similar formal computation gives us a dispersion function for Thick Sprays

$$\mathcal{D}_{\mathrm{TS}}(\omega, k) = 1 - \frac{k^2}{\omega^2} + \frac{k}{\omega} \int_{-\infty}^{+\infty} \frac{v \partial_v f^0(v)}{v - \frac{\omega}{k}} \, \mathrm{d}v$$

Initial condition:

$$\varrho(t=0,x) = 1, \quad u(t=0,x) = 0, \quad f(t=0,x,v) = \frac{1}{\sqrt{2\pi}}(1+\varepsilon\cos(kx))e^{-v^2/2}$$

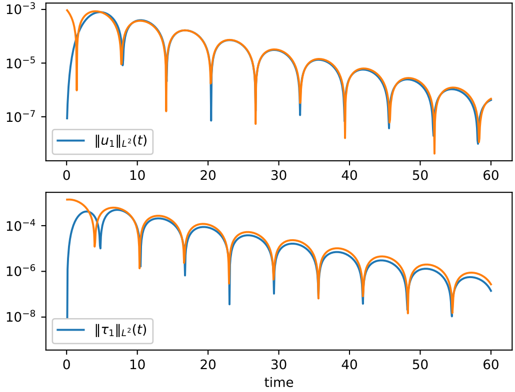


Figure: Decay of the acoustic energy, $\Im(\omega) = -0.13$, $\Re(\omega) = 0.497$

- Presentation of a conservative method to preserve maximum principle for the volume fraction.
- Landau damping phenomenon in the frictionless system.
- Investigate the role of the friction.

A method to recover the maximum principle

Adapt this method in the kinetic case: The constraint is not of the type $a \leq f(t,x) \leq b$ but $a \leq \int_{\mathbf{R}} f(t,x,v)\,\mathrm{d}v \leq b$. After the Prediction step $\tilde{f}^{n+1}(x,v) = f^n(x - \Delta t v, v)$, do

1. Start from a cell x_i where $\tilde{\alpha}_i^{n+1} < \alpha_{\min}$
2. Compute the exceeding mass Δm_i^0. Modify the value, $\forall j$,

$$f_{i,j}^{n+1} = \frac{1-\alpha_{\min}}{\frac{4}{3}\pi r_\star^3} \frac{\tilde{f}_{i,j}^{n+1}}{\sum_k \Delta v_k \tilde{f}_{i,k}^{n+1}}$$

   , so that $\alpha_i^{n+1} = \alpha_{\min}$

3. Start a random walk (S_m), when the walk meet a cell S_m such that $\tilde{\alpha}_{S_m}^{n+1} > \alpha_{\min}$, get rid of as much mass as possible and modify

$$f_{S_m,j}^{n+1} = \min\left(\sum_k \Delta v_k \tilde{f}_{S_m,j}^{n+1} + \Delta m_i^0, \frac{1-\alpha_{\min}}{\frac{4}{3}\pi r_\star^3}\right) \frac{\tilde{f}_{S_m,j}^{n+1}}{\sum_k \Delta v_k \tilde{f}_{S_m,k}^{n+1}}$$

When all the exceeding mass has been distributed, the volume fraction α_i^{n+1} is admissible.

- Necessity to add a small minimum value $\alpha_{\min}$ ($e.g$ 10^{-3}...) because $\alpha = 0$ is not an admissible value, can correspond to a close-packing limit.

Note that no convergence result of this algorithm is known

By construction, this method is conservative

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