Sticky Elastic Collisions and the Effect of Hydrodynamic Interactions

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Outline

- **Part I** : An Introduction to Inertial Particles
- **Part II** : Collisions in Ideal Flows
  - Introduction
  - Sticky Elastic Collisions
  - Hydrodynamic Interactions
  - Conclusions and Perspectives
- **Part III** : Droplet Growth by Coalescence in Turbulent Clouds

Part I : An Introduction to Inertial Particles

Bec, Biferale, Cencini, Falkovich, Lanotte, Toschi, ...

(2005 – now)

Why are we interested in particles?

Pyroclastic flows.

Why are we interested in particles?

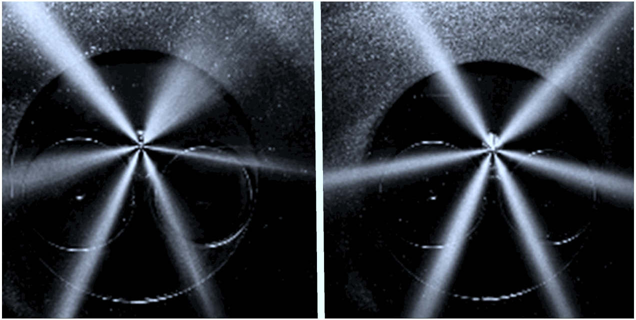
Planktons and marine biology.

Why are we interested in particles?

Pollutant dispersion.

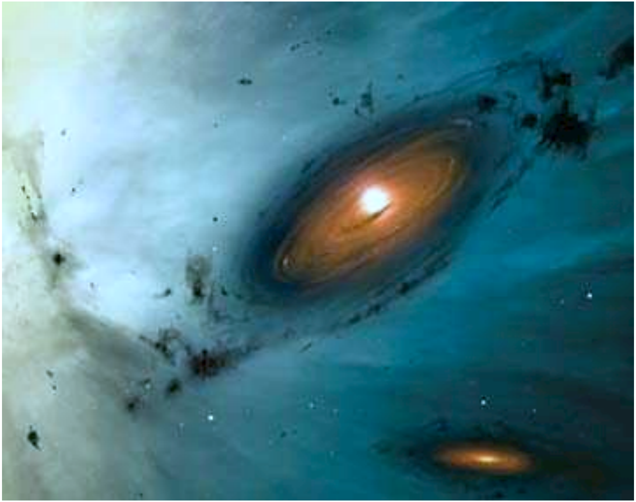
Why are we interested in particles?

Mixing processes in industry.



Why are we interested in particles?

Planetary formation.



Why are we interested in particles?

The physics of cloud formation.

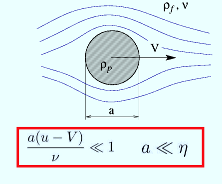
Tracers versus Inertial Particles

- Tracers
  - Same density as the fluid.
  - Point-like.
  - Same velocity as the underlying fluid velocity.
  - Tracer particles have conservative dynamics : Phase space conservation.
- Inertial Particles
  - Density different from that of the fluid.
  - Finite size.
  - Friction (Stokes) and other forces should be included.
  - Velocity different from the underlying fluid velocity.
  - Inertial particles have dissipative dynamics : Uniform contraction in phase space

Single particle dynamics

Single, passive, spherical, inertial, rigid particle of radius a, mass m_p.

$$\rho_p \frac{d\mathbf{v}}{dt} = \rho_f \frac{D\mathbf{u}}{Dt} + (\rho_p - \rho_f)\mathbf{g}$$
$$- \frac{9\nu\rho_f}{2a^2}\left(\mathbf{v} - \mathbf{u} - \frac{a^2}{6}\nabla^2\mathbf{u}\right)$$
$$- \frac{\rho_f}{2}\left(\frac{d\mathbf{v}}{dt} - \frac{D}{Dt}\left[\mathbf{u} + \frac{a^2}{10}\nabla^2\mathbf{u}\right]\right)$$
$$- \frac{9\rho_f}{2a}\sqrt{\frac{\nu}{\pi}}\int_0^t \frac{1}{\sqrt{t-\xi}}\frac{d}{d\xi}(\mathbf{v} - \mathbf{u} - \frac{a^2}{6}\nabla^2\mathbf{u})\mathrm{d}\xi.$$



Here $\mathbf{v}$ represents the particle velocity, $\mathbf{u}$ the fluid velocity, ρ_p the density of the particle, ρ_f the density of the fluid, and ν, a, $\mathbf{g}$ represent the kinematic viscosity of the fluid, the radius of the particle and the acceleration due to gravity, respectively.

Single particle dynamics

- $\rho_f \frac{D\mathbf{u}}{Dt} \longrightarrow$ force by the undisturbed flow;
- $(\rho_p - \rho_f)\mathbf{g} \longrightarrow$ buoyancy;
- $\frac{9\nu\rho_f}{2a^2}\left(\mathbf{v} - \mathbf{u} - \frac{a^2}{6}\nabla^2\mathbf{u}\right) \longrightarrow$ Stokes drag;
- $\frac{\rho_f}{2}\left(\frac{d\mathbf{v}}{dt} - \frac{D}{Dt}\left[\mathbf{u} + \frac{a^2}{10}\nabla^2\mathbf{u}\right]\right) \longrightarrow$ added mass;
- $\frac{9\rho_f}{2a}\sqrt{\frac{\nu}{\pi}}\int_0^t \frac{1}{\sqrt{t-\xi}}\frac{d}{d\xi}(\mathbf{v} - \mathbf{u} - \frac{a^2}{6}\nabla^2\mathbf{u})\mathrm{d}\xi \longrightarrow$ Basset history term.

The derivative $D\mathbf{u}/Dt$ is taken along the path of the fluid element, $D\mathbf{u}/Dt = \partial u/\partial t + (\mathbf{u}\cdot\nabla)\mathbf{u}$. The derivative $d\mathbf{u}/dt$, is taken along the trajectory of the particle $d\mathbf{u}/dt = \partial\mathbf{u}/\partial t + (\mathbf{v}\cdot\nabla)\mathbf{u}$.

Simplifications

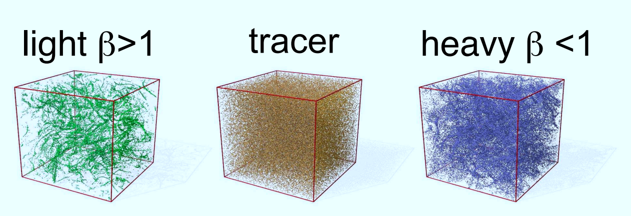
- The Faxen correction $a^2\nabla^2\mathbf{u}$ is of the magnitude $O(a^2u/L)$, and from the assumption, $a << L$, this term's contribution becomes negligible and can be excluded from the equation.
- The Basset history force term which takes into account viscous memory effects becomes less significant and can be dropped, as the particle size is sufficiently small and the concentration of particles is sufficiently low, that they do not modify the flow field or interact with each other.
- Under the low Reynolds number approximation , both the derivatives $D\mathbf{u}/Dt$ and $d\mathbf{v}/dt$ will approximately be the same.
- We assume the buoyancy effects to be negligible.

Working Equations

$$\frac{d\mathbf{x}}{dt} = \mathbf{v};$$
$$\frac{d\mathbf{v}}{dt} = \beta\frac{D\mathbf{u}}{Dt} + \frac{\mathbf{u}-\mathbf{v}}{\tau_p}.$$

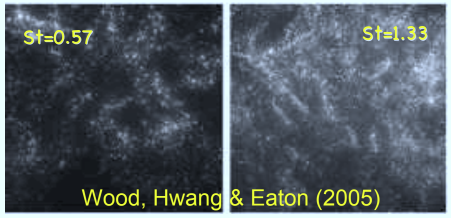
$$\tau_p = \frac{a^2}{3\nu\beta} \quad \tau_f = \frac{L}{U}Re^{-1/2}$$

$$St = \frac{\tau_p}{\tau_f} \quad \beta = \frac{3\rho_f}{\rho_f + 2\rho_p}$$

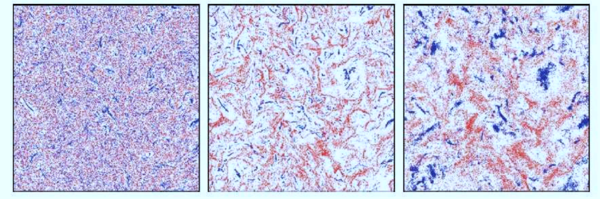


Preferential Concentration

Experiments :

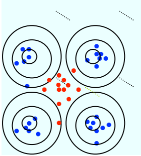


Simulations :



Understanding Preferential Concentration

- Spatial distribution of finite-size massive particles is strongly inhomogeneous (**preferential concentration**) due to inertia.
- Qualitative understanding based on the idea that vortices act as centrifuges ejecting particles heavier than the fluid and trapping lighter ones.



- $\tau_p \to 0$: *uniform distribution*
  - $\dot{\mathbf{x}}_i = \mathbf{u}(\mathbf{x}_i, t)$; $\nabla \cdot \mathbf{u} = 0$; assumption of chaoticity.
- $\tau_p \to \infty$: *uniform distribution*
  - $\tau_f \ll \tau_p$; Langevin equation; ballistic motion.
- Maximum clusterization is achieved for a finite value of τ_p.
- Small scale particle clusters are characterised by the correlation dimension $\mathcal{D}_2$: the probability to find two particles at a distance less than a given r is $P_2^<(r) \sim r^{\mathcal{D}_2}$.

Particles as a nonlinear dynamical system

$$\dot{\mathbf{X}} = \mathbf{V} \qquad \dot{\mathbf{V}} = \beta D_t \mathbf{u}(\mathbf{X}) + \frac{\mathbf{u}(\mathbf{X},t) - \mathbf{V}}{\mathrm{St}} \qquad \mathbf{Z} = (\mathbf{X},\mathbf{V}) \in R^{2d}$$

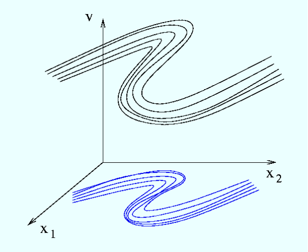
- Well-defined dissipative dynamical system in $2d$-dimensional phase-space :

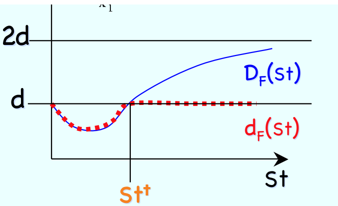
$$\dot{\mathbf{Z}} = \mathbf{F}(\mathbf{Z},t); \qquad \mathbf{F} = (\mathbf{V}, \beta D_t \mathbf{u} + \tfrac{\mathbf{u}-\mathbf{V}}{\mathrm{St}});$$
$$\Longrightarrow \nabla \cdot \mathbf{F} = -\tfrac{d}{\mathrm{St}} < 0.$$

- Inertial particles have dissipative dynamics and evolve onto an attractor : Uniform contraction in phase space
- The fractal dimension of the attractor D_F is expected to be smaller than the phase-space dimension $2d$.

Clustering in physical space

- Tracking particle–positions (clustering) amounts to projecting the fractal, with $D_F < d$, embedded in a $2d$ phase space, onto a d-dimensional space.
- The observed fractal dimension d_F in position space is given by $d_F = \min\{D_F, d\}$.
  - Fractal clustering in physical space with $d_F = D_F$ when $D_F < d$ and $d_F = d$ when $D_F > d$.





Part II : Collisions in Ideal Flows

with J. Bec and S. Musacchio

- Introduction
- Sticky Elastic Collisions
- Hydrodynamic Interactions
- Conclusions and Perspective

Lessons

- Spatial distribution of finite-size massive particles is strongly inhomogeneous (**preferential concentration**) due to inertia.
- Qualitative understanding based on the idea that vortices act as centrifuges ejecting particles heavier than the fluid and trapping lighter ones.
- The equations of motion of small, rigid, spherical particles in a flow is usually derived under the assumptions of
  - no collisions (*ghost-collisions approach*);
  - no particle-to-particle hydrodynamic interactions.
- In the framework of these assumptions, the dynamics of a single particle depends on only two dimensionless parameters : the mass-density ratio between the particle and the flow and the Stokes number.

Introduction : The Model

- Fluid velocity obtained from a solution of the Navier—Stokes equation :

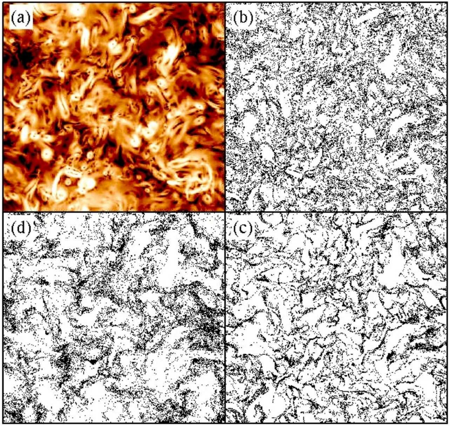
$$\begin{aligned} \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} &= -\nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{f}; \\ \nabla \cdot \mathbf{u} &= 0. \end{aligned}$$

- Particles are much smaller than the Kolmogorov length scale, much *heavier* than the carrier flow, and their slip velocity is associated with a small Reynolds number
- They move with a Stokes drag :

$$\frac{\mathrm{d}\mathbf{V}}{\mathrm{d}t} = -\frac{1}{\tau_{\mathrm{p}}} \left[\mathbf{V} - \mathbf{u}(\mathbf{X}, t)\right]$$

- $\tau_{\mathrm{p}} = 2\rho_p a^2/(9\rho_f \nu)$
- Stokes number *St* is the ratio of the particle-response time scale to the fluid time scale τ.

Introduction : The Model

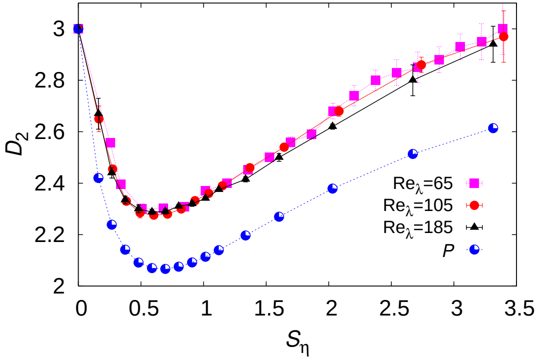


The modulus of the pressure gradient, giving the main contribution to fluid acceleration (a). Particle positions in the same slice are shown for (b) $St_\eta = 0.16$, (c) 0.80 and (d) 3.30.

Bec *et al.*, Phys. Rev. Lett., **98**, 084502, (2007).

The Model : D_2

Small scale particle clusters are characterised by the correlation dimension $\mathcal{D}_2$: the probability to find two particles at a distance less than a given r is $P_2^<(r) \sim r^{\mathcal{D}_2}$.



The correlation dimension $\mathcal{D}_2$ vs St_η for different R_λ.

Bec *et al.*, Phys. Rev. Lett., **98**, 084502, (2007).

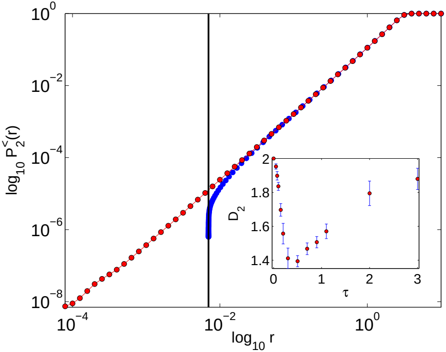
Elastic Collisions

- Trajectory $\mathbf{x}_i(t)$ of a system of N small hard spheres which are in a random fluid field $\mathbf{u}(\mathbf{x}, t)$ and subject to viscous dissipation :

$$\tau \ddot{\mathbf{x}}_i = -\dot{\mathbf{x}}_i + \mathbf{u}(\mathbf{x}_i, t) \quad i \in [1, N].$$

  - $\tau = 2\rho_p a^2/(9\rho_f \nu)$
- Interactions through elastic collisions.
- Dissipative dynamics coupled with elastic collisions.

Elastic Collisions : Consequence

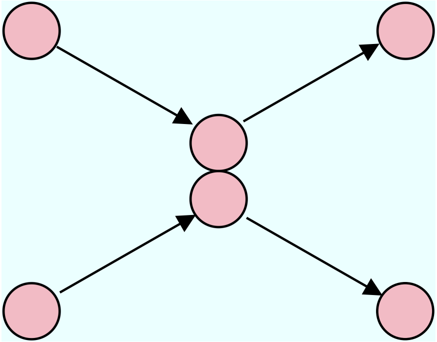


Scaling behaviour of PDFs of inter-particle distance :

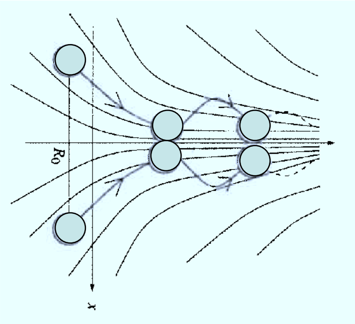
- Clustering : $P_2^<(r) \sim r^{D_2}$
- Collisions : $P_2^<(r - r_c) \sim (r - r_c)^{\alpha+1}$

Elastic Collisions : Large Stokes

- The relative motion of the two particles is almost ballistic.
- Hence $dr = v_{rms} dt$ which leads to $p_2(r) \sim (r - r_c)^0$.
- $\alpha_{\tau \to \mathrm{large}} = 0$.



Sticky Elastic Collisions : Small Stokes



Sticky Elastic Collisions : Small Stokes

- Inter-particle separation : $r = |\mathbf{x}_1 - \mathbf{x}_2|$ and the radial relative velocity $v = (\mathbf{v}_1 - \mathbf{v}_2) \cdot \hat{\mathbf{r}}$:

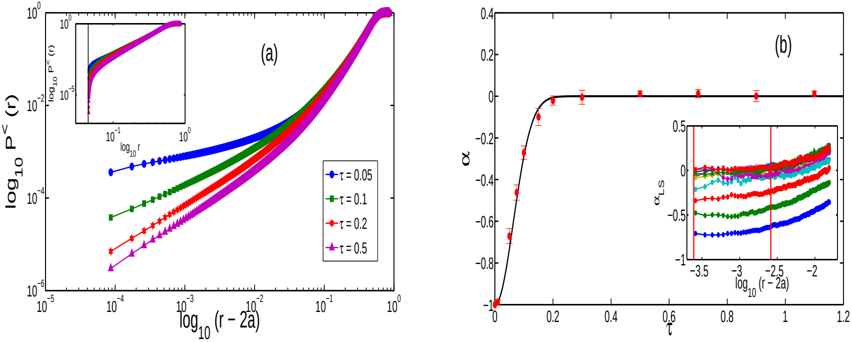
$$\dot{r} = v \ , \quad \tau \dot{v} = -v + 2a\sigma$$

- By making use of suitable asymptotics we obtain :

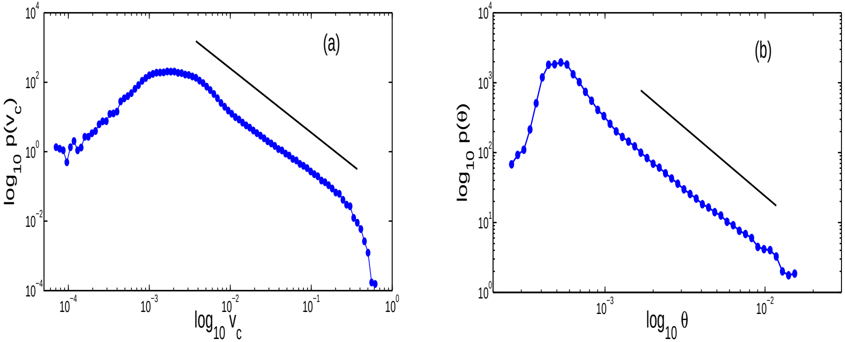
$$\begin{aligned} v_n &\sim 2a\sigma/n \\ \theta_n &\sim \tau/n \\ r_n^*/(2a) - 1 &\sim \sigma\tau/n^2 \\ n_c &\sim exp(t/\tau) \end{aligned}$$

- $p_2(r) \sim (r - r_c)^{-1}$ $\qquad (\alpha_{\tau \to \mathrm{small}} = -1)$
- $p(v_c) \sim v_c^{-2}$
- $p(\theta) \sim \theta^{-2}$

Sticky Elastic Collisions : Statistics



Sticky Elastic Collisions : Statistics



Hydrodynamic Interactions

- Stokes flow around a sphere :

$$\mathbf{u}_s(\mathbf{r},\mathbf{v}) = \left[\frac{3}{4}\frac{a}{r} - \frac{3}{4}\left(\frac{a}{r}\right)^3\right]\frac{\mathbf{r}}{r^2}\left(\mathbf{v}\cdot\mathbf{r}\right) + \left[\frac{3}{4}\frac{a}{r} + \frac{1}{4}\left(\frac{a}{r}\right)^3\right]\mathbf{v}.$$

- Perturbation on the flow due to N particles :

$$\mathbf{u}_i = \sum_{j\neq i}\mathbf{u}_s(\mathbf{r}_{ij},\mathbf{v}_j - \mathbf{U}(\mathbf{x}_j,t) - \mathbf{u_j})$$

- Effective equation of motion :

$$\tau\ddot{\mathbf{x}}_i = -\dot{\mathbf{x}}_i + \mathbf{U}(\mathbf{x}_i,t) + \mathbf{u}_i \quad i\in[1,N].$$

Wang *et al.*, Int. J. Multiphase Flow **35**, 854-867 (2009).

Hydrodynamic Interactions

- One dimensional model $u_1 = -u_2$.
- The perturbed flow :

$$u_1 = \left[\frac{3}{2}\frac{a}{r} - \frac{1}{2}\left(\frac{a}{r}\right)^3\right](v_2 - U_2 - u_2);$$

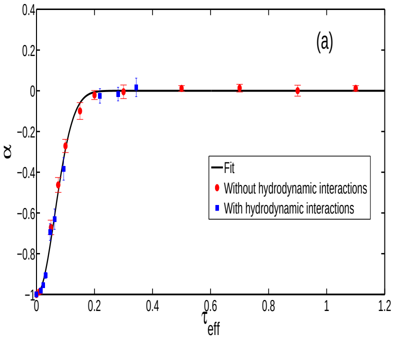
$$r = 2a \implies u_1 = \frac{11}{5}\left(\frac{v}{2} - \sigma a\right).$$

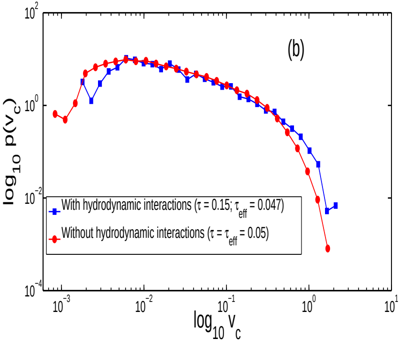
- Model equation :

$$\begin{aligned} \tau \dot{v} &= -v + (U_1 - U_2) + (u_1 - u_2) \\ &= -\frac{16}{5}(v - 2\sigma a) \end{aligned}$$

- $St_{\mathrm{eff}} = \frac{5}{16} St$

Hydrodynamic Interactions

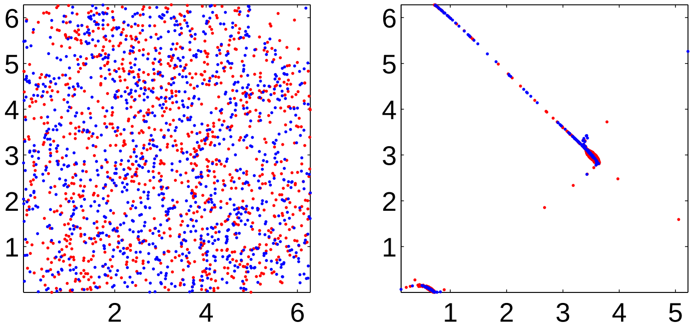




Conclusions and Perspectives

- Collisions have interesting, non-trivial effects on the small-scale clustering of inertial particles.
- Dissipative dynamics coupled with elastic collisions lead to the phenomenon of *sticky elastic collisions*.
- Similarities with granular material.
- Hydrodynamic interactions reduce the effective Stokes number.
- Compressible flows?

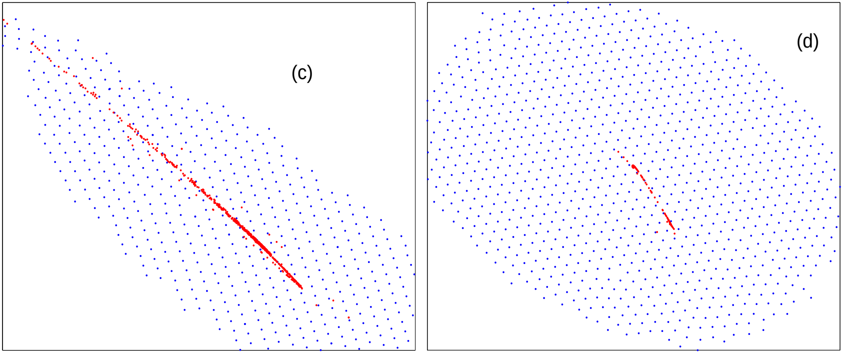
Perspectives : Compressible Flows



Ghost particles

Colliding particles

Perspectives : Compressible Flows



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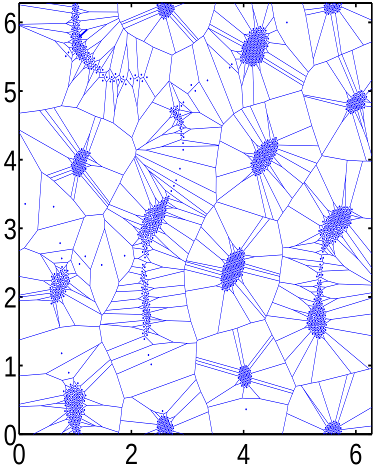
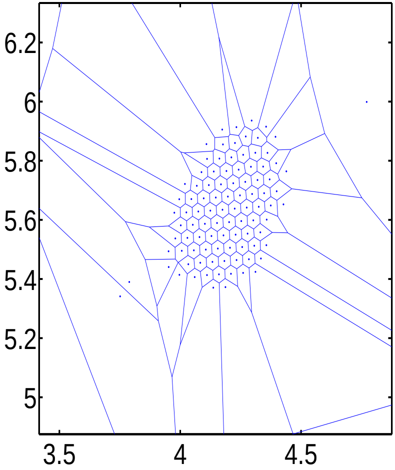
Perspectives : Compressible Flows



Perspectives : Compressible Flows



Part III : Droplet Growth by Coalescence in Turbulent Clouds

with J. Bec and H. Homann

Motivation

The Problem

- Warm clouds consist of small water droplets that do not follow exactly the turbulent airflow but have inertia.
- They thus react with some delay to the fluid motion and feel gravity; hence they distribute non-uniformly in space and can have very large velocity differences.
- Consequently the rate of collision and growth by coalescence of such droplets cannot be predicted by simple arguments and the timescales of precipitation are often under-estimated.
- We investigate this issue by a direct numerical simulation of coalescing particles that are passively transported by a fully-developed homogeneous isotropic turbulent flow.

The model

- Fluid velocity obtained from a solution of the Navier–Stokes equation :

$$\begin{aligned} \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} &= -\nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{f}; \\ \nabla \cdot \mathbf{u} &= 0. \end{aligned}$$

- Particles are much smaller than the Kolmogorov length scale, much *heavier* than the carrier flow, and their slip velocity is associated with a small Reynolds number
- They move with a Stokes drag *and* feel the effect of gravity :

$$\frac{\mathrm{d}\mathbf{V}}{\mathrm{d}t} = -\frac{1}{\tau_\mathrm{p}} [\mathbf{V} - \mathbf{u}(\mathbf{X}, t)] - g\,\mathbf{e}_3$$

- Parallel pseudo-spectral code with a third-order Runge–Kutta time–marching scheme.
- Linear interpolation scheme used to evaluate fluid velocity at the particle locations.

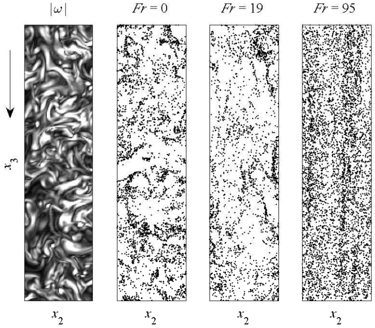
Computational Challenges

- In atmospheric settings, the Kolmogorov dissipative scale η is of the order of $1mm$.
- Hence a 2048^3 simulation represents a cloud of roughly $2m \times 2m \times 2m$.
- Observations in maritime strato-cumuli report typical droplet radii of the order of $10 - 50\mu m$.
- The observed volume fraction of particles are very low: typical numbers of particles per cubic centimeters are in the range 10 to 100, that means between 0.01 and 0.1 particles per cube of size η^3.
- A 2048^3 simulation will thus initially require of the order of one billion particles.

Parameters

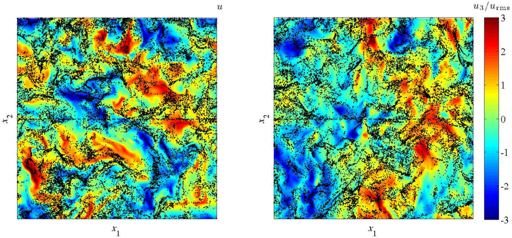
Re_λ	$u_{\rm rms}$	Δt	η	τ_η	L	T_L	N^3	N_p
460	0.189	0.0012	1.45×10^{-3}	0.083	1.85	9.9	2048^3	10×10^8
290	0.185	0.003	2.81×10^{-3}	0.131	1.85	9.9	1024^3	1.28×10^8
127	0.144	0.02	1.12×10^{-2}	0.45	2.11	14.6	256^3	0.08×10^8

Massive parallel simulations on the BlueGene/P system in Julich for 50,000,000 core-hours on 65536 cores.



Key Features

- We get a better understanding of the role of turbulent fluctuations on the coalescence process in warm clouds.
- We focus on the stage where inertial dynamical collisions are important, that is when water droplets are too large to be considered as tracers but too small to be dominated by gravitational settling.
- Our approach consists in investigating this problem in idealized settings (homogeneous and isotropic turbulent airflow with very heavy point particles), but with parameters that are close to those encountered in maritime strato–cumulus clouds.



Conclusions and Perspectives

- Non-trivial scaling laws for various quantities as a function of the Stokes and Froude numbers.
- The dynamics of particles with the inclusion of hydrodynamic interactions?
- Thermodynamics ?

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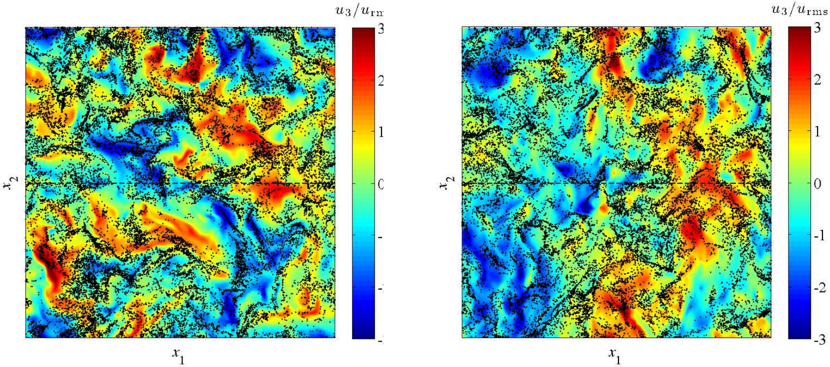
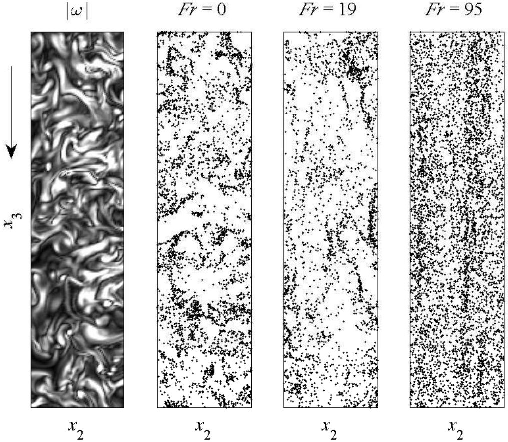
Distribution of particles



Snapshots of the position of particles (black dots), together with the fluid vertical velocity field (colored background) for $St = 1$, $Fr = 0.48$, and $R_\lambda = 127$ in a horizontal (Left) and a vertical (Right) slices, at the same moment of time. Each dashed line represents the other cut.

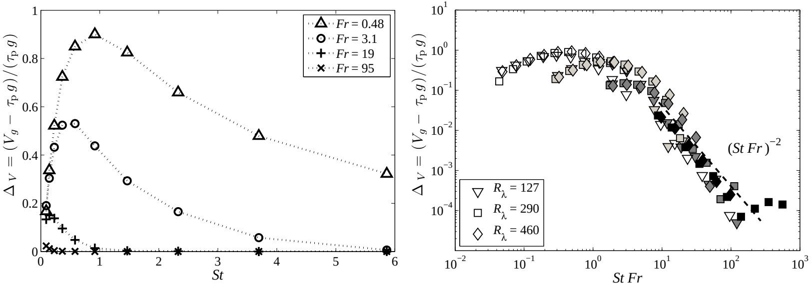
Qualitative effects of gravity



Snapshot of the vorticity modulus (Left; black = low values, white = high values) and of the particle positions for $R_\lambda = 127$, $St = 1$ and three different values of the Froude number in a slice of thickness 10η, width 130η, and height 520η. The vertical arrow indicates the direction of gravity.

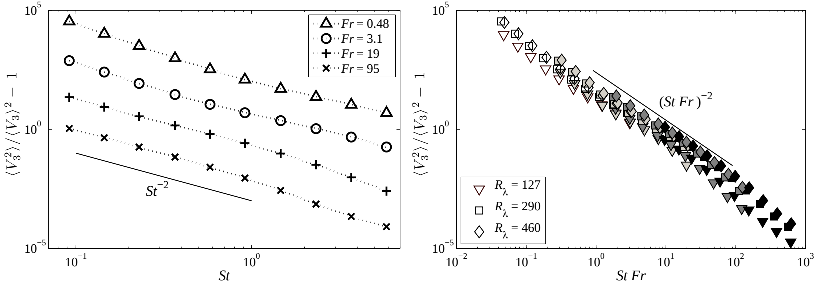
Dynamical quantities : *Settling velocities*

Increase in the particle mean settling velocity is observed: $\Delta_{V3} = \tau_\mathrm{p}\, g - \langle V_3 \rangle > 0$. For large settling velocities (i.e. for $St\, Fr \gg 1$), one observes $\Delta_{V3} \propto (St\, Fr)^{-2}$.



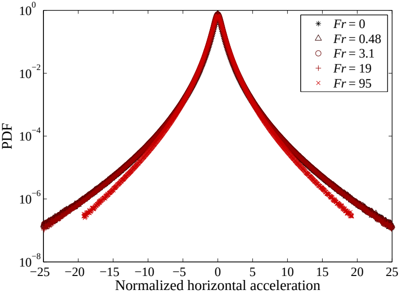
The scaling law can be obtained for large settling velocity $V_g = -\langle V_3 \rangle \implies V_g \gg u_\eta = \eta/\tau_\eta$ by using suitable asymptotics.

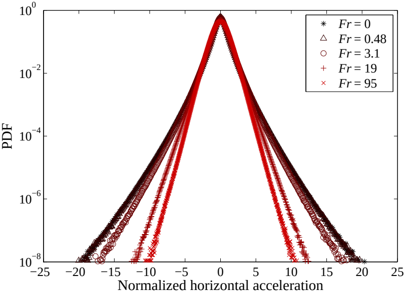
Dynamical quantities : *Settling velocities*



Left: Normalized variance of the particle vertical velocity as a function of St for four different values of the Froude number, as labeled, and $R_\lambda = 290$. Right: same as a function of $StFr$, for three different values of the Reynolds number; the grey level of markers indicates the value of the Froude number, from $Fr = 0.48$ in white to $Fr = 95$ in black.

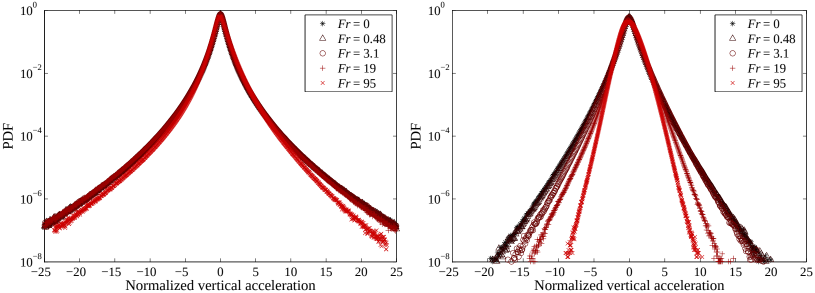
Dynamical quantities : *Acceleration statistics*





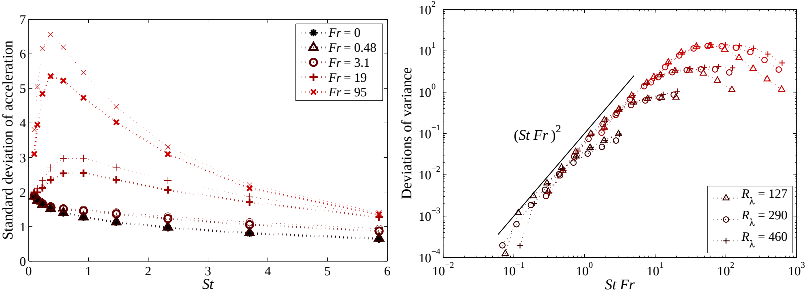
PDF of normalized and centered horizontal acceleration for $St = 0.092$ (Left) and $St = 0.92$ (Right).

Dynamical quantities : *Acceleration statistics*



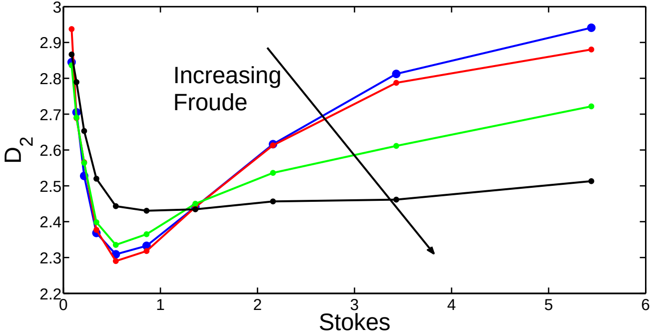
PDF of normalized and centered vertical acceleration for $St = 0.092$ (Left) and $St = 0.92$ (Right).

Dynamical quantities : *Acceleration statistics*



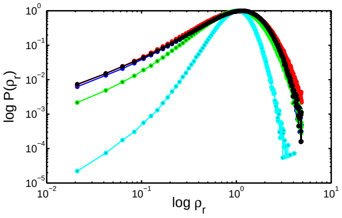
Left: Variance of the vertical and horizontal accelerations as a function of St for different values of Fr. Right: The same as a function of $StFr$ but for different values of Re.

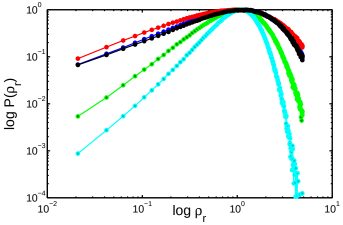
Preferential concentration : *Two-point, small-scale*



Correlation dimension of particle distribution as a function of *St* for different values of *Fr*.

Preferential concentration : *Inertial-range distributions*



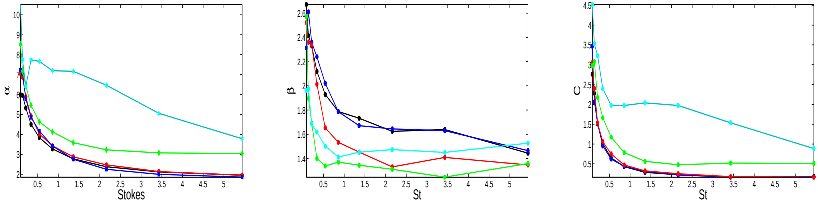


PDF of the coarse-grained density ρ_r for $r = 32\eta$.

Observables directly linked to large deviations of the distribution $p(\rho_r)$:

- The voids relate to the left tail: $p(\rho_r) \propto \rho_r^{\alpha}$;
- the clumps relate to the right tail: $p(\rho_r) \propto \exp(-C\rho_r^{\beta})$.

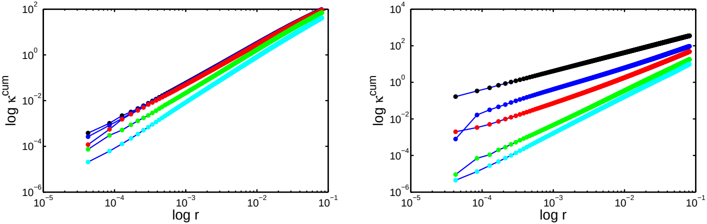
Preferential concentration : *Inertial-range distributions*



Coefficients and exponents α, β and C (from Left to Right) as a function of St for different values of Fr.

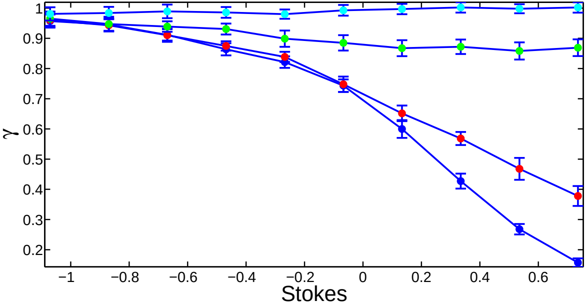
Collision kernel

Relative velocity statistics conditioned on the inter-particle distance:



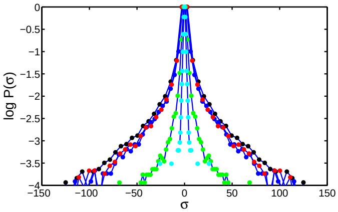
Approaching rate $\kappa(r)$ (cumulative) as a function of the distance between the particle. From Left to right: $St = 0.54$ to $St = 5.44$.

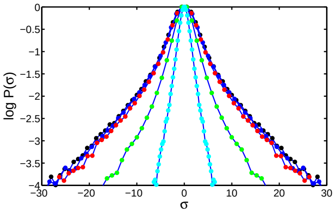
Collision kernel



Exponent of the approaching rate γ (such that $\kappa(r) \propto r^{\gamma}$) as a function of St for different values of Fr.

Longitudinal Velocity Differences





PDF of the longitudinal velocity difference between particles for separations in the dissipative range and for $St = 0.857$.