The 31st Jyväskylä Summer School

Courses in Mathematics and Statistics – MA3

Stochastic modelling and numerical tools around the physics of complex flows

mireille.bossy@inria.fr

Calisto Team

Inria d'Université Côte d'Azur

- Some basic notions of fluid mechanics and the Navier Stokes equations
  - The conservation of mass
  - Incompressibility
  - The momentum equation
  - Acceleration
  - Internal forces
- Complex flows : from laminar flows to turbulent flows
  - Reynolds decomposition
  - Kolmogorov scales
  - The Reynolds Navier Stokes equations
- When *stochasticity* comes in the story : Lagrangian fluctuation
  - Fluid particle
  - Models : Microsclale model view point
  - Brownian motion and Ornstein-Uhlenbeck processes
- Models for turbulent closure : Macroscale view point and PDF approach
  - Fokker Planck equations
  - PDF approaches / Stochastic Lagrangian approaches
- Particle-laden flows

From laminar to turbulent flows.

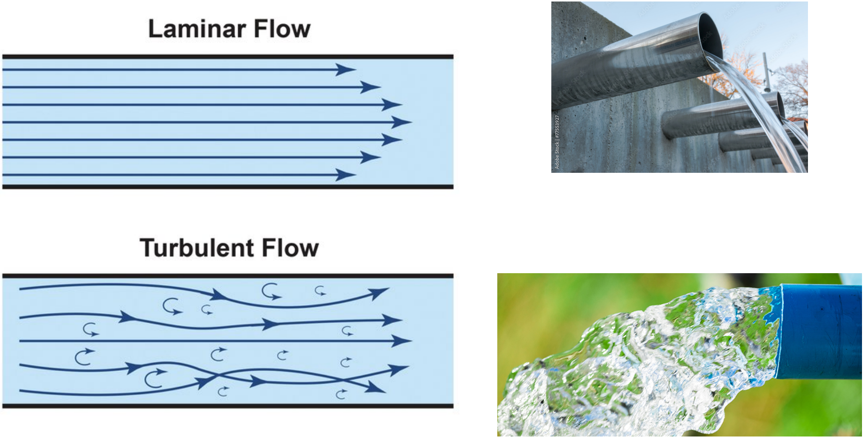


Figure 1: Typical streamlines in laminar (top) or turbulent flows (bottom).

From laminar to turbulent flows.

Figure 2: The smoke of a candle, laminar at the bottom, turbulent at the top.

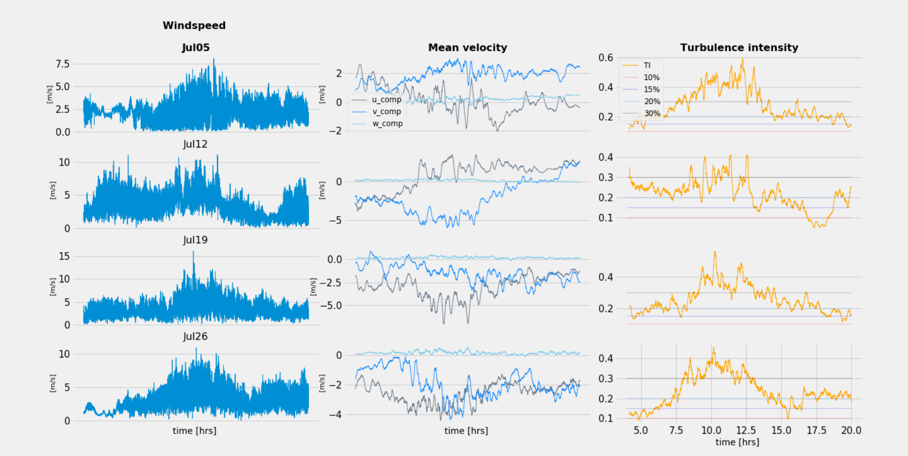


Figure 3: Time series of the measurements of wind velocity vector, taken at a mast of 30 meters height with a sonic anemometer, obtained from the open observation platform of SIRTA (Site Instrumental de Recherche par Télédétection Atmosphérique.

Kolmogorov scales.

In his 1941 theory (called K41), Andrey Kolmogorov introduced the idea that the smallest scales of turbulence are universal (similar for every turbulent flow) and that they depend only on the kinematic viscosity ν, and on the dissipation ε :

- Kolmogorov length scale $\eta = \left(\frac{\nu^3}{\varepsilon}\right)^{1/4}$.
- Kolmogorov time scale $\tau_\eta = \left(\frac{\nu}{\varepsilon}\right)^{1/2}$.
- Kolmogorov velocity scale $u_\eta = (\nu\varepsilon)^{1/4}$.

The dissipation ε is a complex quantity to estimate precisely, but for most of applications, a rough estimation of the Kolmogorov length scale can be obtained by

$$\varepsilon \simeq \frac{U^3}{L}, \quad \text{in engineering application,}$$

$$\varepsilon(t,x) \simeq \frac{u^3}{L}, \text{ in direct measurement, } u = \sqrt{\langle v'v' \rangle}.$$

leading to

$$\eta \simeq \left(\frac{\nu^3 L}{U^3}\right)^{1/4}$$

good enough to get an order of magnitude.

$$\partial_t \langle v_i' v_j' \rangle + \left(\langle v \rangle \cdot \nabla \langle v_i' v_j' \rangle \right)$$
$$= -\sum_{k=1}^{3} \partial_{x_k} \langle v_i' v_j' v_k' \rangle \qquad \underbrace{-\frac{1}{\rho_0} \langle v_j' \partial_{x_i} p' + v_i' \partial_{x_j} p' \rangle}_{\text{velocity pressure gradient tensor } \Pi_{ij}} \qquad + \nu \triangle_x \langle v_i' v_j' \rangle + \frac{p'}{\rho_0} \left(\partial_{x_j} v_i' + \partial_{x_i} v_j' \right)$$
$$+ 2 \underbrace{\nu \sum_{k=1}^{3} \langle \partial_{x_k} v_i' \partial_{x_k} v_j' \rangle}_{\text{dissipation tensor } \varepsilon_{ij}} \qquad \underbrace{- \sum_{k=1}^{3} \left(\langle v_i' v_k' \rangle \partial_{x_k} \langle v_i \rangle + \langle v_j' v_k' \rangle \partial_{x_k} \langle v_j \rangle \right)}_{\text{turbulence production tensor } \mathscr{P}_{ij}}$$

(the second line are the transport terms.)

The two main second order statistics are

1. the half trace of the tensor $\mathscr{R}$ is the turbulent kinetic energy $\mathrm{k}(t,x) := \dfrac{1}{2} \sum_{i=1}^{3} \langle v_i' v_i' \rangle (t,x)$
2. the pseudo-dissipation $\varepsilon(t,x) := \nu \sum_{i,j=1}^{3} \langle \partial_{x_j} v_i' \, \partial_{x_j} v_i' \rangle (t,x)$

similar to the turbulent dissipation (involving the symmetric part of the turbulent velocity gradient tensor instead of the turbulent velocity gradient tensor itself)

$$\varepsilon(t,x) = \tfrac{1}{2} \nu \sum_{i,j=1}^{3} \langle (\partial_{x_j} v_i' + \partial_{x_i} v_j')^2 \rangle (t,x)$$

Tracers trajectories

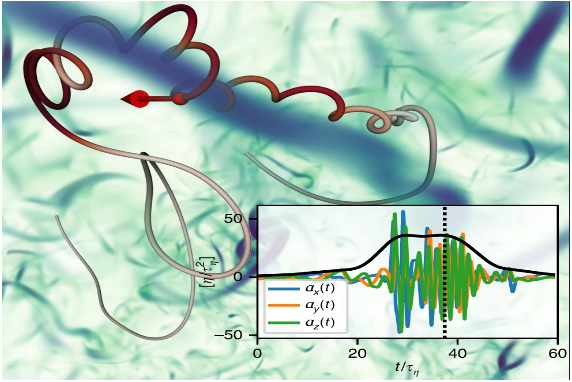


Figure 4: Tracer particle encountering a vortex filament in turbulence. The tracer trajectory is coloured according to its instantaneous acceleration magnitude, and the blue-green volume-rendering corresponds to the intensity of the vorticity field. The particle acceleration components oscillate strongly in time (inset, in Kolmogorov units) when encountering the intense vortex filament. The root of the squared acceleration, coarse-grained over a few Kolmogorov time scales, varies only weakly during such an event (inset, black curve). The dashed line indicates the instant in time at which the vorticity field is visualized and the tracer is rendered as a sphere.

picture borrowed from

Bentkamp, L., Lalescu, C. C., and Wilczek, M. (2019).
Persistent accelerations disentangle lagrangian turbulence. *Nature Communications*.

Temporal Lagrangian autocorrelation

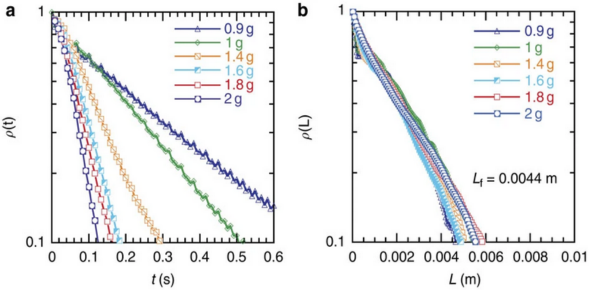


Figure 5: *(a) Temporal Lagrangian autocorrelation function* $\rho^L(\tau)$*, computed for a range of forcing levels in the FWT. This function is decaying approximately exponentially,* $\rho^L(\tau) \simeq \exp(-\tau/T_L)$*, where* T_L *is Lagrangian integral time. (b) Spatial Lagrangian autocorrelation function* $r \mapsto \rho^L(r) = \frac{\langle (V_t(r_0 + r) - \mu) \cdot (V_t(r_0) - \mu)) \rangle}{\langle (V_t(r_0) - \mu)^2 \rangle}$ *computed for the same conditions. As the turbulence energy is increased, Lagrangian integral length remains roughly constant in the broad range of forcing levels.*

picture borrowed from

Francois, N., Punzmann, H., and Shats, M. (2013).

Lagrangian scale of particle dispersion in turbulence. *Nature Communications*.

Exercise

1). Write the Fokker-Planck PDE for the time-marginal laws of (X_t, V_t) and (Y_t) solution of

$$dX_t = V_t\,dt, \quad X_0$$
$$dV_t = \frac{1}{T_L}\left(\langle v\rangle(t, X_t) - V_t\right)dt + \sqrt{C_0\varepsilon}dW_t, \quad V_0, \qquad \text{with Law}(X_0, V_0) = \mu \tag{1}$$
$$dY_t = \langle v\rangle(t, Y_t)dt + \sqrt{C_0\varepsilon}T_L dW_t, \quad X_0 \tag{2}$$

2). Let $(\widetilde{x}_t, \widetilde{u}_t)_{t\geq 0}$ and $(\widetilde{Y}_t)_{t\geq 0}$ be the solutions to the equations (1) and (2) in the case where $\langle v\rangle(t,x) \equiv 0$.
We define $\Gamma_{\mathsf{OU}} : \mathbb{R}^+ \times \mathbb{R}^2 \times \mathbb{R}^2 \mapsto \mathbb{R}$ as the transition density of $(\widetilde{x}_t, \widetilde{u}_t)_{t\geq 0}$ meaning that $\Gamma_{\mathsf{OU}}(t; y, v; x, u) = \mathscr{P}_{y,v}\left((\widetilde{x}_t, \widetilde{u}_t) \in (dx, du)\right)/dxdu$ and $\Gamma_{\mathsf{B}} : \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R} \mapsto \mathbb{R}$ as the transition density of $(\widetilde{Y}_t)_{t\geq 0}$ such that $\Gamma_{\mathsf{B}}(t; y; x) = \dfrac{1}{\sqrt{2\pi\sigma^2 t}}\exp\left(-\frac{1}{2\sigma^2 t}(x-y)^2\right)$.

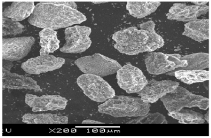
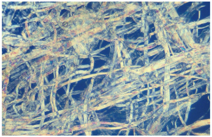
3). Write the Fokker-Planck PDEs for $(t, x, u) \mapsto \Gamma_{\mathsf{OU}}(t; y, v; x, u)$ and $(t, x) \mapsto \Gamma_{\mathsf{B}}(t; y; x)$.

4). Show that the mild equation

$$\rho(t, x, u) = \int_{\mathbb{R}^2} \Gamma_{\mathsf{OU}}(t, y, v; x, u)\mu(dy, dv) \tag{3}$$
$$+ \int_0^t \int_{\mathbb{R}^2} \frac{\partial}{\partial v}\Gamma_{\mathsf{OU}}(t-s, y, v; x, u)\frac{1}{T_L}\langle v\rangle(s, y)\rho(s, y, v)dydv\,ds \tag{4}$$

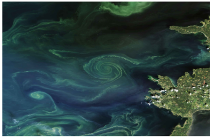
is solution to the Fokker Planck PDE associates to SDE (1).

5). Write the mild equation for $p(t, x)$ the density solution of the Fokker-Planck equation for SDE (2).

Particles in turbulence are important for many industrial and biological applications.
What is important:

- Passive *vs* Active particle
- Size, **Shape**, Inertia, Rheology
- Particle-particle interactions (collisions, agglomerations)
- Additional forces (electrostatics, Brownian motion)



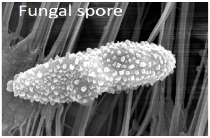
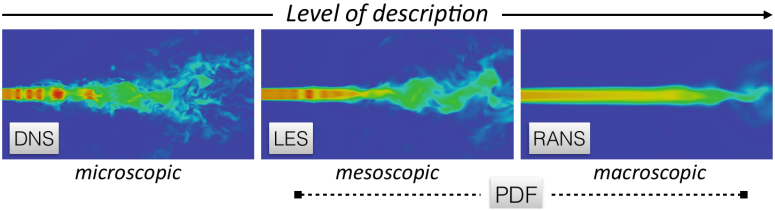


Figure 1. (left) A jet of water directed downward into water with Reynolds number approximately 2300 (obtained in Van Dyke, M. and Van, D., An Album of Fluid Motion, 1982); (right) the same jet simulated in CFD using the RANS approach.

Figure 6: top : Borrowed from ROCKY Blog : Turbulent dispersion model: discover how to account for the turbulence effect on particle trajectories.



- Turbulence scale and flow velocity field.
  The Kolmogorov length scale η_K represents the smallest length scale for fluid motions in a turbulent flow. For most of industrial or environmental flows, $\eta_K \in [50\mu\mathrm{m}, 1\mathrm{mm}]$.

  The flow field $U_f(t, x)$ (governing by the Navier-Stokes equations) is computed :

  ◗ below the scale η_K (Direct Numerical Simulation).⚠ From very expensive to totally prohibitive.

  ◗ above the scale η_K (Engineering application, CFD). Required turbulence modelling: only mean and second order moments velocity are computed $U_f(t, x) = \langle U_f \rangle(t, x) +$ noise.
- Small (spherical) particles. with diameters $d_p \ll \eta_K (\sim 30\mu\mathrm{m})$

  ◗ point-wise approximation is quite reasonable : description is given by Lagrangian equation on center of mass position and velocity $(x_p(t), U_p(t))$.

  ◗ for particles heavier than the fluid (inertial particle: $\rho_p \gg \rho_f$, corresponding to typical size $d_p \geq 5 - 10\mu\mathrm{m}$) the drag force exerted by the fluid is dominant

$$\frac{dU_p}{dt} = \frac{(U_s - U_p)}{\tau_p} + \mathbf{g}, \qquad ⚠\ \tau_p = \tau(\frac{\rho_p}{\rho_f}, d_p, U_f, \ldots), \quad \tau_p(d_p) \nearrow$$

τ_p measures the particle inertia, as the timescale over which particle velocities adjust to **the local fluid velocity seen** U_s.

The particle state vector is now $(x_p(t), U_p(t), U_s(t))$

The velocity seen: $U_s(t) = U_f(t, x_p(t))$.

Modelling the fluid velocity seen by a particle:

$$U_f(t,x) = \langle U_f \rangle(t,x) + \text{noise}(t,x)$$

Modelling coherency requires to adopt Lagrangian point of view also for the fluid :

$$\langle U_f \rangle(t,x) = \langle \mathrm{U}_f(t) | x_f(t) = x) \rangle$$

with a General Langevin Model:

$$\begin{cases} dx_f(t) = \mathrm{U}_f(t)dt, \\ d\mathrm{U}_f^{(i)}(t) = -\partial_{x_i}\langle p \rangle(t, x_f(t))dt + \left(G_{ij}\left(\mathrm{U}_f^{(j)} - \langle \mathrm{U}_f^{(j)} \rangle\right)\right)(t, x_f(t))dt + \sigma_{i,j}(t, x_f(t))dB_t^{(} \end{cases}$$

B is a 3D-Brownian motion.

$$G_{ij} = -\frac{C_R}{2}\frac{\varepsilon}{\mathrm{k}}\delta_{ij} + C_2\frac{\partial \langle \mathrm{U}^{(i)} \rangle}{\partial x_j}, \qquad \sigma_{i,j} = \frac{2}{3}\left(C_R\varepsilon + C_2\mathscr{P} - \varepsilon\right)\delta_{ij},$$

- Mean field approximation for the fluid particle leads to a complex McKean Vlasov SDE, where $\langle \cdot \rangle(t,x) = \mathbb{E}[\cdot | x_f(t) = x]$.
  $\mathbf{u}'(t)$ being the centred Lagrangian velocity $U_f(t) - \langle U_f \rangle(t, x_p(t)$.
  $\mathscr{P} = \frac{1}{2}\mathscr{P}_{ii}$, the turbulent production term $\mathscr{P}_{ij} := -(\langle \mathbf{u}_i'\mathbf{u}_k' \rangle \partial_{x_k}\langle \mathrm{U}^{(i)} \rangle - \langle \mathbf{u}_j'\mathbf{u}_k' \rangle \partial_{x_k}\langle \mathrm{U}^{(j)} \rangle$
  ε is closed with coherent parametrisation involving $\mathrm{k} = \frac{1}{2}\langle \mathbf{u}_i'\mathbf{u}_i' \rangle$.

Langevin model for dispersed particles embedded in a turbulent flows using a dynamic PDF model

- Inertial particle ($\rho_p \gg \rho_f$) :

$$
\begin{aligned}
dx_p(t) &= U_p(t)dt, \\
dU_p(t) &= \frac{1}{\tau_p}(U_s(t) - U_p(t))dt \\
dU_s^i(t) &= -\frac{1}{\rho_f}\partial_{x_i}\langle p\rangle(t, x_p(t))dt \\
&\quad + (\langle U_p^j\rangle - \langle U_f^j\rangle)\partial_{x_i}\langle U_f^j\rangle dt + G^*_{ij}(U_s^j - \langle U_f^j\rangle(t, x_p(t))dt + \sigma_{ij}(t, x_p(t))dB_j
\end{aligned}
$$

$G^*_{ij} = \frac{T_L}{T_L^*}G_{ij}$ where $\frac{T_L}{T_L^*}$ is a model factor. T_L^* is correlation timescale of the velocity of the fluid seen / T_L is the Lagrangian correlation timescale of the velocity.

- Highly inertial particle limit : overdamped dynamics

When $T_L^* \to 0$, and finite τ_p (high inertia), $G^*_{ij} \sim \frac{1}{T_L^*}$,

$$
\begin{aligned}
dx_p(t) &= U_p(t)dt, \\
dU_p^i(t) &= \frac{1}{\tau_p}(\langle U_f^i\rangle(t, x_p(t)) - U_p^i(t))dt \\
&\quad + \frac{1}{\tau_p}G_{ij}^{-1}\frac{1}{\rho_f}\partial_{x_j}\langle p\rangle(t, x_p(t))dt + \frac{1}{\tau_p}(G^{*-1}(\sigma))_{ij}(t, x_p(t))dB_j
\end{aligned}
$$

Langevin model for dispersed particles embedded in a turbulent flows using a dynamic PDF model (II)

- Small-enough particles (colloids, $\rho_p \ll \rho_f$, $d_p \leq 1 - 2\mu\mathrm{m}$). Drag force is complemented with molecular effects and Brownian motion:

$$
\begin{aligned}
dx_p(t) &= U_p(t)dt, \\
dU_p(t) &= \tfrac{1}{\tau_p}(U_s(t) - U_p(t))dt + K_{Brow}(\tau_p)dW(t) \\
dU_s^i(t) &= -\tfrac{1}{\rho_f}\partial_{x_i}\langle p\rangle(t, x_p(t))dt \\
&\qquad + (\langle U_p^j\rangle - \langle U_f^j\rangle)\partial_{x_i}\langle U_f^j\rangle dt + G_{ij}^*(U_s^j - \langle U_f^j\rangle(t, x_p(t))dt + \sigma_{ij}(t, x_p(t))dB_j
\end{aligned}
$$

with K_{Brow} increasing with $1/(\tau_p)^{\frac{1}{2}}$. B and W are assumed independent.

- Generalized Langevin to Einstein limit $\tau_p \to 0$ overdamped dynamics

$$
\begin{aligned}
dx_p(t) &= U_s(t)dt + \tau_p K_{Brow}(\tau_p)dW(t) \\
dU_s^i(t) &= -\tfrac{1}{\rho_f}\partial_{x_i}\langle p\rangle(t, x_p(t))dt \\
&\qquad + G_{ij}^*(U_s^j - \langle U_f^j\rangle(t, x_p(t))dt + \sigma_{ij}(t, x_p(t))dB_j
\end{aligned}
$$