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ACTIVITY REPORT

Project-Team

CALISTO

Stochastic Approaches for Complex Flows and Environment

DOMAIN

Applied Mathematics, Computation and Simulation

THEME

Stochastic approaches

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Project-Team CALISTO

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Computer sciences and digital sciences

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2 Overall objectives

Turbulence modeling and particle dynamics are at play in numerous situations in which inertial particles are transported by turbulent flows. These particles can interact with each other, form aggregates which can fragment later on, and deposit on filters or solid walls. In turn, this deposition phenomenon includes many aspects, from the formation of monolayer deposits to heavy fouling that can clog flow passage sections. Taking into account the potentially complex morphology of these particles then requires to develop new approaches to predict the resulting statistical quantities (turbulent dispersion, formation of aggregates, nature of formed deposits, etc.).

The variety of situations (deposition, resuspension, turbulent mixing, droplet/matter agglomeration, thermal effect) involves specific models that need to be improved. Yet, one of the key difficulties lies in the fact that the relevant phenomena are highly multi-scale in space and time (from chemical reactions acting at the microscopic level to fluid motion at macroscopic scales), and that consistent and coherent models need to be developed together. This raises many challenges related both to physical sciences (i.e. fluid dynamics, chemistry or material sciences) and to numerical modeling.

Through the unique synergy between team members from various disciplines, CALISTO is developing *Stochastic Approaches for complex Flows and Environment* to address the following challenges:

- produce original answers (methodological and numerical) for challenging environmental simulation models, with applications to renewable energy, filtration/deposition technology in industry (cooling of thermal or nuclear power plants) and filtration/deposition, dispersion of materials or active agents (such as biological organisms, micro-robots);
- design new mathematical tools to analyze the fundamental physics of turbulence;
- develop numerical methods to analyze the displacement of micro-swimmers into a range of fluids such as water, non-Newtonian bodily fluids, etc.;
- optimize and control the displacement of artificial micro-swimmers;
- develop stochastic modeling approaches and approximation methods, in the rich context of particle-particle and fluid-particle interactions in complex flows;
- contribute to the field of numerical probability, with new simulation methods for complex stochastic differential equations (SDEs) arising from multi-scale Lagrangian modeling for the dynamics of material/fluid particle dynamics with interaction.

3 Research program

CALISTO is structuring its research according to five interacting axes.

Axis A Complex flows: from fundamental science to applied models.

Axis B Particles and flows near boundaries: specific Lagrangian approaches for large-scale simulations.

Axis C Active agents in a fluid flow.

Axis D Mathematical and numerical analysis of stochastic systems.

Axis E Variability and uncertainty in flows and environment.

3.1 Axis A Complex flows: from fundamental science to applied models

This axis aims at promoting significant advances in the understanding and modeling of realistic dispersed, multiphase turbulent flows. In situations where basic mechanisms are still not fully apprehended, the proposed research aims at bringing out the underlying physics by identifying novel effects and quantifying their impacts. These results will then be used to foster new macroscopic models that are expected to be computationally sufficiently undemanding. These models should also be adaptable to open the way to systematic studies of turbulent suspensions as a function of settings, parameters, system geometry. Such aspects are essential in exploratory researches aimed at optimizing combustion processes, heat transfers, phase changes, or the design of energy-efficient hydraulic or aerodynamic processes.

Accurate modeling of the location, attributes, and effects of particles transported by turbulent flows is key to optimize the design and performance of several processes in industry, in particular in power production. Yet, current macroscopic approaches often oversimplify physical phenomena related to small-scale physics and fail to capture various effects, such as heterogeneous distributions of sizes and shapes, particle deformation, agglomeration, as well as their interactions with boundaries. Improving models remains a huge challenge that requires monitoring spatial and temporal correlations through particle relative dynamics.

Our overall objective here is to design, validate and apply new efficient modeling and simulation tools for fluid-particle systems that account for relative particle motions, two-particle interactions and complex flow geometries. Our methodology consists in simultaneously *(i)* building up a comprehensive microscopic description, *(ii)* developing efficient macroscopic models, and *(iii)* applying these two approaches to study practical situations to compare and validate them.

Continuous exchanges between these two viewpoints make it possible to quickly identify pitfalls in models. Furthermore, fine-scale descriptions will progressively provide suggestions for improvements.

This research axis is currently investigating the following distinct topics

- Models for polydisperse, complex-shaped, deformable particles;
- Particle interactions and size evolution;
- Transfers between the dispersed phase and its environment.

3.2 Axis B - Particles and flows near boundaries: specific Lagrangian approaches for large scale simulations

This research axis aims at developing Lagrangian macroscopic models for single phase and particle-laden turbulent flow simulations. This activity addresses important situations of environmental flows, such as atmospheric boundary layer (ABL), and pollutants, pollen, micro-plastic dispersion and resupension in the atmosphere or river/marine systems. These are situations where boundaries bring additional complexity, in terms of turbulent description, and in terms of the interaction between wall and particles.

In the hierarchy of turbulent models, the Lagrangian stochastic approach (or probability density function (PDF) approach) is distinguished by several important features, mainly: *(i)* it is a stochastic method that resolves the probability density function of some physical relevant variables, needed to provide sufficient statistical information. For example, in the case of single-phase turbulent flows, this method provides the velocity distribution, compatible with the imposed momentum turbulent closure of the considered model. In particular, it delivers the whole tensor of correlations between the flow velocity components in adequacy with the given closure; *(ii)* thanks to its Lagrangian formulation, this approach allows to develop a fully coherent model of a turbulent flow, of particles embedded in it, as well as their interactions.

For two-phase turbulent flows, the combination of fluid-particle approaches with discrete particle approaches –called here Lagrange-Lagrange approaches– appears to be particularly interesting for near boundary flows where interactions with surface boundaries are coming into the problem. Until now, this Lagrangian-Lagrangian modelling approach has never really been explored. The CALISTO in-house SDM software, as a mature fluid-particle Lagrangian simulation code, offers an exciting opportunity to investigate this direction.

This research axis is currently investigating the following distinct topics.

3.2.1 Stand-alone Lagrangian simulations in atmospheric boundary layer (ABL)

The turbulent nature of the atmospheric boundary layer (ABL) contributes to the uncertainty of the wind energy estimation. This has to be taken into account in the modeling approach when assessing the wind power production. The purpose of the Stochastic Downscaling Model (SDM) is to compute the wind at a refined scale in the ABL, from a coarse wind computation obtained with a mesoscale meteorological solver. The main features of SDM reside in the choice of a fully Lagrangian viewpoint for the turbulent flow modeling. This is allowed by stochastic Lagrangian modeling approaches that adopt the viewpoint of a fluid-particle dynamics in a flow. Such methods are computationally inexpensive when one needs to refine the spatial scale. This is a main advantage of the SDM approach, as particles methods are free of numerical constraints (such as the Courant Friedrichs Lewy condition that imposes a limit to the size of the time step for the convergence of many explicit time-marching numerical methods).

A particular attention is now focused on improving stand-alone Lagrangian numerical models in the ABL (such as additional buoyancy model, canopy models). Furthermore, the coupling of fluid particle modeling with phase particle models is of crucial interest for some of our applications.

3.2.2 Advanced stochastic models for discrete particle dispersion and resuspension

As a particle nears a surface, deposition can occur depending on the interactions between the two objects. Deposits formed on a surface can then be resuspended, i.e. detached from the surface and brought back in the bulk of the fluid. Resuspension results from a subtle coupling between forces acting to move a particle (including hydrodynamic forces) and forces preventing its motion (such as adhesive forces, gravity). In the last decades, significant progresses have been achieved in the understanding and modeling of these processes within the multiphase flow community. Despite these recent progresses, particle resuspension is still often studied in a specific context and cross-sectoral or cross-disciplinary exchange are scarce. Indeed, resuspension depends on a number of processes making it very difficult to come up with a general formulation that takes all these processes into account.

Our goal here is to improve deposition law and resuspension law for more complex deposits in turbulent flows, especially towards multilayered deposits. For that purpose, we are improving existing Lagrangian stochastic models while resorting to meta-modeling to develop tailored resuspension law from experimental measurements and fine-scale numerical simulations. We are targeting practical applications such as pollutants in the atmosphere and plastic in marine systems.

3.2.3 Coherent descriptions for fluid and particle phases

Various particles are present in the ABL, such as pollutant, fog or pollen. This surface layer is characterized by various complex terrains (as urban cities or forests), forming the so-called *canopy*. This canopy strongly affects the near-wall turbulent motion as well as the radiative and thermal transfers.

Simulations of two-phase flows requires to couple solvers for the fluid and particle phases. Numerical Weather Prediction (NWP) software usually rely on a Eulerian solver to solve Navier-Stokes equations. Solid particles are often treated using a Lagrangian point of view, i.e. their motion is explicitly tracked by solving Newton's equation of motion, the key difficulty being then to couple these intrinsically different approaches together. In line with the models and numerical methods developed in Sections 3.2.1 and 3.2.2, as an alternative to Eulerian-Lagragian approaches, CALISTO is developing a *new Lagrange-Lagrange formulation* that remains tractable to perform simulations for two-phase turbulent flows. We are particularly interested in *Lagrange-Lagrange models for interactions with surfaces*, as turbulence and collisions with surfaces can significantly affect the concentration of particles in the near-wall region.

3.2.4 Active particles near boundary

Surface effects can lead to the trapping of micro-swimmers near boundaries, as the presence of a boundary breaks both the symmetry of the fluid (leading to strong anisotropy) and the symmetry of the fluid-swimmer system. The better understanding of fluid-particle interactions near boundaries are expected here to help in the design of new control actuation for driving artificial swimmers in confined environments (developed in Axis C).

3.3 Axis C - Active agents in a fluid flow

Active agents are entities immersed into a fluid, capable of converting stored or ambient free energy (for instance through deformation) into systematic movement. Active agents, also called swimmers, can interact with each other as well as with the surrounding medium.

This research axis is devoted to new mathematical modeling approaches to simulate the displacement of swimmers, to get results on control and optimal control associated with them, to study the presence of an additional stochastic effect for driving a swarm of such micro-swimmers.

Modeling approach

The equations of motion of the swimmer derive from its hydrodynamical interactions with the fluid through Newton laws. At a high level of description, this can be described by coupling the Navier-Stokes equations with the hyper-elastic equations describing the swimmer's deformation (in the case of elastic body). In the case of artificial magnetic swimmers, additional contribution representing the action of an external magnetic field on the swimmer needs to be added in the equations of motion. Solving the resulting system of PDEs is a challenging task, since it combines a set of equations deemed to be numerically difficult to solve even when they are decoupled. To overcome these difficulties, CALISTO considers various types of models, ranging from simpler but rough models to more realistic but complex models.

Control and optimal control for swimmers displacement

CALISTO investigates the controllability issues and the optimal control problems related in particular to two situations: the displacement of *(i)* real self-propelled swimmer by assuming that the control is the deformation of its body *(ii)* artificial bio-inspired swimmers that are able to swim using an external magnetic field.

Another line of research concerns optimal path planning in turbulent flow. As a microswimmer swims towards a target in a dynamically evolving turbulent fluid, it is buffeted by the flow or it gets trapped in whirlpools. The general question we want to address is whether such a microswimmer can develop an optimal strategy that reduces the average time or energy it needs to reach a target at a fixed distance.

Stochastic effect on artificial swimmers

CALISTO investigates also the effect of the presence of noise in the response of a micro-robot (to the external magnetic field for instance) by developing new model and related numerical simulation of such systems.

3.4 Axis D - Mathematics and numerical analysis of stochastic systems

This research axis is devoted to fundamental aspects of our models or objects though their mathematical analysis.

Mathematics for fundamental aspects of turbulence and turbulence transport

This research line has the scope of providing a unified description of turbulent flows in the limit of large Reynolds numbers and thus will be applicable to a large range of physical applications. It is conjectured since Kolmogorov and Onsager that the flow develops a sufficiently singular structure to provide a finite dissipation of kinetic energy when the viscosity vanishes. This dissipative anomaly gives a consistent framework to select physically acceptable solutions of the limiting inviscid dynamics. However, recent mathematical constructions of weak dissipative solutions face the problem of non-uniqueness, raising new questions on the relevance to turbulence and on the notion of physical admissibility.

On the one hand, the conservation of kinetic energy is actually not the only symmetry that is broken by turbulence. Various experimental and numerical measurements show significant deviations from simple scaling, time-irreversible fluctuations along fluid elements trajectories, and possibly other broken inviscid symmetries, such as circulation. Still, these anomalies may have a universal nature and, as such, provide new constraints for the design of physically admissible solutions. On the other hand, non-uniqueness could be an intrinsic feature of turbulence. Singular solutions to non-linear problems have an explosive sensitivity leading to spontaneously stochastic behaviors, thus questioning the pertinence of uniqueness and providing a framework to interpret solutions at a probabilistic level. To address such issues and provide unified appreciation, we simultaneously develop three strongly interrelated viewpoints: a) numerical approach, exploiting relevant and efficient fully-resolved simulations; b) new theoretical approaches based on the statistical physics of turbulent flow; c) mathematical construction of "very weak" flows, such as measure-valued solutions to the Euler equations.

Interacting Stochastic Systems, and Mean Field Interactions

A birds flock, a school of fish, a group of fireflies, a crowd in the street, or even the neurons of our brain, are all examples of interacting entities that can suddenly start to behave collectively in a more complex and richer way than their constitutive elements. The mathematical modeling of such phenomena started mainly motivated by biological systems, but lately has gained a lot of attention due to new applications in economics, finance, robotics and even opinion formation in human behavior. CALISTO considers examples of *particle* systems in interaction, possibly under mean field interaction, with the overall goal of analyzing the effect of stochasticity in such system. In particular, we aim to detect and analyze conditions for the emergence of collective behaviors such as collective motions, synchronization and organization with or without the notion of leaders.

Another important example of complex interacting system is given by collisioning particle system under Langevin dynamics. If the case of collisioning systems in the context of gas dynamics –where particles experiment free path between two collision events– and in the context of overdamped Brownian dynamics have been largely studied, until now, situation of a finite number of particles collisioning under a Langevin dynamics is poorly addressed. This last case, describing particles in turbulent flow, is of great interest for CALISTO from both numerical and theoretical view points.

3.5 Axis E - Variability and uncertainty in flows and environment

Variability in wind/hydro simulation at small scale: application to wind/hydro energy

The turbulent nature of the atmospheric boundary layer (ABL) contributes to the uncertainty of the wind energy estimation. This has to be taken into account in the modeling approach when assessing the wind power production. The stochastic nature of the SDM approach developed in Axis B offers some rich perspectives to asses variability and uncertainty quantification issues in the particular context of environmental flows and power extraction evaluation. In particular, as a PDF method, SDM delivers a probability distribution field of the computed entities. Merging such numerical strategy with Sensitivity Analysis (SA)/Uncertainty Quantification (UQ) are potentially fruitful in terms of computational efficiency.

Metamodeling and uncertainty

While building and using computational fluid dynamics (CFD) simulation models, sensitivity analysis and uncertainty quantification methods allow to study how the uncertainty in the output of a model can be apportioned to different sources of uncertainty in the model input. UQ approaches allow to model verification and factor prioritization. It is a precious aid in the validation of a computer code, guidance research efforts, and in terms of system design safety in dedicated application. As CFD code users, we aim at applying UQ tools in our dedicated modeling and workflow simulation. As Stochastic Lagrangian CFD developers, we aim at developing dedicated SA and UQ tools as Stochastic solvers have the ability to support cross Monte Carlo strategy at the basis of SA methodology.

Another goal is to address some control and optimization problems associated with the displacement of swimmers through metamodeling, such as Gaussian process regression model, proved to be efficient for solving optimization of PDEs systems in other contexts.

Anomalies modeling through machine-learned dataset of meteorological observations and forecasts

Stochastic modeling approaches are known to be able to describe the intrinsic variability of a phenomenon, preserving the spatial coherence of variability and interacting with the dynamics of the physical processes involved. The machine learning (or meta model) approach is recognized for these prediction capabilities. It is nowadays everywhere in the forecast data delivered, using past events to de-bias/select the future, when the physical dynamic model becomes too heavy to handle. We aim at intersecting the two approaches to develop methodologies for selecting/enriching future scenarios, starting from the observation that we can not calibrate the model of variability to be associated with a future forecast (distribution of extremes accounts for climatic changes), the same way one calibrates the variability model to be associated with observables.

4 Application domains

Environmental challenges: predictive tools for particle transport and dispersion

Particles are omnipresent in the environment:

- formation of clouds and rain results from the coalescence of tiny droplets in suspension in the atmosphere;
- fog corresponds to the presence of droplets in the vicinity of the Earth's surface, reducing the visibility to below 1 km [24];
- pollution corresponds to the presence of particulate matter in the air. Due to their impact on human health [33], the dispersion of fine particulate matter is of primary concern: PM2.5 and PM10 (particles smaller than 2.5 or 10 μm) and Ultra Fine Particles (UFP) are particularly harmful for human respiratory systems while pollen can trigger severe allergies;
- the dispersion of radioactive particles following their release in nuclear incidents has drawn a great deal of attention to deepen our understanding and ability to model these phenomena [39];
- the dispersion/deposition of ash and soots and their consequences for the environment and health have been highlighted by recent events in France and abroad;
- plastic contamination in oceans impacts marine habitats and human health [27];
- suspension of real micro-swimmers [19] such as sperm cell, bacteria, and in environmental issues with animal flocks attracted intrinsic biological interest[29];
- accretion of dusts is responsible for the formation of planetesimals in astrophysics [28].

These selected examples show that the presence of particles affects a wide range of situations and has implications in public, industrial and academic sectors.

Each of these situations (deposition, resuspension, turbulent mixing, droplet/matter agglomeration, thermal effect) involves specific models that need to be improved. Yet, one of the key difficulties lies in the fact that the relevant phenomena are highly multi-scale in space and time (from chemical reactions acting at the microscopic level to fluid motion at macroscopic scales), and that consistent and coherent models need to be developed together. This raises many issues related both to physical sciences (i.e. fluid dynamics, chemistry or material sciences) and to numerical modeling.

Next generation of predictive models for complex flows

Many processes in power production involve circulating fluids that contain inclusions, such as bubbles, droplets, debris, sediments, dust, powders, micro-swimmers or other kinds of materials. These particles can either be inherent components of the process, for instance liquid drops in sprays and soot formed by incomplete combustion, or external foul impurities, such as debris filtered at water intakes or sediments that can obstruct pipes. Active particles, seen as artificial micro-swimmers, have attracted particular attention for medical applications since they can be used as vehicles for the transport of therapeutics or as tools for limited invasive surgery. In these cases, optimization and control requires monitoring the evolution of their characteristics, their trajectories (with/without driving), and their effects on the fluid with a sufficiently high level of accuracy. These are very challenging tasks given a numerical complexity of the numerical models.

These challenges represent critical technological locks and power companies are devoting significant design efforts to deal with these issues, increasingly relying on the use of macroscopic numerical models. This framework is broadly referred to as "Computational Fluid Dynamics". However, such large-scale approaches tend to oversimplify small-scale physics, which limits their suitability and precision [20]. Particles encountered in industrial situations are generally difficult to model: they are polydisperse, not exactly spherical but of any shape, and deform; they have complex interactions, collide and can agglomerate; they usually deposit or stick to the walls and can even modify the very nature of the flow (e.g. polymeric flows). Extending present models to these complex situations is thus key to improve their applicability, fidelity, and performance.

Models operating in industry generally incorporate rather minimalist descriptions of suspended inclusions. They rely on statistical closures for single-time, single-particle probability distributions, as is the case for the particle-tracking module in the open-source CFD software CODE_SATURNE developed and exploited by EDF R&D. The underlying mean-field simplifications do not accurately reproduce complex features of the involved physics that require higher-order correlation descriptions and modeling. Indeed, predicting the orientation and deformation of particles requires suitable models of the fluid velocity gradient along their trajectories [40] while concentration fluctuations and clustering depend on relative particle dispersion [35, 25]. Estimates of collision and aggregation rates should also be fed by two-particle dynamics [34], while wall deposition is highly affected by local flow structures [36]. Improving existing approaches is thus key to obtain better prediction tools for multiphase flows.

New simulation approach for renewable energy and meteorological/climate forecast

A major challenge of sustainable power systems is to integrate climate and meteorological variability into operational processes, as well as into medium/long term planning processes [23]. Wind, solar, marine/rivers energies are of growing importance, and the demand for forecasts goes hand in hand with it [22, 32]. Numerous methods exist for different forecast horizons [21]. One of the main difficulties is to address refined spatial description. In the case of wind energy, wind production forecasts are submitted to the presence of turbulence in the near wall atmospheric boundary layer. Turbulence increases the variability of wind flows interacting with mill structures (turbine, mast, nacelle), as well as neighboring structures, terrain elevation and surface roughness. Although some computational fluid dynamics models and software are already established in this sector of activity [37] [31], the question of how to enrich and refine wind simulations (from meteorological forecast, or from larger scale information, eventually combined with local measurements) remains largely open.

Though hydro turbine farms are of a less assertive technological maturity than wind farms, simulating hydro turbines farms in rivers and sea channels submitted to tidal effect present similar features and challenges. Moreover in the marine energy context, measures are technically more difficult and more costly, and the demand in weather forecast concerns also the safety in maintenance operations.

At the time scale of climate change, the need for uncertainty evaluation of predictions used in long-term planning systems is increasing. For managers and decision makers in the field of hydrological forecasts, assessing hydropower predictions taking into account their associated uncertainties is a major research issue, as shown by the recent results of the European QUICS project [38]. The term uncertainty here refers to the overall error of the output of a generic model [30]. Translating time series of meteorological forecast into time series of run-of-river hydropower generation necessitates to capture the complex relationship between the availability of water and the generation of electricity. The water flow is itself a nonlinear function of the physical characteristics of the river basins and of the weather variables whose impact on the river flow may occur with a delay.

5 New results

5.1 Axis A – Complex flows: from fundamental science to applied models

5.1.1 Lagrangian stochastic model for the orientation of non-spherical particles in turbulent flow: an efficient numerical method for CFD approach

Participants: Lorenzo Campana, Mireille Bossy, Christophe Henry, Jérémie Bec.

Suspension of anisotropic particles can be found in various industrial applications. Microscopic ellipsoidal bodies suspended in a turbulent fluid flow rotate in response to the velocity gradient of the flow. Understanding their orientation is important since it can affect the optical or rheological properties of the suspension. The equations of motion for the orientation of microscopic ellipsoidal particles were obtained by Jeffery [26]. But so far, this description has always been investigated in the framework of direct numerical simulations (DNS) and experimental measurements. In particular, inertia-free particles, with sizes smaller than the Kolmogorov length, follow the fluid motion with an orientation generally defined by the local turbulent velocity gradient.

In this work, our focus is to characterize the dynamics of these objects in turbulence by means of a stochastic Lagrangian approach. The development of a model that can be used as predictive computational tool in industrial computational fluid dynamics (CFD) codes is highly valuable for practical applications. Models that reach an acceptable compromise between simplicity and accuracy are needed for progressing in the field of medical, environmental and industrial processes.

Firstly, the formulation of a stochastic orientation model is studied in two-dimensional turbulent flow with homogeneous shear, where results are compared with direct numerical simulations (DNS). We address several issues, i.e finding analytical results, the model, scrutinizing the effect of the anisotropies when they are included in the model, and extending the notion of rotational dynamics in the stochastic framework. Analytical results give a reasonable qualitative response, even if the diffusion model is not designed to reproduce the non-Gaussian characteristics of the DNS experiments.

A further extension to the three-dimensional case shows that the implementation of efficient numerical schemes in 3D models is far from straightforward. A numerical scheme has been devised, able to preserve the dynamical features at reasonable computational costs for such highly nonlinear SDEs. The convergence is analyzed, obtaining a strong mean-square convergence of order 1/2 and a weak convergence of order 1.

Eventually, the model and the numerical scheme have been implemented in the open-source CFD CODE_SATURNE software. The model was used to study the orientational and rotational behavior of anisotropic inertia-free particles in an applicative prototype of inhomogeneous turbulence in a channel flow. This application faces two different modeling issues: the first concerns whether and to which extent the model is able to reproduce the DNS experiments in a channel flow; the second is about its numerical implementation within a fully stochastic Lagrangian framework provided by the Lagrangian module of CODE_SATURNE. In this context, the stochastic Lagrangian model for the orientation reproduces with some limits the orientation and rotation statistics of the DNS.

Three related publications are in preparation.

5.1.2 Dynamics and statistics of inertial spheroidal particles in turbulence

Participants: Sofia Allende, Jérémie Bec.

Many industrial processes involve the transport of material inclusions (dust, debris) by a turbulent fluid. Quantifying properties of such particles is essential to optimize the design and performance of these systems. Despite these challenges, the classical approaches used in industry oversimplify the physics at small scale and fail to capture various effects, especially in the case of non-spherical and deformable particles. The improvement of macroscopic models remains to this day a real challenge. In continuation to the collaboration developed between Inria and EDF R&D on models for the transport of non-ideal particles in turbulent flows, we have developed direct numerical simulation tools to provide a microscopic description of the dynamical and statistical properties of inertial non-spherical particles

In this framework we have performed several numerical experiments of rigid ellipsoidal particles (described by the Jeffery equation) passively transported by an incompressible 3D homogeneous isotropic turbulent flow. The idea was to understand the effects of non-sphericity on the statistics of particles velocity, acceleration, rotation and concentration properties. Our results seem to indicate that the translational dynamics of particles solely depends on an angle-averaged Stokes number. Everything happens as if the orientation of the particles is not correlated with its translational dynamics. An article on this topic has been submitted to the Journal of Fluid Mechanics.

5.1.3 Turbophoresis of heavy inertial particles in statistically homogeneous flow

Participants: Jérémie Bec, Robin Vallée.

Dispersed particles suspended in turbulent flows are widely encountered in nature or industry under the form of droplets, dust, or sediments. When they are heavier than the fluid, such particles possess inertia and are ejected by centrifugal forces from the most violent vortical structures of the carrier phase. Once cumulated along particle paths, this small-scale mechanism produces an effective large-scale drift where particles leave the excited turbulent zones and converge to calmer regions to form uneven spatial distributions. This fundamental phenomenon, called *turbophoresis*, has been extensively used to explain why particles transported by non-homogeneous flows concentrate near the minima of the turbulent kinetic energy.

We have shown that turbophoretic effects are just as crucial in statistically homogeneous and isotropic flows. Instantaneous spatial fluctuations of the turbulent activity, despite their uniform average, trigger local fluxes that play a key role in the emergence of inertial-range inhomogeneities in the particle distribution. Direct numerical simulations have been used to thoroughly probe and depict the statistics of particle accelerations and in particular their scale-averaged properties conditioned on the local turbulent activity. They confirm the relevance of the local energy dissipation to describe instantaneous spatial fluctuations of turbulence. This analysis yields an effective coarse-grained dynamics, in which particles detachment from the fluid and their ejection from excited regions are accounted for by a space and time-dependent non-Fickian diffusion.

Such considerations led us to cast inertial-range fluctuations in the particles distributions in terms of a local Péclet number Pe, which measures the relative importance of turbulent advection compared to turbophoresis induced by inertia. Numerical simulations confirm the relevance of this dimensionless parameter to characterize how particle concentration recovers homogeneity at large scales. This approach also explains the presence of voids with inertial-range sizes, and in particular that their volumes have a non-trivial distribution with a power-law tail whose exponent depends on the particle response time. These results are gathered in an article that will be submitted to the Journal of Fluid Mechanics in the coming months.

5.1.4 Modeling of the formation and maturation of soot particle aggregates

Participant: Christophe Henry.

Studying the agglomeration of small nanoparticles (a few nanometers in size) or atomic clusters has remarkable importance for the synthesis of nanoparticles at industrial scale. However, this is a challenge since different physical phenomena have to be considered for instance atomic clusters can experience coalescence upon collisions while larger nanoparticles may experience a rebound after collisions. This means that a sticking probability has to be taken into account. This sticking probability is currently poorly understood especially for nanoparticles formed in flames where changes in agglomeration and flow regimes occur simultaneously.

This study focuses on the aggregation of nascent soot particles, which are very important to predict well soot particle size distribution and morphology in flames. Such nascent soot particles may grow in the reaction-limited aggregation regime (sticking probability $\ll 1$). However, it is currently unknown how fast would be the transition towards diffusion/ballistic-limited aggregation regimes as observed for mature soot (sticking probability close to 1). In this collaborative work, we intend to fill this gap by focusing on numerically simulated soot particles formed in a laminar premixed flame. To this end, a recent fast and accurate Monte Carlo discrete element code called MCAC (developed at CORIA) is used. In these simulations the individual trajectories of particles are integrated in time. The MCAC has been adapted to non-unitary collision and sticking probability considering three different outcomes for interacting aggregates: no collision, sticking or rebound.

Using such fine-scale simulations, we have shown that assuming a unitary sticking and collision probability produces no big changes in the aggregation kinetics, particle size distribution, and aggregate morphology. Meanwhile, the soot particles bulk density was found to affect the aggregation kinetics and particle size distribution. This is an important result for macroscopic models: such effects should be considered in future simulations relying on Population Balance Equations (PBE).

These results have been realized in collaboration with José Moran and Jérôme Yon from CORIA in Rouen. The results were published in Carbon [8] and were presented by José Moran at the French

Conference on Aerosol in January 2021, at the Cambridge Particle Meeting in June 2021 and at the European Aerosol Conference in August 2021 [13, 18].

5.2 Axis B – Particles and flows near boundaries: specific Lagrangian approaches for large-scale simulations

5.2.1 New spatial decomposition method for accurate, mesh-independent agglomeration predictions in particle-laden flows

Participants: Mireille Bossy, Christophe Henry, Kerlyns Martínez Rodríguez.

Computational fluid dynamics simulations in practical industrial/environmental cases often involve non-homogeneous concentrations of particles. In Euler-Lagrange simulations, this can induce the propagation of numerical error when the number of collision/agglomeration events is computed using mean-field approaches. In fact, mean-field statistical collision models allow to sample the number of collision events using a priori information on the frequency of collisions (the collision kernel). Yet, since such methods often rely on the mesh used for the Eulerian simulation of the fluid phase, the particle number concentration within a given cell might not be homogeneous, leading to numerical errors. In this article, we apply the data-driven spatial decomposition (D2SD) algorithm, recently proposed in a previous work reported in [7], to control such error in simulations of particle agglomeration. This D2SD algorithm provides a spatial splitting according to the spatial distribution of particles. More precisely, the D2SD algorithm uses as an input data only the information on the location of the center of gravity of each particle. One of the many advantages of the D2SD algorithm is that the parameters leading to the optimal domain decomposition are automatically tuned through the statistical information coming from the data (position of particles). Thus, there is no bias coming from the choice of arbitrary parameter.

Significant improvements are made to design a fast D2SD version, minimizing the additional computational cost by developing re-meshing criteria. Several options are assessed, introducing a criterion to avoid applying the full version of the D2SD algorithm every time step, or simplifying uniformity tests. The main difficulty is to ensure that the adapted algorithm keeps an appropriate balance between its accuracy and its computational costs.

Through the application to some practical simulation cases, we show the importance of splitting the domain when computing agglomeration events in Euler/Lagrange simulations, so that there is a spatially uniform distribution of particles within each elementary cell. The algorithm is coupled to 3D simulations of particle agglomeration in practical cases with a two-fold objective: first, we assess the accuracy and efficiency of the method in a validation case; second, we illustrate how the D2SD can be applied in a practical case that is representative of situations of interest in the multiphase flow community.

This study is detailed in [6], published in the International Journal of Multiphase Flow.

5.2.2 Evidence of collision-induced resuspension of microscopic particles from a monolayer deposit and new models

Participants: Mireille Bossy, Christophe Henry.

This study aims at bridging the gap between the understanding and modeling of particle resuspension in monolayer deposits and multilayer deposits. More precisely, modeling resuspension is indeed a challenging task owing to its complexity and multiscality. In practice, numerical concepts describing the resuspension at the particle scale, that is in the micron to millimeter size, exist. However, such models have been designed to treat two limit cases: monolayer or multilayer deposits. In the monolayer case, the inter-particle distance L is implicitly assumed to be much greater than the particle diameter D_p ($L \gg D_p$), so that each resuspension event can be treated independently. In the multilayer case where particles sit on top of one another ($L \ll D_p$), resuspension events involve either single particles or clusters of particles depending on the local deposit structure and inter-particle cohesion forces. Yet, a unified description of particle resuspension from monolayer to multilayer deposits is still missing.

The present work bridges the gap by addressing the very special case where the inter-particle distance becomes comparable to the particle diameter ($L \sim D_p$). Experimental investigations performed by co-authors at Technische Universität Dresden (Germany) have revealed two distinct detachment mechanisms. At relatively low flow velocities, few loosely adhering particles move on the wall to eventually collide with neighboring particles resulting in a clustered resuspension. At higher fluid velocities, mostly individual particles resuspend due to their interaction with the turbulent flow.

In line with these new observations, the existing model for particle resuspension from monolayered deposits has been extended to account for the effect of inter-particle collision. Despite its simplicity, this extended model confirms the role played by inter-particle collisions even at relatively low surface coverage while highlighting the importance of initial clustering (which can significantly increase the probability of collision between particles at the local scale).

These results were published in Physical Review Fluids [1] and presented at the Dispersed Two-Phase Flow Conference in October 2021. Another publication is under preparation to further explore the role of adhesive forces.

5.2.3 Effective accretion rates of small inertial particles by a large towed sphere

Participants: Jérémie Bec, Robin Vallée.

The capture of small suspended particles by a streamlined or bluff body is an important process in many natural systems (wind pollination, collection of phytoplancton by passive suspension-feeding invertebrates, planet formation, growth of raindrops by accretion of cloud droplets, riming of supercooled droplets by ice crystals, scavenging of aerosols during wet deposition). Achieving precise predictions requires, on the one hand, elucidating mesoscopic fluid-dynamical effects that determine whether or not impaction occurs, and on the other hand, specifying the microphysical features and processes that affect the outcome of such collisions and a possible capture by the collector.

In collaboration with Christoph Siewert (Deutscher Wetterdienst, Germany), we have studied the collision efficiency of small particles by a large sphere. We found that the rate at which small inertial particles collide with a moderate-Reynolds-number body is strongly affected when these particles are also settling under the effect of gravity. The sedimentation of small particles indeed changes the critical Stokes number above which collisions occur. We explain this by the presence of a shielding effect caused by the unstable manifolds of a stagnation-saddle point of an effective velocity field perceived by the small particles. We also found that there exists a secondary critical Stokes number above which no collisions occur. This is due to the fact that large-Stokes number particles settle faster, making it more difficult for the larger one to catch them up. Still, in this regime, the flow disturbances create a complicated particle distribution in the wake of the collector, sometimes allowing for collisions from the back. We demonstrated that this effect can lead to collision efficiencies higher than unity at large values of the Froude number. An article on this topic has been submitted to Physical Review Fluids.

5.3 Axis C – Active agents in a fluid flow

5.3.1 Finite Element Methods for simulate displacement of flagellated micro-swimmers

Participants: Laetitia Giraldi, Luca Berti.

In collaboration with Vincent Chabannes (IRMA, Strasbourg) and Christophe Prud'Homme (IRMA, Strasbourg), in [2], we propose a numerical method for the finite element simulation of micro-swimmers displacement with a prescribed stroke. We focus on swimmers composed of several rigid bodies in relative motion. Three distinct formulations are proposed to impose the relative velocities between the rigid bodies. We validate our model on the three-sphere swimmer, for which analytical results are available.

This paper was published in *Comptes Rendus – Mathématiques*.

5.3.2 Reinforcement learning with function approximation for 3-spheres swimmer

Participants: Luca Berti, Zakarya El-khyiati, Laetitia Giraldi.

In collaboration with Christophe Prud'Homme (IRMA, Strasbourg) and Youssef Essoussy (IRMA, Strasbourg), the paper [14] investigates the swimming strategies that maximize the speed of the three-sphere swimmer using reinforcement learning methods. First of all, we ensure that for a simple model with few actions, the Q-learning method converges. However, this latter method does not fit a more complex framework (for instance the presence of boundary) where states or actions have to be continuous to obtain all directions in the swimmer's reachable set. To overcome this issue, we investigate another method from reinforcement learning which uses function approximation, and benchmarks its results in absence of walls.

This work was initiated with the internship of Youssef Essoussy. We have also been supported by UCA Fox 2021 School[1] which allows some participant to see each other.

5.3.3 Necessary conditions for local controllability of a particular class of systems with two scalar controls

Participant: Laetitia Giraldi.

In this paper [17] in collaboration with Pierre Lissy (Ceremade, Paris), Jean-Baptiste Pomet (Inria, McTAO) and Clement Moreau (RIMS, Kyoto, Japan), we consider control-affine systems with two scalar controls, such that one control vector field vanishes at an equilibrium state. We state two necessary conditions for local controllability around this equilibrium, involving the iterated Lie brackets of the system vector fields, with controls that are either bounded, small in L^∞ or small in $W^{1,\infty}$. These results were deduced by the behavior of the magnetic flagellated swimmers and they are illustrated with several examples.

The paper is submitted. It was also a chapter of the PhD thesis of Clement Moreau.

5.3.4 Reinforcement learning for the locomotion and navigation of undulatory micro-swimmers in chaotic flow

Participants: Raphaël Chesneaux, Zakarya El Khyiati, Jérémie Bec, Laetitia Giraldi.

We developed a framework to study the motion of vermiform micro-swimmers, self-propelling by undulating their body. Such deformable swimmers have a high potential because of their aptness to carry out a broad set of swimming strategies and to select the most efficient one according to the biological media where they evolve. Many questions are still open on how these micro-swimmers optimize their displacement, in particular when they are embedded in a complex environment. In practice the swimmers navigate in a fluctuating medium comprising walls and obstacles, a fluid flow possibly with non-Newtonian properties or containing other swimmers. In this framework, optimizing their navigation requires dealing with a strongly nonlinear and chaotic high-dimensional dynamics.

Using machine-learning tools, we have developed new methods to tackle this optimization problem where swimming and navigation are tightly bonded. Techniques borrowed from partially-observable Markov decision processes were found to be particularly promising. Combining an efficient locomotion

[1] The 1st edition of the University Cote d'Azur Fall program on Complex Systems 2021, *Mobility, self-organization and swimming strategies*, 18-29 Oct 2021 Nice and Fréjus (France).

strategy with optimal navigation and path-planning is particularly novel in the field. An article demonstrating the efficiency of genetic reinforcement learning for the displacement of undulatory swimmers in two-dimensional flow is currently in preparation and will be submitted in the coming months to Physical Review Letters.

5.4 Axis D – Mathematics and numerical analysis of stochastic systems

5.4.1 Anomalous fluctuations for the Lyapunov exponents of tracers in developed turbulent flow

Participants: Jérémie Bec, Simon Thalabard.

The infinitesimal separation between tracers transported by a turbulent flow is generally characterized in terms of stretching rates and Lyapunov exponents obtained from the integration of the tangent system to the dynamics. We have shown that turbulent intermittency is responsible for long-range correlations in the Lagrangian fluid velocity gradient. This behavior, which does not question the existence of a law of large numbers and of Lyapunov exponents, seriously questions large-deviation approaches that are usually used to characterize the fluctuations of finite-time stretching rates and thus to quantify small-scale turbulent mixing. We propose alternative manners to qualify fluctuations based on generalizations of the central-limit theorem to sums of correlated variables. These results were obtained in the framework of the ANR TILT project and are the subject of a manuscript that will be soon submitted to Physical Review Letters.

These results suggest to introduce new Lagrangian stochastic models for small-scale turbulent mixing that extend traditional diffusive approach to noises with long-range time correlations. Fractional Brownian motion seems a promising candidate.

5.5 Axis E – Variability and uncertainty in flows and environment

5.5.1 Instantaneous turbulent kinetic energy modeling based on Lagrangian stochastic approach in CFD and application to wind energy

Participants: Mireille Bossy, Kerlyns Martínez Rodríguez.

The need of statistical information on the wind, at a given location and on large time period, is of major importance in many applications such as the structural safety of large construction projects or the economy of a wind farm, whether it concerns an investment project, a wind farm operation or its repowering. The evaluation of the local wind is expressed on different time scales: monthly, annually or over several decades for resource assessment, daily, hourly or even less for dynamical forecasting (these scales being addressed with an increasing panel of methodologies). In the literature, wind forecasting models are generally classified into physical models (numerical weather prediction models), statistical approaches (time-series models, machine learning models, and more recently deep learning methods), and hybrid physical and statistical models. At a given site and height in the atmospheric boundary layer, measuring instruments record time series of characteristics of the wind, such as wind speed characterizing load conditions, wind direction, kinetic energy and possibly power production. Such observations should feed into forecasting, but also uncertainty modeling. In this context, probabilistic or statistical approaches are widely used, helping to characterize uncertainty through quantile indicators.

In this work, we construct an original stochastic model for the instantaneous turbulent kinetic energy at a given point of a flow, and we validate estimator methods on this model with observational data examples. Motivated by the need for wind energy industry of acquiring relevant statistical information of air motion at a local place, we adopt the Lagrangian stochastic description of fluid flows to derive, from the 3D+time equations of the physics, a 0D+time-stochastic model for the time series of the instantaneous turbulent kinetic energy at a given position. First, we derive a family of mean-field dynamics featuring the square norm of the turbulent velocity. By approximating at equilibrium the characteristic nonlinear terms of the dynamics, we recover the so called Cox-Ingersoll-Ross process, which was previously suggested in the literature for modeling wind speed. We then propose a calibration procedure for the parameters employing both direct methods (motivating partially the numerical analysis in [3] by the same authors) and Bayesian inference. In particular, we show the consistency of the estimators and validate the model through the quantification of uncertainty, with respect to the range of values given in the literature for some physical constants of turbulence modeling.

This work [15], in collaboration with Jean-Francois Jabir from National Research University HSE Moscow, is now accepted in Journal of Computational Physics. It was also presented ([12]) during the annual meeting of the European Meteorological Society 2021.

5.5.2 Methodology to quantify uncertainties in droplet dispersion in the air

Participants: Christophe Henry, Kerlyns Martínez Rodríguez, Mireille Bossy, Jérémie Bec.

In this work, we resorted to standard uncertainty quantification (UQ) and sensitivity analysis (SA) tools that are available in the open-source software OpenTurns. The present methodology relies on variance-based methods (such as the "Sobol indices" or "variance-based sensitivity indices") to analyze the variability of the numerical results with respect to a number of input parameters (e.g. droplet size, droplet emission velocity, wind velocity). This methodology has been validated on a demonstration case that consisted in a simulation of droplet dispersion in a quiescent flow without evaporation/condensation models. We are currently working on setting up more realistic simulations of droplet dispersion in the air.

This research is described in a short communication in ERCIM News [5], which was done in collaboration with Hervé Guillard from Team Castor as well as Nicolas Rutard and Angelo Murrone from ONERA. This research has actually been carried out through the Inria's Covid Mission Spreading_Factor project 2020, which aimed at setting up a methodology to help quantify the relative importance between the input physical parameters and their impact on droplet dispersion as well as to quantify uncertainties on the output results. The results were also presented at the French Aerosol Conference in January 2021 [11].

5.5.3 Methodology to quantify uncertainties in dispersed two-phase flows

Participants: Aurore Dupré, Christophe Henry, Mireille Bossy.

A similar methodology has been applied to study dispersed two-phase flows. This methodology has actually been developed within the framework of the VIMMP EU project (Virtual Materials Market Place). The objective is to set up a methodology to analyze the sensitivity and then quantify uncertainty in numerical simulations of multiphase flows to a number of input variables. For that purpose, we focused on the case of a point-source dispersion of particles in a turbulent pipe flow. Numerical simulations were performed by coupling a CFD simulation of the turbulent pipe flow (using standard turbulence models) to a particle-tracking simulation (using a stochastic Lagrangian model). The simulations were performed in Code_Saturne CFD software. The simulation workflow is launched using tools from the Salome platform, which allows to handle the coupling of the fluid phase simulation and the particle-phase simulation. The results obtained are then analyzed using existing tools within OpenTurns. For that purpose, a dataset is obtained by running the workflow with a range of input variables (e.g. the fluid velocity, number of particles injected, size of particles) and accounting for the intrinsic stochasticity of each run. Sensitivity analysis techniques (here the Sobol sensitivity indices) were used to identify the key parameters affecting the observed results.

These results were presented at the OpenTurns User Days held in June 2021 [10]. A paper is also in preparation with other partners involved in the VIMMP project (Pascale Noyret, Eric Fayolle and Jean-Pierre Minier from EDF R&D).

5.5.4 Analyzing the Applicability of Random Forest-Based Models for the Forecast of Run-of-River Hydropower Generation

Analyzing the impact of climate variables into the operational planning processes is essential for the robust implementation of a sustainable power system. The work, published in [9], deals with the modeling of the run-of-river hydropower production based on climate variables on the European scale. A better understanding of future run-of-river generation patterns has important implications for power systems with increasing shares of solar and wind power. Run-of-river plants are less intermittent than solar or wind but also less dispatchable than dams with storage capacity. However, translating time series of climate data (precipitation and air temperature) into time series of run-of-river-based hydropower generation is not an easy task as it is necessary to capture the complex relationship between the availability of water and the generation of electricity. This task is also more complex when performed for a large interconnected area. In [9], in collaboration with Valentina Sessa and Edi Assoumou from CMA Mines ParisTech, and Sofia G Simões from Laboratório Nacional de Energia e Geologia in Portugal, a model is built for several European countries by using machine learning techniques. In particular, we compare the accuracy of models based on the Random Forest algorithm and show that a more accurate model is obtained when a finer spatial resolution of climate data is introduced. We then discuss the practical applicability of a machine learning model for the medium term forecasts and show that some very context specific but influential events are hard to capture.

5.6 Other

5.6.1 Selection of microalgue

Participant: Laetitia Giraldi.

The papers [4, 16], in collaboration with Walid Djema and Olivier Bernard (Inria, Biocore) and Sofya Maslovskaya (Paderborn University, Germany), proposes a strategy to separate two strains of microalgae in minimal time. The control is the dilution rate of the continuous photobioreactor. The microalgae dynamics is described by the Droop's model, taking into account the internal quota storage of the cells. Using Pontryagin's principle, we develop a dilution-based control strategy that leads to the most efficient species separation in minimal time. A numerical optimal synthesis –based on direct optimization methods– is performed throughout the paper, in order to determine the structure of the optimal feedback-control law, which is bang-singular. Our numerical study reveals that singular arcs play a key role in the optimization problem since they allow the optimal solution to be close to an associated static optimal control problem. A resulting turnpike-like behavior, which characterizes the optimal solution, is highlighted throughout this work.

6 Bilateral contracts and grants with industry

6.1 Bilateral grants with industry

AVENTAGE **– Towards a very high resolution wind forecast chain on the sailing basin of Marseilles.**

Participants: Mireille Bossy, Thomas Ponthieu.

AVENTAGE is an industrial partnership project with the two French startups SportRizer and RiskWeatherTech. Starting at the end of 2020, the genesis of this project was motivated by the next Paris 2024 Olympic Games, where the sailing events will take place in the Marseilles sailing basin. The reading of the wind is one of the major stakes in the search for performance for the sailing Olympics. However, the exhaustive knowledge of the wind of a body of water is not yet resolved.

AVENTAGE aims to complete the knowledge database of the different local effects in the Marseilles sailing basin, thus facilitating the exploitation of the water body.

A high resolution wind forecast allows to reduce the margin of error in the decision making. This is a determining factor for progress, accelerating learning and supporting the material and technical development underlying performance. To reach a very high resolution of 50 m horizontally, AVENTAGE relies on two distinct and successive downscaling processes to produce its results.

1. An operational processing chain from large-scale weather forecasts (GFS 50 km) up to 1 km resolution. Each day, the SportRIZER & RiskWeatherTech operational chain downloads the 0h00 GFS forecast data for the 0h00+1h to 0h00+48h time frames and performs a downscaling simulation with the WRF model down to 1 km resolution over the Marseilles area.

2. A specific downscaling from the previous operation. To refine the wind simulation up to a resolution of 50 m, this second step relies on the SDM-WindPoS model.

Preliminary results and case studies, as well as detailed methodologies are available on the SDM-WindPos software webpage.

7 Partnerships and cooperations

7.1 International initiatives

7.1.1 STIC/MATH/CLIMAT AmSud project

Participant: Mireille Bossy.

CALISTO was involved in the MATH-AmSUD project Fantastic, ended in 2021, on *statistical inference and sensitivity analysis for models described by stochastic differential equations.* In particular CALISTO was collaborated with Universidad de Valparaíso on the diffusive limit of system of piecewise deterministic Markov processes under mean field interaction.

7.1.2 Participation in other International Programs

Participant: Jérémie Bec.

The team participates in the CNRS IRL IFCAM (Indo-French Center for Applied Mathematics, see website) that provides support for recurrent collaborations with teams at the Indian Institute of Science and the International Center for Theoretical Science in Bangalore. The pandemic however prevented from planning any visit between the French and Indian teams during the year 2021.

7.2 International research visitors

7.2.1 Visits of international scientists

International visits to the team

- In October 2021, Mara Chiricotto came for a 5-day visit in CALISTO. Mara Chiricotto is a Post-Doctoral fellow at the University of Manchester and has an expertise in Molecular Dynamics simulations. Her visit took place in the framework of the VIMMP project. The specific goal was to assist Mireille Bossy and Christophe Henry in the development of a scientific workflow to quantify uncertainty in nano-particle agglomeration using Molecular Dynamics tools. This work is still in progress.

7.2.2 Visits to international teams

Research stays abroad

Jérémie Bec

Visited institution: Göteborg University

Country: Sweden

Dates: Nov. 28 – Dec. 4, 2021

Context of the visit: Preparation of a review article on statistical models for turbulent aerosols

Mobility program/type of mobility: research stay

7.3 European initiatives

7.3.1 FP7 & H2020 projects

Participants: Aurore Dupré, Mireille Bossy, Christophe Henry.

VIMMP (Virtual Materials Market Place) is a EU H2020 project (started in 2018) in the program Industrial Leadership project in Advanced materials. VIMMP is a four-year development for a software platform and simulation market place on the topic of complex multiscale CFD simulations.

As a VIMMP partner, CALISTO is co-working with EDF R&D at designing complex workflows through the EDF's cross-platform SALOME, involving Lagrangian aggregations, fragmentation with CODE_SATURNE. CALISTO also addresses some typical workflow design for uncertainty quantification, and experiments with them in two-phase flow simulation situation. Precisely, we are designing a workflow case of particle dispersion in a turbulent pipe flow, with a selection of physical and numerical inputs as well as observable output. We have performed some sensitivity analysis (based on the Sobol indices method) and meta-modeling (based on polynomial chaos) to asses some main features in term of workflow run in a simulation platform, identifying also the relative HPC needs, and expert supervision needs. This workflow case also served as demonstration case for the development of a common data model (CDM) led by EDR R&D.

7.4 National initiatives

7.4.1 ANR PACE

Participant: Christophe Henry.

Christophe Henry was the coordinator of the PACE project, a MRSEI project funded by the ANR to help prepare European projects. As for PAIRE, the project aims at creating new international and cross-sector collaborations to foster innovative solutions for particle contamination in the environment. This is achieved by bringing together partners in a consortium to submit a research proposal. Submissions have been made to the European MSCA-RISE-2019 and MSCA-RISE-2020 calls. Members of the consortium are now considering the option to submit a research project MSCA-DN (doctoral network) in 2022.

7.4.2 ANR TILT

Participant: Jérémie Bec.

The ANR PRC project TILT (Time Irreversibility in Lagrangian Turbulence) started on Jan. 1, 2021. It is devoted to the study and modeling of the fine structure of fluid turbulence, as it is observed in experiments and numerical simulations. In particular, recall that the finite amount of dissipation of kinetic energy in turbulent fluid, where viscosity seemingly plays a vanishing role, is one of the main properties of turbulence, known as the dissipative anomaly. This property rests on the singular nature and deep irreversibility of turbulent flows, and is the source of difficulties in applying concepts developed in equilibrium statistical mechanics. The TILT project aims at exploring the influence of irreversibility on the motion of tracers transported by the flow. The consortium consists of 3 groups with complementary numerical and theoretical expertise, in statistical mechanics and fluid turbulence. They are located in Saclay, at CEA (Bérengère Dubrulle), in Lyon, at ENSL (Laurent Chevillard, Alain Pumir), and in Sophia Antipolis (Jérémie Bec). A postdoc will be hired by the team on this contract in fall 2022.

7.4.3 ANR NEMO

Participant: Laetitia Giraldi.

The JCJC project NEMO (controlliNg a magnEtic Micro-swimmer in cOnfined and complex environments) was selected by ANR in 2021, and started on Jan. 1, 2022 for four years. NEMO team's is composed of Laetitia Giraldi, Mickael Binois (Inria, Acumes) and Laurent Monasse (Inria, Coffee).

NEMO aims to develop numerical methods to control a micro-robot swimmer in the arteries of the human body. These robots could deliver drugs specifically to cancer cells before they form new tumors, thus avoiding metastasis and the traditional chemotherapy side effects.

NEMO will focus on micro-robots, called Magnetozoons, composed of a magnetic head and an elastic tail immersed into a laminar fluid possibly non-Newtonian. These robots imitate the propulsion of spermatozoa by propagating a wave along their tail. Their movement is controlled by an external magnetic field that produces a torque on the head of the robot, producing a deformation of the tail. The tail then pushes the surrounding fluid and the robot moves forward. The advantage of such a deformable swimmer is its aptness to carry out a large set of swimming strategies, which could be selected according to the geometry or the rheology of the biological media where the swimmer evolves (blood, eye retina, or other body tissues).

Although the control of a such micro-robots has mostly focused on simple unconfined environment, the main challenge is today to design external magnetic fields that allow them to navigate efficiently in complex realistic environments.

NEMO aims to elaborate efficient controls, which will be designed by tuning the external magnetic field, through a combination of Bayesian optimization and accurate simulations of the swimmer's dynamics with Newtonian or non-Newtonian fluids. Then, the resulting magnetic fields will be validated experimentally in a range of confined environments. In such an intricate situation, where the surrounding fluid is bounded laminar and possibly non-Newtonian, optimization of a strongly nonlinear, and possibly chaotic, high-dimensional dynamical system will lead to new paradigms.

7.5 Regional initiatives

Participant: Laetitia Giraldi.

Laetitia Giraldi was the investigator of a project Reboost-2021, from the Academy of excellence "Complex Systems" of the IDEX Université Côte d'Azur, on "Locomotion and optimal navigation of micro-swimmers in complex environements". The project aimed to support the internships of Zakarya El-Khiyati (Inria, CALISTO) and Raphaël Chesneaux (Inria, CALISTO).

7.6 Others

The CALISTO team members are involved in the GdR (CNRS Research network) Turbulence, in the GdR Mascot-NUM on stochastic methods for the analysis of numerical codes, and in the GdR *Théorie et Climat*.

8 Dissemination

Participants: Jérémie Bec, Mireille Bossy, Laetitia Giraldi, Christophe Henry.

8.1 Promoting scientific activities

8.1.1 Scientific events: organisation

Member of the organizing committees

- Jérémie Bec was member of the organizing committee of the conference "Dynamics Days Europe XL" held in Nice in August 2021 (link here).
- Jérémie Bec and Laetitia Giraldi were members of the organizing committee of the first edition of UCA Fall program on Complex Systems devoted to "Mobility, self-organization and swimming strategies" in October 2021 (link here).
- Mireille Bossy was member of the Committee of the "Prix Pierre Lafitte 2021". She is also member of the Steering Committee of the GdR MascotNum.
- Christophe Henry was the organizer of a workshop on "Microplastics in the atmosphere" in November 2021 (details on the program on CALISTO website).

Scientific seminars of the Team

- Since November 2020, the team is organizing a regular seminar every 4 weeks. In 2021, the following researchers were invited to give a presentation (mostly online due to the sanitary situation): Aurore Dupré (CALISTO), Florence Marcotte (Inria, Castor), Grégory Lécrivain (HZDR, Germany), Jérôme Yon and José Moran (CORIA, Rouen), Agnese Seminara (InPhyNi, Nice), Rudy Valette (CEMEF, Mines ParisTech, Sophia Antipolis), Mickael Binois (Inria, Acumes), Areski Cousin (IRMA, Strasbourg and external collaborator in CALISTO), Christophe Brouzet (InPhyNi, UCA, Nice), Angelica Bianco (LaMP, UCA, Clermont), Simon Thalabard (InPhyNi, UCA, Nice).

8.1.2 Scientific events: selection

Member of the conference program committees

- Jérémie Bec was member of the scientific committee of the conference "Fluids & Complexity" held in Nice in November 2021 (link here).

8.1.3 Journal

Member of the editorial boards

- Jérémie Bec acted as a guest editor for a special issue of the Philosophical Transactions of the Royal Society A entitled "Scaling the turbulence edifice" and gathering 25 contributions.

Reviewer - reviewing activities

- Jérémie Bec acted as a reviewer for International Journal of Multiphase flow, Journal of Fluid Mechanics, Journal of Mathematical Physics, Physical Review Fluids.
- Mireille Bossy reviewed project propositions form the generic ANR AAP 2021 and from ANRT. She also acted in 2021 as a reviewer for the following international journals: Annals of Applied Probability, Journal of Computational and Applied Mathematics, IMA Journal of Numerical Analysis, Stochastics and Partial Differential Equations: Analysis and Computations, and Stochastics.
- Laetitia Giraldi reviewed several papers as for instance for Physical Review Fluids, Journal of Fluids Mechanics, IEEE Transactions on Automatic Control.
- Christophe Henry reviewed papers for the following journals in 2021: Talanta (February 2021), Aerosol and Air Quality Research (May 2021), Atmospheric Pollution Research (May 2021) Journal of Aerosol Science (November 2021).

8.1.4 Invited talks

- Mireille Bossy was invited to give a presentation at the *33ème séminaire CEA/GAMNI de mécanique des fluides numérique*, January 25-26,2021. She also gave a plenary talk at the 13th International Conference on Monte Carlo Methods and Applications (MCM 2021, from 16.8 to 20.8.2021). She was an invited speaker at the Conference of Numerical Probability (in honor of Gilles Pagès' 60th birthday) 26-28 May 2021 Paris (France).
- Christophe Henry was invited to give presentations at the OpenTurns User Days (June 2021) and at Helmholtz Zentrum Dresden Rossendorf (in October 2021).
- Laetitia Giraldi was invited to give a presentation at SMAI Congres (June 2021) near Montpellier.

8.1.5 Leadership within the scientific community

- Jérémie Bec is in charge of the Academy of excellence "Complex Systems" of the IDEX Université Côte d'Azur (Decision-making role for funding; Coordination and animation of federative actions; Participation in the IDEX evaluation).
- Mireille Bossy is Chairing of the Scientific Council of the Academy of excellence "Complex Systems" of the IDEX Université Côte d'Azur.

8.1.6 Scientific expertise

- Jérémie Bec was a member of the selection committee for a Professor position in Physics at Université Côte d'Azur.
- Mireille Bossy was the Chair of the selection committee for CRCN and ISFP position at Inria Bordeaux Sud Ouest.

8.1.7 Research administration

- Jérémie Bec is a member of Inria's Comité NICE and of the scientific council of the CNRS GDR "Theoretical challenges for climate sciences".
- Laetitia Giraldi is a member of Inria's Comité NICE, Comité de Suivi Doctoral et du Comité du centre.

8.2 Teaching - Supervision - Juries

8.2.1 Teaching

- Fluid dynamics and turbulence (Jérémie Bec, 6h, Doctoral courses, Mines Paris).
- The physics of turbulent flow (Jérémie Bec, 4h, 2nd-year courses, Mines Paris).
- “Research Trimester” project supervision (Jérémie Bec and Laetitia Giraldi, research project of 2 months followed by 2nd-year students of Mines Paris).
- Microswimming (Laetitia Giraldi, 6h, course, Master 2 cell physics, Université de Strasbourg).
- Khôlle en classes préparatoire MPSI, MP* (Laetitia Giraldi, 2h par semaine scolaire par niveau, Centre International de Valbonne).
- Advanced modeling (Christophe Henry, 50h, Master of Hydrology, Polytech Nice Sophia Université Côte d’Azur).

8.2.2 Supervision

- PhD in progress: Lorenzo Campana, “Stochastic modeling of non-spherical particles in turbulence”; Defense is announced for March 29, 2022; supervised by Mireille Bossy.
- PhD in progress: Zakarya El Khiyati, “Reinforcement learning for the optimal locomotion of micro-swimmers in a complex chaotic environment” started in October 2021; supervised by Jérémie Bec and Laetitia Giraldi.
- PhD in progress: Fabiola Gerosa, “Turbulent fluid-particles coupling and applications to planet formation” started in October 2021; supervised by Jérémie Bec and Héloïse Méheut (Lagrange, Observatoire de la Côte d’Azur).
- PhD defended in March 4, 2021: Sofia Allende Contador, “Dynamics and statistics of elongated and flexible particles in turbulent flows”; supervised by Jérémie Bec.
- PhD defended in March 30, 2021: Robin Vallée, “Suspensions of inertial particles in turbulent flows”; supervised by Jérémie Bec.
- PhD defended in December 13, 2021: Luca Berti, “Mathematical modeling and simulation of magnetic micro-Swimmers”; co-supervised by Laetitia Giraldi and Christophe Prud’Homme (IRMA, Strasbourg).
- M2 Internship: Thomas Ponthieu, “Very high resolution numerical wind simulation. Assessment of the SDM-WindPoS model for use in sports sailing”; March to September 2021; supervised by Mireille Bossy.
- M2 Internship: Zakarya El Khiyati, “Smart strategies for the collective motion of deformable micro-swimmers”, April 2021 to September 2021, supervised by Jérémie Bec and Laetitia Giraldi.
- M2 Internship: Youssef Essoussy (IRMA, Strasbourg),“The locomotion optimization for micro-swimmers using machine learning”, April 2021 to September 2021, supervised by Luca Berti, Laetitia Giraldi and Christophe Prud’Homme (IRMA, Strasbourg).
- M1 Internship: Raphael Chesneaux, “Steering undulatory microswimmers in a moving fluid through machine learning”, December 2020 to February 2021 and June 2021 to August 2021, supervised by Jérémie Bec and Laetitia Giraldi.

8.2.3 Juries

- Jérémie Bec was referee for the Habilitation thesis of Gautier Verhille, *Deformable Objects in Turbulence*, at IRPHE, Aix-Marseille University, June 2021.
- Mireille Bossy served as a referee for the Ph.D. thesis of Arthur Macherey, *Approximation and model reduction for partial differential equations with probabilistic interpretation*, at École Centrale Nante, June 2021.
- Jérémie Bec was examiner for the Ph.D. theses of Pierre Azam (Université Côte d'Azur, September 2021) and Luca Berti (Université de Strasbourg, December 2021).
- Mireille Bossy served as an examiner for the Ph.D. theses of Sofia Allende Contador at Université Côte d'Azur, March 2021, and Camille Choma at Université Le Havre Normandie, July 2021.
- Laetitia Giraldi served as an examiner for the Ph.D. thesis of Maxime Etiévant at Université de Besançon, July 2021.

8.3 Popularization

8.3.1 Interventions

- Christophe Henry was involved in the following popularization events:
  - Café In at Inria Sophia Antipolis Méditerranée in May 2021 (to present the results of Inria's Mission Covid Spreading Factors);
  - Interview of his research activities at Interstice (link here).

9 Scientific production

9.1 Publications of the year

International journals

[1] A. Banari, C. Henry, R. H. Fank Eidt, P. Lorenz, K. Zimmer, U. Hampel and G. Lecrivain. 'Evidence of collision-induced resuspension of microscopic particles from a monolayer deposit'. In: *Physical Review Fluids* 6.8 (Aug. 2021). DOI: 10.1103/PhysRevFluids.6.L082301. URL: https://hal.inria.fr/hal-03467963.

[2] L. Berti, V. Chabannes, L. Giraldi and C. Prud'Homme. 'Modeling and finite element simulation of multi-sphere swimmers'. In: *Comptes Rendus. Mathématique* 359.9 (3rd Nov. 2021), pp. 1119–1127. DOI: 10.5802/crmath.234. URL: https://hal.archives-ouvertes.fr/hal-03023318.

[3] M. Bossy, J. F. Jabir and K. Martínez Rodríguez. 'On the weak convergence rate of an exponential Euler scheme for SDEs governed by coefficients with superlinear growth'. In: *Bernoulli* 27.1 (2021), pp. 312–347. DOI: 10.3150/20-BEJ1241. URL: https://hal.inria.fr/hal-02282168.

[4] W. Djema, L. Giraldi, S. Maslovskaya and O. Bernard. 'Turnpike features in optimal selection of species represented by quota models'. In: *Automatica* (2021). URL: https://hal.archives-ouvertes.fr/hal-03217983.

[5] C. Henry, K. Martinez-Rodriguez, M. Bossy, H. Guillard, N. Rutard and A. MURRONE. 'Social Distancing: The Sensitivity of Numerical Simulations'. In: *ERCIM News*. Special theme: Pandemic Modelling and Simulation 2021.124 (2021). URL: https://hal.inria.fr/hal-03041624.

[6] K. Martínez Rodríguez, M. Bossy and C. Henry. 'Particle agglomeration in flows: fast data-driven spatial decomposition algorithm for CFD simulations'. In: *International Journal of Multiphase Flow* (13th Jan. 2022). URL: https://hal.inria.fr/hal-03180740.

[7] K. Martínez Rodríguez, M. Bossy, R. Maftei, S. Shekarforush and C. Henry. 'New spatial decomposition method for accurate, mesh-independent agglomeration predictions in particle-laden flows'. In: *Applied Mathematical Modelling* 90 (2021), pp. 582–614. DOI: 10.1016/j.apm.2020.08.064. URL: https://hal.inria.fr/hal-02497721.

[8] J. Morán, C. Henry, A. Poux and J. Yon. 'Impact of the maturation process on soot particle aggregation kinetics and morphology'. In: *Carbon* 182 (Sept. 2021), pp. 837–846. DOI: 10.1016/j.carbon.2021.06.085. URL: https://hal-normandie-univ.archives-ouvertes.fr/hal-03281409.

[9] V. Sessa, E. Assoumou, M. Bossy and S. Simões. 'Analyzing the Applicability of Random Forest-Based Models for the Forecast of Run-of-River Hydropower Generation'. In: *Clean Technologies* 3.4 (Dec. 2021), pp. 858–880. DOI: 10.3390/cleantechnol3040050. URL: https://hal.inria.fr/hal-03499725.

Conferences without proceedings

[10] C. Henry, A. Dupré and M. Bossy. 'Sensitivity analysis and uncertainty in CFD simulations of multiphase flow'. In: OpenTurns User day 14 (2021). Paris, France, 21st June 2021. URL: https://hal.inria.fr/hal-03469388.

[11] C. Henry, K. Martinez-Rodriguez, A. MURRONE, N. Rutard, H. Guillard and M. Bossy. 'Sensitivity of droplet dispersion to emission and ambient air properties'. In: CFA2021 - 34ème Congrès Français sur les Aérosols. Paris, France, 26th Jan. 2021. URL: https://hal.inria.fr/hal-03469351.

[12] K. Martínez Rodríguez, M. Bossy and J.-F. Jabir. 'Local turbulent kinetic energy modelling based on Lagrangian stochastic approach in CFD and application to wind energy'. In: EMS Annual Meeting. Virtual format, Germany, 3rd Sept. 2021. DOI: 10.5194/ems2021-399. URL: https://hal.inria.fr/hal-03352876.

[13] J. Morán, C. Henry, A. Poux and J. Yon. 'Impact of the maturation process on soot particle aggregation kinetics and morphology'. In: Cambridge Particle MMeeting. Virtual Conference, United Kingdom, 25th June 2021. DOI: 10.1016/j.carbon.2021.06.085. URL: https://hal-normandie-univ.archives-ouvertes.fr/hal-03351018.

Reports & preprints

[14] L. Berti, Z. El Khiyati, Y. Essousy, C. Prud'Homme and L. Giraldi. *Reinforcement learning with function approximation for 3-spheres swimmer*. 21st Jan. 2022. URL: https://hal.inria.fr/hal-03538754.

[15] M. Bossy, J.-F. Jabir and K. M. Rodriguez. *Instantaneous turbulent kinetic energy modelling based on Lagrangian stochastic approach in CFD and application to wind energy*. 12th Jan. 2021. URL: https://hal.inria.fr/hal-03108031.

[16] W. Djema, L. Giraldi, S. Maslovskaya and O. Bernard. *Turnpike Features in Optimal Selection of Species Represented by Quota Models: Extended Proofs*. RR-9399. Inria - Sophia Antipolis, 8th June 2021, p. 29. URL: https://hal.archives-ouvertes.fr/hal-03253160.

[17] L. Giraldi, P. Lissy, C. Moreau and J.-B. Pomet. *Necessary conditions for local controllability of a particular class of systems with two scalar controls*. 19th Aug. 2021. URL: https://hal.archives-ouvertes.fr/hal-02178973.

Other scientific publications

[18] J. Morán, C. Henry, A. Poux and J. Yon. 'Impact of the maturation process on soot particle aggregation kinetics and morphology'. In: European Aerosol Conference. online presentation, United Kingdom, 30th Aug. 2021. URL: https://hal-normandie-univ.archives-ouvertes.fr/hal-03351023.

9.2 Cited publications

[19] F. Alouges, A. DeSimone, L. Giraldi and M. Zoppello. 'Self-propulsion of slender micro-swimmers by curvature control: N-link swimmers'. In: *International Journal of Non-Linear Mechanics* 56 (2013), pp. 132–141.

[20] S. Balachandar and J. K. Eaton. 'Turbulent Dispersed Multiphase Flow'. In: *Annual Review of Fluid Mechanics* 42.1 (2010), pp. 111–133.

[21] P. Bauer, A. Thorpe and G. Brunet. 'The quiet revolution of numerical weather prediction'. In: *Nature* 525.7567 (2015), pp. 47–55.

[22] E. C. /. E. P. S. Centre. *10 Trends Reshaping Climate and Energy*. 2018.

[23] L. Dubus, S. Muralidharan and A. Troccoli. 'What Does the Energy Industry Require from Meteorology?' In: *Weather & Climate Services for the Energy Industry*. Ed. by A. Troccoli. Cham: Springer International Publishing, 2018, pp. 41–63.

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[25] K. Gustavsson and B. Mehlig. 'Statistical models for spatial patterns of heavy particles in turbulence'. In: *Advances in Physics* 65.1 (2016), pp. 1–57.

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[27] P. Kershaw and C. Rochman. 'Sources, fate and effects of microplastics in the marine environment: part 2 of a global assessment'. In: *Reports and studies-IMO/FAO/Unesco-IOC/WMO/IAEA/UN/UNEP Joint Group of Experts on the Scientific Aspects of Marine Environmental Protection (GESAMP) eng no. 93* (2015).

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[30] A. Montanari. 'What do we mean by 'uncertainty'? The need for a consistent wording about uncertainty assessment in hydrology'. In: *Hydrological Processes: An International Journal* 21.6 (2007), pp. 841–845.

[31] A. Niayifar and F. Porté-Agel. 'Analytical Modeling of Wind Farms: A New Approach for Power Prediction'. In: *Energies* 9.9, 741 (2016).

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[34] A. Pumir and M. Wilkinson. 'Collisional Aggregation Due to Turbulence'. In: *Annual Review of Condensed Matter Physics* 7.1 (2016), pp. 141–170.

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[37] J. Sørensen. 'Aerodynamic Aspects of Wind Energy Conversion'. In: *Annual Review of Fluid Mechanics* 43.1 (2011), pp. 427–448.

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