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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 variery 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, ect.;
- 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 modelling for the dynamics of material/fluid particle dynamics with interaction.

3 Research program

CALISTO will structure 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 modelling 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 need 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).

Particular attention are now bringing on the following direction improving stand-alone Lagrangian numerical model in the ABL such as additiona buoyancy model, canopy models. Further the coupling of fluid particle modelling with phase particle models is a of crutial 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 later on 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 contribute improving deposition law and resuspension law for multilayered deposits in turbulent flows. Starting from Lagrangian stochastic models, developing meta-modelling, taylored from experimental measurements and force-balance Lagrangian model devoted to this problem. 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 *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 entrapment of micro-swimmers near boundaries, as the presence of a boundary breaks the symmetry both of the fluid (leading to strong anisotropy) and 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 calles swimmers, can interact each others 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 approximative to more realistic but complex.

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 swimmer that is 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 fondamental 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 to 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, opinion formation, robotics and even 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 theorietical 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.

Meta modelisation 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 developpers, 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 thought metamodelisation, such as Gaussian process regression model, proved to be efficient for solving optimisation 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 [23];
- 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 [26];

- suspension of real micro-swimmers [18] such as sperm cell, bacteria, and in environmental issues with animal flocks attracted intrinsic biological interest[28];
- accretion of dusts is responsible for the formation of planetesimals in astrophysics [27].

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 [19]. 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, 24]. 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 [22]. Wind, solar, marine/rivers energies are of growing importance, and the demand for forecasts goes hand in hand with it [21, 32]. Numerous methods exist for different forecast horizons [20]. 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 Highlights of the year

Starting in November 2020, CALISTO is created as a joint Project-Team between Inria and CNRS, Cemef, throught the Computing and Fluids (CFL) research group at Cemef CNRS/MINES ParisTech.

6 New software and platforms

The scientific objectives of the team strongly rely on the ability of CALISTO to develop numerical tools and contribute to established or dedicated computational platforms and software. To this purpose, CFD software are in use and futher develop, for modeling development, bench-marking and cross-validation, as well as several open-source Direct Numerical Simulations codes that have to be adapted to CALISTO purpose.

6.1 New software

6.1.1 SDM

SDM is a in-house software of the team. Its development was initiated by the team from a fruitful collaboration with LMD. The very first developments started in 2010, in collaboration with Lemon Team. Inria Chile brought some support in 2012, while we were developing the software module dedicated to wind energy (SDM-WINDPOS), and later with the support of MERIC, we worked on an ocean version (SDM-OCEAPOS).

SDM is now a modulated software composed with SDM_KERNEL based on the numerical solver, SDM-WINDPOS and SDM-OCEAPOS which are dedicated to power wind/hydro farm simulation and SDM-MODELER that allows to specialized SDM-WINDPOS input on real wind computation situation (extraction of IGN maps for the topography definition, extraction of WRF output for the coarse wind prediction to refine, and visualisation). Started in 2019, a 12 man-month *Action Mutuelle de Développement Technologique* is on going on the SDM-MODELER interface.

6.1.2 Channelflow

Channelflow is a spectral code for the Direct Numerical Simulations of incompressible fluids in a channel geometry. It is an open-source software, written in C++ and parallelized. Channelflow 2.0 is developed by the Emergent Complexity in Physical Systems Laboratory (ECPS) at the Swiss Federal Institute of Technology Lausanne (EPFL). The project Channelflow 2.0 is based on the serial Channelflow-1.5 software developed by John. F. Gibson, University of New Hampshire (UNH). The CALISTO team recently contributed to new developments by adding a Lagrangian module to track the motion of inertial particles and flexible fibers in such turbulent channel flows.

6.1.3 LaTu

The numerical software LaTu is an MPI/C++ pseudo-spectral code for the Direct Numerical Simulations of the incompressible Navier–Stokes equations in triply-periodic domains. It is developed under the technical and scientific responsibility of Holger Homann (Laboratoire Lagrange) and contains several Lagrangian modules for the simulation of Lagrangian objects, such as tracers, inertial or finite-size particles. The CALISTO team has recently implemented in LaTu the dynamics of non-spherical particles with inertia to perform state-of-the-art simulations in homogeneous isotropic turbulence that serve as benchmark for the development of macroscopic models.

7 New results

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

7.1.1 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.

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 was obtained by Jeffery[25]. But so far this description has been always investigated in the framework of direct numerical simulations (DNS) and experimental measurements.

In this work, we consider a Lagrangian stochastic model to describe the orientation dynamics of non-spherical particle $\boldsymbol{p}(t)$ which can be coupled with a mean gradient flow velocity $\langle\nabla \boldsymbol{u}\rangle$ solved by a CDF solver with turbulence modelling. In particular, this stochastic Lagrangian orientation model can be easily coupled with classical Lagrangian stochastic transport equation already established [29]. More precisely, the size of the particle is assumed smaller than the Kolmogorov length scale but sufficiently large that its Brownian motion need not be considered. As a result, the local flow around a particle can be considered as inertia-free and Stokes flow solutions can be used to relate particle rotational dynamics to the local velocity gradient. The orientation of ellipsoidal particles can be described as the normalised solution of the linear ordinary differential equation for the separation vector between two fluid tracers, under the action of the velocity gradient tensor.

We develop a numerical scheme for this model that enables to compute the orientation dynamic of ellipsoidal particles for the scale of time-step in use in CFD code. Our method uses the well-known splitting scheme algorithm decoupling the orientation dynamics into their main contributions: stretching and rotation. We analyse the weak and strong convergence both of the global scheme and of their sub-parts. Subsequently, the splitting technique yields a highly efficient hybrid solver coupling a probabilistic and deterministic algorithm. Numerical experiment was implemented to test the scheme for a physical application. Two related publications are in preparation.

This work is a part of the POPART project (see also Section 8.1).

7.1.2 Fiber fragmentation in homogeneous isotropic turbulence

Participants Jérémie Bec, Christophe Henry, Sofia Allende.

We studied the fragmentation of small, inextensible, flexible fibers without inertia, transported by a developed isotropic homogeneous turbulent flow. When these small fibers are fully stretched, they can break through tensile failure, that is, when the tension becomes greater than the internal cohesive forces. Conversely, when they undergo strong compression and buckle, these fibers deform, bend and can then break by flexural failure. In this case, fragmentation occurs when the local curvature exceeds a given threshold.

We performed direct numerical simulations of fluid flow and fiber dynamics to obtain statistics on these two fragmentation processes. Assuming an idealized description of internal fragmentation processes, we have shown that fragmentation rates can be expressed using the probability distribution of turbulent shear rates. Using classical functional approximations for these distributions, we proposed estimates of the tensile and flexural failure rates that we calibrated and validated using numerical simulations. Our analysis emphasizes the central role played by the dimensionless flexibility of fibers in understanding the frequency of fragmentation.

In addition to the fragmentation rates, we obtained results on the size distributions that result from fragmentation. Tensile failure always occurs when the fiber is stretched by the flow and is therefore in a fully straight configuration. The tension is then maximum in its center, so that this type of rupture always produces two fragments of equal size. The situation is more complex in the case of a fracture by bending. Fragmentation occurs when the fiber develops a buckling instability and the resulting break-up process produces several fragments whose sizes depend on the most unstable buckling mode. By performing a linear stability analysis, we obtained estimates of this size distribution as a function of the instantaneous fluid strains. This approach indicates that the number of fragments produced during fracture becomes greater when the fibers are subject to more violent compressions, suggesting the creation of smaller and smaller fragments as the Reynolds number increases. This work, published in [2], provides all the ingredients necessary for the kinetic treatment of the evolution of a fiber population and their fragmentation.

7.1.3 Caustics and large deviations in the dynamics of inertial particles

Participants Jérémie Bec.

The impurities (dust, droplets, organic matter) transported by a flow have a dynamics which cannot be reduced to that of tracers. In particular, they form fractal concentrations, even when the flow is incompressible. Such particles have a finite size and a density different from the fluid which transports them. The description of their movement must therefore take into account their inertia, hence their name of inertial particles.

The fractal nature of the spatial concentrations of inertial particles is quantified by a dimension spectrum that describes how they fill the configuration space. These dimensions are determined by the large deviations of the finite-time Lyapunov exponents (FTLE) i.e, growth rates of infinitesimal volumes defined by very close particle trajectories. The distribution of FTLEs determines the statistical properties of the dynamical fractal attractor to which the particle trajectories converge.

The dynamics of inertial particles take place in the position-velocity phase space and to describe spatial concentrations, volumes must be projected onto the configuration space. In collaboration with Jan Meibohm, Kristian Gustavsson, and Bernhard Mehlig, we studied in [9] how this projection affects the distribution of FTLE. The essential difficulty that we have encountered occurs when the inertial dynamics of phase space generate folds. In that case, the spatial projection is no longer unambiguous, causing the projection of infinitesimal neighborhoods of particles to single points in configuration space. These singular points are catastrophes of the "cusp" (or folds) type, also called "caustics" because of their similarities with random focusing of light in geometric optics. For smooth phase-space manifolds, catastrophes are well listed and lead to finite-time singularities in the spatial density of particles, suggesting that caustics can increase spatial aggregation. We have extended such considerations to the case of non-smooth, fractal manifolds.

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

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

Participants Mireille Bossy, Christophe Henry, Kerlyns Martínez Rodríguez.

This work is mainly motivated by refining the accuracy of the computations of particle agglomeration using population balance equation (PBE)-like algorithms. Indeed, in CFD context, recent developments on numerical simulations of particle agglomeration in complex and turbulent flows increasingly resort to Euler-Lagrange approaches. These methods are coupled with PBE-like algorithms to compute agglomeration inside each cell of the Eulerian mesh. One of the key issues with such approaches is related to the spatially-uniform condition, i.e. agglomeration should be computed on a set of particles that are uniformly distributed locally in each cell. Yet, CFD simulations in realistic industrial/environmental cases often involve non-homogeneous concentrations of particles (due to local injection or accumulation in specific regions). We show that more accurate and mesh-independent predictions of particle agglomeration are made possible by the application of a new data-driven spatial decomposition (D2SD) algorithm. This D2SD algorithm allows the splitting of a domain containing point particles into elementary cells, each cell containing a spatially-uniform distribution of particles. For that purpose, the algorithm relies on the use of statistical information for the spatial distribution of particles and then extracts an optimal spatial decomposition. After evaluating the convergence and accuracy of the algorithm on homogeneous and inhomogeneous cases, this optimal spatial decomposition is applied to study the case of particle agglomeration.

This study is detailled in [8] in collaboration with Radu Maftei and Seyedafshin Shekarforush. This research has also been presented at the French Aerosol Conference in January 2020. Fast versions of the D2SD algorithms have been proposed and validated and will be further discussed in a coming publication.

7.3 Axis C – Active agents in a fluid flow

7.3.1 Micro-swimmers in turbulent flows

Participants Jérémie Bec.

When a micro-swimmer swims toward a target in turbulent fluid, they are shaken by the flow and eventually trapped in eddies. Naively, one might think that it suffices for the swimmer to continuously point his movement towards the target. Can we, however, develop an optimal travel strategy that can reduce the average time required to reach the target? This difficult question, which is of great importance from both fundamental and application point of view, can be tackled using machine learning methods. In collaboration with Jaya Kumar A., A. Verma and R. Pandit from IISc Bangalore, we have shown in [1] that an intelligent swimming strategy using Q-contradictory learning can outperform naïve micro-swimmers.

We have developed a contradictory reinforcement learning scheme for micro-swimmers in statistically homogeneous and isotropic turbulent flows, both in two and three dimensions. We have shown that this scheme allows micro-swimmers to find non-trivial paths allowing them to reach a target in less time than a naive micro-swimmer who constantly tries to swim in the direction of the target. The swimmers' dynamics is rather simple: in addition to advection, they swim with a constant speed in a direction whose orientation is altered by the local vorticity of the flow. Using our contradictory learning scheme, we have shown that in a substantial part of the parameter space, the average time required for micro-swimmers to reach their target is below the average time taken for the following micro-swimmers naive strategy.

7.3.2 Optimal actuation for magnetic micro-swimmers

Participants Laetitia Giraldi.

In collaboration with Yacine El Alaoui-Faris (MCTAO), Jean-Baptiste Pomet (MCTAO), Stéphane Régnier (Sorbonne Université, Paris), in [5], we present an automated procedure for the design of optimal actuation for flagellar magnetic microswimmers based on numerical optimization. Using this method, a new magnetic actuation method is provided which allows these devices to swim significantly faster compared to the usual sinusoidal actuation. This leads to a novel swimming strategy which makes the swimmer perform a 3D trajectory. This shows that a faster propulsion is obtained when the swimmer is allowed to go out-of-plane. This approach is experimentally validated on a scaled-up flexible swimmer.

In this IFAC paper [12], we present a simplified model of a flagellar magnetic micro-swimmer based on shape discretization and the simplification of the hydrodynamical interactions. We numerically solve the optimal control problem of finding the actuating magnetic fields that maximize its horizontal propulsion speed over a fixed time. Depending on the chosen constraints on the control, the optimal trajectories of the swimmer can be planar or three-dimensional. Simulations show the periodicity of the optimal magnetic fields and the shape of the swimmer under optimal actuation. All the simulated magnetic fields outperform the standard sinusoidal actuation method that is prevalent in the literature and in experiments. Moreover, the non-planar actuation patterns leads to novel trajectories for flagellar low-Reynolds swimmers and perform significantly better than planar actuation.

These two results were the core of work of the phD Thesis of Yacine El-Alaoui Faris co-supervised by Laetitia Giraldi.

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

Participants Laetitia Giraldi, Luca Berti.

In collaboration with Vincent Chabannes and Christophe Prud'Homme (IRMA), in [15], we propose a numerical method for the finite element simulation of micro-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.

7.4 Axis D – Mathematics and numerical analysis of stochastic systems

7.4.1 Variational formulations for inviscid fluids and generalized flows

Participants Jérémie Bec.

In collaboration with Simon Thalabard (IMPA, Rio de Janeiro), we studied in [11] the principle of generalized least action and the associated concept of generalized flow introduced by Yann Brenier (*J. Am. Math. Soc.* 1989). This principle extends to a probabilistic framework Arnold's geometric interpretation of ideal fluid mechanics, in which the regular (strong) solutions of the incompressible Euler equations are obtained by minimizing an action on the set of differentiable Lagrangian maps preserving the volumes. While Arnold's framework is based on the deterministic concept of Lagrangian flow, Brenier's principle of least action describes the solutions of Euler's equations in terms of generalized non-deterministic flows, namely probability measures on sets of Lagrangian trajectories.

We proposed a statistical-mechanics interpretation of generalized flows by assimilating them to suitably defined random permutation flows. We solved the principle of least action numerically by a Monte-Carlo method and analyzed the statistics of the obtained generalized flows. We focused on two dimensions of space by considering situations of increasing complexity, ranging from solid rotation and cellular flows, to decaying 2D turbulence.

7.4.2 Butterfly effect and spontaneous stochasticity of singular shear layers

Participants Jérémie Bec.

The butterfly effect is now commonly identified with the extreme sensitivity of deterministic chaotic systems to their initial conditions. However, this is only one facet of the notion of unpredictability introduced by Lorenz. He had in fact predicted that multiscale fluid flows could spontaneously lose their deterministic nature and become intrinsically random. This effect, radically different from chaos, has long remained beyond the reach of physical observations.

In collaboration with Alexei Mailybaev and Simon Thalabard (IMPA, Rio de Janeiro), we revisited this question in [10] for the case of the elementary Kelvin–Helmholtz hydrodynamic instability. We have shown that a spontaneous loss of determinism inherently takes place in initially singular shear layers, making this type of dynamics much less predictable than any chaotic system. We further obtained evidence that the macroscopic flow resulting from this instability exhibits universal statistical properties that are triggered by, but independent of, specific physical properties at microscopic scales. This spontaneous stochasticity is interpreted as an Eulerian counterpart of Richardson's relative dispersion of Lagrangian particles, giving substance to the intrinsic nature of turbulent randomness.

7.5 Axis E – Variability and uncertainty in flows and environment

7.5.1 Instantaneous turbulent kinetic energy modelling 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 modelling. 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 modelling wind speed. We then propose a calibration procedure for the parameters employing both direct methods 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 modelling.

This work, in collaboration with Jean Francois Jabir from National Research University HSE Moscow, is now submitted [16].

7.5.2 Methodology to quantify uncertainties in droplet dispersion in the air

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

The outbreak of COVID-19 has triggered a number of numerical studies to better understand the fate and transport of respiratory droplets in the air due to their potential role in the spreading of a virus. This research aims at developing a methodology to evaluate the variability in numerical simulations of airborne dispersion.

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 analyse 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 work was part of the Inria's Covid Mission project Spreading_Factor (see also Section 8.1). This research is described in a short communication [7], which was done in collaboration with Hervé Guillard from Team Castor as well as Nicolas Rutard and Angelo Murrone from ONERA. The results were also presented at the French Aerosol Conference in January 2021.

7.5.3 Modeling the climate dependency of the run-of-river based hydro power generation using machine learning techniques: an application to French, Portuguese and Spanish cases

A big challenge of sustainable power systems is to integrate climate variability into the operational and long term planning processes. In [17], in collaboration with Valentina Sessa and Edi Assoumou from CMA Mines ParisTech, we focus on the run-of-river based hydro power generation. In particular , we deal with the modeling of this form of power production based on weather variables.

Translating time series of meteorological data (precipitations, snowfall and air temperature) into time series of run-of-river based hydro power 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. Indeed, this kind of hydro power generation is limited by the flow of the river in which the power plants are located. Moreover, the water flow is a nonlinear function of the weather variables and the physical characteristics of the river basins. Finally, the impact of the weather variables on the runoff may occur with a certain delay, whose determination depends on physically based phenomena (e.g., melting snow-local temperature). This work aims at formalizing an efficient technique for the prediction of the run-of-river based hydro power generation. Several well-established regression algorithms based on machine learning are used and compared in terms of correlation coefficient, adjusted coefficient of determination, mean absolute and mean square percentage errors.

We consider three case studies: France, Portugal and Spain. Results indicate that the models based on ensemble of trees and neural networks exhibit the best performance for evaluating both the short term and the long term hydro power generation.

7.6 Other

7.6.1 The role of periodic deformation strategies for locomotion

Participants Laetitia Giraldi.

A periodical cycle of body's deformation is a common strategy for locomotion (see for instance birds, fishes, humans). The aim of the paper [6] in collaboration with Frédéric Jean (ENSTA ParisTech), is to establish that the auto-propulsion of deformable object is optimally achieved using periodic strategies of body's deformations. This property is proved for a simple model using optimal control theory framework.

7.6.2 Selection of microalgue

Participants Laetitia Giraldi.

The paper [4], in collaboration with Walid Djema and Olivier Bernard from Team BIOCORE, 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.

8 Bilateral contracts and grants with industry

8.1 Bilateral grants with industry

Participants Sofia Allende-Contador, Lorenzo Campana, Jérémie Bec, Mireille Bossy, Christophe Henry.

POPART. POPART is an industrial partnership project jointly funded by the IDEX Université Côte d'Azur and EDF.

The aim of POPART is to improve deposition models in turbulent flows and to extend them to the case of particles of any shape, even deformable. Despite recent theoretical and numerical advances, there are still very strong challenges related to a good representation of the dynamics of complex objects in turbulent flows. We address the case of elongated particles, such as fibers, polymers and certain types of algae, generally present in water catchment areas.

We develop both microscopic and macroscopic models for the dynamics of small, flexible, inextensible fibers in a turbulent flow.

This year, the developed 3D macroscopic model for ellipsodis (see also in Section 7.1.1) was implemented within the Lagrangian particle-tracking module of the open-source CFD software CODE_SATURNE developed and exploited by EDF R&D.

Microscopic simulations obtained with Direct Numerical Simulation (DNS) were performed with the computation of the orientation of such fibers in wall-bounded turbulent flows. First comparisons were obtained and reported in [13].

9 Partnerships and cooperations

9.1 International initiatives

9.1.1 Participation in international programs

CALISTO is involved in the MATH-AmSUD project Fantastic on "statistical inference and sensitivity analysis for models described by stochastic differential equations", and in particular collaborates with Universidad de Valparaíso on the diffusive limit of system of piecewise seterministic Markov processes under mean field interaction.

9.2 European initiatives

9.2.1 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, Inria 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. Inria 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 performing some sensitivity analysis (based and Sobol indices) 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. A publication on these approach/experimentation will be soon available.

9.3 National initiatives

9.3.1 ANR PACE

Christophe Henry is 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 already been made to the European MSCA-RISE-2019 and MSCA-RISE-2020 calls.

9.3.2 Inria's Covid Mission

In 2020, Christophe Henry has been the coordinator of the Inria's Covid Mission Spreading_Factor project. This project aims at setting up a methodology to help quantifying the relative importance between the input physical parameters and their impact on droplet dispersion as well as to quantify uncertainties on the output results. It involved several researchers from Team CALISTO (including M. Bossy, J. Bec, K. Martinez-Rodriguez) as well as from other teams (H. Guillard from Team CASTOR and C. Grandmont from Team COMMEDIA) and external partners from ONERA (N. Rutard and A. Murrone). This work led to the establishment of a methodology to analyze the sensitivity of numerical results. This methodology has been tested on a simple demonstration case. A short communication was recently published in ERCIM News [7].

9.3.3 ANR TILT

The PRC project TILT (Time Irreversibility in Lagrangian Turbulence) was selected by ANR in 2020. This project 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 the 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 (B. Dubrulle), in Lyon, at ENSL (L. Chevillard, A. Pumir), and in Sophia Antipolis (J. Bec).

9.4 Regional initiatives

As a complement of ANR PACE, Christophe Henry is the coordinator of the PAIRE project, a TREMPLIN-COMPLEX project funded by University of Côte d'Azur. The project aims at creating new international and cross-sector collaborations to foster innovative solutions for particle contamination in the environment.

Christophe Henry has also been involved as a partner in the PLAISE project, a 12-month project funded by CNRS through the specific call on 'Plastics and Microplastics in marine systems'. The project is focussed on the plastisphere and the impact of colonisation/ageing of microplastics on their sedimentation. It has been coordinated by Maria-Luiza Pedrotti from the Observatory of Oceanography of Villefranche sur Mer (LOV). This led to the development of a simple model for the sedimentation of non-spherical particles in a quiescent fluid. Numerical simulations were performed using the properties measured by partners at LOV (size, mass). Numerical results were shown to accurately reproduce the sedimentation rate observed in laboratory measurements performed at the LOV.

9.5 Others

The Calisto team members are involved in the GdR (CNRS Research network) Turbulence and in the GdR Mascot-NUM on stochastic methods for the analysis of numerical codes.

10 Dissemination

10.1 Promoting scientific activities

10.1.1 Scientific events: selection

Chair of conference program committees Mireille Bossy was chair of the Stochastic Numerics“ session at the Bernoulli-IMS One World Symposium, in August 2020.

Member of the conference program committees Jérémie Bec was a member of the selection commitee of the "Prix de thèse" organized by the Institut des Systèmes Complexes de Paris-Ile de France.

Mireille Bossy was member of the Committee of the "Prix Pierre Lafitte 2020".

Reviewer - reviewing activities Christophe Henry was invited to review two papers in Journal of Aerosol Science and one paper in Chemical Engineering Science in 2020.

Jérémie Bec is a regular reviewer (around 15 reports per year) for *Physical Review, Journal of Fluid Mechanics, International Journal of Multiphase Flow, Journal of Statistical Physics, Journal of Mathematical Physics,...*

Laetitia Giraldi is a regular reviewer (around 5 reports per year) for *Physical Review, Journal of Fluid Mechanics, IEEE Transaction and automated control, ESAIM: COCV* . Laetitia Giraldi was also reviewer of a research project for DFG (Germany).

10.1.2 Invited talks

Mireille Bossy has been invited to give talks at the One World Virtual Seminar Series: Stochastic Numerics and Inverse Problems in October and at the 33ème séminaire CEA/GAMNI de mécanique des fluides numérique.

Laetitia Giraldi has been invited to give talks at the online workshop "Understanding locomotion: Nature-inspired mathematical models" on December 11th, 2020.

10.1.3 Scientific expertise

- Mireille Bossy evaluated a research project submitted to the ANRT and Région Ile-de-France, was member of the hiring committee 26 PR at Université Paris 7 and at Grenoble INP-ENSIMAG/LJK.

- Jérémie Bec was a member of the hiring committee 26/25 MCF at Université Côte d'Azur (LJAD).

- Laetitia Giraldi was a member of the hiring committee 26/25 MCF at Université de Strasbourg. She is also a member of Inria's Comité NICE, Comité de Suivi Doctoral et du Comité du centre.

10.1.4 Research administration

- Jérémie Bec is in charge of the Academy of excellence "Complex Systems" of the IDEX Université Côte d'Azur. He is also a member of Inria's Comité NICE.
- Laetitia Giraldi is a member of Inria's Comité NICE, Comité de Suivi Doctoral et du Comité du centre.

10.2 Teaching - Supervision - Juries

10.2.1 Teaching

- Statistical physics of neural networks (J. Bec, 10h, M2 mathematical engineering, Université Côte d'Azur).
- Predictive tools for complex systems (J. Bec, 6h, Mastère spécialisé HPC-AI, Mines ParisTech).
- Fluid dynamics and turbulence (J. Bec, 4h, Doctoral courses, Mines ParisTech).
- Microswimming (L. Giraldi, 6h, course, Master 2 cell physics, Université de Strasbourg).
- Khôlle en classes préparatoire MPSI, MP* (L. Giraldi, 2h par semaine scolaire par niveau, Centre International de Valbonne).

10.2.2 Supervision

- PhD in progress: Lorenzo Campana, "Stochastic modeling of non-spherical particles transport and deposition by turbulent flows"; started December 2017; supervised by M. Bossy.
- PhD in progress: Sofia Allende Contador, "Dynamics and statistics of elongated and flexible particles in turbulent flows"; started October 2017; supervised by J. Bec.
- PhD in progress: Robin Vallée, "Suspensions of inertial particles in turbulent flows"; started October 2016; supervised by J. Bec.
- PhD : Clément Moreau, "Controllability in finite and infinite dimension and applications to life-inspired nonlinear systems"; started September 2017 ended June 2020; co-supervised by L. Giraldi, P. Lissy and J.-B. Pomet.
- PhD : Yacine El-Alaoui Faris, "Modeling and Optimal Control of Magnetic Micro-Swimmers"; started October 2017 ended December 2020; co-supervised by L. Giraldi, J.-B. Pomet and S. Régnier.
- PhD in progress: Luca Berti, "Mathematical modeling and simulation of magnetic micro-Swimmers"; started October 2018; co-supervised by L. Giraldi and C. Prud'Homme.
- Summer Internship: Sara Capucine Guglielmi, "Boundary and near-wall conditions for the collision between a spheroidal particle and a planar surface"; July & August 2020; supervised by M. Bossy and C. Henry.
- M2 Internship: Gilles Lingam (Observatoire d), "Planetesimal formation: coupling between the gas"; April–September 2020; supervised by J. Bec and H. Meheut (Lagrange, OCA).

10.2.3 Juries

- M. Bossy served as a referee for the HDR of Miguel Martinez, *A contribution to the study and simulation of skew diffusions*, at Université Gustave Eiffel, September 2020.
- M. Bossy served as an examiner for the Ph.D. theses of Sofiane Martel at Université Paris-Est December 2019, Fabio Coppini, Université de Paris, October 2020, and Oumaima Bencheikh at Université Paris-Est, October 2020.
- J. Bec served as a referee for the Ph.D. thesis of Florian Le Roy de Bonneville, INP Toulouse, September 2020, and of Amélie Gay, Aix-Marseille Université, October 2020.

10.2.4 Articles and contents

Laetitia Giraldi was interviewed for Avenir Côte d'Azur and Destimed in January 2020 following the SATT Sud-ESt prize that she was awarded at the end of 2019.

11 Scientific production

11.1 Publications of the year

International journals

[1] J. K. Alageshan, A. K. Verma, J. Bec and R. Pandit. 'Machine learning strategies for path-planning microswimmers in turbulent flows'. In: *Physical Review E* (2020). DOI: 10.1103/PhysRevE.101.043110. URL: https://hal.archives-ouvertes.fr/hal-02362934.

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Conferences without proceedings

[12] Y. El Alaoui-Faris, J.-B. Pomet, S. Régnier and L. Giraldi. 'Comparison of optimal actuation patterns for flagellar magnetic micro-swimmers'. In: IFAC 2020 - 21st IFAC World Congress. Berlin / Virtual, Germany: https://www.ifac2020.org/, 12th July 2020. URL: https://hal.archives-ouvertes.fr/hal-02507327.

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[13] J. Bec, M. Bossy, C. Henry, L. Campana and S. Allende. *Projet POPART :Modélisation du transport et du dépôt de particules non-sphériques par des écoulements turbulentsLivrable n°4*. UCA, Inria; UCA CNRS, 1st Nov. 2020. URL: https://hal.inria.fr/hal-03161688.

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