RESEARCH CENTRE

Inria Centre at Université Côte d'Azur

IN PARTNERSHIP WITH:

CNRS

2023
ACTIVITY REPORT

Project-Team

CALISTO

Stochastic Approaches for Complex Flows and Environment

IN COLLABORATION WITH: Centre de Mise en Forme des Matériaux (CEMEF)

DOMAIN

Applied Mathematics, Computation and Simulation

THEME

Stochastic approaches

Contents

Project-Team CALISTO

Creation of the Project-Team: 2020 November 01

Keywords

Computer sciences and digital sciences

A6.1. – Methods in mathematical modeling

A6.1.1. – Continuous Modeling (PDE, ODE)

A6.1.2. – Stochastic Modeling

A6.2. – Scientific computing, Numerical Analysis & Optimization

A6.2.1. – Numerical analysis of PDE and ODE

A6.2.2. – Numerical probability

A6.2.3. – Probabilistic methods

A6.2.4. – Statistical methods

A6.2.7. – High performance computing

A6.3. – Computation-data interaction

A6.3.5. – Uncertainty Quantification

A6.4.1. – Deterministic control

A6.5. – Mathematical modeling for physical sciences

A6.5.2. – Fluid mechanics

Other research topics and application domains

B3.2. – Climate and meteorology

B3.3.2. – Water: sea & ocean, lake & river

B3.3.4. – Atmosphere

B4.3.2. – Hydro-energy

B4.3.3. – Wind energy

B9.5.2. – Mathematics

B9.5.3. – Physics

1 Team members, visitors, external collaborators

Research Scientists

- Mireille Bossy [Team leader, INRIA, Senior Researcher, HDR]
- Jérémie Bec [CNRS, Senior Researcher, HDR]
- Laetitia Giraldi [INRIA, Researcher]
- Christophe Henry [INRIA, ISFP, HDR]

Post-Doctoral Fellow

- Ciro Sobrinho Campolina Martins [CNRS, Post-Doctoral Fellow, from Feb 2023]

PhD Students

- Zakarya El Khiyati [UNIV COTE D'AZUR]
- Fabiola Gerosa [Université Côte d'Azur, Observatoire de la Côte d'Azur, CNRS, Laboratoire Lagrange]
- Paul Maurer [INRIA]
- Lucas Palazzolo [INRIA, from Oct 2023]
- Nicolas Valade [INRIA]

Interns and Apprentices

- Hao Liu [INRIA, Intern, from May 2023 until Aug 2023, from Technology University Darmstad]
- Lucas Palazzolo [INRIA, Intern, from Mar 2023 until Sep 2023, from Université de Strasbourg]
- Antoine Serres [INRIA, Intern, from Apr 2023 until Jul 2023, from ENS Paris Saclay]

Administrative Assistant

- Sandrine Boute [INRIA]

Visiting Scientists

- Chiara Calascibetta [UNIV ROME III, from Nov 2023, PhD visit]
- Kerlyns Martinez Rodriguez [Universidad de Valparaíso, until Mar 2023]
- Hector Olivero-Quinteros [Universidad de Valparaíso, from Jul 2023 until Jul 2023]

External Collaborators

- Christophe Brouzet [CNRS]
- Nadia Maïzi [ENSMP]
- Antoine Serres [SORBONNE UNIVERSITE, from Jul 2023]
- Eric Simonnet [CNRS]
- Simon Thalabard [UNIV COTE D'AZUR, from Sep 2023]

2 Overall objectives

Particles transported by turbulent flows 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. Such potential complexity is at play in numerous industrial processes involving circulating fluids that contain inclusions (bubbles, droplets, debris, micro-swimmers or other kinds of materials). Active particles, seen as artificial micro-swimmers can be used as vehicles for the transport of therapeutics or as tools for limited invasive surgery. Driving such micro-swimmers requires monitoring the evolution of their characteristics, and their effects on the fluid with a high level of accuracy. On the other hand, sustainable power systems require to integrate climate and meteorological variability into operational processes, as well as into medium/long term planning processes. Moreover, turbulence amplifies the variability of wind/water flows and makes it even more complex to simulate the flow around wind/hydro farms.

These challenges represent critical technological locks. To address them, industrial design increasingly relies on macroscopic numerical models, broadly known as "Computational Fluid Dynamics" (CFD). However, such large-scale approaches are only well deployed on crude particle descriptions (monodisperse sizes, spherical shapes, rigid bodies), with oversimplified small-scale physics. They often rely on statistical closures for single-time, single-particle probability distributions. Yet, these mean-field simplifications do not accurately reproduce complex features of the involved physics, which require more advanced approaches to reproduce higher-order correlations.

Through a unique synergy between team members originating from various disciplines, CALISTO aims at developing/extending state-of-the-art models to these complex situations and thus improve their applicability, fidelity, and performance. Our ambition is to meet the following goals:

- 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), climate and meteorological prediction, and 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, control and optimize the displacement of micro-swimmers in fluids of various natures, ranging from water to non-Newtonian mucus;
- 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 interactions.

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 research axis focuses on complex particles transported by turbulent flows. In practical applications suspended particles often have inertia (such as droplets in clouds or dust in gaseous circumstellar disks), might be non-spherical (like cellulose fibers in paper industry or soot and sand aerosols) and even deformable in some cases (as organic matter in rivers or phytoplankton in the oceans). This brings out a number of questions about the small-scale physical phenomena at play in the turbulent dynamics of such particles, such as their local concentration fluctuations, their relative motion, the effect of spatial and temporal correlations, their aggregation and fragmentation, and how they affect large-scale evolutions (such as mean densities, average rotation, size distributions).

Despite strong interlinks, microscopic phenomena and macroscopic models are most of the time addressed separately in current studies of complex particles in turbulence. From a microscopic viewpoint, fine-scale investigations can rely on particle-resolved direct numerical simulations (PR-DNS) [47], allowing one to track detailed particle-flow couplings (such as fluid-structure interactions). Yet, such approaches quickly become very expensive and point-particle approximations (PP-DNS) are much better adapted to study many-particle systems and particles smaller than the Kolmogorov dissipative scale. From a macroscopic viewpoint, models rely on reduced descriptions of the turbulent flow and particle dynamics. They are implemented either in Euler-Euler frameworks (like two-fluid models [26]) or in hybrid Euler-Lagrange approaches.

The project-team CALISTO has a unique positioning since it combines the expertise of its members across various levels of description (including PP-DNS and hybrid Euler-Lagrange methods) and cross-disciplinary points of view (physicists, mathematicians and engineers). This synergy gives the means to tackle both aspects at once and validate models.

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 direction aims to develop Lagrangian macroscopic models for the simulation of turbulent flows in single-phase and particle-laden conditions.

In many practical applications, suspended particles are indeed moving close to surfaces (like sand / dust / pollen in the atmospheric boundary layer) or even on surfaces (like sediments and gravels in rivers). It is therefore both a great need and a challenge to take into account both the flow and the particles dynamics near boundaries.

The additional difficulties that arise are two-fold: first, the highly anisotropic flow near boundaries induces a much more rich and complex dynamics of particles; second, the physico-chemical interactions between particles and surfaces result in intricate phenomena like resuspension (where particles get detached from the surface and re-entrained by the flow).

As for AXIS A, such phenomena are usually addressed either with a microscopic or a macroscopic viewpoint. This axis further draws from the unique cross-disciplinary skills of each member to tackle this highly multidisciplinary issue (comprising small-scale dynamics, turbulence, chemical engineering and statistical modeling). An additional objective is to come up with a new stochastic Lagrange-Lagrange approach for large-scale simulations, where both the fluid and the particles are described in a coherent and consistent way (by tracking the motion of individual elements thanks to stochastic equations for their dynamics).

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 particle methods have more flexible numerical convergence constraints, allowing a freer choice of time step size relative to the grid in space, in contrast to the limits imposed (as the Courant-Friedrichs-Lewy condition) on the convergence of many explicit time-marching numerical methods. This makes SDM advantageous in terms of computational cost when finer spatial resolutions are required.

Special emphasis is given to enhancing stand-alone Lagrangian numerical models within the Atmospheric Boundary Layer (ABL), including additional buoyancy models and canopy models. Furthermore, the coupling of fluid particle modeling with phase particle models opens up new modeling tools for some of some of the applications we are considering.

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

Simulations of two-phase flows require the coupling of solvers for the fluid and particle phases. Numerical Weather Prediction (NWP) software usually rely on an 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

This research axis deals with the study of self-propelled particles, which have the ability to convert internal or ambient free energy into dynamical motion. Such active agents can be microorganisms, such as bacteria or plankton, as well as artificial devices used for micro-manufacturing, toxic waste disposal, targeted drug delivery or localized medical diagnostics. Many questions remain open on how to control the displacement of these micro-swimmers, in particular for complex flows comprising inhomogeneities, fluctuations, obstacles, walls, or having a non-Newtonian rheology. There is also a need to study the impact of additional stochastic effects in driving a swarm of such micro-swimmers.

Studying and optimizing the displacement of these swimmers is generally done in two successive steps. The first is to find a *locomotion strategy* by choosing the composition, shape, and deformation for an efficient swimming. The second is to define a *navigation strategy* aimed at minimizing the energy needed to reach a target in a given environment. CALISTO's interdisciplinary expertise encompasses optimal control of viscous flows, small-scale fluid-structure interactions, statistical modeling and large-scale turbulent transport. This is a unique opportunity to address locomotion and navigation simultaneously.

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 bodies). 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.

Reinforcement learning

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. In this context, the use of methods borrowed from artificial intelligence has been mainly used for navigation problems in which locomotion mechanisms are oversimplified. Based on recent smart-swimming approach developed in CALISTO, [22] [27], we plan to extend this work to more realistic cases, including for instance other control parameters for the swimmers, the presence of boundaries, of a feedback of the swimmers on the fluid flow, or interactions between swimmers.

3.4 AXIS D- Mathematics and numerical analysis of stochastic systems

Stochastic analysis, and related numerical analysis, together with improved statistical descriptions of highly-nonlinear dynamics are central topics in CALISTO. This research axis encompasses activities aiming, either (a) at strengthening our understanding on the origin and nature of fluctuations that are inherent to turbulent flows, or (b) at providing a coherent framework in response to the various mathematical challenges raised by the development of novel models in other research axes. Addressing these two fundamental aspects concomitantly to more practical and applied objectives is again a hallmark of the team.

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.

Stochastic dynamics : analysis and numerics

Interacting Stochastic Systems and nonlinear SDEs. CALISTO explores 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, our goal is to identify and analyze conditions conducive to the emergence of collective behaviors, including but not limited to collective motions, synchronization, and organization, whether or not involving the concept of leaders.

An 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.

(Numerical) analysis for complex SDEs. This topic stands as a long-term commitment for Calisto. We draw and motivate our objects of study directly from observations and analyses of physical phenomena developed within the team. This approach adds significant value in terms of originality and has the potential for a substantial impact on the addressed problem.

In tandem with modeling activities across all other axes, there is a continuous need to enhance our mathematical toolbox and expertise in dealing with nonlinear Stochastic Differential Equations (SDEs) driven by complex noises, particularly non-Markovian ones. Our objective is to analyze the solutions, explore their asymptotic behavior, and delve into approximation techniques, with a particular emphasis on numerical methods.

3.5 AXIS E- Variability and uncertainty in flows and environment

Uncertainty analysis has evolved as a crucial research topic, especially in predictive systems grappling with an ever-expanding array of parameters.

This analysis effort is particularly pronounced in Computational Fluid Dynamics (CFD), especially in the context of particle-laden turbulent flows. The significance of addressing uncertainty amplifies in environmental applications, prominently in climate-related studies. Our position on these subjects is based on the stochastic modeling of the variability of the phenomena under study.

Integrating uncertainty analysis with solution formulations that already incorporate a statistical approach offers substantial flexibility, both in modeling the sources of uncertainty and in the numerical implementation. Although still in the early stages of development within the team, this line of research enables us to enhance our expertise in essential tools for evaluating our models.

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 assess 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.

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 [31];
- pollution corresponds to the presence of particulate matter in the air. Due to their impact on human health [40], the dispersion of fine particulate matter is of primary concern: PM1, PM2.5 and PM10 (particles smaller than 1, 2.5 or 10 μm) and Ultra Fine Particles (UFP, smaller than 0.1 μm) 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 [46];
- plastic contamination in oceans impacts marine habitats and human health [34];
- suspension of real micro-swimmers [23] such as sperm cell, bacteria, and in environmental issues with animal flocks attracted intrinsic biological interest[36];
- accretion of dusts is responsible for the formation of planetesimals in astrophysics [35].

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 [24]. 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 [48] while concentration fluctuations and clustering depend on relative particle dispersion [42, 32]. Estimates of collision and aggregation rates should also be fed by two-particle dynamics [41], while wall deposition is highly affected by local flow structures [43]. 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 [30]. Wind, solar, marine/rivers energies are of growing importance, and the demand for forecasts goes hand in hand with it [29, 39]. Numerous methods exist for different forecast horizons [25]. 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 [44] [38], the question of how to enrich and refine wind simulations (from meteorological forecast, or from larger scale information, possibly 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 [45]. The term uncertainty here refers to the overall error of the output of a generic model [37]. 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

5.1 HDR

On March 28^{th} 2023, Christophe Henry defended his Habilitation à Diriger des Recherches (HDR) in front of a jury composed of: Eric Climent (IMFT, Toulouse), Rodney Fox (Iowa State University), Elizabeth Guazzelli (Université Paris Diderot), Sergio Chibbaro (Université Paris Saclay), Hervé Guillard (Inria Center of Université Côte d'Azur), Nicolas Mordant (Université Grenoble Alpes) and Aurore Naso (Centrale Lyon). He was awarded his HDR from the Doctorate School on Fundamental and Applied Science (ED-SFA), within Université Côte d'Azur [11].

6 New software, platforms, open data

6.1 New software

6.1.1 CDM-Sci

Name: Common Data Model for Scientific Workflows

Keywords: Databases, Multiphysics modelling

Scientific Description: CDM-Sci provides a unique framework to facilitate coupling/chaining of physical models, which operate at different scales or at different levels of description ranging from molecular dynamics to fluid mechanics, to build multi-physics and multi-scale computational workflows that can be automatically executed. Hence, CDM-Sci is composed of two key ingredients:

1) A common data model for scientific computing: CDM-Sci offers a solution that collects information in a standardized method in the form a query tree designed to identify the physical and numerical models needed in a given situation. This means that each situation to be simulated is first decomposed into a set of physical components, which are defined as either discrete or continuum systems (quantum systems are not addressed in the present version). Then, a physical description is detailed for each component to fully characterize its nature as well as the physical processes at play. This can lead to introducing a number of sub-components which play a specific physical role. Once the physics at stake (variables, laws, evolution equations) is clarified, a numerical description is chosen either in terms of a set of interacting particles or continuous fields for every component or sub-component. By resorting to this combined physical and numerical points of view, the proposed solution offers naturally a way to specify the various numerical softwares needed to simulate the systems of interest. In addition, regardless of whether the workflow requires a single software or to couple several ones, the information exchanged between components, or sub-components, is clearly identified thanks to specific queries. Finally, when the workflow combines several softwares, similar queries allow to identify the information exchanged between them (inputs/outputs identification), as well as the transformations required (mappers) and the format of the data to be exchanged (wrappers).

2) Computational sciences tools for automatic code generation and execution In order to facilitate coding of new models and execution of calculation workflows coupling different models (like discrete and continuum models), new tools for automatic code generation are developed and validated. For that purpose, CDM-Sci relies on a Model Driven Architecture (MDA) development approach, which is based on the assumption that codes can be produced from abstract, human-elaborated modelling diagrams. It allows to generate standardized data to describe models, such as XSD (XML Schema Definition).

Targeted audience: CDM-Sci is of great interest for physics-oriented users as well as computer scientists.

- From the perspective of physics-oriented users, CDM-Sci allows engineers and scientists to go beyond the simulation set-ups they are familiar with by offering them the possibility to explore new multi-scale physics by linking/coupling with models developed in nearby areas.
- From a computer science perspective, CDM-Sci can help experts to understand the needs of engineers/scientists, so that they can adapt existing computational techniques or orient new developments to make them accessible and relevant to engineers/scientists. In short, CDM-Sci bridges the gap between physics-oriented users and computer scientists.

Functional Description: CDM-Sci stands for "Common Data Model for Scientific Simulation Workflows". As a data model, CDM-Sci is a tool that organizes elements of data and standardizes how they relate to one another and to the properties of real-world entities. As applied to scientific simulations, CDM-Sci is specifically designed to organize elements of data corresponding to the physical and numerical information required to set-up scientific simulations. CDM-Sci has been developed to address multi-physics and multi-scale problems (e.g. multiphase flows involving fluid mechanics, surface sciences, material sciences and/or chemistry). CDM-Sci allows naturally such multi-scale models to be mapped into computational workflows, which link/chain scientific softwares operating at different scales. These computational workflows can then be executed on a set of computational resources following an automatic procedure. In short, CDM-Sci provides a common standardized structure (Common Data Model) for the set-up and execution of scientific simulation workflows.

Release Contributions: CDM-Sci has been developed first conceptually (through a documentation in the form of a list, which gives the structure of the query tree). Second, an operational version of this query tree has been implemented in an Eficas catalog. It currently contains all the information to set-up simulations of multiphase flows and, to a lesser extent, some Molecular Dynamics simulation. Since the structure is generic and open, extra information can be added to account for other physical phenomena (e.g. material science, chemistry, electro-magnetism, quantum effects).

URL: https://gitlab.inria.fr/cdm/cdm-sci

Contact: Christophe Henry

Participants: Christophe Henry, Mireille Bossy

Partner: Edf

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: 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 were obtained by Jeffery [33]. 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, in collaboration with Lorenzo Campana former PhD of the team, 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 a 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. A large part of our activity dealt with the dynamics of ellipsoidal particles in turbulent flows, with the main motivation of improving models used in applications. Actually, the translational and rotational dynamics of such non-spherical particles is directly related to their orientation, which has to be properly calculated. Micro- and macroscopic viewpoints were addressed simultaneously.

More precisely, we have introduced a *stochastic Lagrangian model* for the angular dynamics of inertialess spheroids. The model consists of superimposing a short-correlated random component to the large-scale average fluid-velocity gradient. This Lagrangian stochastic approach is implemented in a practical 3D macroscopic model for turbulent transport (currently available in the open-source CFD software CODE_SATURNE) and is published in Computers & Fluids [4].

7.1.2 Approximating the van der Waals interaction potentials between agglomerates of nanoparticles

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 acting at various scales have to be considered: this includes the transport across large distances and short-range attractive forces. The adhesion between complex fractal-like agglomerates is currently still poorly understood due to the complex role of the aggregate morphology.

This study focuses on evaluating the adhesion forces between raspberry-like and fractal-like agglomerates of nanoparticles. For that purpose, we consider only the van der Waals (vdW) interactions, since they are probably one of the most important interaction potentials or forces between nanoparticles and interfaces found in many applications of powder technology (like filtration, impaction, coagulation, agglomerates restructuring, and resuspension). We have developed both analytical and semi-analytical models to predict the agglomerate-molecule and agglomerate-agglomerate vdW interactions. These new models can find multiple applications in practical situations.

This work is the result of a collaboration with José Moran (who did his PhD in Coria, later Post-doc in Carleton University and University of Minnesota), Jérôme Yon (from Coria) and Reza Kholgy (Carleton University), which started in 2021 and has been pursued in 2023. It is published in Advanced Powder Technology in 2023 [9].

7.1.3 Review article on the dynamics of discrete particles in turbulent flows

Participant: Christophe Henry.

The purpose of this work is to review the wide range of situations where small discrete elements, either bubbles, droplets or solid particles, are embedded in turbulent flows. Occurring often at a human scale and in our daily environments, these turbulent dispersed two-phase flows display complex behavior due to the interplay of two fundamental interactions, the fluid-particle and particle-particle interactions, compounded by the turbulence of the carrier flow. This is not a domain where the basic laws are unknown but where the huge number of degrees of freedom involved call for reduced, or coarse-grained, statistical descriptions to be developed. Since we are considering transport and collision phenomena or relaxation processes, it would seem that they can be handled by kinetic theory. In the general case of non-fully resolved turbulent flows, we are however dealing with particles influenced by random media with non-zero time and space correlations. The second aspect of this work is to recognize the limitations of kinetic-based descriptions and to address the challenges driving us to extend the classical framework, for fluid-particle as well as particle-particle interactions. Taking the standpoint provided by the modern formulation of stochastic processes and focusing on the description of the particle phase, this review proposes a step-by-step pedagogical presentation of current models while pointing out new directions and remaining uncharted territories. This is done to provide answers to the question ‘why?’ as much as ‘how?’ and to try to kindle interest into these open and fascinating issues.

This work is a collaboration with Jean-Pierre Minier (EDF R&D, MFEE, Chatou, France). It has been submitted to Review of Modern Physics in 2023 [16].

7.1.4 Clusters of heavy particles in two-dimensional Keplerian turbulence

Participant: Jérémie Bec.

Protoplanetary disks are gaseous systems in Keplerian rotation around young stars, known to be turbulent. They include a small fraction of dust from which planets form. In the incremental scenario for planet growth, the formation of kilometer-size objects (planetesimals) from pebbles is a major open question. Clustering of particles is necessary for solids to undergo a local gravitational collapse. To address this question, we have studied in this work the dynamics of inertial particles in turbulent flows with Keplerian rotation and shear. Two-dimensional direct numerical simulations have been performed to explore systematically two physical parameters: the rotation rate, which depends on the distance to the star, and the particle response time, which relates to their size. Shear was found to drastically affect the characteristics of the turbulent flow destroying cyclones and favoring the survival of anticyclones. Faster Keplerian rotation enhances clustering of particles. For intermediate sizes, particles concentrate in anticyclones. These clusters form in a hierarchical manner and merge together with time. For other parameter values, solids concentrate on fractal sets that get more singular with rotation. The mass distribution of particles was then found to be multifractal with small dimensions at large orders, intriguing for triggering their gravitational collapse. Such results are promising for a precise description and better understanding of planetesimal formation.

This work is a collaboration with Héloïse Méheut (Laboratoire Lagrange, Observatoire de la Côte d’Azur), and Fabiola Gerosa (Laboratoire Lagrange, Observatoire de la Côte d’Azur), PhD student co-advised by J. Bec and H. Méheut. It has been published in the European Physical Journal Plus in 2023 [6].

7.1.5 Velocity and acceleration statistics of heavy spheroidal particles in turbulence

Participant: Jérémie Bec.

Non-spherical particles transported by turbulent flow have a rich dynamics that combines their translational and rotational motions. In this work, the focus was on small, heavy, inertial particles with a spheroidal shape fully prescribed by their aspect ratio. Such particles undergo an anisotropic, orientation-dependent viscous drag with the carrier fluid flow whose associated torque is given by the Jeffery equations. Direct numerical simulations of homogeneous, isotropic turbulence have been performed to study systematically how the translational motion of such spheroidal particles depends on their shape and size. Surprisingly, it was found that the Lagrangian statistics of both velocity and acceleration can be thoroughly described in terms of an effective Stokes number obtained as an isotropic average over angles of the particle’s orientation. Corrections to the translational motion of particles due to their non-sphericity and rotation can hence be fully recast as an effective radius obtained from such a mean.

This work is a collaboration with Sofía Allende (Earth and Climate Research, Earth and Life Institute, Université catholique de Louvain, Belgium). It has been published in the Journal of Fluid Mechanics in 2023 [1].

7.1.6 Review article on statistical models for the dynamics of heavy particles in turbulence

Participant: Jérémie Bec.

When very small particles are suspended in a fluid in motion, they tend to follow the flow. How such tracer particles are mixed, transported, and dispersed by turbulent flow has been successfully described by statistical models. Heavy particles, with mass densities larger than that of the carrying fluid, can detach from the flow. This results in preferential sampling, small-scale fractal clustering, and large collision velocities. To describe these effects of particle inertia, it is necessary to consider both particle positions and velocities in phase space. In recent years, statistical phase-space models have significantly contributed to our understanding of inertial-particle dynamics in turbulence. These models help to identify the key mechanisms and non-dimensional parameters governing the particle dynamics, and have made qualitative, and in some cases quantitative predictions. This article reviews statistical phase-space models for the dynamics of small, yet heavy, spherical particles in turbulence. We evaluate their effectiveness by comparing their predictions with results from numerical simulations and laboratory experiments, and summarize their successes and failures.

This review was written in collaboration with Kristian Gustavsson and Bernhard Mehlig from the University of Gothenburg (Sweden). It will soon appear in the Annual Review of Fluid Mechanics [3].

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

7.2.1 Influence of engineered roughness microstructures on adhesion and turbulent resuspension of microparticles

Participants: Mireille Bossy, Christophe Henry.

From microplastics resuspending into the atmosphere to earth particles left behind during extraterrestrial explorations, the resuspension of microparticles by a turbulent gas flow occurs in many natural, environmental and industrial systems. Wall surfaces, onto which particles initially adhere, are rarely smooth and this surface roughness affects particle resuspension. Available experimental data on particle resuspension have been obtained with substrates, whose surfaces are either unaltered or manually abraded with, for instance, sand blasting. However, the precise role of surface roughness is poorly understood due to the chaotic nature of surface roughness.

This study explores the role of surface roughness using engineered rough surfaces. For that purpose, we rely on surface functionalization, a modern technique allowing the precise fabrication of a wall surface with well-characterized microstructures, hence reducing the asperity randomness associated with conventional abrasion techniques. We present here a new set of reference data, characterizing various functionalized surfaces as well as adhesion force measurements with microparticles and observations of particle resuspension (when particles deposited on these surfaces are exposed to a gas flow). The presented results will primarily contribute to the improvement of resuspension models, which until now rely on a simplified representation of the surface roughness elements.

This is a collaborative work with researchers from the Technical University of Dresden in Germany (especially Grégory Lécrivain and Uwe Hampel) as well as their colleagues from the Helmholtz Center in Friburg. These results are published in Journal of Aerosol Science [2].

7.2.2 Robust algorithms for particle trajectories in complex 3D unstructured meshes

Participants: Christophe Henry.

This work proposes a new algorithm to compute more efficiently and accurately the trajectories of particles in the context of stochastic Lagrangian approaches. The challenges are two-fold: first, the algorithm should remain tractable in complex 3D unstructured meshes; second, given the stochastic nature of the models, a key aspect is to derive estimations of the residence times that do not anticipate the future of the Wiener process. For that purpose, we propose a time-step-robust cell-to-cell integration of particle trajectories, where the main idea is to dynamically update the mean fields used in the time integration by splitting, for each particle, the time step into sub-steps such that each of these sub-steps corresponds to particle cell residence times. This reduces the spatial discretization error. In line with the constraints imposed by stochastic models, the new algorithm relies on a virtual particle, attached to each stochastic one, whose mean conditional behavior provides free-of-statistical-bias predictions of residence times. This new algorithm has been validated on two representative test cases: particle dispersion in a statistically uniform flow and particle dynamics in a non-uniform flow.

This is a collaborative work with researchers from EDF R&D (Martin Ferrand, Guilhem Balvet, Jean-Pierre Minier) and CEREA (Yelva Roustan). The results are published in Monte-Carlo Methods and Applications [12].

7.2.3 Enhanced transport of flexible fibers by pole vaulting in turbulent wall-bounded flow

Participants: Jérémie Bec, Christophe Henry.

Long, flexible fibers transported by a turbulent channel flow sample non-linear variations of the fluid velocity along their length. One of the challenges of the dynamics of flexible fibers in confined flows is related to their interactions with boundaries, which can lead to a range of behavior. In this work, we explore how such fibers tumble and collide with the boundaries and the resulting effect on their near-wall dynamics. Using fine microscopic simulations (based on a Direct Numerical Simulations of the turbulent flow coupled to an explicit tracking of inertialess flexible fibers described with the slender-body theory), we show that as fibers bounce off surfaces, an impulse propels them toward the center of the flow, similar to pole vaulting. As a result, the fibers migrate away from the walls, leading to depleted regions near the boundaries and more concentrated regions in the bulk. These higher concentrations in the center of the channel result in a greater net flux of fibers than what was initially imposed by the fluid. This effect becomes more pronounced as fiber length increases, especially when it approaches the channel height.

This is a collaborative work with Christophe Brouzet (Institute of Physics in Nice). An article has been submitted to Physical Review Letters [13].

7.3 Axis C – Active agents in a fluid flow

This research axis deals with the study of self-propelled particles, which have the ability to convert internal or ambient free energy into dynamical motion. Such active agents can be microorganisms, such as bacteria or plankton, as well as artificial devices used for micro-manufacturing, toxic waste disposal, targeted drug delivery or localized medical diagnostics. Many questions remain open on how to control the displacement of these micro-swimmers, in particular for complex flows comprising inhomogeneities, fluctuations, obstacles, walls, or having a non-Newtonian rheology. Studying and optimizing the displacement of these swimmers is generally done in two successive steps. The first is to find a locomotion strategy by choosing the composition, shape, and deformation for an efficient swimming. The second is to define a navigation strategy aimed at minimizing the energy needed to reach a target in a given environment. CALISTO works rely on cross-disciplinary skills, comprising the optimal control of viscous flows, small-scale fluid-structure interactions, statistical modeling, and large-scale turbulent transport to tackle both aspects, locomotion and navigation, at once.

7.3.1 Mathematical and computation framework for moving and colliding rigid bodies in a Newtonian fluid

Participants: Laetitia Giraldi.

This work is done in collaboration, with Celine Van-Landeghem (IRMA, Université de Strasbourg), PhD student coadvised by L. Giraldi.

We studied numerically the dynamics of colliding rigid bodies in a Newtonian fluid. The finite element method is used to solve the fluid-body interaction and the fluid motion is described in the Arbitrary-Lagrangian-Eulerian framework. To model the interactions between bodies, we consider a repulsive collision-avoidance model, defined by R. Glowinski. The main emphasis in this work is the generalization of this collision model to multiple rigid bodies of arbitrary shape. Our model first uses a narrow-band fast marching method to detect the set of colliding bodies. Then, collision forces and torques are computed for these bodies via a general expression, which does not depend on their shape. Numerical experiments examining the performance of the narrow-band fast marching method and the parallel execution of the collision algorithm are discussed. We validate our model with literature results and show various applications of colliding bodies in two and three dimensions. In these applications, the bodies either move due to gravity, a flow, or can actuate themselves. Finally, we present a tool to create arbitrary shaped bodies in discretized fluid domains, enabling conforming body-fluid interface and allowing to perform simulations of fluid-body interactions with collision treatment in these realistic environments. All simulations are conducted with the Feel++ open source library.

This is collaborative work with Christophe Prud'Homme, Luca Berti, Yannick Hoarau, Vincent Chabannes and Agathe Chouippe. The paper [15] is accepted in Annals of Mathematical Sciences and Applications.

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

Participant: Laetitia Giraldi.

In this paper [7], in collaboration with Pierre Lissy (Ceremade, Paris), Jean-Baptiste Pomet (Inria, McTAO) and Clement Moreau (LS2N, University of Nantes), 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 are illustrated with several examples. This paper is now accepted in ESAIM: Control, Optimisation and Calculus of Variations (ESAIM:COCV).

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

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

This study aimed at finding optimal navigation policies for thin, deformable microswimmers that progress in a viscous fluid by propagating a sinusoidal undulation along their slender body. These active filaments are embedded in a prescribed, non-homogeneous flow, in which their swimming undulations have to compete with the drifts, strains, and deformations inflicted by the outer velocity field. Such an intricate situation, where swimming and navigation are tightly bonded, has been addressed using various methods of reinforcement learning. Each swimmer has only access to restricted information on its configuration and has to select accordingly an action among a limited set. The optimization problem then consists in finding the policy leading to the most efficient displacement in a given direction. It was found that usual methods do not converge and this pitfall has been interpreted as a combined consequence of the non-Markovianity of the decision process, together with the highly chaotic nature of the dynamics, which is responsible for high variability in learning efficiencies. Still, we provided an alternative method to construct efficient policies, which is based on running several independent realizations of Q-learning. This allowed the construction of a set of admissible policies whose properties have been studied in detail and compared to assess their efficiency and robustness. This work has been published in the European Physical Journal E [5].

7.4 Axis D – Mathematics and numerical analysis of stochastic systems

Stochastic analysis, and related numerical analysis, together with improved statistical descriptions of highly-nonlinear dynamics are central topics in CALISTO. This research axis encompasses activities aiming, either (a) at strengthening our understanding on the origin and nature of fluctuations that are inherent to turbulent flows, or (b) at providing a coherent framework in response to the various mathematical challenges raised by the development of novel models in other research axes. Addressing these two fundamental aspects concomitantly to more practical and applied objectives is again a hallmark of the team.

7.4.1 Anomalous dissipation and spontaneous stochasticity in deterministic surface quasi-geostrophic flow

Participants: Jérémie Bec, Simon Thalabard, Nicolas Valade.

Surface quasi geostrophy (SQG) describes the two-dimensional active transport of a temperature field in a strongly stratified and rotating environment. Besides its relevance to geophysics, SQG bears formal resemblance with various flows of interest for turbulence studies, from passive scalar and Burgers to incompressible fluids in two and three dimensions. In the article [10], published in Annales Henri Poincaré in 2023, we substantiated this analogy by considering the turbulent SQG regime emerging from deterministic and smooth initial data prescribed by the superposition of a few Fourier modes. While still unsettled in the inviscid case, the initial value problem is known to be mathematically well-posed when regularized by a small viscosity. In practice, our numerics revealed that in the presence of viscosity, a turbulent regime appears in finite time, which features three of the distinctive anomalies usually observed in three-dimensional developed turbulence: (i) dissipative anomaly, (ii) multifractal scaling, and (iii) super-diffusive separation of fluid particles, both backward and forward in time. These three anomalies point towards three spontaneously broken symmetries in the vanishing viscosity limit: scale invariance, time reversal and uniqueness of the Lagrangian flow, a fascinating phenomenon dubbed spontaneous stochasticity. In the light of previous work on the passive scalar problem, we argued that spontaneous stochasticity and irreversibility are intertwined in SQG, and provided numerical evidence for this connection. Our numerics, though, revealed that the deterministic SQG setting only features a tempered version of spontaneous stochasticity, characterized in particular by non-universal statistics.

7.4.2 Numerical analysis of stochastic system

Strong rate of convergence of approximation scheme for SDEs with superlinear coefficients

Participants: Mireille Bossy.

In collaboration with Kerlyns Martinez (University of Valparaiso), we consider the problem of the approximation of the solution of a one-dimensional SDE with piecewise locally Lipschitz drift and continous diffusion coefficient with polynomial growth. On the basis of the previously proposed (semi-explicit) exponential-Euler scheme [28], we analyze its convergence through its strong approximation error. The main proof arguments developed in this study, based on a stochastic time change technique is rather generic and particularly useful for the strong error control of a Euler type scheme when the polynomial behavior of the coefficients only increases the number of moments to be bound in the dynamics of the error itself. With such a technique we explicit the rather accurate conditions on the parameters of the stochastic equation to get the classical order for the strong convergence rate.

The main objectives of this work are:

(i) extending the C^4 regularity required for the drift b in the weak error analysis to the discontinuous case,

(ii) refining the sufficient control condition on the growth and domination of the drift to achieve the convergence rate,

(iii) investigating the behavior of the scheme near the limit of the Feller zone (the set of coefficients parameters that insures non explosion of solution in finite time with probability one) of the exact process, and the ability of the scheme to capture explosive parameter zone.

Two journal papers are in preparation arround those themes.

On the ε–Euler-Maruyama scheme for time inhomogeneous jump-driven SDEs

Participants: Mireille Bossy, Paul Maurer.

In [14], we consider a class of general SDEs with a jump integral term driven by a time-inhomogeneous random Poisson measure. We propose a two-parameters Euler-type scheme for this SDE class and prove an optimal rate for the strong convergence with respect to the $L^p(\Omega)$-norm and for the weak convergence. One of the primary issues to address in this context is the approximation of the noise structure when it can no longer be expressed as the increment of random variables. We extend the Asmussen-Rosinski approach to the case of a fully dependent jump coefficient and time-dependent Poisson compensation, handling contribution of jumps smaller than ε with an appropriate Gaussian substitute and exact simulation for the large jumps contribution. For any $p \geq 2$, under hypotheses required to control the L^p-moments of the process, we obtain a strong convergence rate of order $1/p$. Under standard regularity hypotheses on the coefficients, we obtain a weak convergence rate of $1/n + \epsilon^{3-\beta}$, where β is the Blumenthal-Getoor index of the underlying Lévy measure. We compare this scheme with the Rubenthaler's approach where the jumps smaller than ε are neglected, providing strong and weak rates of convergence in that case too. The theoretical rates are confirmed by numerical experiments afterwards.

This study is mainly motivated by the simulation of stochastic models, with a focus on investigating Lévy processes, and particularly α-stable processes, arising as the limit distribution of the generalized Central Limit Theorem for independent random variables with infinite variance. We apply this model class for some anomalous diffusion model related to the dynamics of rigid fibres in turbulence studied in [21].

Euler Scheme for a system of Piecewise Deterministic Markov Processes under mean field interaction

Participants: Mireille Bossy.

In collaboration with Hector Olivero-Quintero (University of Valparaiso), and motivated by mathematical models in chemistry, we are working on an Euler time-discretization scheme for a system of mean field interacting particles each of them modeled as Piecewise Deterministic Markov Process. Under suitable hypotheses on the coefficients of the system, we analyze a theoretical rate of convergence. Also, using the strong convergence of the numerical scheme, we recover the convergence of the model to its diffusive approximation. A journal paper is in preparation.

7.4.3 Finite-time Lyapunov exponents of deep neural networks

Participants: Jérémie Bec.

For deep neural networks trained on different classification problems, we explored geometrical structures of finite-time Lyapunov exponents (FTLE) in input space. In fluid mechanics, such Lagrangian coherent structures appear as ridges of large exponents, and they are used with great success to organize the phase space of complex spatiotemporal flow patterns. The same is true for deep neural networks: FTLE ridges partition input space into different regions associated with different classes. Our analysis showed how the network exploits its exponential expressivity to form the ridges. Their sharpness determines how quickly classification errors and prediction uncertainty decreases as one moves away from the ridge. As the width of the network increases, the contrast between ridge and background disappears, leading to a different learning mechanism, random embedding, with qualitative differences regarding classification errors and predictive uncertainties. The transition to this lazy-learning regime occurs for very wide networks. The transition may explain why wider networks are more robust against adversarial attacks: the less important the ridges are for representing the relevant data structures, the harder it is to realize adversarial attacks. The geometrical method presented in our work may extend to other network architectures, such as resnets or transformers, and could help to visualize and understand the mechanisms that allow such neural networks to learn. This study is the subject of a collaboration with Kristian Gustavsson, Hampus Linander, Bernhard Mehlig, and Ludvig Storm (University of Gothenburg) and will soon appear in Physical Review Letters [17].

7.5 Axis E – Variability and uncertainty in flows and environment

7.5.1 Short term predictive models with times-serie based on Lagrangian stochastic approach in CFD and application to wind energy

Participants: Mireille Bossy.

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 [20] in collaboration with Kerlyns Martinez (University of Valparaiso), 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.

We pursue our work by now focusing on a reduced model for the short term prediction of wind gust risk.

7.5.2 Methodology to quantify uncertainties in dispersed two-phase flows

Participants: Christophe Henry, Mireille Bossy.

Within the framework of the VIMMP EU project (Virtual Materials Market Place) that took place between 2017 and 2022, one objective was to set up a methodology to analyze the sensitivity (SA) and then quantify uncertainty (UQ) in numerical simulations of multiphase flows to a number of input variables. For that purpose, a Common Data Model (CDM) has been developed to provide a comprehensive, adequate and standardized structure to collect all the physical and numerical information required to set-up scientific simulation workflows (possibly including various software) while allowing for a systematic analysis of the results obtained using UQ&SA tools.

This collaborative work with partners involved in the VIMMP project (Pascale Noyret, Eric Fayolle and Jean-Pierre Minier from EDF R&D) resulted in the development of the software CDM-Sci (see Section 6). To complement this software, we are in the process of writing a book proposal for Specials Issues in Springer to describe the CDM (both in terms of physics and in terms of implementation) and illustrate it on a few selected examples.

8 Partnerships and cooperations

8.1 International initiatives

Indo-French Center for Applied Mathematics

Participants: Jérémie Bec, Ciro Campolina, Nicolas Valade.

The *Indo-French Center for Applied Mathematics* (**IFCAM**) is a CNRS IRL that provides support for a collaboration on "Turbulence in classical and quantum fluids" with teams at the Indian Institute of Science and the International Center for Theoretical Science in Bangalore. Visits of CALISTO members to Bangalore supported by this initiative took place in January 2023. It is however unclear whether this initiative will be renewed or not.

8.1.1 CEFIPRA project "Polymers in turbulent flows"

Participants: Jérémie Bec.

This bilateral project aims at studying the dynamics of polymers in turbulent flows, with the idea to use Lagrangian approaches to find links between microscopic scales and the rheology of polymer suspensions and macroscopic continuum models. The french PI is Dario Vincenzi (CNRS-LJAD) and the Indian PI is Jason Picardo (IIT Mumbai). The CALISTO team is a partner of the project and received funding to support bilateral visits.

SDE: Theory, Numerics and Applications (RSE Saltire Facilitation Network)

Participants: Mireille Bossy.

Started in 2022, CALISTO takes part to the Royal Society of Edinburgh (RSE) Saltire Facilitation Network on *SDEs: Theory, Numerics and Applications*. This 2 years network project involves mathematicians of 9 European countries on the theme of (numerical) analysis for highly nonlinear SDEs. On the same themes, a submission of an European COST action was submitted this fall.

8.2 International research visitors

8.2.1 Visits of international scientists

Kerlyns Martinez

Status: Associate Professor

Institution of origin: Universidad de Valparaíso

Country: Chile

Dates: from 01/15/2023 to 02/15/2023 and from 12/07/2023 to 02/07/2024

Mobility program: research stay

Hector Quinteros

Status: Associate Professor

Institution of origin: Universidad de Valparaíso

Country: Chile

Dates: from 07/17/2023 to 07/28/2023

Mobility program: research stay

Chiara Calascibetta

Status: PhD

Institution of origin: University of Rome Tor Vergata

Country: Italy

Dates: December 2023

Mobility program: research stay

8.3 National initiatives

8.3.1 ANR PRC 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). Within TILT, a new postdoc joined CALISTO in January 2023.

8.3.2 ANR JCJC 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 is composed of Laetitia Giraldi, Mickael Binois (Inria, Acumes) and Laurent Monasse (Inria, Coffee).

NEMO aims at developing 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 such micro-robots has mostly focused on simple unconfined environments, the main challenge is today to design external magnetic fields that allow them to navigate efficiently in complex realistic environments.

NEMO aims at elaborating 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.

8.3.3 ANR PRC NETFLEX

Participant: Jérémie Bec, Mireille Bossy, Laetitia Giraldi, Christophe Henry, Paul Maurer.

The ANR PRC project NEFFLEX (*Tangles, knots, and breakups of flexible fibers in turbulent fluids*) started on January 1, 2022. NETFLEX is a four-years project that aims at advancing our knowledge on the dynamics of long, flexible, macroscopic fibres in turbulent flows, and to understand and model the processes of fibre fragmentation and aggregation. NETFLEX brings together Université Côte d'Azur (INPHYNI, LJAD), Inria (CALISTO) and Aix-Marseille University (IRPHE). NETFLEX approach combines three levels of description (micro, meso, and macroscopic) and relies on a synergy between mathematical modeling, numerical simulations, and laboratory experiments. It relies on the development of newly designed experiments and a substantial improvement of the mathematical and numerical tools currently used in the study of fibre dynamics. An overall aim is to develop a new framework able to cope with such intricate effects of turbulence and to reproduce the significant observable features in a macroscopic approach.

Improved modeling of turbulent fluctuations and effective transport models for aggregates are among the key issues to be addressed in order to extend the macroscopic models.

Starting in October 2022, Paul Maurer's thesis work on analysis and simulation for temporal intermittency and long-range correlation models is part of this project, and will be applied to the dynamics of flexible particles.

9 Dissemination

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

9.1 Promoting scientific activities

9.1.1 Scientific events: organisation

General chair, scientific chair

- Mireille Bossy is co-chairing with Mickael Binois (ACUMES) the 2024 edition of the Mascot-Num annual conference to be held in Giens peninsula, Hyères, France.
- Jérémie Bec acted as a co-organizer of the European Mechanics Society colloquium "Complex Particles in Turblent Flow" (Nice, May 2023, 45 participants). He was also a co-organizer of the summer school 100 Years of Turbulent Cascades (Nice & Porquerolles, Jun-Jul 2023, 38 partcipants).

Scientific seminars of the Team Calisto is organizing a Periodic Team Seminar every month. In 2023, the following researchers were invited to give a presentation: Michel Orsi (Institut de Physique de Nice, France), Aurore Loisy (IRPHE Marseille, France), Bernhard Vowinckel (TU Dresden, Germany), Ciro Campolina (Team Calisto, Inria, France), Josh Williams (STFC, UKRI, United Kingdom), Luca Moriconi (Universidade Federal do Rio de Janeiro, Brazil), Chiara Calascibetta (University of Rome, Italy)

Workshops In Febuary 2023, CALISTO co-organized with CNRS-IRPHE a three days international workshop on "Complex particles in turbulent flows" with the following speakers: Sylwester Arabas (Jagiellonian University Krakow), Jéremie Bec (CNRS-CEMEF), Mireille Bossy (Inria) Christophe Brouzet (CNRS-InPhyNi), Eric Climent (Toulouse INP), Lionel Gamet (IFPEN), Christophe Henry (Inria), Aurore Naso (CNRS-LMFA), Cristian Marchioli (U. Udine), Bernhard Mehlig (U. Gothenburg), Jean Lou Pierson (IFPEN), Vanessa Teles (IFPEN), Ton van den Bremer (TU Delft), Gautier Verhille (CNRS-IRPHE) , Dario Vincenzi (CNRS-LJAD); Michael Wilczek (U. Bayreuth).

9.1.2 Journal

Reviewer - reviewing activities In 2023 CALISTO team members have been acting as reviewers for various international journals, listed in the following according to each team member.

- Jérémie Bec acted as a reviewer for: Journal of Fluid Mechanics, Journal of Statistical Physics, Physical Review Fluids, Scientific Reports.
- Mireille Bossy acted as a reviewer for BIT Numerical Mathematics, Journal of Computational Physics, Stochastics.
- Laetitia Giraldi acted as a reviewer for Physical Review Fluids and for European Physical Journal E.
- Christophe Henry acted as a reviewer for Aerosol Science and Technology, Journal of Aerosol Science, Powder Technology, Scientific Reports, NPJ Climate and Atmospheric Science, Environmental Impact Assessment Review.

9.1.3 Invited talks

- Mireille Bossy was invited speaker to the following events: RSE Saltire Facilitation Network on SDEs Seminar; MASCOT-NUM Conference (Le Croisic); "Stochastic Computation" workshop at Foundations of Computational Mathematics (FoCM 2023) Conference; workshop on "Stability, mixing and fluid dynamics" at the University of Münster ; RSE Saltire Facilitation Network on SDEs Workshop at University of Strathclyde ; Workshop on "SDEs with low-regularity coefficients: theory and numerics" at the University of Torino;

  She also gave a talk to the following conference: NASPDE 2023 at Eindhoven University of Technology; 14th International Conference on Monte Carlo Methods and Applications MCM2023 (Paris).

- Jérémie Bec was an invited speaker at the conferences “Frontiers in Non-equilibrium Physics” (Chennai, India), “Turbulence: Problems at the Interface of Mathematics and Physics” (Bangalore, India), and at the workshop “Particle Growth in Turbulence” (Stockholm, Sweden).
- Laetitia Giraldi was invited speaker to the Jacques-Louis Lions Spanish-French School on Numerical Simulations in Physics and Engineering at Barcelone in July 2023.

9.1.4 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.

Calisto team members are involved in the scientific/steering committees of several national research networks. This includes the following GdR (CNRS Research network):

- GdR Mascot-NUM on stochastic methods for the analysis of numerical codes,
- GdR Défis théoriques pour les sciences du climat on theoretical aspects for climate science
- GDR Calcul that promotes communication and exchange within the computing community in France.

Calisto team members are also involved as partners in other networks including: GdR Navier-Stokes 2.0 on turbulence, and ASFERA, the French Association on Studies and Research on Aerosols.

9.1.5 Scientific expertise

- Christophe Henry reviewed project propositions from the PAZY foundation (an Israeli research fund that supports scientific projects in the areas of chemistry and materials, engineering and physics).

9.1.6 Research administration

- Since September 2023, Christophe Henry is acting as the local correspondent for the yearly activity reports of all Teams within Inria Center at Université Côte d’Azur.
- Jérémie Bec and Laëtitia Giraldi are members of the “Comité Nice” at Inria Center at Université Côte d’Azur.
- Mireille Bossy is member of the "Bureau du comité des projets" at Inria Center at Université Côte d’Azur.

9.2 Teaching - Supervision - Juries

9.2.1 Teaching

CALISTO scientific staff have been involved in the following teaching activities:

- Assignments (Khôlles) in preparatory schools MPSI, MP* (Laetitia Giraldi, 2h weekly, Centre International de Valbonne).
- Advanced models for hydrology (C. Henry): master students in their final (5^{th}) year within the program “Génie de l’eau” (47h) at the engineering school Polytech’Nice.

9.2.2 Supervision

- PhD in progress: Paul Maurer, “Stochastic models for deformable particle dynamics in turbulence: mathematical analysis and simulation for temporal intermittency and long-range correlation models” started in October 2022; supervised by Mireille Bossy.

- PhD in progress: Nicolas Valade, “Spontaneous stochasticity of quasi-geostrophic surface turbulence” started in October 2022; supervised by Jérémie Bec and Simon Thalabard (INPHYNI, Université Côte d’Azur).

- 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: Celine Van-Landeghem, “numerical methods for locomotion of micro-swimmers in a confined environment” started in October 2021; supervised by Christophe Prud’Homme (IRMA, Strasbourg), Yannick Hoarau 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 in progress: Luca Palazzolo, "Numerical methods for optimising the locomotion of flagellate microswimmers" started in October 2023; supervised by Laetitia Giraldi, Mickael Binois (Inria EPC Acumes) and Christophe Prudhomme (Université de Strasbourg).

- M2 internship : Hao Liu (Technology University Darmstad), "Particle transport in the environment", supervised by Christophe Henry and Mireille Bossy; Luca Palazzolo supervised by Laetitia Giraldi ; Antoine Serres (ENS Paris Saclay) supervised by Jérémie Bec.

9.2.3 Juries

- Jérémie Bec served as an examiner for the Ph.D. thesis of Sumithra Reddy Yerasi (U. Côte d’Azur).

- Laetitia Giraldi served as an examiner for the Ph.D. thesis of Xiao Xie (Nantes university, IMT Atlantique/ LS2N).

9.3 Popularization

9.3.1 Education

CALISTO team members took part in various education activities related to popularization.

- Christophe Henry took part in some of the activities organized by Terra Numerica for young students, including:

  - The event "Stage Math C2+" in June 2023, giving a 1h30 intervention on the "Physics and Mathematics of sand castles" to an audience of 40 students in the first year of upper secondary education (classe de 2nde au Lycée).
  - The event "Stage 3e" in December 2023, giving a 1h intervention on the "Physics and Mathematics of sand castles" to an audience of 11 students in the last year of lower secondary education (classe de 3ème au collège).

9.3.2 Interventions

- Fête de la Science: Every year, a science festival is held across France in autumn where researchers present their activities to the public (especially for kids and young students).

  - Christophe Henry took part in the festival held in Villeneuve-Loubet, in Mouans Sartoux and in Antibes-Juan Les Pins in October 2023, presenting a workshop on the “Physics of sand castles”.

- Complex Days: the Academy “Complex Systems” of Université Côte d’Azur promotes interdisciplinary research on the analysis and applications of complex systems. Since 4 years, the Academy organises an annual event dedicated to its community, called Complex Days. The aim is to bring together young and senior researchers from different backgrounds to exchange ideas and promote new developments in complex systems. In February 2023, CALISTO team members made two contributions:
  - Christophe Henry gave a talk on "Particle and flow dynamics in wall-bounded environments: Modeling & simulation of particle agglomeration" [18].
  - Paul Maurer gave a talk on "Stochastic models driven by a Lévy noise: Application to rods orientation in turbulence" [19].

10 Scientific production

10.1 Publications of the year

International journals

[1] S. Allende and J. Bec. ‘Velocity and acceleration statistics of heavy spheroidal particles in turbulence’. In: *Journal of Fluid Mechanics* 967 (18th July 2023), R4. DOI: 10.1017/jfm.2023.508. URL: https://inria.hal.science/hal-04304086.

[2] A. Banari, K. Graebe, M. Rudolph, E. Mohseni, P. Lorenz, K. Zimmer, R. Hübner, C. Henry, M. Bossy, U. Hampel and G. Lecrivain. ‘Influence of engineered roughness microstructures on adhesion and turbulent resuspension of microparticles’. In: *Journal of Aerosol Science* 174 (Nov. 2023), p. 106258. DOI: 10.1016/j.jaerosci.2023.106258. URL: https://inria.hal.science/hal-04232948.

[3] J. Bec, K. Gustavsson and B. Mehlig. ‘Statistical models for the dynamics of heavy particles in turbulence’. In: *Annual Review of Fluid Mechanics* 56 (2024). DOI: 10.1146/annurev-fluid-032822-014140. URL: https://hal.science/hal-04058674.

[4] L. Campana, M. Bossy and C. Henry. ‘Lagrangian stochastic model for the orientation of inertialess non spherical particles in turbulent flows: an efficient numerical method for CFD approach’. In: *Computers and Fluids* 257 (May 2023), p. 105870. DOI: 10.1016/j.compfluid.2023.105870. URL: https://inria.hal.science/hal-03862286.

[5] Z. El Khiyati, R. Chesneaux, L. Giraldi and J. Bec. ‘Steering undulatory micro-swimmers in a fluid flow through reinforcement learning’. In: *European Physical Journal E: Soft matter and biological physics* 46.6 (June 2023), p. 43. DOI: 10.1140/epje/s10189-023-00293-8. URL: https://hal.science/hal-04058675.

[6] F. A. Gerosa, H. Meheut and J. Bec. ‘Clusters of heavy particles in two-dimensional Keplerian turbulence’. In: *The European Physical Journal Plus* 138 (2023), p. 9. DOI: 10.1140/epjp/s13360-022-03585-8. URL: https://hal.science/hal-03868249.

[7] 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’. In: *ESAIM: Control, Optimisation and Calculus of Variations* 30.4 (2024). DOI: 10.1051/cocv/2023073. URL: https://hal.science/hal-02178973.

[8] C. Henry, J.-P. Minier and S. Brambilla. ‘Particle resuspension: challenges and perspectives for future models’. In: *Physics Reports* 1007 (11th Jan. 2023), pp. 1–98. DOI: 10.1016/j.physrep.2022.12.005. URL: https://inria.hal.science/hal-03909063.

[9] J. Morán, J. Yon, C. Henry and M. R. Kholghy. 'Approximating the van der Waals interaction potentials between agglomerates of nanoparticles'. In: *Advanced Powder Technology* 34.12 (Dec. 2023), p. 104269. DOI: 10.1016/j.apt.2023.104269. URL: https://normandie-univ.hal.science/hal-04285994.

[10] N. Valade, S. Thalabard and J. Bec. 'Anomalous dissipation and spontaneous stochasticity in deterministic surface quasi-geostrophic flow'. In: *Annales Henri Poincaré* (23rd Feb. 2023). DOI: 10.1007/s00023-023-01284-3. URL: https://hal.science/hal-03868221.

Doctoral dissertations and habilitation theses

[11] C. Henry. 'Modeling particle-laden flows'. Université Cote d'Azur; ED SFA, 28th Mar. 2023. URL: https://inria.hal.science/tel-04178774.

Reports & preprints

[12] G. Balvet, J.-P. Minier, C. Henry, Y. Roustan and M. Ferrand. *A time-step-robust algorithm to compute particle trajectories in 3-D unstructured meshes for Lagrangian stochastic methods*. 15th Mar. 2023. DOI: 10.1515/mcma-2023-2002. URL: https://edf.hal.science/hal-04059629.

[13] J. Bec, C. Brouzet and C. Henry. *Enhanced transport of flexible fibers by pole vaulting in turbulent wall-bounded flow*. 20th Nov. 2023. URL: https://hal.science/hal-04296840.

[14] M. Bossy and P. Maurer. *On the ε-Euler-Maruyama scheme for time inhomogeneous jump-driven SDEs*. 17th Jan. 2024. URL: https://inria.hal.science/hal-04404438.

[15] C. V. Landeghem, L. Berti, V. Chabannes, C. Prud'Homme, A. Chouippe, Y. Hoarau and L. Giraldi. *Mathematical and computation framework for moving and colliding rigid bodies in a Newtonian fluid*. 2023. URL: https://hal.science/hal-04101291.

[16] J.-P. Minier and C. Henry. *The dynamics of discrete particles in turbulent flows: open issues and current challenges in statistical modeling*. 2023. DOI: 10.48550/arXiv.2311.01921. URL: https://inria.hal.science/hal-04355292.

[17] L. Storm, H. Linander, J. Bec, K. Gustavsson and B. Mehlig. *Finite-time Lyapunov exponents of deep neural networks*. 21st June 2023. URL: https://inria.hal.science/hal-04304090.

10.2 Other

Scientific popularization

[18] C. Henry. 'Particle and flow dynamics in wall-bounded environments: Modeling & simulation of particle agglomeration'. In: *Complex Days*. Complex Days. Complex Days 3. Nice, France, 7th Feb. 2023. URL: https://hal.science/hal-04043157.

[19] P. Maurer. 'Stochastic models driven by a Lévy noise: Application to rods orientation in turbulence'. In: *Complex Days*. Complex Days. Complex Days 3. Nice, France, 2023. URL: https://hal.science/hal-04042978.

10.3 Cited publications

[20] 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'. In: *Journal of Computational Physics* (1st Sept. 2022). DOI: 10.1016/j.jcp.2021.110929. URL: https://hal.inria.fr/hal-03108031.

[21] L. Campana, M. Bossy and J. Bec. 'Stochastic model for the alignment and tumbling of rigid fibres in two-dimensional turbulent shear flow'. In: *Physical Review Fluids* 7.12 (2022), p. 124605. URL: https://hal.inria.fr/hal-03718232.

[22] 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). https://arxiv.org/abs/1910.01728 - 8 pages, 10 figures. DOI: 10.1103/PhysRevE.101.043110. URL: https://hal.archives-ouvertes.fr/hal-02362934.

[23] 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.

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

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

[26] F. Berthelin, T. Goudon and S. Minjeaud. 'Multifluid flows: a kinetic approach'. In: *Journal of Scientific Computing* 66.2 (2016), pp. 792–824. DOI: 10.1007/s10915-015-0044-1.

[27] L. Berti, Z. E. Khiyati, Y. Essousy, C. Prud'homme and L. Giraldi. 'Reinforcement learning with function approximation for 3-spheres swimmer'. In: *IFAC-PapersOnLine* 55.16 (2022). 18th IFAC Workshop on Control Applications of Optimization CAO 2022, pp. 1–6. DOI: https://doi.org/10.1016/j.ifacol.2022.08.072. URL: https://www.sciencedirect.com/science/article/pii/S2405896322011624.

[28] 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). https://arxiv.org/abs/1904.09441, pp. 312–347. DOI: 10.3150/20-BEJ1241. URL: https://hal.inria.fr/hal-02282168.

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

[30] 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.

[31] *Fog, Glossary of Meteorology*. Tech. rep. American Meteorological Society, 2017.

[32] 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.

[33] G. B. Jeffery. 'The motion of ellipsoidal particles immersed in a viscous fluid'. In: *Proc. Royal Soc. Lond. A* 102.715 (1922), pp. 161–179.

[34] 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).

[35] J. J. Lissauer. 'Planet formation'. In: *Annual review of astronomy and astrophysics* 31.1 (1993), pp. 129–172.

[36] M. C. Marchetti, J. Joanny, S. Ramaswamy, T. Liverpool, J. Prost, M. Rao and R. Simha. 'Hydrodynamics of soft active matter'. In: *Reviews of Modern Physics* 85.3 (2013), p. 1143.

[37] 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.

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

[39] E. E. Agency. *Adaptation challenges and opportunities for the European energy system Building a climate-resilient low-carbon energy system*. 2019.

[40] W. H. Organization et al. 'Ambient air pollution: A global assessment of exposure and burden of disease'. In: (2016).

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

[42] B. Sawford. 'TURBULENT RELATIVE DISPERSION'. In: *Annual Review of Fluid Mechanics* 33.1 (2001), pp. 289–317.

[43] A. Soldati and C. Marchioli. 'Physics and modelling of turbulent particle deposition and entrainment: Review of a systematic study'. In: *International Journal of Multiphase Flow* 35.9 (2009). Special Issue: Point-Particle Model for Disperse Turbulent Flows, pp. 827–839.

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

[45] A. K. Sriwastava and A. M. A. M. Moreno-Rodenas. *QUICS - D.1.1 Report on uncertainty frameworks; QUICS - D.4.2 Report on application of uncertainty frameworks, potential improvements*. Tech. rep. USFD and TUD, 2017.

[46] M. Stempniewicz, E. M. Komen and A. de With. 'Model of particle resuspension in turbulent flows'. In: *Nuclear Engineering and Design* 238.11 (2008), pp. 2943–2959.

[47] M. Uhlmann. 'An immersed boundary method with direct forcing for the simulation of particulate flows'. In: *Journal of Computational Physics* 209.2 (2005), pp. 448–476. DOI: 10.1016/j.jcp.2005.03.017.

[48] G. A. Voth and A. Soldati. 'Anisotropic Particles in Turbulence'. In: *Annual Review of Fluid Mechanics* 49.1 (2017), pp. 249–276.