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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

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Project-Team CALISTO

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Keywords

Computer sciences and digital sciences

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2 Overall objectives

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

The variety of situations (deposition, resuspension, turbulent mixing, droplet/matter agglomeration, thermal effect) involves specific models that need to be improved. Yet, one of the key difficulties lies in the fact that the relevant phenomena are highly multi-scale in space and time (from chemical reactions acting at the microscopic level to fluid motion at macroscopic scales), and that consistent and coherent models need to be developed together. This raises many challenges related both to physical sciences (i.e. fluid dynamics, chemistry or material sciences) and to numerical modeling. 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 the unique synergy between team members from various disciplines, CALISTO is developing *Stochastic Approaches for complex Flows and Environment* to address the following challenges:

- produce original answers (methodological and numerical) for challenging environmental simulation models, with applications to renewable energy, filtration/deposition technology in industry (cooling of thermal or nuclear power plants), 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;
- optimize and control the displacement of artificial micro-swimmers;
- develop stochastic modeling approaches and approximation methods, in the rich context of particle-particle and fluid-particle interactions in complex flows;
- contribute to the field of numerical probability, with new simulation methods for complex stochastic differential equations (SDEs) arising from multi-scale Lagrangian modeling for the dynamics of material/fluid particle dynamics with 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 axis aims at promoting significant advances in the understanding and modeling of realistic dispersed, multiphase turbulent flows. In situations where basic mechanisms are still not fully apprehended, the proposed research aims at bringing out the underlying physics by identifying novel effects and quantifying their impacts. These results will then be used to foster new macroscopic models that are expected to be computationally sufficiently undemanding. These models should also be adaptable to open the way to systematic studies of turbulent suspensions as a function of settings, parameters, system geometry. Such aspects are essential in exploratory researches aimed at optimizing combustion processes, heat transfers, phase changes, or the design of energy-efficient hydraulic or aerodynamic processes.

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

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

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

This research axis is currently investigating the following distinct topics

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

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

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

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

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

This research axis is currently investigating the following distinct topics.

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

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

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

3.2.2 Advanced stochastic models for discrete particle dispersion and resuspension

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

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

3.2.3 Coherent descriptions for fluid and particle phases

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

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

3.2.4 Active particles near boundary

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

3.3 AXIS C- Active agents in a fluid flow

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

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

Modeling approach

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

Control and optimal control for swimmers displacement

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

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

Stochastic effect on artificial swimmers

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

3.4 AXIS D- Mathematics and numerical analysis of stochastic systems

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.

Mathematics for fundamental aspects of turbulence and turbulence transport

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

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

Interacting Stochastic Systems and nonlinear SDEs

CALISTO considers examples of *particle* systems in interaction, possibly under mean field interaction, with the overall goal of analyzing the effect of stochasticity in such system. In particular, we aim to detect and analyze conditions for the emergence of collective behaviors such as collective motions, synchronization and organization with or without the notion of leaders.

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.

The modeling activities carried out in CALISTO require to develop continuously our mathematical toolbox and expertise on nonlinear SDEs driven by complex noises, in particular non-Markovian ones. We are particularly concerned with strong and weak solution behaviors, long-time behaviors, approximation techniques including numerical ones, and the study of singular situations arising for instance from boundary conditions.

3.5 AXIS E- Variability and uncertainty in flows and environment

Uncertainty has become a very important research topic for predictive systems involving an ever increasing number of parameters. This analysis effort is particularly present in CFD, all the more so when dealing with particle-laden turbulent flows. It becomes critical for environmental applications, among which we can mention in the first place climate uncertainty. Our position on these subjects is based on the stochastic modeling of the variability of the phenomena under study. Crossing the analysis in uncertainty with solution formulations that already incorporate a statistical approach allows a great flexibility, both in modeling the uncertainty sources and in numerical implementation. This line of research allows us to enhance our expertise on essential tools for the evaluation of 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 asses variability and uncertainty quantification issues in the particular context of environmental flows and power extraction evaluation. In particular, as a PDF method, SDM delivers a probability distribution field of the computed entities. Merging such numerical strategy with Sensitivity Analysis (SA)/Uncertainty Quantification (UQ) are potentially fruitful in terms of computational efficiency.

Metamodeling and uncertainty

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

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

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

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

4 Application domains

Environmental challenges: predictive tools for particle transport and dispersion

Particles are omnipresent in the environment:

- formation of clouds and rain results from the coalescence of tiny droplets in suspension in the atmosphere;
- fog corresponds to the presence of droplets in the vicinity of the Earth's surface, reducing the visibility to below 1 km [26];
- pollution corresponds to the presence of particulate matter in the air. Due to their impact on human health [35], the dispersion of fine particulate matter is of primary concern: PM2.5 and PM10 (particles smaller than 2.5 or 10 μm) and Ultra Fine Particles (UFP) are particularly harmful for human respiratory systems while pollen can trigger severe allergies;
- the dispersion of radioactive particles following their release in nuclear incidents has drawn a great deal of attention to deepen our understanding and ability to model these phenomena [41];
- the dispersion/deposition of ash and soots and their consequences for the environment and health have been highlighted by recent events in France and abroad;
- plastic contamination in oceans impacts marine habitats and human health [29];
- suspension of real micro-swimmers [19] such as sperm cell, bacteria, and in environmental issues with animal flocks attracted intrinsic biological interest[31];
- accretion of dusts is responsible for the formation of planetesimals in astrophysics [30].

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

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

Next generation of predictive models for complex flows

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

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

Models operating in industry generally incorporate rather minimalist descriptions of suspended inclusions. They rely on statistical closures for single-time, single-particle probability distributions, as is the case for the particle-tracking module in the open-source CFD software CODE_SATURNE developed and exploited by EDF R&D. The underlying mean-field simplifications do not accurately reproduce complex features of the involved physics that require higher-order correlation descriptions and modeling. Indeed, predicting the orientation and deformation of particles requires suitable models of the fluid velocity gradient along their trajectories [42] while concentration fluctuations and clustering depend on relative particle dispersion [37, 27]. Estimates of collision and aggregation rates should also be fed by two-particle dynamics [36], while wall deposition is highly affected by local flow structures [38]. 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 [25]. Wind, solar, marine/rivers energies are of growing importance, and the demand for forecasts goes hand in hand with it [24, 34]. Numerous methods exist for different forecast horizons [22]. 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 [39] [33], the question of how to enrich and refine wind simulations (from meteorological forecast, or from larger scale information, eventually combined with local measurements) remains largely open.

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

At the time scale of climate change, the need for uncertainty evaluation of predictions used in long-term planning systems is increasing. For managers and decision makers in the field of hydrological forecasts, assessing hydropower predictions taking into account their associated uncertainties is a major research issue, as shown by the recent results of the European QUICS project [40]. The term uncertainty here refers to the overall error of the output of a generic model [32]. Translating time series of meteorological forecast into time series of run-of-river hydropower generation necessitates to capture the complex relationship between the availability of water and the generation of electricity. The water flow is itself a nonlinear function of the physical characteristics of the river basins and of the weather variables whose impact on the river flow may occur with a delay.

5 New software and platforms

5.1 New software

5.1.1 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).

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

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6 New results

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

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

Participants: Jérémie Bec, Mireille Bossy, Lorenzo Campana, 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 [28]. But so far, this description has always been investigated in the framework of direct numerical simulations (DNS) and experimental measurements. In particular, inertia-free particles, with sizes smaller than the Kolmogorov length, follow the fluid motion with an orientation generally defined by the local turbulent velocity gradient.

In this work, our focus is to characterize the dynamics of these objects in turbulence by means of a stochastic Lagrangian approach. The development of a model that can be used as 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 [8]. In 2D flow with a mean shear, comparison with DNS allowed a precise calibration of this approach and emphasized the role played by the coherent structures of the flow in the particles angular dynamics [4]. These promising Lagrangian stochastic approaches were then extended to 3D cases and implemented in a practical macroscopic model for turbulent transport [12] (currently available in the open-source CFD software CODE_SATURNE).

6.1.2 Clusters of heavy particles in two-dimensional Keplerian turbulence

Participants: Jérémie Bec.

In collaboration with Fabiola Antonietta Gerosa and Héloïse Meheut, (Observatoire de la Côte d'Azur – Lagrange), we have studied particles in flows with a homogeneous shear, motivated by the formation of planets and the small-scale dynamics of the gas-dust mixture in Keplerian rotation around the star.

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 studied the dynamic of inertial particles in turbulent flows with Keplerian rotation and shear. Two-dimensional direct numerical simulations are 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. We found that in such situations shear drastically affects the characteristics of the turbulent flow destroying cyclones and favoring the survival of anticyclones [13]. Faster rotation enhances clustering of particles in anticyclones, especially for intermediate particle sizes. These clusters form in a hierarchical manner and merge together with time. For parameter values falling outside this regime, solids still concentrate on fractal sets. The mass distribution of particles is 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.

6.1.3 Modeling of the formation and maturation of soot particle aggregates

Participant: Christophe Henry.

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

This study focuses on the aggregation of nascent soot particles, which are very important to predict well soot particle size distribution and morphology in flames. Such nascent soot particles may grow in the reaction-limited aggregation regime (sticking probability $\ll 1$). However, it is currently unknown how fast would be the transition towards diffusion/ballistic-limited aggregation regimes as observed for mature soot (sticking probability close to 1). In this collaborative work, we intend to fill this gap by focusing on numerically simulated soot particles formed in a laminar premixed flame. To this end, a recent fast and accurate Monte Carlo discrete element code called MCAC (developed at CORIA) is used. In these simulations the individual trajectories of particles are integrated in time. The MCAC has been adapted to non-unitary collision and sticking probability considering three different outcomes for interacting aggregates: no collision, sticking or rebound. Using such fine-scale simulations, we have shown that assuming a unitary sticking and collision probability produces no big changes in the aggregation kinetics, particle size distribution, and aggregate morphology. Meanwhile, the soot particles' bulk density was found to affect the aggregation kinetics and particle size distribution. This is an important result for macroscopic models: such effects should be considered in future simulations relying on Population Balance Equations (PBE).

This work is a collaboration with José Moran and Jérôme Yon from Coria which started in 2021 and has been pursued in 2022. It was presented at the French Congress on Aerosol in 2022 [17].

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

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

Participants: Mireille Bossy, Christophe Henry.

Computational fluid dynamics simulations in practical industrial/environmental cases often involve non-homogeneous concentrations of particles. In Euler-Lagrange simulations, this can induce the propagation of numerical error when the number of collision/agglomeration events is computed using mean-field approaches. In fact, mean-field statistical collision models allow to sample the number of collision events using a priori information on the frequency of collisions (the collision kernel). Yet, since such methods often rely on the mesh used for the Eulerian simulation of the fluid phase, the particle number concentration within a given cell might not be homogeneous, leading to numerical errors. In this article, we apply the data-driven spatial decomposition (D2SD) algorithm, recently proposed in a previous work reported in [18], to control such error in simulations of particle agglomeration. This D2SD algorithm provides a spatial splitting according to the spatial distribution of particles. More precisely, the D2SD algorithm uses as input data only the information on the location of the center of gravity of each particle. One of the many advantages of the D2SD algorithm is that the parameters leading to the optimal domain decomposition are automatically tuned through the statistical information coming from the data (position of particles). Thus, there is no bias coming from the choice of arbitrary parameters.

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

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

This study is detailed in [7] in collaboration with Kerlyns Martinez (University of Valparaiso), published in the International Journal of Multiphase Flow.

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

Participants: Mireille Bossy, Christophe Henry.

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

The collaboration with researchers from Technische Universität Dresden in Germany (especially Grégory Lécrivain) has been pursued this year. The results obtained last year revealed the role of inter-particle collisions on particle resuspension even for monolayer deposits at intermediate surface coverage (where $L \sim D_p$) [21]. These results have been presented at the French Congress on Aerosol in 2022 [16]. Drawing on these results, more systematic analysis of the images obtained by experimental observations performed at TUD have been carried out. The idea is to extract detailed information on the outcome of each collision that happens between particles at the surface, especially to monitor the kinetic energy and momentum of both particles involved in the collision. By comparing these values, the objective is to determine if collisions at the surface conserve the kinetic energy and momentum (as is the case for elastic collisions in the bulk of a fluid) and, if not, to evaluate the loss of kinetic energy and/or momentum. These works are still in progress due to the difficulties encountered in the precision of the image analysis techniques (used to extract the particle positions at subsequent times).

6.2.3 Challenges in the modeling of particle resuspension

Participants: Christophe Henry.

The purpose of this work is to review the current challenges in the field of particle resuspension. In particular, we analyze the physics at play in particle resuspension in order to bring insights into the rich complexity of this common but challenging concern. This is performed by starting from a range of practical observations and experimental data. We then work our way through the investigation of the key mechanisms which play a role in the overall process. At the core of this analysis are descriptions of these physical phenomena and the different ways through which they are intertwined to build up various models used to provide quantitative assessment of particle resuspension. The physics of particle resuspension implies to hold together processes occurring at extremely different space and time scales. This raises questions on what makes up a model and one objective of the present work is to clarify the essence of a modeling approach.

This collaborative work with researchers from Los Alamos National Laboratory (Sara Brambilla) and from EDF R&D (Jean-Pierre Minier) is published in Physics Reports [6].

6.3 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.

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

Participants: Laetitia Giraldi.

In collaboration with Lucas Berti (IRMA, Strasbourg), Vincent Chabannes (IRMA, Strasbourg) and Christophe Prud'Homme (IRMA, Strasbourg), in [10], we consider the problem of moving rigid bodies in a Newtonian fluid. The fluid-solid problem is solved using the finite element method, and the solution is based on the Arbitrary-Lagrangian-Eulerian description of the fluid with conforming treatment of moving interfaces. Numerical experiments are discussed, and the results are validated with the literature. The results are obtained with the Feel++ open source library.

6.3.2 Reinforcement learning with function approximation for 3-spheres swimmer

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

In collaboration with Christophe Prud'Homme (IRMA, Strasbourg) and Youssef Essoussy (IRMA, Strasbourg), the paper [11] investigates the swimming strategies that maximize the speed of the three-sphere swimmer using reinforcement learning methods. First of all, we ensure that for a simple model with few actions, the Q-learning method converges. However, this latter method does not fit a more complex framework (for instance the presence of boundary) where states or actions have to be continuous to obtain all directions in the swimmer's reachable set. To overcome this issue, we investigate another method from reinforcement learning which uses function approximation, and benchmarks its results in absence of walls.

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

Participant: Laetitia Giraldi.

In this paper [14] in collaboration with Pierre Lissy (Ceremade, Paris), Jean-Baptiste Pomet (Inria, McTAO) and Clement Moreau (RIMS, Kyoto, Japan), we consider control-affine systems with two scalar controls, such that one control vector field vanishes at an equilibrium state. We state two necessary conditions for local controllability around this equilibrium, involving the iterated Lie brackets of the system vector fields, with controls that are either bounded, small in L^∞ or small in $W^{1,\infty}$. These results were deduced from the behavior of the magnetic flagellated swimmers and they are illustrated with several examples.

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

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

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

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

Using machine learning tools, we have developed new methods to address this optimisation problem where swimming and navigation are closely related. Techniques borrowed from partially-observable Markov decision processes were found to be particularly promising. Combining an efficient locomotion strategy with optimal navigation and path-planning is particularly novel in the field. An article demonstrating the efficiency of genetic reinforcement learning for the displacement of undulatory swimmers in two-dimensional flow is currently in preparation and will be submitted in the coming months to Physical Review Letters.

6.4 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.

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

Participants: Jérémie Bec, Simon Thalabard.

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

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

6.4.2 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. This analogy is here substantiated 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 regularised by a small viscosity. In practice, numerics reveal 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 that Krzysztof Gawedzki dubbed spontaneous stochasticity. In the light of Gawedzki's work on the passive scalar problem, in [15], we argue that spontaneous stochasticity and irreversibility are intertwined in SQG, and provide numerical evidence for this connection. Our numerics, though, reveal that the deterministic SQG setting only features a tempered version of spontaneous stochasticity, characterised in particular by non-universal statistics.

6.4.3 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 non-globally Lipschitz drift and diffusion coefficients behaving as x^{α} , with $\alpha > 1$. On the basis of the previously proposed (semi-explicit) exponential-Euler scheme [23], we analyse 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. A journal paper will be submitted soon.

6.5 Axis E – Variability and uncertainty in flows and environment

6.5.1 Instantaneous turbulent kinetic energy modeling 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 [3] 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. First, we derive a family of mean-field dynamics featuring the square norm of the turbulent velocity. By approximating at equilibrium the characteristic nonlinear terms of the dynamics, we recover the so-called Cox-Ingersoll-Ross process, which was previously suggested in the literature for modeling wind speed. We then propose a calibration procedure for the parameters employing both direct methods and Bayesian inference. In particular, we show the consistency of the estimators and validate the model through the quantification of uncertainty, with respect to the range of values given in the literature for some physical constants of turbulence modeling.

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

6.5.2 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), one objective is 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 new software CDM-Sci (see Section 5). An article is in preparation to describe the CDM and illustrate it on a few selected examples.

7 Bilateral contracts and grants with industry

7.1 Bilateral grants with industry

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

Participants: Mireille Bossy.

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

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

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

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

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

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

8 Partnerships and cooperations

8.1 International initiatives

IFCAM

Participants: Jéremie Bec, Nicolas Valade.

IFCAM: *Indo-French Center for Applied Mathematics* 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. With the pandemic, the 2022 planed visit was postponed in January 2023.

SDE:TNA (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 is under preparation.

8.2 European initiatives

8.2.1 H2020 projects

Participant: Mireille Bossy, Christophe Henry.

VIMMP (Virtual Materials Market Place) is a EU H2020 project (started in January 2018 and ended in June 2022) in the program Industrial Leadership project in Advanced materials. VIMMP is a development project for a software platform and simulation market place on the topic of complex multiscale CFD simulations. As a VIMMP partner, CALISTO is co-working with EDF R&D at designing complex workflows through the EDF's cross-platform SALOME, involving Lagrangian aggregations, fragmentation with CODE_SATURNE. CALISTO also addresses some typical workflow design for uncertainty quantification, and experiments with them in two-phase flow simulation situation.

Design of a standardized method for multi-physics simulations. Within the framework of the European VIMMP project, CALISTO members have been co-working with EDF R&D at designing a standardized method (in the form of a query tree) that allows to collect all the physical and numerical information required to set-up scientific workflows for multi-physics simulations. During this final phase of the project, the CDM-Sci software (see section 5) has been illustrated on a scientific workflow used to compute particle aggregation in a turbulent pipe flow (using the open-source CFD code CODE_SATURNE). A publication is in preparation.

8.2.2 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.

8.2.3 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.

8.2.4 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 flow, 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 modelling 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

Chairing / Organizing events

- Mireille Bossy chaired and co-organized the *EMRSIM 2022 Conference* on simulation and optimization for marine renewable energy, which was held in Roscoff (May 2022).

Scientific seminars of the Team

- Since November 2020, CALISTO is organizing a Periodic Team Seminar every 4 weeks.
  In 2022, the following researchers were invited to give a presentation: Raphael Chetrite (LJAD, Nice), Michel Bergmann (Team Memphis, Inria, Bordeaux), Roxane Letournel (Safran, Chateaufort), Guillaume Cordonnier (Team GraphDeco, Inria, Sophia Antipolis), Valentina Sessa (CMA, Mines ParisTech, Sophia Antipolis), Eric Simonnet (InPhyNi, Nice), Sebastian Jara (University of Valparaiso, Chile), Nicolas Valade (Team Calisto, Inria, Sophia Antipolis), Sugan Murugan (ICTS, Bengalore, India).

9.1.2 Journal

Member of the editorial boards

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

Reviewer - reviewing activities

- Mireille Bossy acted in 2022 as a reviewer for the following international journals: Stochastics, Journal of Mathematical Analysis and Applications; ESAIM: M2AN, IMA Journal of Numerical Analysis.
- Christophe Henry acted as a reviewer for Acta Mechanica, Journal of Aerosol Science and Physical Review Fluids.

9.1.3 Invited talks

- Jérémie Bec was invited speaker to the following events: *Atmospheres, Oceans, Earths* – Unifying perspectives on geophysical and environmental multiphase flows (Santa Barbara, October 2022); Challenges and benchmarks for AI in complex fluids and flows (Rome, July 2022); Complex Lagrangian problems of particles in flows (Bangalore, March 2022), Modelling and analysis of turbulent transport, mixing and scaling (Cambridge, March 2022); Stochastic approaches to turbulence in hydrodynamical equations (Banff, March 2022).
- Mireille Bossy was invited speaker to the following events: International Seminar on SDEs and Related Topics (February 2022), RSE Saltire Facilitation Network on SDEs Seminar (February 2022), RSE Saltire Facilitation Network on SDEs Workshop (August 2022).

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, and 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

- Mireille Bossy reviewed project propositions from the generic ANR AAP 2022 and from H2020-MSCA-COFUND.

9.2 Teaching - Supervision - Juries

9.2.1 Teaching

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

- Stochastic modeling and numerical tools around the physics of complex flows (M. Bossy) a 10h course as guest lecturer to the 31st International Jyväskylä Summer School (advance graduate and PhD students).
- Fluid dynamics and turbulence (J. Bec): Doctoral Mines Paris (6h), ICTS (12h).
- The physics of turbulent flow (J. Bec): 2nd-year Mines Paris (4h).
- Microswimming (L. Giraldi): Master 2 cell physics Université de Strasbourg (6h).
- 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" (58h) 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.
- PhD in progress: Zakarya El Khiyati, "Reinforcement learning for the optimal locomotion of microswimmers in a complex chaotic environment" started in October 2021; supervised by Jérémie Bec and Laetitia Giraldi.
- PhD in progress: Fabiola Gerosa, "Turbulent fluid-particles coupling and applications to planet formation" started in October 2021; supervised by Jérémie Bec and Héloïse Méheut (Lagrange, Observatoire de la Côte d'Azur).
- PhD defended in March 29, 2022: Lorenzo Campana, "Stochastic modeling of non-spherical particles in turbulence"; supervised by Mireille Bossy.
- M2 Internship: Belgacem Othman (Sorbonne University, Paris), "Particle resuspension: modeling the effect of inter-particle collisions", supervised by Christophe Henry.
- M2 Internship: Paul Maurer (Sorbonne University), "Stochastic dynamics of particles in turbulence", supervised by Mireille Bossy.
- M2 Internship: Nicolas Valade (Mines ParisTech), "Spontaneous stochasticity of quasi-geostrophic surface turbulence", supervised by Jérémie Bec.
- M2 Internship: Carlamaria Cosenza (Politecnico di Torino), "Simulation of the dynamics of inertial particles in model flows", supervised by Jérémie Bec.
- M2 Internship: Hao Liu (Technology University Darmstad), "Numerical methods for optimizing the locomotion of flagellated microswimmers", supervised by Laetitia Giraldi and Jérémie Bec.
- M1 Internship: Mateo Ghezal (Université Paris-Saclay), "Tangent velocity of a reflected Langevin process and related bridge of the Brownian integral", supervised by Mireille Bossy.

9.2.3 Juries

- Mireille Bossy served as an examiner for the Ph.D. theses of Roxane LETOURNEL (CentralSupÉlec, February 2022), Rémi GERARD (Mines ParisTech, July 2022), Jean Michel MASEO (Université Côte d'Azur, November 2022).

9.3 Popularization

9.3.1 Interventions

- General audience talks (within Inria):
  The communication team within Inria Centre at Université Côte d'Azur is organizing general audience talks where researchers present some of their activities to staffs&researchers from the Inria centre.
  - Christophe Henry gave a presentation in February 2022 at Café In about the "Physics of sand castles".
  - Laetitia Giraldi gave a presentation in March 2022 at Café In about the "Scallop theorem".
- 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 Valbonne (Terra Numerica) and in Mouans Sartoux in October 2022, presenting a workshop on the "Physics of sand castles".

10 Scientific production

10.1 Publications of the year

International journals

[1] J. Bec, G. Krstulovic, T. Matsumoto, S. Sankar Ray and D. Vincenzi. 'Editorial: Scaling the Turbulence Edifice (part 2)'. In: *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences* 380.2219 (21st Mar. 2022). DOI: 10.1098/rsta.2021.0102. URL: https://hal.science/hal-03853666.

[2] J. Bec, G. Krstulovic, T. Matsumoto, S. S. Ray and D. Vincenzi. 'Editorial: Scaling the Turbulence Edifice'. In: *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences* 380.2218 (7th Mar. 2022). DOI: 10.1098/rsta.2021.0101. URL: https://hal.science/hal-03853659.

[3] 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.

[4] 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.

[5] M. Gupta, P. Chaudhuri, J. Bec and S. S. Ray. 'Turbulent route to two-dimensional soft crystals'. In: *Physical Review E* (2022). URL: https://hal.science/hal-02362959.

[6] C. Henry, J.-P. Minier and S. Brambilla. 'Particle resuspension: challenges and perspectives for future models'. In: *Physics Reports* (2022). URL: https://hal.inria.fr/hal-03909063.

[7] K. Martínez Rodríguez, M. Bossy and C. Henry. 'Particle agglomeration in flows: fast data-driven spatial decomposition algorithm for CFD simulations'. In: *International Journal of Multiphase Flow* 149 (Apr. 2022), p. 103962. DOI: 10.1016/j.ijmultiphaseflow.2021.103962. URL: https://hal.inria.fr/hal-03180740.

Doctoral dissertations and habilitation theses

[8] L. Campana. 'Stochastic modelling of non-spherical particles in turbulence'. Université Côte d'Azur, 29th Mar. 2022. URL: https://hal.science/tel-03666030.

Reports & preprints

[9] G. Barrué, R. Di Dio, Z. El Khiyati, Y. Guguen and R. Tayewo. *Report SEME for SCALIAN*. IRMAR - Université Rennes 1; Université Bretagne Sud; Université Cote d'Azur, May 2022, pp. 1–4. URL: https://hal.science/hal-03674181.

[10] L. Berti, V. Chabannes, L. Giraldi and C. Prud'Homme. *FLUID-RIGID BODY INTERACTION USING THE FINITE ELEMENT METHOD AND ALE FORMULATION: FRAMEWORK, IMPLEMENTATION AND BENCHMARKING*. 31st Oct. 2022. URL: https://hal.science/hal-03835136.

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

[12] 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*. 21st Nov. 2022. URL: https://hal.inria.fr/hal-03862286.

[13] F. A. Gerosa, H. Meheut and J. Bec. *Clusters of heavy particles in two-dimensional Keplerian turbulence*. 23rd Nov. 2022. URL: https://hal.science/hal-03868249.

[14] 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*. Sept. 2022. URL: https://hal.science/hal-02178973.

[15] N. Valade, S. Thalabard and J. Bec. *Anomalous dissipation and spontaneous stochasticity in deterministic surface quasi-geostrophic flow*. 23rd Nov. 2022. URL: https://hal.science/hal-03868221.

Other scientific publications

[16] A. Banari, C. Henry and G. Lécrivain. *EVIDENCE OF COLLISION-INDUCED EFFECTS IN PARTICLE RESUSPENSION*. Paris, France, 9th May 2022. DOI: 10.25576/ASFERA-CFA2022-27862. URL: https://hal.inria.fr/hal-03812861.

[17] J. Morán, R. M. R. Kholghy, C. Henry and J. Yon. 'Van der Waals interaction forces between raspberry-like Agglomerates of Nanoparticles'. In: CFA 2022 - Congres Français sur les Aérosols. Paris, France, 9th May 2022. URL: https://hal-normandie-univ.archives-ouvertes.fr/hal-03665520.

10.2 Cited publications

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

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[21] A. Banari, C. Henry, R. H. F. Eidt, P. Lorenz, K. Zimmer, U. Hampel and G. Lecrivain. 'Evidence of collision-induced resuspension of microscopic particles from a monolayer deposit'. In: *Physical Review Fluids* 6.8 (2021), p. L082301.

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[23] 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.

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

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

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