My research interests concern the theoretical modelling and the development of computational methods for problems in Fluid Dynamics, including particle laden turbulent flows, thermal convection, the dynamics and rheology of complex fluids (such as polymer solutions and soft-glassy materials) and active matter. During my scientific career I have acquired a thorough knowledge of theoretical methods (kinetic theory, perturbative methods for non-linear field theories, statistical closures for non-linear PDEs, stochastic methods, phenomenological modelling) and numerical techniques (pseudospectral methods, finite differences schemes, lattice Boltzmann algorithms, molecular dynamics, parallel computing). I have been trained to run massive simulations on the most powerful architecture for high performance computing in Europe, handling complex codes and large state-of-the-art databases. I have also had the opportunity to have direct experience with experimental measurements of turbulent thermal convection and flowing foams. Among my major scientific achievements, it is worth mentioning: the first measurement of the statistics of life times of vortex filaments in turbulent flows [1]; the development of a closure model for heavy particle pairs dispersion in turbulence [2]; the development of the first thermodynamically consistent thermal lattice Boltzmann method for multiphase fluids [3]; the discovery of the mechanism of mixing arrest in stratified Rayleigh-Taylor turbulence and its phenomenological modelling in terms of a statistical closure of the equations [3, 4]; the derivation of a scaling law for the front propagation speed in turbulent reactive mixing under unsteady conditions [5]; the first numerical simulation study of model self-propelled-colloids/chemotactic bacteria with fully resolved hydrodynamic and chemotactic interactions [6]; the derivation of a scaling law for the heat flux (Nusselt number) in turbulent Poiseuille-Rayleigh-Bénard flows [7]; the first experimental measurement of the distribution of plastic events in a Poiseuille flow of a foam [8, 9]. My wish is now to push my research further, to cutting-edge problems where, due to the convergence of diverse complex phenomena, a heterogeneous expertise is needed. I will focus on unexplored situations where the flow regime of complex or active fluids is turbulent. As discussed later on in these statements, this is far from being a purely speculative problem, having, instead, many geophysical, industrial and environmental applications. I plan to develop novel theoretical concepts and unconventional numerical tools which will lead, on a long term perspective, to the establishment of a unique *in silico* laboratory of biofluid and complex fluid dynamics. To this aim I will make use of:

- a Eulerian-Lagrangian code consisting of a fully dealiased 3d pseudospectral solver for the incompressible Navier-Stokes equations and of a ODE-solver for the Maxey-Riley equation [10] ruling the point-particle dynamics;
- a multiphysics package based on the lattice Boltzmann method, featuring: temperature dynamics, non-ideal equation of state (phase transition and coexistence), multiple components, Lagrangian dynamics of finite size resolved particles and point-like particles.

I. TURBULENT DYNAMICS OF ACTIVE FLUIDS

Active fluids, or active matter more in general, are ubiquitous in Nature, around us and inside [11, 12]. Flocks of birds, swarms of microrobots, bacterial colonies, oceanic plankton are instances of such systems. They consist of collections of elements immersed in a fluid, characterized by the common feature of being able to convert stored or ambient free energy into systematic movement, thus being intrinsically out-of-equilibrium. As such, they display a rich and striking phenomenology, including self-organisation, pattern formation, coordinated motion, etc. Since the pioneering work of Vicsek and coworkers on flocking, the last two decades have witnessed an upsurge of agent-based and continuum models trying to capture such collective behaviour. Birds flocks, fish schools or phytoplankton blooms, fly and swim often in a turbulent environment, notwithstanding almost all approaches have overlooked the dynamics of the fluid matrix, leaving its role as a major challenge. My interest is to study the effect of turbulence on the complex spatiotemporal evolution of active systems, and in particular on the capability and stability of animal flocking/schooling, and on the dynamics of populations of microorganisms (e.g. bacteria, plankton).

A. Flock models in turbulence

Possible sources of external perturbations to flocking are generically modelled as random noise in agent-based models, coarse-grained into diffusive terms for field equations in continuum approaches [11, 13, 14]. Fluid motion around birds/fish in a flock/school is far more complex than random noise, however the study of flock models in realistic flow fields is basically unexplored [15]. The forefront research that I wish to pursue consists, as a first step, of exploiting direct numerical simulations of homogeneous isotropic turbulence seeded with self-propelled particles, representing the active agents. The Navier-Stokes equations will be integrated by means of pseudo-spectral algorithms on tri-periodic cubic domains, while the Lagrangian dynamics of particles will be ruled by an equation of Maxey-Riley type [10], equipped with an extra term describing the ability of performing autonomous motion. Each particle carries an intrinsic (or *proper*) velocity vector with constant magnitude (i.e., the speed at which an isolated *animal* would travel, in absence of disturbances): the direction of such proper velocity is updated at every time step in such a way to align, with a certain characteristic relaxation time, to the average direction of neighbouring particles. The neighbours can be selected in term of either a metric criterion (those elements within a fixed distance), as proposed in the original Vicsek model [13], or a topological one (fixed number of closest elements), as recently suggested by experimental evidences from starling flocks [16]. This conceptual duplicity and the huge parameter space open a number of key questions, like: How does the topology and stability of a flock depend on the interaction rule? Can the interaction be related to hydrodynamic correlations among agents? How is the capability to form and mantain a flock affected by variation of parameters (e.g., turbulence level, proper particle velocity, particle inertia, alignment relaxation time)? Is there an optimal number of elements in a flock as a function of these parameters? Is it possible to derive a continuum (hydrodynamic) model for flock dynamics? How do flocks respond to turbulent structures? The last question motivates the introduction of an algorithmic way for animals to adapt to the environment. This feature will be implemented integrating the Eulerian-Lagrangian fluid dynamic solver with a *reinforcement learning* scheme (as, e.g., a Q-learning algorithm [17, 18]). According to the paradigm of reinforcement learning, an agent *learns* progressively how to act through a trial-and-error interaction with the environment, updating an action-value function (capturing the matured *experience*, or the *intelligence* of the agent) by means of a series of steps in which it gains a numerical *reward* corresponding to a certain action performed to reach a certain final state, given the initial state. The procedure will be used in conjuction with the interaction rules for the proper particle velocity (stated above) or in their place, thus resulting in an effective communication among individuals induced by fluid motion and filtered by reinforcement learning. On the other hand the learning algorithm will be exploited in numerical simulations where the Navier-Stokes equations for the fluid will be coupled with an advection-diffusion equation for a scalar field which can be a drive for animals coordinated motion, thus mimicking, e.g., the effect of temperature or of the terrestrial magnetic field in migratory movement.

B. Population dynamics in turbulence

In Nature, organisms are rarely distributed uniformly or at random, they form instead some sort of spatial patterns. This is due to various causes: environment inhomogeneities, externally induced drift, population competition for nutrients, or predation that result in spatially patchy structures. This spatial variance in the environment creates diversity in communities of organisms, as well as in the variety of the observed biological and ecological events. These observations are at the base of modern population dynamics and spatial ecology research. Most microorganisms live in inhomogeneous environments characterized by, e.g., spatially varying growth rates and/or diffusion constants. In order to face such heterogeneity, many microorganisms have developed the capability to propel themselves (e.g. by rotating helical flagella) in response to external stimuli: the most ubiquitous of such behaviours is *chemotaxis* [19], that is the ability to sense and direct movement in response to gradients of chemical species. The ocean is one of the largest reservoirs of bacteria and *plankton*. There, populations of these microorganisms are wildly advected by oceanic currents and turbulence. While turbulence acts, as it is well known, as a very efficient mixing mechanism for passive particles, the interplay between the dynamics of the population (characterized by swimming and birth/death processes) and turbulent transport may lead to formation of persistent patches; such *localization* events may influence significantly the fixation of a gene mutation at the edge of a growing population [20]. The studies of population dynamics in presence of convecting drift or turbulence have been limited so far to simple cases: steady flow in a prescribed geometry, [21, 22], random vortices model in a two-dimensional space [23], even one-dimensional shell-models of turbulence [24], or two-dimensional simulations [25], and typically neglecting chemotaxis. I propose to investigate, quantitatively, the effect of turbulence on the population dynamics by means of state-of-the-art, high resolution, pseudo-spectral simulations of turbulent flows coupled to models describing populations dynamics. Populations will be modelled in terms of a density field coupled with a concentration field (representing the chemical species after which bacteria chase, e.g., nutrients) according to the Keller-Segel (KS) model. An unprecented novelty of my approach will be the inclusion of a reaction-like term in the KS equations accounting for birth/death processes; a logistic type quadratic term will be used, as in the Fischer-Kolmogorov-Petrovsky-Piskunov equation [26, 27]. The equations for the density of bacteria and the chemical field will be integrated numerically by means of a finite-difference scheme. The description of chemotaxis in terms of an explicite chemical field dynamics allows to capture an essential feature, i.e. the fact that turbulence affects population dynamics also indirectly, through the stirring/mixing of such field: if, on one hand, its spreading by turbulence can favour the uptake of nutrients by bacteria, on the other a too strong turbulence level may mix the field below the threshold of capabilty of gradient-sensing by the microorganisms [28]. This investigations will provide insight on some unresolved challenges like: How does the degree of localisation depend on birth/death rates, diffusivities, chemotactic affinity, Reynolds number? Is there a critical Reynolds number for optimal chemotaxis?

II. TURBULENT HEAT TRANSFER IN COMPLEX FLUIDS

Heat transfer in fluids is a complex phenomenon, of utmost importance for several physical problems, of technological or natural origin: from climatology, to oceanography and geophysics, to industrial flows in heat exchangers [29–31]. The problems are even more challenging if, instead of a single (simple) fluid, one uses as the heat carrier a a system undergoing phase transitions, a liquid mixture, a solution or a suspension (generally speaking, a multicomponent system); notwithstanding, these are not just hypothetical complications, but actual examples of technological relevance. My aim is, then, to broaden the knowledge on the heat transfer properties of fluid systems, extending it to the case of *complex fluids* confined in *complex geometries*. By complex fluids I mean, here, basically multiphase fluids and liquids with additives (e.g. polymer solutions, suspensions of solid micro-/nano-particles).

A. Multiphase fluids

Thermal convection in multiphase fluids can be of great relevance for many industrial and natural problems. Besides the emergence of strong NOB effects, one has to cope, in this case, with the (non-linear) non-equilibrium thermodynamics of the phase transition. Despite having been boiling known since long time as an effective mechanism for heat transfer [32], there are issues, such as the influence of phase-coexistence, nucleation and/or bubble coalescence in the total heat flux, which are still far from being understood. In an actual experiment all the above processes occur at the same time and it is next to impossible to separately quantify their relative importance. I plan to exploit numerical simulations for this purpose. Ideally, a simulation should be able to resolve individual bubbles and to follow their evolution but, with the present capabilities, this great level of detail is sometimes dramatically simplified using point-like bubble models in which the interaction of the individual bubbles with the surrounding liquid is parametrized [33]. I propose to use, instead, a numerical method based on a lattice Boltzmann model for non-ideal fluids, where one can get naturally, through a suitable choice of internal forces, the stable formation of diffuse interfaces between liquid and gas/vapour phases, thus enabling the simulation of hydrodynamic equations containing the stresses arising from the density gradients (diffuse interface hydrodynamics) and any desired wettability properties at the boundaries [34]. This provides a general scheme of two-phase hydrodynamics involving the gas-liquid transition in non-uniform temperature profiles and, possibly, with non-trivial contact angles (i.e. triple contact lines) at the boundaries, which are known to play a major role on, e.g., two-phase pressure drop of flow boiling. The aim is to perform controlled numerical simulations of the heat transfer mechanism in a liquid with a mean temperature close to its boiling point, with full scale resolved vapour/gas diffuse interfaces. Here, bubbles and droplets can nucleate, deform, grow or shrink through evaporation and condensation and react back on the flow both thermally and mechanically [35].

B. Nanofluids

A nanofluid is a colloidal suspension of nano-sized particles (typically metal oxides, such as CuO or Al_2O_3) in a liquid (water, oil, ethylene glycol, among the most used); nanofluids are characterized by a notably enhanced thermal conductivity (up to 60%) with respect to that of the base fluid, even for a few percent concentration [38]. Thanks to these properties, nanofluids have gained a considerable engineering interest in the last years, as, for example, work fluids in heat exchangers. It has been noticed [39], moreover, that, under certain conditions, various phenomena, like, e.g., particle clusters formation or fluid-solid interfacial thermal (Kapitza) resistance, can significantly alter the heat transfer properties, which escape any attempt of theoretical predictions by simple effective medium arguments. Modelling can be even more difficult under flow conditions [40] (which is, anyhow, a situation of utmost relevance in technological applications). I propose to develop a Eulerian-Lagrangian approach for the simulation of thermal (possibly multiphase) flows in nanofluids. In this model the system is described as a continuum phase (the solvent, with an associated Eulerian velocity field) seeded with dispersed finite size particles (following a Lagrangian dynamics). The feedback of particles on the fluid velocity and temperature fields is taken into account through the setting of suitable boundary conditions for the momentum [41] and heat flux at the particle surface; in this way it is possible, for example, to incorporate the effect of the Kapitza resistance, when needed. On the other hand, collective effects (particles aggregation) have not to be added artificially by hand, but they may rather emerge naturally from the interplay between the particle dynamics and the underlying fluid flow topology (as it is known to happen in standard turbulence, where inertial particles clustering has been extensively studied experimentally and numerically, and characterized with tools borrowed from dynamical systems theory) [42]. Moreover, introducing non-ideal fluid behaviour, as discussed in the previous point, will enable to attack complex phenomena emerging in boiling nanofluids.

C. Polymer solutions

It is well recognized (reproduced in experiments and simulations and, somehow, epxlained theoretically) that adding small amounts of polymers to turbulent fluids in wall-bounded domain can significantly reduce the drag (Toms, 1949). However, much less is known about which can be the effect of polymer additives on the heat transfer properties of a thermally driven turbulent system. Recently theoretical/numerical [36] and experimental [37] studies have addressed this problem, however the picture is not yet fully clear and theoretically debated. I plan to develop a numerical approach where the hydrodynamics of the solvent is coupled to a coarse-grained field model of the polymer dynamics (e.g. Oldroyd, FENE-P models) and I will perform state-of-the-art numerical simulations, both in the natural and forced convection configurations, with variable roughness at the walls, in order to tune the contribution of the boundary layers to have an insight on the transition between the two regimes. To achieve a more realistic description an unprecedented feature (in turbulent thermal convection studies) will be introduced, that is a temperature-dependent "feedback" of the polymers, accounting for the thermal degradation of the chain molecules.

III. INFLUENCE OF THERMALLY INDUCED INERTIA ON MULTIPHASE FLOWS

The transport on inertial particles, such as droplets, bubbles, ashes, dusts, etc, by turbulent flows is an ubiquitous phenomenon in Nature, playing a crucial role in manifold problems of geophysical, environmental and industrial interest (see, e.g., [42] and references therein). This has motivated a huge amount of experimental, theoretical and numerical works on particle laden turbulent flows focusing, typically, on issues like the spatial distribution (on fractal sets) of particles, the dynamics an statistics of pair and multi-particle dispersion or the statistical properties of small scale quantities such as velocity fluctuations, acceleration, curvature of particle trajectories. In the huge majority of these studies particles have no effect (feedback) on the carrier fluid; the original ideas that I want to develop concern the case where such effect stems from the particles carrying a heat content, i.e. being there temperature differences between particles and the fluid. Few studies have addressed this problem for a single particle or a pair in simple flows and in simple geometries [43]. These studies have shown that the convective flow surrounding the particles can fundamentally change the particle behavior in terms of sedimentation velocity (as in *thermal levitation*) and of interaction with neighbouring particles or boundaries. Interestingly, one can imagine that, even in laminar flows, if the temperature difference between particle and fluid is high enough, locally the Reynolds number can be large thus triggering non-trivial inter-particle correlations (i.e. a collective dynamics). For particles in a buoyant plume, such as that of volcanic ashes, the heat content of the particles may be critical for the energetics, and can, under some circumstances be a dominant source even when compared with latent heat of vapour condensation [44, 45]. Also relevant in this respect are the settling characteristics of a field of hot particles in a turbulent flow field under gravity. The particle thermal inertia, describing the relation between the timescale of cooling of the particle and the thermal timescale of the fluid flow, provide an estimate for the tendency to equilibrate or lag beyond the surrounding fluid temperature and may be a critical parameter in determining particles influence on the temporal and geometrical plume dynamics. My plan is to develop a theoretical understanding of the influence of thermal inertia on the dynamics of individual and clouds of particles in three-dimensional turbulent thermal flows. To this aim I will performed state-of-the-art numerical simulations using a thermal lattice Boltzmann method with finite size resolved particles, equipped with a solver for the Lagrangian dynamics of point-like particles. The problem will be tackled, numerically, at two levels of resolution for particles. When a single particle or pairs are considered, in simple setups such as under gravity or in a laminar shear, these will be treated as finite size objects at whose surfaces a proper boundary condition for the exchange of momentum and heat with the fluid is set (in the spirit of Ladd's bounce-back-on-links algorithm [41]). The goal is to formulate a phenomenological model for single particle dynamics building up on hints from the numerics; in other words the question is: Can the effect of particle-fluid thermal mismatch be described in terms of an effective force to be added in the Maxey-Riley equation [10] for point-particles? The development of such a high-risk tool open the way to new challenges, allowing to extend the study to point-particles. In this case, massive simulations will be run with large numbers (billions) of particles (initially homogeneously distributed or emitted from localised point-like sources [46], mimicking, e.g., a volcanic eruption) enabling to address, with unprecedented statistics, problems related to the dynamics of hot/cold clouds of particles like: How does thermal inertia affect particle spatial distribution and dispersion? How do thermally inertial particles affect turbulent Eulerian structeres (e.g. vortex filaments)? How does a cloud settle under gravity? The latter question suggests to explore the turbulent mixing dynamics of a cloud with clear fluid, unveiling intriguing analogies with Rayleigh-Taylor turbulence. Overall the results of these investigations must be expected to have high impact on fields as diverse as cloud physics, the formation, rise and settling of volcanic ash plumes and industrial processes involving thermal multiphase flows, amongst others.

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