Summary for the PhD thesis
“Particle motion and gradient dynamics in turbulent flows: Theory and Numerical Simulations”

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The dynamics of fluid and inertial particles in turbulence is the main topic of this thesis. The work is divided in two parts. The first part deals with the theoretical investigation of turbulent flows, which constitute a major open problem in classical mechanics. We begin with the analysis of the turbulent energy cascade across the scales of statistically steady and isotropic turbulence. The energy cascade is a signature of time-irreversibility of turbulence and it has important implications on the motion of fluid and inertial particles in turbulent flows. An expression for the average cascade is derived in terms of coarse-grained Vortex Stretching and Strain Self Amplification, starting from the two-point energy balance and taking to account compressibility issues by introducing an incompressible filtered velocity increment. The role of Vortex Stretching and Strain Self Amplification mechanisms is examined in detail by studying the Lagrangian dynamics of the velocity gradient in the strain-rate eigenframe. The equations for the velocity gradient dynamics along the fluid particle trajectory are unclosed due to the non-locality of the pressure Hessian contribution and viscous stress. The non-local part of the pressure Hessian plays a key role in preventing singularities of the gradients but its statistical relation to local velocity gradients is not yet fully understood. A symmetry for the non-local pressure Hessian is proposed, which allows for a reduction of its dimensionality and complexity. The proposed gauge symmetry allows to transform the three-dimensional pressure Hessian into a two-dimensional tensor leaving the one-point dynamics of the velocity gradient invariants unchanged. The aim of this part is to provide a little insight into the turbulent dynamics relying on geometry and statistical analysis of results from Direct Numerical Simulations of Navier-Stokes turbulence. In the second part the dynamics of inertial particles in turbulence is considered, with focus on momentum, heat and mass transfer in particle-laden flows. The Nonuniform Fast Fourier Transform (NUFFT) is proposed as an efficient tool to perform numerical simulations of two-way coupled particle-laden flows. The NUFFT has been employed in various research areas but not yet in the field of particles in turbulence. Here it is shown that the NUFFT algorithm suits very well to the point-particle model. Details on the accuracy and parallel scaling of a pseudo-spectral code equipped with the NUFFT algorithm for the Direct Numerical Simulation of two-way coupled flows are presented. Then, numerical experiments of two-way coupled particle-laden flows are carried out with focus on the thermal coupling. Several results are presented to characterize the fluid and particle temperature statistics, focus is put on the scale scale-dependence of two-particle statistics and thermal caustics is observed. A novel characterization of the interaction between the temperature gradients and inertial particles is also introduced. Finally, the condensational growth of water droplets in atmospheric clouds is studied, with focus on the effect of the droplet thermal inertia and on the influence of the large-scale forcing scheme. It is shown that temperature fluctuations can enhance the droplet condensational growth and that the details of the external forcing can play a relevant role, despite the broad scale separation between the droplet size and the forced scale. A more detailed overview of the Fortran-MPI code employed for the Direct Numerical Simulations of two-way coupled particle-laden flows, developed by the candidate during the PhD period, is in the Appendix. The most relevant modules of the parallel code are reported and described.