Large Eddy Simulations of Turbulent Single-Phase and Dispersed Two-Phase Flows

Michał Rajek, M.Sc. Eng.

Doctoral advisor: **Prof. Jacek Pozorski**

General introduction

Turbulent dispersed two-phase flows with a particulate phase in the form of solid particles, droplets or bubbles represent a significant part of flows relevant to many environmental phenomena and industrial processes. It should be emphasized that the turbulent transport of the particulate phase still poses a major challenge in both theoretical and computational contexts. The reason for this can be partly attributed to the inherent non-linearity of this process and the wide range of spatial and temporal scales associated with both the underlying turbulence and the particulate phase itself. Things become even more complex if one considers not only gravitational effects, chemical reactions or phase transition, but also momentum exchange between the phases, collisions and coalescence within the dispersed phase, and other particle-particle interactions. Although in certain cases far-reaching simplifications can be introduced, a more profound understanding of the physics underlying particulate two-phase flows requires a multidisciplinary approach, combining not just theoretical predictions, mathematical modeling or laboratory and real-world experiments, but also numerical methods and high-performance computing. Despite significant developments in experimental methods, both inevitable limitations of measuring instruments and other technical constraints often make it challenging, or even unfeasible, to perform experiments relevant to turbulent dispersed two-phase flows. For this very reason, future advancements in this very matter will probably be contingent on further developments not only in mathematical and numerical modeling but also experimental methods. On the other hand, it should be emphasized that a rapid growth of computing power has contributed greatly to the development of the foregoing fields, and thus has opened up entirely new perspectives for studying the dispersed two-phase flows.

Background and motivation

The so-called "warm" rain formation is an example of a two-phase process in which an insufficient description of the turbulent transport of the particulate phase causes significant discrepancies between model predictions and reality. Warm rain occurs when the average temperature throughout the cloud is above the freezing point. It accounts for approximately 30% of the total rainfall on Earth. It is well established that cloud droplets effectively grow by the diffusion of water vapor until they reach approximately 5 µm to (numerical range) 20 µm in radius, from where further growth is triggered by collision-coalescence. On the other hand, gravity-induced collisions are most pronounced for cloud droplets that have exceeded approximately 60 µm to (numerical range) 80 µm in radius. This essentially leaves a gap in the description of the mechanism governing the growth of cloud droplets. Based on an extensive literature on this very issue, one can conclude that the growth of droplets having approximately 20 µm to (numerical range) 60 µm in radius is driven by cloud turbulence and aerodynamic interactions between the them. Although the turbulent atmosphere is a truly multiscale phenomenon in which the characteristic length scales can vary from millimeters up to several hundred kilometers, a more profound understanding of the warm rain formation can be attained through modeling the microphysical processes, that is, at length scales comparable to the smallest ones in a turbulent flow.

One of the essential tools commonly used for studying particulate two-phase flows are the so-called Direct Numerical Simulations (DNS) in which the full Navier-Stokes equations governing the motion of a Newtonian fluid (possibly incompressible, as in this work) are solved without any simplifications. Turbulent atmosphere in microscale is often modeled as homogeneous and isotropic, sometimes also statistically stationary. The latter property is usually achieved by introducing a forcing term in the momentum balance equation, whose sole purpose is to compensate for the energy dissipation. At this point, it should be emphasized that while the forcing term is artificial, it attempts, from a physical perspective, to model specific mechanisms facilitating the generation of turbulence. Indeed, in real flows, kinetic energy production typically results from, e.g., the mean pressure or temperature gradients. This clearly indicates the anisotropy of the flow, whereas the inevitable presence of boundaries also implies its inhomogeneity. For these very reasons, isotropic turbulence is to some extent unphysical yet experimentally accessible mathematical model of a real turbulent flow. For instance, the so-called grid turbulence generated in a wind tunnel can be considered an example of freely decaying isotropic turbulence, whereas at certain length scales, a channel flow (assuming, e.g., a constant pressure gradient) can be considered an example of statistically stationary isotropic turbulence; however in both cases, the aforementioned approximations hold only close to the respective center lines.

The DNS allows for simulating cloud microphysical processes at length scales varying from millimeters up to several meters. Starting in the early 1970s, isotropic turbulence has most commonly been solved using the pseudo-spectral approach with a computational domain being a cube of certain size. Isotropy can be ensured by imposing both zero-mean flow and periodic boundary conditions. In addition to that, statistical stationarity can be achieved by forcing specific Fourier modes in either deterministic or stochastic manner; however, it should be emphasized that none of the commonly used forcing terms can be implemented experimentally. Owing to the fact that cloud droplets are initially much smaller than the smallest flow scales in a turbulent flow, these entities can be safely approximated by point particles. In this case the Lagrangian particle tracking is coupled with the DNS leading to the so-called point-particle DNS (PP-DNS). Despite far-reaching simplifications, this model has contributed greatly to the understanding of various phenomena relevant not only to cloud microphysics but also other types of processes.

A significant development in both experimental and numerical methods has been observed over the past years. Recent studies focused on turbulent dispersed two-phase flows allow to conclude that the point-particle approximation may be insufficient, and thus can lead to pronounced discrepancies between numerical simulations and experiments (or even real-world observations). At this point, it should be emphasized that in the case of single-phase flows, the DNS results are usually in excellent agreement with experimental data. For this very reason, the method itself has attained the status of a numerical experiment over the past decades. It is also worth mentioning that both significant development of numerical methods and exponential growth of computing power have given rise to the so-called particle-resolved DNS (PR-DNS) in which all details of turbulence, particularly including the flow around each particle, are resolved. This allows one to determine the hydrodynamic forces exerted on a moving particle more accurately. Unfortunately, due to significant computational cost associated with this approach, the PR-DNS allows to account for a relatively small number of particles. It appears that due to invaluable practical significance, the PP-DNS will remain the method of choice for studying particulate two-phase flows. It is also anticipated that further insights into the physics underlying these flows will result from the combined developments in mathematical modeling, experimental techniques and numerical simulations using the PP-DNS, however with enhancements following from the PR-DNS.

Due to the lack of both the mean flow and a well-defined characteristic dimension, isotropic turbulence is most often characterized by means of the Reynolds number based on the Taylor microscale λ, which is associated with the spatial correlation of the velocity field. The computational cost of the DNS still prevents one from studying turbulent flows at Reynolds numbers relevant to cloud turbulence where $Re_\lambda \sim 10000$. Unfortunately, in the case of single-phase turbulence, the current state-of-the-art DNS is approximately at $Re_\lambda \sim 2500$, with the spatial resolution of $\sim 32786^3$ nodes, whereas the PP-DNS is currently at $Re_\lambda \sim 600$, with the computational grid of $\sim 4096^3$ nodes and approximately 1024^3 point particles in order to obtain the appropriate volume fraction of the dispersed phase. Considering the practical significance, it seems that one of the most important achievements in the field of computational fluid dynamics is the development of the so-called Large Eddy Simulations (LES). In this method, only the large, energy-containing flow scales are resolved. With increasing Reynolds number, small-scale turbulence is expected to exhibit universal scaling properties regardless of the complexity of a turbulent flow, and hence can be filtered out, eventually leading to significant computational savings. The impact of the unresolved part of turbulence is usually accounted for statistically; however, different, more explicit approaches are equally often of interest. Although the LES is widely used in various industrial applications, it has not gained much attention in studying the fundamental aspects relevant to the dynamics of inertial particles suspended in a turbulent flow. It should be emphasized that in the case of single-phase turbulence, the spatial filtering can be compensated relatively easily, whereas in the case of two-phase flows, the lack of small-scale turbulence also impacts inertial particle dynamics, and thus may imply the need for more advanced modeling. The scientific literature covering this very matter remains limited and, in most cases, primarily concerned with reconstructing specific particle statistics obtained using the PP-DNS. It does not provide any insights into more practical capabilities of either the LES or the PP-LES, particularly within the range of parameters they were originally designed for.

Abstract

It should be emphasized that all simulations performed in this work are of general purpose, and thus can be potentially used to quantify different physical processes provided that relevant dimensionless numbers remain unchanged. However, mostly to provide a more physically-oriented context, this work was devoted to the application of the PP-LES in research concerning particle-laden turbulent flows, specifically within the range of parameters relevant to cloud turbulence. This dissertation is essentially composed of two parts concerning the DNS and the LES of respectively the single-phase turbulence and the particle-laden one.

In the first part, a new pseudo-spectral code for either decaying or forced isotropic

turbulence was developed. In the latter case, it has been indicated that frequently reported forcing parameters can lead to artificially correlated velocity fields by amplifying the influence of periodic boundary conditions. For this very reason, the results of numerical simulations differ significantly from the model predictions. It has been shown that specific forcing parameters can be selected so that both the longitudinal and transverse velocity autocorrelation functions take correct forms, particularly vanishing at separations equal to approximately half the size of the computational box. Depending on the Stokes number, that is, a measure of particle inertia, this property can have a significantly beneficial impact on particle dynamics. In addition to the above, this research study indicates that for a given spatial resolution, the Reynolds number based on the Taylor microscale strongly depends on the selected range of forced Fourier modes, which can lead to incorrect conclusions regarding the required spatial resolution of the DNS. Recently, many research studies have been devoted to developing the so-called autonomous LES in which all model parameters are determined from the resolved velocity field. Partly for this very reason, in this work a new approach to model the impact of the small-scale turbulence on the resolved one was developed based on a scale-dependent eddy-viscosity determined by minimizing the instantaneous difference between the resolved and reference (imposed) energy spectrum functions. It has been indicated that within the range of parameters appropriate for LES, the new approach accurately models the impact of unresolved small-scale turbulence. This part also outlines certain prerequisites (or necessary conditions) for considering the LES a tool for studying turbulent flows at high Reynolds numbers, particularly concerning the selection of model parameters and the spatial resolution of the LES itself.

The second part, concerning the motion of inertial particles suspended in a turbulent flow, was devoted to assessing the capability of the LES to capture certain particle-related phenomena, e.g., the preferential concentration and the preferential sweeping. In this part, particle dynamics was quantified by, e.g., the settling speed enhancement, the probability density function of the second invariant of the velocity gradient tensor sampled at particle locations, the spectrum of the particle number density, the radial distribution function and the radial relative velocity. For instance, the two latter statistics are of significant importance for accurate parametrization of droplet collisions, which is essential to improving the quality of mesoscale numerical weather prediction models. It has been indicated that as long as the ratio between the spatial resolution of the DNS and the LES is on the order of 4, certain particle statistics in the LES remain in exceptionally good qualitative and satisfactory quantitative agreement with the DNS. Recent studies have revealed that in addition to the clustering at length scales comparable to the smallest resolved ones in a turbulent flow, inertial particles also exhibit a tendency to cluster at length scales relevant to the inertial subrange. It has been shown that the new model allows to statistically quantify this phenomenon with outstandingly good quantitative agreement with the DNS. The results indicate that the LES enriched with the new statistical parametrization of small-scale turbulence allows for studying turbulent dispersed two-phase flows within the range of parameters relevant to turbulent atmosphere.

It appears that the advent of both petascale and exascale simulations has opened entirely new possibilities for the use of the LES for studying turbulent single-phase and dispersed two-phase flows, specifically within the range of Reynolds numbers unreachable by now. Despite inevitable deficiencies of the method itself, the results indicate that this approach creates the potential for further advancements in the understanding of the physics underlying turbulent dispersed two-phase flows. Although all simulations considered in this work have been performed using a personal general-purpose computer, it appears that a natural extension of this research is to adapt the current pseudo-spectral code to large-scale computing.