



UNIVERSITÀ
DEGLI STUDI
DI PADOVA

Sede Amministrativa: Università degli Studi di Padova

Centro di Ateneo di Studi e Attività Spaziali “Giuseppe Colombo” - CISAS

PhD Course: Sciences, Technologies and Measurements for Space

Curriculum: Sciences and Technologies for Aeronautics and Satellite Applications - STASA

HIGH-FIDELITY SIMULATION AND MODELING OF TURBULENT DISPERSED MULTIPHASE FLOWS

Coordinatore: Ch.mo Prof. Francesco Picano

Supervisore: Ch.mo Prof. Francesco Picano

Co-Supervisore: Ch.mo Prof. Federico Dalla Barba

Dottorando: Xiang'en Kong

Abstract

Particulate-laden flow refers to a two-phase fluid flow in which one phase is continuous (referred to as the carrier phase) and the other phase consists of fine, insoluble, and typically dilute particles (known as the dispersed or particulate phase). An example of particulate flow is the transport of fine aerosol particles in air, where aerosols represent the dispersed phase and air serves as the carrier phase. Two-phase flow modeling has a wide range of applications in both engineering and scientific disciplines, including atmospheric pollution dispersion, fluidization in combustion processes, and aerosol deposition in pharmaceutical sprays. Accurately predicting the behavior of these flows is essential for optimizing engineering applications and understanding environmental phenomena. This understanding can be achieved through experimental studies and numerical simulations. However, numerical simulations are often hindered by the complexity of turbulent interactions between the carrier phase and the dispersed particles. In this context, the present paper focuses on the development of a novel numerical approach that combines a semi-stochastic model based on the Langevin equation with drift correction and the Wall Modelling Large Eddy Simulation (WM-LES) framework for simulating particle-laden turbulent channel flows in one-way coupling conditions. A comprehensive description of the theoretical framework and its numerical implementation is provided. The paper presents various statistical velocity properties of both the carrier and dispersed phases. The results demonstrate that the proposed method accurately reproduces particle dynamics across a range of Reynolds and Stokes numbers, in comparison with reference data obtained from direct numerical simulations. The model effectively captures key aspects of particle behavior, including velocity fluctuations, the accuracy of particle velocities near the wall, and the expected logarithmic distribution of axial velocities in the logarithmic region. Additionally, the method successfully replicates particle concentration trends both near the fluid wall and within the bulk flow region. The author believes that these findings underscore the potential of the semi-stochastic WM-LES framework to enhance the accuracy and efficiency of particle-laden flow simulations, offering valuable insights into turbulent particle dynamics.

Contents

1	Introduction	4
2	State of the art	11
2.1	Turbulent flows: theoretical aspects and modeling	11
2.1.1	Theoretical aspects	11
2.1.2	Simulation: DNS, RANS and LES	17
2.2	Particle-laden Turbulent Flows	29
2.2.1	DNS for particle-laden turbulent flows	32
2.2.2	RANS for particle-laden turbulent flows	42
2.2.3	LES for particle-laden turbulent flows	44
2.3	Stochastic Modeling in Turbulence Simulations	49
2.3.1	Development of stochastic models	49
2.3.2	Langevin equations in turbulence simulations	54
3	Numerical Methods and Models	75
3.1	Governing Equations for the Carrier Phase	75
3.2	Modeling of the Dispersed Phase	77
4	Model Validation and Results Analysis	84
4.1	Computational Domain and Simulation Setup	84
4.2	Statistics of the carrier phase – Validation of the WM-LES im- plementation	86
4.3	Statistics of the dispersed phase	87
5	Final remarks and future perspectives	96
A	Sensitivity of the semi-stochastic WM-LES model from the interface parameters	98

CHAPTER 1

Introduction

Particle-laden, turbulent multiphase flows are fundamental to a wide range of natural and industrial processes, including atmospheric transport of aerosols [3], sediment transport [22, 4], and pollutant dispersion [11, 10]. Accurately predicting the behavior of these flows is crucial for optimizing engineering applications and understanding environmental phenomena. However, the complexity of turbulent interactions between the carrier phase and the dispersed particles poses significant modeling challenges. Large-Eddy Simulation (LES) provides a powerful tool to capture turbulence dynamics by resolving large-scale structures while modeling the effects of smaller, unresolved scales, thus reducing the computational cost of such simulations. However, when applied to wall-bounded flows, standard LES requires extremely fine grids near solid boundaries, making computations still prohibitively expensive in many cases of practical interest. Wall-modeled LES (WM-LES) offers a more feasible alternative by incorporating wall models to approximate near-wall turbulence, significantly reducing computational costs.

In the context of particle-laden flows, the accuracy of WM-LES depends not only on the turbulence model for the carrier phase but also on the representation of subgrid-scale velocity fluctuations sampled by the particles and the reconstruction of near-wall turbulence. Developing reliable modeling approaches within the WM-LES framework is essential to capturing key phenomena such as turbophoresis, preferential concentration, and particle deposition. In this context, this study aims to advance the modeling of particle-laden turbulent flows in WM-LES by addressing the challenges associated with near-wall turbulence reconstruction and its impact on particle dynamics.

In the context of particle-laden turbulent flows, modeling the transport and dispersion of the dispersed phase requires an appropriate formulation of the forces acting on the particles. These forces depend on the relative motion

between the carrier phase velocity at the particle location and the particle velocity itself. However, no exact formulation exists for these forces in a turbulent flow. A widely used reference is the expression derived by Maxey and Riley [12] for an isolated, small particle in a Stokes flow, which has become the standard approach in deterministic Direct Numerical Simulation (DNS) studies. In such cases, the entire turbulent velocity field of the carrier phase is fully resolved, and various interpolation schemes are employed to determine the gas velocity at particle locations. However, in the context of LES, the velocity field is only partially resolved, meaning that evaluating the particle forces based solely on the resolved flow field would neglect the effects of unresolved velocity fluctuations on particle motion. To address this limitation, additional modeling strategies are required to account for subgrid-scale turbulence effects on the particle dynamics. Additional complexity arises in the frame of WM-LES, where the entire velocity field in the near-wall region should be modeled.

In the last decades, many researchers have contributed to the advancement of both Wall-Resolved Large-Eddy Simulation (WR-LES) and WM-LES for particle-laden turbulent flows. These efforts have focused on improving the accuracy of particle behavior predictions, particularly in challenging regions such as the near-wall area, where traditional methods often struggle due to high particle concentrations and complex turbulence structures. In the simulation of two-phase flows at low Reynolds numbers, WR-LES combined with the Lagrangian point-force method has demonstrated the ability to produce results that align well with DNS and experimental observations [2, 14, 20, 6]. Different models have been designed to account for subgrid-scale turbulence. Broadly speaking, two types of models have been developed to account for missing subgrid-scales in the particle equation of motion. The first type involves stochastic models, either by adding broadband stochastic noise to the Navier-Stokes equation for the continuous phase [8], or by introducing an additional velocity term in the particle equation of motion [15]. The second type uses approximate deconvolution of the filtered fluid velocity to estimate the unfiltered velocity, which is then applied in the particle equation of motion [9].

Bini and Jones [2] developed a stochastic model for subgrid-scale fluid velocity contributions, capturing the non-Gaussian behavior of particle acceleration observed in experiments and DNS. They achieved this using a nonlinear stochastic differential equation for the particle-fluid relative velocity. Later, they applied this approach to a droplet-laden spatially developing mixing layer.

Pozorski and Apte [14] studied the impact of using the filtered velocity field in particle motion equations within homogeneous isotropic turbulence.

They focused on the changes in preferential concentration patterns of particles and proposed a stochastic Langevin model for the subgrid contributions to fluid velocity. This model, based on subgrid-scale turbulence kinetic energy, successfully reconstructs the particle turbulence kinetic energy.

More recently, Wu et al. [20] propose a machine-learned subgrid-scale model applied to LES of heavy particles in isotropic turbulence, with a particular focus on particles with varying Stokes numbers. The model, based on the gene expression programming method, is tested for the first time in multiphase problems. The results show that the proposed model significantly improves predictions of particle statistics, including particle acceleration, velocity, and clustering, compared to traditional models.

Hausmann et al. [6] developed a modeling framework for LES of particle-laden turbulent flows that captures the interactions between the particle and fluid phases on both the resolved and subgrid-scales. Unlike most existing subgrid-scale models, the proposed framework accounts for the influence of subgrid-scale velocities on particle acceleration and also considers the impact of particles on the turbulent fluid flow. Even if subgrid-scale plays a role in the modeling of turbulent, particle-laden flows, there are different conditions under which the latter can be neglected. When the particle relaxation time is much larger than the typical turbulent flow time scales and the smallest time scales resolved in the LES, the subgrid scales of the fluid velocity have been shown to have a minimal influence on particle motion [16, 19, 21]. In such cases, the effects of unresolved turbulence on particle dynamics are negligible, and a subgrid model for the particle equation of motion is unnecessary. Armenio et al. [1] showed through both a priori and a posteriori studies that subgrid scales had little effect on particle motion, particularly in cases where the particle relaxation time is significantly larger than the turbulence time scales. Moreover, Wang and Dalla Barba [17] assessed the reliability of LES neglecting the subgrid-scale fluctuations for different LES resolutions of turbulent sprays laden with droplets demonstrating that, in many cases, these can be successfully neglected, at least for what concerns the reproducibility of mean droplet motion and evaporation.

In turbulent flows bounded by walls, the gradient in turbulence intensity along the wall-normal direction causes inertial particles to migrate toward the wall, leading to increased particle concentrations in the near-wall region. Accurately capturing this effect poses a challenge for WM-LES, as the small-scale structures and sharp gradients characteristic of the viscous sublayer and buffer region are not explicitly resolved in this modeling approach. As a result, WM-LES is often viewed as less suitable for predicting turbophoresis compared to

more detailed methods. Compared to WR-LES, the literature on WM-LES for particle-laden flows is relatively limited, reflecting the additional complexities involved in modeling subgrid-scale particle dynamics near the wall. To the best of the authors knowledge, the first effort to develop an advanced model for WM-LES of particle-laden flows was presented by Johnson et al. [7], who specifically addressed these challenges in the context of turbophoresis. In particular, using a DNS-tuned interpolation kernel below the first grid point has been shown to improve the prediction of particle concentration profiles within the WM-LES framework. Recently, Fazeli et al. [5] assess the performance of WM-LES using an algebraic equilibrium wall model for internal turbulent flows, with and without particles, in 90° bent pipes. They compare the results with experimental data, DNS, and other numerical approaches, including standard LES and Reynolds-averaged Navier-Stokes (RANS) with a Reynolds stress model (RSM). Their findings indicate that, despite the limitations of equilibrium wall models in nonequilibrium flows, WM-LES accurately predicts particle deposition efficiency for Stokes numbers greater than 0.5 but performs less accurately for smaller Stokes numbers.

Finally, Wang et al. [18] presented a new wall model for LES of particle-laden flow over an erodible bed. The model incorporates conserved momentum flux and Prandtl's mixing length for turbulent viscosity, alongside empirical expressions for particle mass flux, saltating height, and a correction coefficient. The model's performance is tested against WR-LES with Lagrangian particle tracking, showing superior predictions of particle statistics compared to other methods.

In this context, WM-LES for particle-laden turbulent flows requires further development to enhance the reliability and universality of the models. This work aims to address the gap in the literature by proposing a more general modeling approach to tackle the problem. The carrier phase is described by the three-dimensional, incompressible Navier-Stokes equations, solved using implicit filtering along with a Wall Adapting Local Eddy (WALE) viscosity subgrid-scale model [13] and an equilibrium wall model to reconstruct near-wall stresses. Particle dynamics are modeled with the classical point-particle approach, while a semi-stochastic model is employed to reconstruct the carrier-phase velocity fluctuations sampled by the discrete phase in the near-wall region, where LES resolution is limited. This model is based on Langevin equations with drift correction for the streamwise and spanwise velocity components, while the wall-normal velocity is reconstructed separately similarly to what has been proposed in Johnson et al. [7].

Bibliography

- [1] V. Armenio, U. Piomelli, and V. Fiorotto. Effect of the subgrid scales on particle motion. *Physics of Fluids*, 11(10):3030–3042, 1999.
- [2] M. Bini and W.P. Jones. Large-eddy simulation of particle-laden turbulent flows. *Journal of Fluid Mechanics*, 614:207–252, 2008.
- [3] Silvia M Calderón, Juha Tonttila, Angela Buchholz, Jorma Joutsensaari, Mika Komppula, Ari Leskinen, Liqing Hao, Dmitri Moiseev, Iida Pullinen, Petri Tiitta, et al. Aerosol–stratocumulus interactions: towards a better process understanding using closures between observations and large eddy simulations. *Atmospheric Chemistry and Physics*, 22(18):12417–12441, 2022.
- [4] G. DAlessandro, Z. Hantsis, C. Marchioli, and U. Piomelli. Accuracy of bed-load transport models in eddy-resolving simulations. *International Journal of Multiphase Flow*, 141:103676, 2021.
- [5] M. Fazeli, H. Emdad, M.M. Alishahi, and S. Rezaeiravesh. Wall-modeled large eddy simulation of 90 bent pipe flows with/without particles: A comparative study. *International Journal of Heat and Fluid Flow*, 105:109268, 2024.
- [6] M. Hausmann, F. Evrard, and B. van Wachem. Large eddy simulation model for two-way coupled particle-laden turbulent flows. *Physical Review Fluids*, 8(8):084301, 2023.
- [7] P.L. Johnson, M. Bassenne, and P. Moin. Turbophoresis of small inertial particles: theoretical considerations and application to wall-modelled large-eddy simulations. *Journal of Fluid Mechanics*, 883:A27, 2020.
- [8] A.K. Kuczaj and B.J. Geurts. Mixing in manipulated turbulence. *Journal of Turbulence*, 7:N67, 2006.
- [9] J.G.M. Kuerten. Subgrid modeling in particle-laden channel flow. *Physics of fluids*, 18(2), 2006.
- [10] X.Y. Li, H. Wang, J. Chen, S. Endo, G. George, B. Cairns, S. Chellappan, X. Zeng, S. Kirschler, and C. et al. Voigt. Large-eddy simulations of marine boundary layer clouds associated with cold-air outbreaks during the activate campaign. part i: Case setup and sensitivities to large-scale forcings. *Journal of the atmospheric sciences*, 79(1):73–100, 2022.

- [11] M.L. Lu and J.H. Seinfeld. Study of the aerosol indirect effect by large-eddy simulation of marine stratocumulus. *Journal of the atmospheric sciences*, 62(11):3909–3932, 2005.
- [12] M.R. Maxey and J.J. Riley. Equation of motion for a small rigid sphere in a nonuniform flow. *The Physics of Fluids*, 26(4):883–889, 1983.
- [13] Franck Nicoud and Frédéric Ducros. Subgrid-scale stress modelling based on the square of the velocity gradient tensor. *Flow, turbulence and Combustion*, 62(3):183–200, 1999.
- [14] Jacek Pozorski and Sourabh V Apte. Filtered particle tracking in isotropic turbulence and stochastic modeling of subgrid-scale dispersion. *International Journal of Multiphase Flow*, 35(2):118–128, 2009.
- [15] O. Simonin, E. Deutsch, and J.P. Minier. Eulerian prediction of the fluid/particle correlated motion in turbulent two-phase flows. *Applied Scientific Research*, 51:275–283, 1993.
- [16] WSJ Uijttewaal and RVA1027 Oliemans. Particle dispersion and deposition in direct numerical and large eddy simulations of vertical pipe flows. *Physics of Fluids*, 8(10):2590–2604, 1996.
- [17] J. Wang and F. Dalla Barba. Assessment of the parcel model in evaporating turbulent diluted sprays within a large-eddy-simulation approach. *International Journal of Multiphase Flow*, 169:104609, 2023.
- [18] P. Wang, Z. Chen, N. Jin, and X. Zheng. Wall model for large eddy simulations accounting for particle effect. *International Journal of Multiphase Flow*, page 105152, 2025.
- [19] Q. Wang and K.D. Squires. Large eddy simulation of particle deposition in a vertical turbulent channel flow. *International Journal of Multiphase Flow*, 22(4):667–683, 1996.
- [20] Q. Wu, Y. Zhao, Y. Shi, and S. Chen. Large-eddy simulation of particle-laden isotropic turbulence using machine-learned subgrid-scale model. *Physics of Fluids*, 34(6), 2022.
- [21] F. Yeh and U. Lei. On the motion of small particles in a homogeneous isotropic turbulent flow. *Physics of Fluids A: Fluid Dynamics*, 3(11):2571–2586, 1991.

- [22] Hai Zhu, Ling-ling Wang, and Hong-wu Tang. Large-eddy simulation of suspended sediment transport in turbulent channel flow. *journal of hydrodynamics*, 25(1):48–55, 2013.

CHAPTER 2

State of the art

This chapter provides an overview of the theoretical aspects and modeling techniques used in studying turbulent flows, including Direct Numerical Simulation (DNS), Reynolds-Averaged Navier-Stokes (RANS), and Large Eddy Simulation (LES). It also discusses the modeling of particle-laden turbulent flows and how these simulation methods are applied to such systems. Furthermore, the section explores the development of stochastic models, particularly focusing on the use of Langevin equations in turbulence simulations to account for random fluctuations, providing a comprehensive understanding of current advancements in turbulence and particle interaction modeling.

2.1 Turbulent flows: theoretical aspects and modeling

2.1.1 Theoretical aspects

Turbulence, in fluid mechanics, refers to a type of fluid motion characterized by chaotic variations in pressure and velocity, in contrast to laminar flow [97]. The majority of fluid motions occurring both in nature and engineering applications are turbulent [143]. In natural environments, turbulence dominates the transport of particles in multiphase flows and is associated with various environmental issues, such as sandstorms, smog pollution, riverbed and coastal erosion, as well as the suspension and deposition of sediments [103, 115, 121, 53, 50]. In engineering, turbulence-induced vibrations pose structural safety concerns [125], leading to phenomena such as aircraft turbulence, severe oscillations in large bridges, and tall buildings. Turbulence increases frictional resistance and energy loss, which in turn limits the range of aircraft and reduces the efficiency of

crude oil pipelines [133]. Additionally, turbulence plays a crucial role in affecting both mixing and combustion efficiencies [86]. In the medical field, the wall shear stress caused by turbulence is closely linked to physiological changes, offering valuable insights for disease diagnosis [23]. Moreover, the enhanced diffusivity associated with turbulence can elevate the risk of viral transmission, particularly in crowded environments [149, 15]. Given these diverse impacts, understanding and predicting turbulence is of significant practical importance.

The issue of turbulence, due to its significance in physics, has always attracted considerable attention. As early as the 15th century, Leonardo da Vinci made observations and accumulated empirical knowledge about turbulent phenomena [85]. In the late 19th century, Reynolds, in his two classic papers, initiated the scientific study of turbulence through pipe flow experiments and Reynolds decomposition [116, 117]. Since then, turbulence research has drawn contributions from numerous renowned scientists and Nobel laureates, including Rayleigh, Heisenberg, Onsager, Landau, Feynman, Chandrasekhar, Lee Tsung-Dao, Alvin, Magoshi, and Parisi. The strong nonlinearity, spatiotemporal multiscale coupling, non-local characteristics, and the coexistence of randomness and order make turbulence the last unsolved problem in classical physics [41].

Mathematically, the Navier-Stokes equations, as the governing equations for the evolution of turbulence, present a major challenge to the development of mathematical science, particularly regarding the solvability and the behavior of its solutions, which is unlikely to be resolved in the short term [141]. Turbulence, in physical terms, involves both momentum transport in physical space and the cascading of energy across different scales. The study of these nonequilibrium, complex systems has led to profound shifts in scientific understanding. From a physical standpoint, there are still two major unresolved mysteries in turbulence. The first concerns the origin of turbulence, particularly the critical Reynolds number that marks the transition from laminar flow to turbulence, as well as the underlying mechanism behind this transition. Heisenberg [52] and Lin Jiaqiao [77] proved the instability of parabolic velocity profiles, and recently, Wei Dongyi [151] confirmed that the transition phenomenon depends on both the Reynolds number and initial conditions, further validating the Trefethen conjecture [144]. The second is the statistical theory of developed turbulence – the universality of statistical moments of all orders i.e., all moments together uniquely determine all the information about turbulence, which has recently been listed as one of the 125 frontier scientific problems [120].

Turbulence arises when excessive kinetic energy within a fluid flow over-

comes the damping effects of the fluid's viscosity. As a result, turbulence is more likely to occur in fluids with low viscosity. Generally, in turbulence, unsteady vortices of varying sizes emerge, interacting with one another, which increases the resistance generated by frictional effects. As a result, more energy is needed to pump fluid through pipes. The onset of turbulence can be predicted using the dimensionless Reynolds number. The Reynolds number is defined as: $Re = \frac{UL}{\nu}$, where U and L represent the characteristic flow velocity and length scale, respectively, and ν is the kinematic viscosity of the fluid [128].

Tennekes and Lumley [142] outlined several key characteristics of turbulence in their book *A First Course in Turbulence*, including irregularity, diffusivity, high Reynolds numbers, three-dimensional vorticity fluctuations, dissipation, continuity, and the fact that turbulence is a property of the flow rather than the fluid itself. One of the most notable features of turbulence is its irregularity or randomness, and it is very difficult to describe turbulence using completely deterministic methods. As shown in Fig. 2.1, the velocity measured by a probe in the turbulent field exhibits random characteristics. Typically, turbulence is characterized through statistical or time-averaged approaches, such as Reynolds averaging or spectral analysis, which provide a stationary description of the flow rather than its instantaneous dynamics. While such approaches are effective for describing the mean features of turbulent flows, they may obscure the dynamic interactions and transient behaviors that are crucial in multiphase or particle-laden turbulence. Although turbulence is always chaotic and disordered, not all chaotic flows can be classified as turbulence. For instance, while magma flow may display chaotic behavior, it does not necessarily qualify as turbulence. A defining feature of turbulence is its diffusivity, which enables fluids to mix rapidly and enhances the transfer of momentum, heat, and mass. Although turbulence may appear random at first glance, a flow cannot be considered truly turbulent unless its velocity fluctuations are accompanied by diffusion. Turbulent flows are inherently dissipative, with kinetic energy converted into heat through viscous shear stress; without external energy input, they decay rapidly. They typically arise under high Reynolds number conditions, driven by the complex interplay between viscous forces and convection. Turbulence also exhibits rotational behavior, as indicated by nonzero vorticity, with processes such as the stretching of three-dimensional vortices playing a central role. Moreover, turbulence is a continuous phenomenon, since even its smallest vortices remain much larger than molecular scales. Importantly, turbulence is a property of fluid flow rather than of the fluid itself. Whether in liquids or gases, flows at high Reynolds numbers display similar dynamic characteristics.

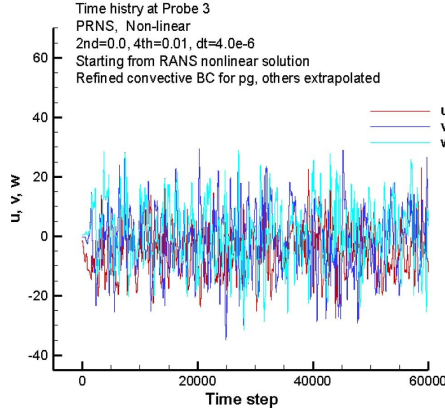


Figure 2.1: Velocity time history at probe location in turbulent flow [122]

The most widely accepted turbulence theory is based on the "energy cascade" concept proposed by Kolmogorov [64, 63], as shown in Fig. 2.2,. The energy cascade describes the transfer of energy from large-scale motions to small-scale motions (referred to as the forward energy cascade). This energy transfer between different scales can only occur in nonlinear systems. Strictly speaking, energy transfer in the cascade happens locally, only between scales that are very close to each other. According to this theory, turbulence consists of vortices of different sizes, each with a certain amount of energy, which depends on its size. Larger vortices break down into smaller vortices, and this process occurs in a chain-like manner. Newly formed smaller vortices undergo similar breakdown processes, transferring their energy to even smaller vortices. This chain-like breakdown continues until the smallest possible vortices scale is reached. At this scale, the molecular viscosity can effectively dissipate turbulent kinetic energy as heat (dissipation is the process through which mechanical energy is converted into thermal energy via friction).

In turbulence, the largest vortices contain the most kinetic energy, while energy dissipation primarily occurs in the smallest vortices, driven by the fluid's viscosity. Kolmogorov hypothesized that at sufficiently high Reynolds numbers, the large separation between the energy-containing and dissipative scales gives rise to an intermediate range – the inertial subrange – within which the turbulent fluctuations exhibit statistically isotropic behavior. In this region, the equilibrium characteristics of the flow depend solely on the rate of energy dissipation at the smallest scales. This dissipation rate can be expressed in terms of the strain rate fluctuations in turbulence and the kinematic viscosity of the fluid. At equilibrium, the rate of turbulent kinetic energy generation at the large scales equals the rate of energy dissipation at the small scales.

The energy spectrum of turbulence, $E(k)$, depends on the turbulent kinetic

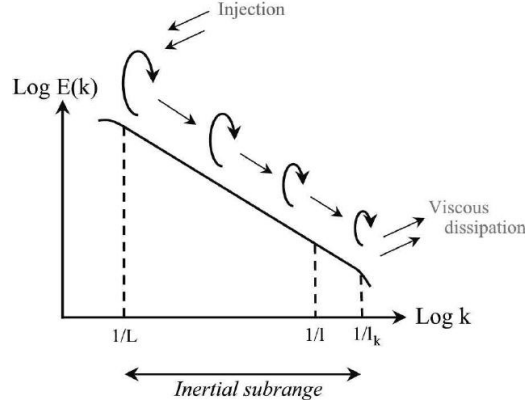


Figure 2.2: Energy cascade. Source: Wikipedia https://en.wikipedia.org/wiki/Energy_cascade

energy per unit mass of fluid [109]:

$$\frac{1}{2} (\overline{u_i u_i}) = \int_0^\infty E(k) dk. \quad (2.1)$$

Here, u_i represents the velocity component of the fluctuations, with the overline indicating the ensemble average. The expression is summed over i . k is the wavenumber. Therefore, the energy spectrum $E(k)$ represents the turbulent kinetic energy located between the wavenumber intervals k and $k + dk$. Larger vortices correspond to lower wavenumbers, while smaller vortices have higher wavenumbers. Because diffusion is the Laplacian of velocity, the rate of dissipation can be expressed as an energy spectrum:

$$\varepsilon = 2\nu \int_0^\infty k^2 E(k) dk. \quad (2.2)$$

Here, ν is the kinematic viscosity of the fluid. From this equation, it can be observed that although the kinetic energy is primarily present in the low-wavenumber motions (large vortices), the dissipation mainly occurs in the high-wavenumber motions (small vortices).

The energy transfer from low wavenumbers to high wavenumbers is called energy cascade. It transfers turbulent energy from large-scale motions to small-scale motions, which is eventually dissipated by viscosity. The range of scales between these, known as the inertial subrange, can be derived from Kolmogorov's hypothesis to yield the universal form of the energy spectrum:

$$E(k) = C\varepsilon^{2/3} k^{-5/3}. \quad (2.3)$$

A large body of experimental evidence under a variety of conditions supports this conclusion. The values measured in the experiments were $C = 1.5$ [109]. The smallest turbulent vortices are characterized by Kolmogorov's micro-length scale (η) and time scale (t_η), which are defined as:

$$\eta = \left(\frac{\nu^3}{\varepsilon} \right)^{1/4} \quad (2.4)$$

$$t_\eta = \left(\frac{\nu}{\varepsilon} \right)^{1/2} \quad (2.5)$$

Additionally, the size of the largest vortices, also known as the integral length scale, is defined as proportional to the size of the geometry under consideration.

Navier-Stokes equations are a set of partial differential equations that describe the motion of fluid. The equations are named after the French physicist Claude-Louis Navier and the Irish physicist George Stokes. The Navier-Stokes equations describe the momentum and mass conservation properties that a Newtonian fluid must satisfy during motion. In some applications of the Navier-Stokes equations, they are listed alongside the equation of state to illustrate the relationship between fluid pressure, temperature, and density. By solving the Navier-Stokes equations, one can obtain the full spatiotemporal turbulence spectrum involved in the flow field. The flow of non-reacting, isentropic Newtonian fluids is governed by the Navier-Stokes equations in conjunction with the mass conservation equation [40].

$$\frac{Du_i}{Dt} = a_i = f_i - \frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \left(\frac{\partial^2 u_i}{\partial x_j \partial x_j} + \frac{1}{3} \frac{\partial}{\partial x_i} \frac{\partial u_j}{\partial x_j} \right) \quad (2.6)$$

$$\frac{D\rho}{Dt} + \rho \frac{\partial u_j}{\partial x_j} = 0 \quad (2.7)$$

Where $\frac{D}{Dt}$ denotes the Lagrangian (or total or material) derivative, u_i is the fluid velocity, a_i is the fluid acceleration, f_i is the forcing term, $\frac{\partial p}{\partial x_i}$ is the pressure gradient, ρ is the fluid density, ν is the fluid kinematic viscosity, $\frac{\partial^2 u_i}{\partial x_j \partial x_j}$ is the velocity Laplacian, and $\frac{\partial u_j}{\partial x_j}$ is the velocity divergence. The fluid acceleration is the Lagrangian derivative of the velocity:

$$a_i = \frac{Du_i}{Dt} = \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \quad (2.8)$$

, making it inherently a Lagrangian quantity. This means it can only be directly measured using Lagrangian measurement techniques.

Nevertheless, it can be decomposed into two components: the local acceler-

ation (the partial time derivative of velocity) and the advective acceleration (or transport terms, i.e., the partial spatial derivatives of the velocity multiplied by the transport velocity; see Equation 2.8).

For turbulence simulation, based on the concept of energy cascade, the direct numerical solution of the Navier-Stokes equations requires very small time and spatial steps to resolve all the spatiotemporal turbulence scales. This computationally intensive method is referred to as Direct Numerical Simulation (DNS) in the literature. To reduce this immense computational cost, statistical analysis methods can be employed to simplify the solution of turbulence. The time-dependence of turbulence and its broad range of timescales suggest that statistical averaging methods can be used to approximate the treatment of random fluctuations. However, time averaging introduces previously unknown correlations, which arise due to the nonlinear terms in the governing equations. The simulation of these correlations constitutes the classical closure problem in turbulence modeling.

Based on this statistical approach, the Large eddy simulation (LES) method [76, 119] can directly simulate the large-scale turbulence structures, while the small-scale turbulence is modeled using subgrid models. The advantage of this method lies in its ability to directly resolve high-energy large vortices (anisotropic turbulence) while simplifying the simulation of smaller vortices. It is feasible to accurately simulate these vortices using this approach because the smaller-scale turbulence can be considered isotropic and independent of flow conditions and boundary effects. With advancements in computer technology in recent years, the use of the LES method to solve industrial problems has gained increasing acceptance.

Another method that utilizes statistical averaging in time is known as the Reynolds-Averaged Navier-Stokes (RANS) equations [117]. The key to this method is to decompose the flow components into time-averaged components and fluctuating components, and then substitute them into the original equations, followed by time-averaging the resulting equations. Currently, the RANS method is the most popular approach for addressing turbulence problems in industrial applications.

2.1.2 Simulation: DNS, RANS and LES

Among all the numerical techniques and models available today, DNS, LES, and RANS simulation represent the three main approaches, and they stand as the three historical pillars of turbulence numerical simulation.

In DNS, all the significant turbulence scales are directly resolved without

the need for any modeling. As a result, DNS can predict turbulence with an accuracy comparable to laboratory experiments, and is often referred to as a numerical experiment. However, the separation between large-scale and small-scale turbulence dictates the computational effort required, limiting the application of DNS to low Reynolds numbers and simplified flow regions, thus confining it to academic research.

In contrast, in RANS simulations, the entire turbulence spectrum is modeled by estimating the effect of turbulent motions on the mean field through turbulence models, significantly reducing the computational workload required for turbulence simulations even in high Reynolds number and complex flow domains. However, the uncertainty introduced by turbulence models requires careful preliminary evaluation when used in new applications, and very accurate predictions of turbulence can generally only be achieved after fine-tuning model coefficients.

LES offers a compromise between accuracy and computational cost by introducing filtering techniques to simulate only the computationally intensive small-scale part of the turbulence spectrum, known as the subgrid model, while explicitly calculating the largest scales. LES is considered a high-fidelity turbulence simulation technique, capable of providing accurate results for a wide range of flows without the need for the fine-tuning of closure models as in RANS.

Figure 2.3 presents a visual comparison of DNS, LES, and RANS simulations for a turbulent jet, showing the corresponding velocity fields. Clear differences and similarities can be observed among the three approaches. The DNS result provides the highest level of flow detail, accurately resolving the full range of turbulent scales. The LES result captures the dominant large-scale structures but filters out the smallest eddies due to limited grid resolution. In contrast, the RANS result represents only the mean velocity distribution derived from ensemble averaging, without resolving any instantaneous turbulent motions. This comparison highlights the trade-off between computational cost and physical fidelity, with RANS being the most economical but least detailed, and DNS offering the most complete turbulence representation at the highest computational expense.

Fig. 2.4 presents the velocity history at a point downstream of the turbulent separation region in the turbulent jet flow, as provided by LES and RANS techniques, in a conceptual manner. Starting with the raw DNS signal, as expected, it contains a wide range of turbulence frequencies, from low-frequency modulations associated with large-scale structure motion to high-frequency oscillations generated by the transfer of energy from large-scale to small-scale

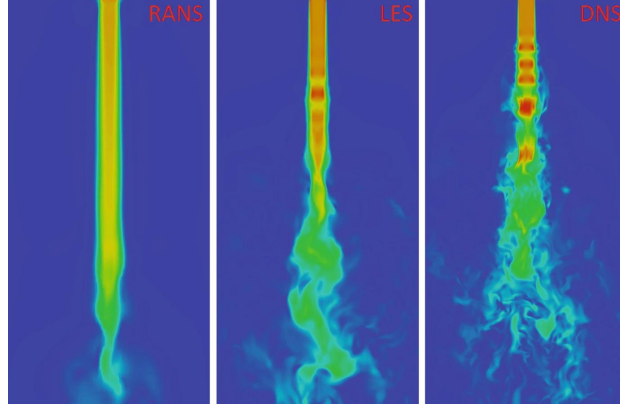


Figure 2.3: Velocity distribution for a turbulent jet using RANS (LHS), LES (middle), and DNS (RHS) [118]

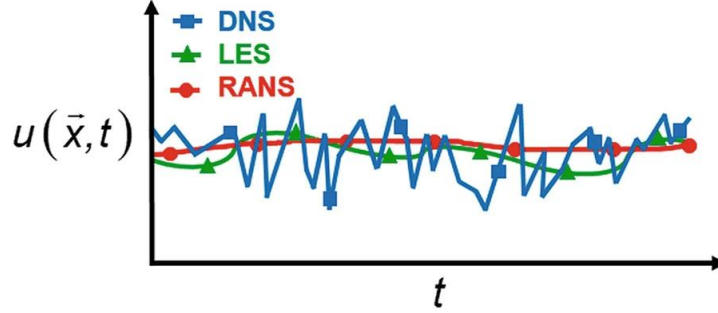


Figure 2.4: A comparison of RANS, LES, and DNS instantaneous velocities [118]

disturbances. The corresponding LES signal is obtained by spatially averaging the raw DNS profile, accurately representing the low-frequency modulations while filtering out most of the high-frequency oscillations. On the other hand, within the RANS framework, only the average value of the DNS signal can be estimated.

Direct Numerical Simulations (DNS)

In 1972, Orszag and Patterson [102] conducted the first DNS of homogeneous isotropic turbulence, which is considered a pioneering study in the field of turbulence. Later, Kim et al. [60] used DNS to study wall-bounded turbulence, focusing on wall-bounded turbulence at a friction Reynolds number of $Re_\tau = 180$. They reported particle tracking flow visualization results, revealing the structure and dynamics of near-wall turbulence. Following this, Moser et

al. [98] expanded their work by increasing the friction Reynolds number Re_τ to 590 and reported the quasi-asymptotic behavior of turbulence statistics, suggesting that wall-bounded turbulence exhibits universal behavior at sufficiently high Reynolds numbers. Subsequently, Lee and Moser [75] extended Re_τ to 5200, providing reliable data for high-Reynolds-number wall-bounded turbulence. The resolution of the simulations met or exceeded current standards, with minimal statistical error and agreement with DNS and experimental data for $Re_\tau \leq 2000$. At high Reynolds numbers, the flow displayed a distinct logarithmic region, and the von Karman constant κ was found to be 0.384 ± 0.004 , clearly confirming the existence of this logarithmic profile for the first time.

Chong et al. [25] explored the topological characteristics of vortex motions in the flow, focusing on the turbulence structures associated with the attached vortex model. Their study provided direct evidence for the role of vortex structures in the turbulent boundary layer and demonstrated the potential of DNS data to validate the attached vortex hypothesis. Philippe et al. [132] used DNS to investigate empirical scaling laws for wall-bounded turbulence, exploring the relationship between Reynolds stress and wall distance (y^+) and friction Reynolds number (Re_τ) for different flow types (such as channel flow, Couette flow, and pipe flow). The study emphasized the normalized turbulence characteristics and proposed several empirical formulas to describe these features. Their work provided strong support for empirical scaling laws for wall-bounded turbulence through DNS data while also emphasizing the need for further research, particularly in three-dimensional flows and under different pressure gradient conditions.

DNS has also been widely applied to other types of classical flows to study the similarity and asymptotic behavior of wall-bounded turbulence under simple shear flow conditions. Spalart et al. [131] employed DNS to simulate the turbulent boundary layer of a flat plate with zero pressure gradient, investigating the turbulent behavior across a Reynolds number range from $Re_\theta = 225$ to $Re_\theta = 1410$. The results showed that at higher Reynolds numbers, the turbulence statistics and models exhibited significant Reynolds number dependence, while the effects at lower Reynolds numbers were relatively weak. The detailed turbulence data provided by DNS is crucial for validating and improving existing turbulence models, particularly at high Reynolds numbers.

Wu et al. [152] simulated the flat plate boundary layer with nominal zero pressure gradient to explore the process of transition from laminar to turbulent flow. The Reynolds number range for the simulation was from 80 to 940, with the transition occurring at approximately $Re_\theta = 750$, and local disturbances from the free stream were introduced during the simulation, triggering the for-

mation of turbulence. The study showed that the hairpin vortex structure in the turbulent boundary layer played a critical role in the generation of turbulence, and this finding provides important reference value for future turbulence models and theoretical studies.

Eggels et al. [34] compared DNS results with experimental data to investigate the characteristics of fully developed turbulent pipe flow, especially the turbulence statistics differences between different geometries (axisymmetric pipe flow and planar channel flow). The study found significant differences in turbulence statistics between axisymmetric pipe flow and planar channel flow, particularly in terms of the uniform flow profile and turbulence fluctuation statistics. The "wall laws" for pipe flow exhibited more complex behavior compared to those for planar channel flow. Differences between pipe and channel flow were particularly evident in higher-order statistics (such as skewness and kurtosis), especially in the skewness and kurtosis of normal velocity fluctuations. The study indicated that the influence of axisymmetric pipe geometry on flow is more complex than that of planar channel geometry. Although higher-order statistics are difficult to obtain accurately, numerical simulations and experimental results showed high consistency in lower-order statistics and energy budget analysis, demonstrating the effectiveness of numerical simulations in capturing turbulence behavior.

Pirozzoli et al. [106] used DNS to study the characteristics of pipe flow at a friction Reynolds number $Re_\tau \approx 6000$. The DNS data supported the classical logarithmic layer theory, particularly at higher friction Reynolds numbers, where the velocity distribution and friction factor closely matched the theoretical values. The study showed that the centerline velocity and friction velocity of the pipe flow converge at high Reynolds numbers, supporting the notion that pipe flow tends to approach a fully developed flow state. The findings challenge traditional balance assumptions, highlighting the imbalance between turbulence production and dissipation in the outer layer, and indicating that pipe flow at high Reynolds numbers exhibits complex turbulent features.

Large-Eddy Simulations (LES)

In 1963, Smagorinsky [126] first applied spatial filtering to the fluid flow equations. Subsequently, Deardorff [28] used this spatial filtering technique to study three-dimensional turbulent plane Poiseuille flow under high Reynolds number conditions, simulating the subgrid-scale effects in turbulence and modeling them with a vortex coefficient proportional to local velocity deformation. By calculating turbulence statistics and comparing them with experimental data,

the study examined the different vortex structures in turbulence and their characteristics, focusing on the calculated vortex shapes, turbulence energy balance, and variations of longitudinal and transverse vortices.

In 1982, Moin and Kim [96] conducted a numerical study on turbulent channel flow, with a focus on simulating large-scale turbulence. Based on a Reynolds number of $Re = 13800$, the study was the first to apply LES methods, performing numerical integration of the three-dimensional time-dependent Navier-Stokes equations to simulate the statistical characteristics of the flow and its time dependence. The results indicated that LES could effectively simulate turbulent channel flow and provide a valuable supplement to experimental data, particularly in capturing the flow characteristics near the wall. The paper also discussed models for small-scale turbulence and calculated the analytical components of the Reynolds stress equations, highlighting the significance of these results for the development of phenomenological turbulence models for complex flows.

The LES filter can be applied to both spatial and temporal fields, $\phi(x, t)$, performing spatial filtering, temporal filtering, or both simultaneously. The filtered field is denoted by vertical bars, as defined in [109]:

$$\overline{\phi(x, t)} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi(r, \tau) G(x - r, t - \tau) d\tau dr \quad (2.9)$$

Here G is the filter convolution kernel and the above equation can also be written as:

$$\overline{\phi} = G * \phi. \quad (2.10)$$

The filter kernel G has a characteristic cutoff length scale Δ and a cutoff time scale τ_c , below which quantities ϕ' are eliminated. Therefore, ϕ can be expressed as:

$$\phi = \overline{\phi} + \phi' \quad (2.11)$$

For incompressible flows, the continuity equation is filtered to obtain the filtered incompressible continuity equation:

$$\frac{\partial \overline{u}_i}{\partial x_i} = 0 \quad (2.12)$$

The momentum equation is filtered to obtain the filtered incompressible mo-

mentum equation:

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} (\bar{u}_i \bar{u}_j) = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \nu \frac{\partial}{\partial x_j} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + 2\nu \frac{\partial}{\partial x_j} \bar{S}_{ij} \quad (2.13)$$

Where $\bar{p}$ is the filtered pressure field, $\bar{S}_{ij}$ is the strain rate tensor calculated using the filtered velocity, and $\overline{(u_i u_j)}$ is the nonlinear filtered convective term, which is the most critical term in LES. Leonard [76] decomposed $\overline{(u_i u_j)}$ into two terms, namely:

$$\overline{u_i u_j} = \tau_{ij} + \bar{u}_i \bar{u}_j \quad (2.14)$$

where τ_{ij} is the residual stress tensor. Thus, the filtered incompressible momentum equation can be expressed as:

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} (\bar{u}_i \bar{u}_j) = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + 2\nu \frac{\partial}{\partial x_j} \bar{S}_{ij} - \frac{\partial \tau_{ij}}{\partial x_j} \quad (2.15)$$

Leonard again decomposes τ_{ij} into three terms:

$$\tau_{ij} = L_{ij} + C_{ij} + R_{ij} \quad (2.16)$$

Where L_{ij} is the Leonard tensor, representing the interactions between large scales; $R_{ij} = \overline{(u'_i u'_j)}$ represents the interactions at the subgrid scale; and $C_{ij} = \overline{(u_i u'_j)} + \overline{(u'_j u_i)}$ is the Clark tensor, representing the cross-scale interactions between large and small scales.

The filtering equation for the passive scalar ϕ can be expressed as follows:

$$\frac{\partial \bar{\phi}}{\partial t} + \frac{\partial}{\partial x_j} (\bar{u}_j \bar{\phi}) = \frac{\partial \bar{J}_\phi}{\partial x_j} + \frac{\partial q_j}{\partial x_j} \quad (2.17)$$

Where $J_\phi = D_\phi \frac{\partial \phi}{\partial x_i}$ represents the diffusion flux of ϕ , and $q_j = \bar{\phi} \bar{u}_j - \overline{\phi u_j}$ represents the sub-filter flux of ϕ .

The Smagorinsky model is a turbulence closure scheme introduced to represent the effects of unresolved, sub-grid scale motions in numerical simulations of the atmospheric general circulation. It parameterizes the eddy viscosity and diffusivity as proportional to the square of a characteristic length scale (related to grid spacing) and the magnitude of the local strain rate of the resolved flow. In this way, regions with strong velocity shear produce larger diffusion, mimicking the cascade of energy from large to small scales and preventing the artificial buildup of energy at the grid scale. This approach provided one of

the first effective means of incorporating small-scale turbulent processes into primitive equation models and later became a foundational method for large eddy simulation (LES) in fluid dynamics. The Smagorinsky model [126] has the following limitations: excessive dissipation, inaccurate asymptotic behavior in the near-wall region, and a strong dependence of the model constants on the specific problem. Germano et al. [44] proposed a new dynamic subgrid-scale eddy viscosity model to address the shortcomings of existing subgrid-scale stress models in rotational flows, shear flows, near solid boundaries, and transitional regions. The coefficients of this model are dynamically computed rather than preset. Specifically, the model is based on an algebraic relationship between the subgrid-scale stress and the stress at two different filtering levels. It can reduce the subgrid-scale stress to zero in laminar flow and near solid boundaries and exhibit correct asymptotic behavior in the near-wall region of turbulent boundary layers. Through testing the model on transitional flows and turbulent channel flow using LES, the results showed good agreement with the data from DNS. In comparisons, the new dynamic model demonstrates superior performance over the traditional Smagorinsky model and other models with damping functions, especially in the cases of transitional flows and fully developed turbulence.

The dynamic model has a certain level of complexity, and to address this issue, researchers have proposed alternative models. Yoshizawa [154] transformed the Smagorinsky model into an subgrid-scale (SGS) model that considers both convective and transport effects by using the subgrid energy equation. This model improves upon the traditional Smagorinsky model by introducing a variable Smagorinsky coefficient, addressing the limitations of the standard model in handling different types of turbulence, such as the inability of fixed constants to adapt to various flow conditions. Nicoud and Ducros [99] introduced a new subgrid-scale stress model (the WALE model), which is based on the square of the velocity gradient tensor. Compared with the classical Smagorinsky model, it has several advantages:

1. **Local strain and rotation rate:** The new model identifies all turbulence structures related to kinetic energy dissipation by incorporating local strain and rotation rate.
2. **Turbulent viscosity near the wall:** The model naturally drives turbulent viscosity to zero near the wall, eliminating the need for dynamic constant adjustments or damping functions to compute wall-bounded flow.

3. **Pure shear flow:** In pure shear cases, the model generates zero turbulent viscosity, enabling it to simulate the laminar-to-turbulent transition induced by linear instability modes.

The model was validated through two typical turbulent flow cases: free-decaying isotropic turbulence and turbulent pipe flow. The experimental results showed that the WALE model could accurately reproduce the desired characteristics (such as turbulence transition and scaling near the wall), with its computational results closely matching experimental data, demonstrating the model's potential in complex flows. Overall, the WALE model has shown great applicability and efficiency in LES for wall-bounded turbulence, flow transitions, and complex geometries, providing a more practical alternative to the dynamic Smagorinsky model, particularly in situations where multiscale filtering is unnecessary.

Tabor et al. [139] categorized the methods for generating LES inlet conditions into two types. The first is the Precursor Simulation Method, which involves conducting a separate, pre-calculated turbulence simulation to generate a database of turbulence data, which is then used as the inlet condition for the main simulation. This method uses actual turbulence data, ensuring the physical realism of the inlet conditions. The second is the Synthesis Method, which constructs a random field to simulate the characteristics of turbulence without directly simulating the turbulence itself. It uses mathematical techniques, such as Fourier transforms, wavelet transforms, or other stochastic processes, to generate turbulence-like fluctuations.

In LES, fully resolving the small-scale turbulent structures in the near-wall region remains computationally expensive, which significantly limits the application of LES in complex industrial geometries and high Reynolds number flows. By introducing wall models, the computational cost of LES simulations can be significantly reduced, as wall models are used to represent the internal region of the turbulent boundary layer, which is typically the most computationally demanding part [105]. Choi and Moin [24] re-estimated the number of grid points required for LES, particularly for high Reynolds number boundary layer flows. The authors corrected Chapman's grid point estimation method from 1979 using high-precision formulas, providing more accurate results. The study found that for LES with wall modeling, the required grid points follow a power-law relationship with Reynolds number $N_{\text{wm}} \sim Re^{2/7} L_x$, indicating a closer relationship between the grid points and the flow direction length L_x and Reynolds number Re . For DNS, the required grid points follow the relationship $N_{\text{DNS}} \sim Re^{37/14} L_x$, which indicates that the computational demand

for DNS is much higher than for LES, especially under high Reynolds number conditions. The study emphasized the practical importance of wall modeling in high Reynolds number flows, noting that wall modeling can significantly reduce computational costs, with a reduction of several orders of magnitude compared to fully resolving the wall in LES.

Goc et al. [47] used the equilibrium wall model, assuming the boundary layer to be in a state of equilibrium, which is suitable for high Reynolds number flows. In this model, the turbulent structures in the wall region are assumed to be in local equilibrium, simplifying the direct resolution of complex vortices. When dealing with high Reynolds number aircraft flows, directly resolving wall vortices requires extremely fine grids, which not only increases computational costs but may also lead to numerical instability. WMLES, through wall modeling techniques, effectively reduces the required grid resolution while maintaining high-accuracy simulation of large-scale vortices. Their study successfully achieved high-precision predictions of complex high-lift configuration aircraft flows using WMLES, particularly showing significant advantages in simulating large-scale separation and wind tunnel effects. The paper also demonstrates the feasibility of WMLES in aerospace engineering, especially in providing fast and accurate simulation predictions during the design cycle, offering a new direction for high-performance aerodynamic simulations in aircraft design.

Reynolds-Averaged Navier-Stokes Simulations (RANS)

Since the 1970s, researchers have begun conducting numerical simulations of turbulence based on the Reynolds-averaged Navier-Stokes equations. In 1972, Hanjali and Launder [51] proposed a new turbulence model aimed at achieving closure of the turbulence equations through approximate transport equations for the Reynolds stress tensor and the turbulence energy dissipation rate. Initially, the model used seven transport equations to describe turbulent quantities, but in practical applications, it was simplified to six constants and solved through experiments. The core of the model is the improved approximation of the pressure-strain rate correlation term, which successfully predicted the level of stress components in plane homogeneous turbulence, particularly the anisotropy in the transverse normal stress components.

In 1974, Launder and Spalding [72] proposed a two-equation model based on turbulence kinetic energy k and turbulence energy dissipation rate ε , focusing on the model's effectiveness in practical applications, especially in flows near solid walls. This model effectively provides accurate predictions in various turbulent flow situations, particularly in capturing the turbulent characteris-

tics in the near-wall region.

As shown below, the Reynolds-Averaged NavierStokes (RANS) equations capture the time-averaged dynamics of fluid flow.

$$\frac{\partial U_i}{\partial x_i} = 0 \quad (2.18)$$

$$\frac{\partial}{\partial x_j} (U_j U_i) = -\frac{1}{\rho} \frac{\partial P}{\partial x_i} + \nu \frac{\partial^2 U_i}{\partial x_j \partial x_j} - \frac{\partial}{\partial x_j} (R_{ij}) \quad (2.19)$$

P and U_i represent the mean pressure and mean velocity of the fluid, respectively. $R_{ij} = \overline{u_i u_j}$ is the Reynolds stress tensor. In general, the time-averaged transport equation for a scalar is:

$$\frac{\partial}{\partial x_j} (U_j \Phi) = \nu \frac{\partial^2 \Phi}{\partial x_j \partial x_j} - \frac{\partial}{\partial x_j} (f_j) \quad (2.20)$$

In this context, Φ represents the mean scalar field, and $f_j = \overline{u_j \Phi}$ denotes the vector of turbulent scalar fluxes.

R_{ij} is a newly introduced unknown quantity that requires closure. Prandtl proposed the first closure model:

$$R_{ij} = 2\nu_t S_{ij} - \frac{2}{3} \delta_{ijk}, \quad S_{ij} = \frac{1}{2} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \quad (2.21)$$

In this context, ν_t represents the eddy viscosity, and $k = \frac{1}{2} \overline{u_i u_i}$ denotes the turbulent kinetic energy, where u_i denotes the fluctuating component of the velocity field, and the overbar $\overline{(\cdot)}$ represents an ensemble average.

Subsequently, a series of turbulence models were proposed by researchers. Spalart and Allmaras [130] introduced a one-equation turbulence model for aerodynamic flows, known as the SpalartAllmaras model. This model was constructed through empirical methods and dimensional analysis, based on a transport equation for turbulence viscosity, and includes a destruction term that depends on the distance from the wall. Unlike earlier one-equation models, this model is local (i.e., the solution at a given point does not depend on the solutions at other points), making it compatible with arbitrary grid structures and applicable to both two-dimensional and three-dimensional Navier-Stokes solvers. The model is robust with respect to wall modeling and numerical stability, achieves rapid convergence, and facilitates a smooth laminar-to-turbulent transition, especially in boundary layers subject to large pressure gradients.

Launder and Spalding [72] proposed the two-equation model, the $k - \varepsilon$ model. This model calculates turbulent flow by solving two transport equations: one for turbulent kinetic energy k , and the other for turbulent dissipation rate ε . This approach enables the model to simulate various turbulent flow conditions with relatively low computational cost. The $k - \varepsilon$ turbulence model is one of the most widely used models today. Its balanced approach between computational efficiency and physical realism makes it widely applicable to various engineering problems.

Wilcox introduced the $k - \omega$ two-equation model, where k still represents turbulent kinetic energy, and ω is the specific dissipation rate, which represents the rate of turbulent kinetic energy dissipation per unit time. The $k - \varepsilon$ model is generally less accurate when predicting turbulent boundary layers under adverse pressure gradients, especially in cases involving compressible flows, separated flows, surface roughness, or mass injection. In contrast, the $k - \omega$ model shows superior predictive capabilities in boundary layers with adverse pressure gradients, compressible boundary layers, and free shear flows. The model uses more suitable closure coefficients and can directly integrate through the viscous sublayer without relying on wall functions. However, further improvements in the model's constitutive relationships are still needed, particularly in addressing anisotropy, stream curvature, and boundary layer separation effects.

The models mentioned above are based on the Boussinesq hypothesis, which uses eddy viscosity to calculate the Reynolds stress tensor, and are therefore referred to as Eddy Viscosity Models (EVM). However, these models may lead to significant errors in flows where turbulence stress anisotropy plays a prominent role. This is due to the linear relationship between the Reynolds stress tensor and the mean strain rate assumed in the Boussinesq hypothesis, which fails to accurately predict vortex flows [89, 79]. The quadratic Speziale-Sarkar-Gatski (SSG) model proposed by Speziale et al. [134] introduces nonlinearities in the anisotropic tensor, which are only of a quadratic form. Through calibration against existing experimental data, the SSG model performs better than the Launder-Reece-Rodi (LRR) model, especially in complex turbulent flows such as rotating shear flows. However, some defects in the SSG model still exist in rotating shear flows, which are related to the model's structure and cannot be overcome by adding more complex nonlinear terms.

The Reynolds Stress Model (RSM) proposed by Launder et al. [73] primarily focuses on the closure of Reynolds stresses in turbulent flows, aiming to provide a more accurate turbulence model for complex flow situations. By improving the pressure-strain correlation, handling secondary strain terms, and

modifying the turbulence energy dissipation equation, the RSM can effectively simulate complex turbulent flows. It shows strong predictive capabilities under various flow conditions, particularly when dealing with inhomogeneous turbulence and complex strain fields. However, the model constants still require further optimization, and the assumptions regarding energy dissipation processes need to be refined to enhance its applicability in a broader range of applications.

2.2 Particle-laden Turbulent Flows

Particle-laden turbulent flows refer to the phenomenon in which a large number of solid particles or droplets are suspended in a turbulent flow. This flow represents a typical two-phase system, in which the continuous (carrier) phase transports the dispersed particles or droplets. Since the particles or droplets are generally small and can move with the fluid, they are influenced by the turbulence, resulting in a highly complex and variable flow state. The behavior of particle-laden turbulent flows is characterized by significant diversity and complexity, primarily due to the differences between the particle and fluid properties, the multiple couplings between the dispersed and continuous phases, and the large scale differences. These factors introduce numerous control parameters, making particle-laden turbulent flows a major challenge in numerical modeling [16].

The interaction between particles and the fluid primarily involves two important mechanisms:

1. Particle-fluid interaction: Particles are influenced by the turbulence in the flow, which is manifested in phenomena such as particle acceleration, rotation, and collisions.
2. The effect of turbulence enhancement: The presence of particles alters the turbulence motion, which in turn affects the flow structure and the distribution of turbulence energy.

The main forces acting on particles in turbulent flows include drag forces, viscous forces, gravity, buoyancy, and inter-particle collision forces. The motion of particles depends on the velocity of the fluid, the intensity of the turbulence, and the physical properties of the particles themselves (such as density, size, and shape).

When the mass fraction of the dispersed phase is low, it is reasonable to assume a unidirectional coupling between the phases, meaning the dynamics

of the particle phase are influenced by the carrier phase, but the dynamics of the carrier phase are not affected by the particle phase. However, when the mass fraction of the dispersed phase is high, the dynamic interaction between the phases becomes significant, and bidirectional coupling effects must be considered.

When using the Lagrangian method to model the dispersed phase, a very large computational capacity may be required to track a sufficiently large particle sample for statistical convergence when the particle number is very high. Moreover, if the particle mass is relatively light, their motion behaves more like that of a second fluid. In such cases, it is more appropriate to use the Eulerian method to model the dispersed phase.

Fig. 2.5 illustrates the different dynamical regimes describing the transport process of spherical particles in turbulence, presented in a three-dimensional space. The phase space of this figure is defined by three main parameters: particle size, the density ratio between the particle and the fluid, and the solid-phase volume fraction. These parameters reflect the varying motion characteristics of particles within turbulent flows. The diagram is based on the three parameters: $\frac{D_p}{\eta}$, $\frac{\rho_p}{\rho_f}$, and Φ_V . Here, $\frac{D_p}{\eta}$ represents the ratio of particle size to turbulent scale, where D_p is the diameter of the spherical particles and η is the Kolmogorov scale. The ratio of particle size to turbulent scale influences the dynamic response of the particles. Smaller particles closely follow the fluid flow, whereas larger particles are more strongly influenced by turbulence structures, which modify their trajectories. $\frac{\rho_p}{\rho_f}$ is the density ratio between the particle and the fluid, where ρ_p is the particle density and ρ_f is the fluid density. This ratio describes the settling behavior of the particles and their interactions with the fluid. When the density ratio is large, the particles settle faster; when the density ratio is close to 1, the interaction between the particles and the fluid becomes more complex, particularly in the presence of gravity. Φ_V represents the solid-phase volume fraction. An increase in particle concentration significantly affects the behavior of turbulence, leading to various fluid dynamic phenomena, such as interactions between particles and their impact on the turbulent flow. These parameters describe how particle behavior changes across different turbulent regimes. The figure displays several distinct regions in the phase space, each representing a different dynamical regime based on particle size, density ratio, and volume fraction.

Fig. 2.5 divides the dynamic regimes into multiple categories based on the combination of different parameters, which include the following:

1. **Inertial Clustering:** For particles with inertia, they tend to cluster in

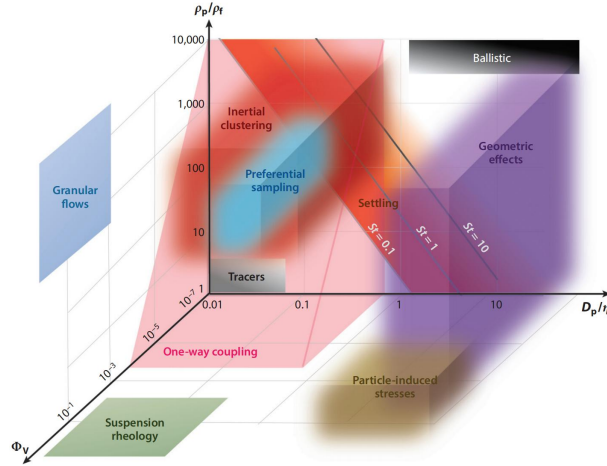


Figure 2.5: The three-dimensional view of different fluid dynamics regimes for the transport of spherical particles in turbulence. [16]

specific regions due to factors such as strain rates in the fluid turbulence. Smaller particles (with a smaller Stokes number) are especially prone to exhibit this clustering phenomenon, particularly in regions of weak turbulence or low vorticity. The inertial characteristics of the particles, such as the Stokes number, determine the strength and extent of the clustering.

2. **Preferential Sampling:** Preferential sampling refers to the tendency of particles to concentrate in specific regions of turbulence. For example, particles are more likely to be found in regions with higher strain rates and less likely in the centers of vortices. This phenomenon helps explain the spatial distribution of particles.
3. **One-way Coupling:** In one-way coupling, the motion of the particles does not significantly affect the turbulence. This regime typically occurs when particle concentration is low, and the particles have minimal influence on the turbulent characteristics of the fluid. In such cases, the particles act as small tracers within the fluid.
4. **Geometric Effects:** For larger particles, the local deformation of the fluid (such as vortex structures in turbulence) has a more pronounced effect on the particle motion. These geometric effects become more significant as the particle size increases, especially when the particle size approaches or exceeds the microscopic scales of turbulence. In such cases, particles begin to induce geometric deformation in the fluid, impacting the turbulence structure and dynamics.

5. **Particle-induced Stresses:** When the particle concentration is high, interactions between particles lead to stresses that are exerted on the fluid. As the particle concentration increases, these particle-induced stresses become stronger, affecting the regulation of turbulence and fluid dynamics.

2.2.1 DNS for particle-laden turbulent flows

Maxey [87] provides a comprehensive review of particle-laden flow simulation methods, including Resolved Simulations, Immersed Boundary Method, Point Particle Methods, Meshless Methods, and Lattice Boltzmann Method. The Resolved Simulations method solves the fluid dynamics equations directly, accurately describing the motion of solid particles in the fluid, using the Navier-Stokes equation with particles. In this method, the particle motion is driven by fluid forces, and the interactions between particles can also be considered. One of the most significant recent advances is the rapid adoption of Particle Resolved Direct Numerical Simulation (PR-DNS) methods [16]. PR-DNS combines traditional DNS with particle dynamics simulation, precisely addressing particle behavior in turbulence. Unlike conventional DNS, PR-DNS not only simulates the fluid motion but also explicitly accounts for the motion and interactions of each particle. Each particle in the simulation has a defined position and trajectory, capturing the precise interactions between particles and the fluid. This method solves the Navier-Stokes equations of the fluid directly, without the need for turbulence models, enabling highly accurate descriptions of fluid details. PR-DNS simulates the motion, collision, settling, and aggregation of particles through their interaction with the fluid. During the simulation, the motion of the particles affects the fluid flow, while the fluid flow also alters the particle trajectories. Since each particle requires precise simulation, PR-DNS generally demands significant computational resources, especially when the particle number is large or the fluid conditions are complex. The Immersed Boundary Method addresses complex fluid-particle interaction problems by handling the boundaries between fluid and particles. Uhlmann [145] proposed a direct forcing immersed boundary method for simulating freely suspended particles. By treating the particles as point particles and estimating the fluid forces acting on them, this method is typically used in low-concentration particle suspension systems and is particularly effective for small particles. The Lagrangian method can describe fluid motion at different levels of detail. If, in addition to detailed flow around each particle, the method also resolves all scales from the fluid motion to the Kolmogorov scale,

it is referred to as Point Particle Direct Numerical Simulation (PP-DNS) [80]. Meshless Methods, such as Smoothed Particle Hydrodynamics (SPH), do not rely on traditional grids and are suited for more complex particle shapes and fluid interactions, providing better simulation of non-homogeneous flows and high-concentration suspensions. The Lattice Boltzmann Method is a weakly compressible fluid simulation technique based on gas molecular dynamics, capable of efficiently simulating particle-laden flows. This method has advantages such as a simple structure and ease of parallel computation, making it particularly suitable for simulating particles in low Reynolds number flows. Each of these methods has its own characteristics, and the choice of an appropriate simulation method depends on factors such as particle size, concentration, and the Reynolds number of the flow.

For simulations involving a large number of particles, the Point Particle Method is a standard approach [80]. When the particle size is smaller than the Kolmogorov scale, it can be treated as a point particle, with equations solved for each individual particle. One important parameter in this method is the relaxation time, which represents the time constant for the exponential decay of the particle velocity due to drag forces. A very short relaxation time for a particle indicates that its velocity is approximately equal to the local instantaneous fluid velocity, allowing the particle to be treated as a tracer. On the other hand, if a particle has a long relaxation time, it means that the particle's velocity lags behind the fluid velocity, and its velocity must be solved using Newton's second law.

The Maxey-Riley-Gatignol (MRG) equation of motion forms the basis of the Point Particle Method. This equation describes the forces acting on a spherical particle moving in an unsteady, homogeneous, and viscous fluid. The equation of motion is not applied when particles are considered passive tracers. The equation of motion is given by:

$$\frac{d\mathbf{x}_i(t)}{dt} = \mathbf{v}_i \quad (2.22)$$

where $\mathbf{x}_i$ denotes the position of the i th particle and $\mathbf{v}_i$ denotes the velocity of the i th particle.

For passive particles, their equations of motion are expressed as:

$$m_i \frac{d\mathbf{v}_i(t)}{dt} = \sum \mathbf{F}_i \quad (2.23)$$

$$\mathbf{v}_i = \mathbf{u}(\mathbf{x}_i(t), t) \quad (2.24)$$

where m_i denotes the mass of the i th particle, $\mathbf{u}(\mathbf{x}_i(t), t)$ denotes the velocity of the fluid, and $\mathbf{F}_i$ denotes all the forces on the particle.

MRG equation of motion is expressed as:

$$m_i \frac{d\mathbf{v}_i(t)}{dt} = \mathbf{F}_B + \mathbf{F}_{PG} + \mathbf{F}_{AM} + \mathbf{F}_D + \mathbf{F}_{hist} \quad (2.25)$$

In this equation, $\mathbf{F}_B$ represents the buoyancy force, $\mathbf{F}_{PG}$ denotes the force due to the undisturbed velocity field, also known as the pressure gradient force, $\mathbf{F}_{AM}$ refers to the added mass force, $\mathbf{F}_D$ is the drag force, and $\mathbf{F}_{hist}$ represents the Basset history force. The validity of the MRG equation of motion requires that the particle size is much smaller than the Kolmogorov length scale. For particles with larger sizes, Faxen correction terms can be applied to account for the size effects. The study by Homann and Bec [55] illustrates the influence of these correction terms on larger particles.

Buoyancy force is expressed as:

$$\mathbf{F}_B = (\rho_i - \rho_f)V_i\mathbf{g} \quad (2.26)$$

where ρ_i denotes the density of the i th particle, ρ_f denotes the density of the fluid, V_i denotes the volume of the i th particle, and $\mathbf{g}$ denotes the acceleration of gravity.

The force by the undisturbed velocity field is expressed as:

$$\mathbf{F}_{PG} = m_{f,i} \frac{D\mathbf{u}_i}{Dt} \quad (2.27)$$

The added mass force is expressed as:

$$\mathbf{F}_{AM} = \frac{1}{2}\rho_f V_i \left(\frac{D\mathbf{u}_i}{Dt} - \frac{d\mathbf{v}_i(t)}{dt} \right) \quad (2.28)$$

The drag force is expressed as:

$$\mathbf{F}_D = m_i \frac{(\mathbf{u}(\mathbf{x}_i(t), t) - \mathbf{v}_i)}{\tau_i} (1 + 0.15Re_i^{0.687}) \quad (2.29)$$

where τ_i denotes the particle relaxation time of the i -th particle, which characterizes the response of the particle velocity to the local fluid velocity fluctuations. For low particle Reynolds numbers, τ_i can be approximated by the Stokes relaxation time,

$$\tau_i = \frac{\rho_p d_p^2}{18\mu},$$

where ρ_p is the particle density, d_p is the particle diameter, and μ is the dynamic viscosity of the fluid. Re_i denotes the number of particle Reynolds of the i th particle, and the expressions of these two parameters will be described in detail in the next section.

The Basset history force is expressed as:

$$\mathbf{F}_{hist} = \frac{3}{2} (\pi \rho_f \mu)^{1/2} d_i^2 \int_0^t \frac{d}{d\tau} (\mathbf{u}_i(\tau) - \mathbf{v}_i(\tau)) \frac{1}{(t - \tau)^{1/2}} d\tau \quad (2.30)$$

Some of these forces can be simplified or neglected depending on the characteristics of the particles. For instance, the study by Armenio and Fiorotto [4] found that for small and heavy particles (i.e. $\rho_i \gg \rho_f$), the pressure gradient force, added mass force, and Basset history force are relatively small compared to the drag force and can be ignored. Similarly, research by Ling et al. [78] indicated that for small and heavy particles, gravity and drag forces dominate. Due to the high computational cost of the Basset history force, it is typically neglected; however, studies [27, 101] have shown that it significantly influences particle kinematics and clustering. Prasath et al. [113] proposed a new numerical method that accurately solves the Maxey-Riley equation including the Basset history force, without increasing storage costs. This method is suitable for numerical simulations of smooth flows and is particularly effective for analyzing particle behavior in complex flows.

The Lagrangian particle tracking (LPT) method can be classified into one-way coupling, two-way coupling, and four-way coupling. One-way coupling refers to a scenario where, at low particle volume fractions, the effect of particles on turbulence is negligible. In this case, particle motion is influenced by turbulence, but the turbulence characteristics are not significantly altered by the presence of particles. Two-way coupling occurs when the particle volume fraction increases, and particles start to influence the turbulence, thereby altering its structure. In this regime, the interaction between particles and turbulence becomes more complex, with particle motion being influenced by turbulence, while particle motion also affects the turbulence characteristics. Four-way coupling refers to the situation where, at sufficiently high particle volume fractions, there are not only two-way effects between particles and turbulence but also collisions between particles (i.e., particle-particle interactions), further complicating the turbulence dynamics. Four-way coupling represents the intricate interactions between particles, turbulence, and particles.

Elghobashi [37] provided a classification diagram for the different stages

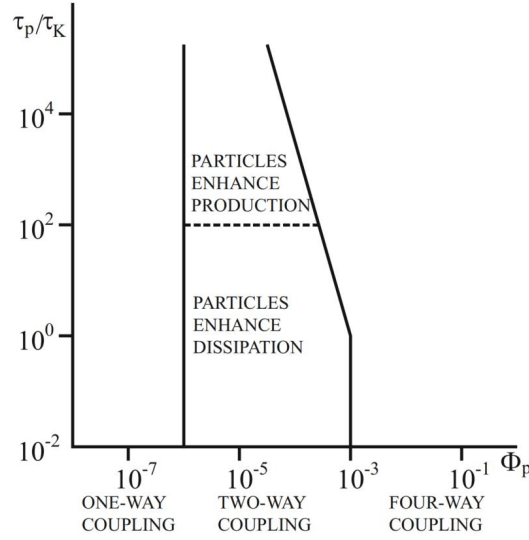


Figure 2.6: Map of regimes of interaction between particles and turbulence. [37]

of particle-turbulence interaction in particle-laden turbulent flows, as shown in Fig. 2.6. The diagram plots particle concentration (volume fraction) against particle response time ratio on the vertical and horizontal axes, respectively, to delineate the various coupling regimes. When particle concentration is very low (e.g. $\Phi_p < 10^{-6}$), the effect of particles on turbulence is negligible, and this is considered the "unidirectional coupling" regime. As particle concentration increases, the influence of particles on turbulence becomes more significant, eventually transitioning into the "two-way coupling" or "four-way coupling" regimes. Particle size (i.e., particle response time) and concentration not only affect the turbulence dissipation (energy loss) and turbulence energy production but also influence the structure of turbulence and particle dispersion behavior. For example, smaller particles (with shorter response times) may enhance turbulence energy and lead to greater turbulence dissipation, while larger particles may promote vortex formation and increase turbulence production.

One-way coupling

In 1974, Riley and Patterson [104] studied the diffusion behavior of scalar particles (such as tracer particles) in isotropic turbulence using numerical integration methods. This may be the first study to apply the point particle method in this context. By injecting a large number of passive tracer particles into a stable three-dimensional turbulent velocity field, they successfully reproduced the entire process of particle transport from initial advection with

the flow to the later stages exhibiting normal diffusion.

In 1988, Yeung and Pope [153] systematically established a particle tracking framework for extracting Lagrangian information from DNS results, and comprehensively evaluated interpolation accuracy, time step size, and statistical errors. This development contributed to the extension of turbulent flow numerical simulations from an Eulerian to a Lagrangian perspective. In 1989, McLaughlin applied the Maxey-Riley equation (including Stokes drag and Saffman lift) to simulate particle motion. The particles were rigid spheres with initial velocities matching the local fluid velocities, neglecting interactions between particles and electrostatic effects. The study validated the inertial mechanism of particle deposition, highlighted the role of shear lift in the viscous sublayer, and found that particle deposition was related to the initial distance from the wall, relaxation time, and particle density.

Bernard et al. [9] conducted a DNS of particle paths in turbulent channel flow, providing a detailed analysis of the origin of Reynolds stresses and their relationship with fluid particle motion. The simulation, conducted for a Reynolds number $R_\tau = 173.2$, involved two observation planes ($y^+ = 15.8$ and $y^+ = 37.5$) and tracked 3204 particle paths (including both forward and backward). A second-order Runge-Kutta method and three-dimensional linear interpolation were used to compute the paths, and the particle paths were graphically displayed along with Lagrangian statistical analysis (e.g., correlation function R_{uv}). The study revealed that Reynolds stress cannot be fully explained by gradient transport alone, as a small fraction of particle paths (approximately 2 – 3%) contributed more than 30% of the total Reynolds stress. These paths exhibited spiral or arc-shaped motion closely associated with the traditional sweep-ejection structure and displayed strong nonlinear and three-dimensional vortical dynamics. The Lagrangian particle tracking method provided a powerful tool for understanding turbulent momentum transport and may offer insights for improving future turbulence models.

Kontomaris et al. [65] introduced a particle tracking algorithm that made significant breakthroughs in both accuracy and computational efficiency, providing a robust numerical tool for studying complex turbulent fields using Lagrangian methods. This is particularly useful for research on channel flow and turbulence near wall regions and has important implications for studies of aerosol diffusion and pollutant transport.

In the study of particles in turbulent channel flow, Marchioli et al. [81] carried out benchmark tests on particle diffusion in low Reynolds number wall-bounded turbulent flows through an international multi-institution collaboration. The research used DNS and LPT methods, comparing results obtained

with different numerical schemes. They established the first particle diffusion database that includes both DNS and LPT steady-state simulations, filling a long-standing gap in such data. The study found that, despite using identical physical settings and initial conditions, differences in numerical methods, interpolation strategies, and time step sizes still led to notable discrepancies in particle concentration and velocity statistics, particularly in predicting particle concentration peaks near the wall. However, the overall trends were consistent, indicating that the reliability of the data was acceptable. For key statistics such as mean velocity, velocity fluctuations, and Reynolds stresses, the results from multiple groups showed good consistency. For Gaussian Stokes number particles ($St = 25$), the predictions from different groups were more consistent, indicating that larger particle inertia reduced simulation uncertainty.

Marchioli et al. [83] also investigated the behavior of particles in non-rotating pipe flow. Their study revealed that in vertical pipe turbulence, particle wall migration is constrained by the instantaneous effects of turbulent structures (sweeping and ejection). Particles with different inertial properties exhibited distinct deposition mechanisms, with accumulation occurring in the near-wall region. The presence of lift forces weakened particle deposition, especially for smaller particles.

Esch and Kuerten [147] examined the motion of particles in rotating pipe flow, focusing on the impact of rotation on particle separation efficiency, particularly under different flow conditions (laminar, turbulent, and unsteady laminar flows). The study showed that in rotating pipe flows, turbulence primarily affects the collection efficiency for larger particles, with a reduction in their capture capability. In contrast, the collection efficiency for smaller particles was almost unaffected by turbulence.

In recent years, research on particle motion in homogeneous isotropic turbulence has been steadily advancing. Squires and Eaton [135] employed DNS to investigate the influence of turbulence structure in forced homogeneous isotropic turbulence on particle concentration distribution and analyze the modulation effects of particles on turbulence energy and structure under varying mass loadings. Their study found that particle distribution exhibits structural selectivity. In homogeneous isotropic turbulence, moderately inertial light particles tend to accumulate in regions of low vorticity and high strain rate, while extremely light or heavy particles tend to distribute uniformly. Particles not only modulate turbulence energy, but as mass loading increases, turbulence energy and viscous dissipation decrease significantly, with particles acting as an additional dissipation source for turbulence. Eaton and Fessler [136] studied the non-uniform distribution of particles under the influ-

ence of forced homogeneous isotropic turbulence. Their research demonstrated that preferential enrichment is a common phenomenon that depends on the structure of the turbulence, and it is observed in almost all particle-turbulence interaction systems. The presence of this phenomenon depends on the vortex structure rather than random disturbances. The Stokes number is critical in predicting particle behavior. When the Stokes number is between 0.1 and 1, the interaction between particles and turbulence is most pronounced, making it easier to form enrichment regions. Particle distribution also has a feedback effect on the flow field itself. At certain particle concentrations (e.g., when the mass ratio reaches 1), particles can modulate the turbulence structure, altering its scale and intensity. Elghobashi and Truesdell [36] studied the diffusion characteristics of particles in decaying homogeneous isotropic turbulence, revealing differences in the movement behavior of particles and fluid points and surrounding fluid in turbulence, and explored the effects of inertia and gravity on the statistical properties of particle diffusion. The particle dynamics model considered factors such as Stokes drag, Basset force, added mass force, and buoyancy.

Extensive research has also been conducted on the dynamics of particles in wall-bounded turbulent flows. Reeks [114] studied the statistical behavior of discrete particles in non-uniform turbulence and proposed a new transport equation. It was found that turbulence migration shares a similar physical mechanism with thermophoresis, where particles are driven by local "energy gradients" (turbulence intensity or velocity variance), causing migration that reflects thermodynamic properties. Marchioli and Soldati [82] studied the migration and separation mechanisms of heavy particles in the turbulence boundary layer, focusing on the particle aggregation phenomena in the near-wall region and their relationship with the turbulence structure. The study revealed that particle migration and separation in the turbulence boundary layer are highly dependent on the near-wall coherent structures, and the peak particle concentration mainly results from the long-term retention and turbulent diffusion effects in the low-speed regions. Understanding the interaction mechanism between turbulence structures and particles is crucial for improving the control of particle deposition, resuspension, and mixing efficiency in industrial processes.

Two-way coupling

As shown in Fig. 2.6, Elghobashi [37] stated that when Φ_V exceeds 10^{-6} , the system can be considered as two-way coupling. Extensive studies have

been conducted on bidirectional coupling. Eaton [33] combined DNS and LES methods to simulate the gas-particle flow under varying particle concentrations, particle sizes, and turbulence conditions. The motion of the particles is influenced by the drag force from the gas flow, and the feedback effects of the particles on the turbulence are also incorporated into the simulation. The study found that the presence of particles in the airflow significantly alters the turbulence characteristics, particularly when the particle size is close to the small scale of the turbulence, where the attenuation effect of particles on turbulence becomes more pronounced. Particles not only affect the energy distribution of turbulence but may also enhance energy in the small-scale turbulence. Capecelatro and Desjardins [22] proposed a numerical method based on an Euler-Lagrange strategy for simulating particle-carrier fluid flow. This method first derived a volume-filtered equation for the carrier phase suitable for variable-density flow and discussed in detail the unresolved terms, particularly the interaction terms between the fluid and particle phases, ensuring these terms correctly converge during grid refinement. To handle particle collisions, a modified soft-sphere model was used, and parallel computation was optimized to improve computational efficiency. Gualtieri et al. [49] proposed a new method, the Exact Regularized Point Particle (ERPP) method, to simulate the momentum exchange between phases in multiphase flow. The method captures the interaction between particles and fluid by studying the unstable Stokes flow around small rigid spheres, thus avoiding singularity problems in particle models. The ERPP method uses regularization techniques to localize the disturbance caused by the particles to the fluid, effectively avoiding the computational complexity caused by a large number of particles in traditional methods. Horwitz and Mani [57] argued that under two-way coupling, the presence of particles alters the fluid velocity, leading to lower drag force predictions based on traditional Stokes drag calculations. Therefore, they proposed a correction method to calculate the undisturbed fluid velocity, instead of directly using the disturbed velocity obtained from calculations. Numerical experiments showed that the proposed correction method significantly reduced the calculation error for particle settling in stagnant fluids and agreed with the analytical solution. Ireland and Desjardins [58] introduced the volume-filtered Euler-Lagrange method to resolve fluid disturbances at the particle scale and avoid grid dependency issues. The proposed drag force correction method significantly improved the prediction accuracy of particle settling velocity, particularly at low particle Reynolds numbers. The correction method demonstrated good adaptability in the choice of filter size and resolution, with the best results achieved when the filter size-to-particle diameter ratio reached

2. Balachandar et al. [5] proposed a self-induced velocity correction method to improve the estimation of drag force in Euler-Lagrange point particle simulations. The paper applied steady and unsteady models for different Reynolds and Stokes numbers and verified that the unsteady model could accurately predict self-induced velocity disturbances in various scenarios. The unsteady model is more suitable for rapidly changing fluids and feedback forces. The proposed self-induced velocity correction model does not rely on a specific drag force expression and can be widely applied in various EL point particle simulations, including rigid particles, droplets, and bubbles.

Four-way coupling

According to Elghobashi [37], when Φ_V exceeds 10^{-3} , four-way coupling must be considered. Zhao et al. [155] studied the behavior of non-spherical particles in turbulent channel flows, focusing particularly on the effects of particle shape and Stokes number on the flow. A four-way coupled Lagrangian point particle method was used, with the fluid phase at low Reynolds number ($Re_\tau = 150$) modeled using DNS, while the particles were tracked individually. The study revealed the complex behavior of non-spherical particles in turbulent channel flows and clarified the influence of particle shape and Stokes number on the turbulence structure of the fluid. Particle collisions are typically simulated using nearest-neighbor list methods and stochastic collision models [80]. Hoomans et al. [56] studied the formation of bubbles and waves in a gas fluidized bed using discrete particle simulations, employing a hard-sphere method to model the motion of individual spherical particles in a two-dimensional fluidized bed, considering particle collisions and friction. The discrete particle model directly calculated the two-dimensional motion of each particle and simulated the interaction between the particles and the gas phase. The collision process in the model was based on the conservation of momentum and involved two empirical parameters: the restitution coefficient and the friction coefficient. Particle collisions were processed sequentially, simulating the fluid dynamics of the gas-solid two-phase flow. Verman [148] investigated the turbulence characteristics in gas-solid pipeline flow. The study mainly involved simulating the gas phase flow using DNS while modeling solid particles using the Lagrangian method, considering the effects of particle collisions. Notably, the paper discussed the impact of wall roughness on the simulation of turbulence characteristics, showing that wall roughness is crucial for fitting experimental data. Oesterle and Petitjean [100] proposed a new Lagrangian simulation method for modeling particle collisions in gas-solid flows. The core of their approach is to com-

pute the trajectory of individual particles and introduce simulated particle collisions during the calculation. The probability of collision occurrence was predicted through an iterative process, with the probability depending on local concentration and particle velocity. Unlike traditional dilute-phase flow simulations, this method does not require computing the simultaneous trajectories of multiple particles, thereby avoiding high computational costs and making it suitable for moderate concentration gas-solid flows. Sundaram and Collins [137] used DNS to study the collision frequency of particles in turbulence, simulating heavy particles suspended in turbulence and examining how turbulence parameters and particle properties affect collision rates. The particle volume fraction was kept within a small range (around 10^{-4}) to ensure the system remained in the dilute limit. A pseudo-spectral algorithm was used to update the fluid velocity, and the forces on the particles were approximated using Stokes drag. The simulation considered the finite volume of particles, requiring the inclusion of particle collisions. Wang et al. [150] studied the statistical mechanics description and modeling of inertial particle collisions in turbulence, focusing on the particle collision rate in turbulent gas flows and proposing contributions from turbulent transport effects and accumulation effects to the collision rate. They quantified the effects of turbulent transport and accumulation on particle collision rates. Turbulent transport effects are mainly related to the particle's inertial response time and the integral time scale of the flow field, while accumulation effects arise from the dissipative flow structures in turbulent regions, causing inhomogeneous local particle concentration distributions. Berlemont et al. [8] explored two Lagrangian methods for modeling particle collisions: a multi-particle tracking method and a single-particle method based on stochastic processes, emphasizing the key role of particle-particle velocity correlation in the collision process. Sommerfeld [129] used a stochastic Lagrangian model to simulate particle collisions and evaluated the model's effectiveness by comparing it with experimental data. The results indicated that the stochastic Lagrangian model showed good accuracy in simulating particle collisions in turbulence, effectively capturing the collision process and agreeing with existing experimental data.

2.2.2 RANS for particle-laden turbulent flows

Similar to single-phase flows, fluid flow can also be statistically described using the RANS equations. This significantly reduces the computational effort required for statistically steady turbulence, as only the average flow quantities need to be computed once, while the solution of the particle motion equa-

tions can be completed in the post-processing stage [80]. In this approach, a stochastic turbulence dispersion model is required to describe the impact of turbulence on particle motion. There are two types of stochastic turbulence dispersion models: one uses information from the RANS solution, such as Reynolds stress or turbulence kinetic energy, while the other is based on the probability density function (PDF) method.

Burry and Bergeles [20] introduced a particle simulation model combining the Lagrangian particle tracking method with the RANS method by incorporating the anisotropic characteristics of turbulence. The RANS method is used to simulate fluid turbulence and solve the averaged flow equations for the continuous phase. The Reynolds stress model (RSM) describes the irregular fluctuations and pressures in turbulence, allowing for a more accurate prediction of particle motion in anisotropic turbulence. Graham and James [48] studied the predictive ability of the vortex interaction model for particle diffusion under homogeneous isotropic stable turbulence (HIST) conditions. The core of the study was to analyze the motion and diffusion characteristics of non-fluid particles in turbulence using the vortex interaction model. The model assumes that particles interact with vortices in turbulence, and the velocity, length, and lifetime of the vortices are treated as random variables. Pozorski and Minier [112] used the PDF framework to analyze dispersed-phase turbulent flow. The PDF framework combines the variables of both the fluid and particles, providing a statistical modeling method at an intermediate level. By deriving the particle dynamics equations, the stochastic differential equation (SDE) method was employed, which helps describe particle motion in turbulence and clarifies the interaction between particle and fluid velocities. To address the effect of fluid velocity on particles, the paper proposed a Langevin equation model that considers the relationship between fluid velocity and particle motion. A. Tanire and Arcen [140] introduced the Generalized Langevin Model (GLM), which is mathematically consistent with the Reynolds stress transport equations, avoiding inconsistencies in standardized models and making it suitable for low-inertia particle conditions.

Minier et al. [93] proposed a set of standards and guidelines for the Lagrangian stochastic model applied to both single-phase and dispersed two-phase flows. The fluid dynamics background analysis mainly focuses on how to use the RANS equations to describe turbulent flow, particularly in the context of the Lagrangian stochastic model framework, and how to capture the characteristics of fluid turbulence. The authors combined the Lagrangian stochastic model with the RANS equations to describe the motion of fluid particles in turbulence, especially within complex flow structures. In this model,

the motion of fluid particles is influenced not only by the macroscopic flow field (such as the average velocity field) but also by the microscopic random fluctuations induced by turbulence. These fluctuations, which are typically not captured directly by the RANS equations due to the complexity of turbulence, are addressed by introducing a random force term in the Lagrangian stochastic model. In two-phase flows, particle motion is influenced not only by fluid turbulence but can also feedback and affect the turbulence structure. For example, in particle suspension flows or droplet-gas flows, the presence of particles alters the fluid dynamics, impacting the energy distribution and transport of turbulence. Therefore, the Lagrangian stochastic model is capable of capturing these complex fluid-particle interactions and provides a more detailed turbulence description than traditional RANS methods.

2.2.3 LES for particle-laden turbulent flows

In LES for point particles, similar to single-phase flow, the filtered fluid velocity can be used. In such simulations, the fluid velocity at the particle's location is not precisely known but only a filtered velocity is available. In certain applications, the unresolved scales of the fluid velocity have a significant impact on particle motion. Therefore, in addition to introducing subgrid models into the governing fluid equations, the influence of subgrid models must also be considered in the particle motion equations [80]. When the particle relaxation time is significantly larger than both the characteristic time scales of turbulence and the smallest time scale resolved in LES, the effect of the subgrid scales on particle motion can be neglected. In this case, there is no need to introduce a subgrid model into the particle motion equations [146]. However, if the particle relaxation time is close to the Kolmogorov time scale, neglecting subgrid scales significantly affects vortex migration in turbulent channel flows with particles, thereby impacting the accuracy of LES [69].

To account for the effects of subgrid scales, two different models have been proposed. The first model applies a random model by introducing broadband random noise into the Navier-Stokes equations for the continuous phase or by adding extra velocity terms in the particle motion equations. The second model approximates the deconvolved filtered fluid velocity to obtain the unfiltered fluid velocity and applies it in the particle motion equations [80].

Amiri et al. [2] used three stochastic models to simulate the effect of subgrid scale velocity fluctuations on particle motion. Model 1 is for isotropic flow without SGS temporal correlation, where SGS velocity is assumed to follow a Gaussian distribution and is randomly sampled. This model is suitable for

cases where the particle response time is much larger than the SGS vortex time scale (i.e., when particle inertia is high). Model 2 is for isotropic flow with SGS temporal correlation, considering the Lagrangian time correlation of SGS velocity along the particle trajectory. This model is suitable for small particles or cases where the time step is close to the SGS time scale. Model 3 is for anisotropic flow with SGS temporal correlation, which builds on Model 2 by introducing an anisotropic adjustment factor for SGS turbulence. This model significantly outperforms the other two models in predicting the turbulence intensity of small particles near the wall.

Pascal and Olivier [39] studied the impact of subgrid-scale fluid turbulence on the collision statistics of heavy particles. First, DNS was used to compute the fluid velocity field, and combined with particle trajectory simulations, the small-scale fluid fluctuations in particle motion were analyzed. Subsequently, particle trajectories were calculated using filtered fluid velocity fields, and the effects of subgrid fluid turbulence on particle statistical characteristics, including turbulence diffusion, kinetic energy, particle aggregation efficiency, relative particle velocity, and collision frequency, were evaluated. The study showed that particle inertia has a minimal effect on subgrid fluid turbulence, especially in terms of subgrid Lagrangian integration time scales. In extreme cases, the impact of particle inertia on subgrid fluid becomes negligible. The particle diffusion coefficient is less influenced by subgrid turbulence, primarily dominated by turbulence vortices with high energy content. For particles with a large subgrid Stokes number (long particle response time), subgrid turbulence has little effect on particle aggregation and collision frequency. For particles with a smaller Stokes number (shorter response time), the effect of subgrid turbulence vortices is more significant, particularly in particle aggregation and collision frequency. For particles with a large subgrid Stokes number, the LES method can accurately simulate gas-solid turbulent flow without the need for additional subgrid fluid turbulence modeling. For particles with a smaller Stokes number, subgrid turbulence needs to be modeled using stochastic force models, such as the Langevin equation. This study provides an important theoretical foundation for applying LES methods in gas-solid turbulent flows, particularly in simulating particle motion and collisions while accounting for subgrid fluid turbulence effects.

Bini and Jones [12] proposed a model based on SDE to describe the Lagrangian velocity increments of particles, especially in cases where only low-frequency turbulence field data are available. Since traditional Langevin equations do not adequately capture the non-Gaussian statistical features observed in experiments, a nonlinear drift and diffusion SDE model was introduced and

compared with experimental data. This nonlinear model better describes the statistical characteristics of particle acceleration in turbulence, including the commonly observed heavy tail and non-Gaussian distributions in experiments. Furthermore, a class of nonlinear SDE models with different parameters was proposed, which can match experimental results by adjusting the parameters, providing a more precise description. This improved nonlinear model not only applies to experimental data but also has broad potential for use in particle diffusion modeling in LES.

Pozorski and Apte [111] studied the numerical simulation of particle motion in isotropic turbulence and proposed a stochastic modeling method for SGS particle diffusion. The study focused on the impact of spatial filtering on particle motion, particularly in filtering methods commonly used in LES, as well as the influence of subgrid-scale turbulence on particle statistical properties, including preferential concentration. Through a preliminary analysis of particle-laden forced isotropic turbulence using DNS, the effects of subgrid-scale motion on particles with different inertias were investigated, and a scheme for reconstructing the residual flow field using a stochastic Langevin model was proposed. The study found that neglecting subgrid-scale fluctuations significantly affects the preferential concentration of particles. The proposed stochastic Langevin model can accurately recover the turbulence kinetic energy of particles, and for larger inertial particles, the subgrid-scale filtering effect can be well simulated using this model. However, for smaller inertial particles, the model struggles to recover the small-scale patterns of the particle distribution.

In 2004, Kuerten and Vreman [69] first introduced the inverse filtering model to correct the subgrid effects in LES and explored how to predict vortex effects (i.e., vortex clustering) in turbulent particle motion using LES. The study found that by introducing inverse filtering, LES could significantly improve the prediction accuracy of vortex clustering, bringing the LES results closer to the DNS results, especially in the diffusion-impaction regime. The inverse filtering method not only improved the prediction of vortex clustering but also enhanced the diffusion characteristics of particles.

Shotorban and Mashayek [124] used an approximate deconvolution method to simulate the effects of SGS turbulence on particles in LES. The approximate deconvolution method reconstructs the instantaneous velocity of the fluid phase through deconvolution, compensating for the subgrid-scale effects on particles that are filtered out in LES. By applying the deconvolved velocity to the particle momentum equation, the fluid velocity is reconstructed. The study used homogeneous shear turbulence as a test scenario and compared the

effects of different levels of approximate deconvolution ($N=0, 1, 2$) on particle statistics. Two testing methods were used to evaluate the model: A priori testing, where the effectiveness of the approximate deconvolution was evaluated by filtering the velocity from DNS results, and A posteriori testing, where the approximate deconvolution was applied in LES and compared with DNS results. The study found that reconstructing the fluid phase velocity through approximate deconvolution significantly improves the prediction of particle statistics, especially when the particle time constant is small. The approximate deconvolution method effectively improves the accuracy of LES predictions for particle number density and turbulence kinetic energy (TKE). In the A priori test, after reconstructing the fluid velocity using deconvolution, the LES predictions closely matched the DNS results, while LES without accounting for subgrid effects performed poorly. In the A posteriori test, the approximate deconvolution method successfully recovered the turbulence diffusion of particles, especially in the earlier stages of simulation.

Marchioli et al. [84] studied two candidate models: one based on fractal interpolation and the other based on approximate deconvolution, aiming to improve particle dynamics modeling in turbulent dispersion flows, particularly by incorporating SGS effects in the Lagrangian equations of particle motion. The velocity field reconstructed by fractal interpolation better matches DNS data, particularly for fluctuations in the wall-normal component, thereby improving the accuracy of LES in predicting turbulence-driven particle clustering effects. The approximate deconvolution model improves fluid and particle velocity fluctuations by recovering SGS turbulence kinetic energy, but in coarse-grid LES, the deconvolution leads to an overestimation of velocity fluctuations, which affects the prediction of particle velocity fluctuations.

Gobert [45] analyzed three SGS models for particle-fluid flow in LES and proposed an analytical method based on statistical moments (such as the mean and variance of particle velocity and position) for evaluation. These models include the approximate deconvolution method (ADM) and two stochastic models based on the Langevin equation. The study found that for large Stokes numbers, the ADM model performs better, while for small Stokes numbers, the Langevin-based models perform better. Later, Gobert and Manhart [46] introduced the Spectrally Optimized Interpolation (SOI) model. This model optimizes the interpolation kernel function to make the fluid velocity spectrum perceived by the particle as close as possible to the target spectrum, improving the traditional ADM model. The core idea is to use particle interpolation errors to construct a particle-LES model and correct the fluid spectrum perceived by the particle through interpolation optimization. Compared to the

traditional ADM model, the SOI model more accurately captures the impact of unresolved scales on particle dynamics. The study validated the SOI model's effectiveness through DNS and LES simulations in homogeneous isotropic turbulence. The SOI model showed significantly higher accuracy in particle-LES simulations compared to the ADM model, especially in coarse-grid cases. SOI not only provides a more precise description of particle motion but also has a computational cost similar to that of fourth-order interpolation.

Bianco et al. [11] studied the inherent errors introduced by filtering operations in LPT during LES. The focus was on the filtering errors in particle motion, with a comparison to the results from DNS, using DNS as the reference standard. Various filter types and widths (such as cutoff and top-hat filters) were applied, and statistical analysis was performed on the filtering errors with respect to particle inertia and different wall distances. Three different Stokes numbers ($St = 1, 5, 25$) were used, with a focus on the influence of filter width on error distribution. The study found that filtering errors are random and exhibit clear non-Gaussian characteristics, particularly near the wall. The filtering errors depend not only on particle inertia but also on filter width. As the filter width increases, the variance of the errors grows, and the non-Gaussian characteristics become more pronounced. The influence of particle inertia on filtering errors is significant. In some cases (e.g., $St = 5$), inertial particles exhibit the strongest response to filtering errors, with larger error peaks. In the flow, inertial particles respond differently to turbulence structures of various scales, which amplifies the error magnitude. Near the wall, the peaks of filtering errors are more prominent, especially in the "buffer layer" of the flow, where the errors show significant negative values, indicating an overestimation of fluid drag. The error distribution is highly skewed with sharp peaks, suggesting that error fluctuations have intermittent characteristics. The PDF shows significant non-Gaussianity in filtering errors at different wall positions, particularly near the wall. As the filter width increases, the PDF tail broadens, showing stronger skewness and peakness.

Michaek et al. [91] proposed a Hybrid Stochastic-Deconvolution Model, which combines the deconvolution model with a stochastic subgrid-scale model to describe particle motion in unresolved flows. The model combines the ADM with a stochastic model for subgrid scales. The primary method is based on prior results from DNS for particle transport, particularly applied in channel flow at $Re_\tau = 950$. The coefficients of the stochastic part of the model (such as RMS values and Lagrangian correlation time) are based on DNS results, while the basic part of the model is based on LES resolved flow. The study showed that the Hybrid Stochastic-Deconvolution Model significantly improves

accuracy in LES particle motion simulations, especially in predicting particle concentration near walls and turbulent particle clustering.

2.3 Stochastic Modeling in Turbulence Simulations

2.3.1 Development of stochastic models

Foundations and early development of probability theory

The foundations of stochastic methods can be traced back to the early 20th century. In 1933, Russian mathematician Andrey Kolmogorov published his book *Foundations of the Theory of Probability* [62], which introduced the axiomatic foundation of modern probability theory. In this work, he provided a rigorous mathematical framework for probability theory, establishing an axiomatic system for probability spaces and laying the groundwork for the study of stochastic processes. Kolmogorov's axiomatic definition provided strict mathematical tools for random events and processes, allowing researchers to analyze and derive the laws of random phenomena in a systematic way. The core idea of Kolmogorov's axiomatic probability theory is that by defining a probability space (including the sample space, events, and probability measures), random phenomena can be effectively described, and through numerical methods of probability, the foundation of modern statistics was gradually formed. This theory provided a solid mathematical foundation for later studies in turbulence, treating it as a random process.

In 1941, Kolmogorov proposed the statistical theory of turbulence [64], which centers around using structure functions and energy spectra to describe the statistical characteristics of turbulence. The basic idea of this theory is that the energy transfer across different scales in turbulent flow can be described by statistical laws, and under certain conditions, these laws exhibit self-similarity, meaning their statistical properties remain unchanged across different scales. In 1941, Kolmogorov introduced the concept of the energy cascade process in turbulence, where the energy in turbulent flow progressively transfers from large scales to small scales and ultimately dissipates as thermal energy through viscous dissipation. This theory provided a clear framework for the statistical description of turbulence. Specifically, his proposed "structure function" as a method of describing turbulence, highlighted how velocity differences in turbulence change with distance, and how these differences can be quantita-

tively described using statistical measures like the root-mean-square velocity difference.

In Kolmogorov's theory, turbulence is viewed as a nearly stationary, homogeneous random process. While this theory has been successful in many applications, it also faces some limitations, such as its inability to fully explain complex phenomena like two-dimensional turbulence or intermittency. To address issues such as scalar transport, two-dimensional turbulence, and other turbulence-related problems, researchers have developed results in random dynamical systems, the ergodic theory of stochastic differential equations (SDE), Langevin dynamics, and Malliavin calculus [110].

The introduction of the stochastic Burgers equation

The Burgers equation, as a simplified form of the Navier-Stokes equations, has been widely applied in turbulence research. Originally proposed by Bateman in 1915 and further developed by Burgers in 1948, the Burgers equation has played an important role in fluid dynamics and the stochastic modeling of turbulence [110]. By introducing the Burgers equation, researchers are able to study fluctuations and dissipation phenomena in fluid dynamics and turbulence using a more simplified model. Although the Burgers equation is similar in form to the Navier-Stokes equations, it is a simplified nonlinear equation with fewer variables and a simpler structure, making it an important tool in the study of turbulence and stochastic modeling.

The Burgers equation is expressed as:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} \quad (2.31)$$

In the Burgers equation, $u(x, t)$ represents the fluid velocity, and ν is the viscosity coefficient (or diffusion coefficient), which represents the fluid's viscous effects. The equation combines the advection term $u \frac{\partial u}{\partial x}$ and the diffusion term $\nu \frac{\partial^2 u}{\partial x^2}$, describing the changes in the fluid velocity.

The Burgers equation essentially models the fluctuations in fluid flow, and is particularly significant in the study of incompressible fluids or approximately incompressible fluids. It can also be considered one of the fundamental equations for describing energy transport, dissipation, and turbulence generation in turbulent phenomena.

The classic version of the Burgers equation is a deterministic equation, but turbulence is inherently stochastic and lacks the complexity needed to describe the features of incompressible turbulence [13]. As a result, researchers

gradually introduced stochastic differential equations (SDE) to describe random disturbances in turbulence. This extension allows the Burgers equation to better simulate the random fluctuations, anomalies, and unpredictability in turbulence.

The stochastic version of the Burgers equation typically includes a random disturbance term, such as using a Wiener process (white noise) to model external random disturbances [88, 10, 59, 10]. This random disturbance term is typically expressed by introducing a stochastic source term (such as noise), allowing the equation to not only account for viscous and nonlinear effects but also capture the irregular fluctuations induced by random disturbances in turbulence.

The typical form of the stochastic Burgers equation is:

$$\frac{\partial}{\partial t}u + u\frac{\partial}{\partial x}u = \nu\frac{\partial^2}{\partial x^2}u + f \quad (2.32)$$

where $f(x, t)dt = \sum_k f_k(x)dW_k(t)$ is an additive noise and $W_k(\cdot)$ are independent Wiener process. This randomised version of the Burgers' equation allows researchers to take into account more complex stochastic and non-linear behaviours in the modelling of turbulence and thus better simulate real phenomena in turbulent flows.

Introduction of the stochastic Navier-Stokes equation

The unpressurised Navier-Stokes equations in the presence of random external forces or noise are the core model for describing real turbulence [110]:

$$\frac{\partial u}{\partial t} + (u \cdot \nabla)u = -\nabla p + \nu \nabla^2 u + \sum_k g_k dW_k \quad (2.33)$$

$$\nabla \cdot u = 0 \quad (2.34)$$

In this equation, u is the velocity field, p is the pressure field, ν is the viscosity coefficient, g_k is the noise coefficient, and dW_k represents the Wiener process (random noise). By introducing the noise term $g_k dW_k$, the equation incorporates randomness into fluid motion, simulating random external disturbances in turbulence. This equation is a SDE, and the existence and uniqueness of its solution depend on the intensity of the random disturbance and the boundary conditions. Under certain conditions, solutions to the stochastic Navier-Stokes equation exist, particularly in Sobolev spaces. For both two-dimensional and three-dimensional Navier-Stokes equations, the existence and

uniqueness of local strong solutions have been proven; however, the existence of a global solution for the three-dimensional case remains an open problem. The issue of ergodicity has also been addressed for stochastic Navier-Stokes equations. Under certain conditions, the solution of the system tends to a steady state, with ergodic theory indicating that the solution will approach a stationary random process. The pioneering work of Bensoussan-Temam laid the foundation for local/global strong solutions in the two-dimensional case, and the results were later extended to three dimensions by Brzeniak-Peszat, Kim, and others [7, 19, 61, 92, 32]. The existence of Markov solutions in the weak (martingale) sense and the unique invariant measure is discussed in subsequent studies by Da Prato-Zabczyk [42, 95, 26, 1]. Additionally, the forward-backward SDE systems based on variational principles provide paths for numerical algorithms.

Kraichnan stochastic flow model

The passive scalar advection model proposed by Kraichnan in 1968 uses a time white noise velocity field, making it one of the few analytically solvable turbulence models [67]. Its anomalous scaling can be systematically explained through renormalization group and operator product expansion [3]. The model reveals phenomena such as inverse energy cascade in two-dimensional turbulence, with classic references including Kraichnan's own analysis of the inertial range in 2D turbulence [66] and Tabeling's experimental review [138].

The core assumption of the Kraichnan model is that the velocity field has white noise properties in time, meaning the components of the velocity field are independent in time and exhibit homogeneity and isotropy. This assumption simplifies the complex motion in real fluids, making the model an idealized description in turbulence research.

In this model, the autocorrelation function of the velocity field satisfies the following conditions:

$$\langle u_i(t, x) u_j(t', x') \rangle = \delta(t - t') D_{ij}(x, x') \quad (2.35)$$

where $D_{ij}(x, x') = D_{ij}(|x - x'|)$. Here, $u_i(t, x)$ represents the velocity component of the fluid at position x and time t , and $D_{ij}(x, x')$ is the spatial autocorrelation function, typically a uniform function in one or two dimensions.

The Kraichnan model uses the Lagrangian method to track the motion of particles in the fluid. In the Lagrangian method, each fluid particle is treated as an independent tracking object, and its trajectory is determined by the action

of the velocity field. For each fluid particle, its motion follows the following equation:

$$dR(t; t_0, x_0) = u(t, R(t))dt \quad (2.36)$$

In this equation, $R(t; t_0, x_0)$ represents the particle's position, x_0 is the particle's initial position, and $u(t, R(t))$ is the velocity field. The equation is based on the assumption that the velocity field is white noise in time, leading to the typical randomness of particle motion. By introducing the autocorrelation function and time independence, the Kraichnan model further simplifies the random motion of particles and, by calculating their statistical properties, investigates transport phenomena and instabilities in turbulence.

The equation that the Kraichnan model uses to describe the scalar transport process is typically a reaction-diffusion equation, in the form of:

$$\frac{\partial \Phi}{\partial t} + (u \cdot \nabla) \Phi = D \nabla^2 \Phi + S(x, t, \Phi) \quad (2.37)$$

In this equation, Φ is the scalar field (such as temperature or concentration), D is the diffusion coefficient, and $S(x, t, \Phi)$ is the source or consumption term. This equation is used to simulate the diffusion and transport processes of scalar quantities in turbulence.

To further simplify and analyze, the Kraichnan model assumes that the velocity field is white noise in time, and that the autocorrelation function of the velocity takes the following form:

$$D_{ij}(x, x') = \delta(x - x') \quad (2.38)$$

Through this assumption, the Kraichnan model obtains a relatively simple analytical solution, making it an important theoretical tool in turbulence research.

One of the main contributions of the Kraichnan model is its description of the statistical properties and transport phenomena in turbulence. By studying the structure function of the scalar field Φ , the model reveals the characteristics of material transport in turbulence. The form of the structure function is:

$$S_n(\Delta x, t) \sim \langle |\Phi(x + \Delta x, t) - \Phi(x, t)|^n \rangle \quad (2.39)$$

where Δx is the scale of the space and n is the order of the structure function. An important property of the Kraichnan model is that under this model, the structure function has different power law behaviours at different scales,

exhibiting typical turbulence characteristics.

Overall, the Kraichnan model not only provides a simplified framework for theoretical research but has also been widely applied in turbulence simulation and prediction. The model's simplified nature makes it widely used in numerical simulations of high-dimensional turbulence problems, especially in the study of two-dimensional turbulence. By using the Kraichnan model, researchers are able to more accurately predict the statistical behavior of turbulence, laying the foundation for further studies.

Langevin / path integral stochastic modelling

The Langevin/path integral stochastic model combines the Langevin equation with the path integral method to describe dynamic systems under random disturbances. The Langevin equation is typically used to describe the motion of particles under the influence of external random forces, while the path integral method provides a global perspective on the system's trajectory, particularly suited for the statistical analysis of random processes.

By converting the two-dimensional Euler equation or quasi-geostrophic fluid system into stochastic Langevin dynamics and applying the Martin-Siggia-Rose path integral framework, it becomes possible to study large deviations, instantons, and nonequilibrium statistical mechanics. Bouchet, Laurie, and Zaboronski provided a comprehensive discussion and application of this method [14].

A detailed description of the Langevin equation will be provided in the next section.

Overall, the introduction and development of stochastic methods represent a significant breakthrough in turbulence research. From Kolmogorov's probability theory to modern stochastic differential equations, and the Langevin equation, stochastic methods have enabled researchers to gain a deeper understanding and simulation of the complex dynamic behavior of turbulence from the perspective of statistical physics. With the improvement of computational capabilities and continuous advancements in stochastic numerical methods, significant progress has also been made in the numerical simulation and experimental research of turbulence.

2.3.2 Langevin equations in turbulence simulations

The developments in thermodynamics at the end of the 19th century and the beginning of the 20th century established the connection between the macro-

scopic world and the atomic world. Einstein [35] and Smoluchowski [127] independently proposed the theory of Brownian motion in 1905 and 1906, explaining that the random motion of measurable particles in a fluid is a manifestation of atomic motion. In 1908, Langevin [71] introduced the Langevin equation, further linking thermal fluctuations with macroscopic fluid dynamics. He proposed a new random force model to describe the motion of particles subjected to random disturbances, particularly when influenced by collisions and drag forces in a fluid.

The Langevin equation was written by Langevin (for one Cartesian component of velocity and Langevin force) as follows:

$$M \frac{dV}{dt} = -\zeta V + X(t) \quad (2.40)$$

where V is the particle's velocity, ζ is the viscous drag coefficient, typically representing the resistance of the fluid to the particle's motion. $X(t)$ is the random noise term, typically modeled using the Wiener process (Brownian motion), representing the random collisions and disturbances of the fluid molecules on the particle.

The Langevin equation divides the force acting on a Brownian particle into two parts: one is the drag related to the viscous fluid (Stokes drag), and the other is the random force $X(t)$ associated with random collisions in the atomic world. The random force has zero mean and is independent of the particle's velocity.

The original form of the Langevin equation is linear. Kolmogorov [123] extended it to a nonlinear equation without violating the reversibility constraints:

$$M \frac{dV}{dt} = -\zeta V(t) - \nabla \Phi + X(t) \quad (2.41)$$

where $V(t) = \frac{dr}{dt}$. This is equivalent to adding a force on the right-hand side of the Langevin equation, which is the negative gradient of the potential $\Phi(r)$ at the position r of the Brownian particle. This extended equation can explain the observed anomalous Brownian motion.

In the standard Brownian motion of a mesoscopic-sized sphere in a fluid, the mass density of the sphere and the surrounding fluid are of the same order of magnitude. In this case, the viscous force can no longer be replaced by the standard Stokes expression, and the dependence of the frictional force on history must be considered [107]. This is achieved by replacing the instantaneous

friction in the Langevin equation with a convolution term:

$$M \frac{dV}{dt} = - \int_0^t dt' \Gamma(t - t') V(t') + X(t) \quad (2.42)$$

where the kernel $\Gamma(t)$ is to be derived by solving Stokes' equation.

The Langevin equation was initially used to explain Brownian motion, describing how particles suspended in a liquid are affected by random collisions with surrounding molecules, leading to irregular random motion. Over time, the Langevin equation has gradually been introduced into turbulence research, becoming an important tool for analyzing the microscopic dynamics and stochastic fluctuations in turbulence. The Langevin equation allows for the introduction of random disturbance terms when describing the microscopic motion in fluids, thus providing an effective method for stochastic modeling in turbulence research. In particular, the Langevin equation has shown its unique advantages in simulating irregular fluctuations, random vortices, and energy dissipation in turbulence.

Turbulence is a highly complex, nonlinear flow phenomenon with multi-scale characteristics. In turbulence, fluid motion is not only characterized by macroscopic velocity field changes but also involves numerous small-scale vortices, random fluctuations, and irregularities. While traditional Navier-Stokes equations can describe the macroscopic behavior of turbulence, they often fall short in capturing the microscopic stochastic fluctuations and unpredictability within turbulence. The Langevin equation, by introducing random noise terms, provides a more detailed mathematical framework for the microscopic dynamics of turbulence. Small-scale vortices and the motion of fluid particles in turbulence are often influenced by external disturbances, and the randomness and noise terms in the Langevin equation are used to simulate these stochastic fluctuations. Through the Langevin equation, researchers can account for the effects of random disturbances on the microscopic behavior of fluids during turbulence simulations, allowing for a more accurate description of irregular fluctuations, energy dissipation, and other phenomena in turbulence.

Krasnoff and Peskin [68] discussed the Langevin model for turbulent diffusion and proposed an improved method to describe particle motion in turbulence. The model considers the interaction between pressure and viscous stress and analyzes single-particle and two-particle diffusion in turbulence. The model derives the Lagrangian time micro-scale and integral scale in turbulence and relates them to the properties of the Eulerian field. The study shows that the Langevin model effectively describes the relative velocity and diffusion

behavior of two particles in turbulence, providing reasonable approximations even at lower Reynolds numbers. In Pope's research [108], the Langevin equation was successfully applied to velocity modeling in homogeneous turbulence. The Langevin equation was used to simulate the velocity evolution of particles in turbulence, particularly under homogeneous turbulence conditions. By numerically solving the Langevin equation, the velocity time series of fluid particles were obtained, allowing for the analysis of velocity distribution and turbulence intensity in turbulence. The Langevin equation was further extended to propose a model for turbulence frequency (or turbulence dissipation rate) and used to describe the frequency variations of turbulent particles. The extension of the Langevin equation enables a more comprehensive description of various physical quantities in turbulence, including the coupling of velocity and frequency.

Heppe and Burkhard [54] proposed a new stochastic model for relative turbulent diffusion based on the generalized Langevin equation, considering different turbulence scales, including viscous scale, inertial scale, and integral scale. The authors used a nonlinear projection method to derive the generalized Langevin equation from the Navier-Stokes equations, describing the velocity difference between two fluid particles. This equation captures the instantaneous non-Gaussian characteristics of turbulence and the effects of the viscous range.

Mito et al. [94] introduced spatially varying Lagrangian time scales and joint Gaussian random forcing functions into the Langevin equation to adapt to the non-homogeneous turbulent flow field. These modifications allow the equation to more accurately describe particle diffusion in non-homogeneous turbulence, especially in regions with significant variations in the flow field. Laval et al. [74] proposed a turbulence simulation method aimed at describing turbulence behavior using a sub-filter model in LES. By modeling the turbulent force (represented by the turbulence Lamb vector) as two contribution terms, one part determined by classical eddy viscosity, and the other part derived dynamically using a generalized (stochastic) Langevin equation, the LES-Langevin model provides a more accurate description of energy transfer, energy decay, and inter-scale energy transport than traditional eddy viscosity-based LES models under similar computational conditions.

Dehbi [29] proposed a particle diffusion prediction method based on the Lagrangian continuous random walk (CRW) model, specifically for turbulent particle diffusion in complex wall-bounded geometries. The study combined CFD simulations with Eulerian statistical data provided by DNS and used a standardized Langevin equation to describe the effect of turbulence inho-

mogeneity on particle motion. The model included drift velocity corrections, making it particularly suitable for considering particle inertia, and avoided the non-physical issues common in traditional random walk models. Later, Dehbi [30] introduced a model based on the stochastic Langevin equation to describe particle diffusion in turbulent flows, especially considering the effects of thermal diffusion on particle behavior. In this model, particle motion is influenced by three main forces: drag force, gravity, and thermal diffusion force. The model effectively captures the influence of turbulence and thermal diffusion on particle diffusion, enabling accurate predictions of particle deposition behavior by considering turbulence fluctuations and thermal diffusion.

Brouwers [17] studied the random motion of fluid particles in turbulence induced by wall surfaces, particularly using the Langevin equation for modeling. By modeling the random motion of fluid particles with the Langevin equation, the study analyzed the relationship between particle acceleration and small-scale turbulence and found that the Langevin equation is applicable to high Reynolds number turbulence. The study showed that the damping term in the traditional Langevin equation lacks uniqueness in anisotropic turbulence and proposed a solution based on the Onsager symmetry, further deriving the specific form of the damping term for wall-induced turbulence. Experiments confirmed that the asymmetry of the damping term had negligible statistical effects on particle displacement.

Kuerten and Brouwers [70] applied the Langevin equation to describe particle motion in turbulence, especially for calculating Lagrangian statistical quantities. By introducing colored noise corrections and considering finite viscosity effects, and comparing extensively with DNS results, the Langevin model was shown to accurately describe the particle motion characteristics in turbulence, particularly in regions far from the wall.

Brouwers [18] employed Lagrangian Kolmogorov K-41 theory to mathematically model turbulence, proposing the Langevin equation to describe the statistical velocity characteristics of fluid particles. Using the C-10 expansion method, they derived the diffusion equation describing turbulence transport processes. The equation describes the statistical velocity of fluid particles in turbulence under high Reynolds number conditions, considering the particle velocity attenuation function and Gaussian white noise excitation terms, with all coefficients derived from the C-10 expansion. Based on the Langevin equation, the authors derived the diffusion equation for the position diffusion of tagged fluid particles and validated its consistency with DNS results.

Dhariwal et al. [31] used DNS and PDF-based Langevin simulations to analyze the relative velocity and position between particle pairs. They evolved the

relative velocity and separation of particle pairs using the Langevin equation and simulated the relative motion of multiple particle pairs. Three forms of diffusion rates were considered in the simulations: CF1, CF2, and CF3. CF1: The Eulerian correlation function of the two-time fluid relative velocity based on DNS-calculated data. CF1 is the most accurate model as it relies entirely on DNS data without further approximations. CF2: A diffusion rate derived from analytical assumptions, assuming the variation in relative velocity is primarily caused by the convective effects of large-scale vortices. CF2 has the advantage of being analytically derived, but may introduce bias for small Gaussian numbers. CF3: An improved model of CF2, considering the response of particle pair centroids, aiming to better capture the effects of large-scale vortices in turbulence.

Callaham et al. [21] proposed a new framework to ensure the statistical consistency of the model through forward and adjoint Fokker-Planck equations, addressing the challenges presented by time-dependent forcing forces (such as vortices and turbulence) in traditional methods. The Langevin regression, combined with sparse regression and optimization of the Fokker-Planck equation, can identify nonlinear dynamical features of the system, even when the system's random disturbances do not adhere to the classical Gaussian white noise assumption.

Gallo et al. [43] introduced a coupled lattice model (CML) based on the Langevin equation to study the velocity distribution function (VDF) of turbulent flows at different spatial scales. The study showed that the probability density function (PDF) of velocity fluctuations in turbulence could be well fitted by the κ -distribution, and there was a significant relationship between the κ -parameter, spatial scale k , and turbulence intensity (represented by the Reynolds number Re).

Benella et al. [6] studied dynamical scale turbulence in weakly collisional plasmas, particularly at the sub-ion scale. The researchers proposed a framework where turbulence energy transfer is viewed as a scale-dependent Langevin process, linking the drift term in the Langevin equation to the scale characteristics of fluctuations, explaining global scale invariance at the sub-ion scale. The study showed that fluctuations exhibit a uniform energy distribution within this scale range, and the drift term directly relates to the most probable Hlder exponent.

Farndell et al. [38] used Langevin dynamics simulations to study polymer conformations in high shear flows and turbulent flows, particularly for their application in nuclear waste treatment. The study investigated the behavior of polymers in turbulent shear flows by varying shear rates to find the optimal

shear rate for promoting flocculation. The research employed Langevin dynamics based on the FENE model and DNS methods to simulate the dynamics of polymer chains, and validated the results by comparing with experimental data, analyzing polymer homogeneity and extensibility.

Michael et al. [90] proposed a new method based on the generalized Langevin equation (GLE) to simulate Brownian motion with hydrodynamic memory effects and to apply it in a continuous framework. This method does not rely on molecular dynamics to determine the hydrodynamic memory kernel but optimizes the kernel in real-time through a multiphase DNS framework. This allows simulations over a wide range of particle-fluid density ratios, from 1 to 1000, and accurately captures particle diffusion characteristics in various environments.

The introduction of the Langevin equation provides an effective stochastic modeling tool for turbulence research. By incorporating random noise terms, the Langevin equation can simulate irregular fluctuations, random vortices, and energy dissipation processes in turbulence, aiding researchers in analyzing the microscopic dynamics of turbulence. Despite some challenges, the advantages of the Langevin equation in multi-scale modeling, stochastic modeling, and numerical simulations make it an indispensable tool in turbulence research.

Bibliography

- [1] Sergio Albeverio, Franco Flandoli, Yakov G Sinai, and Franco Flandoli. An introduction to 3d stochastic fluid dynamics. *SPDE in Hydrodynamic: Recent Progress and Prospects: Lectures given at the CIME Summer School held in Cetraro, Italy August 29–September 3, 2005*, pages 51–150, 2008.
- [2] A Elhami Amiri, S Kazemzadeh Hannani, and F Mashayek. Large-eddy simulation of heavy-particle transport in turbulent channel flow. *Numerical Heat Transfer, Part B: Fundamentals*, 50(4):285–313, 2006.
- [3] NV Antonov. Renormalization group, operator product expansion and anomalous scaling in models of turbulent advection. *Journal of Physics A: Mathematical and General*, 39(25):7825, 2006.
- [4] Vincenzo Armenio and Virgilio Fiorotto. The importance of the forces acting on particles in turbulent flows. *Physics of fluids*, 13(8):2437–2440, 2001.

- [5] S Balachandar, Kai Liu, and Mandar Lakhote. Self-induced velocity correction for improved drag estimation in euler–lagrange point-particle simulations. *Journal of Computational Physics*, 376:160–185, 2019.
- [6] Simone Benella, Mirko Stumpo, Tommaso Alberti, Oreste Pezzi, Emanuele Papini, Emiliya Yordanova, Francesco Valentini, and Giuseppe Consolini. Linking the langevin equation to scaling properties of space plasma turbulence at sub-ion scales. *Physical Review Research*, 5(4): L042014, 2023.
- [7] Alain Bensoussan and Roger Temam. Equations stochastiques du type navier-stokes. *Journal of Functional Analysis*, 13(2):195–222, 1973.
- [8] Alain Berlemont, P Achim, and Z Chang. Lagrangian approaches for particle collisions: The colliding particle velocity correlation in the multiple particles tracking method and in the stochastic approach. *Physics of fluids*, 13(10):2946–2956, 2001.
- [9] Peter S Bernard, Mohamed F Ashmawey, and Robert A Handler. An analysis of particle trajectories in computer-simulated turbulent channel flow. *Physics of Fluids A: Fluid Dynamics*, 1(9):1532–1540, 1989.
- [10] Lorenzo Bertini, Nicoletta Cancrini, and Giovanni Jona-Lasinio. The stochastic burgers equation. *Communications in Mathematical Physics*, 165:211–232, 1994.
- [11] Federico Bianco, Sergio Chibbaro, Cristian Marchioli, MARIA VITTORIA Salvetti, and Alfredo Soldati. Intrinsic filtering errors of lagrangian particle tracking in les flow fields. *Physics of Fluids*, 24(4), 2012.
- [12] M Bini and WP Jones. Particle acceleration in turbulent flows: A class of nonlinear stochastic models for intermittency. *Physics of Fluids*, 19(3), 2007.
- [13] Alexandre Boritchev and Sergei Kuksin. *One-dimensional turbulence and the stochastic Burgers equation*, volume 255. American Mathematical Soc., 2021.
- [14] Freddy Bouchet, Jason Laurie, and Oleg Zaboronski. Langevin dynamics, large deviations and instantons for the quasi-geostrophic model and two-dimensional euler equations. *Journal of Statistical Physics*, 156: 1066–1092, 2014.

- [15] Lydia Bourouiba. Turbulent gas clouds and respiratory pathogen emissions: potential implications for reducing transmission of covid-19. *Jama*, 323(18):1837–1838, 2020.
- [16] Luca Brandt and Filippo Coletti. Particle-laden turbulence: progress and perspectives. *Annual Review of Fluid Mechanics*, 54(1):159–189, 2022.
- [17] JJH Brouwers. Langevin equation of a fluid particle in wall-induced turbulence. *Theoretical and Mathematical Physics*, 163:677–695, 2010.
- [18] JJH Brouwers. Statistical models of large scale turbulent flow. *Flow, Turbulence and Combustion*, 97:369–399, 2016.
- [19] Z Brzezniak and Szymon Peszat. Strong local and global solutions for stochastic navier-stokes equations. *Infinite dimensional stochastic analysis*, pages 85–98, 1999.
- [20] D Burry and G Bergeles. Dispersion of particles in anisotropic turbulent flows. *International journal of multiphase flow*, 19(4):651–664, 1993.
- [21] Jared L Callaham, J-C Loiseau, Georgios Rigas, and Steven L Brunton. Nonlinear stochastic modelling with langevin regression. *Proceedings of the Royal Society A*, 477(2250):20210092, 2021.
- [22] Jesse Capecelatro and Olivier Desjardins. An euler–lagrange strategy for simulating particle-laden flows. *Journal of Computational Physics*, 238: 1–31, 2013.
- [23] Jeng-Jiann Chiu and Shu Chien. Effects of disturbed flow on vascular endothelium: pathophysiological basis and clinical perspectives. *Physiological reviews*, 91(1):327–387, 2011.
- [24] Haecheon Choi and Parviz Moin. Grid-point requirements for large eddy simulation: Chapmans estimates revisited. *Physics of fluids*, 24(1), 2012.
- [25] Min S Chong, Julio Soria, Anthony E Perry, J Chacin, Brian J Cantwell, and Y Na. Turbulence structures of wall-bounded shear flows found using dns data. *Journal of Fluid Mechanics*, 357:225–247, 1998.
- [26] Giuseppe Da Prato and Jerzy Zabczyk. *Stochastic equations in infinite dimensions*, volume 152. Cambridge university press, 2014.

- [27] Anton Daitche and Tamás Tél. Memory effects are relevant for chaotic advection of inertial particles. *Physical review letters*, 107(24):244501, 2011.
- [28] James W Deardorff. A numerical study of three-dimensional turbulent channel flow at large reynolds numbers. *Journal of Fluid Mechanics*, 41(2):453–480, 1970.
- [29] A Dehbi. Turbulent particle dispersion in arbitrary wall-bounded geometries: A coupled cfd-langevin-equation based approach. *International Journal of Multiphase Flow*, 34(9):819–828, 2008.
- [30] A Dehbi. A stochastic langevin model of turbulent particle dispersion in the presence of thermophoresis. *International Journal of Multiphase Flow*, 35(3):219–226, 2009.
- [31] Rohit Dhariwal, Sarma L Rani, and Donald L Koch. Stochastic theory and direct numerical simulations of the relative motion of high-inertia particle pairs in isotropic turbulence. *Journal of Fluid Mechanics*, 813: 205–249, 2017.
- [32] Lihuai Du and Ting Zhang. Local and global strong solutions to the stochastic incompressible navier-stokes equations in critical besov space. *Journal of Mathematical Analysis and Applications*, 481(1):123472, 2020.
- [33] John K Eaton. Two-way coupled turbulence simulations of gas-particle flows using point-particle tracking. *International Journal of Multiphase Flow*, 35(9):792–800, 2009.
- [34] Jack GM Eggels, Friedemann Unger, MH Weiss, Jerry Westerweel, Ronald J Adrian, Rainer Friedrich, and Frans TM Nieuwstadt. Fully developed turbulent pipe flow: a comparison between direct numerical simulation and experiment. *Journal of Fluid Mechanics*, 268:175–210, 1994.
- [35] Albert Einstein. Über die von der molekularkinetischen theorie der wärme geforderte bewegung von in ruhenden flüssigkeiten suspendierten teilchen. *Annalen der physik*, 4, 1905.
- [36] S Elghobashi and GC Truesdell. Direct simulation of particle dispersion in a decaying isotropic turbulence. *Journal of Fluid Mechanics*, 242: 655–700, 1992.

- [37] Said Elghobashi. On predicting particle-laden turbulent flows. *Applied scientific research*, 52:309–329, 1994.
- [38] Lauren Farndell, Lee Mortimer, and Michael Fairweather. Langevin dynamic simulations for polymer conformation in shear and turbulent flows. In *AIP Conference Proceedings*, volume 3308, page 020008. AIP Publishing LLC, 2025.
- [39] Pascal Fede and Olivier Simonin. Numerical study of the subgrid fluid turbulence effects on the statistics of heavy colliding particles. *Physics of Fluids*, 18(4), 2006.
- [40] Simone Ferrari, Riccardo Rossi, and Annalisa Di Bernardino. A review of laboratory and numerical techniques to simulate turbulent flows. *Energies*, 15(20):7580, 2022.
- [41] Richard Phillips Feynman. The feynman lectures on physics. (*No Title*), 1:46, 1963.
- [42] Franco Flandoli and Bohdan Maslowski. Ergodicity of the 2-d navier-stokes equation under random perturbations. *Communications in mathematical physics*, 172:119–141, 1995.
- [43] Iván Gallo-Méndez and Pablo S Moya. Langevin based turbulence model and its relationship with kappa distributions. *Scientific Reports*, 12(1): 2136, 2022.
- [44] Massimo Germano, Ugo Piomelli, Parviz Moin, and William H Cabot. A dynamic subgrid-scale eddy viscosity model. *Physics of Fluids A: Fluid Dynamics*, 3(7):1760–1765, 1991.
- [45] Ch Gobert. Analytical assessment of models for large eddy simulation of particle laden flow. *Journal of Turbulence*, (11):N23, 2010.
- [46] Christian Gobert and Michael Manhart. Subgrid modelling for particles by spectrally optimised interpolation (soi). *Journal of Computational Physics*, 230(21):7796–7820, 2011.
- [47] Konrad A Goc, Oriol Lehmkuhl, George Ilhwan Park, Sanjeeb T Bose, and Parviz Moin. Large eddy simulation of aircraft at affordable cost: a milestone in computational fluid dynamics. *Flow*, 1:E14, 2021.

- [48] DI Graham and PW James. Turbulent dispersion of particles using eddy interaction models. *International Journal of Multiphase Flow*, 22(1):157–175, 1996.
- [49] Paolo Gualtieri, Francesco Picano, Gaetano Sardina, and Carlo Massimo Casciola. Exact regularized point particle method for multiphase flows in the two-way coupling regime. *Journal of Fluid Mechanics*, 773:520–561, 2015.
- [50] K Gustavsson and B Mehlig. Statistical models for spatial patterns of heavy particles in turbulence. *Advances in Physics*, 65(1):1–57, 2016.
- [51] Kemal Hanjalić and Brian E Launder. A reynolds stress model of turbulence and its application to thin shear flows. *Journal of fluid Mechanics*, 52(4):609–638, 1972.
- [52] Werner Heisenberg. On stability and turbulence of fluid flows. Technical report, 1951.
- [53] Christophe Henry, Jean-Pierre Minier, and Sara Brambilla. Particle re-suspension: Challenges and perspectives for future models. *Physics Reports*, 1007:1–98, 2023.
- [54] Burkhard MO Heppe. Generalized langevin equation for relative turbulent dispersion. *Journal of Fluid Mechanics*, 357:167–198, 1998.
- [55] Holger Homann and Jeremie Bec. Finite-size effects in the dynamics of neutrally buoyant particles in turbulent flow. *Journal of Fluid Mechanics*, 651:81–91, 2010.
- [56] BPB Hoomans, JAM Kuipers, Willem J Briels, and Willibrordus Petrus Maria van Swaaij. Discrete particle simulation of bubble and slug formation in a two-dimensional gas-fluidised bed: a hard-sphere approach. *Chemical Engineering Science*, 51(1):99–118, 1996.
- [57] JAK Horwitz and Ali Mani. Accurate calculation of stokes drag for point-particle tracking in two-way coupled flows. *Journal of Computational Physics*, 318:85–109, 2016.
- [58] Peter J Ireland and Olivier Desjardins. Improving particle drag predictions in euler-lagrange simulations with two-way coupling. *Journal of Computational Physics*, 338:405–430, 2017.

- [59] Arnulf Jentzen, Diyora Salimova, and Timo Welti. Strong convergence for explicit space–time discrete numerical approximation methods for stochastic burgers equations. *Journal of Mathematical Analysis and Applications*, 469(2):661–704, 2019.
- [60] John Kim, Parviz Moin, and Robert Moser. Turbulence statistics in fully developed channel flow at low reynolds number. *Journal of fluid mechanics*, 177:133–166, 1987.
- [61] Jong Uhn Kim. Strong solutions of the stochastic navier-stokes equations in 3. *Indiana University mathematics journal*, pages 1853–1886, 2010.
- [62] A.N. Kolmogorov and A.T. Bharucha-Reid. *Foundations of the Theory of Probability: Second English Edition*. Dover Publications, New York, 2018.
- [63] Andrei Nikolaevich Kolmogorov. Dissipation of energy in the locally isotropic turbulence. *Proceedings of the Royal Society of London. Series A: Mathematical and Physical Sciences*, 434(1890):15–17, 1991.
- [64] Andrei Nikolaevich Kolmogorov. The local structure of turbulence in incompressible viscous fluid for very large reynolds numbers. *Proceedings of the Royal Society of London. Series A: Mathematical and Physical Sciences*, 434(1890):9–13, 1991.
- [65] K Kontomaris, TJ Hanratty, and JB McLaughlin. An algorithm for tracking fluid particles in a spectral simulation of turbulent channel flow. *Journal of Computational Physics*, 103(2):231–242, 1992.
- [66] Robert H Kraichnan. Inertial ranges in two-dimensional turbulence. *Physics of fluids*, 10(7):1417, 1967.
- [67] Robert H Kraichnan. Small-scale structure of a scalar field convected by turbulence. *The Physics of Fluids*, 11(5):945–953, 1968.
- [68] E Krasnoff and RL Peskin. The langevin model for turbulent diffusion. *Geophysical Fluid Dynamics*, 2(1):123–146, 1971.
- [69] JGM Kuerten and AW1187 Vreman. Can turbophoresis be predicted by large-eddy simulation? *Physics of Fluids*, 17(1):011701–011701, 2005.
- [70] Johannes GM Kuerten and JJH Brouwers. Lagrangian statistics of turbulent channel flow at $re\tau = 950$ calculated with direct numerical simulation and langevin models. *Physics of fluids*, 25(10), 2013.

- [71] Paul Langevin et al. Sur la théorie du mouvement brownien. *CR Acad. Sci. Paris*, 146(530-533):530, 1908.
- [72] Brian Edward Launder and Dudley Brian Spalding. The numerical computation of turbulent flows. In *Numerical prediction of flow, heat transfer, turbulence and combustion*, pages 96–116. Elsevier, 1983.
- [73] Brian Edward Launder, G Jr Reece, and W Rodi. Progress in the development of a reynolds-stress turbulence closure. *Journal of fluid mechanics*, 68(3):537–566, 1975.
- [74] J-P Laval and Bérengère Dubrulle. A les-langevin model for turbulence. *The European Physical Journal B-Condensed Matter and Complex Systems*, 49:471–481, 2006.
- [75] Myoungkyu Lee and Robert D Moser. Direct numerical simulation of turbulent channel flow up to. *Journal of fluid mechanics*, 774:395–415, 2015.
- [76] Athony Leonard. Energy cascade in large-eddy simulations of turbulent fluid flows. In *Advances in geophysics*, volume 18, pages 237–248. Elsevier, 1975.
- [77] CC Lin. On the stability of two-dimensional parallel flows. *Proceedings of the national academy of sciences*, 30(10):316–324, 1944.
- [78] Y Ling, M Parmar, and S Balachandar. A scaling analysis of added-mass and history forces and their coupling in dispersed multiphase flows. *International journal of multiphase flow*, 57:102–114, 2013.
- [79] Zhengliang Liu, Jinyu Jiao, Ying Zheng, Qikai Zhang, and Lufei Jia. Investigation of turbulence characteristics in a gas cyclone by stereoscopic piv. *AIChE journal*, 52(12):4150–4160, 2006.
- [80] JG M. Kuerten. Point-particle dns and les of particle-laden turbulent flow-a state-of-the-art review. *Flow, turbulence and combustion*, 97:689–713, 2016.
- [81] Ch Marchioli, A Soldati, JGM Kuerten, B Arcen, A Taniere, G Golden-soph, KD Squires, MF Cargnelutti, and LM Portela. Statistics of particle dispersion in direct numerical simulations of wall-bounded turbulence: Results of an international collaborative benchmark test. *International Journal of Multiphase Flow*, 34(9):879–893, 2008.

- [82] Cristian Marchioli and Alfredo Soldati. Mechanisms for particle transfer and segregation in a turbulent boundary layer. *Journal of fluid Mechanics*, 468:283–315, 2002.
- [83] Cristian Marchioli, Andrea Giusti, Maria Vittoria Salvetti, and Alfredo Soldati. Direct numerical simulation of particle wall transfer and deposition in upward turbulent pipe flow. *International journal of Multiphase flow*, 29(6):1017–1038, 2003.
- [84] Cristian Marchioli, Maria Vittoria Salvetti, and Alfredo Soldati. Appraisal of energy recovering sub-grid scale models for large-eddy simulation of turbulent dispersed flows. *Acta mechanica*, 201:277–296, 2008.
- [85] Ivan Marusic and Susan Broomhall. Leonardo da vinci and fluid mechanics. *Annual Review of Fluid Mechanics*, 53(1):1–25, 2021.
- [86] Assaad R Masri. Challenges for turbulent combustion. *Proceedings of the Combustion Institute*, 38(1):121–155, 2021.
- [87] Martin Maxey. Simulation methods for particulate flows and concentrated suspensions. *Annual Review of Fluid Mechanics*, 49(1):171–193, 2017.
- [88] Sara Mazzonetto and Diyora Salimova. Existence, uniqueness, and numerical approximations for stochastic burgers equations. *Stochastic Analysis and Applications*, 38(4):623–646, 2020.
- [89] Shiqi Meng, Xiaoheng Li, Xiaokang Yan, Lijun Wang, Haijun Zhang, and Yijun Cao. Turbulence models for single phase flow simulation of cyclonic flotation columns. *Minerals*, 9(8):464, 2019.
- [90] Anand Joseph Michael, Andreas Mark, Srdjan Sasic, and Henrik Ström. Generalized langevin dynamics in multiphase direct numerical simulations using hydrodynamically optimized memory kernels. *Physics of Fluids*, 37(3), 2025.
- [91] WR Michałek, JGM Kuerten, JCH Zeegers, Raoul Liew, J Pozorski, and BJ Geurts. A hybrid stochastic-deconvolution model for large-eddy simulation of particle-laden flow. *Physics of Fluids*, 25(12), 2013.
- [92] Remigijus Mikulevicius and Boris L Rozovskii. Stochastic navier–stokes equations for turbulent flows. *SIAM Journal on Mathematical Analysis*, 35(5):1250–1310, 2004.

- [93] Jean-Pierre Minier, Sergio Chibbaro, and Stephen B Pope. Guidelines for the formulation of lagrangian stochastic models for particle simulations of single-phase and dispersed two-phase turbulent flows. *Physics of Fluids*, 26(11), 2014.
- [94] Yoichi Mito and Thomas J Hanratty. Use of a modified langevin equation to describe turbulent dispersion of fluid particles in a channel flow. *Flow, turbulence and combustion*, 68:1–26, 2002.
- [95] Manil T Mohan, K Sakthivel, and Sivaguru S Sritharan. Ergodicity for the 3d stochastic navier–stokes equations perturbed by lévy noise. *Mathematische Nachrichten*, 292(5):1056–1088, 2019.
- [96] Parviz Moin and John Kim. Numerical investigation of turbulent channel flow. *Journal of fluid mechanics*, 118:341–377, 1982.
- [97] Faith A Morrison. *An introduction to fluid mechanics*. Cambridge University Press, 2013.
- [98] Robert D Moser, John Kim, Nagi N Mansour, et al. Direct numerical simulation of turbulent channel flow up to $Re = 590$. *Phys. fluids*, 11(4): 943–945, 1999.
- [99] Franck Nicoud and Frédéric Ducros. Subgrid-scale stress modelling based on the square of the velocity gradient tensor. *Flow, turbulence and Combustion*, 62(3):183–200, 1999.
- [100] B Oesterle and A Petitjean. Simulation of particle-to-particle interactions in gas solid flows. *International journal of multiphase flow*, 19(1): 199–211, 1993.
- [101] Stefano Olivieri, Francesco Picano, Gaetano Sardina, Daniele Iudicone, and Luca Brandt. The effect of the basset history force on particle clustering in homogeneous and isotropic turbulence. *Physics of fluids*, 26(4), 2014.
- [102] Steven A Orszag and GS Patterson Jr. Numerical simulation of three-dimensional homogeneous isotropic turbulence. *Physical review letters*, 28(2):76, 1972.
- [103] Thomas Pähtz, Abram H Clark, Manousos Valyrakis, and Orencio Durán. The physics of sediment transport initiation, cessation, and entrainment across aeolian and fluvial environments. *Reviews of Geophysics*, 58(1):e2019RG000679, 2020.

- [104] GS Patterson and JJ Riley. Diffusion experiment with numerically integrated isotropic turbulence. *Phys. Fluids*, 17(2), 1974.
- [105] Ugo Piomelli and Elias Balaras. Wall-layer models for large-eddy simulations. *Annual review of fluid mechanics*, 34(1):349–374, 2002.
- [106] Sergio Pirozzoli, Joshua Romero, Massimiliano Fatica, Roberto Verzicco, and Paolo Orlandi. One-point statistics for turbulent pipe flow up to. *Journal of fluid mechanics*, 926:A28, 2021.
- [107] Yves Pomeau and Jarosław Piasecki. The langevin equation. *Comptes Rendus. Physique*, 18(9-10):570–582, 2017.
- [108] SB Pope. Lagrangian pdf methods for turbulent flows. *Annu. Rev. Fluid Mech.*, 23:63, 1994.
- [109] Stephen B Pope. Turbulent flows. *Measurement Science and Technology*, 12(11):2020–2021, 2001.
- [110] Ali Poursina, Ali Pourjamal, and Ali Bozorg. Stochastic approach to turbulence: A comprehensive review. *arXiv preprint arXiv:2211.12918*, 2022.
- [111] Jacek Pozorski and Sourabh V Apte. Filtered particle tracking in isotropic turbulence and stochastic modeling of subgrid-scale dispersion. *International Journal of Multiphase Flow*, 35(2):118–128, 2009.
- [112] Jacek Pozorski and Jean-Pierre Minier. Probability density function modeling of dispersed two-phase turbulent flows. *Physical Review E*, 59(1):855, 1999.
- [113] S Ganga Prasath, Vishal Vasan, and Rama Govindarajan. Accurate solution method for the maxey–riley equation, and the effects of basset history. *Journal of Fluid Mechanics*, 868:428–460, 2019.
- [114] MW Reeks. The transport of discrete particles in inhomogeneous turbulence. *Journal of aerosol science*, 14(6):729–739, 1983.
- [115] Yan Ren, Hongsheng Zhang, Xiaoye Zhang, Wei Wei, Qianhui Li, Bingui Wu, Xuhui Cai, Yu Song, Ling Kang, and Tong Zhu. Turbulence barrier effect during heavy haze pollution events. *Science of the Total Environment*, 753:142286, 2021.

- [116] Osborne Reynolds. Xxix. an experimental investigation of the circumstances which determine whether the motion of water shall be direct or sinuous, and of the law of resistance in parallel channels. *Philosophical Transactions of the Royal society of London*, (174):935–982, 1883.
- [117] Osborne Reynolds. Iv. on the dynamical theory of incompressible viscous fluids and the determination of the criterion. *Philosophical transactions of the royal society of london.(a.)*, (186):123–164, 1895.
- [118] S. Rodriguez. *LES and DNS Turbulence Modeling*. Springer, Cham, 2019. doi: 10.1007/978-3-030-28691-0_5.
- [119] Pierre Sagaut. *Large eddy simulation for incompressible flows: an introduction*. Springer Science & Business Media, 2005.
- [120] S Sanders. 125 questions: Exploration and discovery. *Science/AAAS Custom Publishing Office: Washington, DC, USA*, 2021.
- [121] Christopher R Sherwood, Ap Van Dongeren, James Doyle, Christie A Hegermiller, Tian-Jian Hsu, Tarandeep S Kalra, Maitane Olabarrieta, Allison M Penko, Yashar Rafati, Dano Roelvink, et al. Modeling the morphodynamics of coastal responses to extreme events: What shape are we in? *Annual review of marine science*, 14(1):457–492, 2022.
- [122] T-H Shih, JP Moder, and N-S Liu. Nonlinear subscale turbulent models for very large eddy simulation of turbulent flows. *Shock Waves*, 29(8): 1155–1179, 2019.
- [123] AN Shiryayev. On the reversibility of the statistical laws of nature. *Selected Works of AN Kolmogorov: Volume II Probability Theory and Mathematical Statistics*, pages 209–215, 1992.
- [124] Babak Shotorban and Farzad Mashayek. Modeling subgrid-scale effects on particles by approximate deconvolution. *Physics of Fluids*, 17(8), 2005.
- [125] Emil Simiu and DongHun Yeo. *Wind effects on structures: Modern structural design for wind*. John Wiley & Sons, 2019.
- [126] Joseph Smagorinsky. General circulation experiments with the primitive equations: I. the basic experiment. *Monthly weather review*, 91(3):99–164, 1963.

- [127] Marian Smoluchowski. The kinetic theory of brownian molecular motion and suspensions. *Ann. Phys*, 21:756–780, 1906.
- [128] Arnold Sommerfeld. A contribution to hydrodynamic explanation of turbulent fluid motions. In *Int. Congr. Math*, volume 3, pages 116–124, 1908.
- [129] Martin Sommerfeld. Validation of a stochastic lagrangian modelling approach for inter-particle collisions in homogeneous isotropic turbulence. *International Journal of Multiphase Flow*, 27(10):1829–1858, 2001.
- [130] Philippe Spalart and Steven Allmaras. A one-equation turbulence model for aerodynamic flows. In *30th aerospace sciences meeting and exhibit*, page 439, 1992.
- [131] Philippe R Spalart. Direct simulation of a turbulent boundary layer up to $Re_\theta = 1410$. *Journal of fluid mechanics*, 187:61–98, 1988.
- [132] Philippe R Spalart and Hiroyuki Abe. Empirical scaling laws for wall-bounded turbulence deduced from direct numerical simulations. *Physical Review Fluids*, 6(4):044604, 2021.
- [133] Philippe R Spalart and J Douglas McLean. Drag reduction: enticing turbulence, and then an industry. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 369(1940):1556–1569, 2011.
- [134] Charles G Speziale, Sutanu Sarkar, and Thomas B Gatski. Modelling the pressure–strain correlation of turbulence: an invariant dynamical systems approach. *Journal of fluid mechanics*, 227:245–272, 1991.
- [135] Kyle D Squires and John K Eaton. Particle response and turbulence modification in isotropic turbulence. *Physics of Fluids A: Fluid Dynamics*, 2(7):1191–1203, 1990.
- [136] Kyle D Squires and John K Eaton. Preferential concentration of particles by turbulence. *Physics of Fluids A: Fluid Dynamics*, 3(5):1169–1178, 1991.
- [137] Shivshankar Sundaram and Lance R Collins. Collision statistics in an isotropic particle-laden turbulent suspension. part 1. direct numerical simulations. *Journal of Fluid Mechanics*, 335:75–109, 1997.

- [138] Patrick Tabeling. Two-dimensional turbulence: a physicist approach. *Physics reports*, 362(1):1–62, 2002.
- [139] Gavin R Tabor and MH Baba-Ahmadi. Inlet conditions for large eddy simulation: A review. *Computers & Fluids*, 39(4):553–567, 2010.
- [140] Anne Taniere and Boris Arcen. Prediction of a particle-laden turbulent channel flow: Examination of two classes of stochastic dispersion models. *International journal of multiphase flow*, 60:1–10, 2014.
- [141] Terence Tao. Finite time blowup for an averaged three-dimensional navier-stokes equation. *Journal of the American Mathematical Society*, 29(3):601–674, 2016.
- [142] Hendrik Tennekes and John Leask Lumley. *A first course in turbulence*. MIT press, 1972.
- [143] Francis CK Ting and James T Kirby. Dynamics of surf-zone turbulence in a spilling breaker. *Coastal Engineering*, 27(3-4):131–160, 1996.
- [144] Lloyd N Trefethen, Anne E Trefethen, Satish C Reddy, and Tobin A Driscoll. Hydrodynamic stability without eigenvalues. *Science*, 261(5121):578–584, 1993.
- [145] Markus Uhlmann. Interface-resolved direct numerical simulation of vertical particulate channel flow in the turbulent regime. *Physics of Fluids*, 20(5), 2008.
- [146] WSJ Uijttewaai and RVA1027 Oliemans. Particle dispersion and deposition in direct numerical and large eddy simulations of vertical pipe flows. *Physics of Fluids*, 8(10):2590–2604, 1996.
- [147] BPM Van Esch and JGM Kuerten. Direct numerical simulation of the motion of particles in rotating pipe flow. *Journal of Turbulence*, (9):N4, 2008.
- [148] AW Vreman. Turbulence characteristics of particle-laden pipe flow. *Journal of fluid mechanics*, 584:235–279, 2007.
- [149] Jietuo Wang, Federico Dalla Barba, Alessio Roccon, Gaetano Sardina, Alfredo Soldati, and Francesco Picano. Modelling the direct virus exposure risk associated with respiratory events. *Journal of the Royal Society Interface*, 19(186):20210819, 2022.

- [150] Lian-Ping Wang, Anthony S Wexler, and Yong Zhou. Statistical mechanical description and modelling of turbulent collision of inertial particles. *Journal of Fluid Mechanics*, 415:117–153, 2000.
- [151] Dongyi Wei and Zhifei Zhang. Transition threshold for the 3d couette flow in sobolev space. *Communications on Pure and Applied Mathematics*, 74(11):2398–2479, 2021.
- [152] Xiaohua Wu and Parviz Moin. Direct numerical simulation of turbulence in a nominally zero-pressure-gradient flat-plate boundary layer. *Journal of Fluid Mechanics*, 630:5–41, 2009.
- [153] PK Yeung and SB Pope. An algorithm for tracking fluid particles in numerical simulations of homogeneous turbulence. *Journal of computational physics*, 79(2):373–416, 1988.
- [154] Akira Yoshizawa. Eddy-viscosity-type subgrid-scale model with a variable smagorinsky coefficient and its relationship with the one-equation model in large eddy simulation. *Physics of Fluids A: Fluid Dynamics*, 3(8):2007–2009, 1991.
- [155] F Zhao, WK George, and Berend GM van Wachem. Four-way coupled simulations of small particles in turbulent channel flow: The effects of particle shape and stokes number. *Physics of Fluids*, 27(8), 2015.

CHAPTER 3

Numerical Methods and Models

3.1 Governing Equations for the Carrier Phase

The mechanics of the carrier phase is described by the three-dimensional, incompressible formulation of the Navier-Stokes equations,

$$\nabla \cdot \tilde{\mathbf{u}} = 0 \quad (3.1)$$

$$\frac{\partial \tilde{\mathbf{u}}}{\partial t} + \tilde{\mathbf{u}} \cdot \nabla \tilde{\mathbf{u}} = -\frac{\nabla \tilde{p}}{\rho_f} + \nabla \cdot (\nu_{tot}(\nabla \tilde{\mathbf{u}} + \nabla \tilde{\mathbf{u}}^T)) \quad (3.2)$$

where $\tilde{\mathbf{u}}$ is the filtered fluid velocity field, $\tilde{p}$ the hydrodynamic pressure and ρ_f the density of the fluid; implicit filtering is employed. The total viscosity ν_{tot} is given by the sum of the molecular, kinematic viscosity, ν_f , and turbulent viscosity, ν_t , $\nu_{tot} = \nu_f + \nu_t$. The equations are solved within a rectangular prism, discretized using a fixed, uniform, and equispaced Cartesian grid. Pressure field is stored at the cell centers, while velocities are stored at the center of cell faces to prevent odd-even decoupling between pressure and velocity [1]. Boundary conditions are imposed on the sides of the Eulerian domain using ghost nodes. A Wall-Adapting Local Eddy (WALE) viscosity model [8] is used for the sub-grid scale fluid fluctuations. WALE model efficiently imposes a vanishing eddy viscosity close to the wall without the need of dumping functions. In Einstein index notation ν_t is given by [8]:

$$\nu_t = (C_w \Delta)^2 \frac{(G_{i,j} G_{i,j})^{3/2}}{(S_{i,j} S_{i,j})^{5/2} + (G_{i,j} G_{i,j})^{5/4}}, \quad (3.3)$$

where the model constant is assumed to be $C_w = 0.565$ [8] whereas,

$$G_{i,j} = S_{i,k}S_{k,j} + \Omega_{i,k}\Omega_{k,j} - \frac{1}{3}\delta_{i,j}(S_{m,n}S_{m,n} - \Omega_{m,n}\Omega_{m,n}) \quad (3.4)$$

with,

$$S_{i,j} = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right), \quad (3.5)$$

$$\Omega_{i,j} = \frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_j} - \frac{\partial \tilde{u}_j}{\partial x_i} \right). \quad (3.6)$$

The local, equivalent grid size, Δ , is assumed to be $\Delta = (\Delta x \Delta y \Delta z)^{1/3}$.

A wall-model (WM) is used near to the wall by modifying the total viscosity, ν_{tot} . The WM is based on an algebraic equilibrium model that is able to impose no-penetration and no-slip conditions together with the proper wall stress [2]. The WM provides an estimate of the local wall stress, τ_w , based on the local filtered LES velocity, u_I , at an interface located at around two or three Eulerian points away from the wall in order to minimize the log-layer mismatch effect and improve the accuracy of the WM-LES, see e.g., De Vanna et al. [2]. The Reichardt's wall law is used for velocity extrapolation and stress reconstruction [9]:

$$\frac{\tilde{U}_I}{u_\tau} = \frac{1}{k} \log(1 + kY_I^+) + C_k \left(1 - e^{-\frac{Y_I^+}{11}} - \frac{Y_I^+}{11} e^{-\frac{Y_I^+}{3}} \right), \quad (3.7)$$

$$Y_I^+ = \frac{Y_I u_\tau}{\nu_f}. \quad (3.8)$$

The non-linear, algebraic Eq. 3.7-3.8 are solved via a Newton-Raphson algorithm in order to find u_τ , given the filtered velocity $\tilde{U}_I$ at the distance Y_I from the wall. Then, the correct wall stress is computed as:

$$\tau_w = \rho_f u_\tau^2. \quad (3.9)$$

The numerical velocity gradient at the wall, $\frac{\partial \tilde{u}}{\partial y}|_w$, is computed and the kinematic viscosity at the wall is corrected as:

$$\nu_{tot,w} = \frac{\tau_w}{\rho_f \frac{\partial \tilde{u}}{\partial y}|_w}. \quad (3.10)$$

It should be noted that the velocity gradient at the wall, $\frac{\partial \tilde{u}}{\partial y}|_w$, is computed using wall tangential velocity component evaluated at the first grid point away

from the wall and ghost nodes. Finally, the ghost nodes of viscosity field are modified in order to impose the correct wall-viscosity, $\nu_{tot,w}$, and correct the stress distribution on the wall.

The numerical algorithms employed in this work have been build upon the opens-source code CaNS by Costa [1]. Eq. 3.1-3.2 are numerically integrated in time by means of a low-storage, third-order Runge-Kutta algorithm using a pressure-correction scheme. Second-order finite difference stencils are used to discretize differential operator in space, thus guaranteeing an overall second-order temporal and spatial accuracy [1]. Finally, it is worth noting that, the pressure Poisson equation is solved with the method of eigenfunction expansions. This approach allows for very efficient FFT-based solvers in problems with different combinations of homogeneous pressure boundary conditions [1]. In the following the symbol Δt will refer to the finite time-step from time t^n to t^{n+1} whereas the notation Δt_r will be used to refer to the r^{th} Runge-Kutta sub-time-steps. The coefficients of the Runge-Kutta algorithm are: $\alpha_{RK} = \{8/15, 5/12, 3/4\}$, $\beta_{RK} = \{0, -17/60, -5/12\}$ and $\gamma_{RK} = \alpha_{RK} + \beta_{RK}$.

3.2 Modeling of the Dispersed Phase

The point-particle equations are employed to describe the dispersed phase dynamics in a one-way coupling regime:

$$\frac{d\mathbf{v}_p}{dt} = f(Re_p) \frac{\mathbf{u}_p - \mathbf{v}_p}{\tau_p}, \quad (3.11)$$

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p, \quad (3.12)$$

where $\mathbf{v}_p$ is the particle velocity, $\mathbf{x}_p$ is the particle position, $\mathbf{u}_p$ the fluid velocity field evaluated at the particle position, $\mathbf{x}_p$, and τ_p is the particle relaxation time:

$$\tau_p = \frac{\rho_p}{\rho_f} \frac{d_p^2}{18\nu_f}, \quad (3.13)$$

with ρ_p the particle density and d_p the particle diameter. To account for particle finite inertia it is adopted the factor $f(Re_p) = 1 + 0.15Re_p^{0.687}$ based on the Schiller-Naumann relation [7], with $Re_p = |\mathbf{v}_p - \mathbf{u}_p|d_p/\nu_f$ the particle Reynolds number.

The main problem in Eq. 3.11 is that the fluid velocity at particle position $\mathbf{u}_p$ is not fully known. To calculate the fluid velocity sampled by the particle,

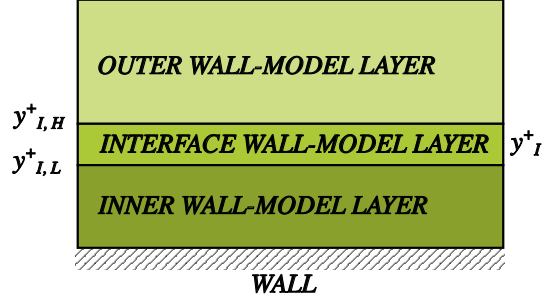


Figure 3.1: Schematics of domain decomposition near the walls as a function of the distance from the wall.

we split the domain into three different regions as sketched in Fig. 3.1. In viscous units, an inner layer where $y^+ \leq y_{I,L}^+$, an interface layer where $y_{I,L}^+ < y^+ < y_{I,H}^+$ and an outer layer where $y^+ \geq y_{I,H}^+$. The interface separating the outer and inner layer is considered to be located in the middle of the interface layer at y_I^+ . In turn, the interface layer is defined by the boundaries located at $y_{I,L}^+ = y_I^+ - \Delta_I^+/2$ and $y_{I,H}^+ = y_I^+ + \Delta_I^+/2$, with Δ_I^+ the interface thickness expressed in internal units. The different distances from the wall that define the different layers will be discussed in chapter 4, whereas, in Appendix A, it will be shown that the final model is quite insensitive from the chosen values.

Away from the wall, i.e., $y^+ > y_{I,H}^+$, the filtered fluid velocity, $\tilde{\mathbf{u}}_p$, can be extracted at particle position from the Eulerian flow dynamics. On the other hand, in the inner layer, i.e., $y^+ < y_{I,L}^+$, where the equilibrium wall model is employed, only an estimate of the mean velocity is known, $\bar{\mathbf{u}}_p$. Hence, we can write the fluid velocity at particle position as a function of the particle distance from the wall, y_p^+ :

$$\mathbf{u}_p = \begin{cases} \bar{\mathbf{u}}_p + \mathbf{u}'_p, & y_p^+ \leq y_{I,L}^+ \\ \sqrt{\alpha}\tilde{\mathbf{u}}_p + (1 - \sqrt{\alpha})\bar{\mathbf{u}}_p + \sqrt{1 - \alpha}\mathbf{u}'_p, & y_{I,L}^+ < y_p^+ < y_{I,H}^+ \\ \tilde{\mathbf{u}}_p + \mathbf{u}''_p, & y_p^+ \geq y_{I,H}^+ \end{cases} \quad (3.14)$$

According to Wang and Dalla Barba [10], in the present work we assume negligible the sub-grid contribution $\mathbf{u}''_p$ in the outer region; we compute the filtered fluid velocity at particle position from the Eulerian flow dynamics by using trilinear interpolation. On the contrary, we use a semi-stochastic model for the velocity fluctuation $\mathbf{u}'_p$ in the inner layer. Finally, in the interface layer, the fluid velocity sampled at the particle position is computed as a combination of the velocity in the inner and outer layer by means of the parameter α , which goes smoothly from zero to unity going from the inner to outer layer. It is

worth noting that, this specific relation employed to combined the velocity fluctuations ensure a continuity in the standard deviation of the fluctuation fields moving away from the wall. To ensure a smooth transition the parameter α is computed as in the following:

$$\alpha = \begin{cases} 0, & y_p^+ = y_{I,L}^+ \\ 3a^2 - 2a^3, & y_{I,L}^+ < y_p^+ < y_{I,H}^+ \\ 1, & y_p^+ = y_{I,H}^+ \end{cases}, \quad (3.15)$$

where the parameter a varies linearly from zero to one within the interface layer.

In the inner layer, we assume that the fluid velocity fluctuations, $\mathbf{u}'_p$ can be estimated by using the following stochastic model by Dehbi [3] along the flow and span-wise directions, respectively:

$$d\left(\frac{u'_p}{\sigma_x}\right) = -\left(\frac{u'_p}{\sigma_x}\right) \frac{dt}{\tau_L} + \sqrt{\frac{2}{\tau_L}} d\xi_x + s_p \frac{D_x}{\sigma_x} \frac{dt}{1 + Stk}, \quad (3.16)$$

$$d\left(\frac{w'_p}{\sigma_z}\right) = -\left(\frac{w'_p}{\sigma_z}\right) \frac{dt}{\tau_L} + \sqrt{\frac{2}{\tau_L}} d\xi_z, \quad (3.17)$$

where u'_p is the component of $\mathbf{u}'_p$ along the flow direction and w'_p that along the span-wise direction. The symbols σ_x and σ_z refer the root-mean-square of velocity fluctuation components along the flow and span-wise directions, respectively. The variables $d\xi_x$ and $d\xi_z$ are modeled as a series of uncorrelated Gaussian random numbers with zero mean and variance equal to the time increment, dt . The parameter s_p is defined to be equal to one and positive for the lower wall and negative for the upper wall of the channel. The Stokes number, Stk , is defined as:

$$Stk = \frac{\tau_p}{\tau_L}, \quad (3.18)$$

with the Lagrangian fluid time scale τ_L computed as a function of the La-

grangian integral scale, T_L [6, 11, 3]:

$$\tau_L = \frac{T_L}{\beta} \left(1 - (1 - \beta) \left(1 + \frac{\tau_p}{T_E} \right)^{-0.4(1+0.01)\frac{\tau_p}{T_E}} \right), \quad (3.19)$$

$$T_L = T_L^+ \frac{\nu_f}{u_\tau^2}, \quad (3.20)$$

$$T_L^+ = \begin{cases} 10 & y_p^+ < 5 \\ 7.122 + 0.5731y_p^+ - 0.00129y_p^{+2}, & 5 < y_p^+ < 200 \end{cases} \quad (3.21)$$

where T_E is the fluid Eulerian integral time scale and $\beta = T_L/T_E$. In this work the value of β is taken to be $\beta = 0.356$, as given by Wang and Stock [11], and is used to compute T_E from T_L . Finally, the particle drift is corrected according to the drift correction term, represented by the last terms on the right-hand-side of Eq. 3.16, D_x :

$$D_x = \frac{\partial \overline{u'_p v'_p}}{\partial y}, \quad (3.22)$$

where v'_p is the component of $\mathbf{u}'_p$ along the wall-normal direction.

We tried to use a corresponding stochastic model along the wall-normal direction to describe velocity fluctuations. However, it leads to the arising of a spurious preferential concentration of particles in correspondence of the interface layer (not shown). This spurious behavior was observed independently from the thickness of the interface layer. We attribute the issue to the interaction of inertial memory of particle velocity and the different regions of the model that increase the resident time near the interface. Indeed, if a particle exits the interface layer towards the outer one experiencing a positive fluctuation, it can be immediately forced back into the interface layer by "random" negative fluctuations induced by the carrier in the outer layer. On the contrary if a particle resident in the inner layer experiences negative fluctuations, these will force the particle to maintain its position for longer times. To avoid these issues, inspired by the model proposed in Johnson et al. [5], we consider along the wall-normal direction velocity fluctuations sampled by the particles as modulated by the fluctuations of the carrier phase, $v_{p,I}$, located above the particle at the interface location, y_I^+ :

$$v'_p = f(y_p^+)v_{p,I} + s_p k f(y_p^+) \frac{df(y^+)}{dy^+} \bigg|_{y_p^+} \frac{\Delta t_r}{1 + Stk} + N, \quad (3.23)$$

where we considered the following modulating function:

$$f(y^+) = \sqrt{\frac{y^+ \left(4 \left(1 - e^{-\frac{C_1}{y^+ C_2}} \right)^{C_3} \right)}{y_I^+ \left(4 \left(1 - e^{-\frac{C_1}{y_I^+ C_2}} \right)^{C_3} \right)}}, \quad (3.24)$$

with the constants $C_1 = 2.536$, $C_2 = 0.578$ and $C_3 = 0.403$. This modulating

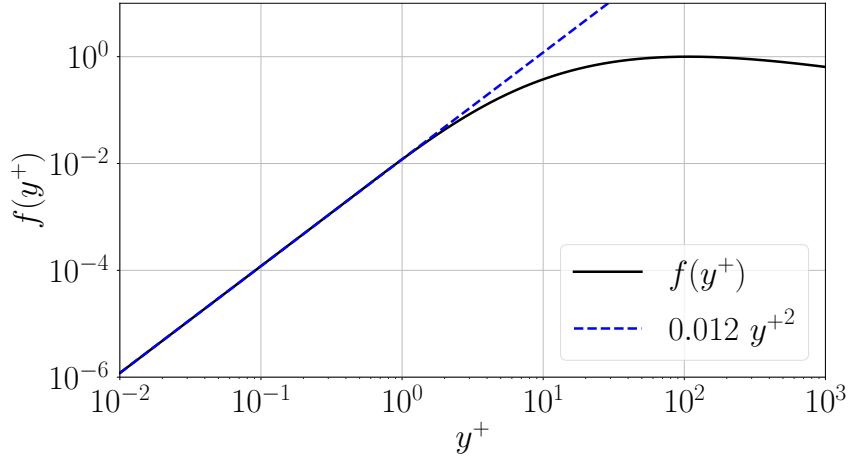


Figure 3.2: Representation of the modulating function provided by Eq. 3.24 as a function of the distance from the wall in internal units, y^+ , assuming $y_I^+ = 100$.

function allows us to preserve a quadratic scaling of the root-mean-square of velocity fluctuations near the wall as sketched in Fig. 3.2 and assumes unity value at the interface location, y_I^+ . Eq. 3.23 mimics the form of Eq. 3.16 and includes a drift correction term with a proportionality constant k , which has been empirically set to be $k = 100$. In addition, a random Gaussian noise, N , of zero mean and variance proportional to $u_\tau/25$ is added to the right-hand-side of Eq. 3.23. It is worth noting that, the intensity of k , which was set empirically, does not affect significantly the model but ensure a more correct turbophoretic behavior of particles near the walls. In addition, since the model without the noise N is deterministic in this direction, this stochastic noise mimics the randomness of small scale fluid motions.

Eq. 3.11-3.12 are evolved in time using the same Runge-Kutta scheme adopted for the carrier phase. On the other hand, an implicit Euler algorithm is used to advance in time Eq. 3.16-3.17 across each of the sub-steps of the main Runge-Kutta algorithm for the time increment Δt_r . The Lagrangian

time scale, τ_L is evaluated according to Eq. 3.19, whereas the variables $d\xi_x$ and $d\xi_z$ are modeled as a series of uncorrelated Gaussian random numbers with zero mean and variance equal to the finite time increment Δt_r . It is also worth remarking that the finite time increment in the right-hand-side of Eq. 3.16-3.17-3.23 is set to be equal to the sub-time-step Δt_r . In addition, when a particle transits from the outer layer to the interface one the velocity fluctuations are initialized as the local velocity fluctuations sampled from the Eulerian carrier phase. Finally, lookup tables are used together with linear

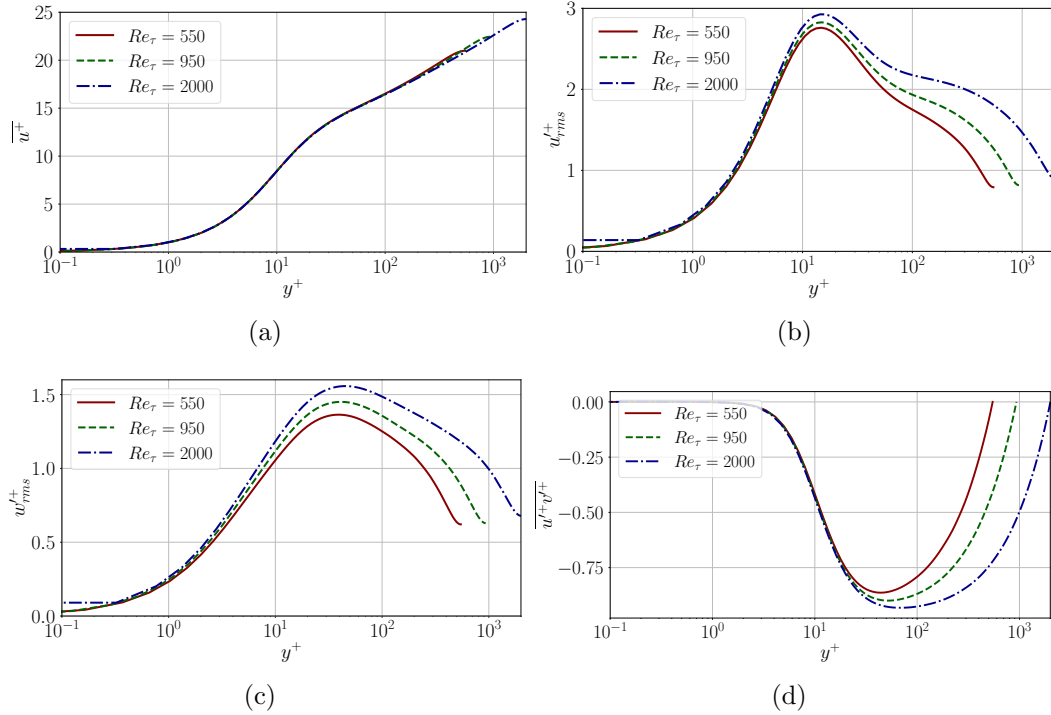


Figure 3.3: Statistics of velocity field of a turbulent channel flow from the DNS by Hoyas and Jiménez [4]. (a) Mean axial velocity profile. (b) Mean axial velocity fluctuations. (c) Mean span-wise velocity fluctuations. (d) Reynolds stresses. Each quantity is expressed in viscous units as a function of the distance from the wall. The statistics refer to three different friction Reynolds numbers, $Re_\tau = 550$, $Re_\tau = 950$ and $Re_\tau = 2000$, where $Re_\tau = u_\tau \delta / \nu_f$, being δ the channel semi-height.

interpolation for what concerns the estimation of the drift coefficient given by Eq. 3.22, the root-mean-square of particle fluctuations appearing in Eq. 3.16-3.17, σ_x and σ_z , and the axial component of the mean velocity, $\bar{u}_p$. In the present work, data for lookup tables have been obtained at different friction Reynolds numbers from the Direct Numerical Simulation (DNS) of turbulent channel flow by Hoyas and Jiménez [4] and are provided in Fig. 3.3.

Bibliography

- [1] P. Costa. A fft-based finite-difference solver for massively-parallel direct numerical simulations of turbulent flows. *Computers & Mathematics with Applications*, 76(8):1853–1862, 2018.
- [2] F. De Vanna, M. Cogo, M. Bernardini, F. Picano, and E. Benini. Unified wall-resolved and wall-modeled method for large-eddy simulations of compressible wall-bounded flows. *Physical Review Fluids*, 6(3):034614, 2021.
- [3] A. Dehbi. Validation against dns statistics of the normalized langevin model for particle transport in turbulent channel flows. *Powder Technology*, 200(1-2):60–68, 2010.
- [4] S. Hoyas and J. Jiménez. Reynolds number effects on the reynolds-stress budgets in turbulent channels. *Physics of Fluids*, 20(10), 2008.
- [5] P.L. Johnson, M. Bassenne, and P. Moin. Turbophoresis of small inertial particles: theoretical considerations and application to wall-modelled large-eddy simulations. *Journal of Fluid Mechanics*, 883:A27, 2020.
- [6] G.A. Kallio and M.W. Reeks. A numerical simulation of particle deposition in turbulent boundary layers. *International journal of multiphase flow*, 15(3):433–446, 1989.
- [7] Z. Naumann and L. Schiller. A drag coefficient correlation. *Z. Ver. Deutsch. Ing*, 77(318):e323, 1935.
- [8] Franck Nicoud and Frédéric Ducros. Subgrid-scale stress modelling based on the square of the velocity gradient tensor. *Flow, turbulence and Combustion*, 62(3):183–200, 1999.
- [9] H. Reichardt. Vollständige darstellung der turbulenten geschwindigkeitsverteilung in glatten leitungen. *ZAMM-Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik*, 31(7):208–219, 1951.
- [10] J. Wang and F. Dalla Barba. Assessment of the parcel model in evaporating turbulent diluted sprays within a large-eddy-simulation approach. *International Journal of Multiphase Flow*, 169:104609, 2023.
- [11] L.P. Wang and D.E. Stock. Dispersion of heavy particles by turbulent motion. *Journal of the Atmospheric Sciences*, 50(13):1897–1913, 1993.

CHAPTER 4

Model Validation and Results Analysis

4.1 Computational Domain and Simulation Setup

In this chapter, the numerical results from three different semi-stochastic, Wall-Modeled Large Eddy Simulations (WM-LESs) of a turbulent channel flow laden with solid particles at varying friction Reynolds numbers, $Re_\tau = 500$, $Re_\tau = 1000$ and $Re_\tau = 2000$ will be presented. In each case, the computational domain is a prism of dimensions $L_x \times L_y \times L_z = 6\delta \times 2\delta \times 3\delta$ along the streamwise, wall-normal, and spanwise directions, respectively, where δ is the channel semi-height. The domain is discretized using a uniform Cartesian grid with $N_x \times N_y \times N_z = 48 \times 48 \times 48$ nodes. The grid resolution is deliberately kept low to challenge the proposed model at its limits. Periodic boundary conditions are applied in the streamwise and spanwise directions, while no-slip and no-penetration boundary conditions are enforced on the upper and lower boundaries of the domain. A bulk Reynolds number, $Re_b = U_b 2\delta / \nu_f$, where U_b is the streamwise bulk velocity, is maintained by applying a pressure gradient to ensure a constant volumetric flow rate. A sketch of the computational domain is presented in Fig. 4.1. As previously stated, three different simulations are considered at varying friction Reynolds numbers, as reported in Tab. 4.1. In each of the three simulations, the flow is laden with $N_p = 150000$ point particles, a number chosen to minimize computational cost while ensuring a sufficiently large sample for statistical analysis. More specifically, for each simulations, three subsets of 50000 particles with different Stokes number, $Stk^+ = \tau_p / t_\tau$, are examined. The latter is based on the viscous time scale, $t_\tau = l_\tau / u_\tau$, where $l_\tau = \nu_f / u_\tau$ is the viscous length, $u_\tau = \sqrt{\tau_w / \rho_f}$ the friction velocity, and τ_w the mean wall stress. The density ratio is fixed to $\rho_p / \rho_f =$

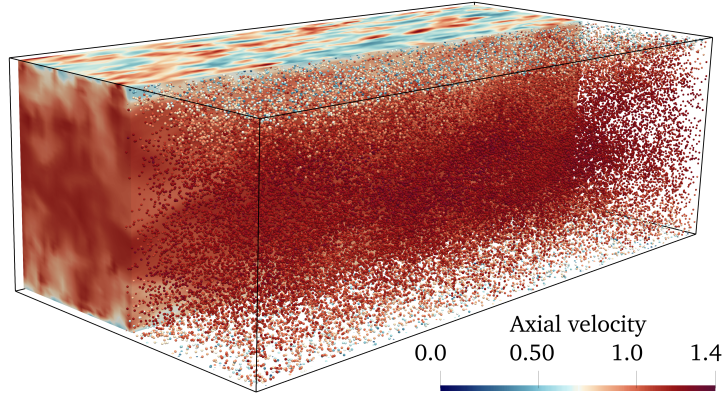


Figure 4.1: Sketch of the computational domain.

Simulation	Re_b	Re_τ	$d_p/(2\delta)$	d_p^+	Stk^+
Sim 1	18100	500	$8.164 \cdot 10^{-5}$	0.0816	1
			$2.582 \cdot 10^{-4}$	0.2582	10
			$8.165 \cdot 10^{-4}$	0.8165	100
Sim 2	40000	1000	$4.083 \cdot 10^{-5}$	0.0816	1
			$1.291 \cdot 10^{-4}$	0.2582	10
			$4.083 \cdot 10^{-4}$	0.8165	100
Sim 3	87100	2000	$2.041 \cdot 10^{-5}$	0.0816	1
			$6.455 \cdot 10^{-5}$	0.2582	10
			$2.041 \cdot 10^{-4}$	0.8165	100

Table 4.1: Summary of simulation parameters, including Reynolds numbers, $Re_b = U_b 2\delta / \nu_f$, $Re_\tau = u_\tau \delta / \nu_f$, and particle properties. The particle diameter, d_p , is scaled by the channel height, 2δ , whereas the particle diameter $d_p^+ = d_p / l_\tau$, with l_τ the viscous length. The Stokes number is defined as $Stk^+ = \tau_p / t_\tau$, with t_τ the viscous time scale.

2700. Tab. 4.1 provides also the particle properties for each of the considered cases.

Regarding the WM of the carrier phase, the velocity is extrapolated to reconstruct the wall stresses starting from two Eulerian points away from the wall, aiming to minimize the log-layer mismatch. The interface points where the velocity is interpolated according to Eq.3.7 are $Y_I^+ \simeq 40$ for $Re_\tau = 500$, $Y_I^+ \simeq 80$ for $Re_\tau = 1000$, and $Y_I^+ \simeq 160$ for $Re_\tau = 2000$. Conversely, for the dispersed phase, the interface is set according to Tab.4.2, unless otherwise specified. It is worth noting that, the semi-stochastic WM for particles is applied within the entire region where the WM for the carrier phase is active (i.e. $y^+ \leq Y_I^+$) and beyond, in order to avoid sampling of spurious velocity at particle positions.

Re_τ	$y_{I,L}^+$	$y_{I,H}^+$
500	40	50
1000	80	100
2000	160	200

Table 4.2: Interface values for different friction Reynolds numbers.

For two of the three cases considered in this work, we also performed DNS as a reference. Specifically, we carried out DNSs of a turbulent channel flow laden with point particles at $Re_\tau = 500$ and $Re_\tau = 1000$, using the same Stokes numbers as in the LES cases. In the reference DNSs, the computational domain extends over $L_x \times L_y \times L_z = 10\delta \times 2\delta \times 3\delta$ along the flow, wall-normal, and spanwise directions, respectively, and is discretized using $N_x \times N_y \times N_z = 1216 \times 512 \times 640$ nodes. The grid is stretched in the wall-normal direction to ensure sufficient resolution of the viscous sublayer, with a minimum grid spacing of $\Delta y_{min}^+ \simeq 0.1$ at the wall.

We begin by analyzing the velocity field statistics of the carrier phase, evaluating the consistency of mean profiles and fluctuations against reference data. This comparison validates the accuracy of the adopted modeling approach and characterizes the main turbulent properties of the flow. The analysis then shifts to the statistics of the dispersed phase.

4.2 Statistics of the carrier phase – Validation of the WM-LES implementation

Fig. 4.2, Fig. 4.3, and Fig. 4.4 show a comparison between the mean axial velocity profiles and velocity fluctuations from the semi-stochastic WM-LES and reference DNS data at $Re_\tau = 500$, $Re_\tau = 1000$, and $Re_\tau = 2000$, respectively. The mean axial velocity from the WM-LES closely follows the expected logarithmic profile, showing good agreement with the DNS data. A minor deviation from the logarithmic law is observed in term of slope. Similarly, the root mean square of the velocity fluctuations in all three directions is consistent with the DNS results. However, some underestimation of the fluctuations, especially in the wall-normal and spanwise directions, is observed. These discrepancies can be attributed to the coarser grid resolution in the semi-stochastic WM-LES. Despite this, the overall agreement confirms the accuracy of the proposed approach in capturing the main turbulent features of the flow. Although the lower grid resolution could be seen as a limitation, it was intentionally chosen to test the models performance under such conditions.

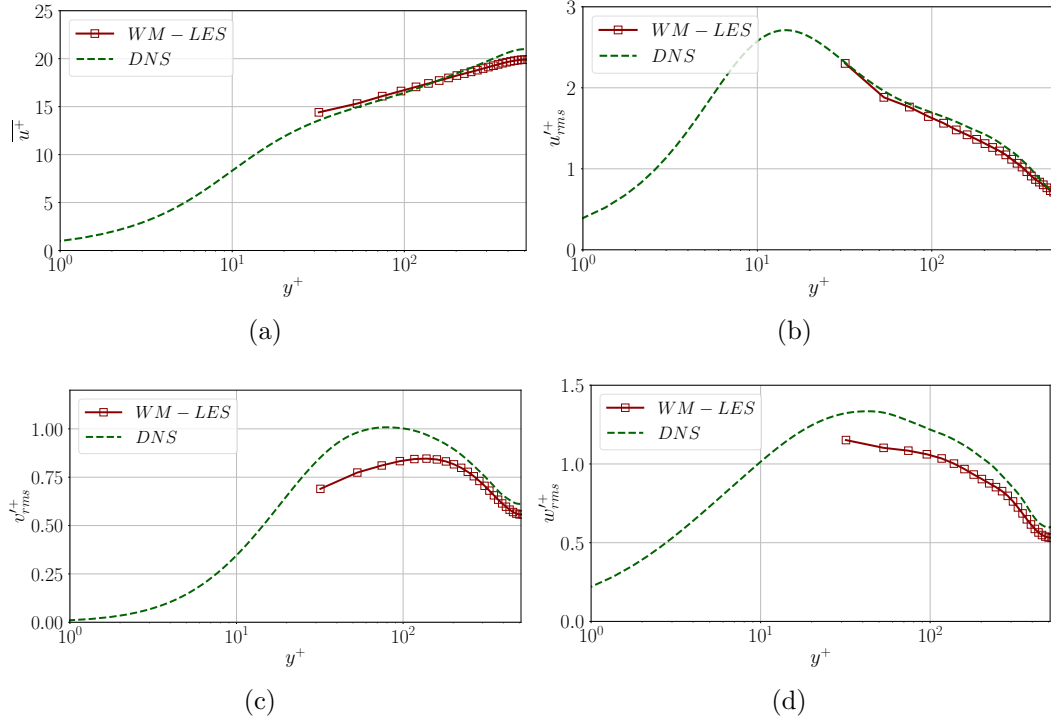


Figure 4.2: Statistics of velocity field (carrier phase) of the turbulent channel flow from wall-modelled LES at $Re_\tau = 500$, where $Re_\tau = u_\tau \delta / \nu_f$, being δ the channel semi-height. (a) Mean axial velocity profile. (b) Mean axial velocity fluctuations. (c) Mean wall-normal velocity fluctuations. (d) Mean span-wise velocity fluctuations. The statistics are also compared with the reference data from DNS.

The agreement in mean velocity profiles and velocity fluctuation statistics, despite the discrepancies due to the low grid resolution, supports the ability of the proposed modeling approach to capture the key turbulent characteristics of the flow while keeping the computational costs low.

4.3 Statistics of the dispersed phase

In this section, we present the analysis of the statistics of the dispersed phase. To compute the velocity statistics and concentration, the domain has been discretized along the wall-normal direction by dividing it into a specified number of bins, $N_b = 100$, distributed according to a hyperbolic tangent function. The size of the j^{th} bin, $\Delta y_{b,j}^+$, starting from the wall, is given by the following

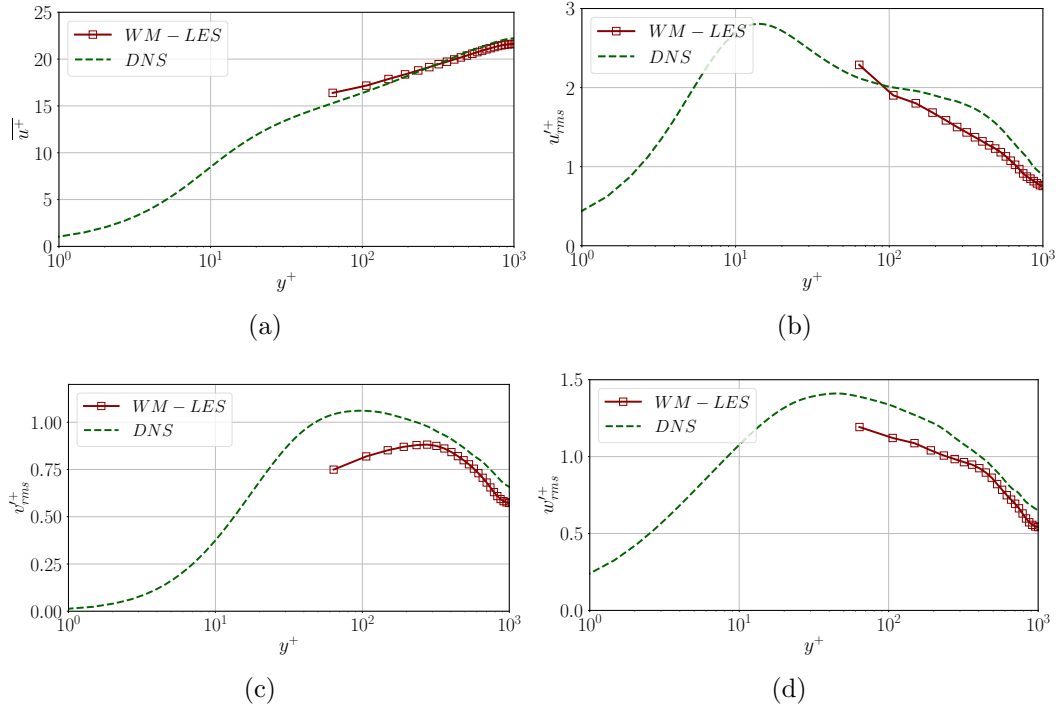


Figure 4.3: Statistics of velocity field (carrier phase) of the turbulent channel flow from wall-modelled LES at $Re_\tau = 1000$, where $Re_\tau = u_\tau \delta / \nu_f$, being δ the channel semi-height. (a) Mean axial velocity profile. (b) Mean axial velocity fluctuations. (c) Mean wall-normal velocity fluctuations. (d) Mean span-wise velocity fluctuations. The statistics are also compared with the reference data from DNS.

relation:

$$\Delta y_{b,j}^+ = \frac{Re_\tau}{\tanh(\gamma)} \left(\tanh\left(\frac{\text{real}(j)}{\text{real}(N_b)}\right) - \tanh\left(\frac{\text{real}(j-1)}{\text{real}(N_b)}\right) \right), \quad (4.1)$$

with the factor $\gamma = 1.5$ and $1 \leq j \leq N_b$, $j \in \mathcal{N}$. After splitting the domain into bins, for each time step, each particle is assigned to a bin based on its position, and the Lagrangian properties of the particles are associated with the corresponding bin. Finally, the Lagrangian properties within each bin are averaged based on the number of particles in that bin. The simulation is run with a time step $\Delta t/t_0 = 5 \cdot 10^{-3}$ for a total time of $t/t_0 = 750$. Statistical data were collected from $t/t_0 = 375$ to the end of the simulation at intervals of $\Delta t_{stats}/t_0 = 0.5$, where the timescale t_0 is defined as $t_0 = h/U_b$, with h the channel height and U_b the bulk velocity.

We begin the analysis of the dispersed phase statistics by examining the mean axial velocity profiles, shown in Fig. 4.5, as a function of the distance

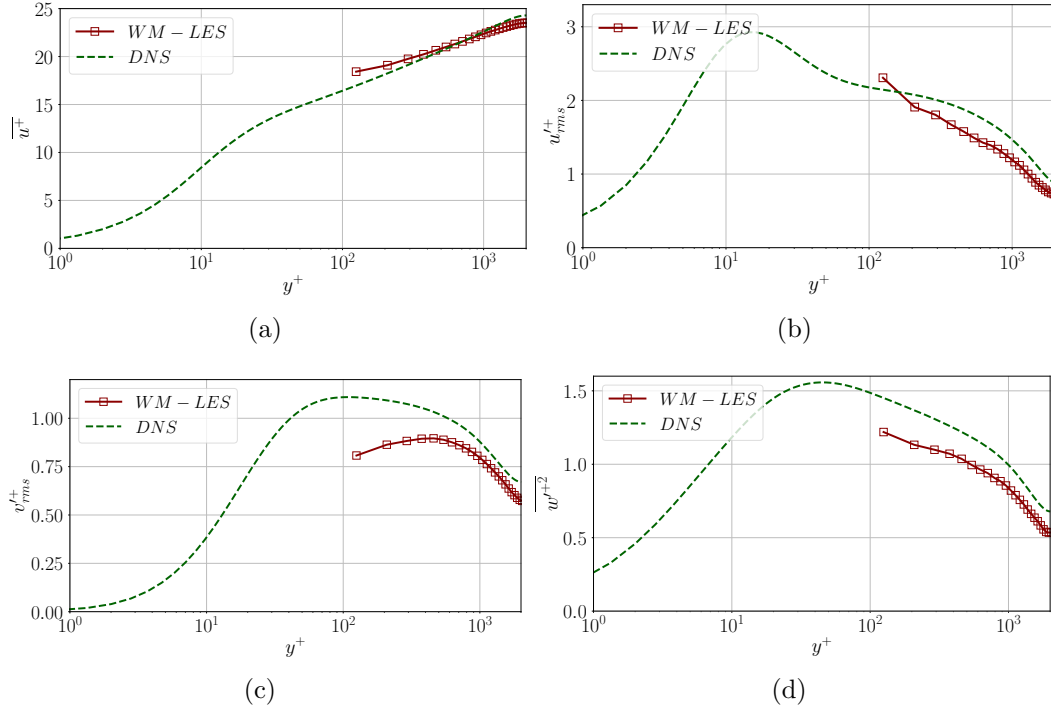


Figure 4.4: Statistics of velocity field (carrier phase) of the turbulent channel flow from wall-modelled LES at $Re_\tau = 2000$, where $Re_\tau = u_\tau \delta / \nu_f$, being δ the channel semi-height. (a) Mean axial velocity profile. (b) Mean axial velocity fluctuations. (c) Mean wall-normal velocity fluctuations. (d) Mean span-wise velocity fluctuations. The statistics are also compared with the data from the DNS by Hoyas and Jiménez [1].

from the wall for $Re_\tau = 500$, $Re_\tau = 1000$, and $Re_\tau = 2000$. As expected, the velocity profiles exhibit a logarithmic trend in the logarithmic region, confirming consistency with the theoretical behavior of turbulent channel flows.

For the first two cases, the semi-stochastic model predictions align closely with the DNS results across all Stokes numbers and over the entire range of distances from the wall. This agreement demonstrates the models ability to accurately capture the dynamics of the dispersed phase along the flow direction. It is worth noting that, in all cases, the velocity profiles show a minor deviation from the Eulerian phase trend in correspondence with the interface layer, before recovering in the near-wall region to match the DNS trend imposed by the semi-stochastic model. In particular, a small velocity overshoot is barely noticeable within the interface region. The presence of such a feature can be attributed to interpolation effects or numerical artifacts arising from the interface treatment, but its negligible magnitude suggests that it does not

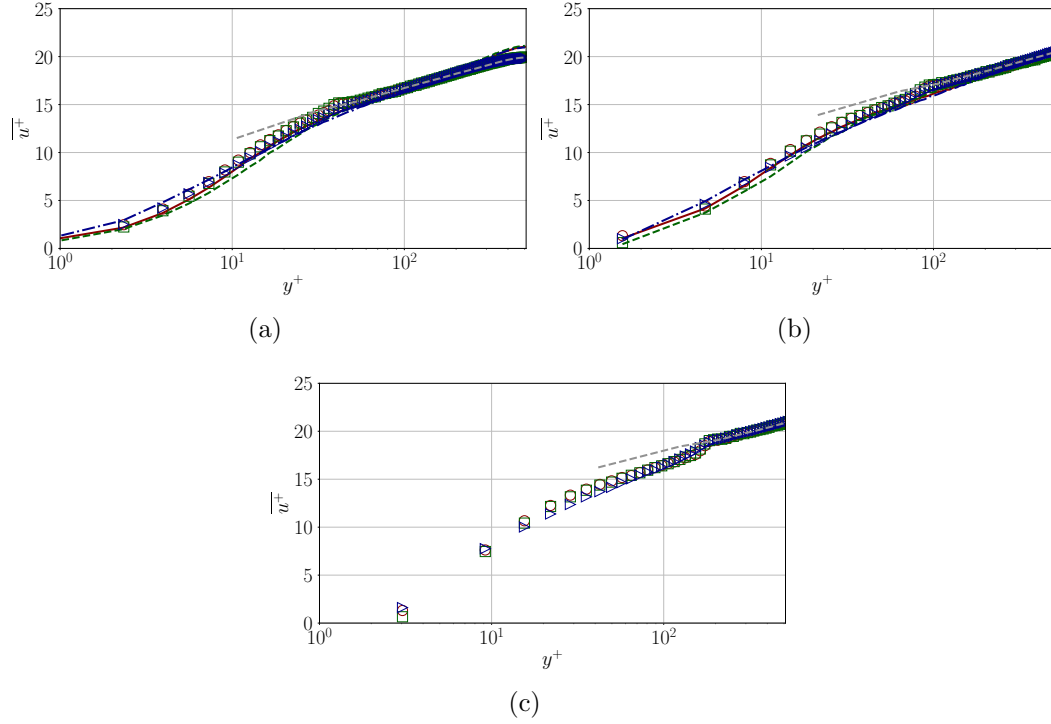


Figure 4.5: Mean axial velocity profiles of particles computed using the binning described in Eq. 4.1. Symbols represent the WM-LES datasets, while lines correspond to the reference DNS datasets, available for the first two cases. Three Stokes numbers, Stk^+ , are considered: 1 (red circles and solid red line), 10 (green squares and dashed green line), and 100 (blue triangles and dash-dotted blue line). Different panels show the results for different friction Reynolds numbers: (a) $Re_\tau = 500$, (b) $Re_\tau = 1000$, and (c) $Re_\tau = 2000$. All the quantities are expressed in viscous units. The light-grey, dashed curve represents the corresponding statistics of the carrier phase.

compromise the reliability of the model's predictions.

Next, we present in Fig. 4.6 the root mean square of axial velocity fluctuations of particles as a function of the distance from the wall for $Re_\tau = 500$, $Re_\tau = 1000$, and $Re_\tau = 2000$. In each case, the statistical trends of the dispersed phase closely follow those of the carrier phase in the outer layer, where the Eulerian statistics are used to drive the motion of the particles. Conversely, in the inner region, particle velocity fluctuations progressively deviate from the Eulerian trend and recover a behavior more similar to the DNS results, owing to the action of the semi-stochastic model. The only notable exception occurs in the near-wall behavior of the case with $Stk^+ = 100$. In this scenario, the DNS results exhibit a more pronounced deviation from the corresponding semi-stochastic WM-LES predictions. Although we cannot provide direct evidence,

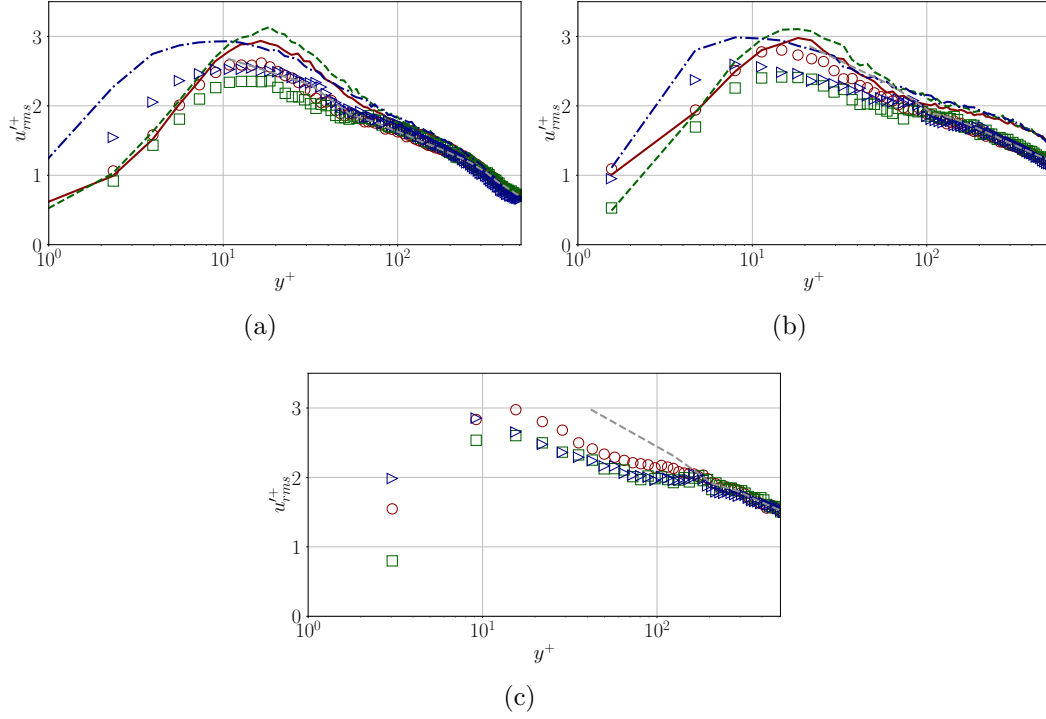


Figure 4.6: Root mean square of axial velocity fluctuations of particles computed using the binning described in Eq. 4.1. Symbols represent the WM-LES datasets, while lines correspond to the reference DNS datasets, available for the first two cases. Three Stokes numbers, Stk^{+} , are considered: 1 (red circles and solid red line), 10 (green squares and dashed green line), and 100 (blue triangles and dash-dotted blue line). Different panels show the results for different friction Reynolds numbers: (a) $Re_{\tau} = 500$, (b) $Re_{\tau} = 1000$, and (c) $Re_{\tau} = 2000$. The light-grey, dashed curve represents the corresponding statistics of the carrier phase.

we hypothesize that this discrepancy is due to inertial effects captured by the DNS but not fully reproduced by our model. A further possible source of the discrepancy observed for $Stk^{+} = 100$ lies in the simplified wall-normal velocity fluctuation model introduced in Eq. 3.23. This formulation assumes a linear relaxation-type response of particles to the sampled wall-normal fluctuations, which is adequate for low and moderate Stokes numbers. However, at high inertia, particles respond more slowly to rapid wall-normal variations and exhibit a more pronounced phase lag with respect to the fluid velocity. These nonlinear and frequency-dependent effects are not explicitly represented in Eq. 3.23. As a result, the model may underestimate wall-normal fluctuation intensities in the near-wall region, thereby contributing to the mismatch with DNS for $Stk^{+} = 100$. This suggests that future improvements may require extending

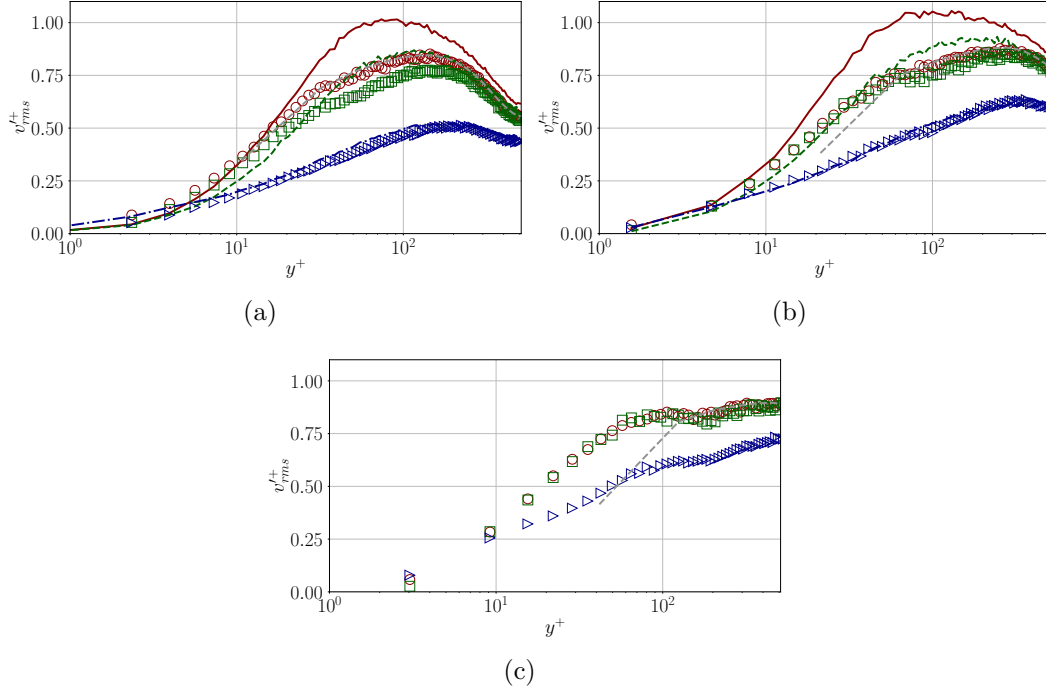


Figure 4.7: Wall-normal root mean square velocity fluctuations of particles computed using the binning described in Eq. 4.1. Symbols represent the WM-LES datasets, while lines correspond to the reference DNS datasets, available for the first two cases. Three Stokes numbers, Stk^+ , are considered: 1 (red circles and solid red line), 10 (green squares and dashed green line), and 100 (blue triangles and dash-dotted blue line). Different panels show the results for different friction Reynolds numbers: (a) $Re_\tau = 500$, (b) $Re_\tau = 1000$, and (c) $Re_\tau = 2000$. The light-grey, dashed curve represents the corresponding statistics of the carrier phase.

Eq. 3.23 to incorporate inertia-dependent decorrelation or frequency-selective response behavior. More specifically, in DNS, highly inertial particles migrating from the outer layer toward the wall retain higher-intensity fluctuations, which, upon reaching the near-wall region, contribute to an increase in velocity fluctuation statistics. Our model, however, does not entirely capture this mechanism, leading to a slight underprediction of fluctuations for this particular Stokes number. Despite this localized discrepancy, the model accurately predicts the overall trend of axial velocity fluctuations across all considered cases, capturing the key features of the dispersed phase dynamics.

Analogous considerations can be made for the wall-normal and spanwise root mean square velocity fluctuations, reported in Fig.4.7 and Fig.4.8, respectively. In these cases, the consistency between the considered cases and the reference DNS data is even more evident. It is also worth noting that, as

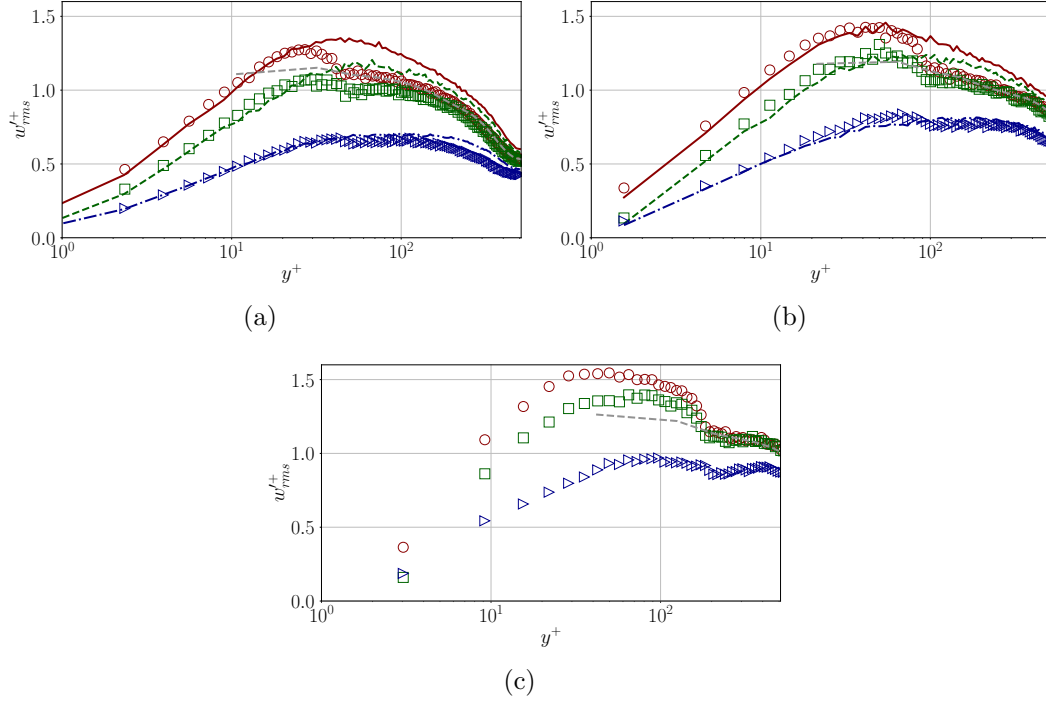


Figure 4.8: Spanwise root mean square velocity fluctuations of particles computed using the binning described in Eq. 4.1. Symbols represent the WM-LES datasets, while lines correspond to the reference DNS datasets, available for the first two cases. Three Stokes numbers, Stk^+ , are considered: 1 (red circles and solid red line), 10 (green squares and dashed green line), and 100 (blue triangles and dash-dotted blue line). Different panels show the results for different friction Reynolds numbers: (a) $Re_\tau = 500$, (b) $Re_\tau = 1000$, and (c) $Re_\tau = 2000$. The light-grey, dashed curve represents the corresponding statistics of the carrier phase.

previously discussed, the low resolution employed in the semi-stochastic WM-LES is responsible for the underestimation of velocity fluctuations in the outer region, where the Eulerian statistics are used to force the point-particle dynamics. This underestimation of fluctuations, in turn, leads to a corresponding underestimation of the velocity fluctuations of the Lagrangian phase in this region. On the other hand, near the wall, the semi-stochastic model allows for an accurate representation of the Lagrangian dynamics of the particles. This confirms that, considering the limitations due to grid resolution, the model effectively captures the key statistical features of the dispersed phase both along the span-wise and wall-normal directions.

Finally, we present the results of particle distribution in terms of concentration over the binning of the domain described by Eq. 4.1. The concentration profiles are normalized by the reference concentration, C_0 , which corresponds

to a random, uniform distribution of particles in space along all three directions. It is worth noting that, under this assumption, the normalized concentration would be unity for tracers, i.e., particles with low Stokes numbers.

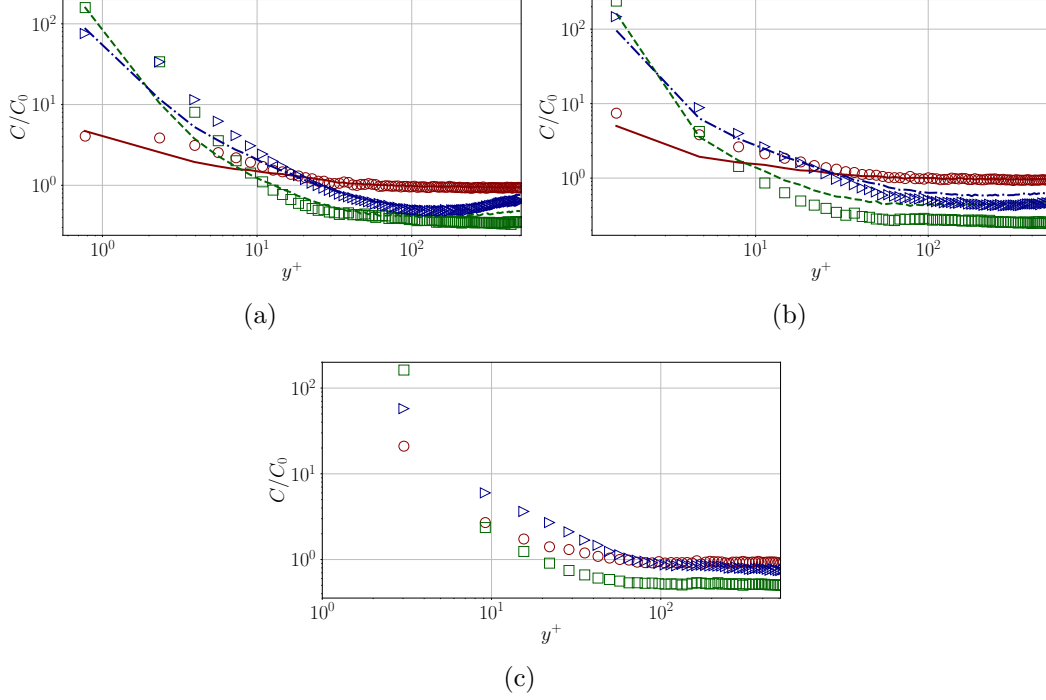


Figure 4.9: Mean normalized concentration of particles computed using the binning described in Eq. 4.1. Symbols represent the WM-LES datasets, while lines correspond to the reference DNS datasets, available for the first two cases. Three Stokes numbers, Stk^+ , are considered: 1 (red circles and solid red line), 10 (green squares and dashed green line), and 100 (blue triangles and dash-dotted blue line). Different panels show the results for different friction Reynolds numbers: (a) $Re_\tau = 500$, (b) $Re_\tau = 1000$, and (c) $Re_\tau = 2000$.

For all the Stokes and Reynolds numbers considered, turbophoresis leads to an accumulation of particles near the wall, as expected. The model fully captures the inertial effects on turbophoresis, with lighter particles exhibiting lower accumulation and heavier ones showing a stronger concentration near the wall. We observe that, for low Stokes numbers, i.e., $Stk^+ \leq 10$, the particle concentration profiles obtained from the semi-stochastic WM-LESs closely follow the reference DNS data both in the near-wall region and in the bulk flow. On the other hand, for higher Stokes numbers, some discrepancies appear in the bulk region, while the near-wall behavior remains well-predicted. Even if we cannot provide any evidence, we infer that, the reduction in accuracy of the semi-stochastic WM-LES model for higher Stokes numbers in the bulk region

could be attributed to the way particle dynamics are coupled with the Eulerian flow field. For low Stokes numbers, particles behave almost like tracers, meaning their motion is strongly influenced only by the local, instantaneous fluid velocity. Since the semi-stochastic WM-LES approach captures the large-scale structures and mean flow properties of the carrier phase in the bulk region, the resulting particle concentration profiles remain consistent with the DNS data across the entire channel in this case. However, for higher Stokes numbers, inertial effects become more significant. In these cases, particles respond more slowly to fluid velocity fluctuations and tend to maintain their momentum over longer distances. This means that their distribution is influenced not only by local turbulence but also by their prior history of motion, including their interactions with coherent turbulent structures. In the bulk region, when the resolution is lower and subgrid-scale fluctuations are not explicitly resolved, the model might not fully capture the transport mechanisms responsible for the redistribution of inertial particles. As a result, discrepancies arise between the WM-LES and DNS data in this region. Despite this, the near-wall behavior remains well-predicted because the semi-stochastic model correctly accounts for the enhanced turbophoretic drift that dominates particle accumulation in this area. Near the wall, turbulent fluctuations are weaker, and the dominant effect is the progressive drift of particles toward the boundary, which is well handled by the model.

Bibliography

- [1] S. Hoyas and J. Jiménez. Reynolds number effects on the reynolds-stress budgets in turbulent channels. *Physics of Fluids*, 20(10), 2008.

CHAPTER 5

Final remarks and future perspectives

This study investigates the integration of a semi-stochastic model, based on the Langevin equation with drift-correction, into the Wall-Modeled Large-Eddy Simulation (WM-LES) framework for simulating particle-laden turbulent channel flows. For the carrier phase, the three-dimensional, incompressible Navier-Stokes equations are solved using implicit filtering. A WALE model is used to account for the effects of the sub-grid scales of the turbulent motion on the resolved ones. An equilibrium wall model, based on algebraic equations, is employed to correct the stress field near the walls. The motion of the dispersed phase is described using the classical point-particle approach, while a semi-stochastic model, based on Langevin equations, reconstructs the velocity fluctuations sampled by the particles in the near-wall region, where the Eulerian velocity field is affected by the low resolution of the LES and wall modeling. The results demonstrate that the proposed semi-stochastic WM-LES approach successfully and accurately reproduces particle velocity statistics across a range of Reynolds and Stokes numbers. In particular, the model provides a reliable approximation of particle dynamics in turbulent flow, capturing average velocity fluctuations, recovering the expected logarithmic profiles for the axial velocity component in the logarithmic region, and accurately predicting near-wall particle velocities. Additionally, the model efficiently reproduces the trends in particle concentration both near the wall and in the bulk region of the flow. While the model captures the key features of the particle motion and concentration, some minor discrepancies are observed in particle concentration predictions for higher Stokes numbers. In particular, the model tends to slightly underestimate particle concentration in the bulk region, a limitation that may stem from the inability to fully account for inertial effects at high Stokes numbers and the low resolution employed for the simulations. Despite these limitations, the present study highlights the potential of this modeling

approach for improving computational efficiency while maintaining accuracy in predicting particle motion and concentration. In conclusion, the findings of this study contribute valuable insights into the modeling of particulate flows in turbulent systems. Future work should focus on refining the semi-stochastic model to better capture inertial effects at high stokes numbers, and exploring its potential in a wider range of flow configurations. This approach could prove beneficial in industrial and environmental applications, such as sediment transport, mixing, and pollutant dispersion.

APPENDIX A

Sensitivity of the semi-stochastic WM-LES model from the interface parameters

In this appendix, a sensitivity analysis of the model proposed in this paper is presented, focusing on the position of the model interface. To this end, three different cases are considered, with the interface located at $y_I^+ = 70$, $y_I^+ = 90$, and $y_I^+ = 110$, respectively. The interface thickness is fixed in all cases and set to $\Delta I^+ = 20$. The analysis is reported for the case with $Re_\tau = 1000$ and two Stokes numbers, $Stk^+ = 1$ and $Stk^+ = 100$, as the results for other configurations show similar trends. The outcomes of the sensitivity analysis are illustrated in Fig. A.1. Overall, no significant differences are observed across the considered interface positions. Only minor discrepancies appear near the wall for the concentrations of lower Stokes number case, which are not considered to have a meaningful impact on the overall accuracy of the model.

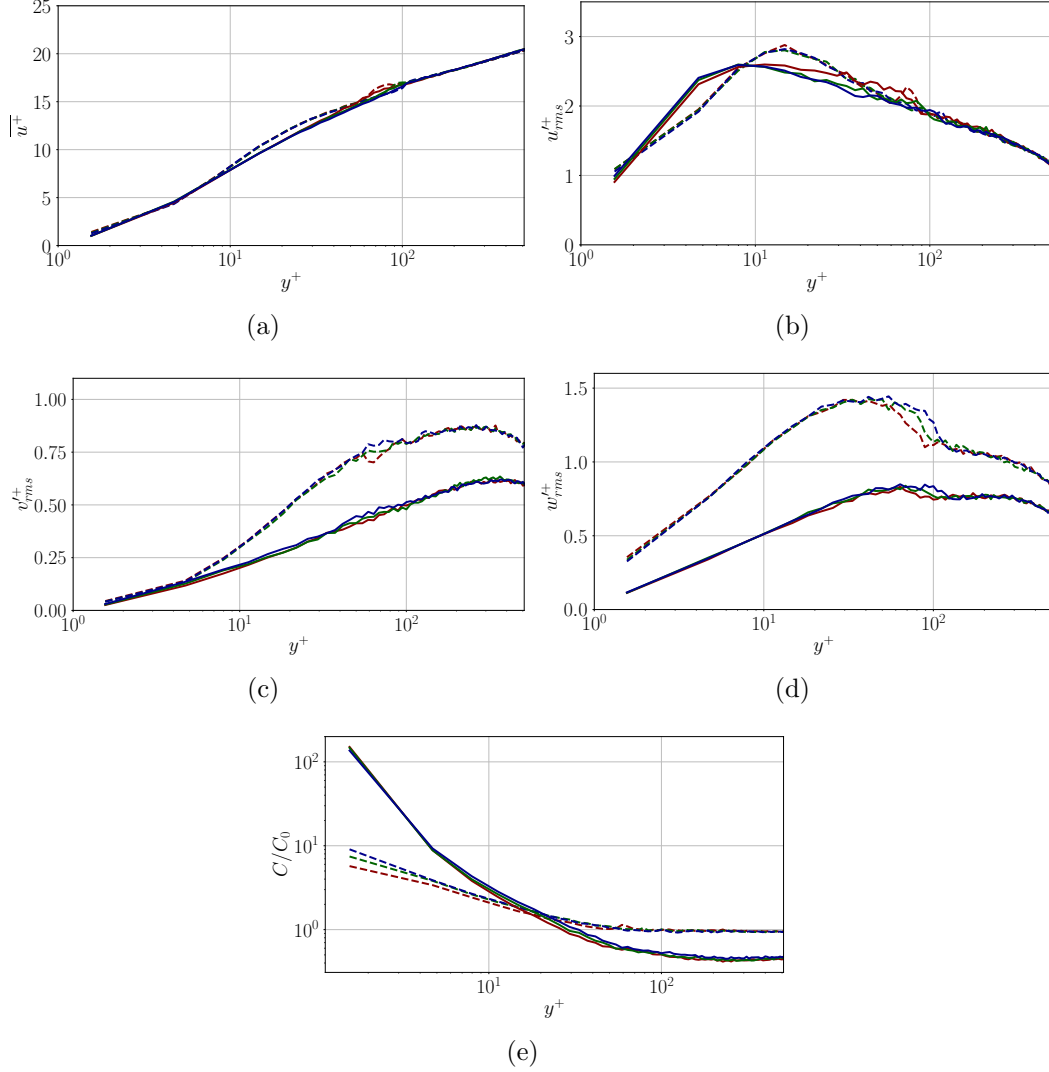


Figure A.1: Velocity statistics (panels a-d) and particle concentration (panel e) at two different Stokes numbers for $Re_\tau = 1000$: $Stk^+ = 1$ (dashed lines) and $Stk^+ = 100$ (solid lines). Red, green, and blue lines correspond to three different interface positions set at $y_I^+ = 70$, $y_I^+ = 90$, and $y_I^+ = 110$, respectively. The interface thickness is fixed in all cases and set to $\Delta I^+ = 20$.