UNIVERSITÀ DEGLI STUDI DI PADOVA

High-fidelity Simulation and Modeling of Turbulent Dispersed Multiphase Flows

Xiang’en Kong - 38th Cycle

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Admission to the final exam - 11/09/2025

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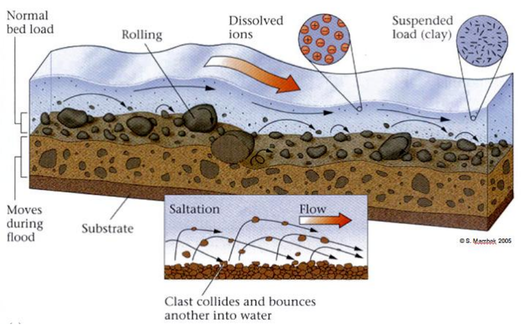
Motivation

Particle/Droplet-laden multiphase flows

Sediment transport



Marshak, S. (2004). Essentials of geology..

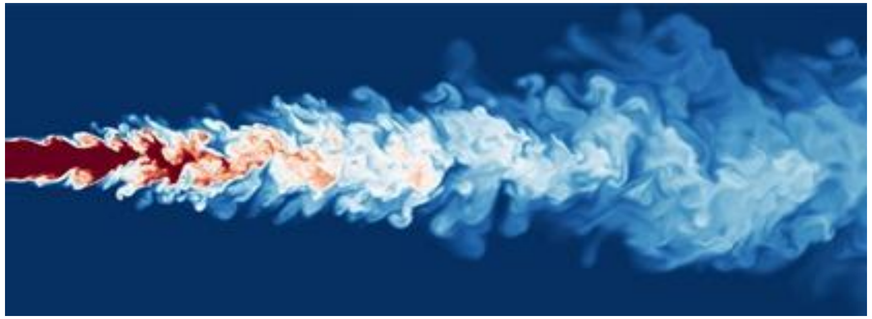
Volcanos

https://www.timeforkids.com/g34/volcanoes-2/

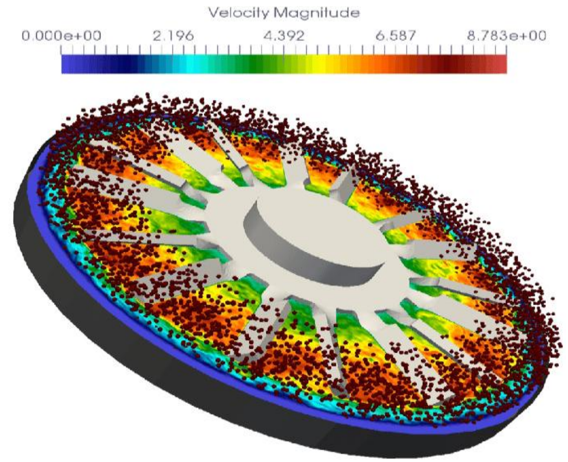
Biological flows

https://www.jillcarnahan.com/2025/02/24/

Turbulent sprays and clouds



Dynamic cross-flow filtration

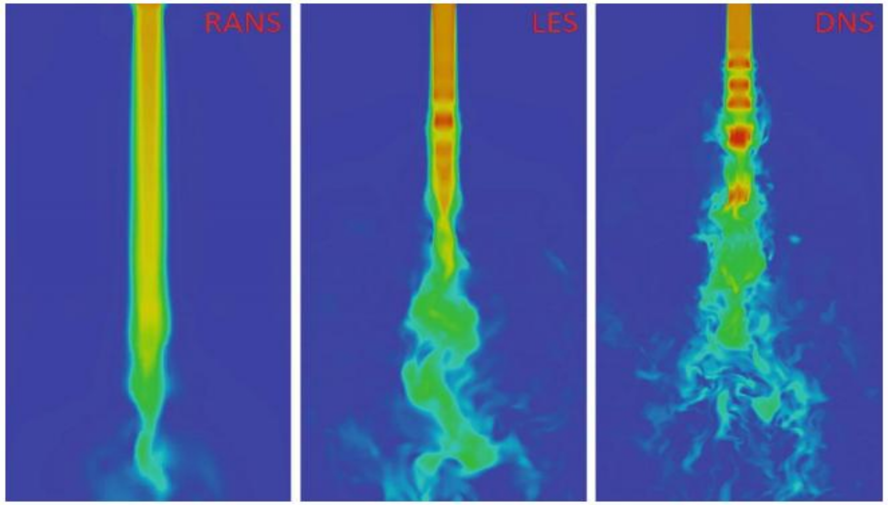


Krause, M (2020). Computers & Mathematics with Applications. 81. 10.1016/j.camwa.2020.04.033.

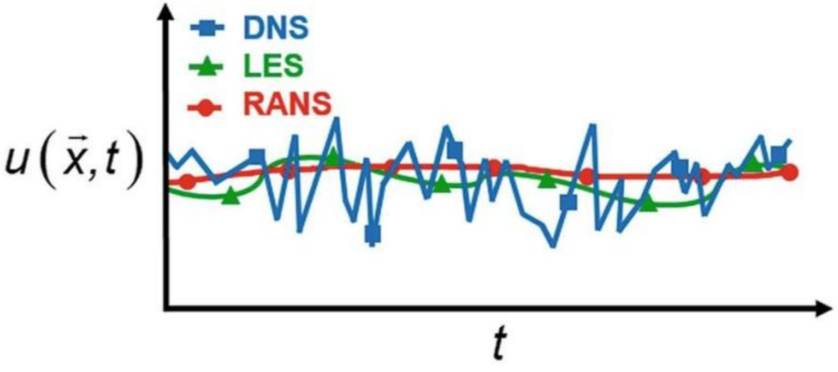
- Particle/Droplet-laden, turbulent multiphase flows refer to the phenomenon in which a large number of solid particles or droplets are suspended in a turbulent flow.
- Particle/Droplet-laden, turbulent multiphase flows are fundamental to a wide range of natural and industrial processes
- **Accurately predicting the behavior of these flows is crucial for optimizing engineering applications and understanding environmental phenomena**

Introduction: Turbulent simulation method

A visual comparison of DNS, LES, and RANS simulations for a turbulent jet



Velocity time history at probe in turbulent flow



T-H Shih, JP Moder, and N-S Liu.(2019). Shock Waves.

➢ Flow Field Comparison

•**DNS**: Captures full turbulence details, instantaneous structures match experiments.
•**LES**: Reproduces large-scale structures, but small-scale details are blurred.
•**RANS**: Only shows mean flow field, instantaneous structures are lost.

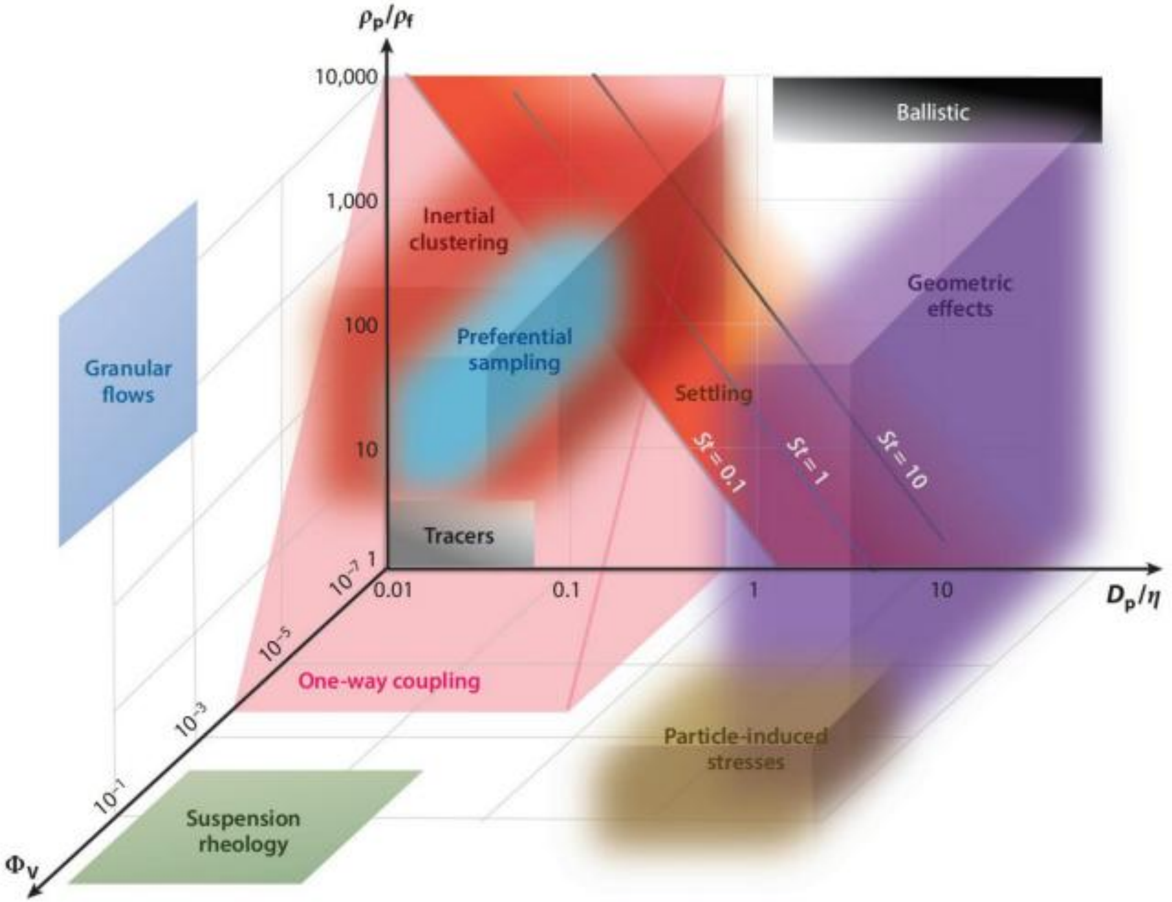
➢ Velocity Signal Comparison

•**DNS**: Contains full frequency range, from low-frequency large-scale to high-frequency small-scale.
•**LES**: Retains low-frequency large-scale modulations, filters out most high-frequency components.
•**RANS**: Provides only the mean value, no instantaneous variations.

➢ Computational Cost Comparison

DNS > LES > RANS

Introduction: Particle-laden turbulent flow simulation method



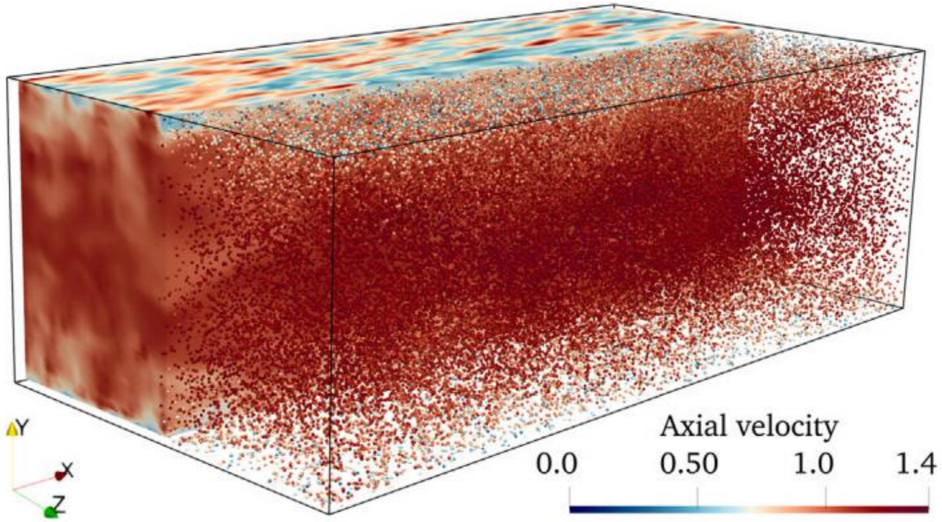
Luca Brandt and Filippo Coletti.(2022) Annual Review of Fluid Mechanics

- D_p/η -- the ratio of particle size to turbulent scale, D_p is s the diameter of the spherical particles, η is the Kolmogorov scale in turbulence
- $\rho_p/\ \rho_f$ -- the density ratio between the particle and the fluid
- Φ_V -- the solid-phase volume fraction, which is the proportion of the particles in the total fluid volume

The transport of spherical particles in turbulence can be categorized into distinct dynamical regimes, determined by specific parameter combinations.

Objectives

- Simulation of particle-laden flows in the frame of Wall-Modelled Large Eddy Simulation (WM-LES)
- Development and improvement of wall models for point-particles



A sketch of the computational domain

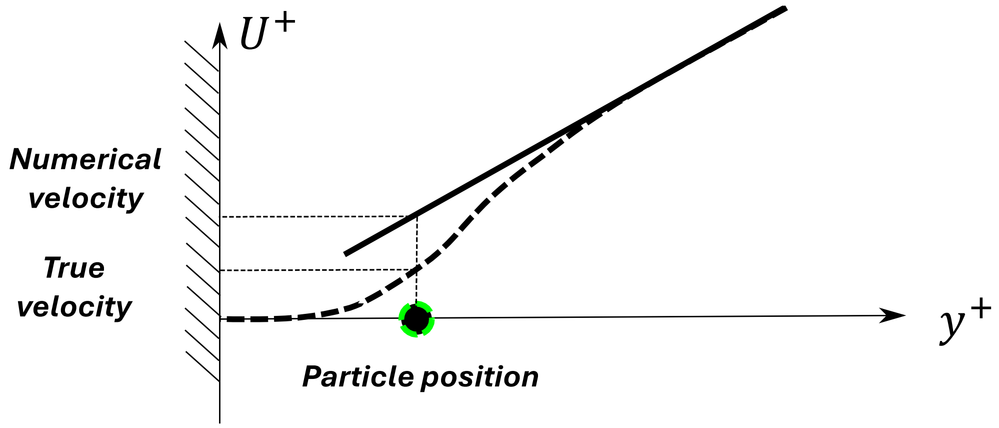
Overview of WM-LES approach

CARRIER PHASE

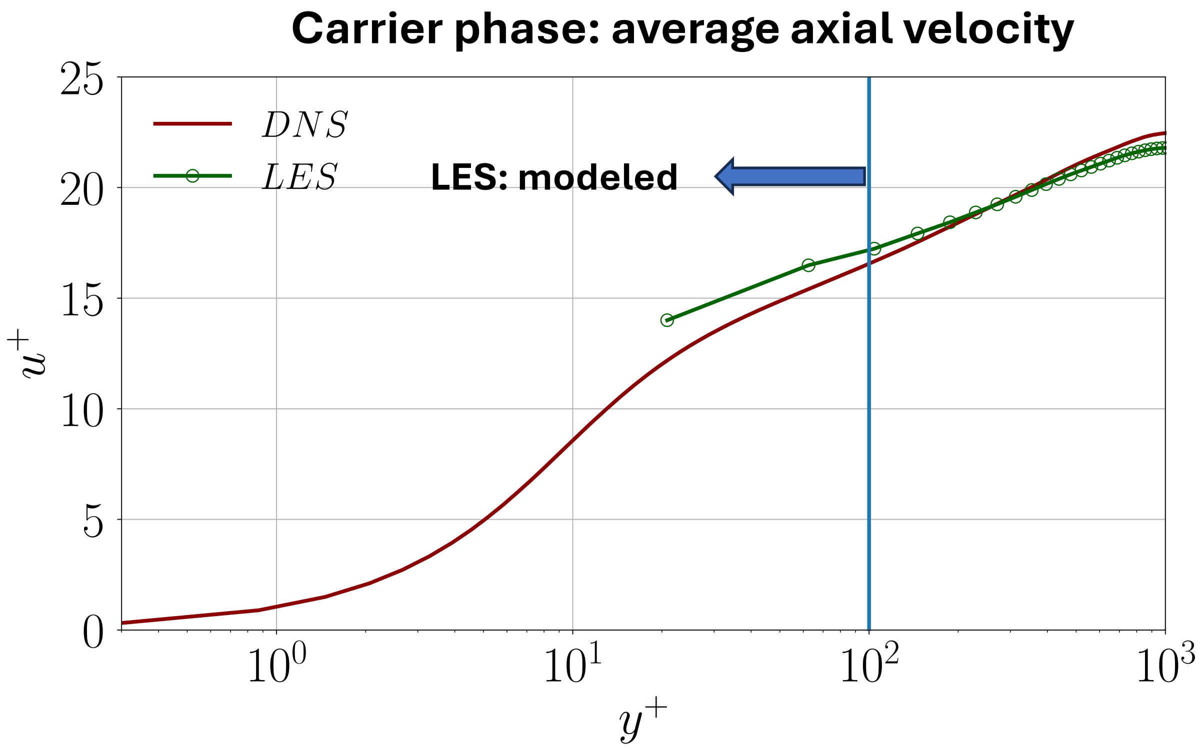
- LES: Wall Adapting Local Eddy-viscosity (WALE) model
- WM: velocity profile modelled within the unresolved boundary layer. Artificial viscosity added to correct wall stresses.

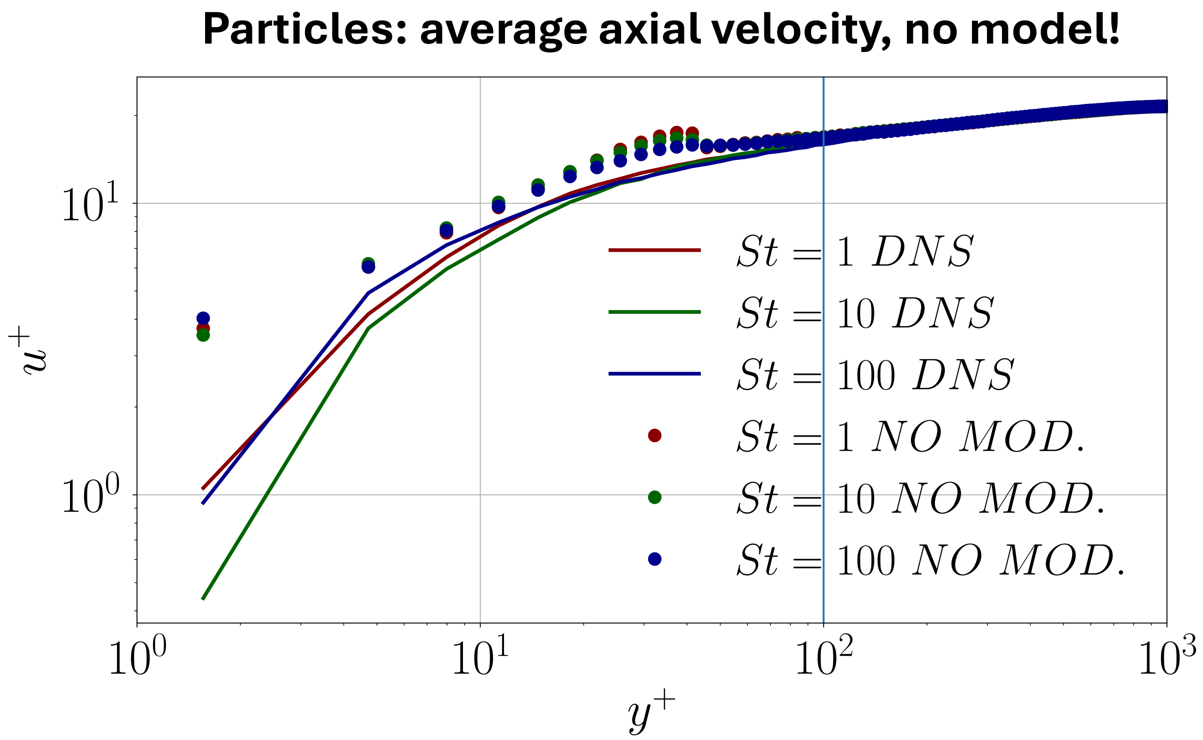
PARTICLES

- Classical point-particles equations
- SGS fluctuations are neglected
- **Necessity for special treatment of velocity computation within the unresolved boundary layer**



Wall-model LES without particle model





Computational domain and simulation setup

WM-LES

- $N_x \times N_y \times N_z = 48 \times 48 \times 48$

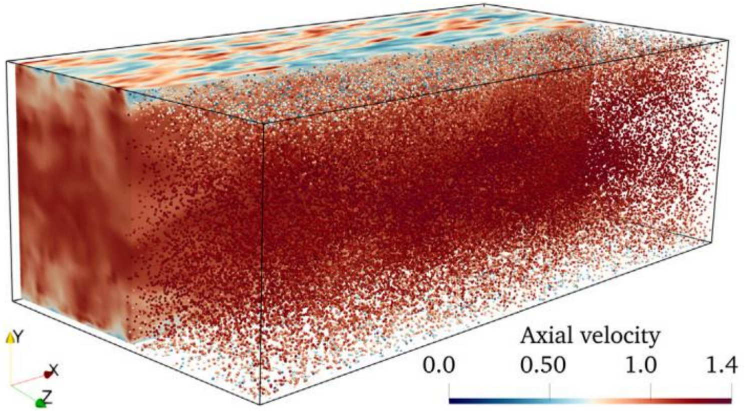
  LOW RES!!!

- $L_x \times L_y \times L_z = 6\delta \times 2\delta \times 3\delta$
- $Re_\tau = 500, 1000, 2000$
- $N_p = 150000$
- $Stk^+ = 1, 10, 100$

PRELIMINARY REFERENCE DNS

- $N_x \times N_y \times N_z = 1216 \times 512 \times 640$
- $L_x \times L_y \times L_z = 10\delta \times 2\delta \times 3\delta$
- $\Delta y^+_{min} \simeq 0.1$
- $Re_\tau = 500, 1000$
- $N_p = 150000$
- $Stk^+ = 1, 10, 100$

Note:
δ -- Channel half-height; Re_τ -- friction Reynolds numbers;
N_p -- Number of point particles; Stk^+ -- particle Stokes number



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More simulation setup details for WM-LES

CISAS G. COLOMBO

STMS

Summary of simulation parameters

Case	Re_b	Re_τ	$d_p/(2\delta)$	d_p^+	Stk^+	Φ	Ψ
Sim 1	18 100	500	$8.164 \cdot 10^{-5}$	0.0816	1	$3.2 \cdot 10^{-9}$	$8.6 \cdot 10^{-6}$
			$2.582 \cdot 10^{-4}$	0.2582	10	$1.0 \cdot 10^{-7}$	$2.7 \cdot 10^{-4}$
			$8.165 \cdot 10^{-4}$	0.8165	100	$3.2 \cdot 10^{-6}$	$8.6 \cdot 10^{-3}$
Sim 2	40 000	1000	$4.083 \cdot 10^{-5}$	0.0816	1	$4.0 \cdot 10^{-10}$	$1.1 \cdot 10^{-6}$
			$1.291 \cdot 10^{-4}$	0.2582	10	$1.3 \cdot 10^{-8}$	$3.5 \cdot 10^{-5}$
			$4.083 \cdot 10^{-4}$	0.8165	100	$4.0 \cdot 10^{-7}$	$1.1 \cdot 10^{-3}$
Sim 3	87 100	2000	$2.041 \cdot 10^{-5}$	0.0816	1	$5.0 \cdot 10^{-11}$	$1.4 \cdot 10^{-7}$
			$6.455 \cdot 10^{-5}$	0.2582	10	$1.6 \cdot 10^{-9}$	$4.3 \cdot 10^{-6}$
			$2.041 \cdot 10^{-4}$	0.8165	100	$5.0 \cdot 10^{-8}$	$1.4 \cdot 10^{-4}$

Grid spacing along the streamwise, Δx, wall-normal, Δy, and spanwise, Δz, directions, respectively.

Simulation	Re_b	Re_τ	Δx^+	Δy^+	Δz^+	Δx	Δy	Δz
Sim 1	18 100	500	63	21	31	0.0625	0.0208	0.0313
Sim 2	40 000	1000	126	42	62	0.0625	0.0208	0.0313
Sim 3	87 100	2000	252	84	124	0.0625	0.0208	0.0313

Note:

$\boldsymbol{d_p}$ -- Particle diameter;

$\boldsymbol{Re_b}$-- Bulk Reynolds numbers;

$\boldsymbol{d_p^+}$-- $d_p^+ = d_p/l_\tau$, $l_\tau$is viscous length;

$\boldsymbol{Stk^+}$ -- particle Stokes number

$\boldsymbol{\Phi}$ --Volume fractions of the dispersed phase;

$\boldsymbol{\Psi}$ -- Mass fractions of the dispersed phase;

Numerical Methodology
Governing equations of the carrier phase
WM-LES

Navier-Stokes (incompressible)

$$\nabla \cdot \tilde{u} = 0$$
$$\frac{\partial \tilde{u}}{\partial t} + \tilde{u} \cdot \nabla \tilde{u} = -\frac{\nabla \tilde{p}}{\rho_f} + \nabla \cdot \left(\nu_{tot} (\nabla \tilde{u} + \tilde{u}^T) \right)$$

$\nu_{tot} = \nu_f + \nu_t$ Total viscosity

ν_f Molecular, kinematic viscosity

ν_t Turbulent viscosity

Wall-Adapting Local Eddy (**WALE**) viscosity model

Wall-model (WM)

WM: velocity profile modelled within the unresolved boundary layer. **Artificial viscosity added to correct wall stresses:**

Law of the wall

$$\frac{\tilde{U}_I}{u_\tau} = f(y^+) \longrightarrow u_\tau \longrightarrow \tau_w = \rho_f u_\tau^2$$

$$\tau_w, \left. \frac{\partial \tilde{u}}{\partial y} \right|_w \longrightarrow \nu_{tot,w} = \frac{\tau_w}{\left. \frac{\partial \tilde{u}}{\partial y} \right|_w}$$

Local velocity gradient

Viscosity added to ghost nodes

Numerical Methodology

Governing equations of the dispersed phase

$$\frac{d\boldsymbol{v}_p}{dt} = f(Re_p)\frac{\boldsymbol{u}_p - \boldsymbol{v}_p}{\tau_p}$$

$$\frac{d\boldsymbol{x}_p}{dt} = \boldsymbol{v}_p$$

One-way coupling

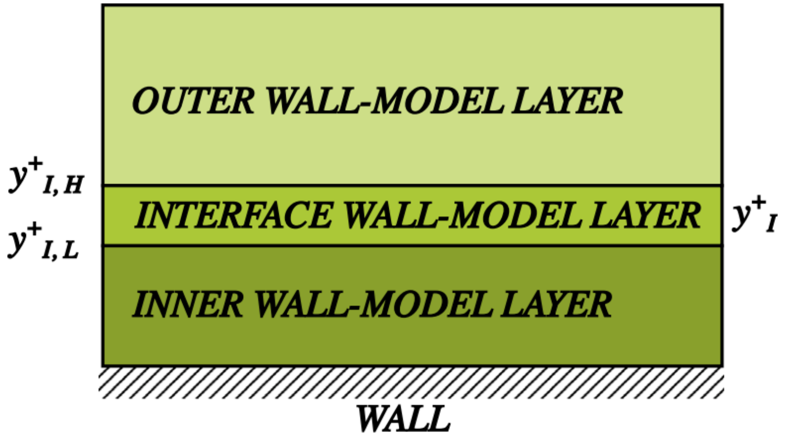
$$\tau_p = \frac{\rho_p}{\rho_f}\frac{d_p^2}{18\nu_f}$$

Particle relaxation time

$$f(Re_p) = 1 + 0.15 Re_p^{0.687}$$

Based on the Schiller–Naumann relation

$$Re_p = \frac{|v_p - u_p| d_p}{\nu_f}$$



$y^+_{I,L} = y^+_I - \Delta^+_I/2$

$y^+_{I,H} = y^+_I + \Delta^+_I/2$

Δ^+_I is the interface thickness

$$u_p = \begin{cases} \bar{u}_p + u'_p, & y^+_p \le y^+_{I,L} \\ \sqrt{\alpha}\,\tilde{u}_p + (1-\sqrt{\alpha})\bar{u}_p + \sqrt{1-\alpha}\,u'_p, & y^+_{I,L} < y^+_p < y^+_{I,H} \\ \tilde{u}_p + u_p\varepsilon, & y^+_p \ge y^+_{I,H} \end{cases}$$

$$\alpha = \begin{cases} 1, & y^+_p = y^+_{I,H} \\ 3t^2 - 2t^3, & y^+_{I,L} < y^+_p < y^+_{I,H} \\ 0, & y^+_p = y^+_{I,L} \end{cases}$$

Numerical Methodology
Governing equations of the dispersed phase

Streamwise direction component of u'_p

-- $u'_{p,1}$

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

Spanwise direction component of u'_p

-- $u'_{p,3}$

$$d\left(\frac{u'_{p,3}}{\sigma_z}\right) = -\left(\frac{u'_{p,3}}{\sigma_x}\right)\frac{dt}{\tau_L} + \sqrt{\frac{2}{\tau_L}}\, d\xi_z$$

Damping terms **Stochastic terms**

Drift correction terms

- σ_x, σ_z RMS of velocity fluctuations
- $d\xi_x$,$d\xi_z$ Gaussian random numbers with zero mean and variance dt
- τ_L Lagrangian time scale
- s_p is defined to be equal to one and positive for the lower wall and negative for the upper wall of the channel.
- $Stk = \frac{\tau_p}{\tau_L}$
- $D_x = \frac{\partial \overline{u'_{p,1} u'_{p,2}}}{\partial y}$

Dehbi, A. (2008). **Turbulent particle dispersion in arbitrary wall-bounded geometries: A coupled CFD-Langevin-equation based approach**. *International Journal of Multiphase Flow*, *34*(9), 819-828.

Dehbi, A. (2010). **Validation against DNS statistics of the normalized Langevin model for particle transport in turbulent channel flows**. *Powder Technology*, *200*(1-2), 60-68.

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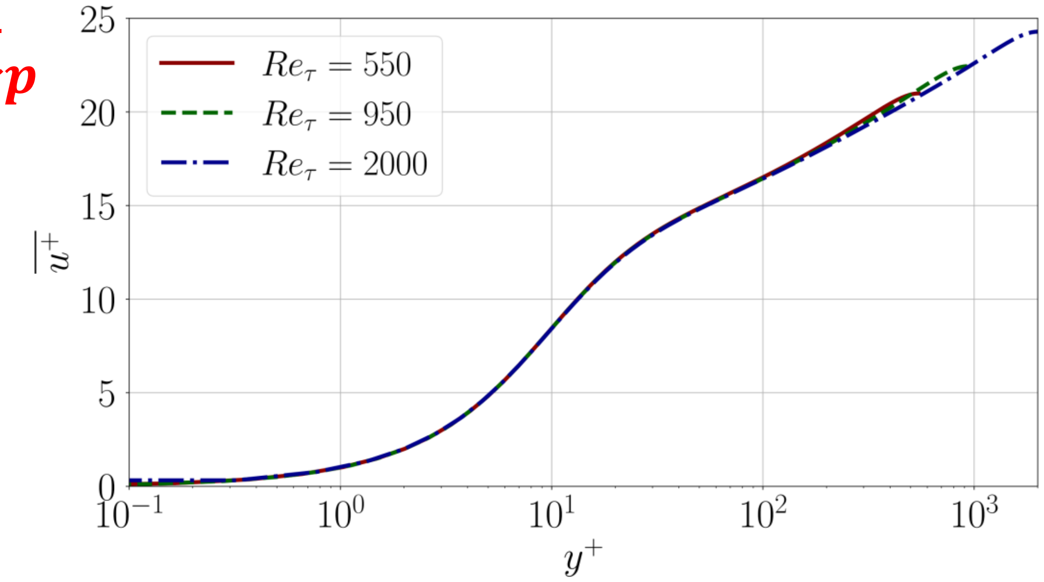
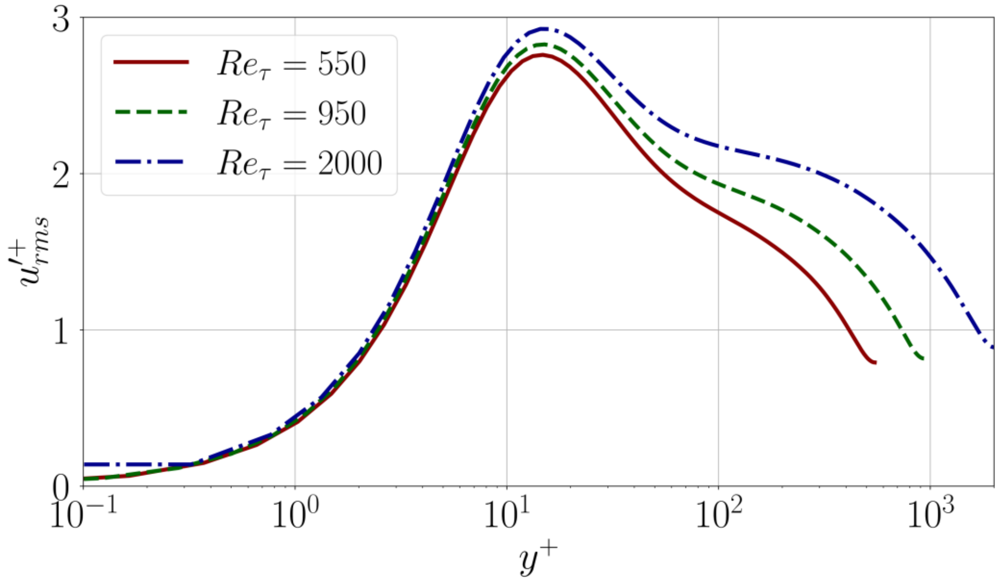
Data for look up table

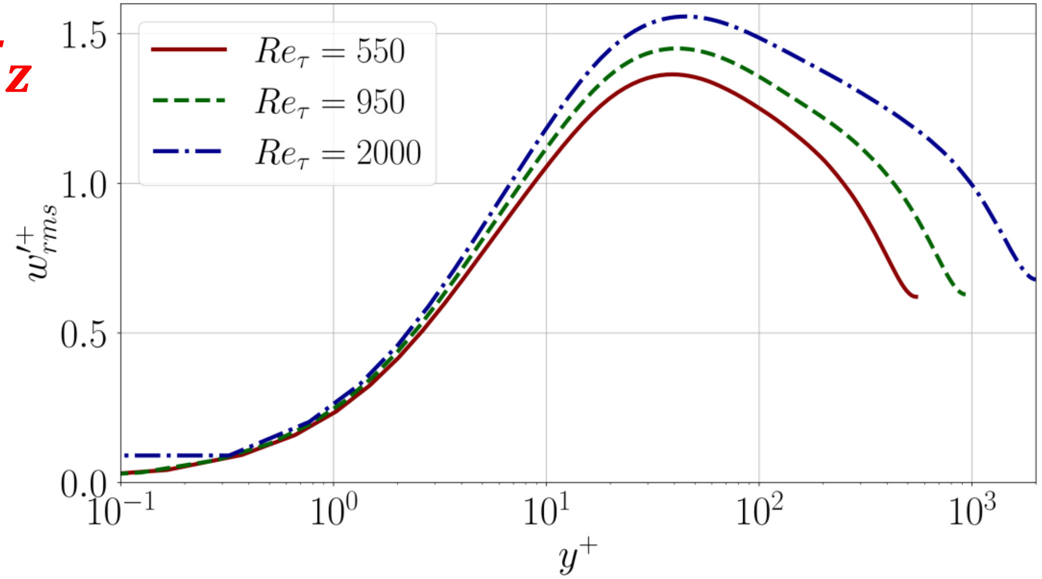
$\bar{u}_p$



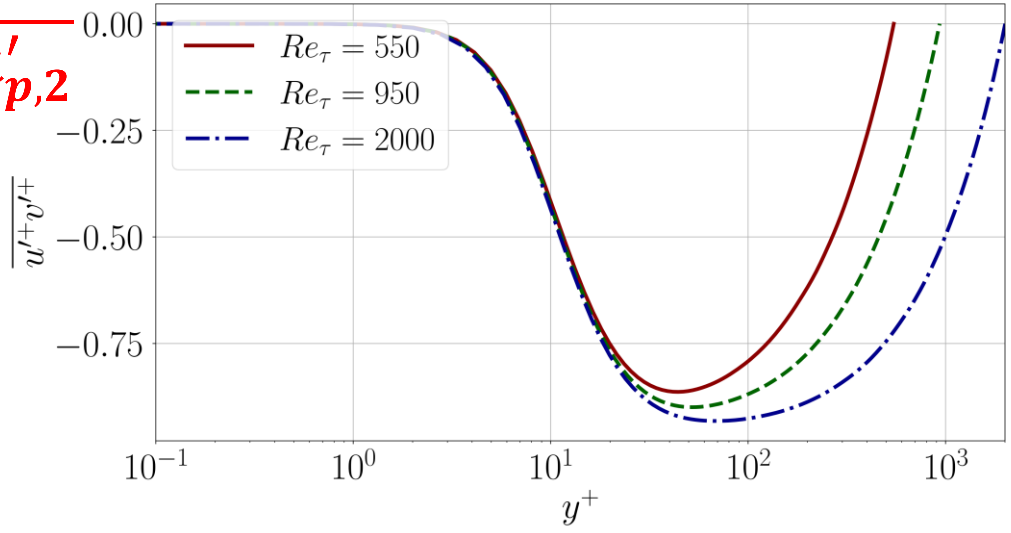
σ_x



σ_z



$\overline{u'_{p,1}u'_{p,2}}$



Hoyas and Jiménez (2008)

Numerical Methodology
Governing equations of the dispersed phase

Wall-normal direction component of u_p' -- $u_{p,2}'$

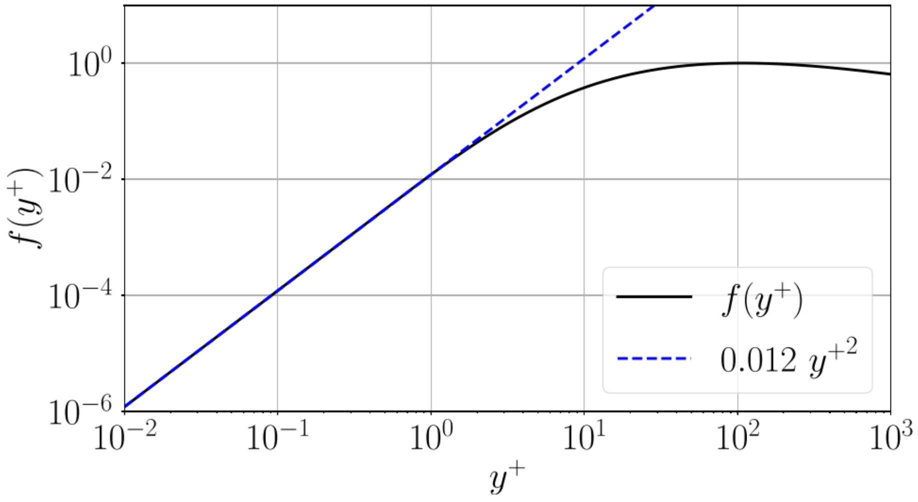
$$u_{p,2}' = f(y_p^+)u_{p,2,I} + s_p k f(y_p^+) \frac{df(y^+)}{dy^+}\bigg|_{y_p^+} \frac{\Delta t_r}{1+Stk} + N$$

Modulating function

Fluctuations of the carrier phase, $u_{p,2,I}$, located above the particle at the interface location, y_I^+

Drift correctionterm, imitates the drift correction idea in the Langevin equation in the tangential direction

Zero-mean Gaussian noise is used to inject small-scale randomness in this direction to avoid the model being completely deterministic in the normal direction.



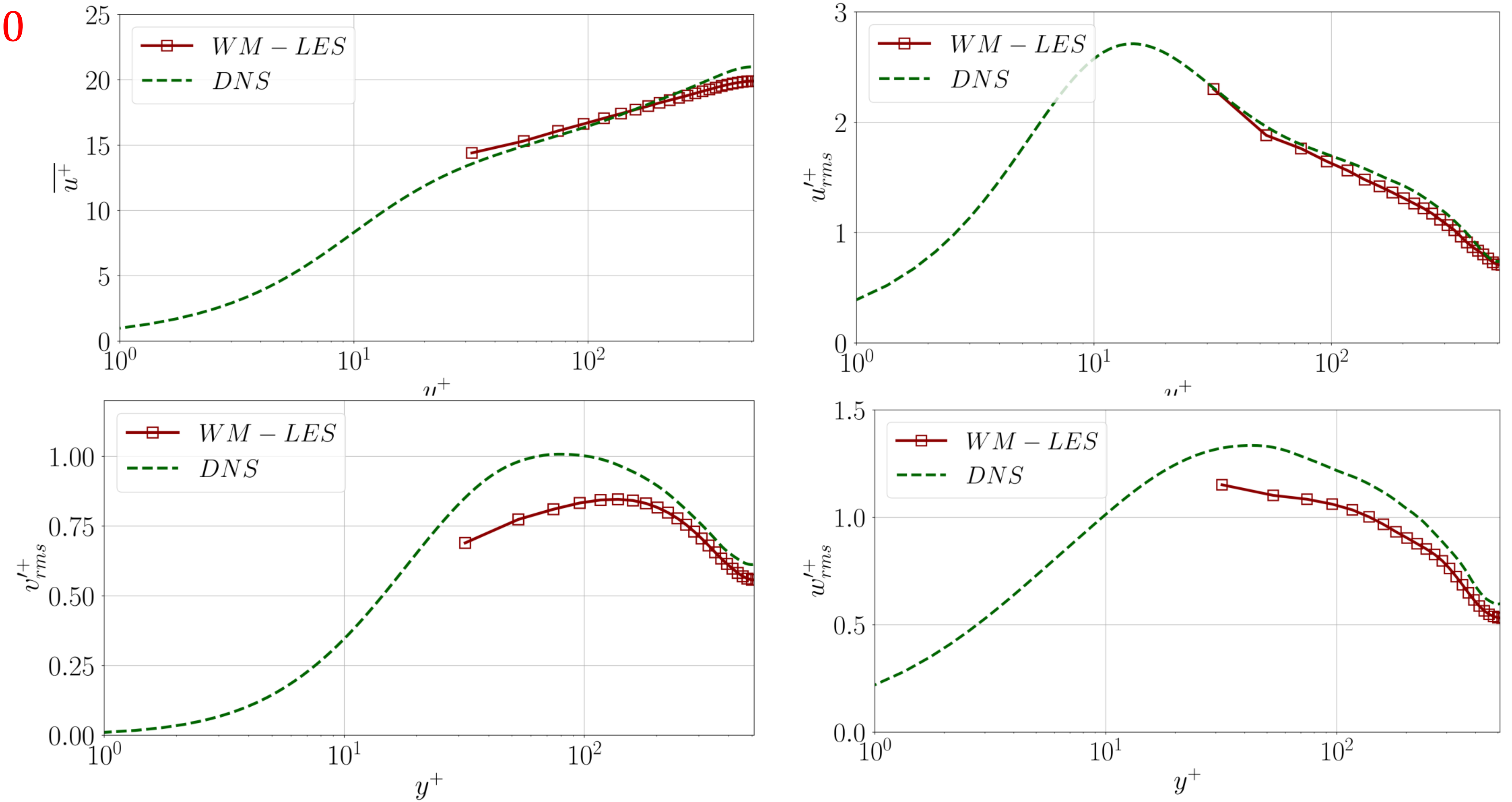
$$f(y^+) = \sqrt{\frac{y^{+4}\left(1-e^{-\frac{C_1}{y^{+C_2}}}\right)^{C_3}}{y_I^{+4}\left(1-e^{-\frac{C_1}{y^{+C_2}}}\right)^{C_3}}}$$

C_1=2.536, C_2 =0.578, C_3 =0.403

Johnson, P.L., et al 2020. J. Fluid Mech. 883, A27

Result: *Statistics of the carrier phase*

$Re_\tau = 500$



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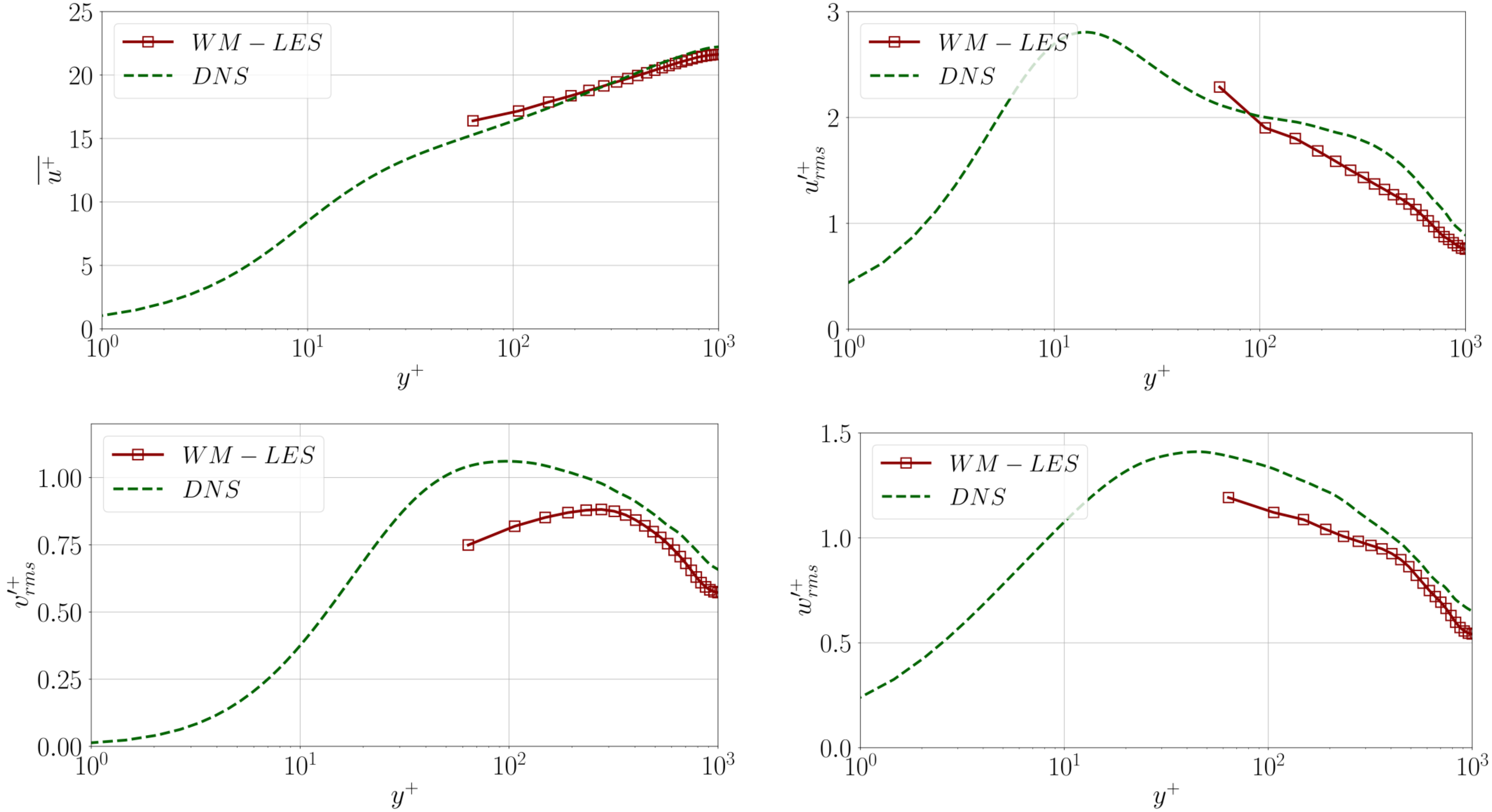
Result： *Statistics of the carrier phase*

$Re_\tau = 1000$



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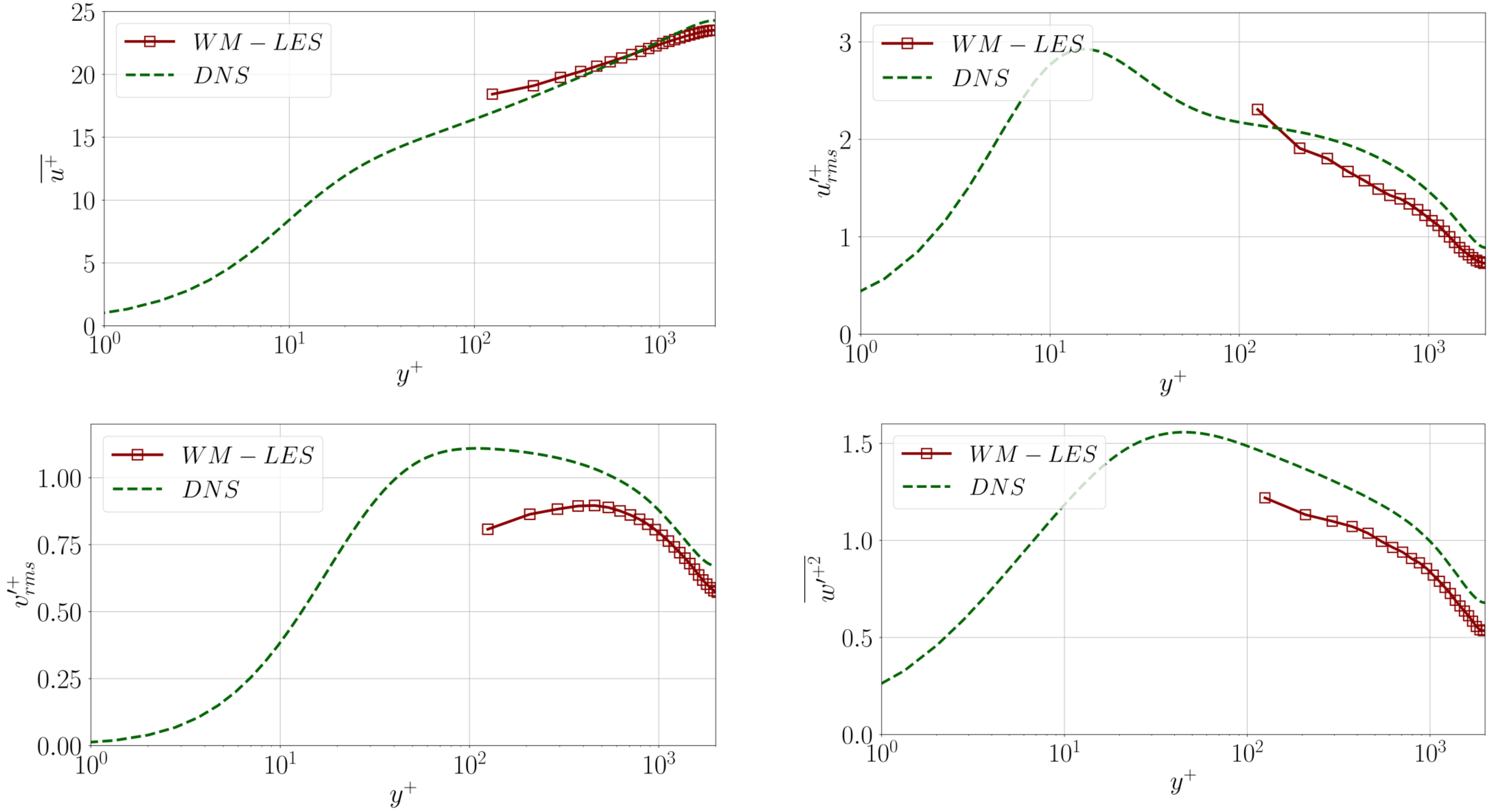
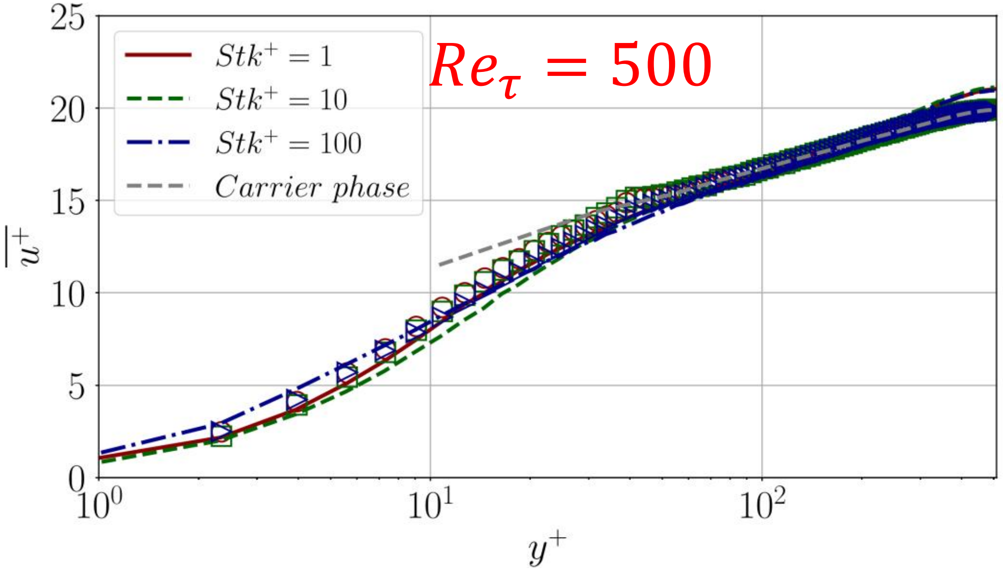
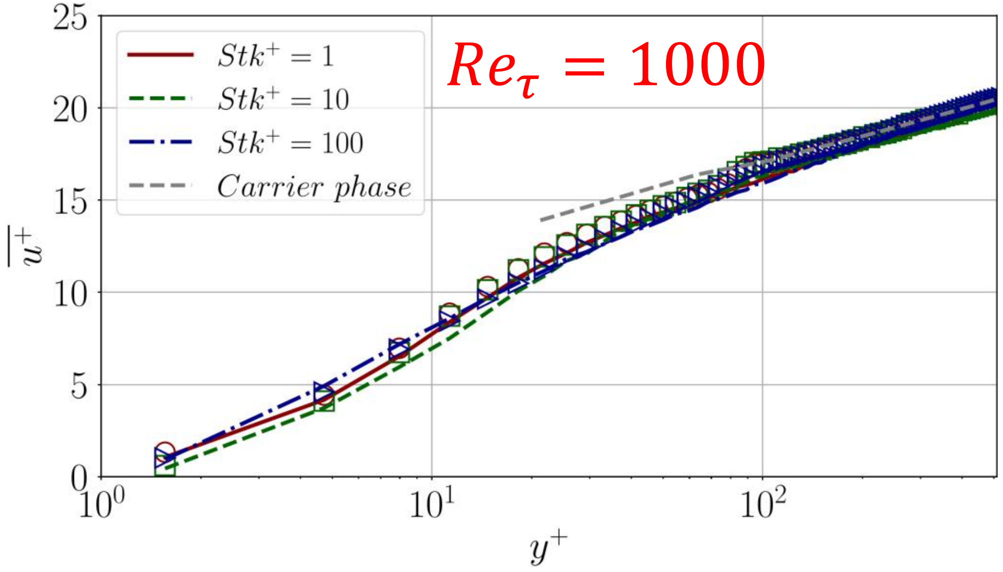
Result: *Statistics of the carrier phase*

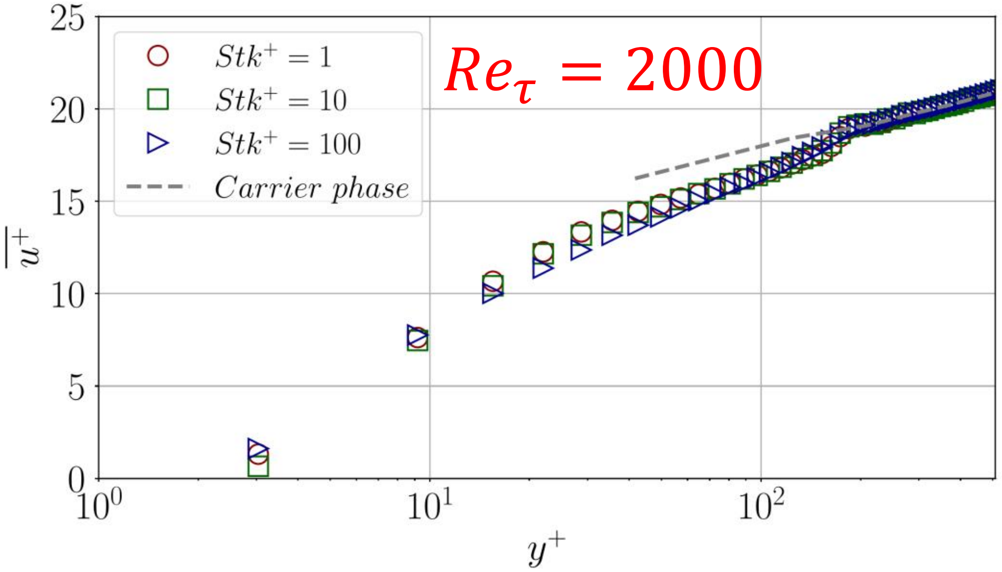
$Re_\tau = 2000$



Result: *Statistics of the dispersed phase* -- Mean axial velocity profiles of particles

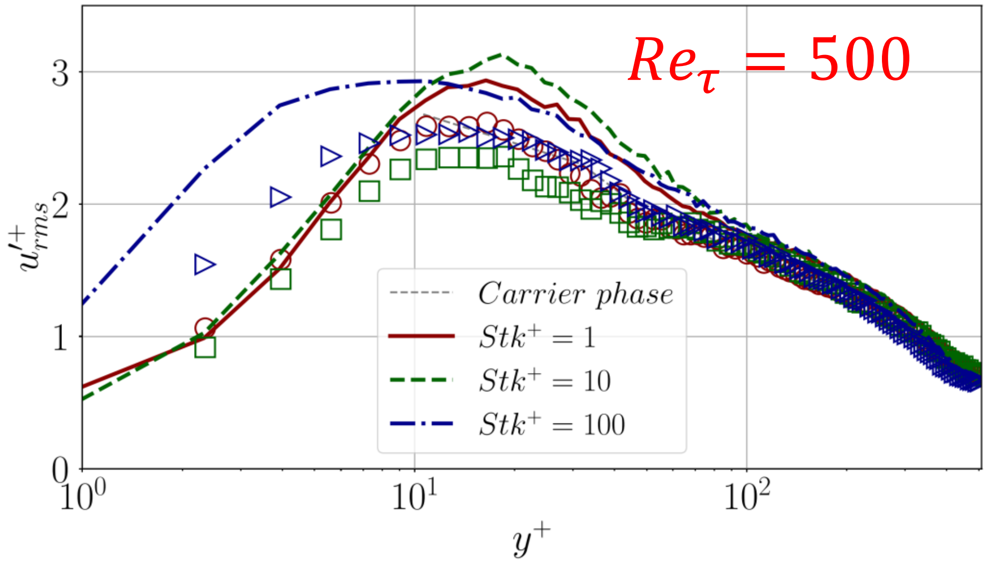


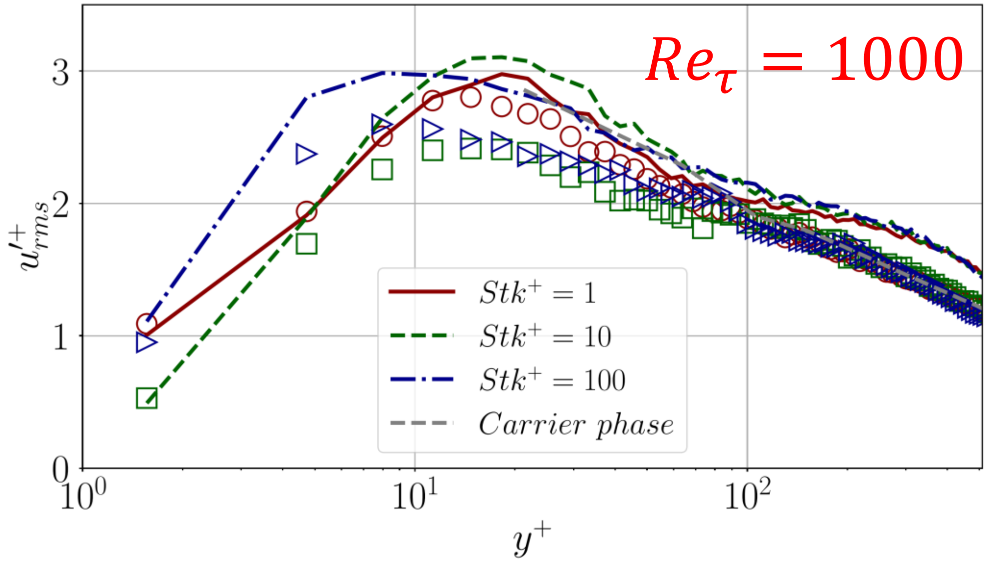


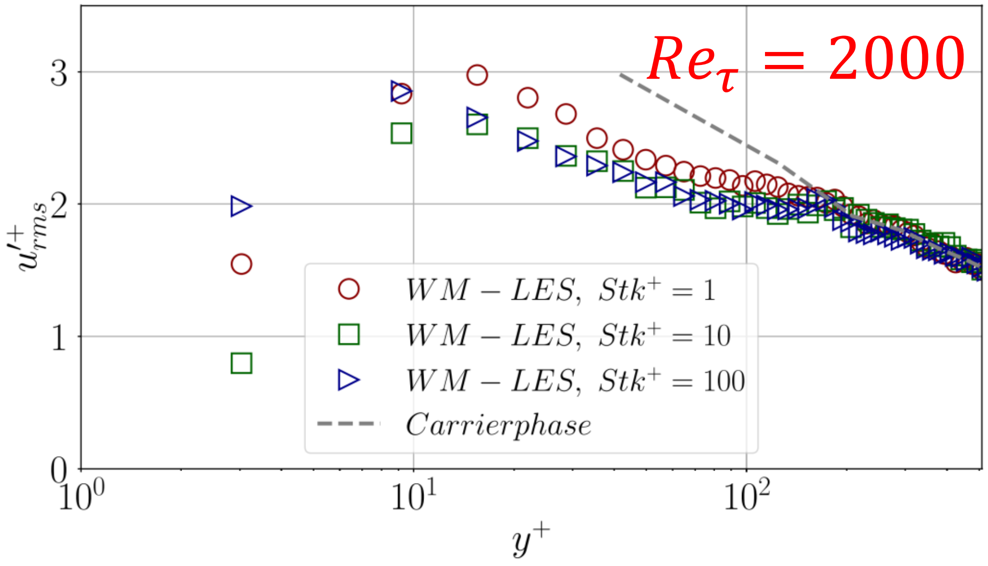


- Successfully captured the distribution pattern of the logarithmic law area
- Highly consistent with DNS data under different Stokes numbers
- The model has the ability to accurately capture the dynamics of the dispersed phase along the streamwise direction.

Result: *Statistics of the dispersed phase* -- Root mean square of axial velocity fluctuations of particles







- The model can accurately reproduce the distribution of particle axial velocity fluctuations, especially in the case of low and medium inertia particles, where it is highly consistent with DNS.
- However, for high inertia particles, the near-wall fluctuation level is slightly underestimated, reflecting the limitation of the model in capturing the inertial memory effect.

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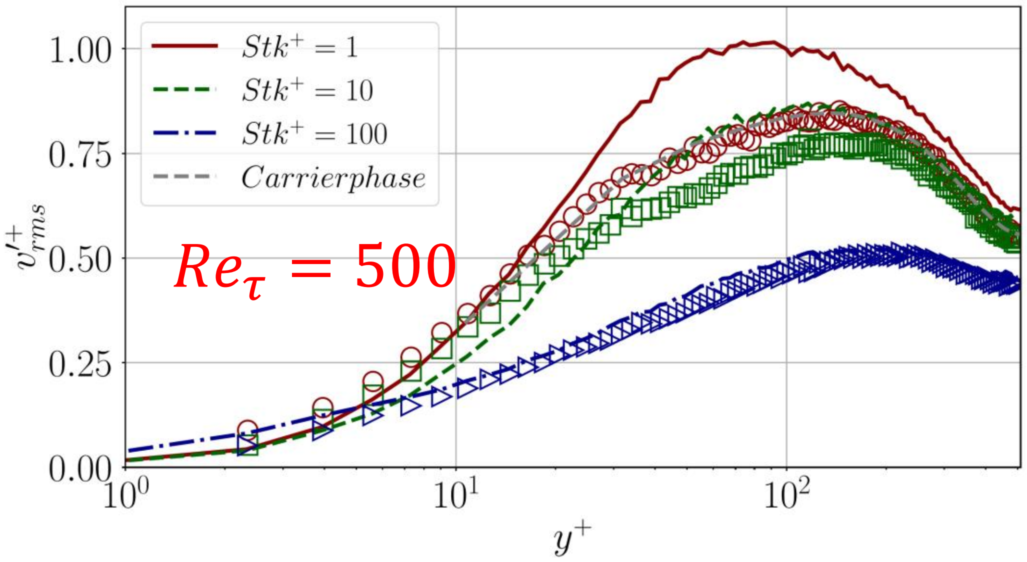
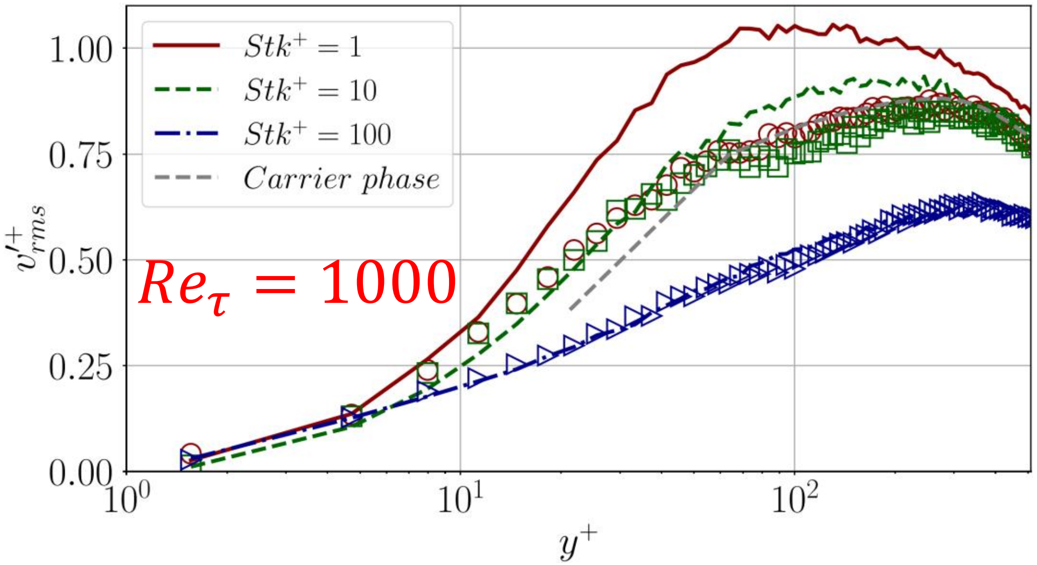
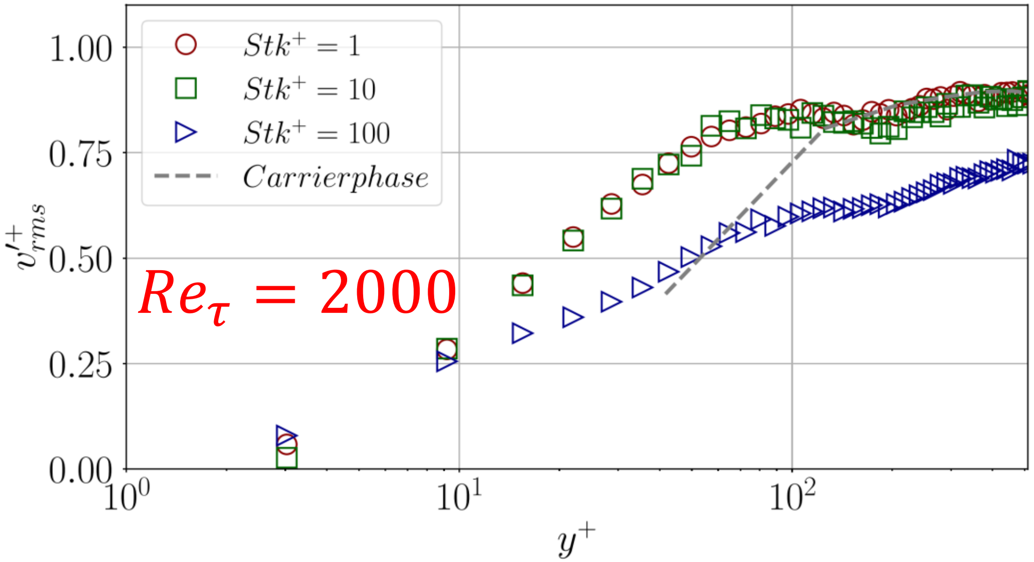
Result: *Statistics of the dispersed phase* -- Wall-normal root mean square velocity fluctuations of particles

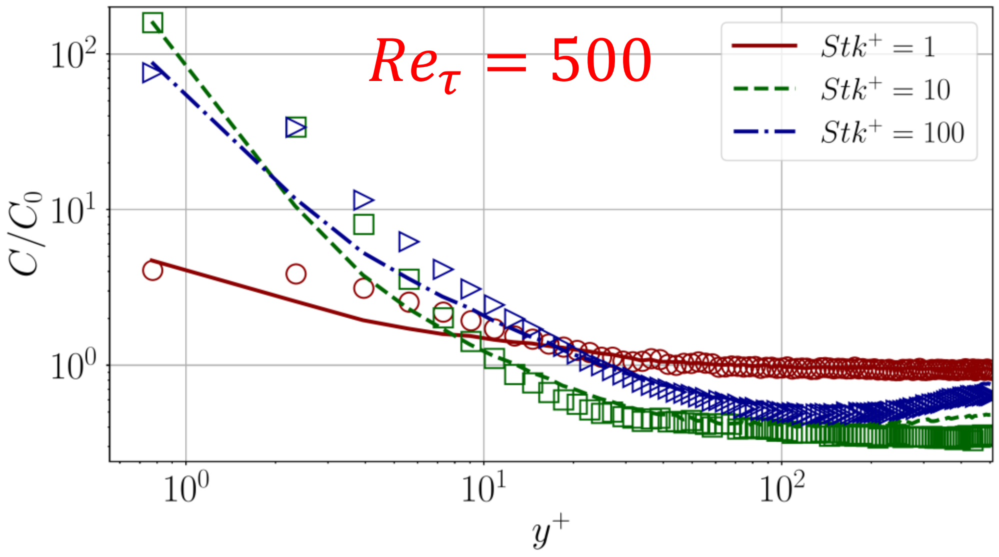


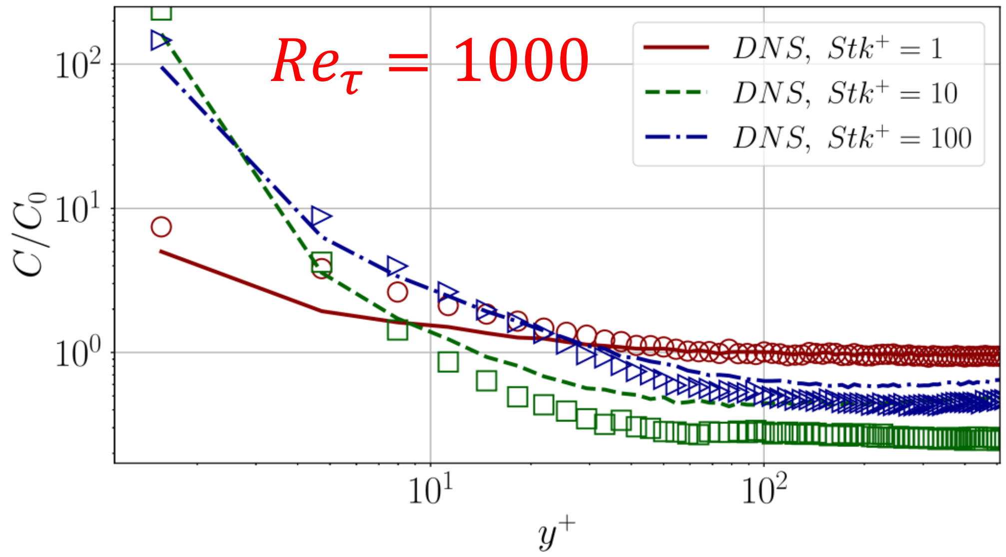


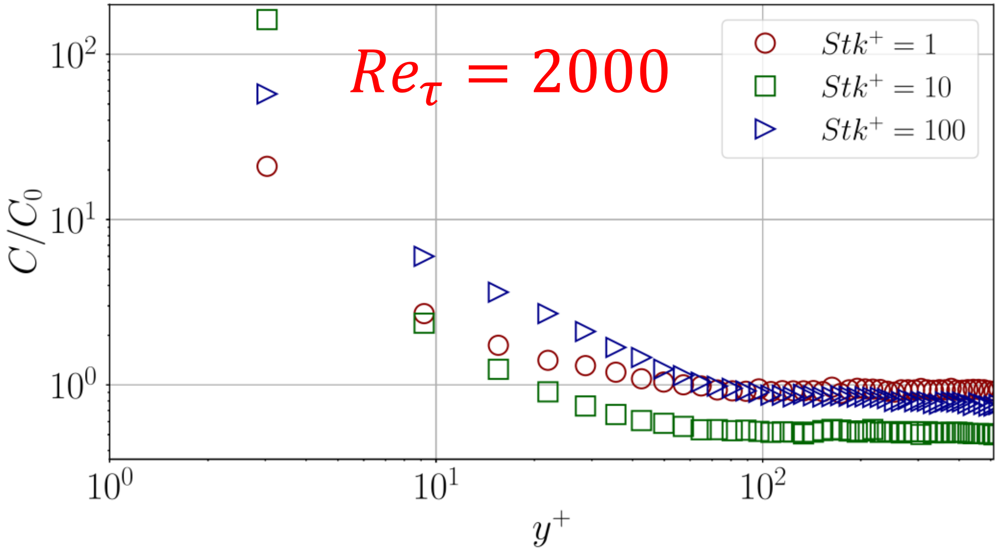


- The model can well reproduce the particle normal fluctuation distribution, especially the accurate prediction under medium and high inertia
- However, it underestimates the fluctuation level of low-inertia particles in the outer layer, which is attributed to the insufficient turbulent kinetic energy of the carrier phase in the outer layer.

Result: *Statistics of the dispersed phase* -- Mean normalized concentration of particles







- The model successfully reproduces particle near-wall accumulation, with particularly accurate predictions for low- and intermediate-inertia particles.
- However, for high-inertia particles, certain discrepancies appear in the outer-layer concentration distribution, mainly because the model does not fully capture particle inertia-memory effects and the influence of large-scale flow structures.

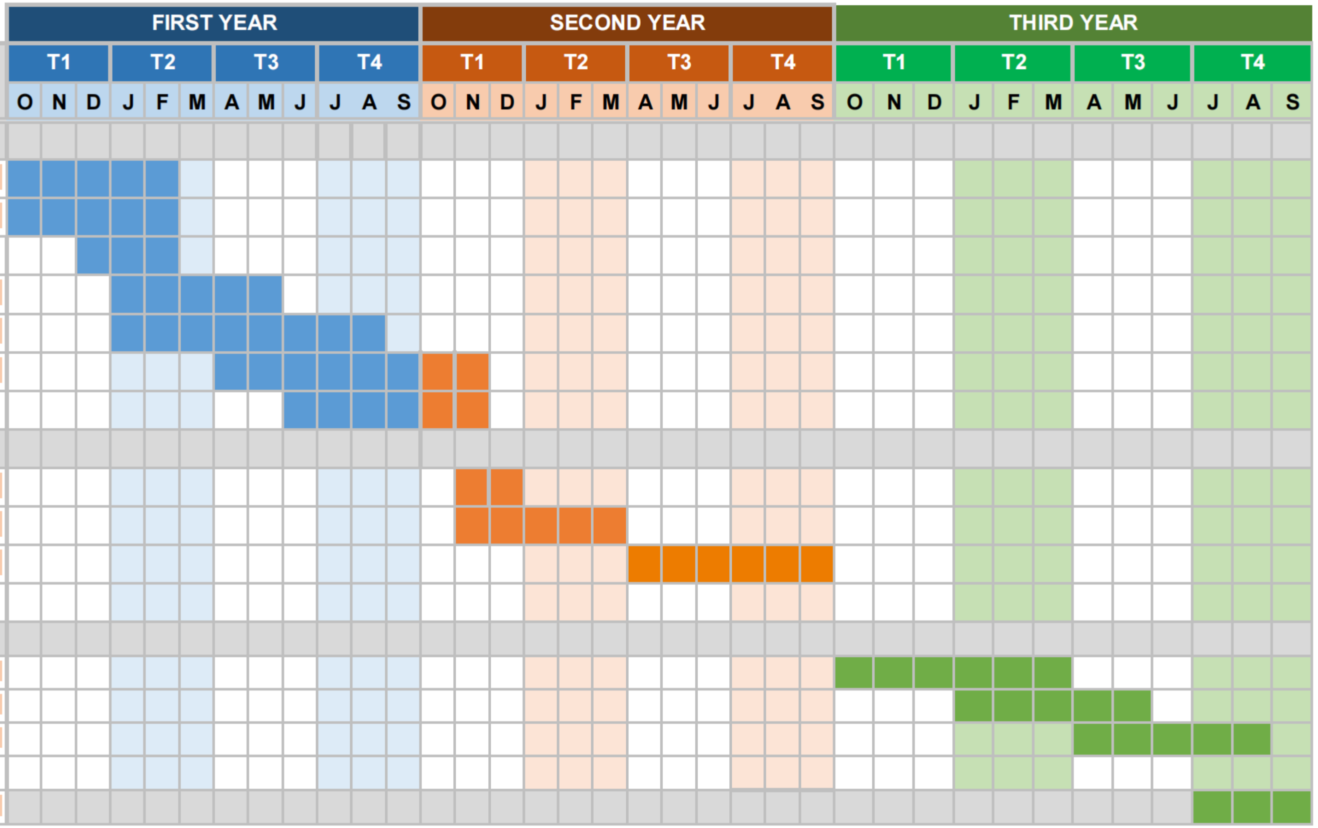
Final remarks and conclusions

- A **semi-stochastic wall-modelled LES (WM-LES)** approach was proposed for particle-laden turbulent channel flow.
- The method combines **DNS-informed lookup tables** with a **Langevin-based stochastic model** to reconstruct near-wall velocity fluctuations.
- Validated against DNS at $\boldsymbol{Re_\tau = 500, 1000}$, the model accurately predicts:
    1. Mean particle velocity (log-law region well reproduced)
    2. Velocity fluctuations (especially streamwise and wall-normal RMS)
    3. Near-wall concentration profiles (turbophoresis captured)
- **Discrepancies** remain for high-inertia particles in the outer layer due to limited resolution of WM-LES and unrepresented inertia-memory effects.
- The approach provides a **computationally efficient framework** for wall-bounded turbulent particle-laden flows at high Reynolds numbers.
- Future work: extend to **two-way coupling** and **complex geometries**.

GANTT CHART

PHD STUDENT	Xiang'en Kong	DATE	28/08/2025
PHD THESIS	High-fidelity simulation and modeling of turbulent dispersed mu	ADMISSION TO	Final Examination

WBS NUMBER	TASK TITLE	% OF TASK COMPLETE
1	Bibliographical Research	
1.1	Learning fluid mechanics and the turbulent flows theory	100%
1.2	Literature reviews on turbulent spray dynamics	100%
2	OpenFOAM Simulation	
2.1	Training for OpenFOAM	100%
2.2	Non-reactive spray simulation in LES standard	100%
2.3	Reactive spray simulation in LES standard	100%
EVENT	**Admission to Year Ⅱ**	
3	Definition of WM-LES Model and Machine-learning Algorithm for Particle Transport	
3.1	Learning the principles and algorithms of machine learning as well as deep learning	100%
3.2	Stochastic modeling for particles transport in wall-modeled Large Eddy Simulation	100%
3.3	Machine-learning algorithms for particle-laden flow near the wall	100%
EVENT	**Admission to Year Ⅲ**	
4	Definition of Machine-learning Algorithm for Spray Droplets Transport	
4.1	Machine-learning algorithms testing for particle-laden flow near the wall	100%
4.2	Machine-learning algorithms for spray droplets transport	100%
4.3	Machine-learning algorithms testing for non-reactive spray	100%
EVENT	**Admission to Final Examination**	
5	Writing Thesis and Reports	100%



Thanks for the attention

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