UNIVERSITÀ DEGLI STUDI DI PADOVA

High-fidelity simulation and modeling of turbulent sprays

Xiang'en Kong - 38th Cycle

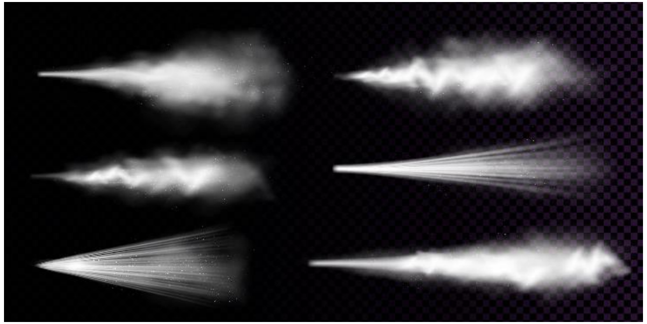
Supervisor: Prof. Francesco Picano

Co-supervisor: Prof. Federico Dalla Barba

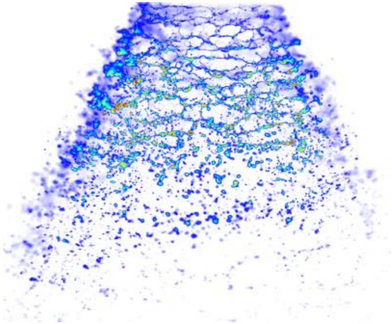
Meeting - 16/09/2024

Motivation

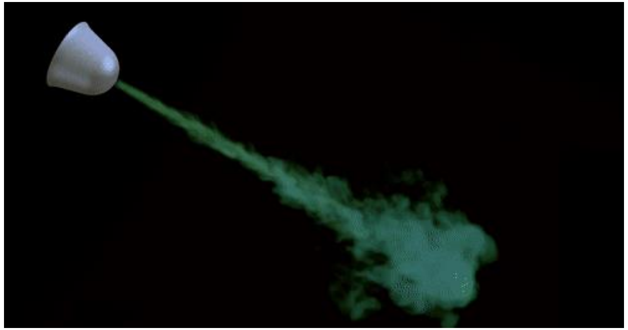
Spray:



https://www.freepik.com/free-vector/white-dust-spray-isolated-transparent-background-realistic-set-smoke-powder-with-particles-splash-from-aerosol-stream-spraying-cosmetic-fragrance-deodorant_10308169.htm

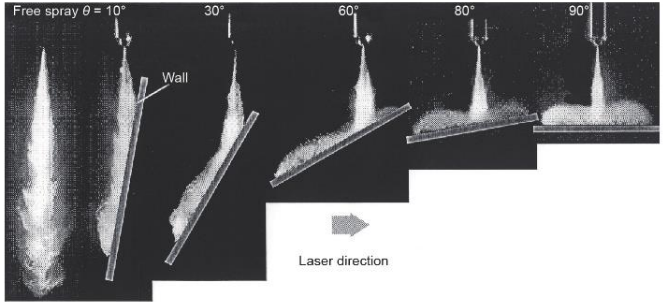


https://spray-imaging.com/

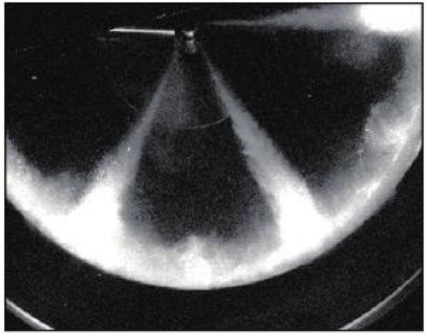


https://gfycat.com/impartialminoramericanbobtail-flamelet-generated-manifolds-large-eddy-simulation

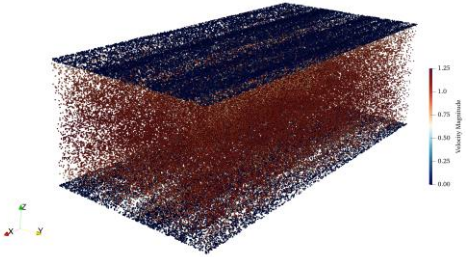
Particles in Wall-Bounded Turbulent Flows:



doi: 10.1016/j.eng.2019.04.010

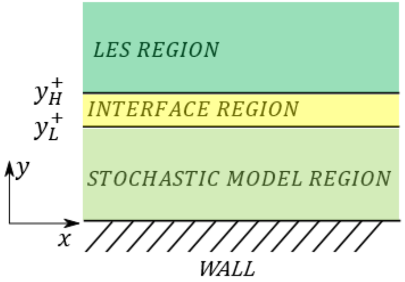


doi: 10.1016/j.eng.2019.04.010

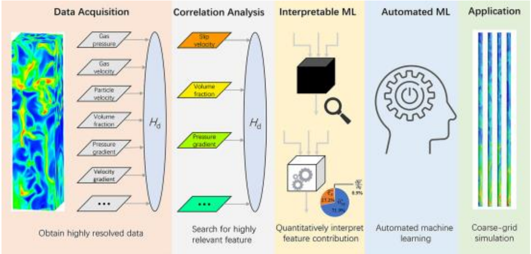


Main Tasks

Task 1:
Modeling dispersed phase transport in Wall-Model Large-Eddy-Simulations



Task 2:
Near-wall transport of dispersed multiphase flows simulation using Machine-learning algorithms



j.partic.2022.12.004

Task 3:
Simulation of dispersed multiphase flows (spray, particle-laden channel) using physics-based and machine-learning algorithms

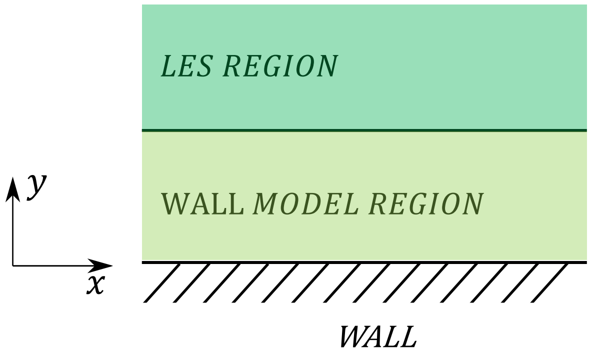
Task 1:Numerical Methodology

- **DNS:**
Accurate simulation, but very computationally expensive

- **RANS:**
Low computational cost but lack of fidelity

- **LES:**
Better accuracy than RANS but high computational cost for high Reynolds numbers wall bounded flows

- **Wall-Model Large-Eddy-Simulations (WM-LES)**
Better accuracy than RANS with lower computational cost at wall than LES



Task 1:Parameter Setting for Simulation

WM-LES

- $N_x \times N_y \times N_z = 48 \times 48 \times 48$ LOW RES!!!
- $L_x \times L_y \times L_z = 6h \times 2h \times 3h$
- $Re_\tau = 1000$
- $N_p = 300000$
- $St^+ = 1, 10, 100$
- Wall-modelled layer $y^+ < 100$ both for carrier and discrete phase (below 2.5 nodes)

$$Re_\tau = \frac{u_\tau h}{v} \qquad St^+ = \frac{\tau_p}{\tau^+}$$

PRELIMINARY REFERENCE DNS

- $N_x \times N_y \times N_z = 1216 \times 512 \times 640$
- $L_x \times L_y \times L_z = 10h \times 2h \times 3h$
- $\Delta y^+_{min} \simeq 0.5$
- $Re_\tau = 1000$
- $N_p = 300000$
- $St^+ = 1, 10, 100$

Task 1:WM-LES Approach

Navier-Stokes (incompressible) (WM-LES)

$$\nabla \cdot \tilde{\boldsymbol{u}} = 0$$

$$\rho \frac{\partial \tilde{u}}{\partial t} = -\nabla p + \nabla \cdot \left[2(\mu + \mu_{SGS}) \tilde{E} \right]$$

μ_{SGS}: Sub-grid viscosity with **WALE**

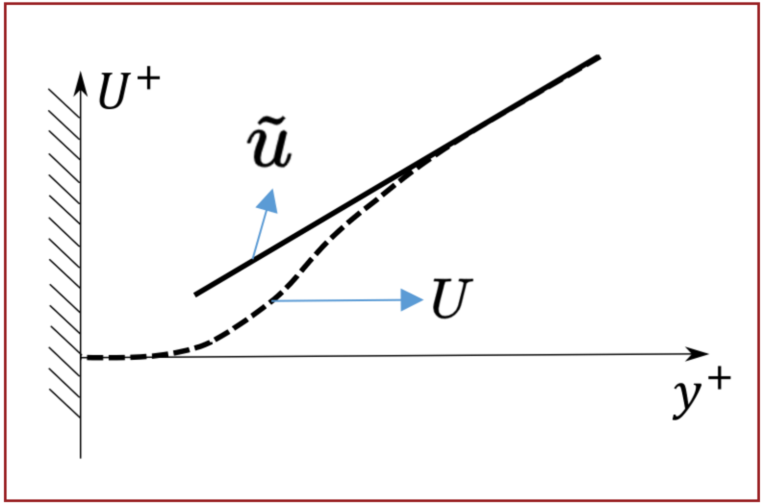
$\tilde{E}$: Deformation tensor

Lagrangian Point-particle equations

$$\frac{dv}{dt} = f_p \frac{u - v}{\tau_p} \qquad u = \tilde{u} + u''$$

If $u'' = 0$, SGS fluctuation is neglected

Algebraic Wall-model



Task 1:WM-LES Stochastic model

Lagrangian Point-particle equations

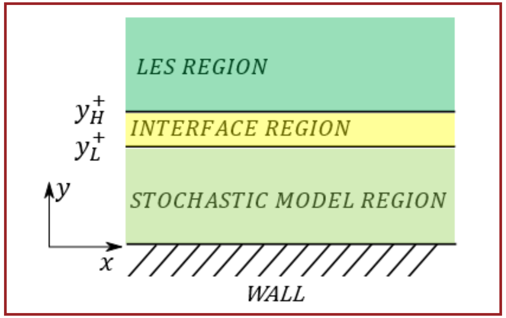
$$\frac{dv}{dt} = f_p \frac{u - v}{\tau_p}$$

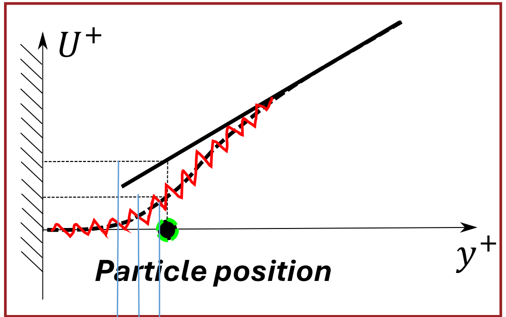
$$u = U + u_{STO}$$

$$f_p = 1 + 0.15 Re_p^{0.687}$$

$$Re_p = \frac{2||u - v||r_p}{\nu}$$

- u fluid velocity at particle
- v point-particle velocity
- U averaged fluid velocity fields
- u_{STO} stochastic velocity fluctuations at the particle positions
- τ_p particle relaxation time
- SGS fluctuations are neglected





The normalized Langevin equations

$$d\left(\frac{u_{STO}}{\sigma_x}\right) = -\left(\frac{u_{STO}}{\sigma_x}\right)\frac{dt}{\tau_l} + \sqrt{\frac{2}{\tau_l}}d\xi_x + \frac{\partial\left(\frac{\overline{uv}}{\sigma_x}\right)}{\partial y}\frac{dt}{1+St}$$

$$d\left(\frac{v_{STO}}{\sigma_y}\right) = -\left(\frac{v_{STO}}{\sigma_y}\right)\frac{dt}{\tau_l} + \sqrt{\frac{2}{\tau_l}}d\xi_y + \frac{\partial\sigma_y}{\partial y}\frac{dt}{1+St}$$

$$d\left(\frac{w_{STO}}{\sigma_z}\right) = -\left(\frac{w_{STO}}{\sigma_z}\right)\frac{dt}{\tau_l} + \sqrt{\frac{2}{\tau_l}}d\xi_z$$

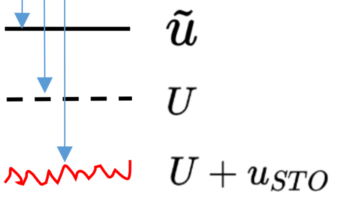
$\sigma_x, \sigma_y, \sigma_z$ RMS of velocity fluctuations

Drift correction terms

$St = \tau_p/\tau_l$

Lagrangian time scale

Gaussian random numbers with zero mean and variance dt

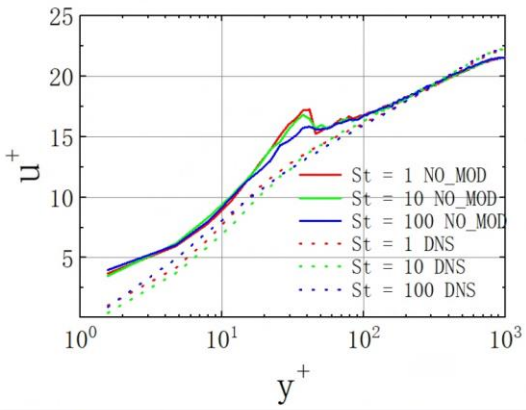


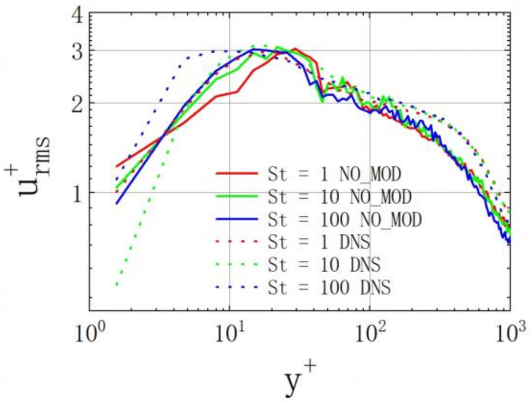
$$u_{CMB} = \sqrt{\alpha}u_{LES} + (1 - \sqrt{\alpha})u_{AVG} + \sqrt{1-\alpha}u_{STO}$$

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.

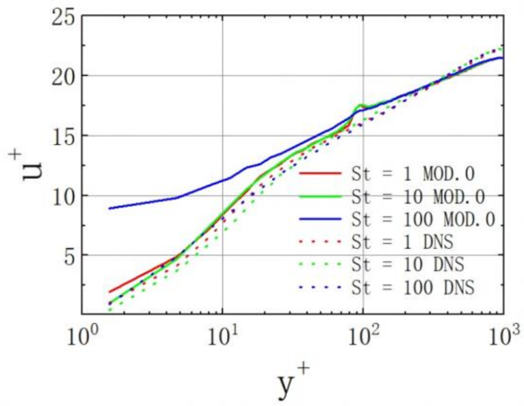
Task 1: Velocity Statistics

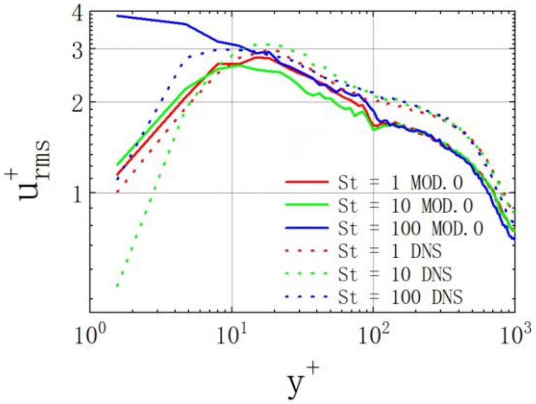
NO MODEL





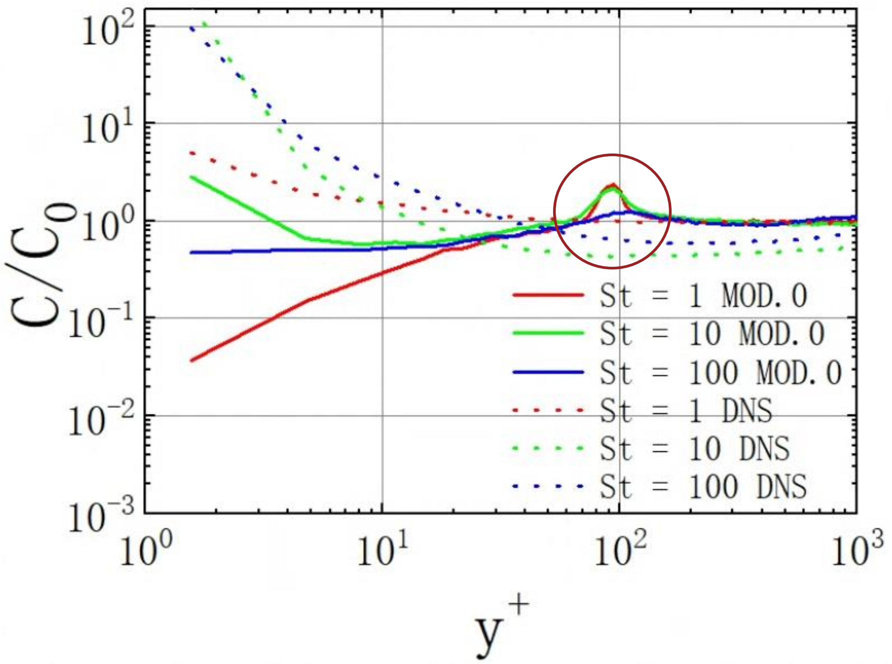
STOCHASTIC MODEL

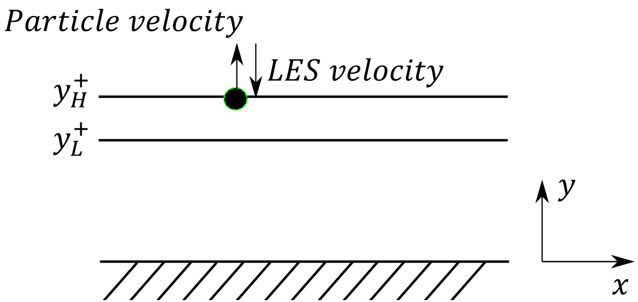




- For all Stokes numbers, there are apparent difference in velocity and u_{RMS} !

Task 1:STOCHASTIC MODEL CONCENTRATION

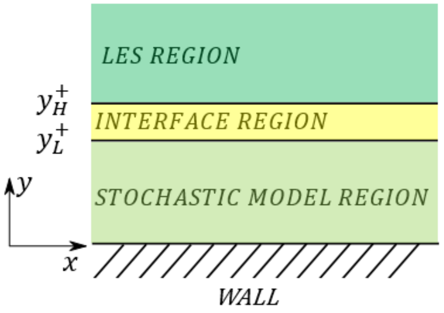


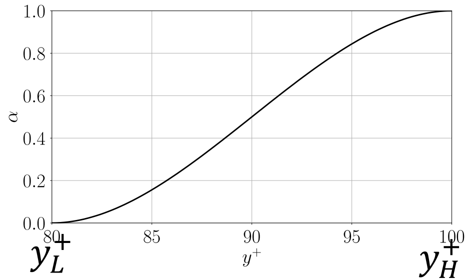


Particles going outside of interface may encounter fluid velocity fluctuations with opposite sign (phase opposition) thus stopping the particles at the interface for longer time!

In the interfacial region, the normalized concentrations of all Stokes peaked and deviated from DNS results!

Task 1:WM-LES—A Semi-stochastic Approach 1/2





$$\alpha = \begin{cases} 1, & y^+ \geq y_H^+ \\ 3t^2 - 2t^3, & y_L^+ \leq y^+ < y_H^+ \\ 0, & y^+ < y_L^+ \end{cases}$$

$$t = 1 + \frac{\left(y^+ - y_L^+ - (y_H^+ - y_L^+)\right)}{y_H^+ - y_L^+}$$

For streamwise and spanwise velocity

$$\frac{dv}{dt} = f_p \frac{u - v}{\tau_p}$$

$$f_p = 1 + 0.15 Re_p{}^{0.687}$$

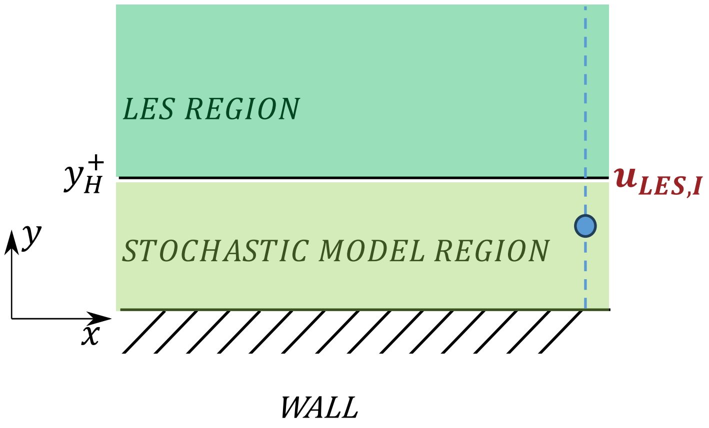
$$Re_p = \frac{2||u - v||r_p}{\nu}$$

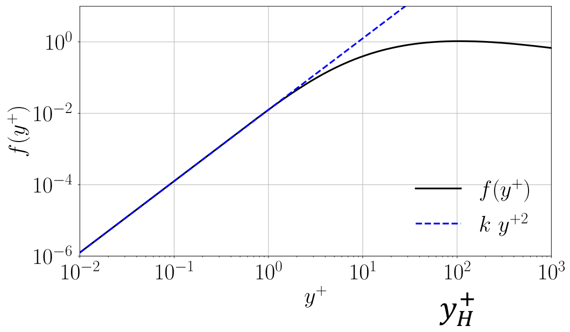
$$u = \begin{cases} \tilde{u} + u'', & y_p^+ \geq y_H^+ \\ u_{CMB}, & y_L^+ \leq y_p^+ < y_H^+ \\ U + u_{STO}, & y_p^+ < y_L^+ \end{cases}$$

$$u_{CMB} = \sqrt{\alpha}\tilde{u} + \left(1 - \sqrt{\alpha}\right)U + \sqrt{1 - \alpha} u_{STO}$$

The difference between previous and present model lies in the method of calculating normal velocity.

Task 1:WM-LES—A Semi-stochastic Approach 2/2





For normal velocity: Modulated from the interface LES value

$$\frac{dv}{dt} = f_p \frac{u-v}{\tau_p}$$

$$f_p = 1 + 0.15 {Re_p}^{0.687}$$

$$Re_p = \frac{2||u-v||r_p}{\nu}$$

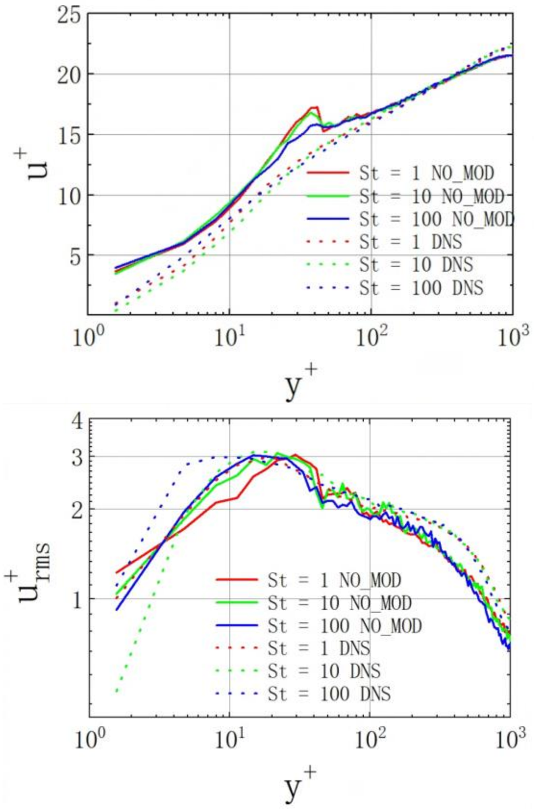
$$u = \begin{cases} \tilde{u} + u'', & y_p^+ \geq y_H^+ \\ u_{FUN}, & y_p^+ < y_H^+ \end{cases}$$

$$u_{FUN} = f(y_p^+) u_{LES,I} + k f(y_p^+) \frac{df(y^+)}{dy^+}\bigg|_{y_p^+} \frac{\Delta t}{1+St^+} + N$$

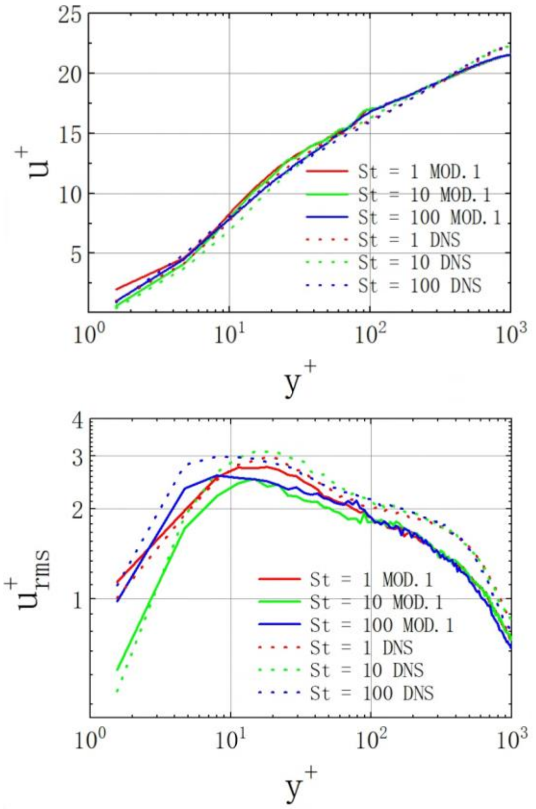
- $u_{LES,I}$ interpolated from LES velocity field at the interface at y_H^+ (above particle)
- Function $f(y^+)$ such that:
  - $f(y_H^+) = 1$
  - Quadratic trend near zero
  - Derivative modulated by Stokes $St^+ = \tau_p/\tau^+$

Task 1: SEMI-STOCHASTIC—Velocity Statistics

NO MODEL

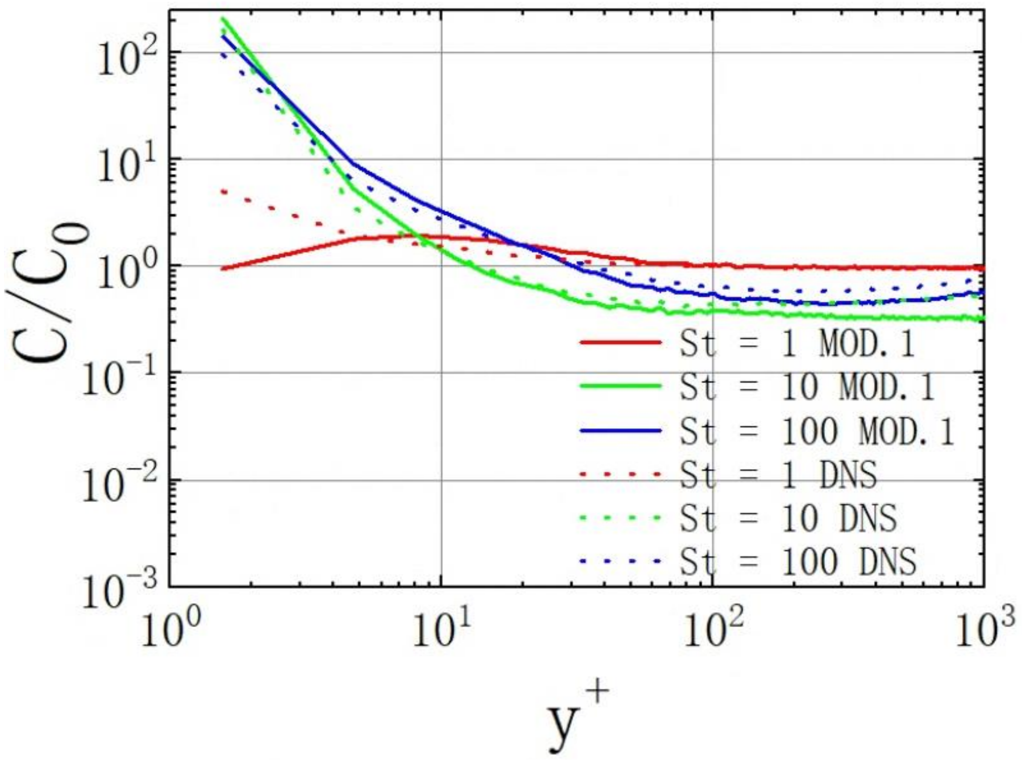


SEMI-STOCHASTIC



- Much better agreement!
- OBS: Lower velocity statistics due to low resolution in LES!

Task 1:SEMI-STOCHASTIC – Concentrations



- Much better agreement of normalized concentrations!

Summary of The Research Activity & Perspective Plan

I. We developed a model for the near-wall numerical treatment of point-particle/droplet-laden flows in Wall-Modelled Large Eddy Simulation (WM-LES). Models **blending a stochastic approach**, i.e. the Langevin equations, **with properly rescaled LES velocity fields along the wall-normal direction**

II. A machine learning model will be developed for the high-fidelity simulation of **particle-laden flow near the wall**

III. A machine learning model will be developed for the high-fidelity simulation of **turbulent sprays**

GANTT CHART

PHD STUDENT	Xiang'en Kong	DATE	06/09/2024
PHD THESIS	High-fidelity simulation and modeling of turbulen	ADMISSION TO	Year Ⅲ

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	30%
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	0%
4.2	Machine-learning algorithms for spray droplets transport	0%
4.3	Machine-learning algorithms testing for non-reactive spray	0%
EVENT	**Admission to Final Examination**	
5	Writing Thesis and Reports	0%

Thanks for the attention

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