Inertial particles in wall-bounded turbulence: turbophoresis, wall-modeled large-eddy simulations, and super-particle collisions

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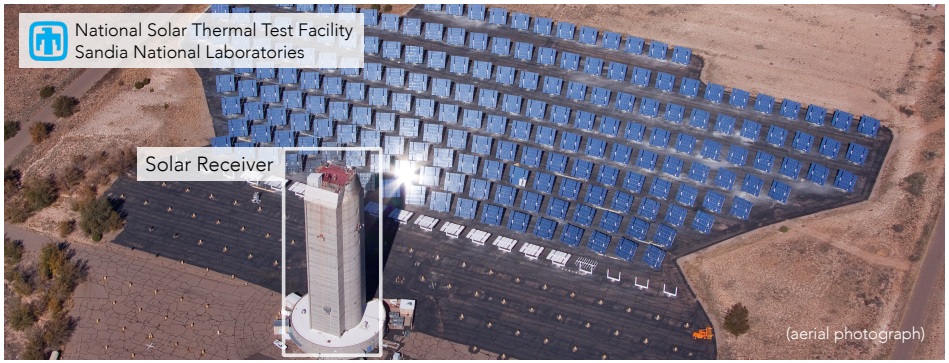
Stanford PSAAP II (https://exascale.stanford.edu)

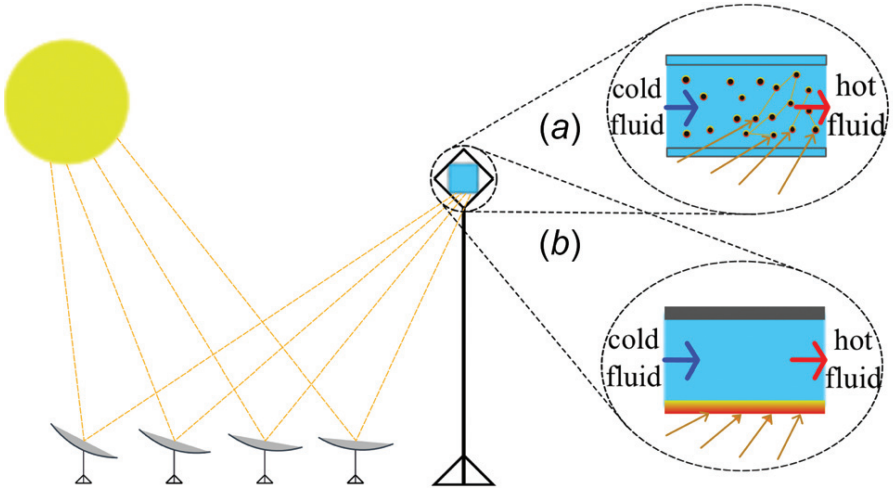
Predictive **S**cience **A**cademic **A**lliance **P**rogram

Concentrated solar power



Crescent Dunes Solar Energy Facility (Nevada)

Particle-based solar receivers

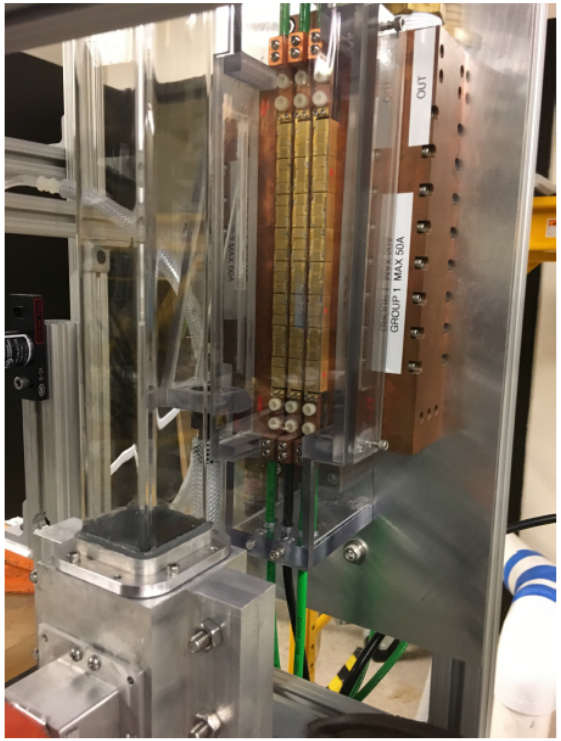


Pouransari & Mani (2017)

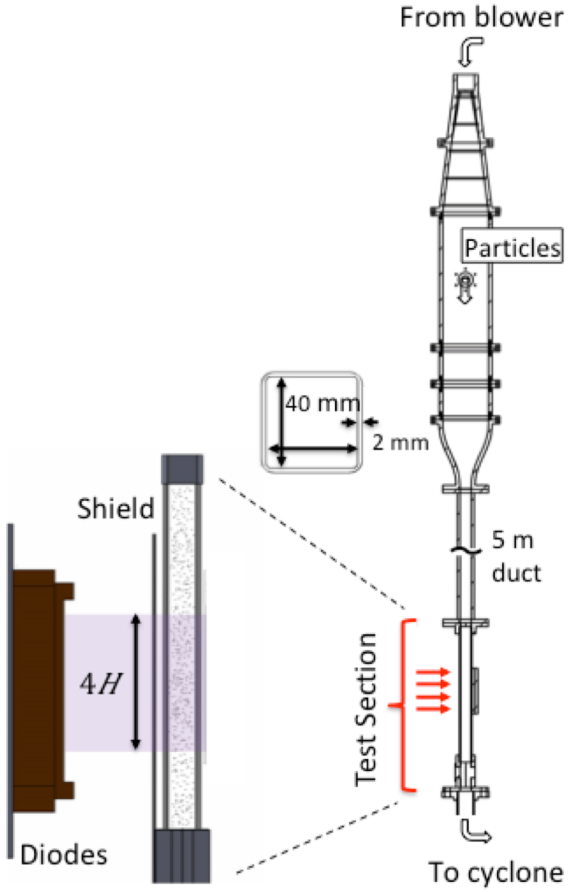
Predictive multiphysics simulations

- fluid dynamics (turbulence)
- radiation
- particle transport

Lab-scale experiment



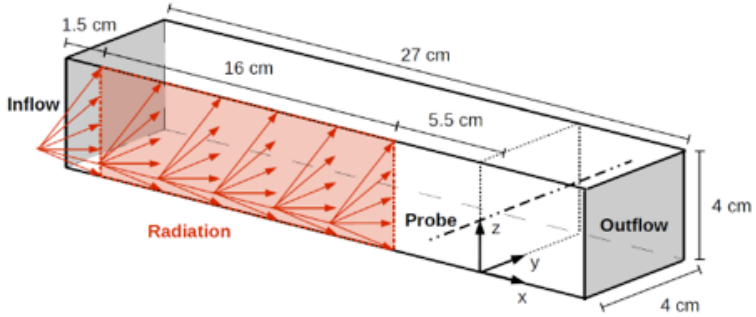
- Air flow duct
  - 4 cm square duct
  - $U_{bulk} \approx 8$ m/s
  - $Re_\tau \approx 600$
- Nickel particles
  - $d_p \approx 8$ - 15 μm
  - $d_p^+ \approx 0.2$ - 0.4
  - $St^+ \approx 20$ - 60
- Laser diode array
  - 1 - 2 kW



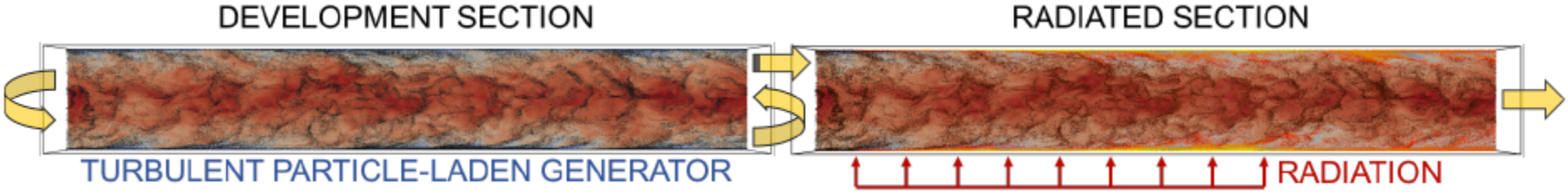
Close experimental-computational collaboration for modeling & validation.

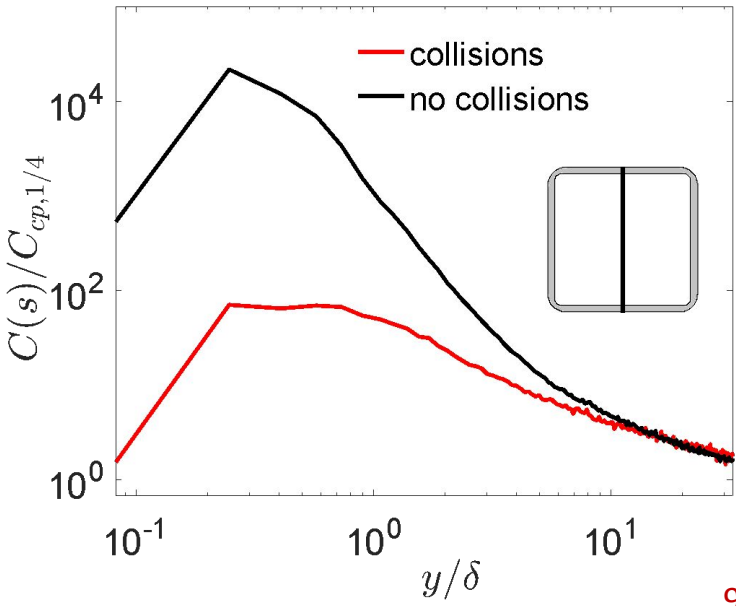
- particle concentration
- gas & particle velocities
- gas temperature
- radiation transmission

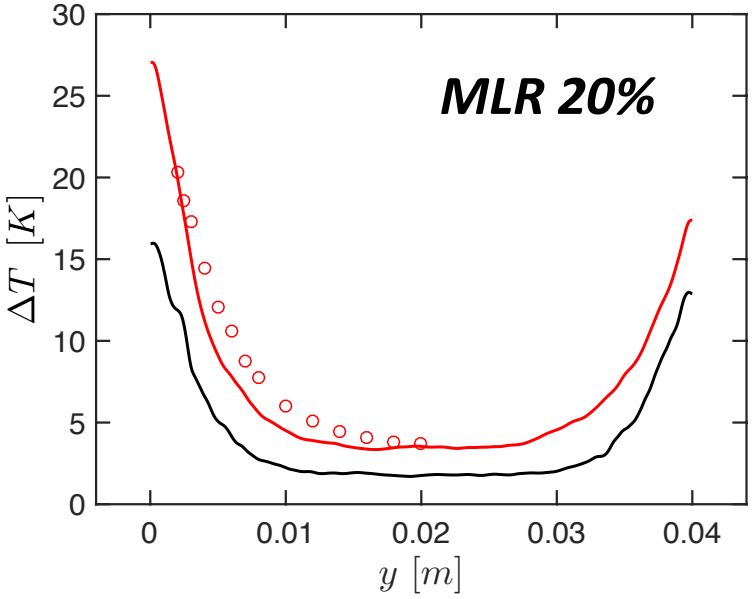
Validation: DNS with point-particles



- staggered Cartesian mesh (2nd order)
- low Mach compressible
- point-particle, Schiller-Naumann drag
- discrete ordinates method (DOM)







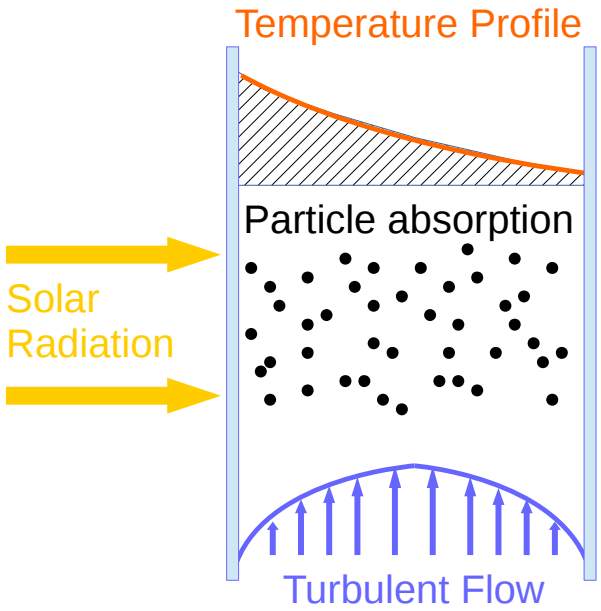
Outline

1. Turbophoresis
2. Wall-modeled LES
3. Super-particle collisions

Particle-based solar receivers

- Radiation absorbed by suspended particles
- Ideal case, uniform $n(x)$:

$$\boxed{I(x) = I_0 \exp(-\sigma n A_p x)}$$



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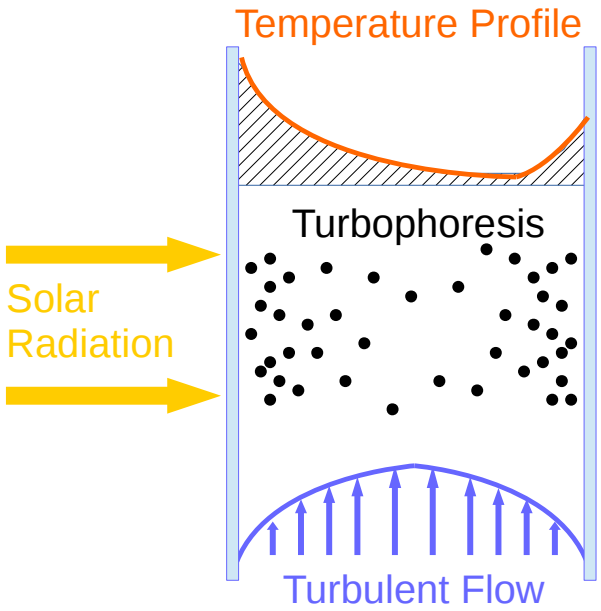

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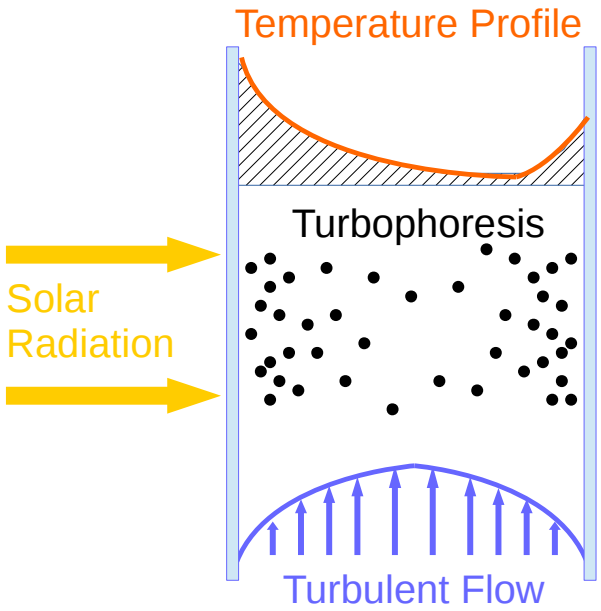
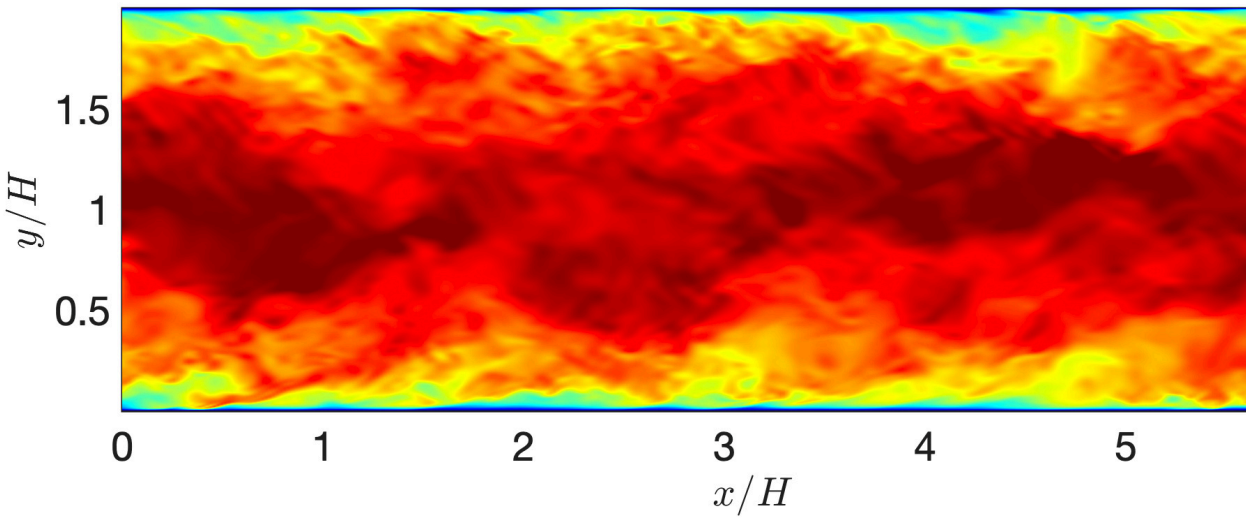


Turbophoresis: the tendency for particles to migrate in the direction of decreasing turbulence level (Caporaloni 1975; Reeks 1983)

- in a wall-bounded flow, particles migrate toward walls

Turbophoresis in a channel flow

- Particles: $\frac{d\mathbf{v}}{dt} = \frac{\mathbf{u}-\mathbf{v}}{\tau_p}$, where $\tau_p = \frac{\rho_p d_p^2}{18\mu_f}$; define $St^+ = \tau_p^+$



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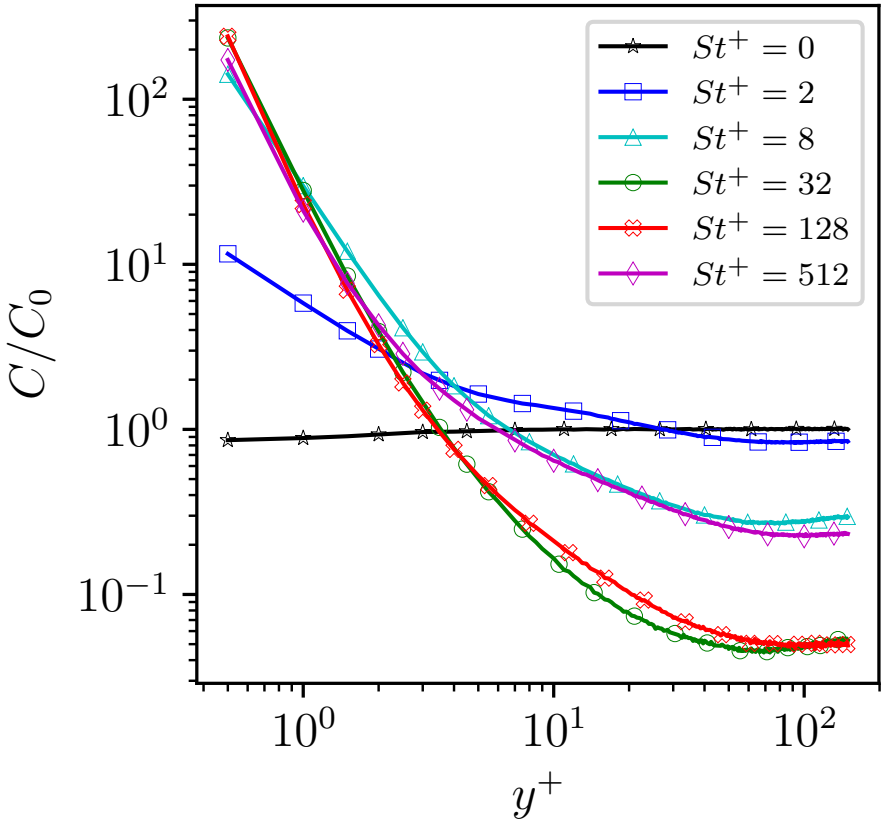

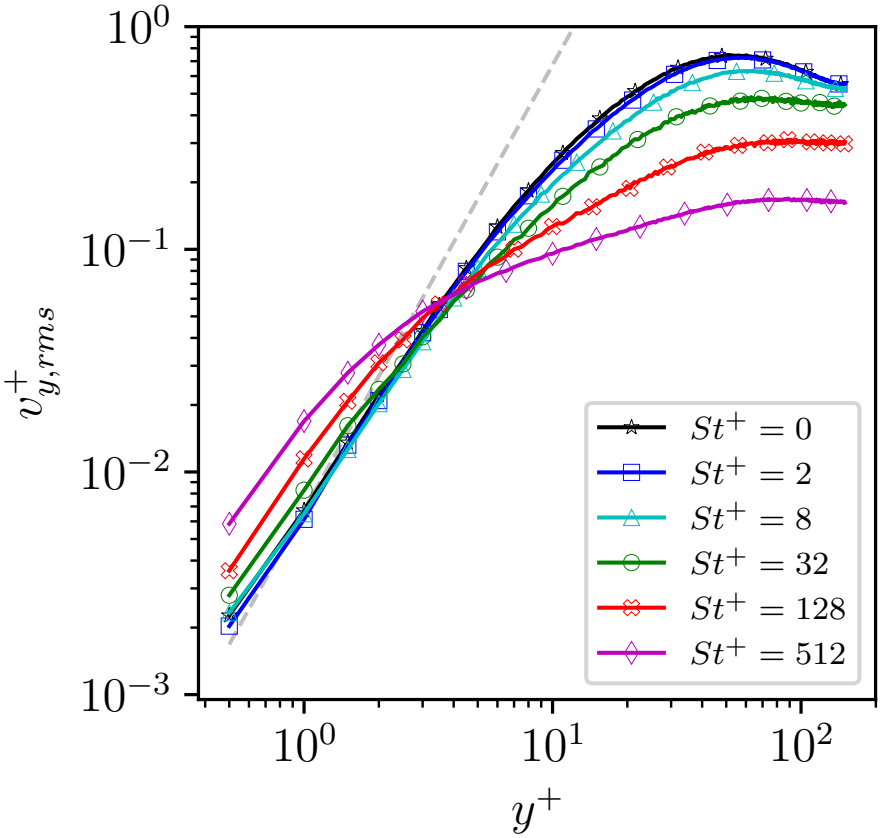

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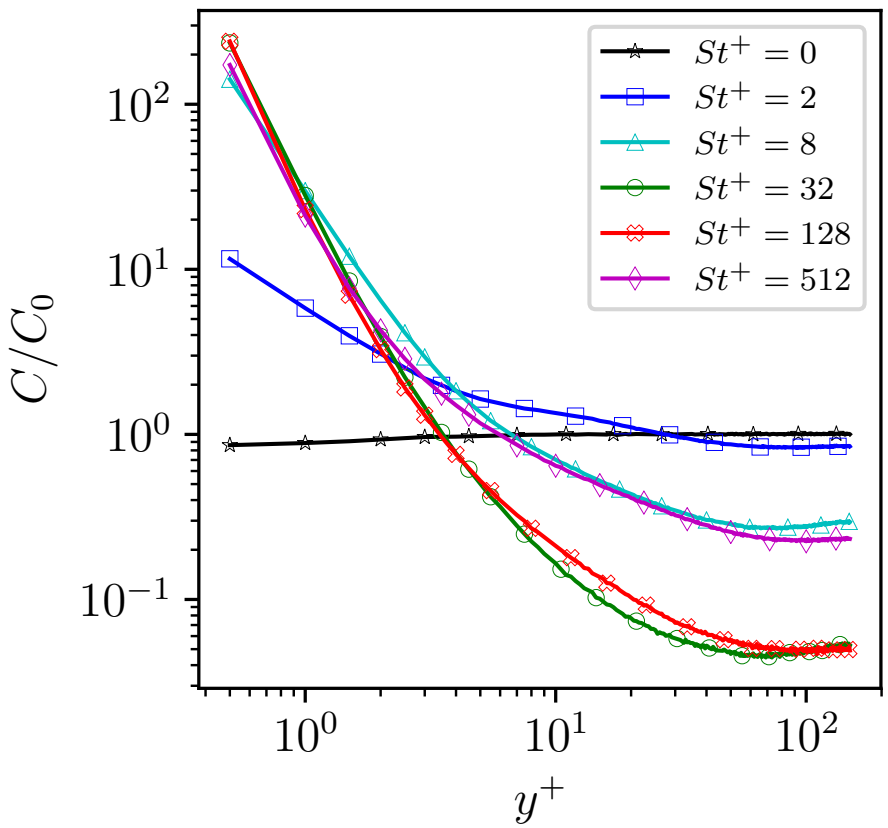

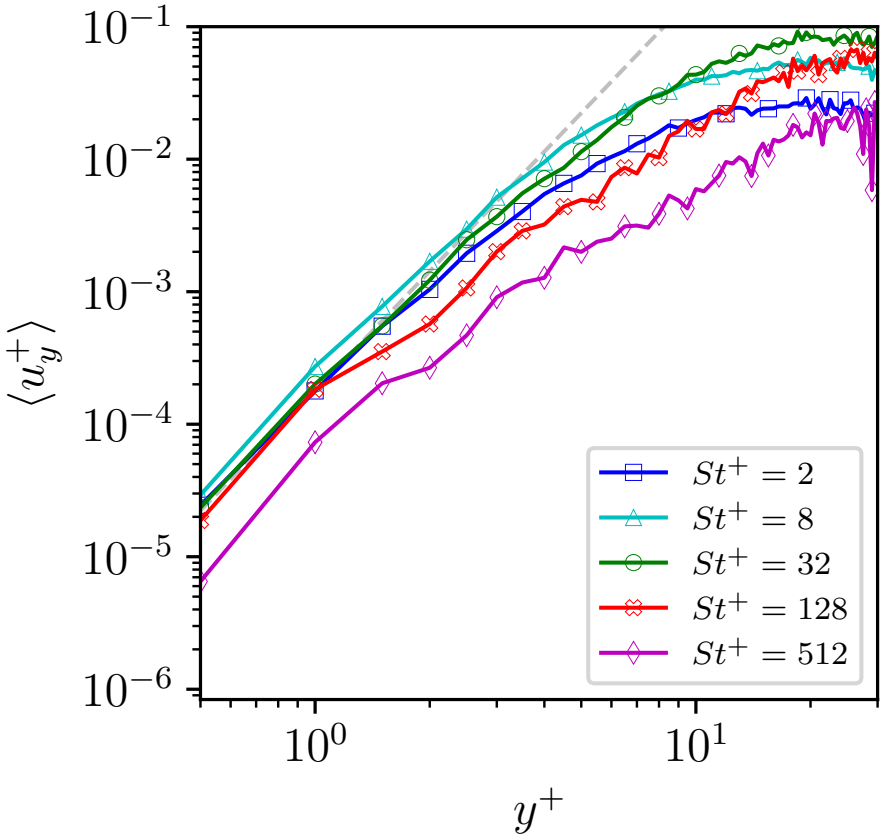

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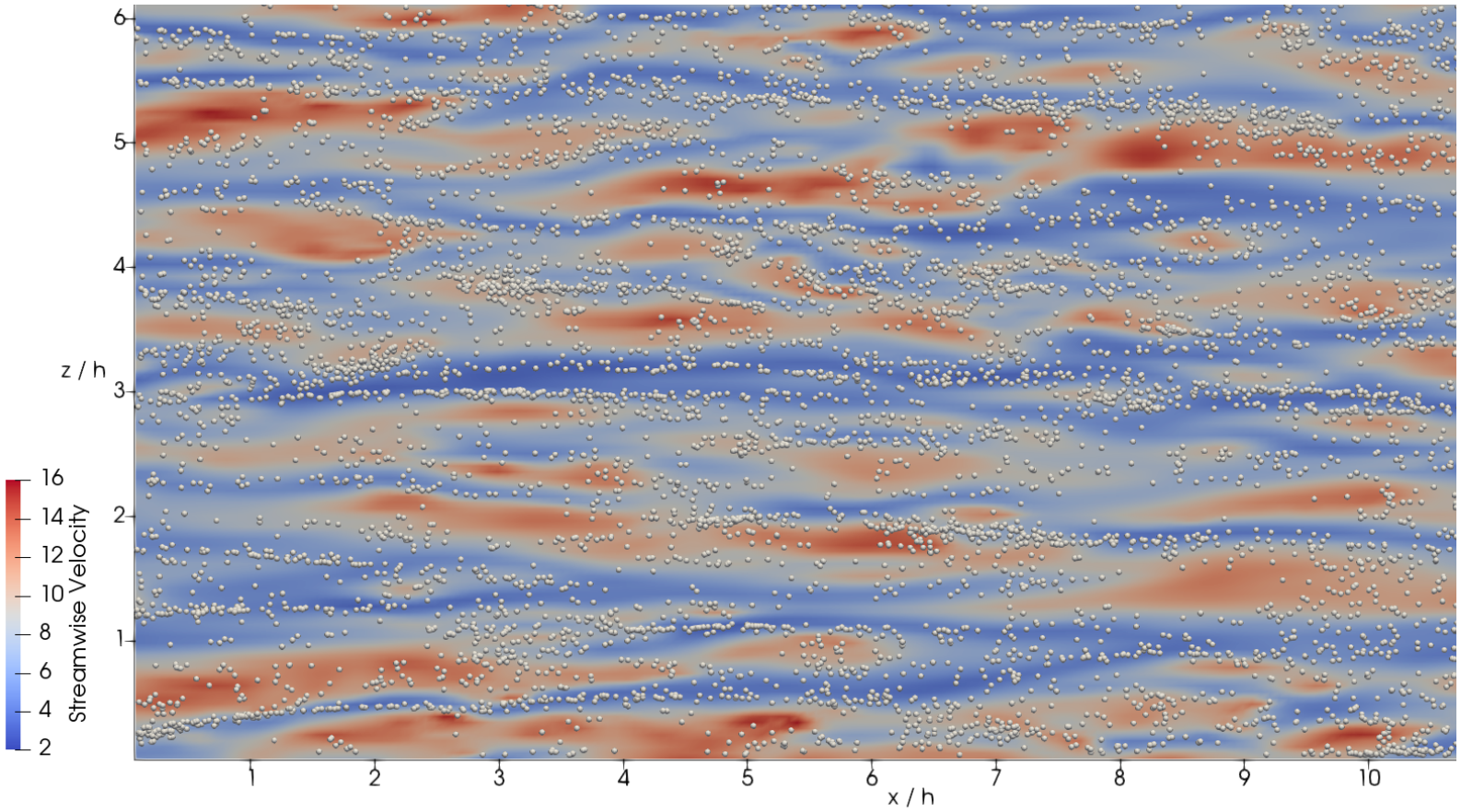

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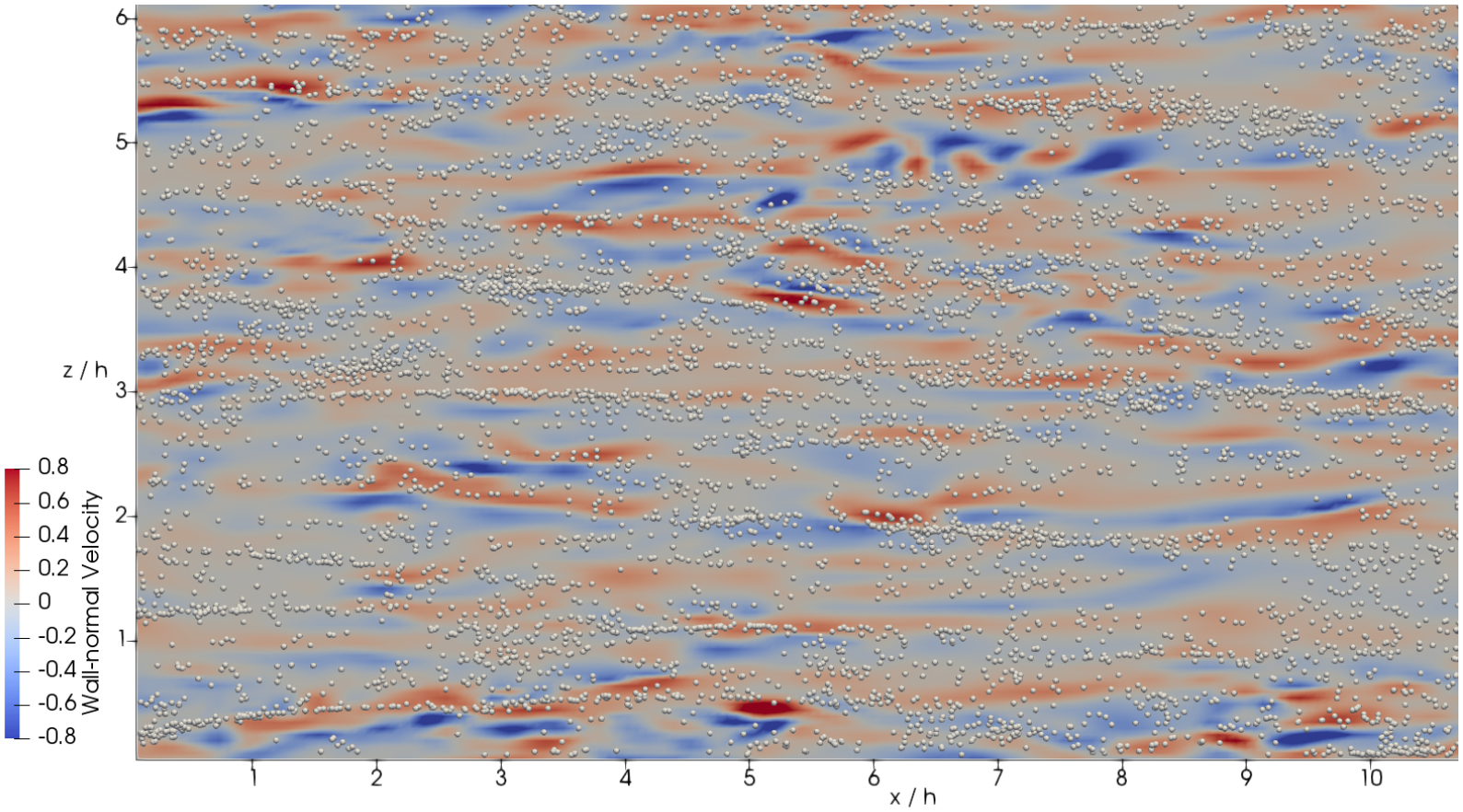

Turbophoresis vs. biased sampling

- Formal solution of momentum conservation:

$$C(y) = \mathcal{N} \exp \left(\underbrace{\frac{1}{\tau_p} \int^y \frac{\langle u_y | \eta \rangle}{\langle v_y^2 | \eta \rangle} d\eta}_{\text{biased sampling}} - \underbrace{\int^y \frac{d \ln \langle v_y^2 | \eta \rangle}{d\eta} d\eta}_{\text{turbophoresis}} \right)$$

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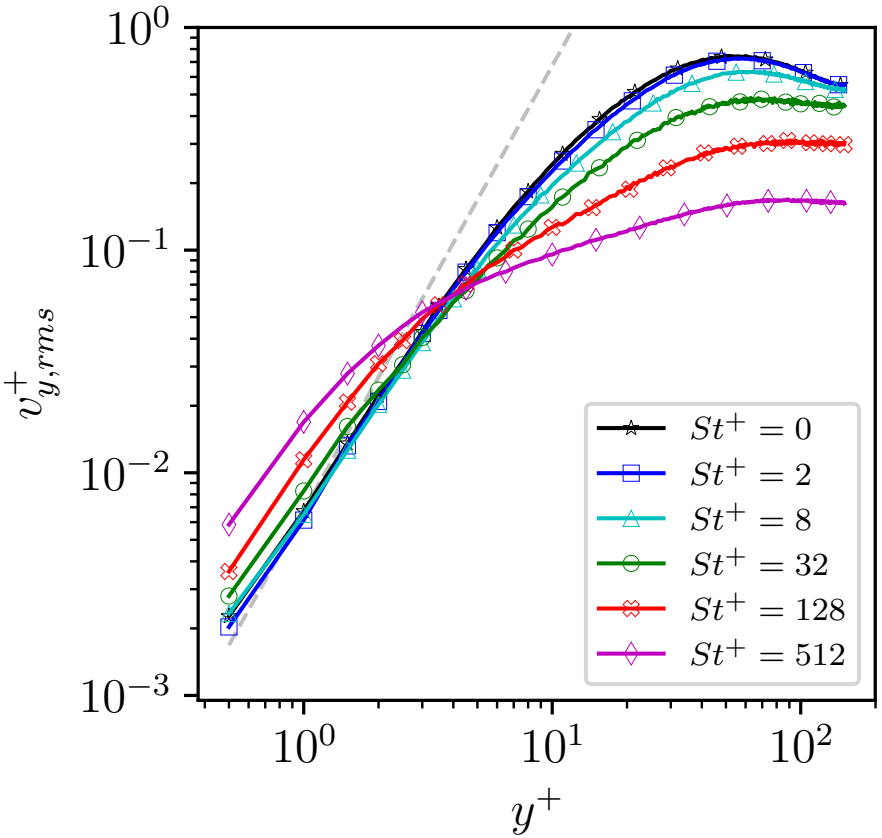

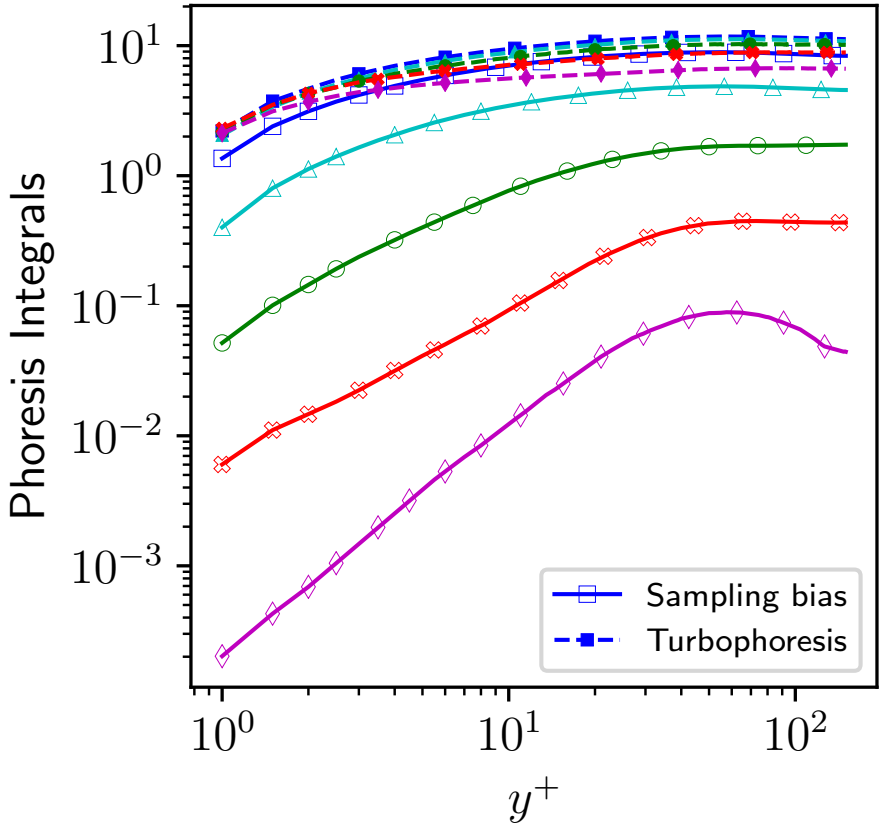

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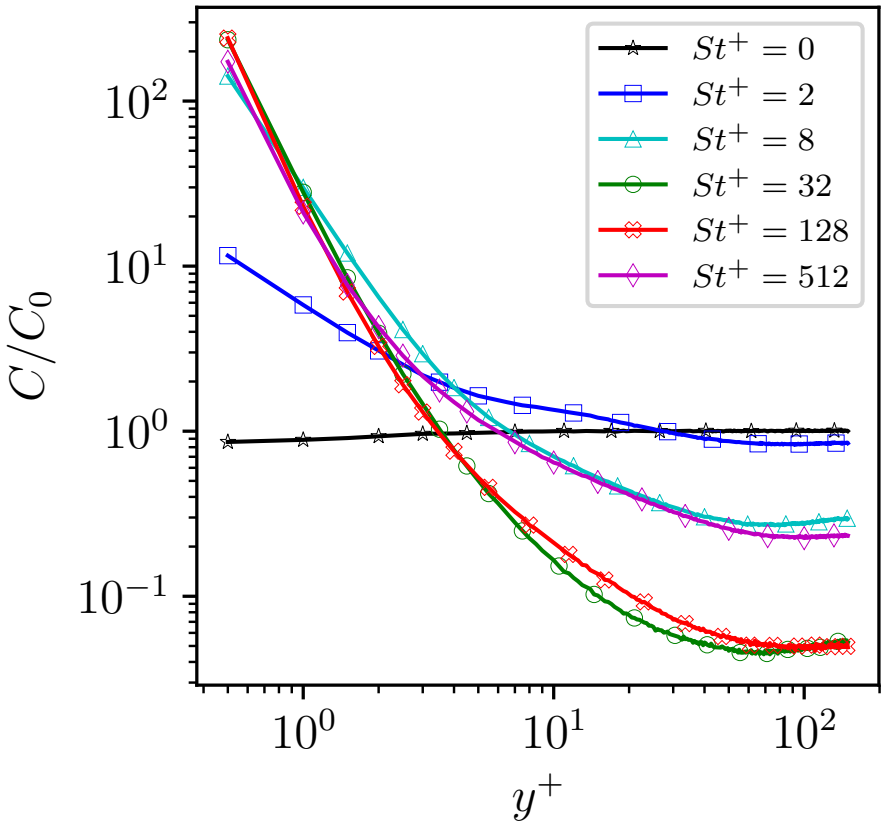

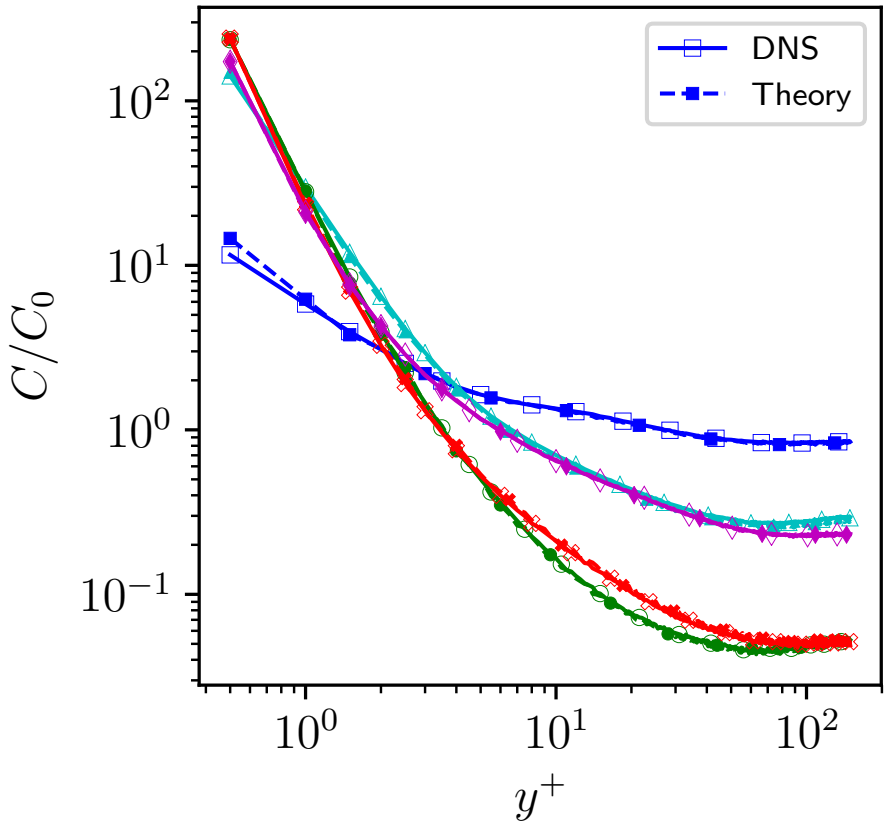

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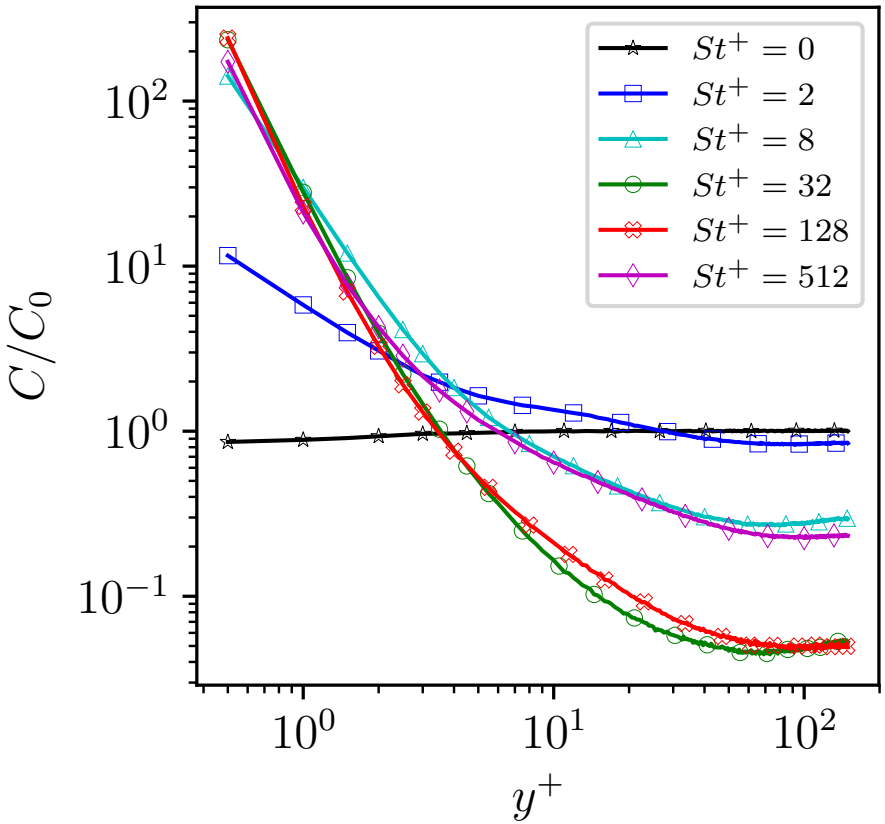

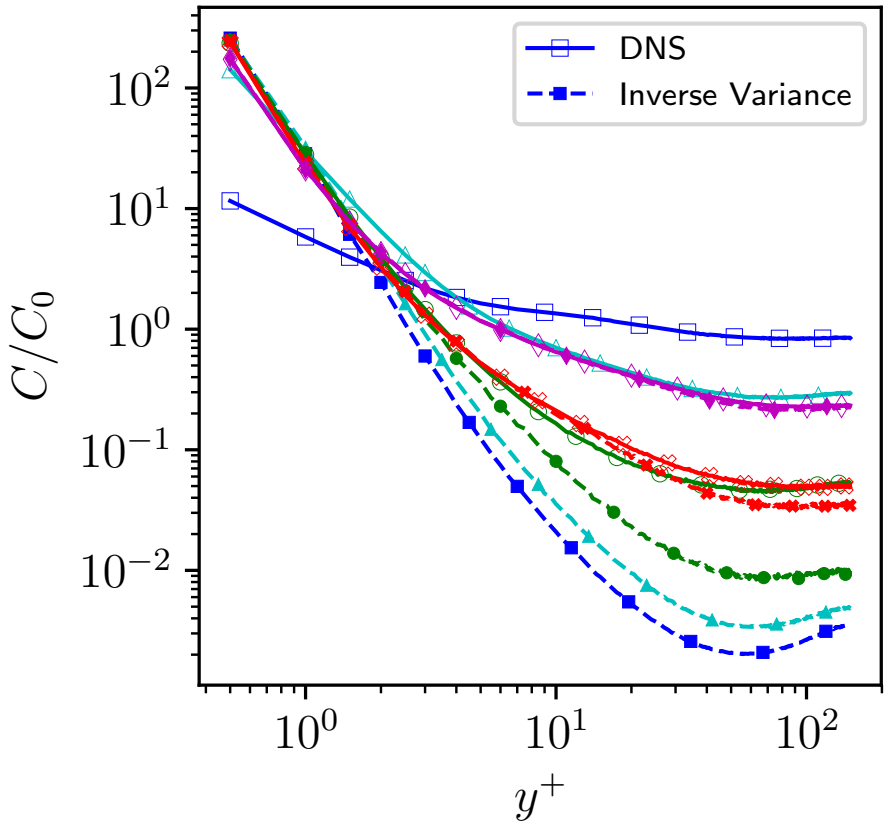

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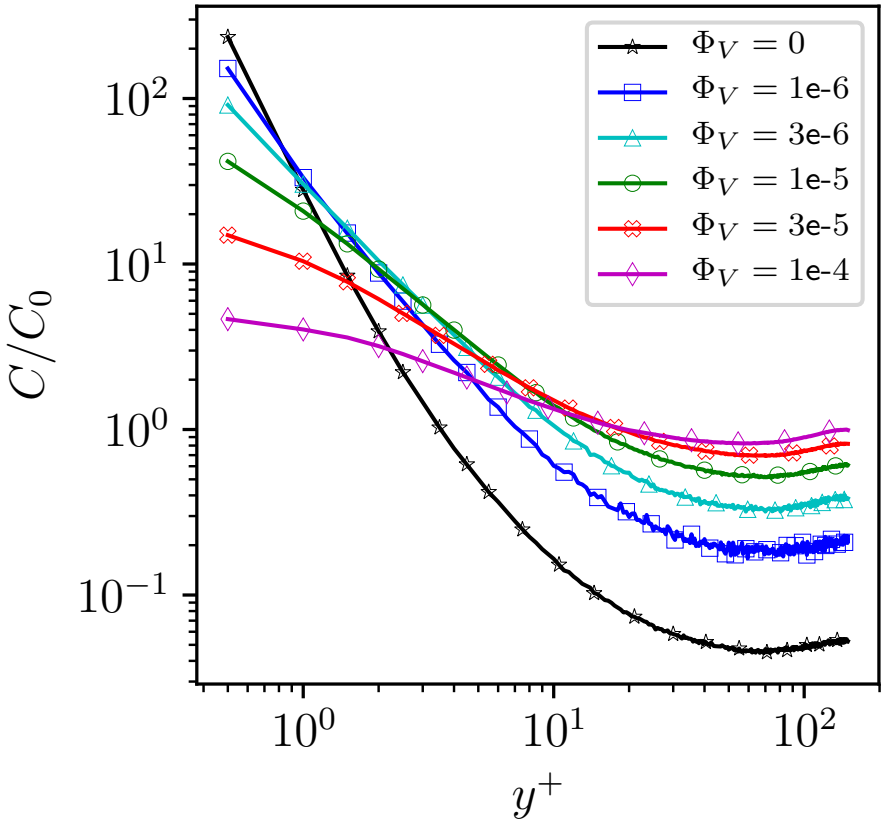

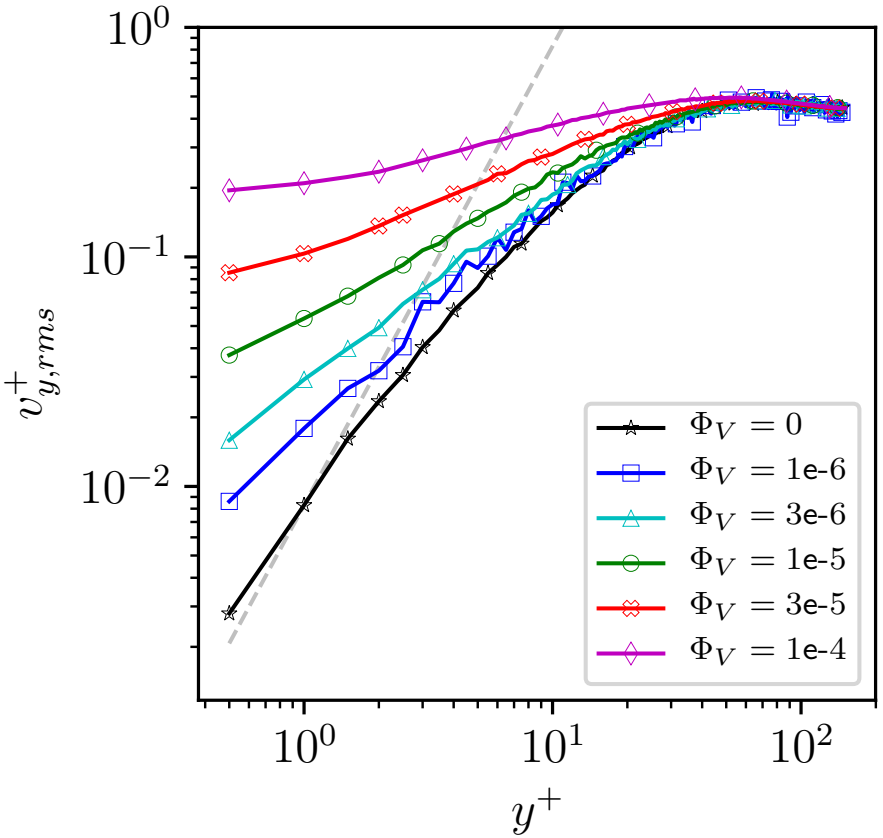

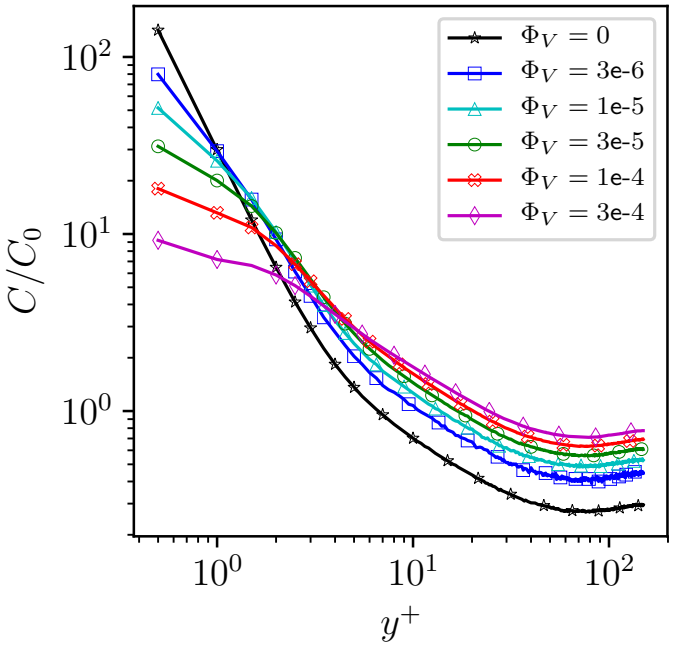

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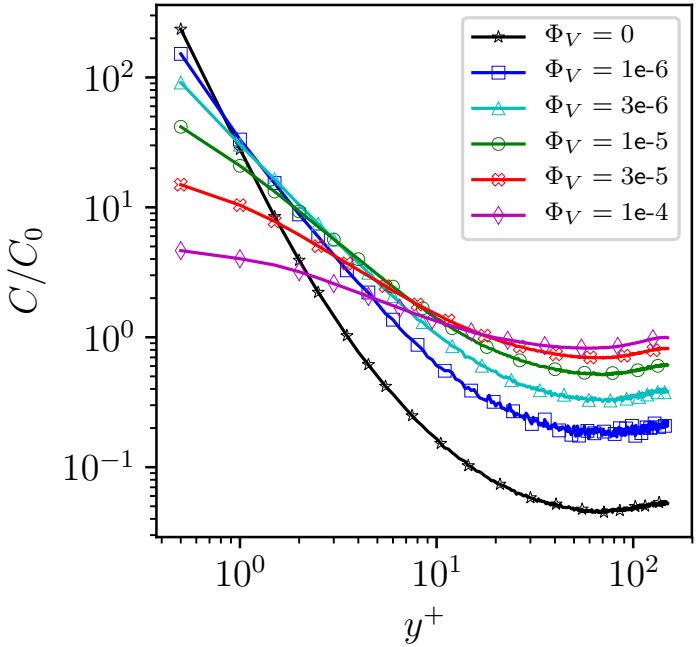

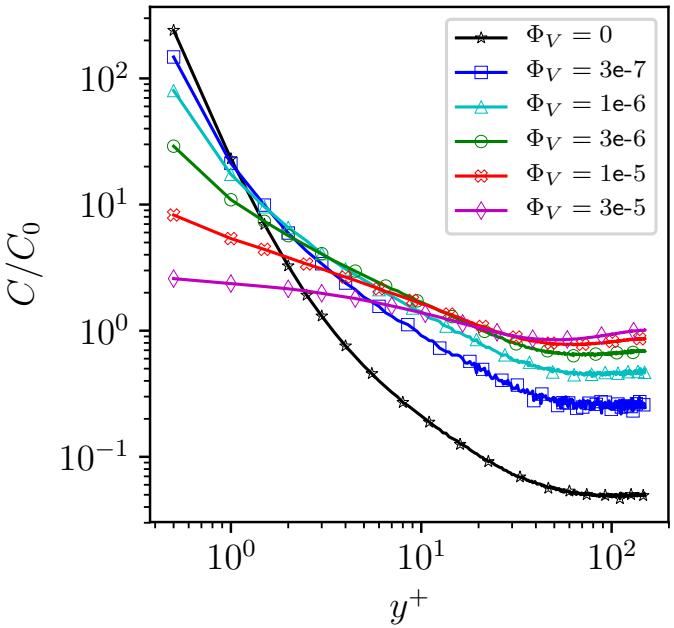

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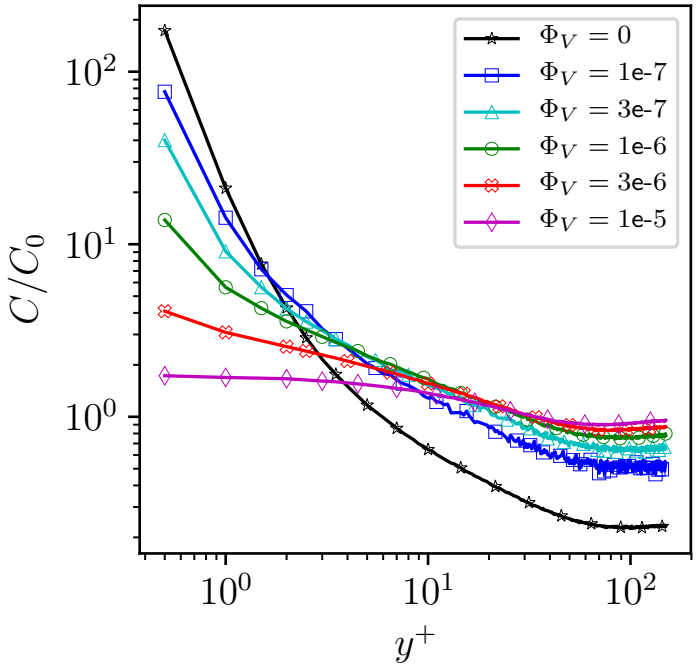

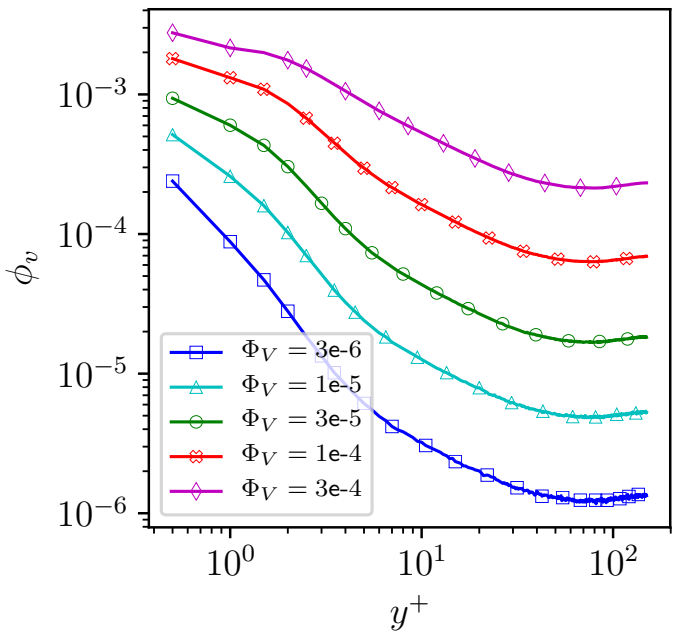

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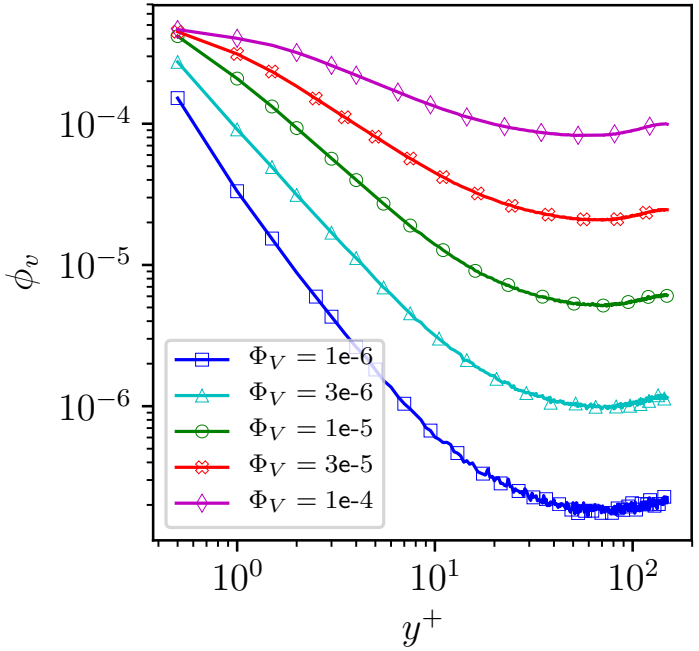

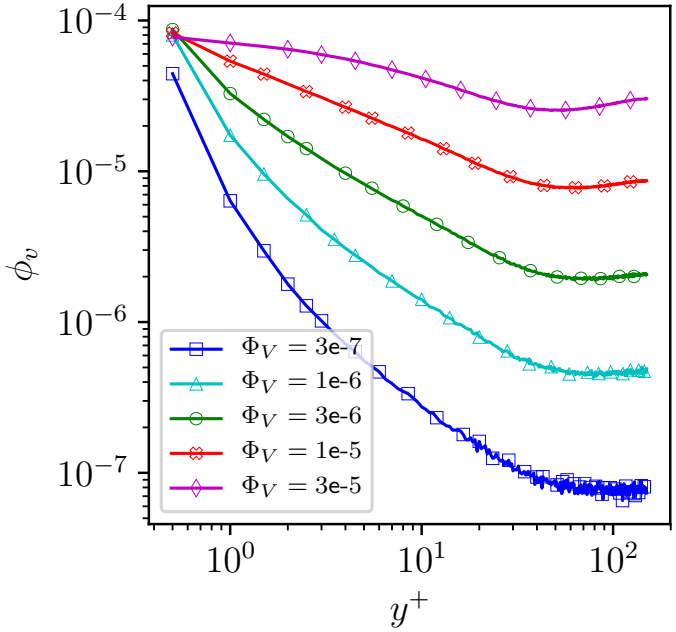

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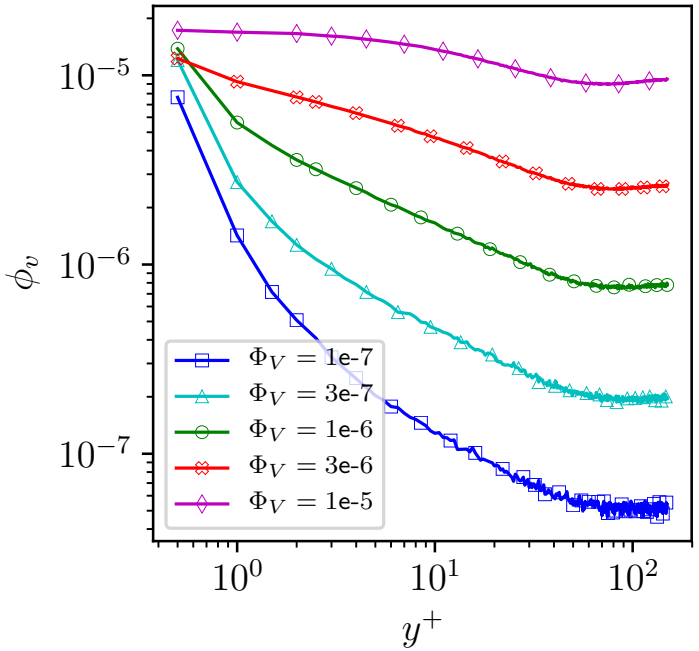

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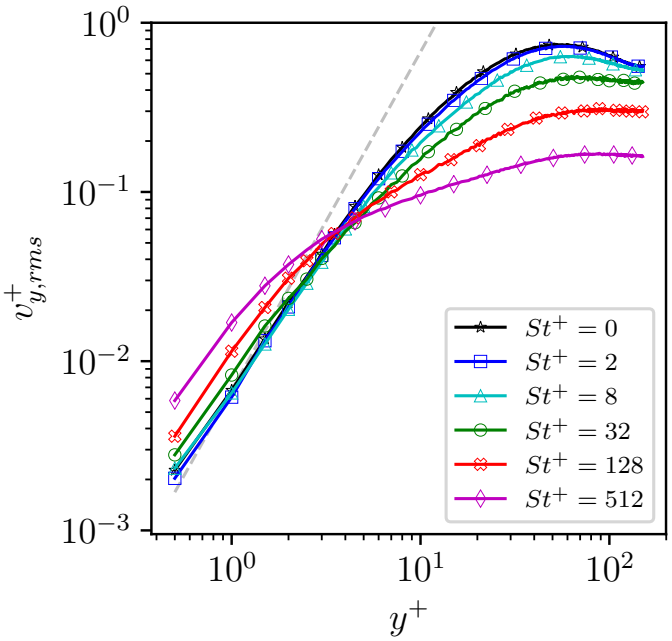

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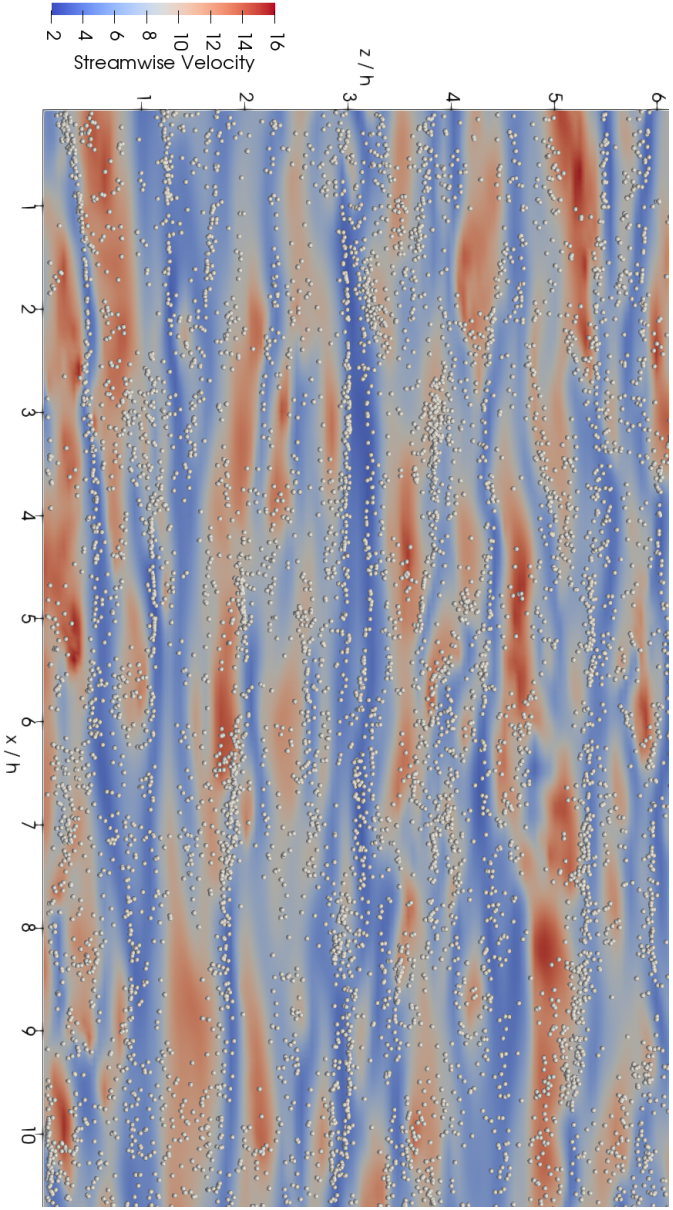

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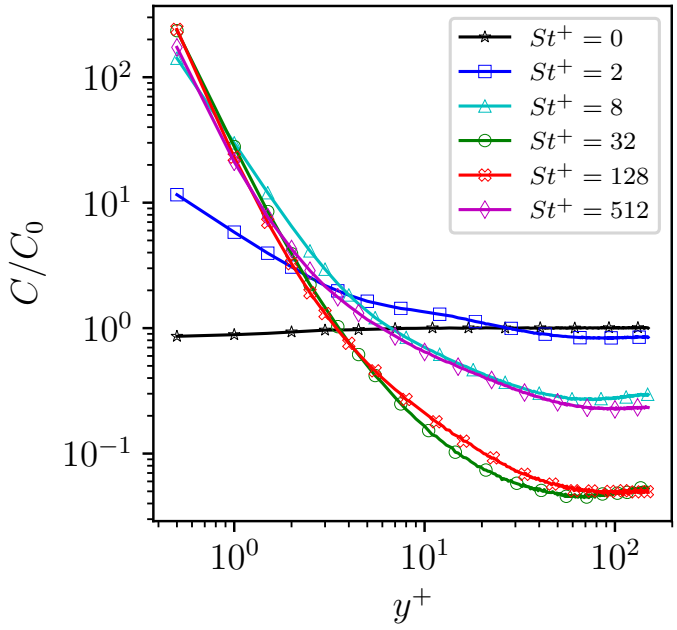

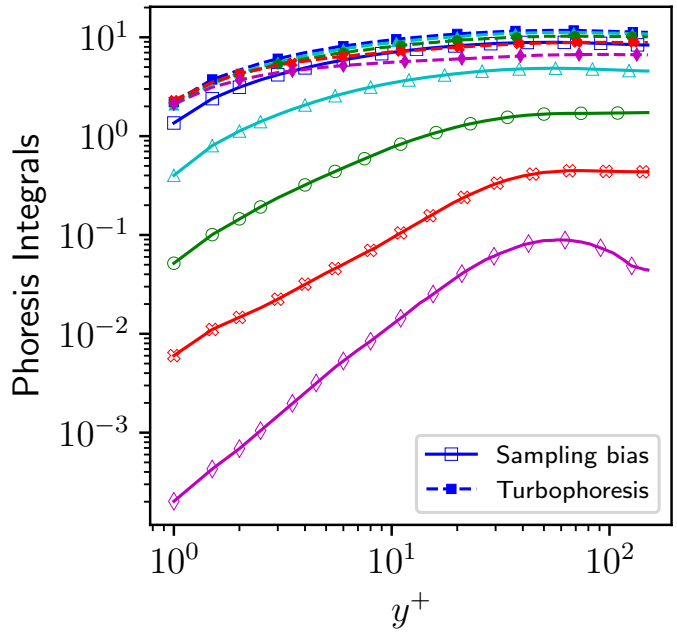

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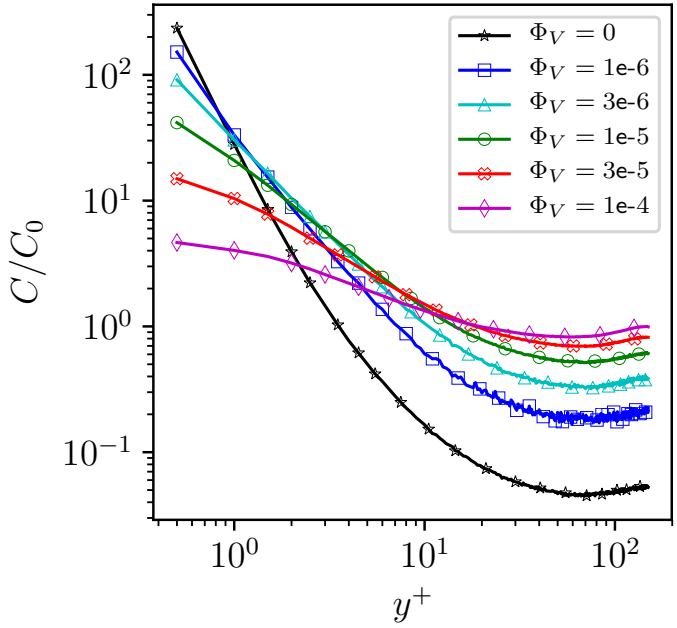
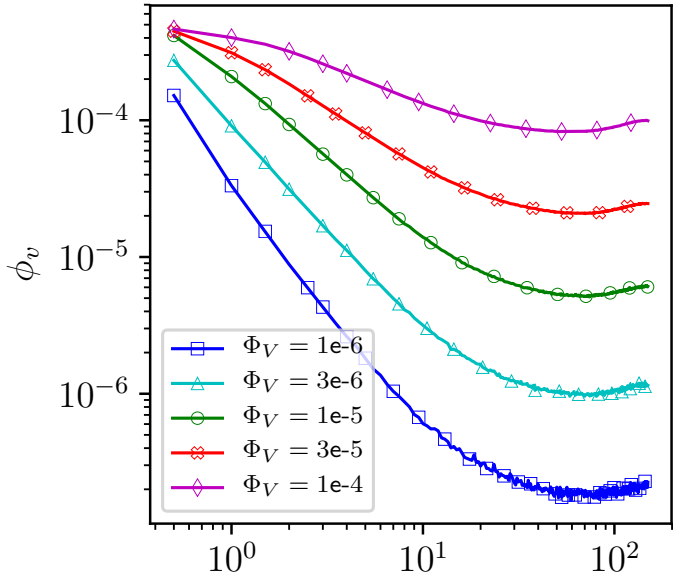
- Collisions decrease turbophoresis
  - enforce max near-wall ϕ_v
  - what does this mean for super-particles?





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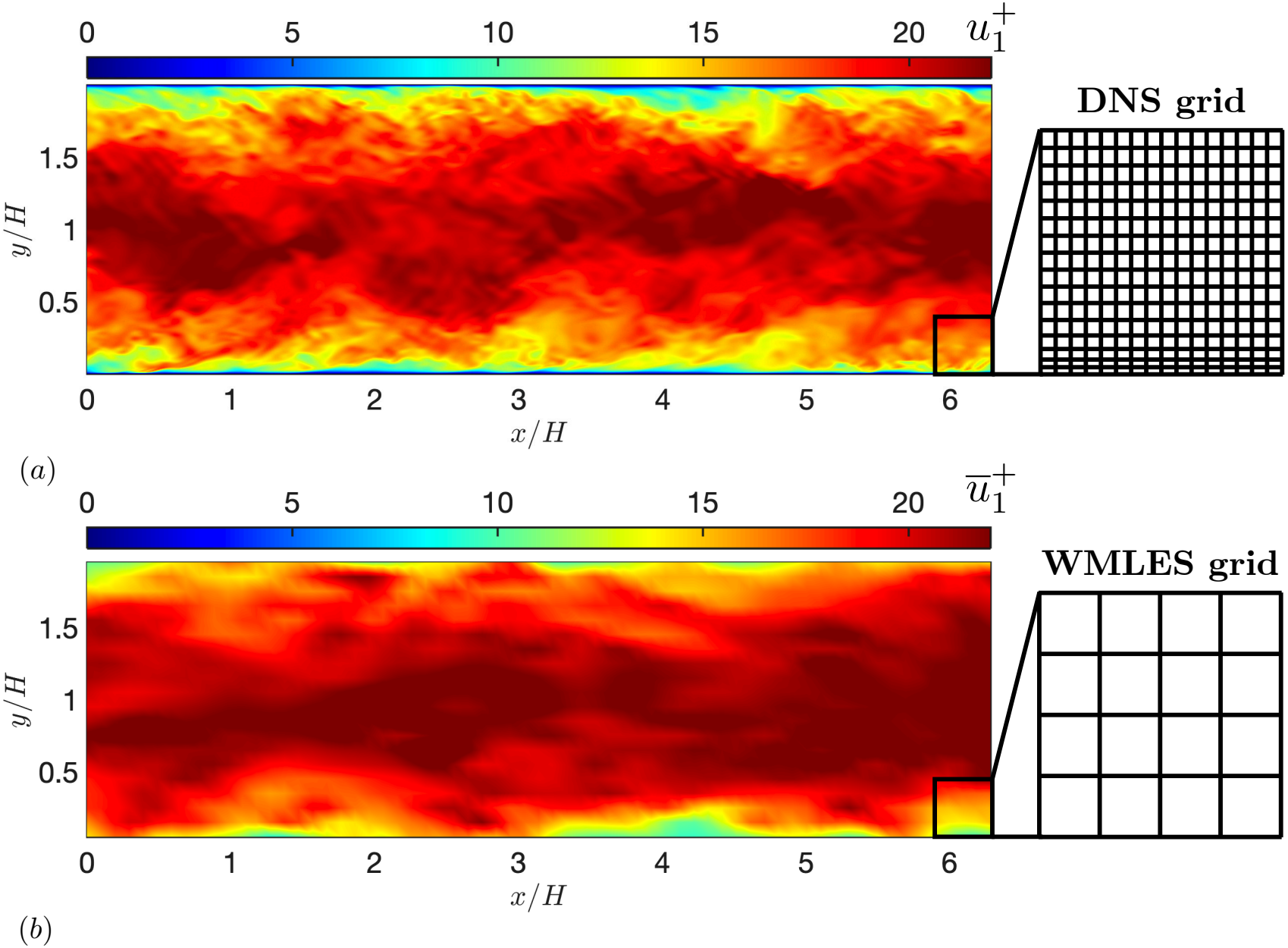
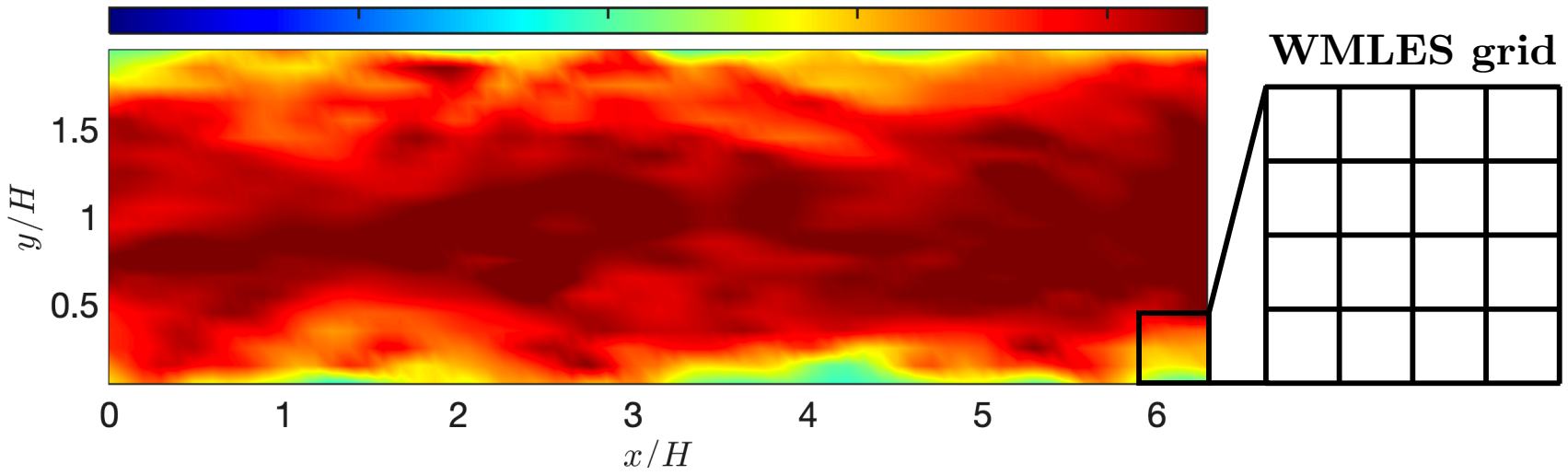


Wall-modeled LES



$$\frac{\partial \widetilde{\mathbf{u}}}{\partial t} + \widetilde{\mathbf{u}} \cdot \nabla \widetilde{\mathbf{u}} = -\nabla \widetilde{p} + \nu \nabla^2 \widetilde{\mathbf{u}} - \nabla \cdot \sigma, \qquad \nabla \cdot \widetilde{\mathbf{u}} = 0,$$

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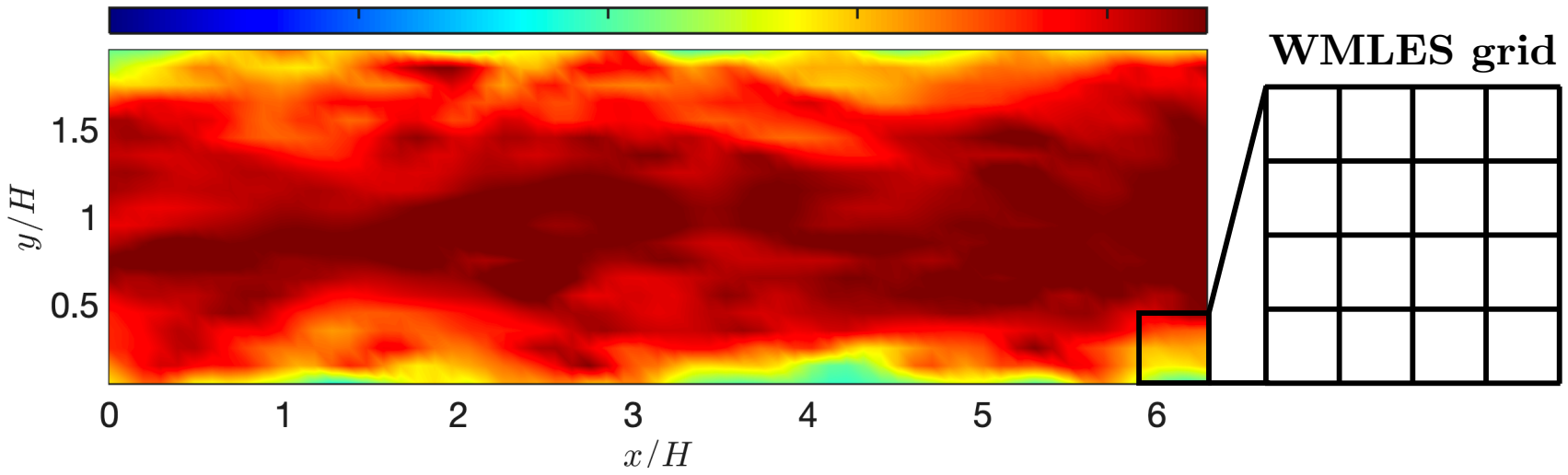

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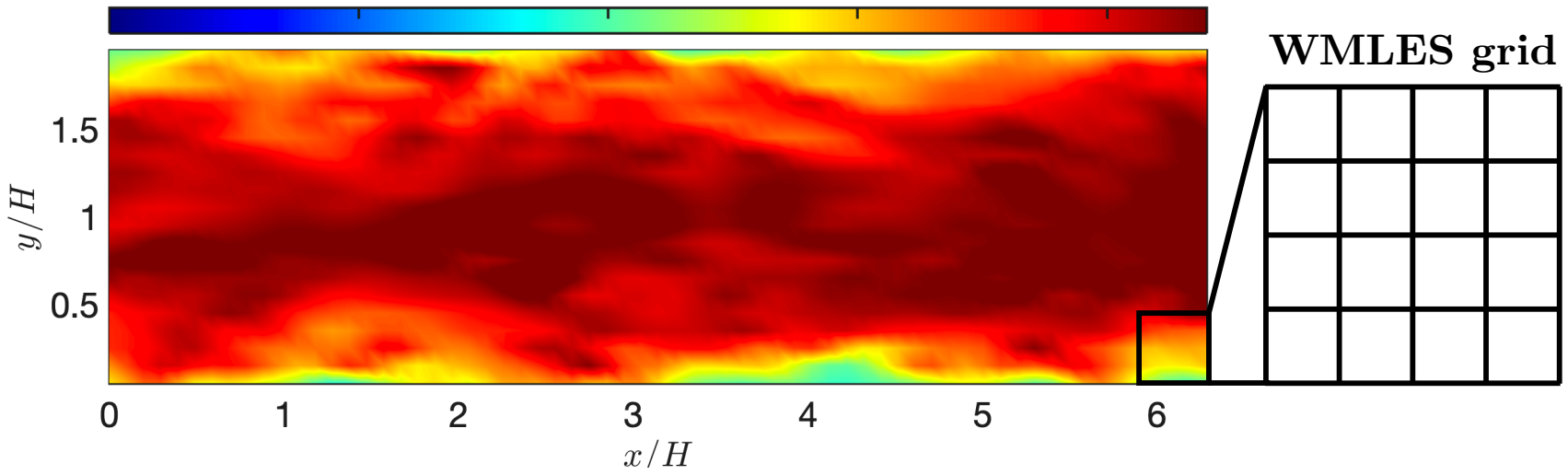
- staggered mesh, 2nd-order central differencing
- dynamic Smagorinky SGS stress, $\sigma_{ij} = -2(C_s \Delta)^2 |\widetilde{\mathbf{S}}| \widetilde{S}_{ij}$
- algebraic equilibrium wall-model, $u_{\|}(y_{1/2}) = u_* \left[\frac{1}{\kappa} \ln \left(\frac{y_{1/2} u_*}{\nu_f} \right) + B \right],$

Advecting particles in wall-modeled LES



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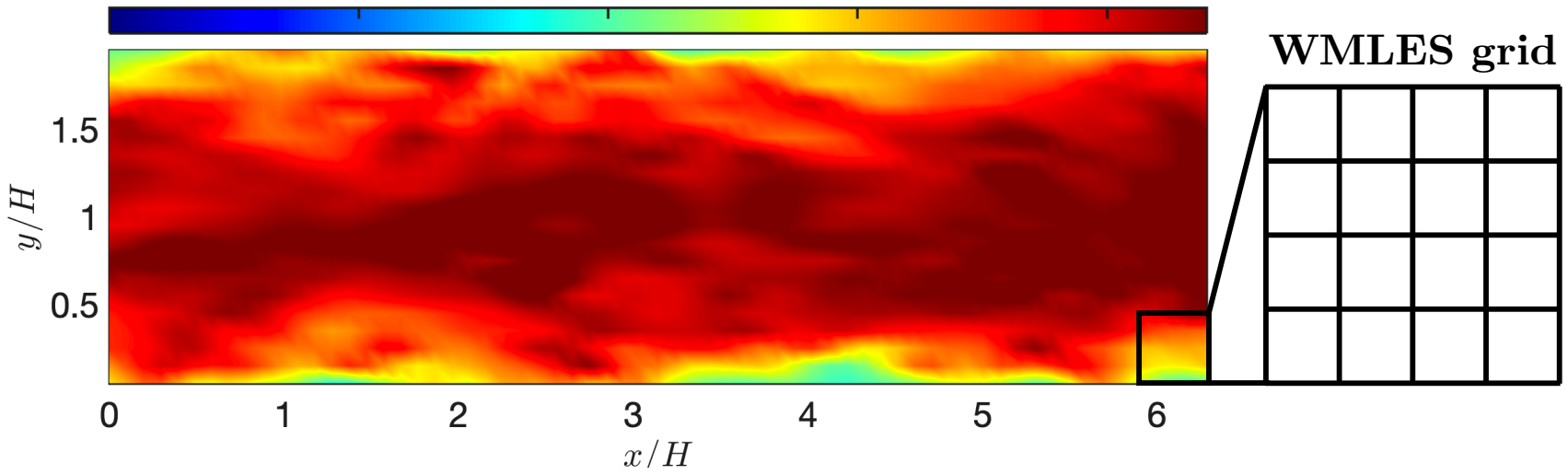

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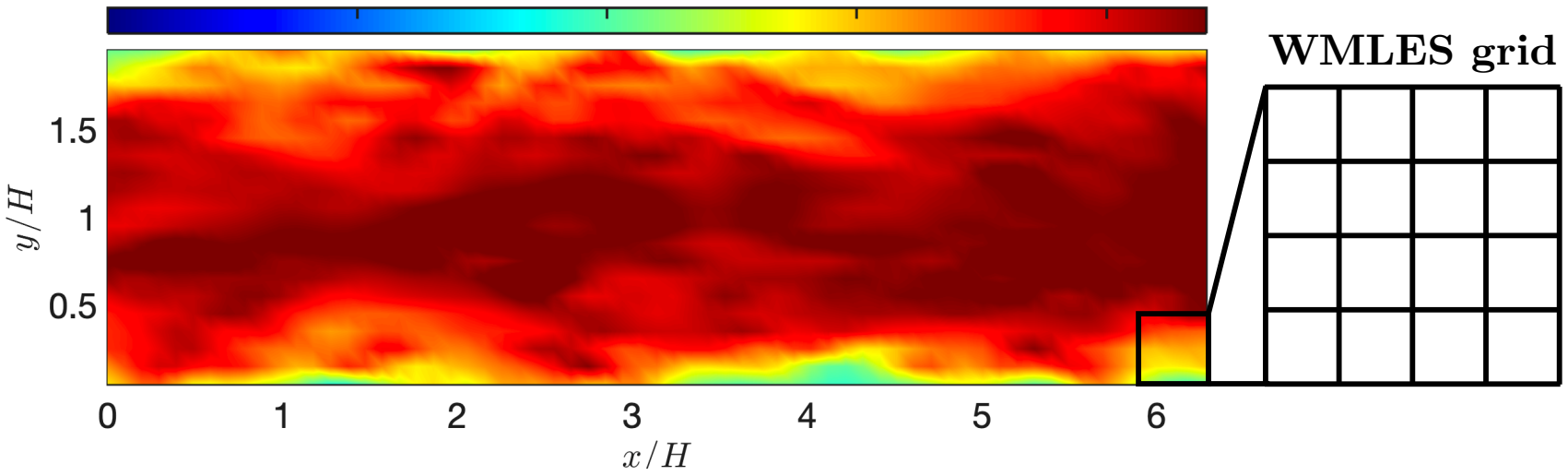

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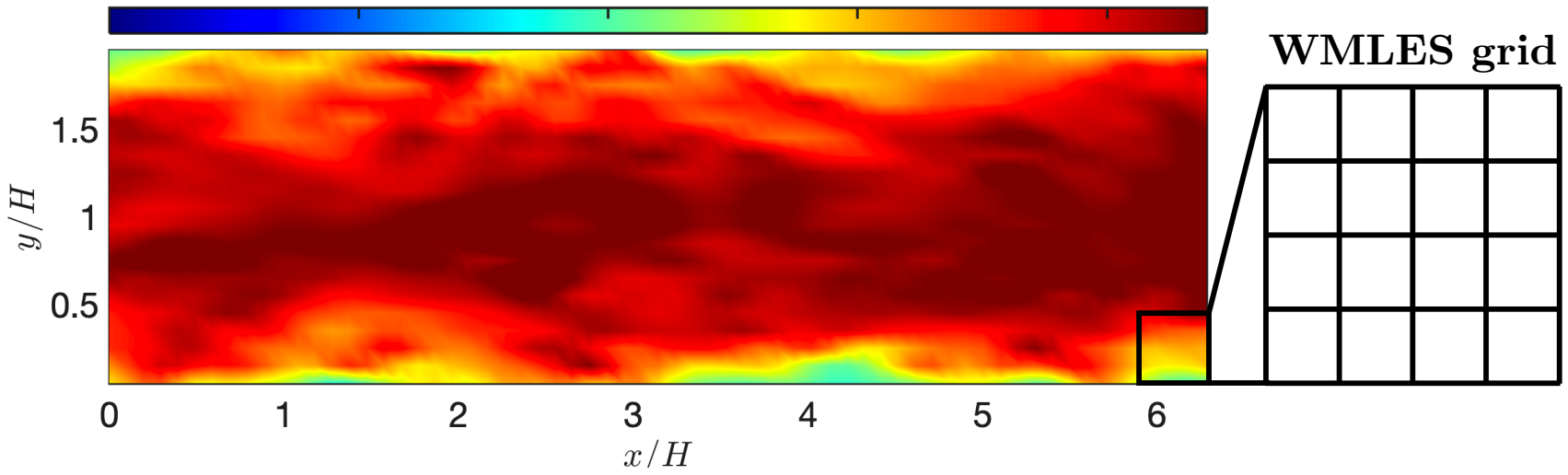

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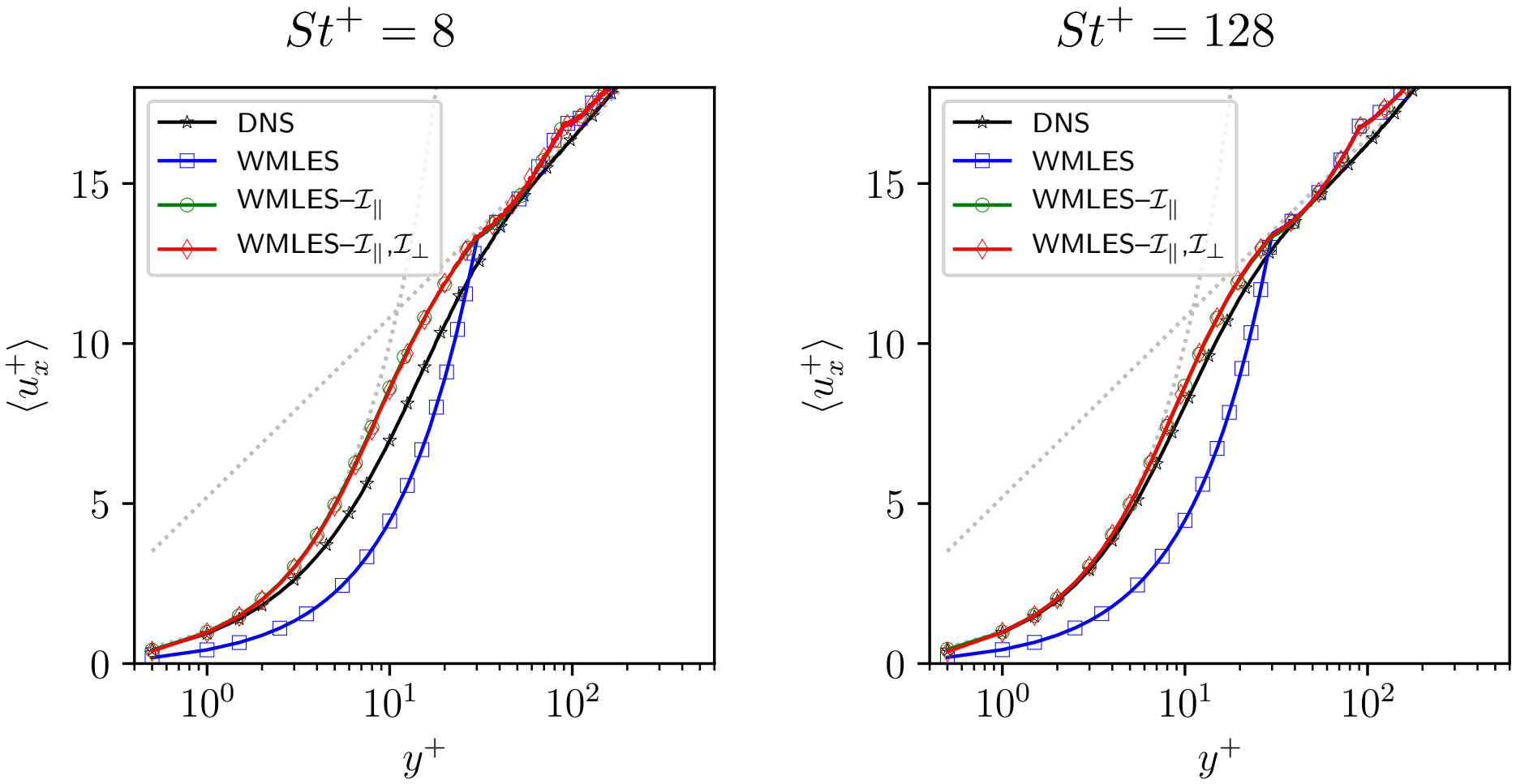
- how important is $\mathbf{u}'$ vs. specialized interpolation

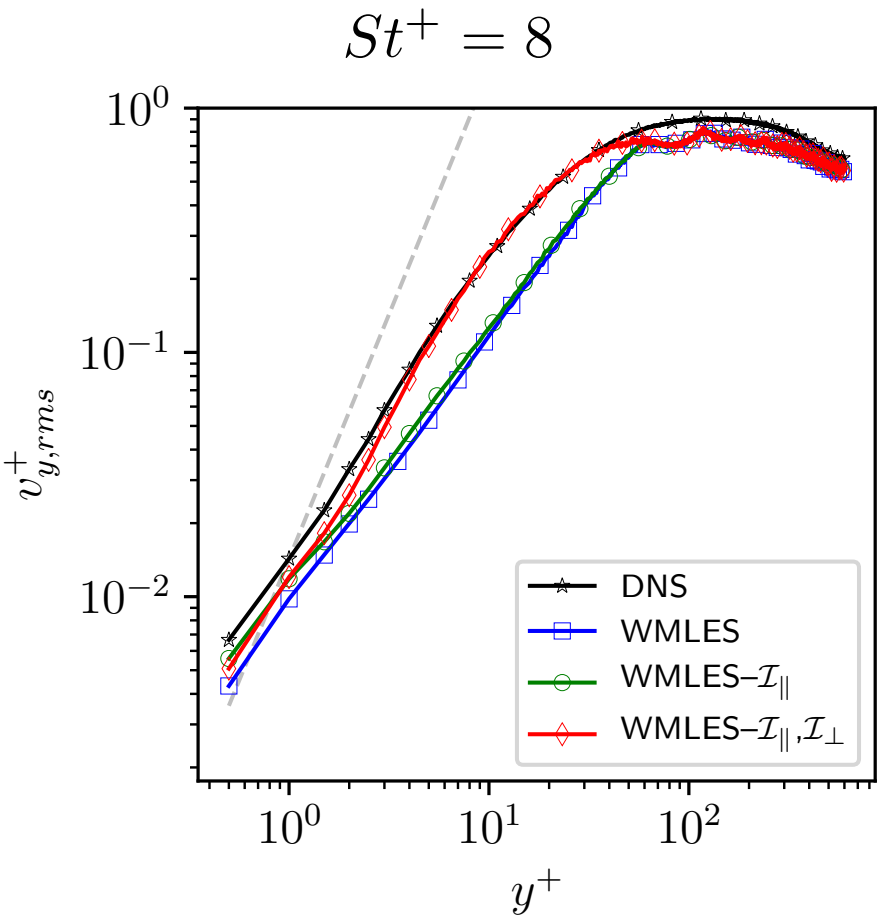
Interpolating streamwise velocity

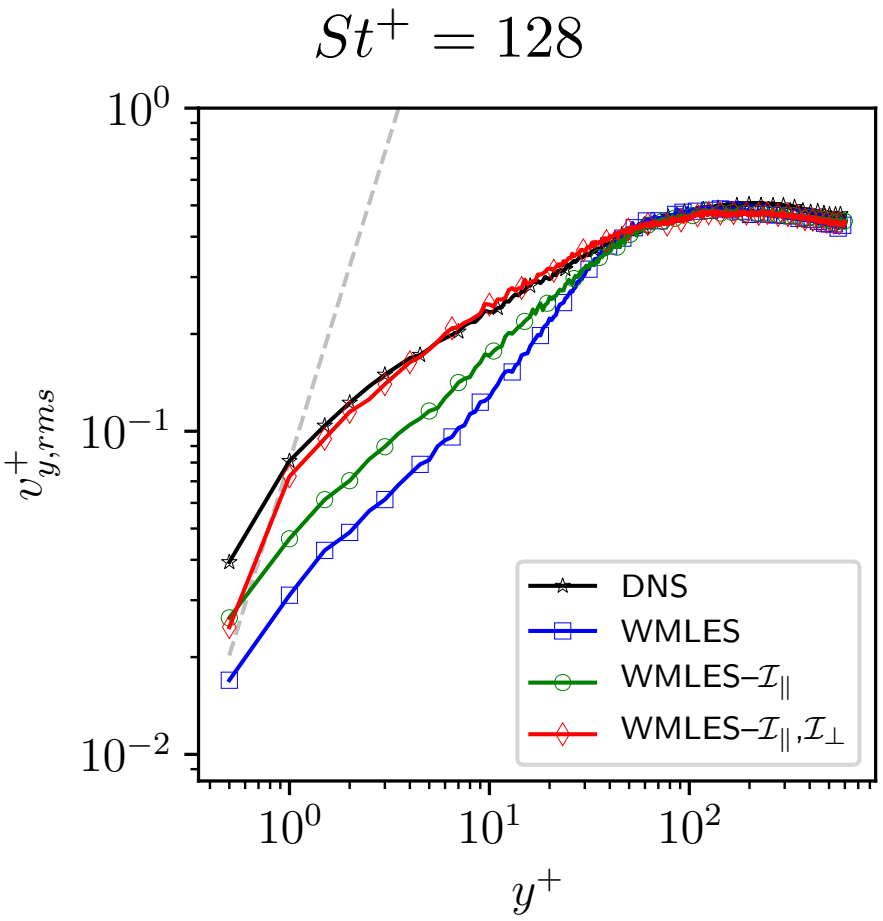


Biased sampling of low speed streaks reduces mean streamwise velocity.

- Less important at higher St^+

Interpolating wall-normal velocity

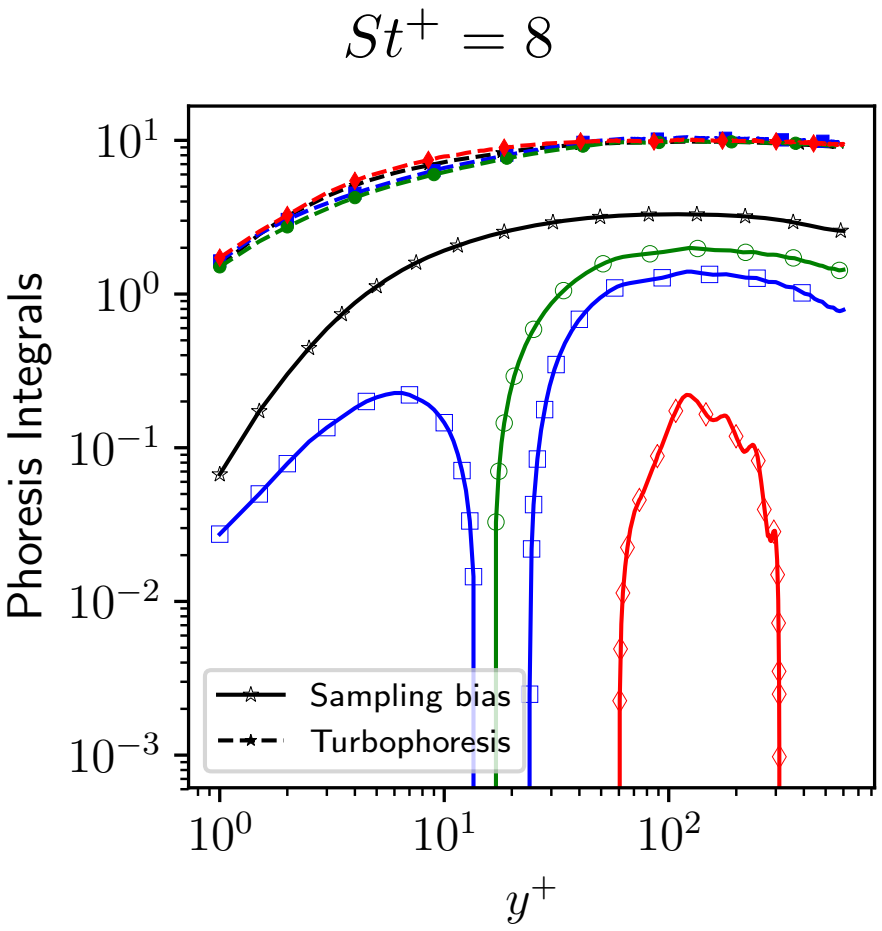


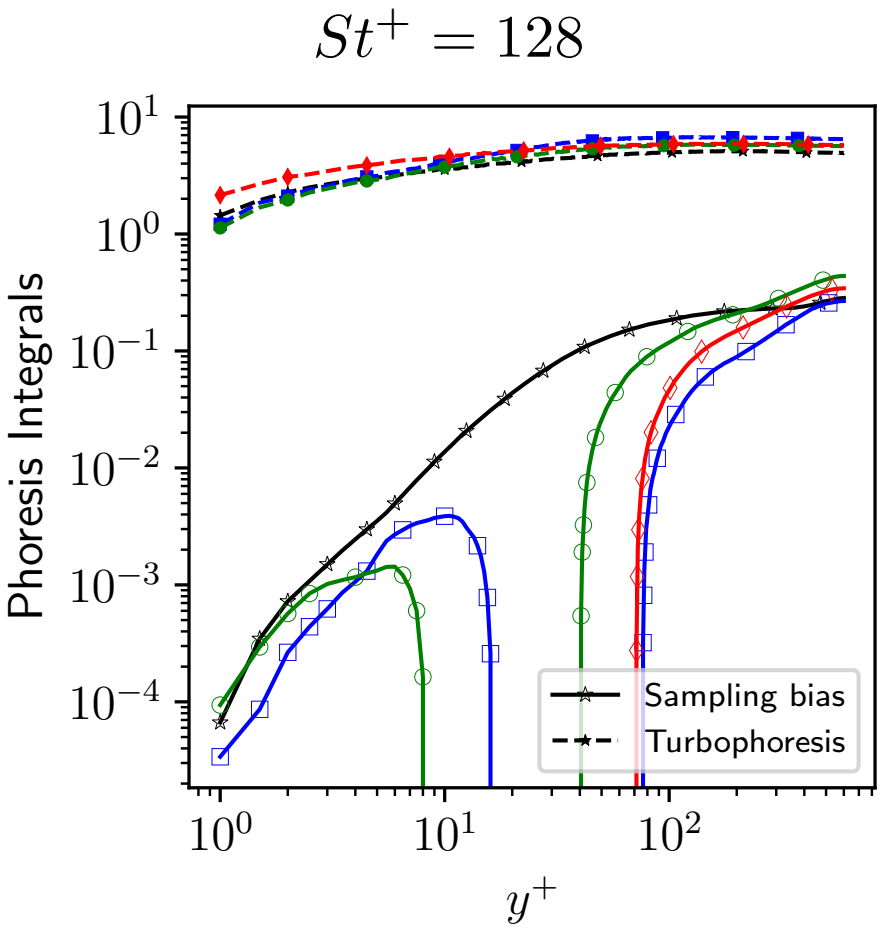


DNS-informed wall-normal velocity $\rightarrow$ more accurate turbophoresis.

- Not trivial, because $v_y \neq u_y$

Biased sampling in wall-modeled LES

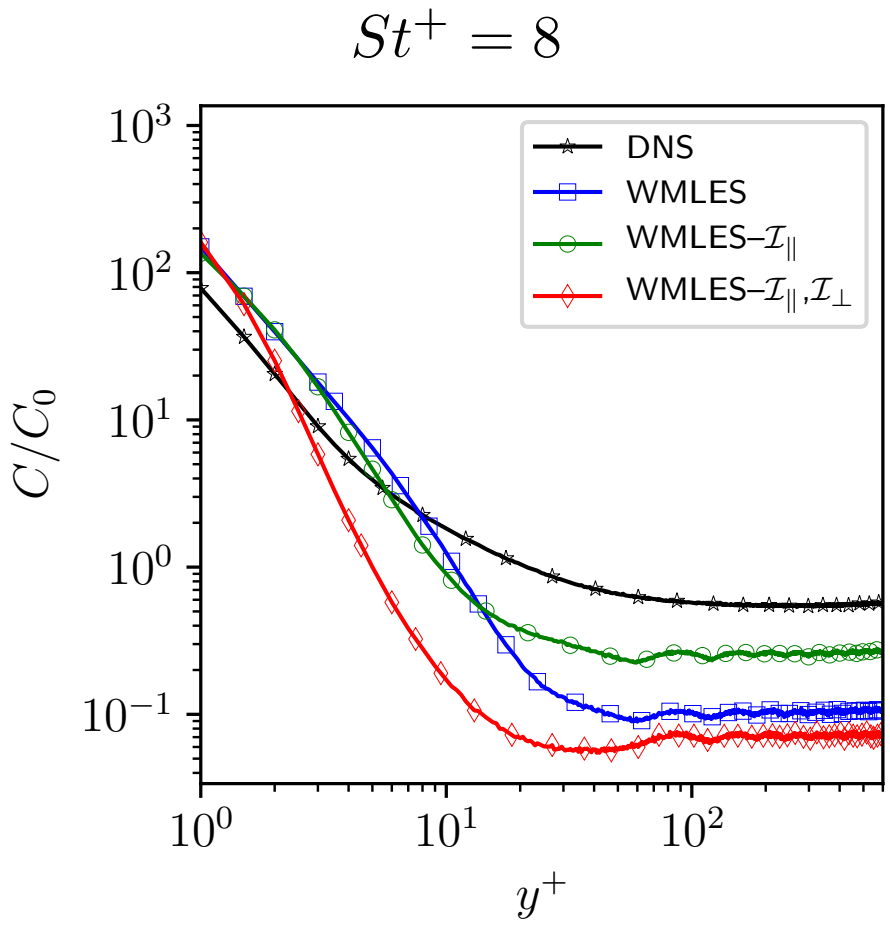


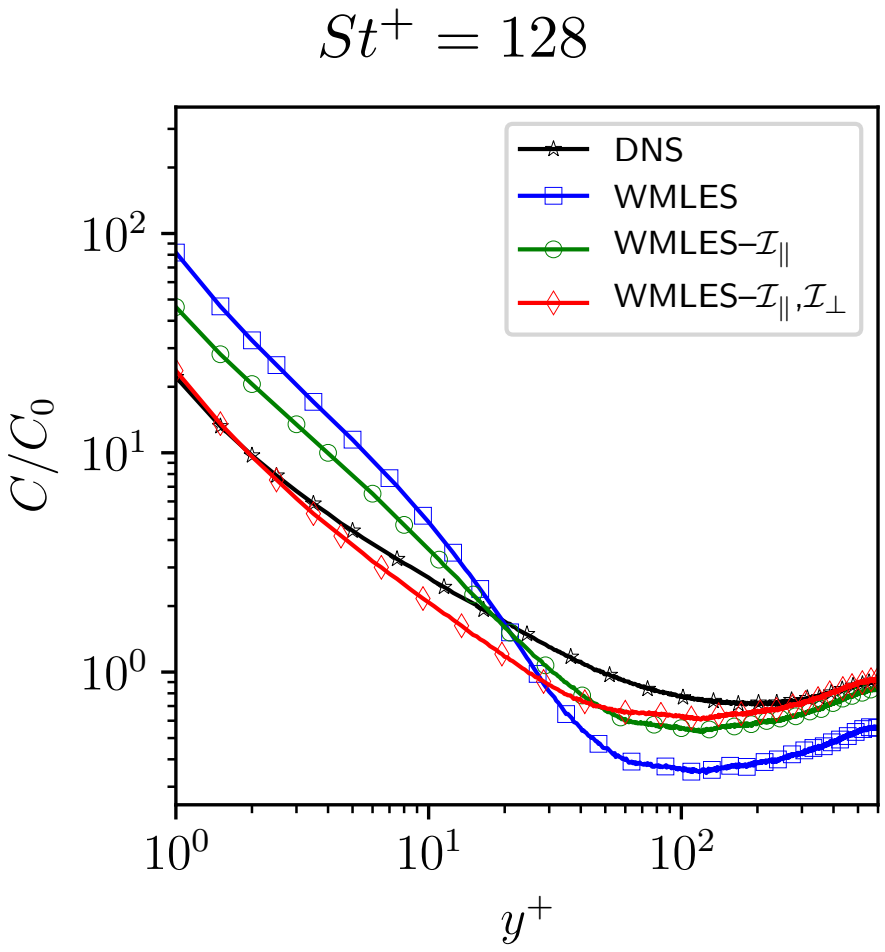


Less near-wall flow structures, WMLES under-predicts biased sampling.

- Likely worse at higher Re_τ
- However, biased sampling less important at larger St^+

Concentration profiles in wall-modeled LES





Physics-based interpolation helpful at $St^+ = 128$, small biased sampling.

- Clear need for $\mathbf{u}'$ at $St^+ = 8$ (future work)

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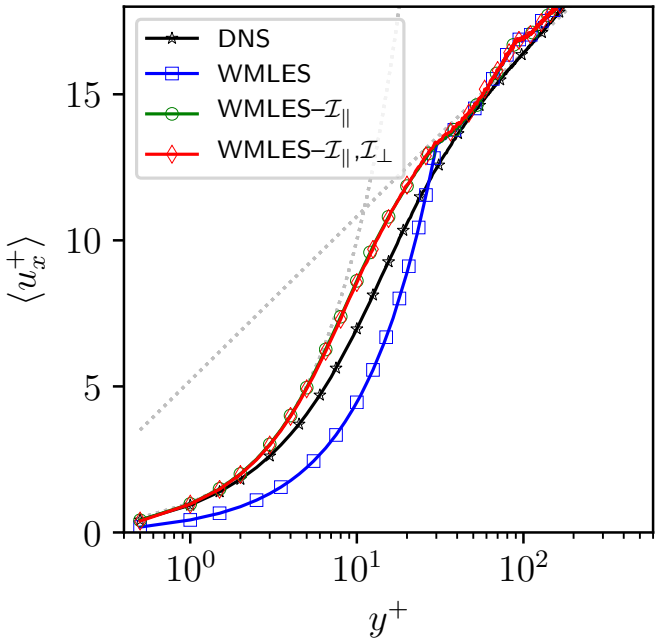

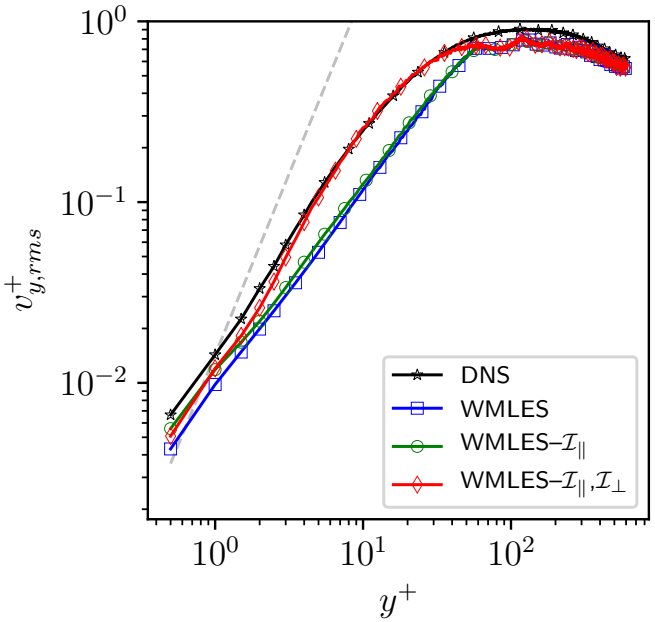

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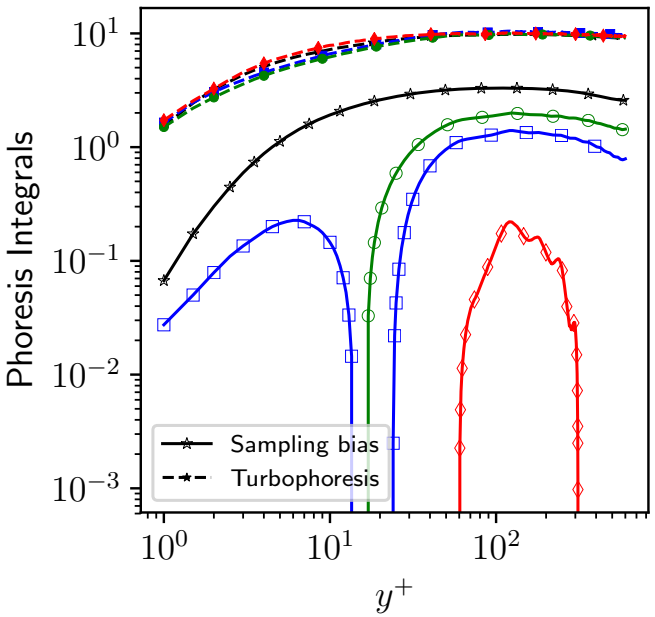

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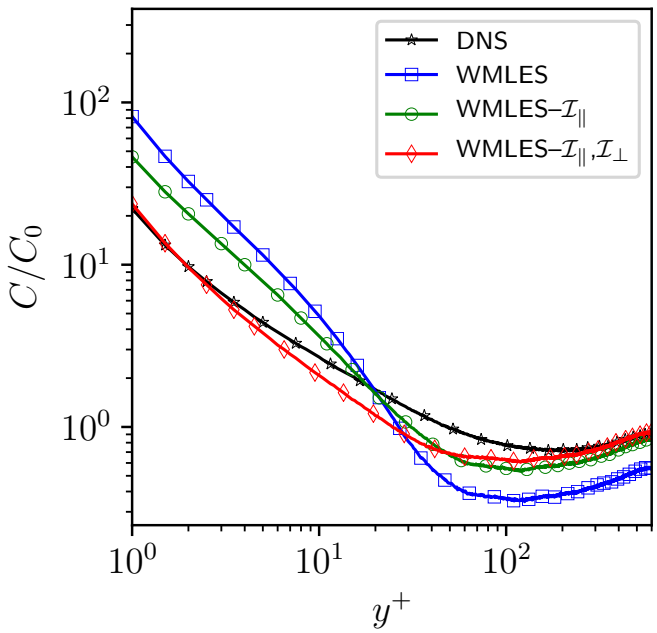

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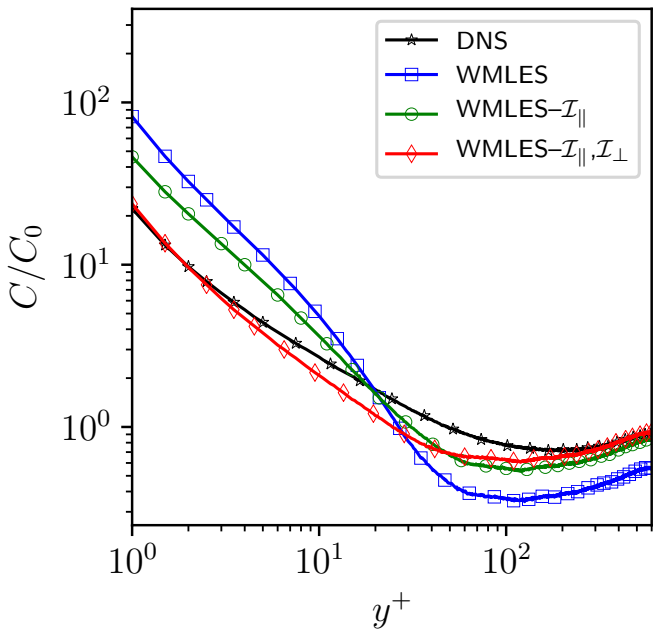
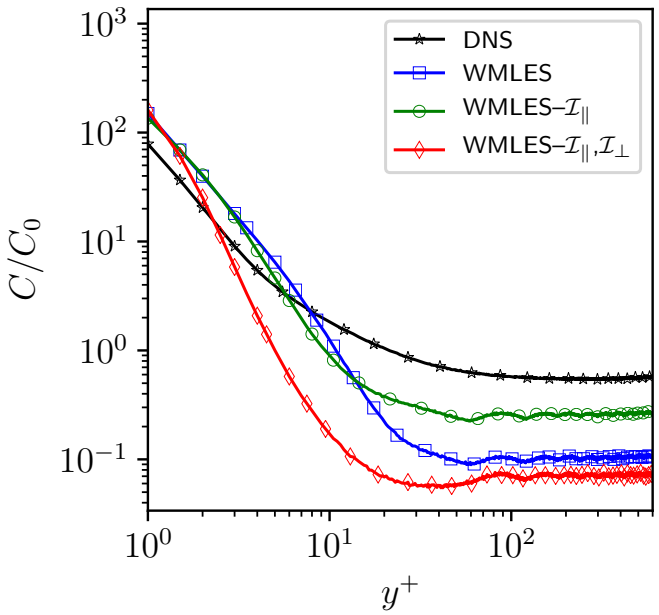
- Low St^+
  - biased sampling is key
  - future work: represent $\mathbf{u}'$



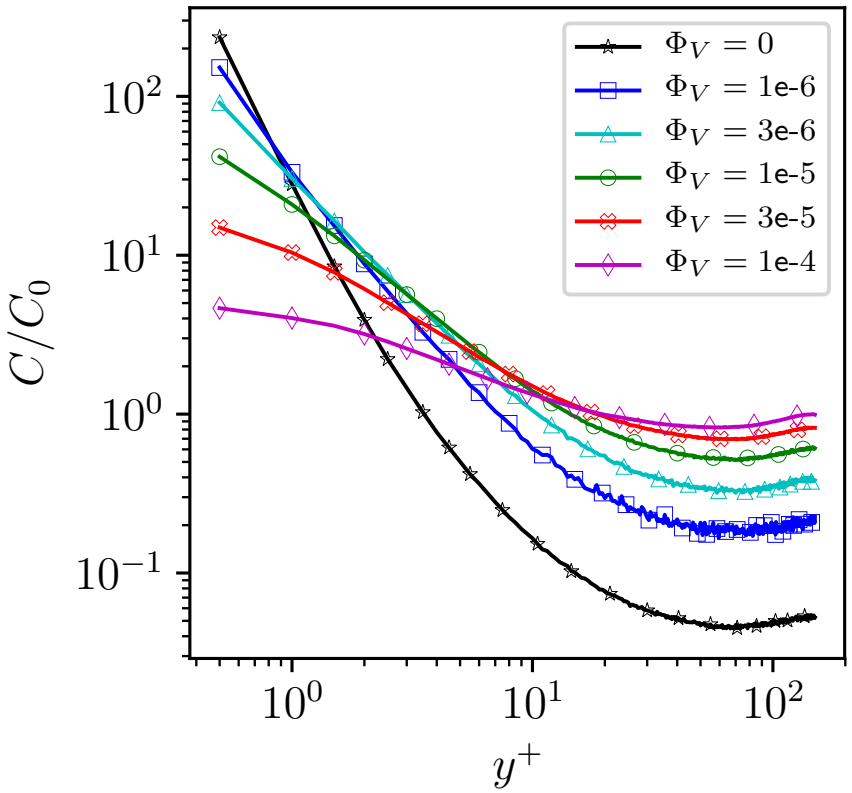


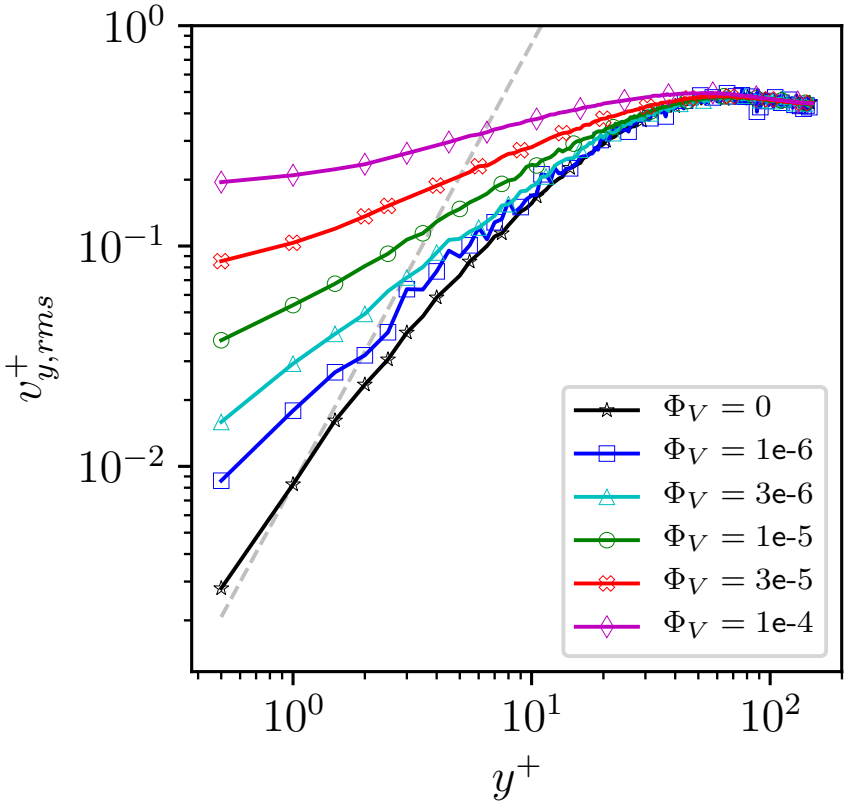
Outline

1. Turbophoresis
2. Wall-modeled LES
3. Super-particle collisions

Particle-Particle Collisions & Turbophoresis

- As global volume fraction (Φ_V) increases, particle-particle collisions redistribute and transfer fluctuation energy (e.g. at $St^+ = 32$ below)





Concentration profile is very sensitive to volume fraction.

Multifidelity Uncertainty Quantification (UQ)[1]

[1] H. R. Fairbanks, L. Jofre, G. Geraci, G. Iaccarino, A. Doostan. Bi-fidelity approximation for uncertainty quantification and sensitivity analysis of irradiated particle-laden turbulence. Under review in Journal of Computational Physics.

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- vary 14 input uncertainties

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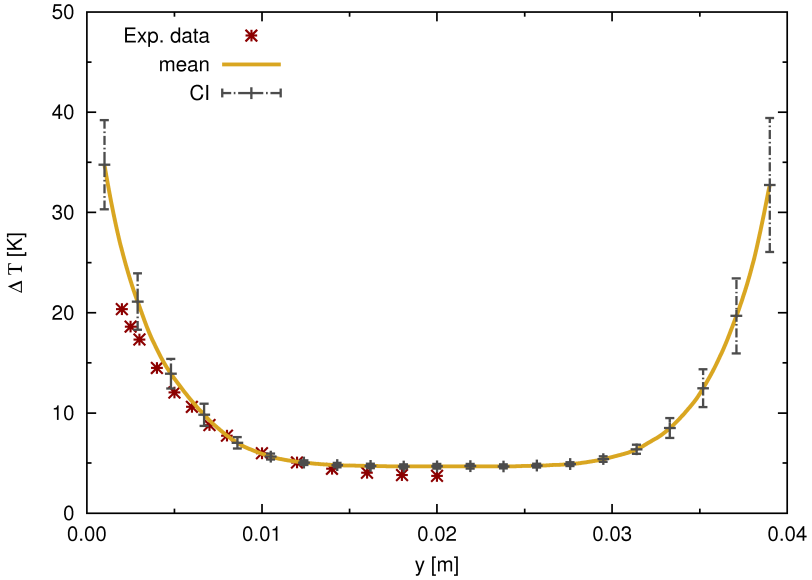

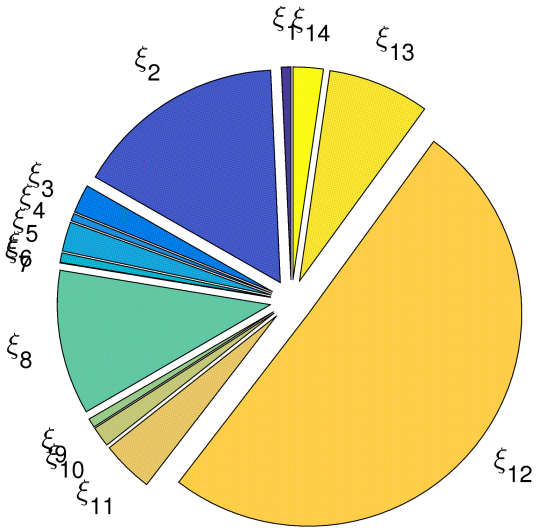

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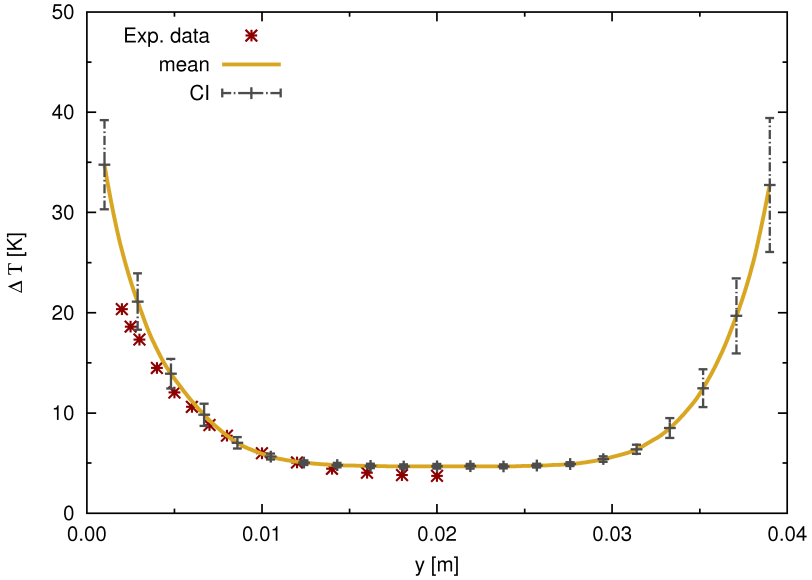
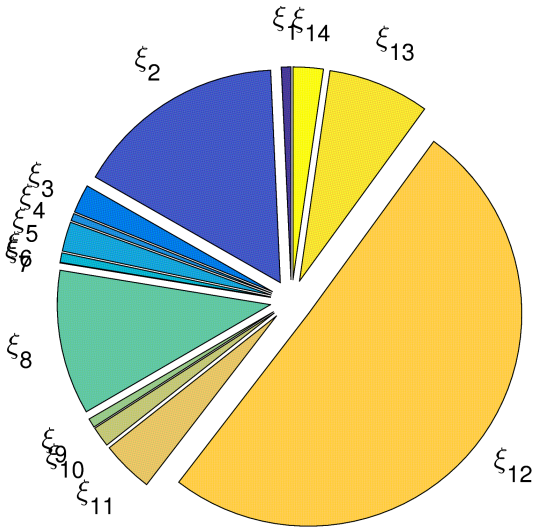
- LES (dynamic Smagorinsky)
- coarser $\times 10$ in dx, dy, dz, dt
- reduction $\times 10$ in # of particles (deterministic collisions)





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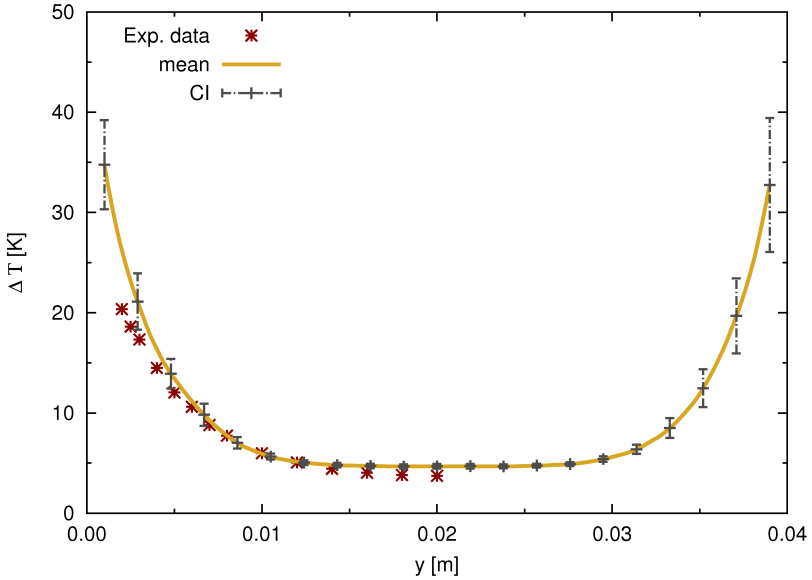

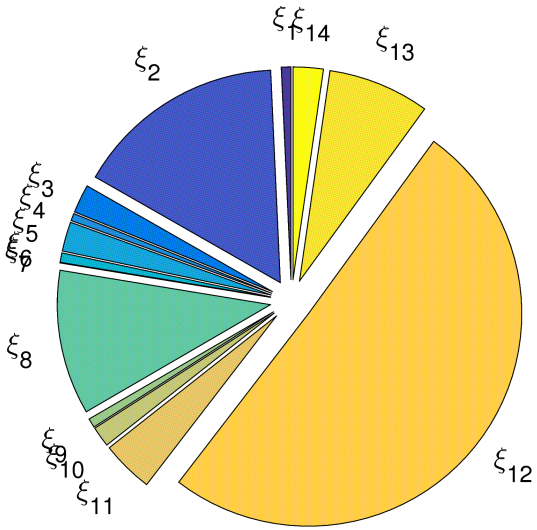

Low fidelity susceptible to volume fraction sensitivity.

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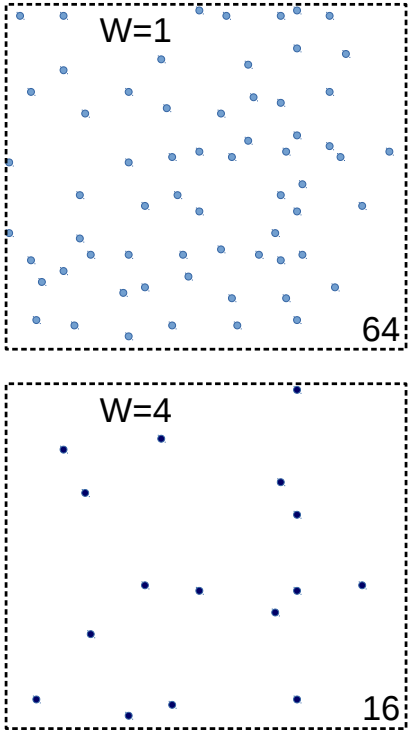
A Super-Particle Approach

- $\dot{\mathbf{x}}^{(i)} = \mathbf{v}^{(i)}, \qquad \dot{\mathbf{v}}^{(i)} = \mathbf{a} \overset{e.g.}{=} \frac{\mathbf{u}(\mathbf{x}^{(i)},t) - \mathbf{v}^{(i)}}{\tau_p}$



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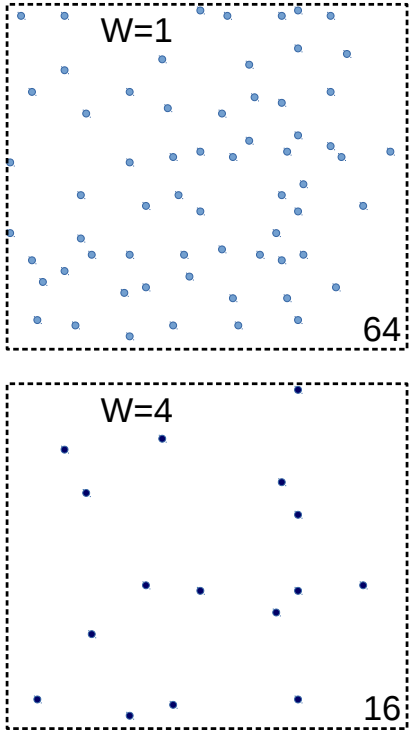

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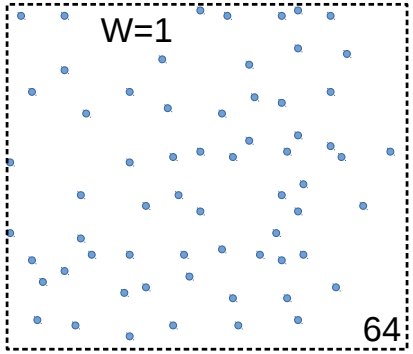

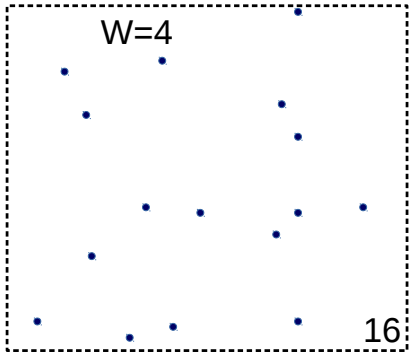

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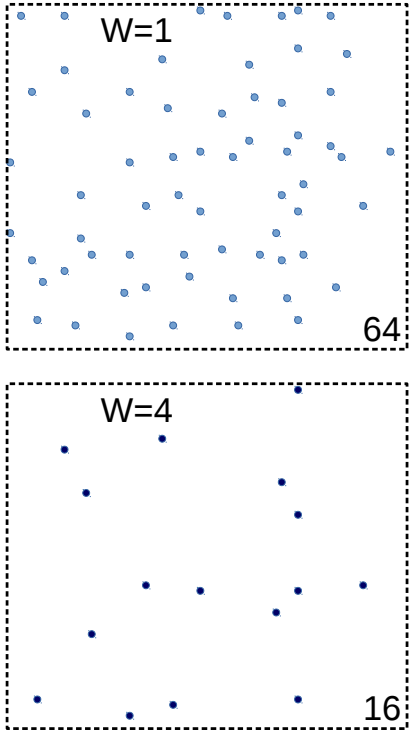
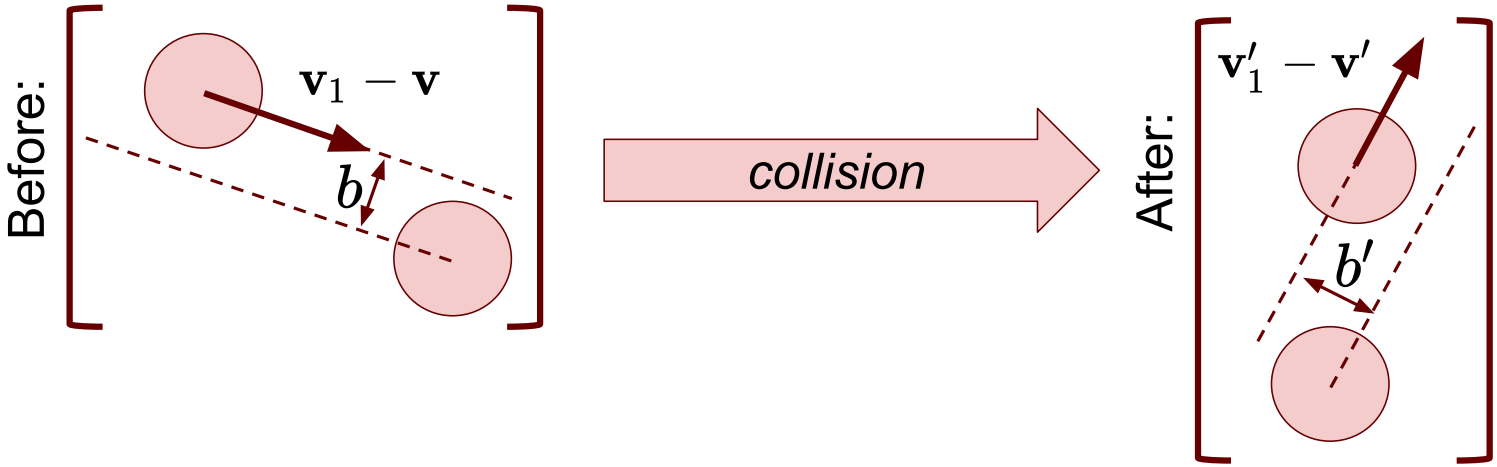
- $\dot{f}_{coll} \sim N_p^2 \; d_p^2 \; v_{rel} \; / \; W$



Invariance with W is broken by collision term, $\dot{f}_{coll}$.



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- Correct by changing collision diameter: $\dot{f}_{coll} \sim N_p^2 \frac{d_c^{2+h}}{W}$
- For invariance with W: $d_c = d_p \, W^{1/(2+h)}$
  - Relative velocity via restitution coefficient: $e_c = e_p \, W^{-h/(2+h)}$

Collision Scaling

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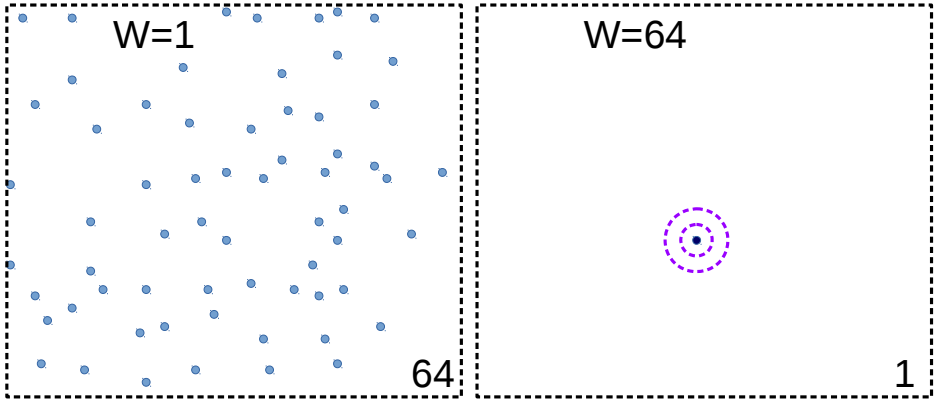
- Example: $W = 64$
  - low St, 'smooth', ($\alpha = 1/3$, 'const. vol. frac.'): $d_c = 4d_p$
  - high St, 'ballistic', ($\alpha = 1/2$, 'const. swept vol.'): $d_c = 8d_p$



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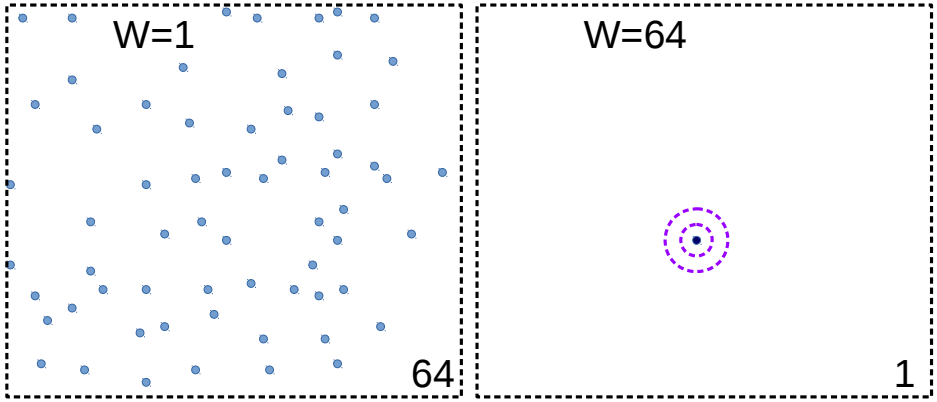
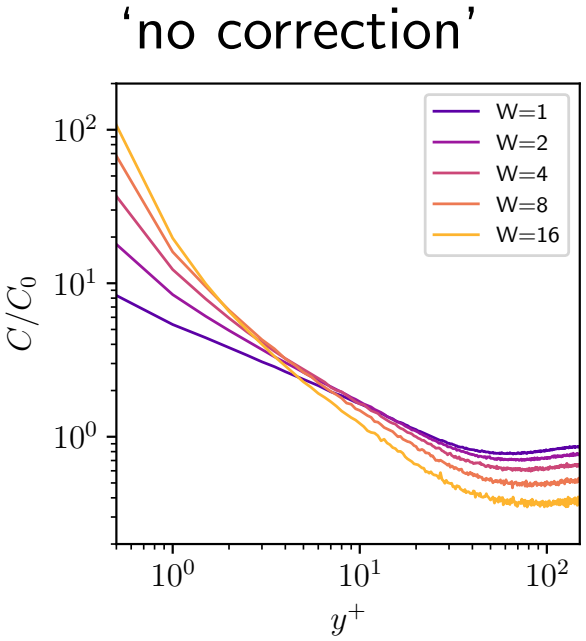


Effective collision diameter scaling should depend on St^+.

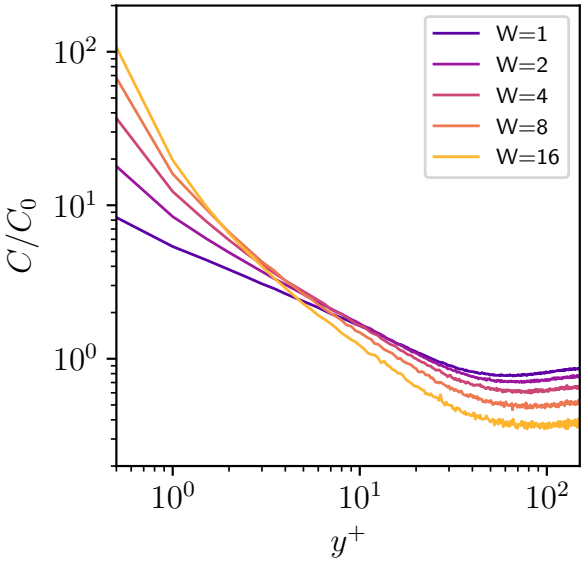
Results for $St^+ = 128$ ($\Phi_V = 1 \times 10^{-5}$)



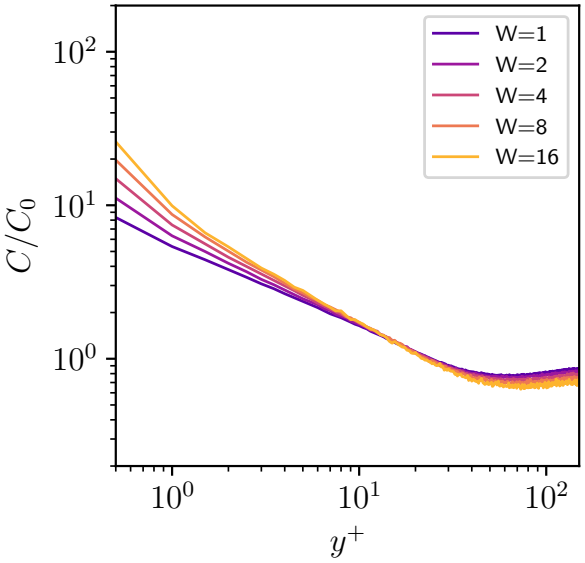
Results for $St^+ = 128$ ($\Phi_V = 1 \times 10^{-5}$)

$h = 1$

'no correction'



'smooth'



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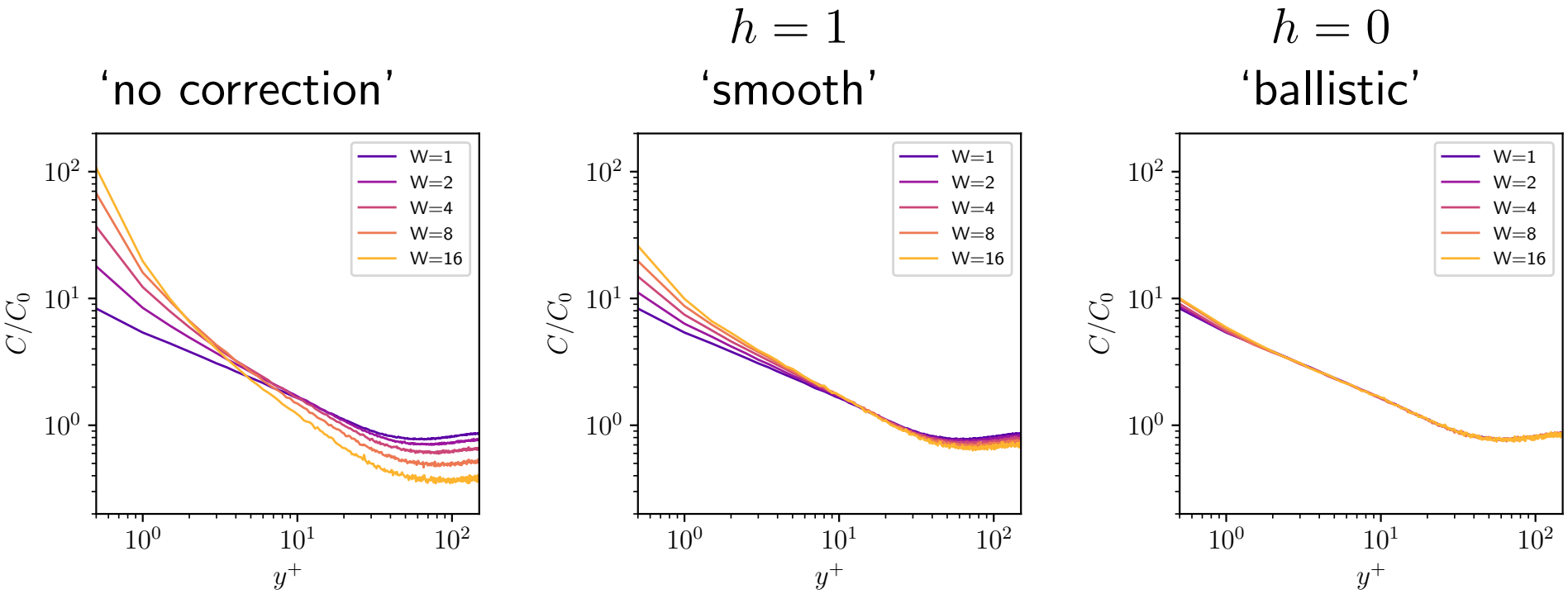

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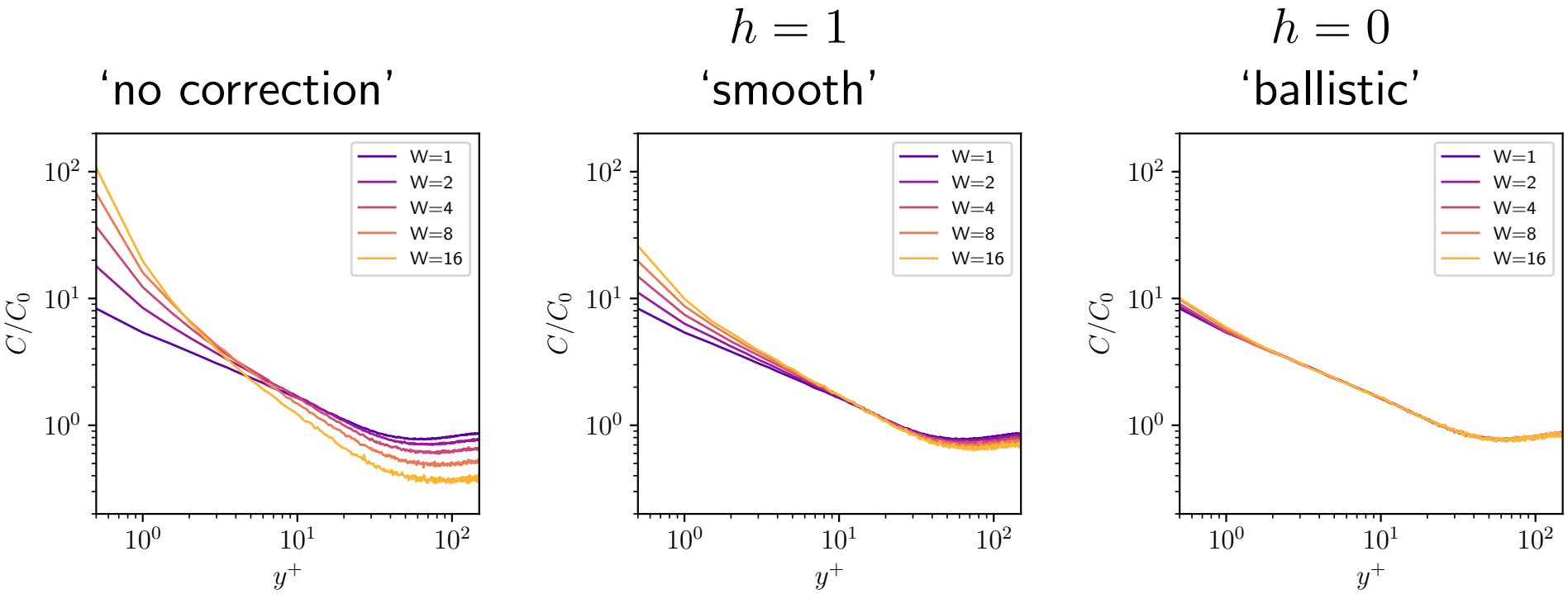
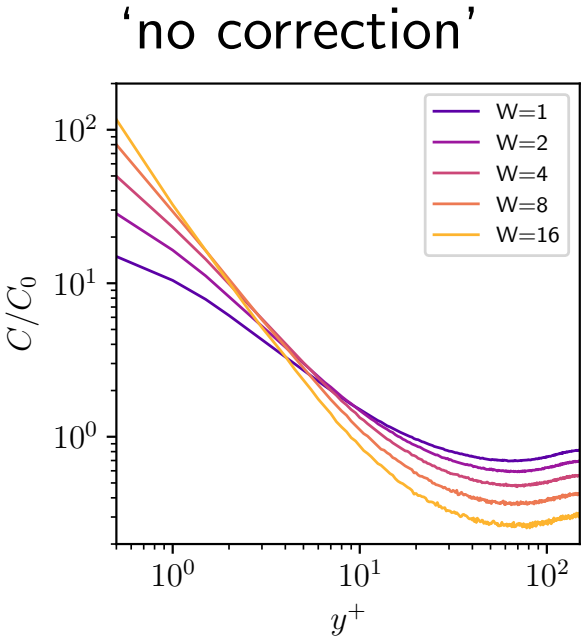


At $St^+ = 128$, the 'ballistic' scaling, $h = 0$, seems effective.

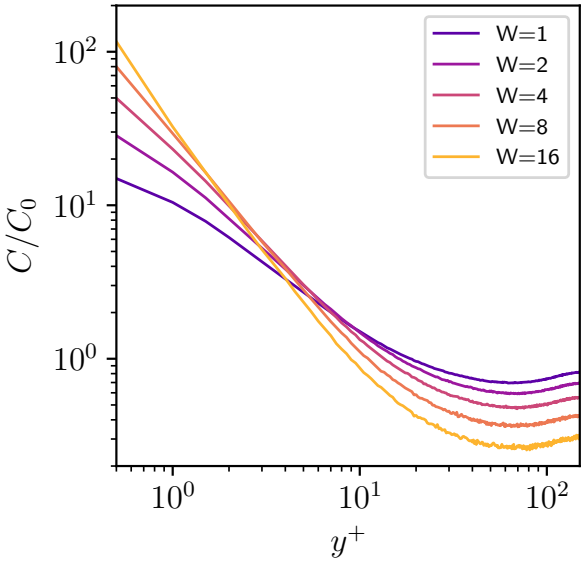
Results for $St^+ = 32$ ($\Phi_V = 3 \times 10^{-5}$)



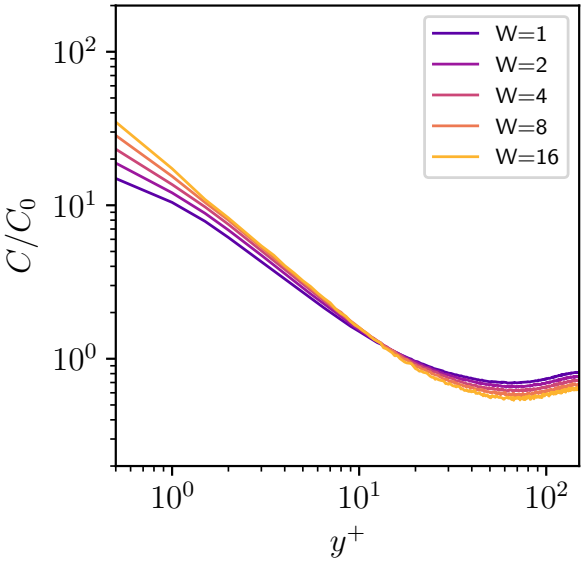
Results for $St^+ = 32$ ($\Phi_V = 3 \times 10^{-5}$)

$h = 1$

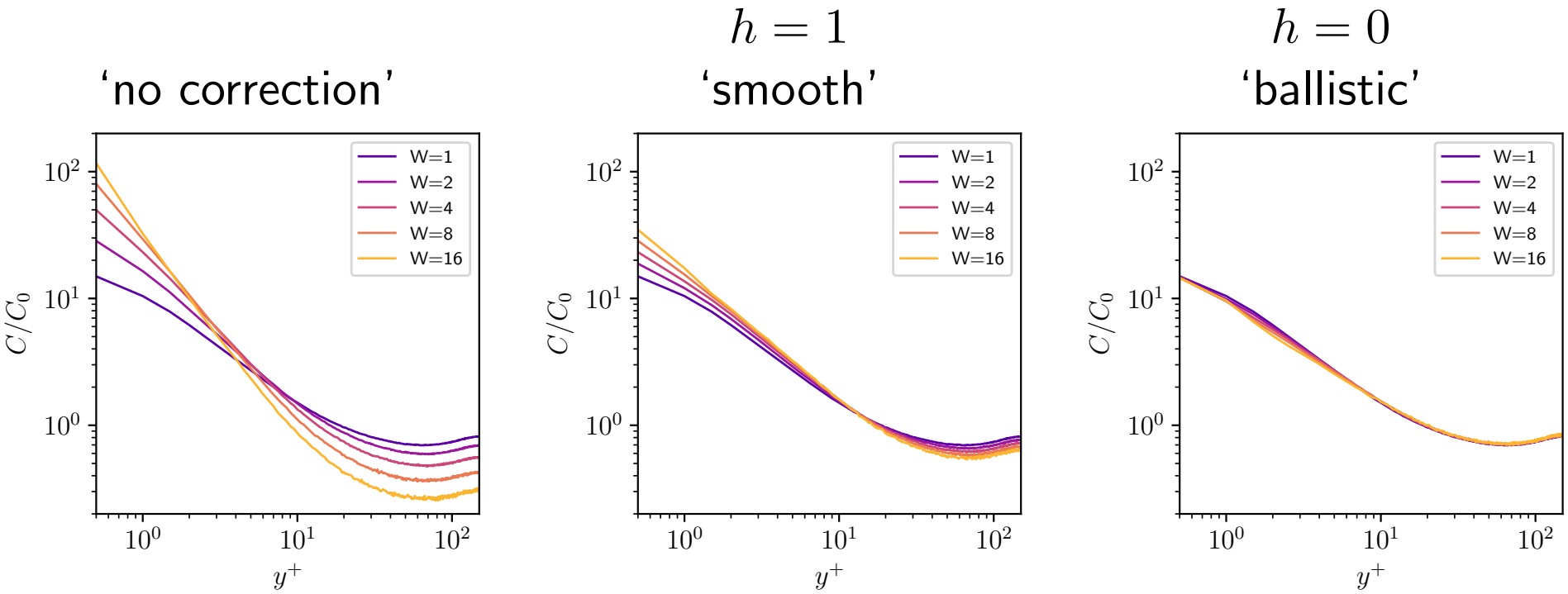
'no correction'



'smooth'



Results for $St^+ = 32$ ($\Phi_V = 3 \times 10^{-5}$)



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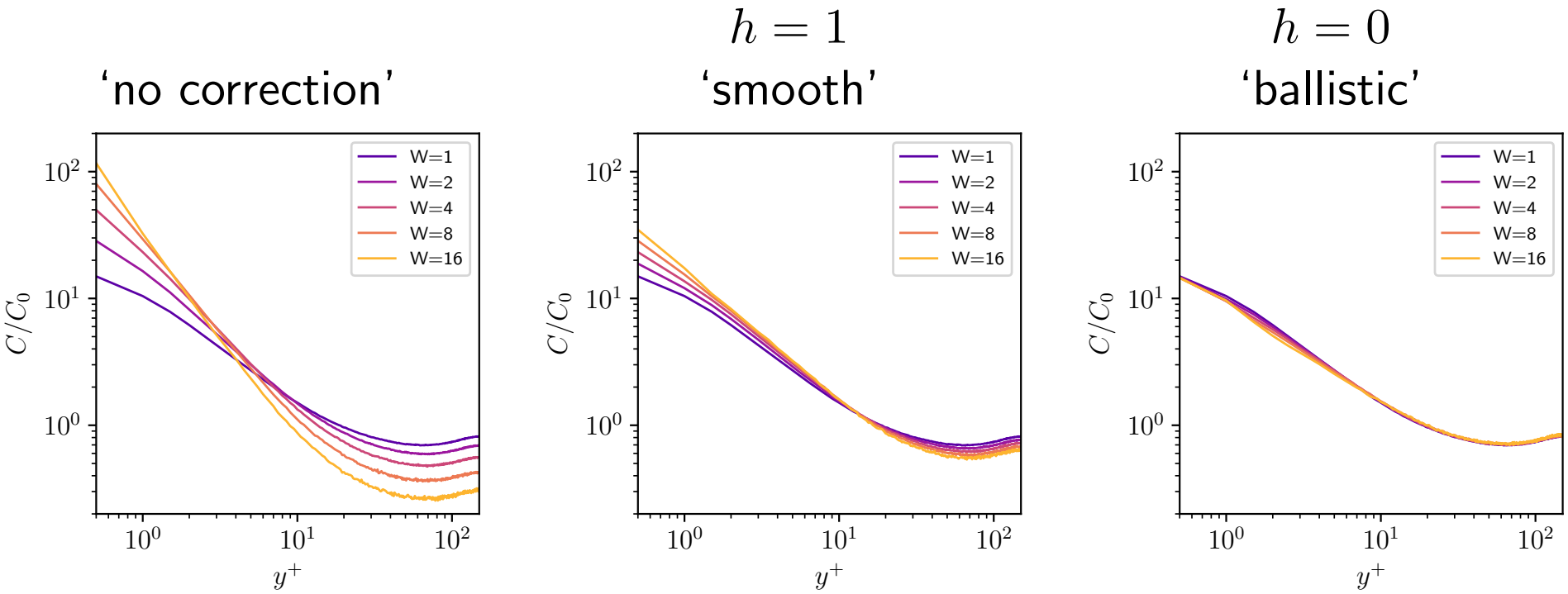
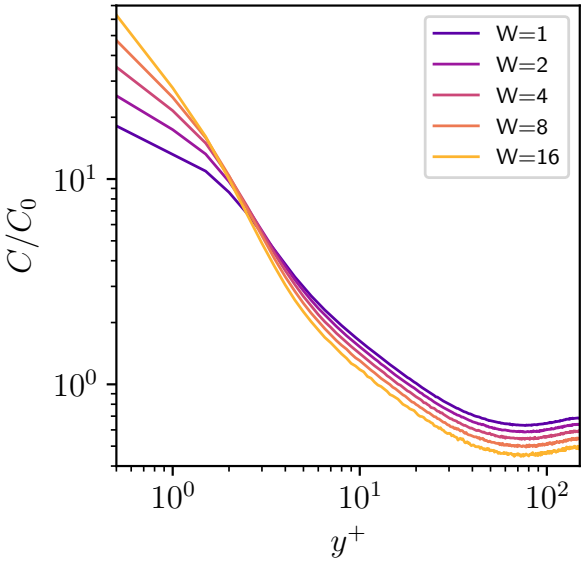


At $St^+ = 32$, the 'ballistic' scaling, $h = 0$, seems effective.

Results for $St^+ = 8$ ($\Phi_V = 1 \times 10^{-4}$)

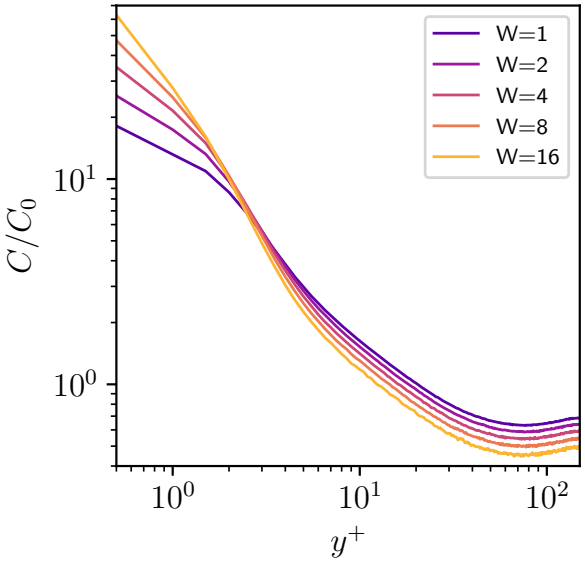
'no correction'



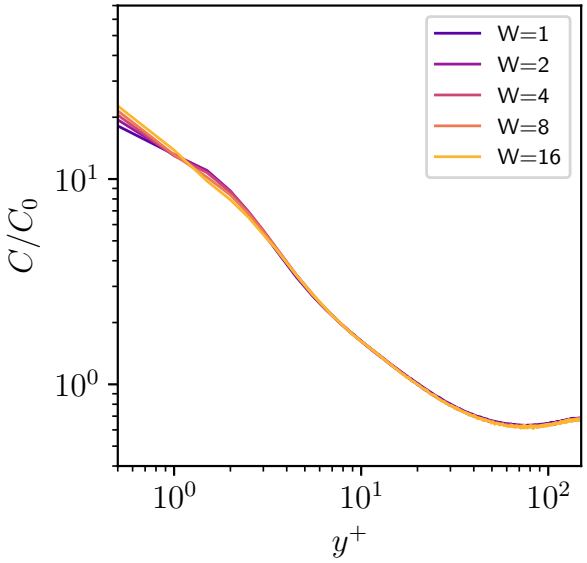
Results for $St^+ = 8$ ($\Phi_V = 1 \times 10^{-4}$)

$h = 1$

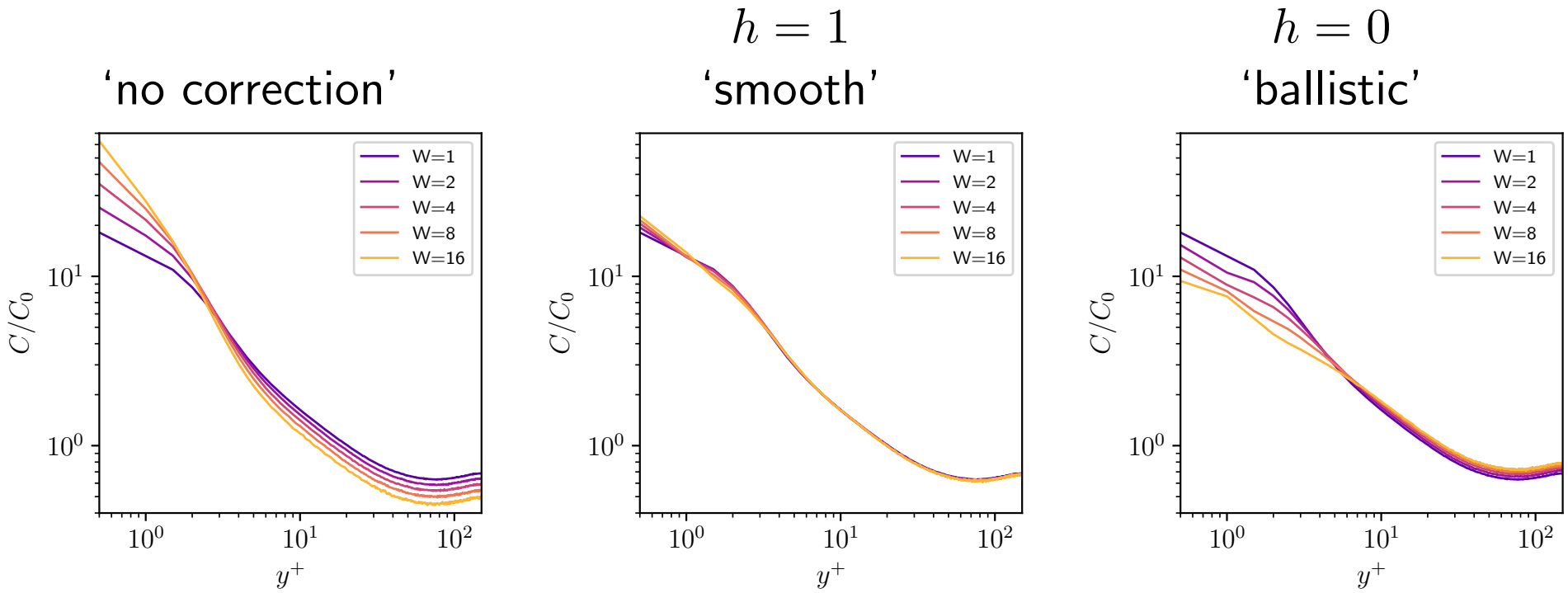
'no correction'



'smooth'



Results for $St^+ = 8$ ($\Phi_V = 1 \times 10^{-4}$)



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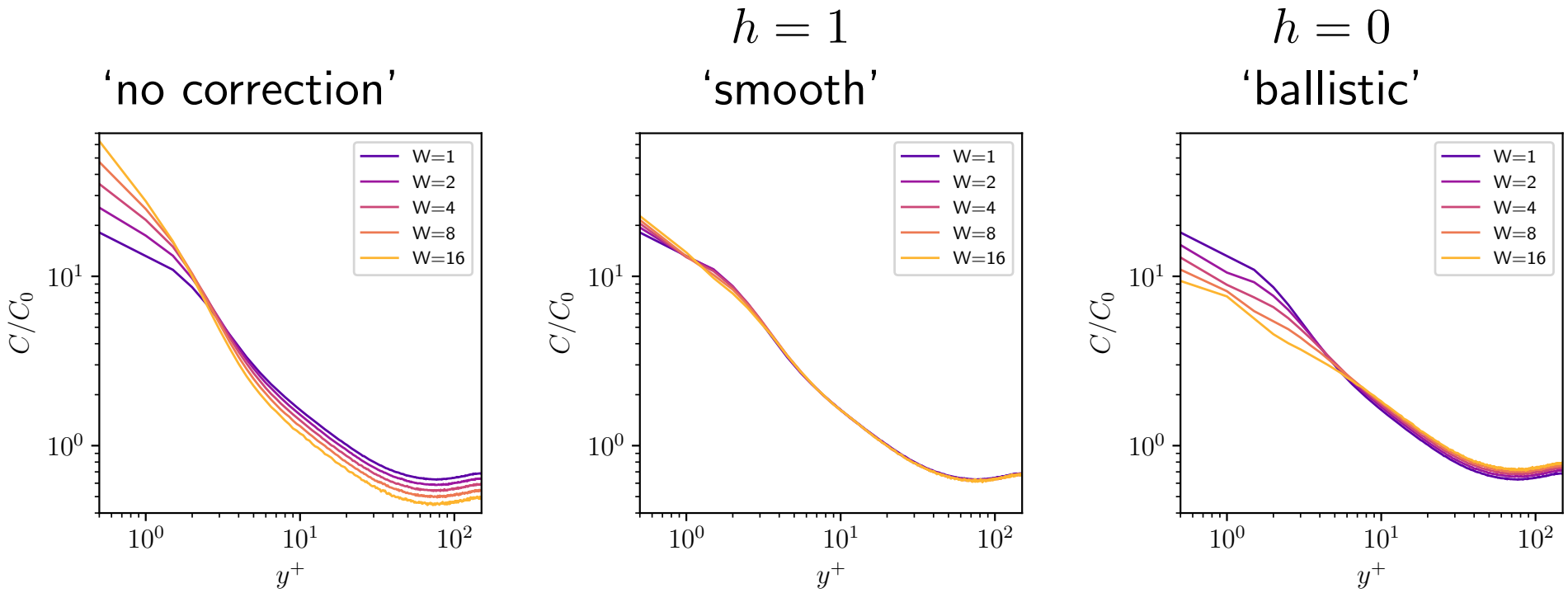
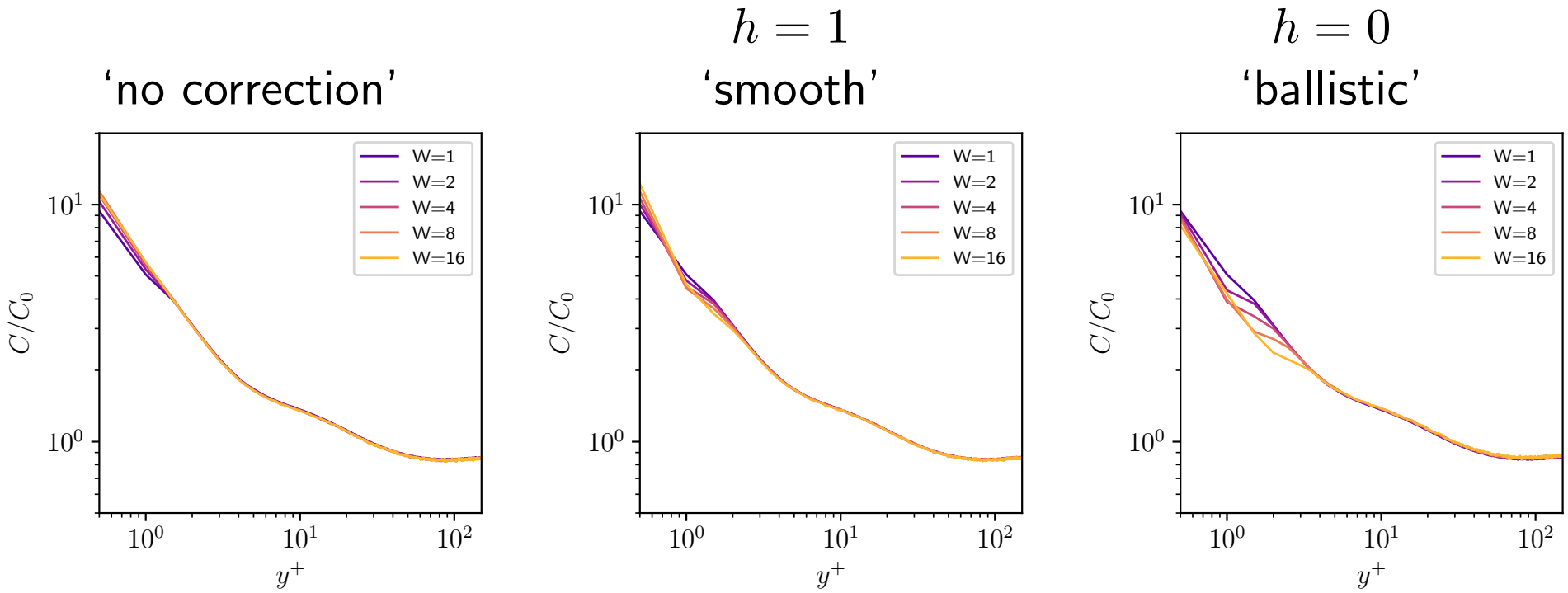


At $St^+ = 8$, the 'smooth' scaling, $h = 1$, seems better.

Results for $St^+ = 2$ ($\Phi_V = 1 \times 10^{-4}$)



At $St^+ = 2$, low sensitivity to collisions.

Local model for h

Limiting behaviors confirmed:

- $h = 0$ works better for $St^+ \geq 32$
- $h = 1$ works better for $St^+ \leq 8$

For each collision, detect h based on:

$$b = \frac{|v_{rel}|\tau_p}{d_c - d_p} = \frac{\text{stopping distance}}{\text{additional distance travelled to collision}}$$

Limiting behaviors are:

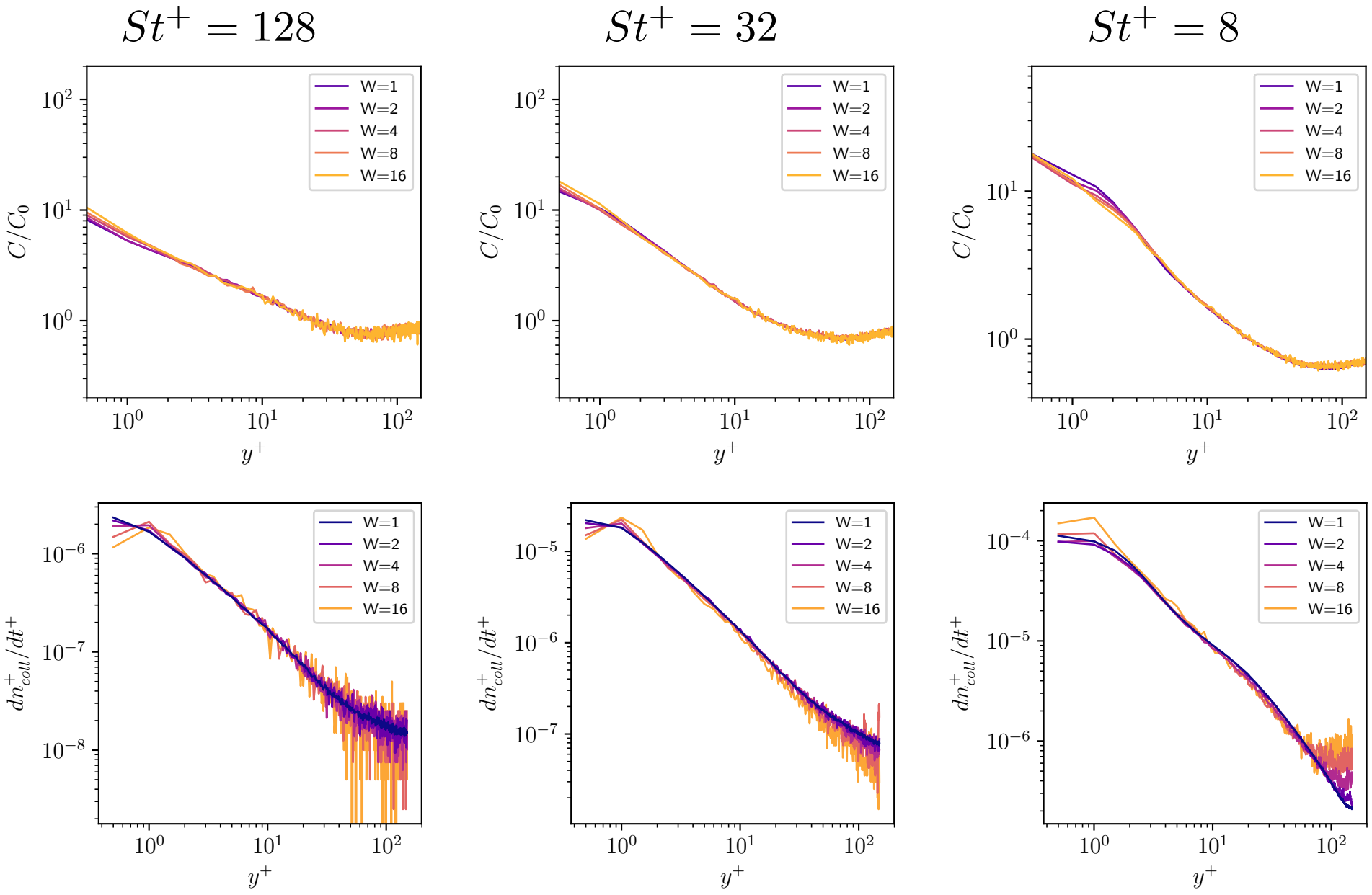
- $b \to 0$: slaved to relative flow velocity, 'smooth', $h = 1$
- $b \to \infty$: 'ballistic', $h = 0$

Proposed form:

$$h = \exp\left(-\frac{b}{b_{tr}}\right)$$

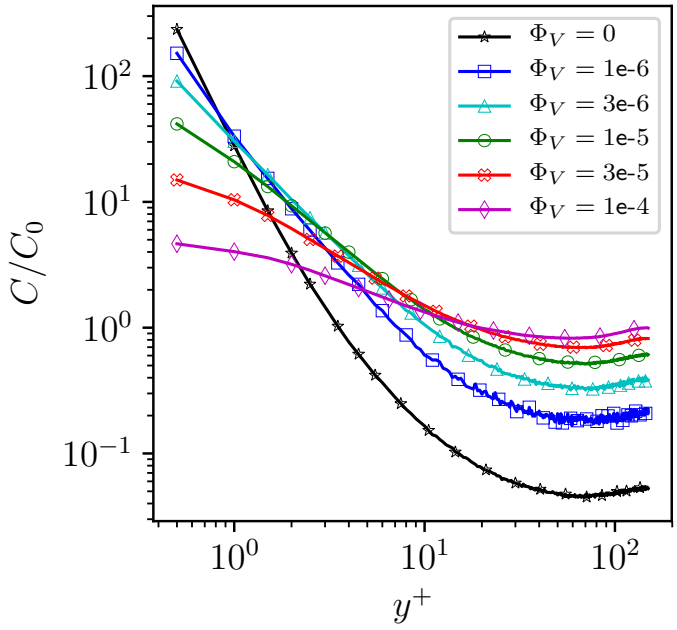
with one free parameter, b_{tr}, to be determined empirically.

Results for $b_{tr} = 32$



Super-particle collisions summary

- Super-particle approach: $N_c < N_p$
  - turbophoresis sensitive to Φ_V
  - broken invariance of statistical evolution with $W = N_p/N_c$



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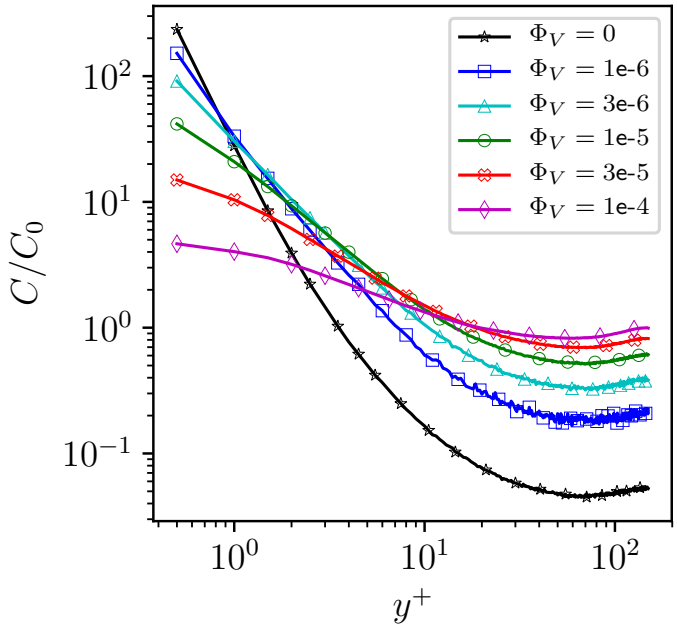
  - retain deterministic collisions



Super-particle collisions summary

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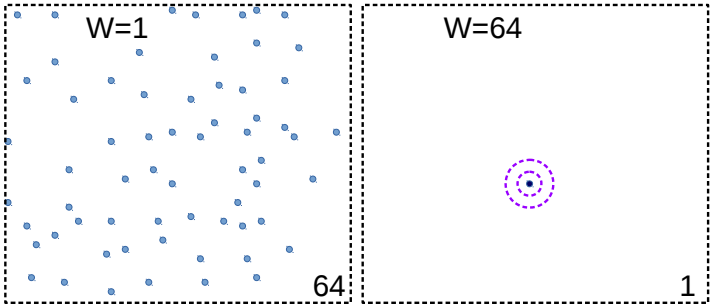
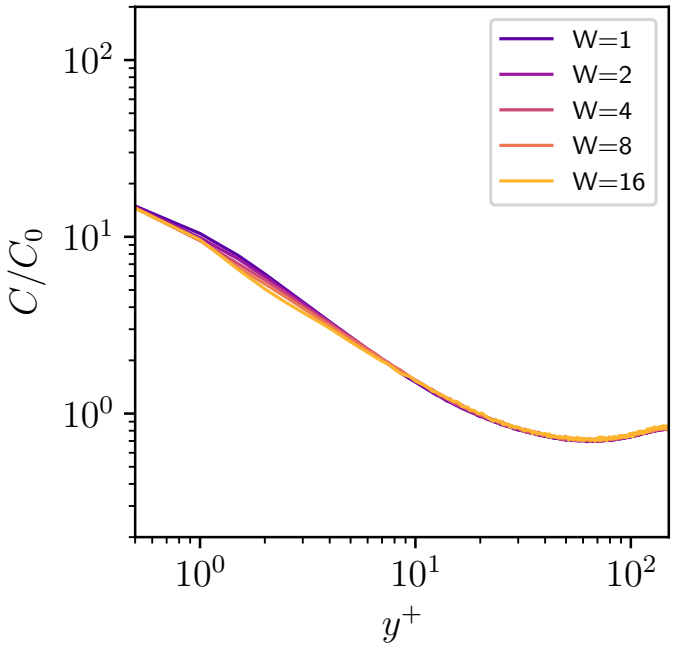
- Two limits, two scalings
  - large St^+: $d_c \sim W^{1/2}$
  - small St^+: $d_c \sim W^{1/3}$





Super-particle collisions summary

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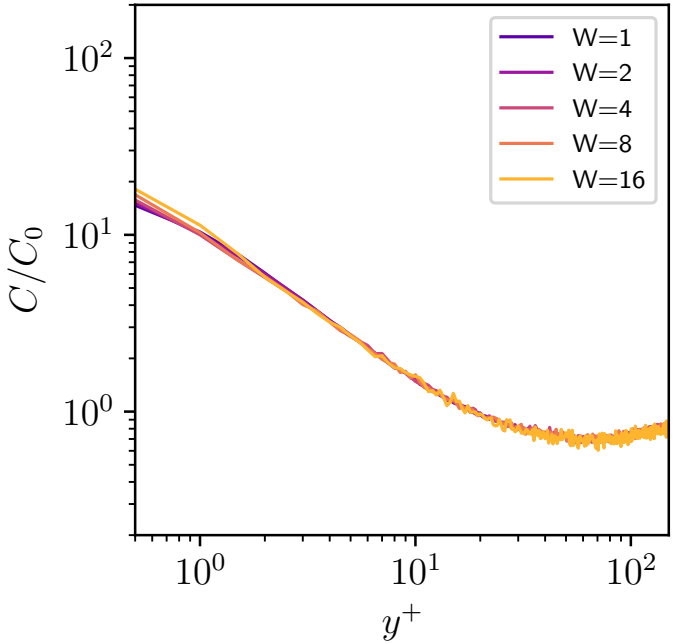
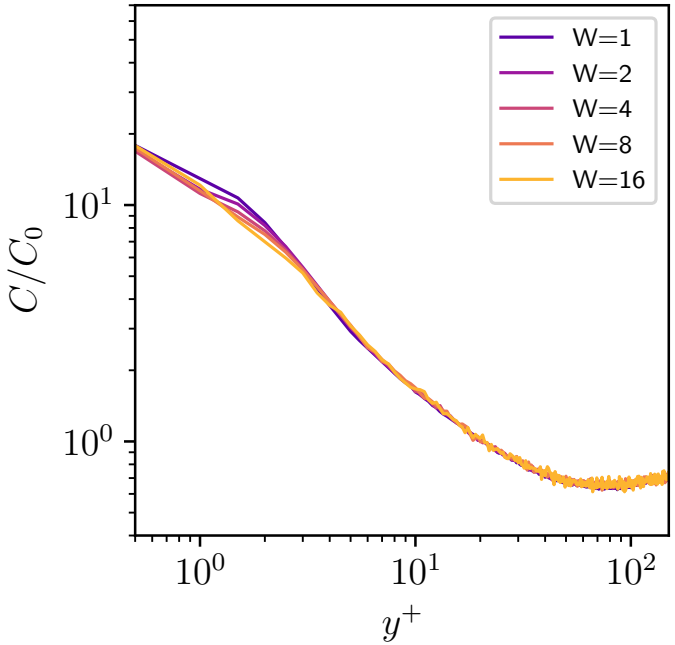
  - retain deterministic collisions
- Two limits, two scalings
  - large St^+: $d_c \sim W^{1/2}$
  - small St^+: $d_c \sim W^{1/3}$
- Determine h for each collision
  - $h = h(|v_{rel}|, \tau_p)$
  - $d_c \sim W^{1/(2+h)}$
  - $e_c \sim W^{-h/(2+h)}$
  - effective across all St^+





Acknowledgements

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- WMLES collaborator: Maxime Bassenne
- PSAAP UQ and super-particles: Lluis Jofre
- PSAAP validation simulations: Thomas Jaravel, Mahdi Esmaily, etc...

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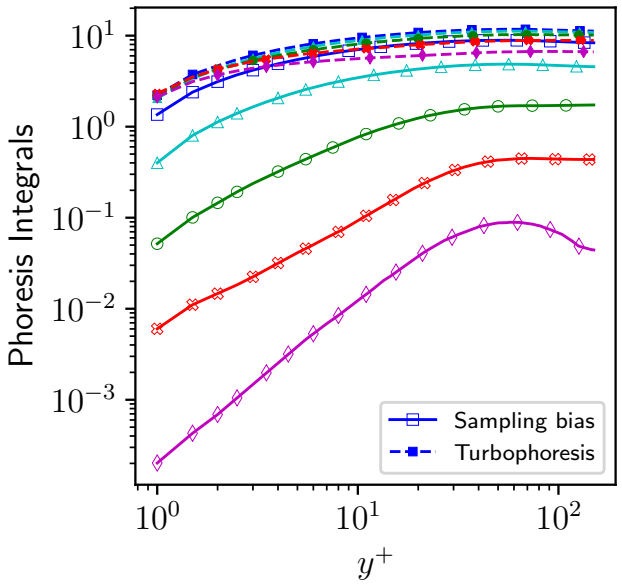
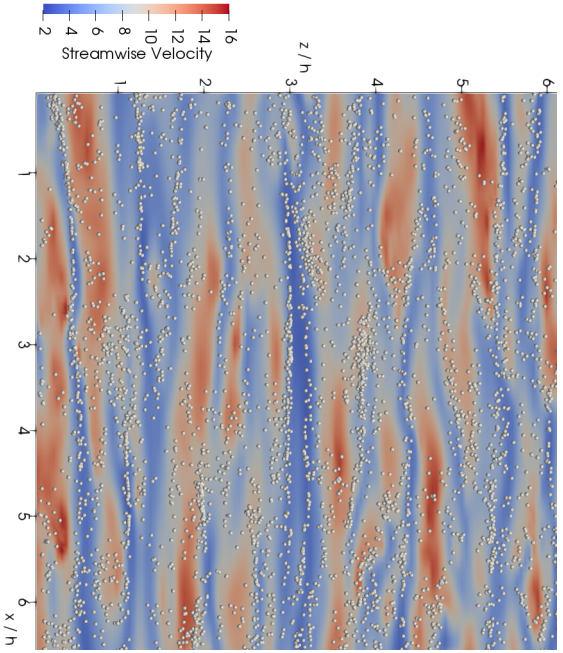
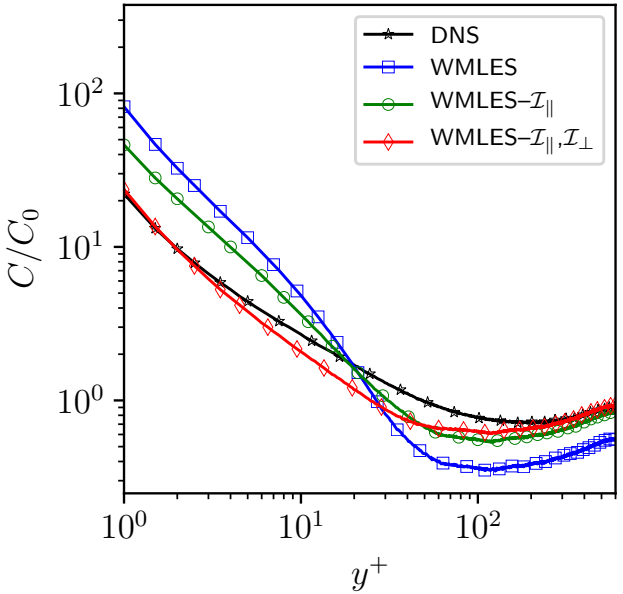
Thank you for your attention! Any questions?

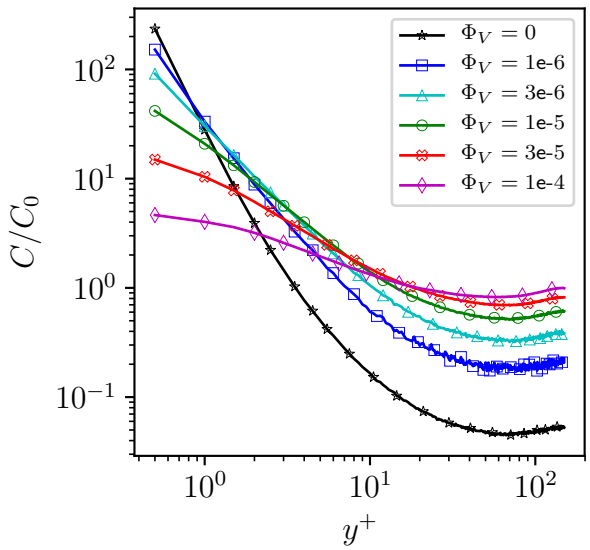
Turbophoresis, biased sampling, and wall-modeled LES

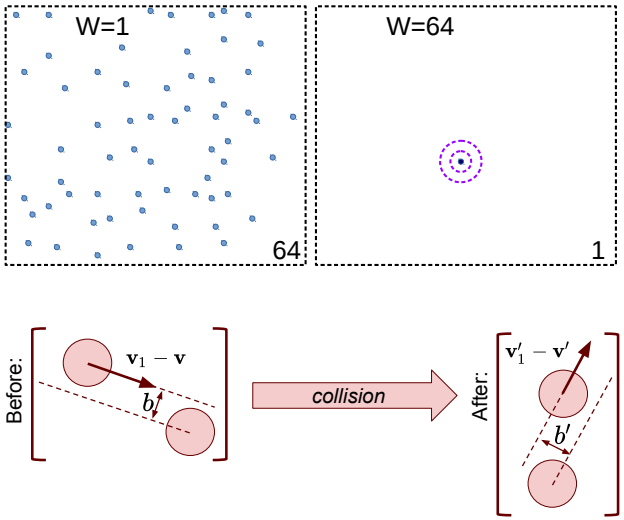


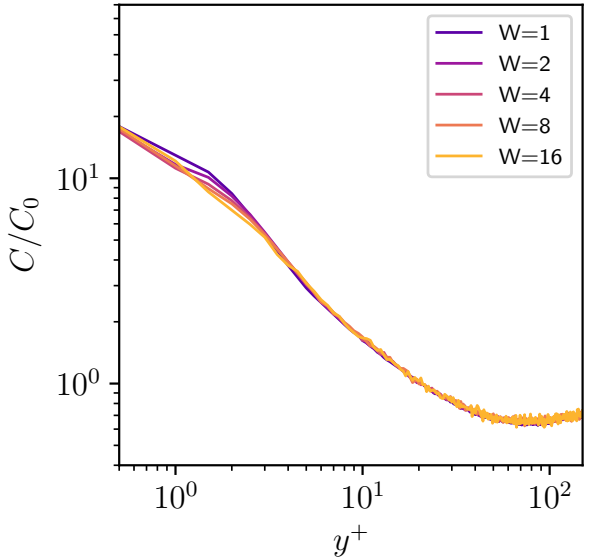




Turbophoresis, particle-particle collisions, and super-particles

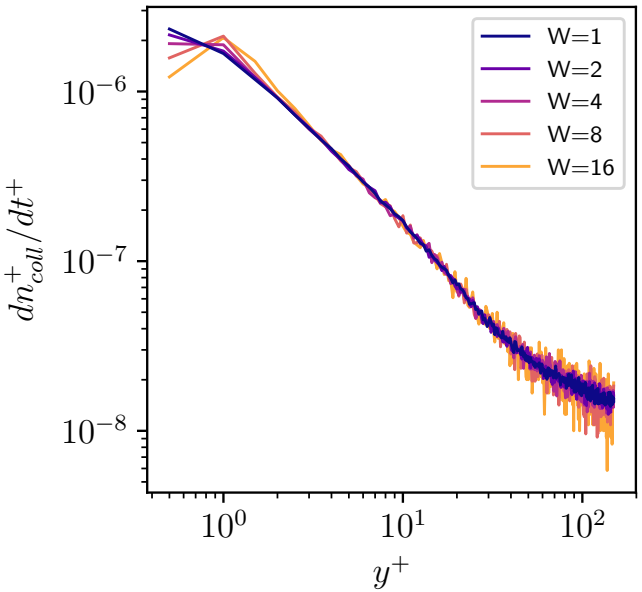






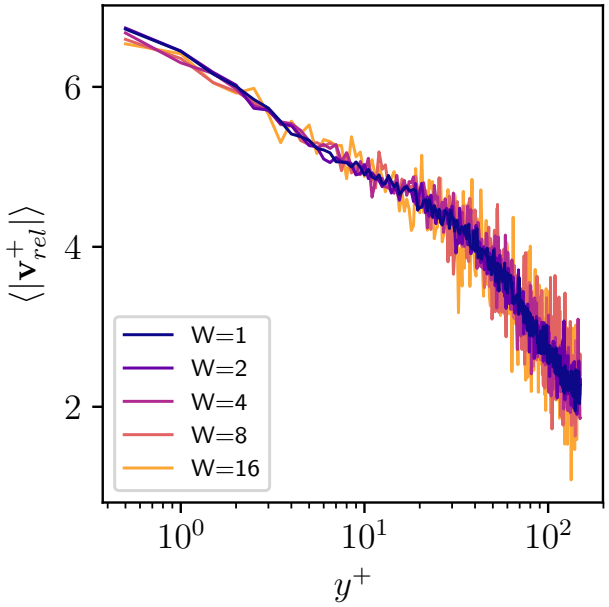
Backup slides

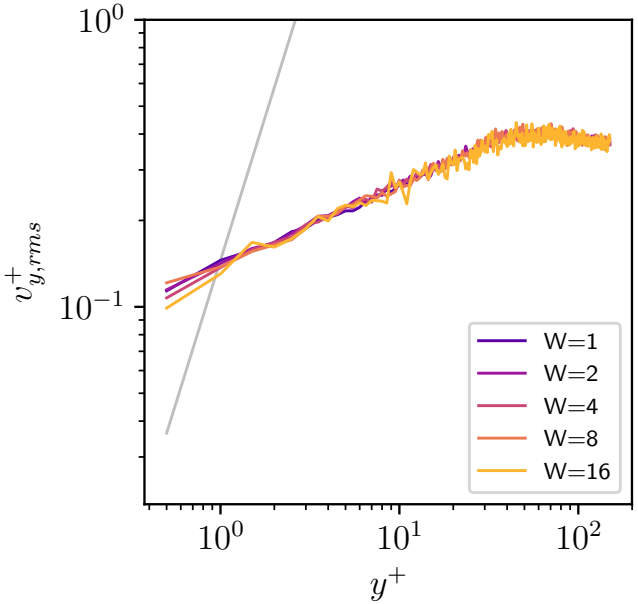
A Closer Look: $St^+ = 128$, $h = 0$ (ballistic correction)



← Collision freq.

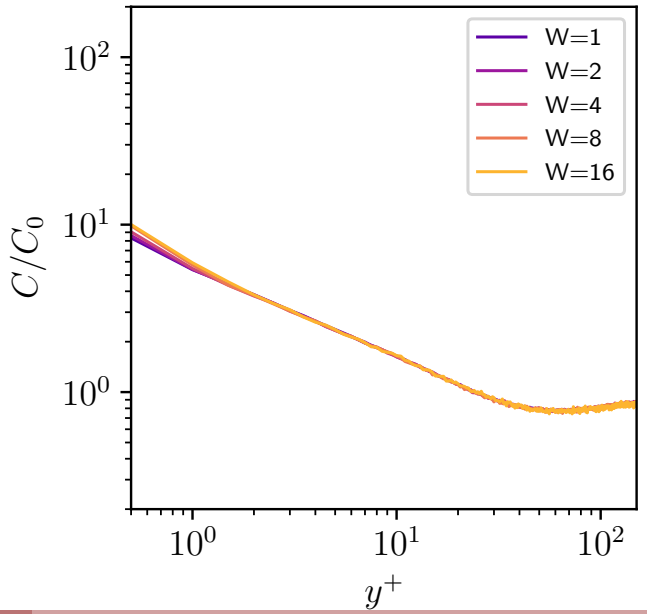
Collision vel. →



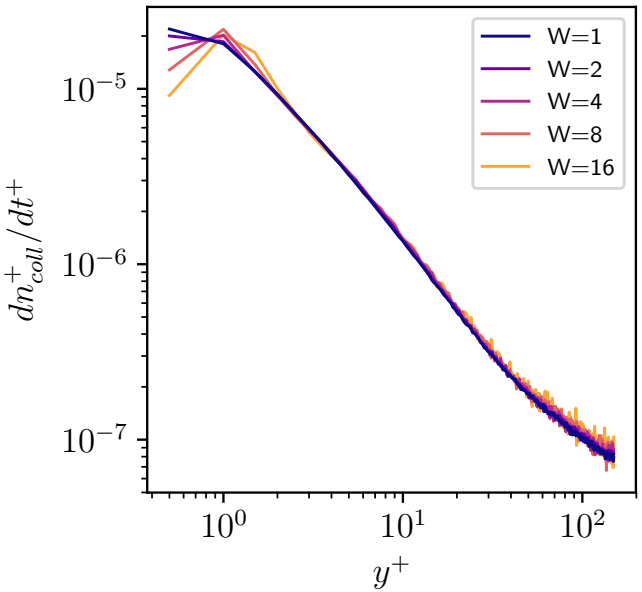


← Particle vel. RMS

Concentration →



A Closer Look: $St^+ = 32$, $h = 0$ (ballistic correction)



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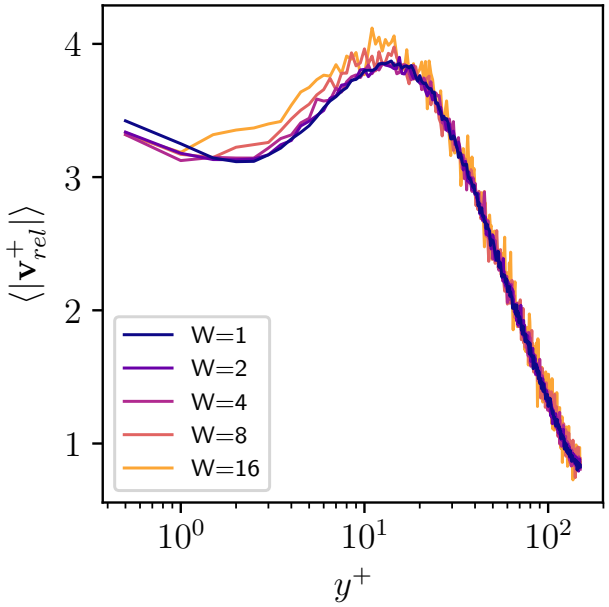

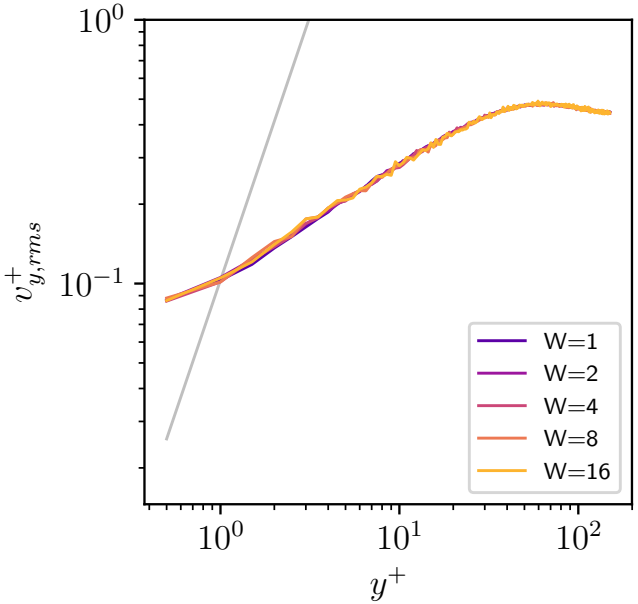

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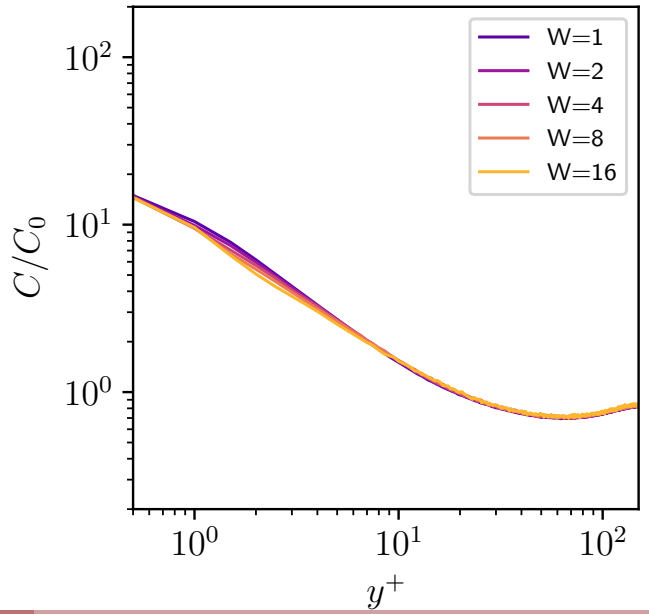
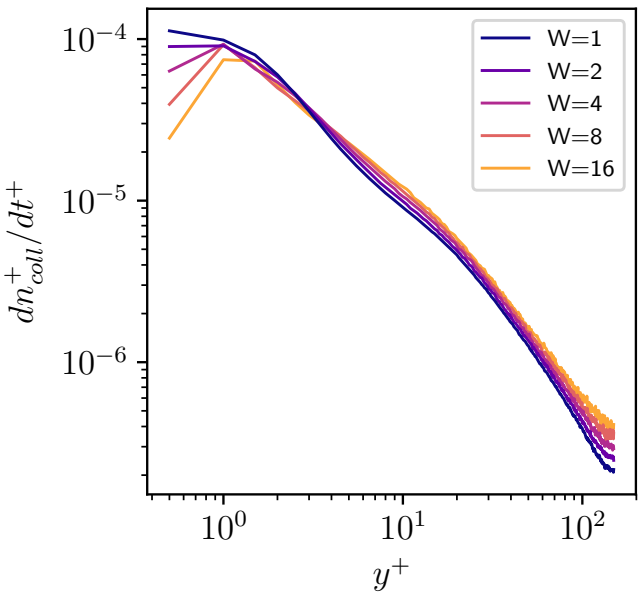
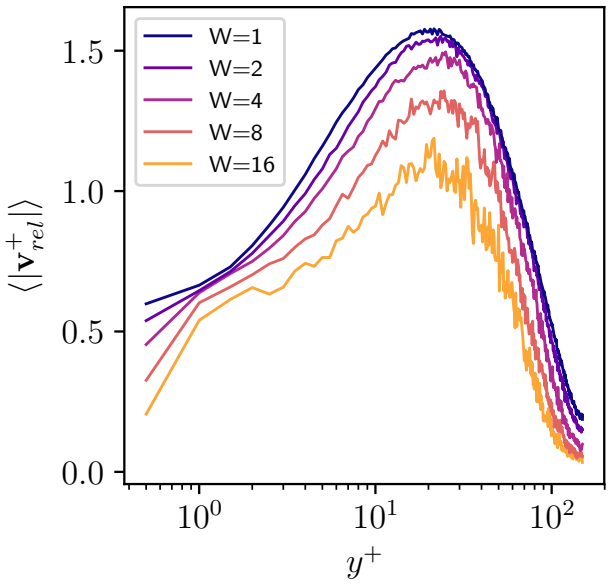


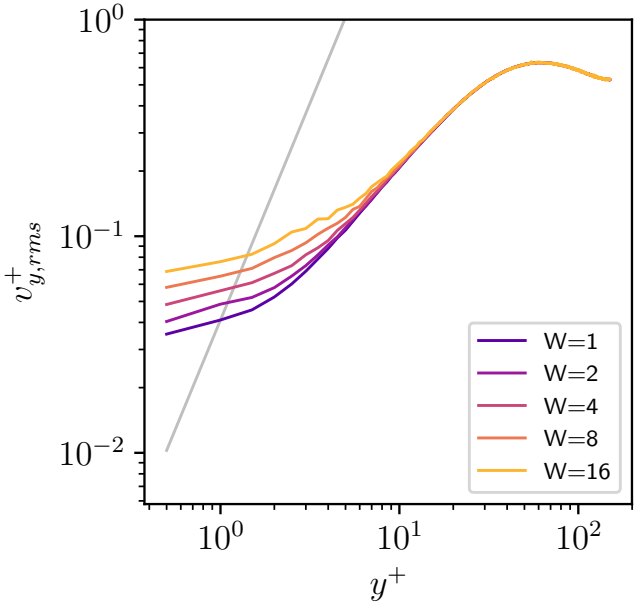
A Closer Look: $St^+ = 8$, $h = 1$ (smooth correction)



← Collision freq.

Collision vel. →





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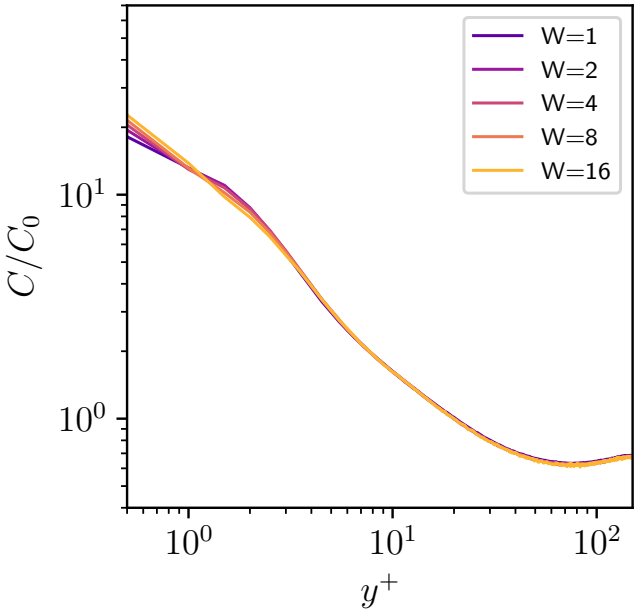
Concentration →