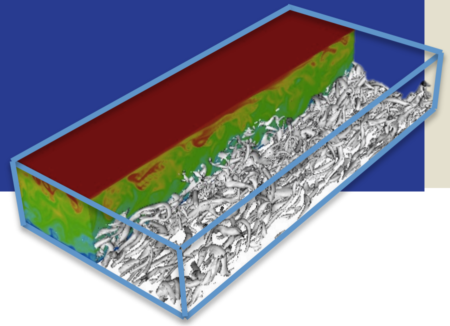


COMETE Training School on Direct numerical simulation of solid particles, droplets and bubbles in turbulence

Multiphase Flow Laboratory

University of Udine

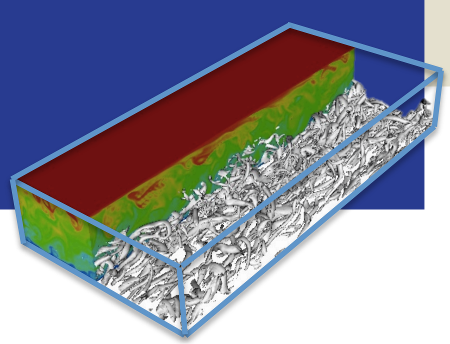
Simulation approaches to HPC of multiphase turbulent flows

Cristian Marchioli

University of Udine & CISM

Wien 11-13 February 2020

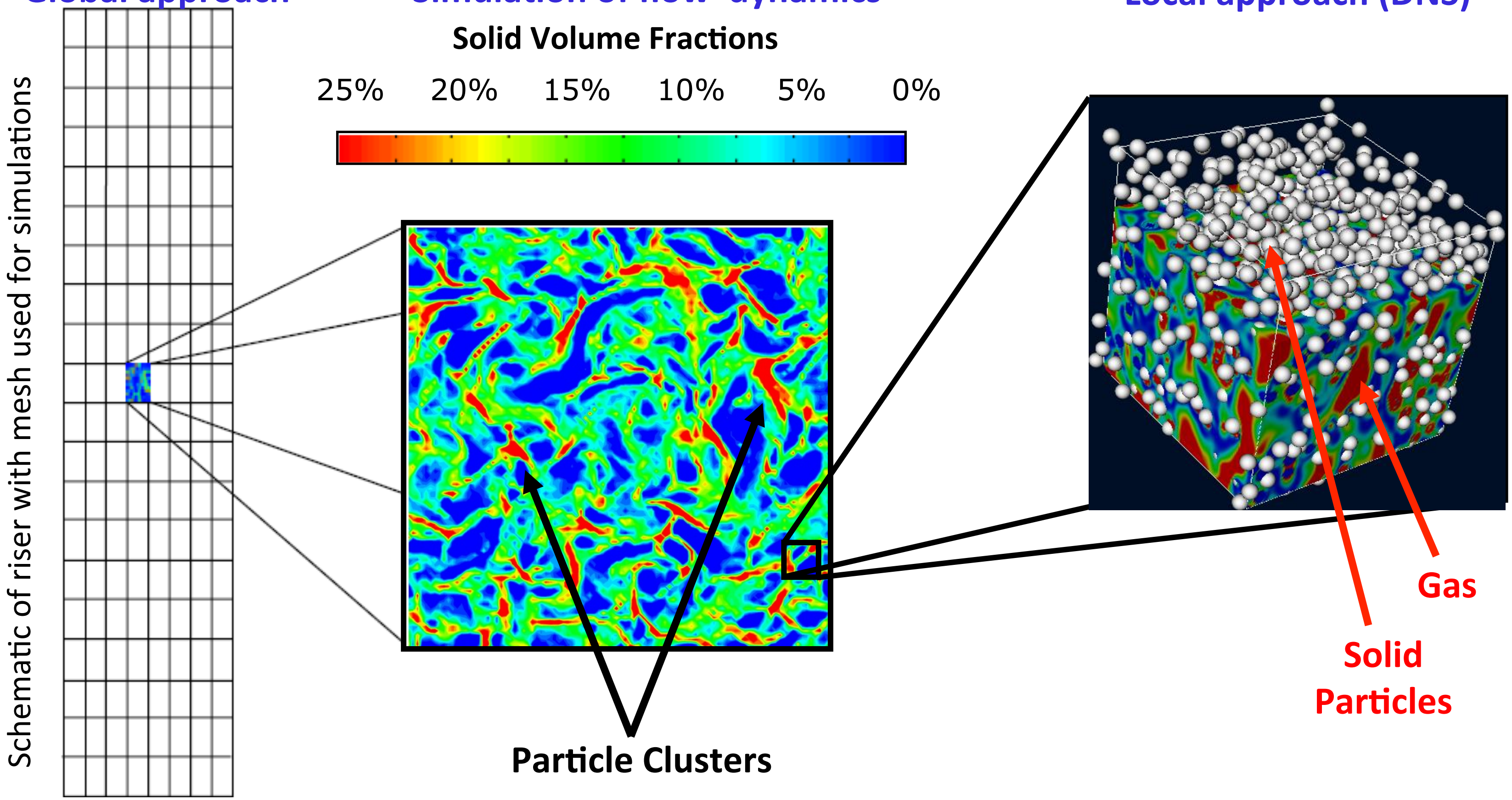
COMETE



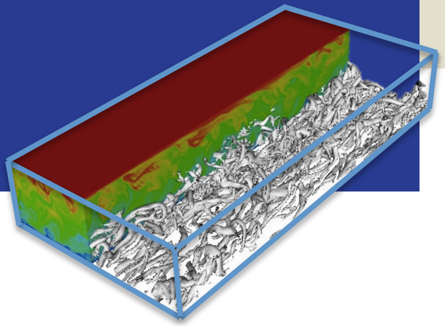
Particle-laden flows are multi-scale & require hierarchic approaches

Multiphase Flow Laboratory
University of Udine

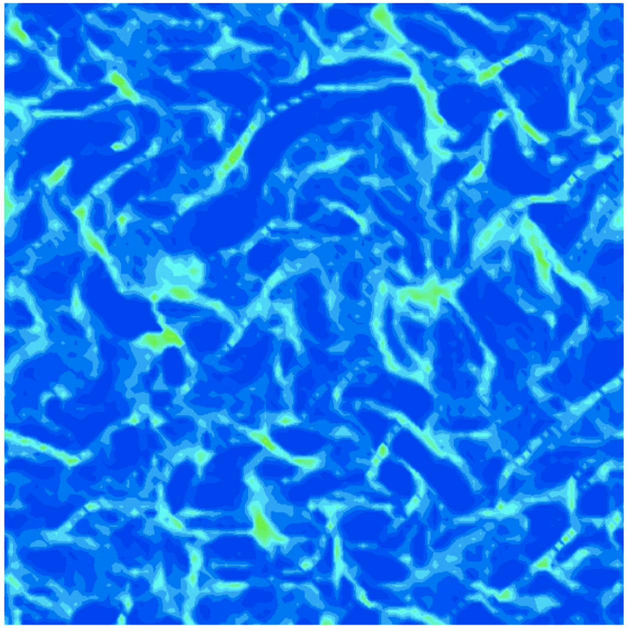
Global approach | Simulation of flow dynamics | Local approach (DNS)



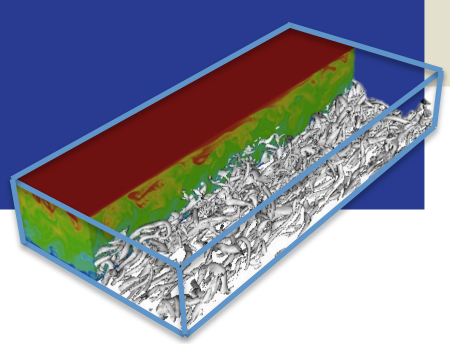
Macro-scale (cm-m) **Meso-scale** (mm–cm) **Micro-scale** (μm)



What’s common to (almost) all particle-laden turbulent flows?



Are we looking at a particle-laden flow or at the bottom of a swimming pool on a sunny summer day?



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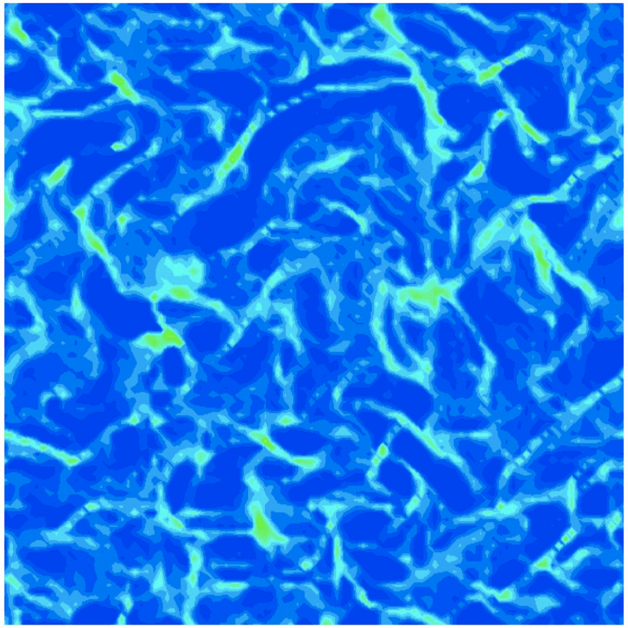
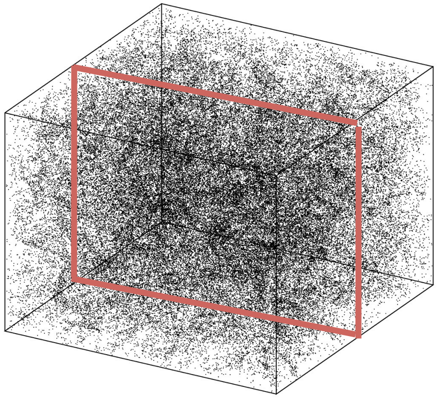
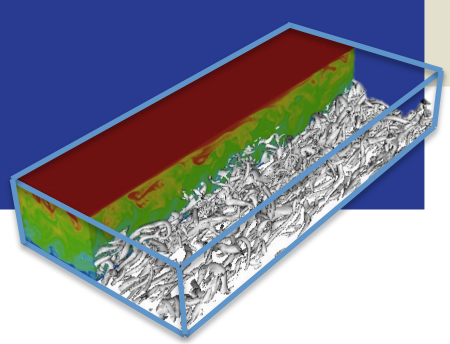




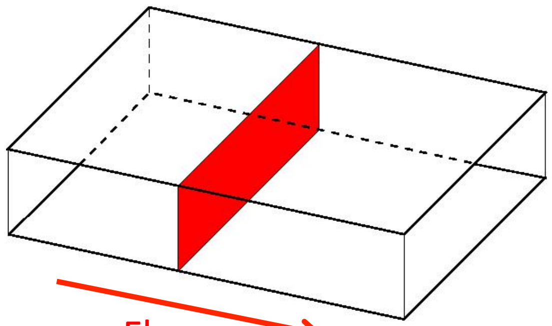
Particle number density in homogeneous isotropic turbulence (Re_{λ}=51, St=1)

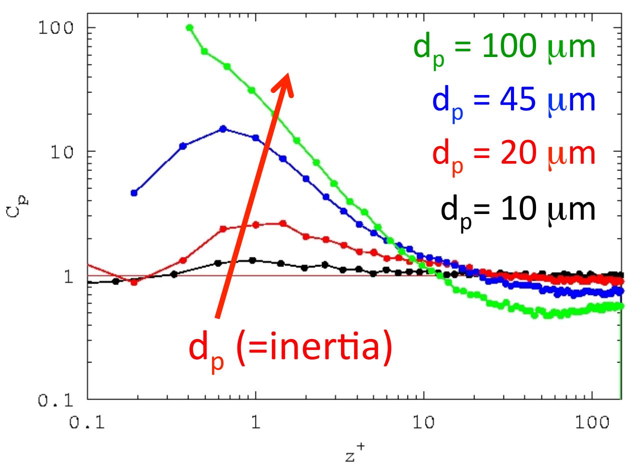
Particles concentrate preferentially in high-strain, low-vorticity regions due to their inertia

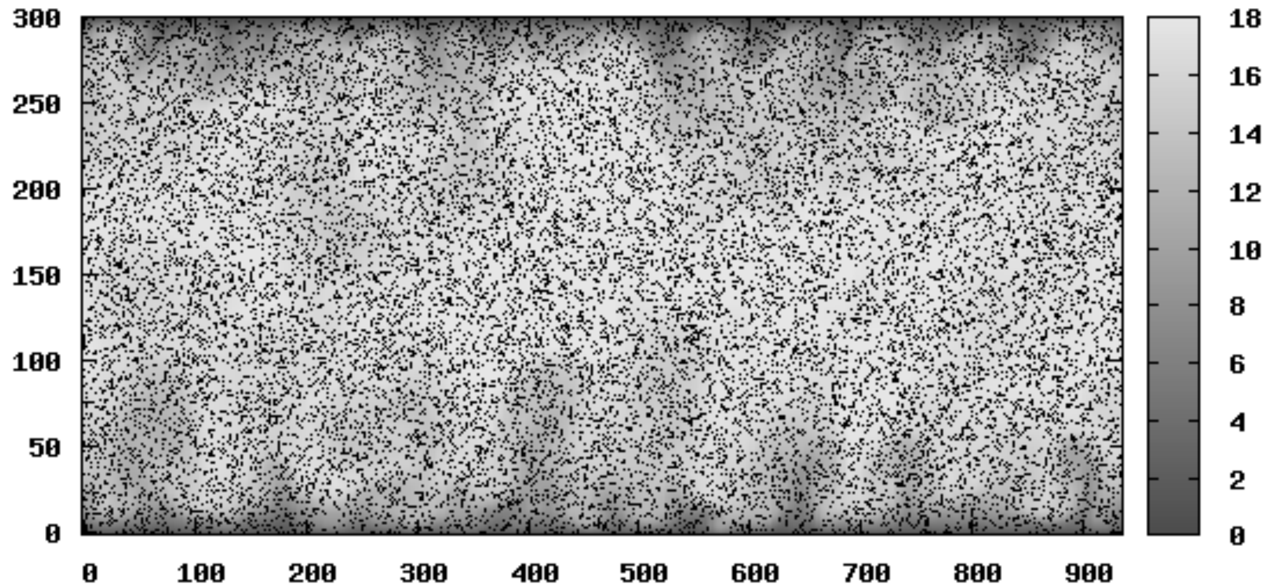


Near-wall particles-turbulence interactions

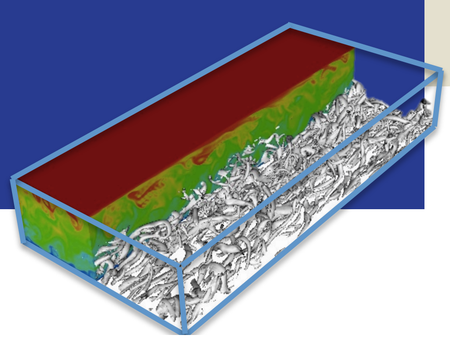
In wall-bounded flows inertial particles concentrate preferentially but also accumulate at the wall



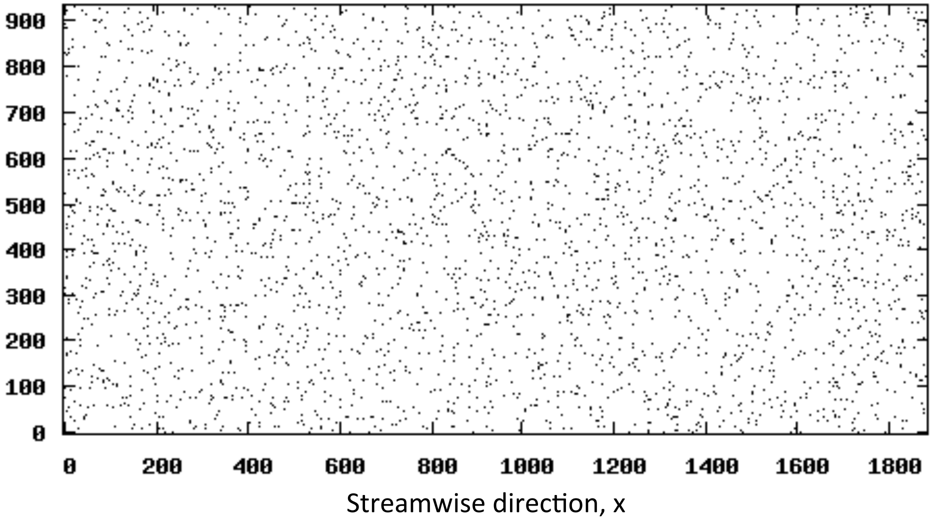


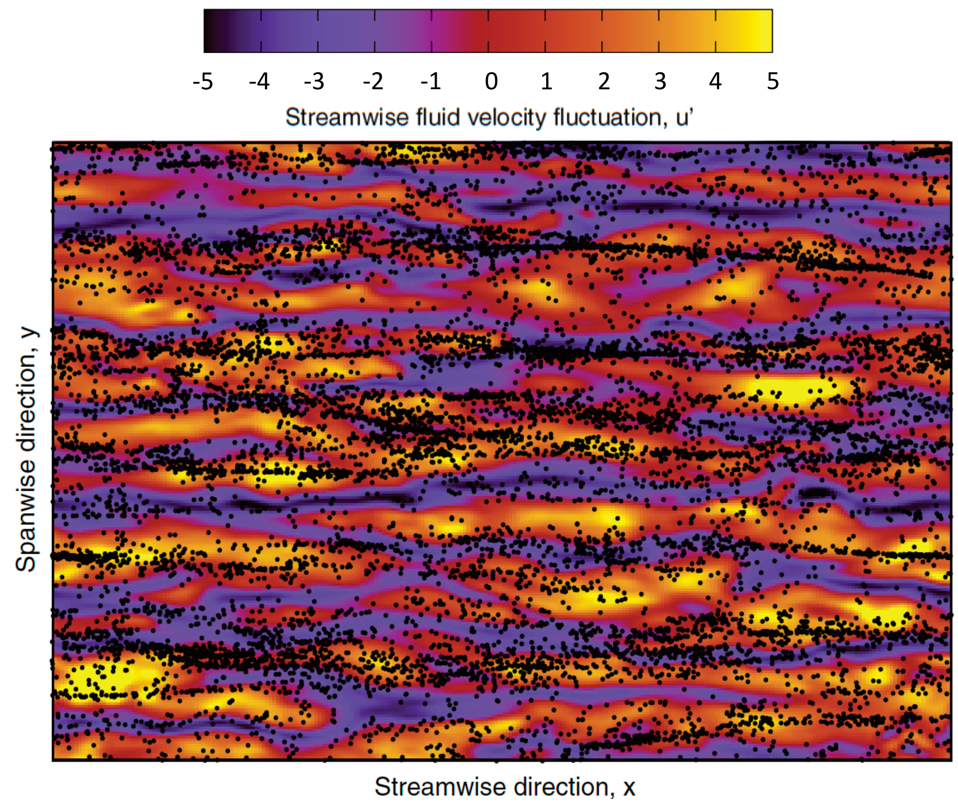


Time evolution of particle distribution in a turbulent channel (Re_H=9000, d_p=100 μm)



Near-wall particles-turbulence interactions





In bounded flows, inertial particles concentrate preferentially but also accumulate at the wall, segregating into low-speed fluid streaks

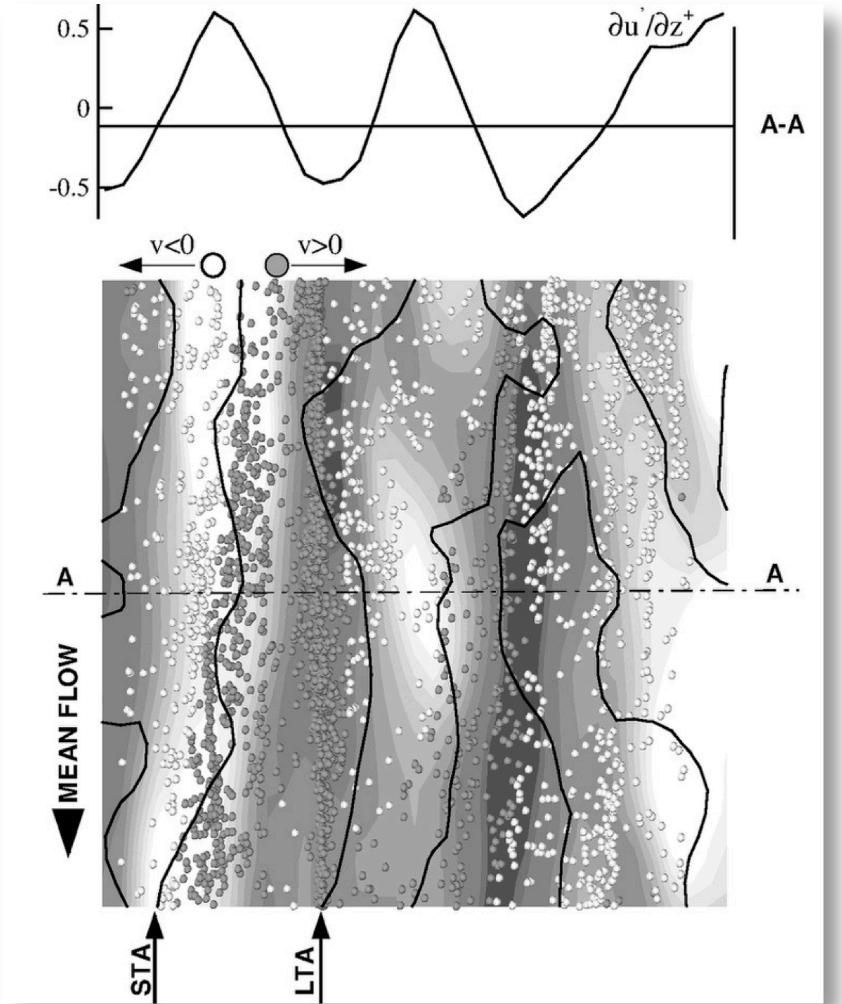
Near-wall particles-turbulence interactions

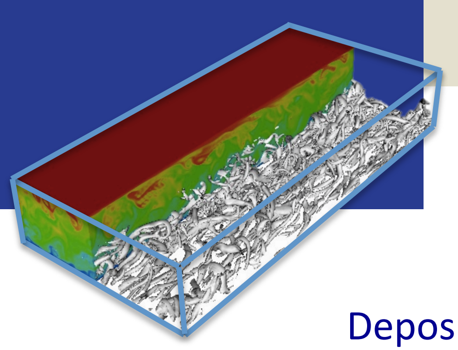
Instantaneous particle distribution in the viscous sublayer (ref. case: St=25 Particles in TCF at Re=150)

Particles tend to sample:

STA (Short Term Accumulation): regions where particles reach the near-wall layer

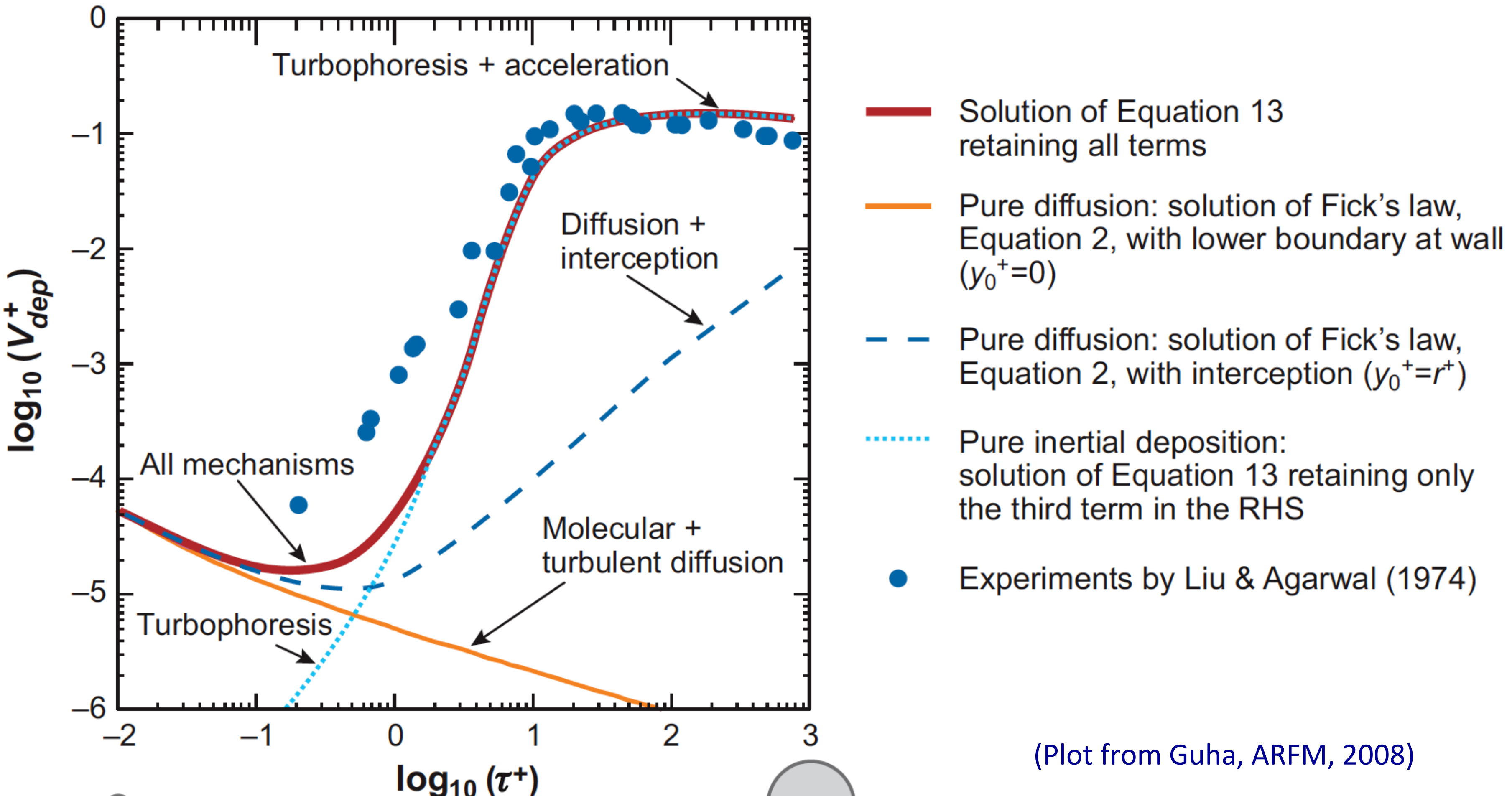
LTA (Long Term Accumulation): regions where particles remain trapped



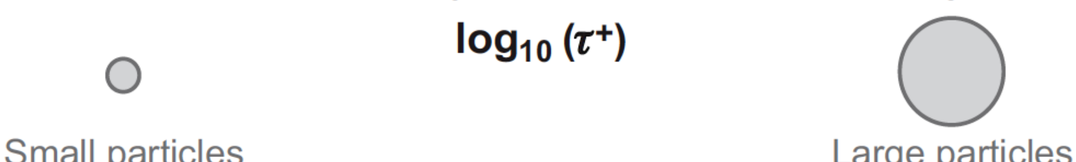


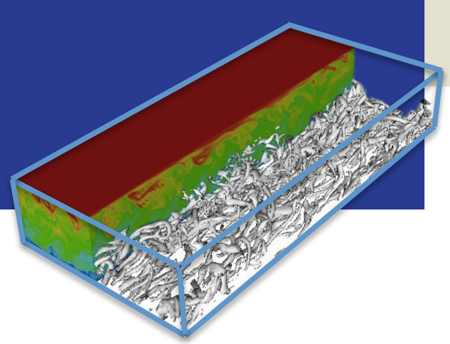
Near-wall particles-turbulence interactions

Deposition & re-entrainment rates also change depending on particle inertia



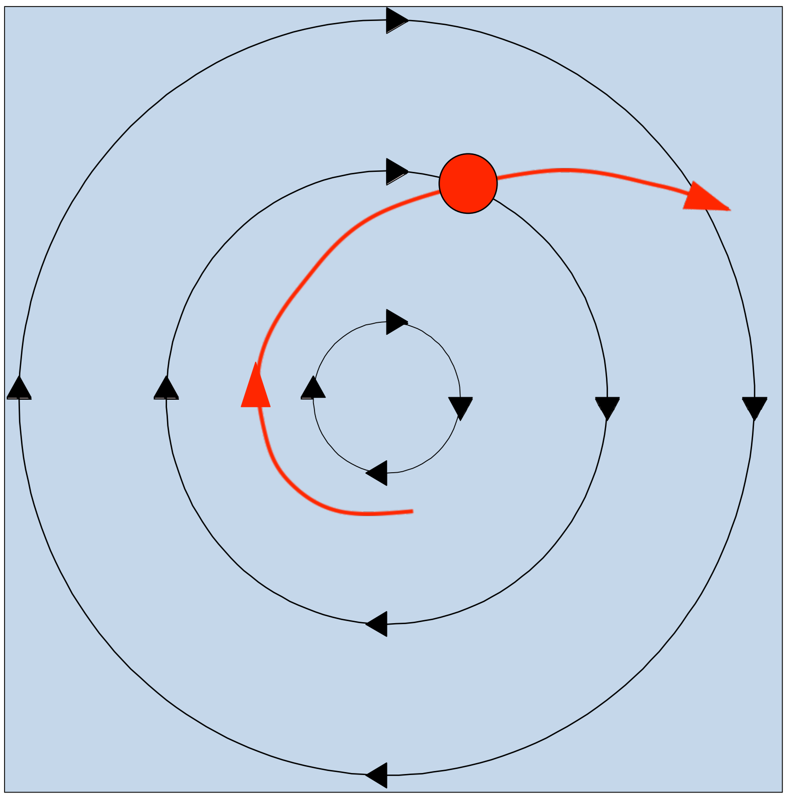
(Plot from Guha, ARFM, 2008)





What's common to (almost) all particle-laden turbulent flows?

My answer is: particles tend to deviate from fluid streamlines!



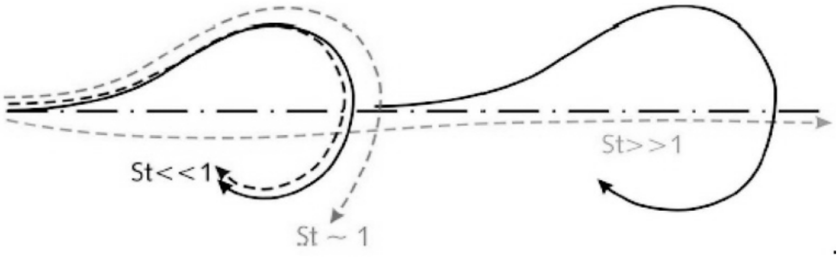
Source of bias: particle inertia!

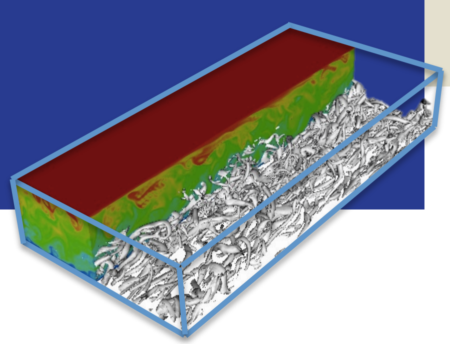
Deviations depend on the particle response time to the underlying flow field:

Particle Relaxation Time: $\tau_p = \frac{\rho_p d_p^2}{18\mu}$

Flow Time Scale: τ_f

Particle Stokes number: $St = \frac{\tau_p}{\tau_f}$

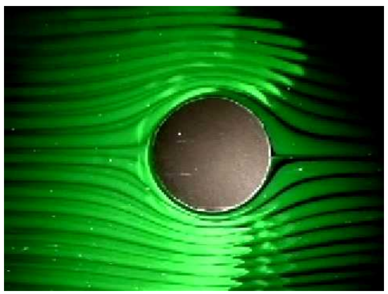




A numerical approach to study preferential concentration

The simplest dynamical model to study “inertia-driven” preferential concentration considers small **pointwise** spherical particles (only source of bias is inertia!)

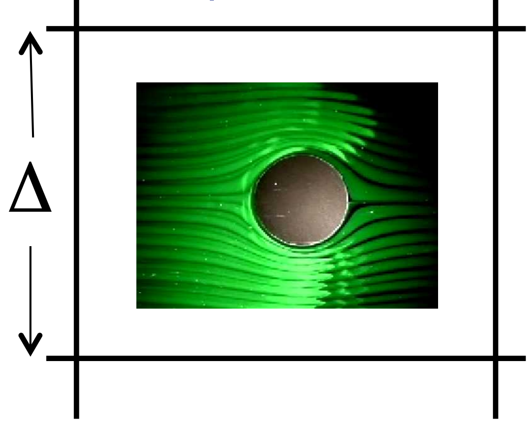
No wake (Stokes flow)



$$\mathrm{Re}_p = \frac{\mathrm{u}_{rel}\mathrm{L}}{\nu} << 1$$

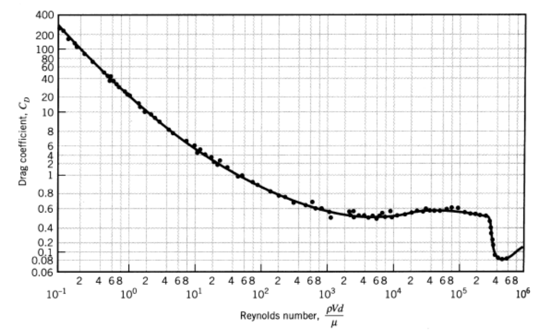
Enough to know $\mathbf{x}_p$ and $\mathbf{v}_p$!

D << η , Δ (pointwise)

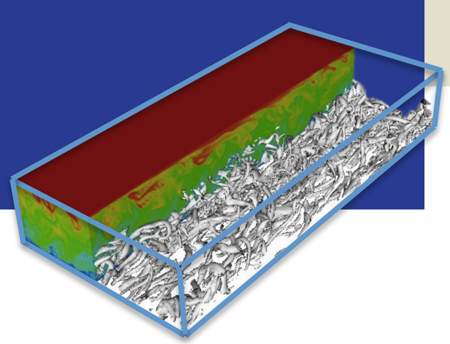


$$\frac{\mathrm{d}\mathbf{x}_p}{\mathrm{d}t} = \mathbf{v}_p, \quad m_p \frac{\mathrm{d}\mathbf{v}_p}{\mathrm{d}t} = \sum_i \mathbf{F}_i$$

Force model: Drag

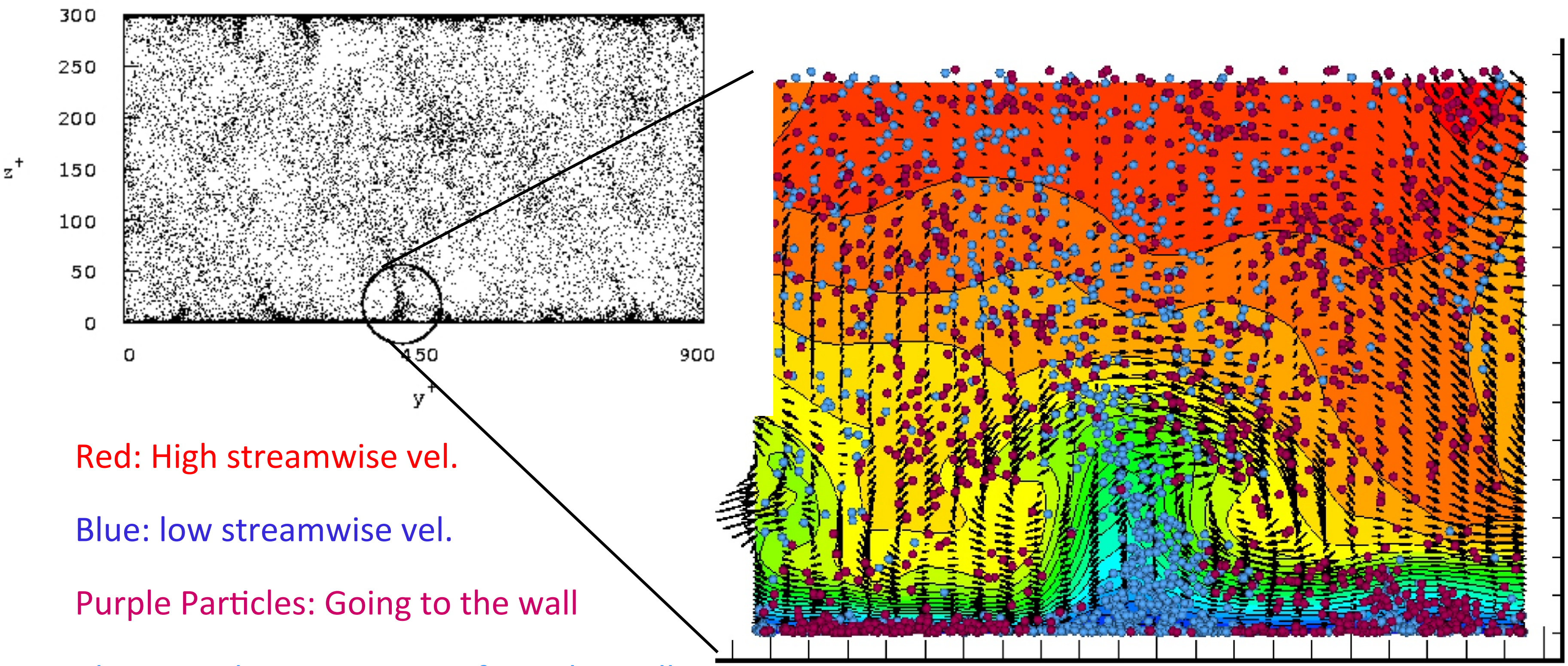


$$C_D(\mathrm{Re}_p) = \frac{\mathbf{F}_\mathrm{D}}{\frac{1}{2}\rho \mathbf{u}_\mathrm{rel}^2 \mathrm{A}_\mathrm{p}}$$



Phenomenology of preferential concentration of small particles

Physics learned from this simple model (in DNS):
Qualitative explanation of particle deposition/entrainment in DILUTE turbulent boundary layers

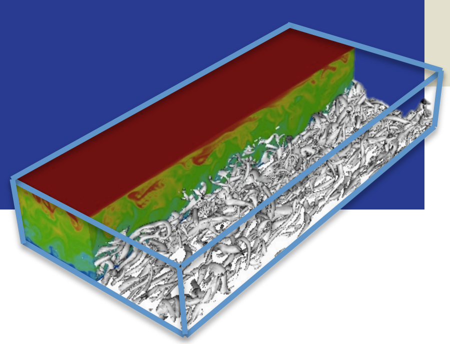


Red: High streamwise vel.

Blue: low streamwise vel.

Purple Particles: Going to the wall

Blue Particles: Going away from the wall



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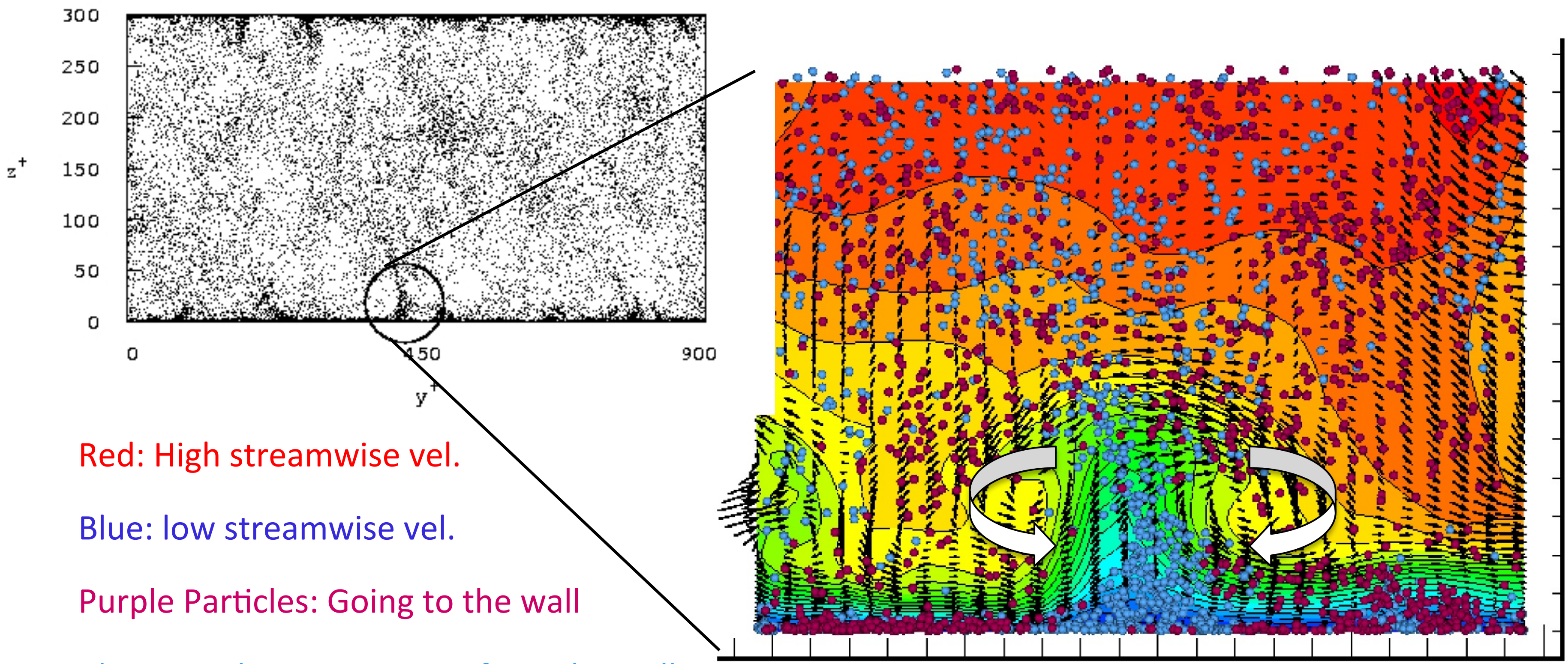

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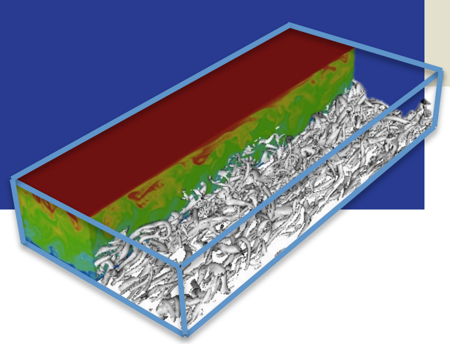

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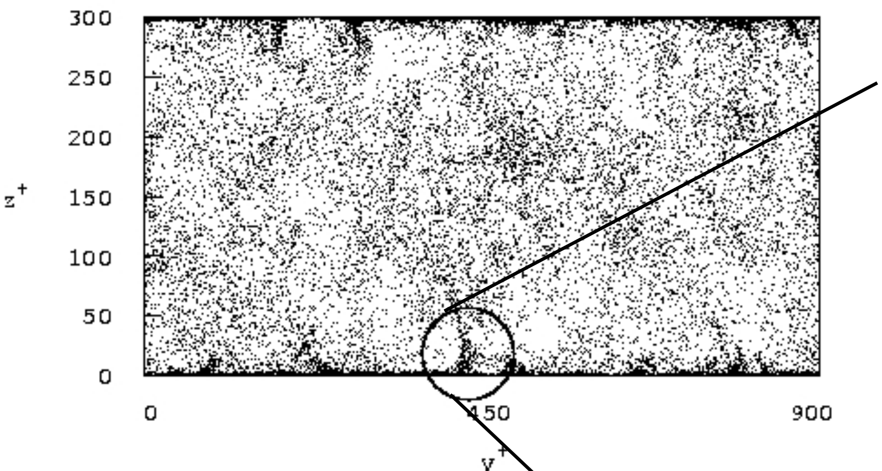
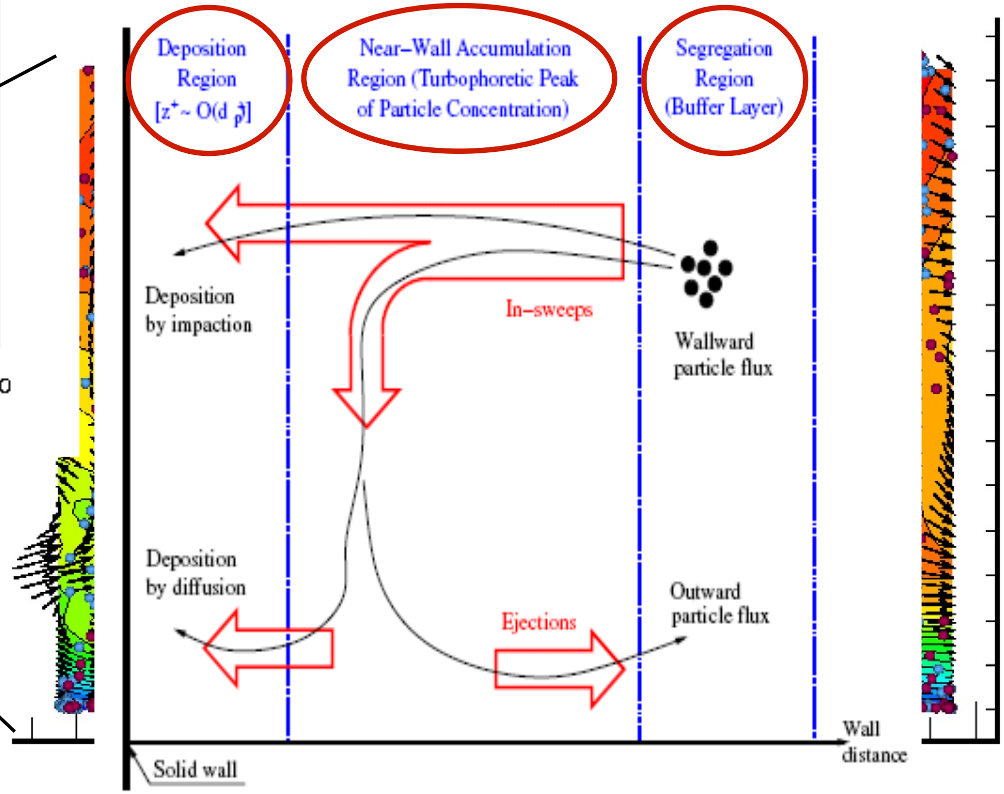


STRUCTURES → SEGREGATION → ACCUMULATION → DEPOSITION



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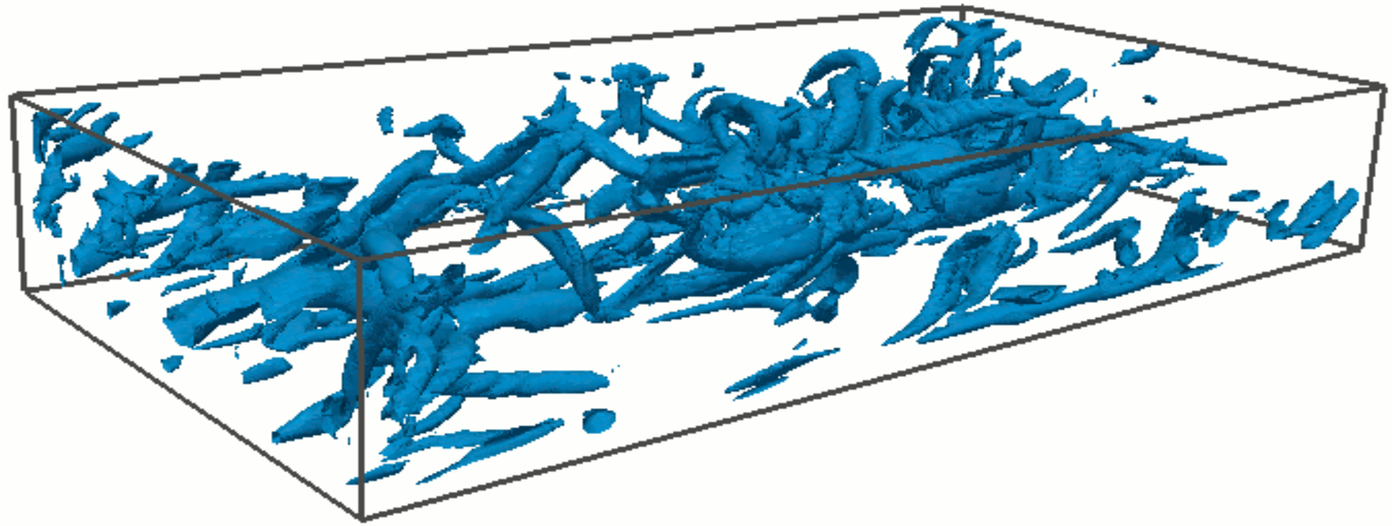
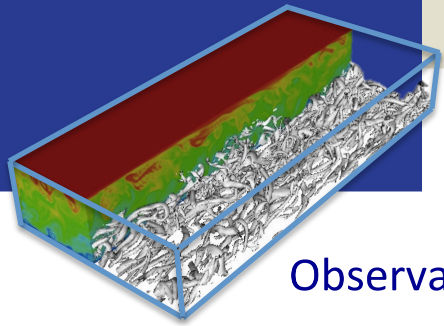
Interlude: Coherent structures in TBL

A (perhaps) naive question you might want to ask ("but were afraid to") is: what is a coherent structure?

Formal definition of CS: some spatio-temporally compact region of the flow over which some macroscopic quantity - such as velocity, vorticity or kinetic energy - is strongly correlated (see F. Waleffe, R.J. Adrian and co-workers).

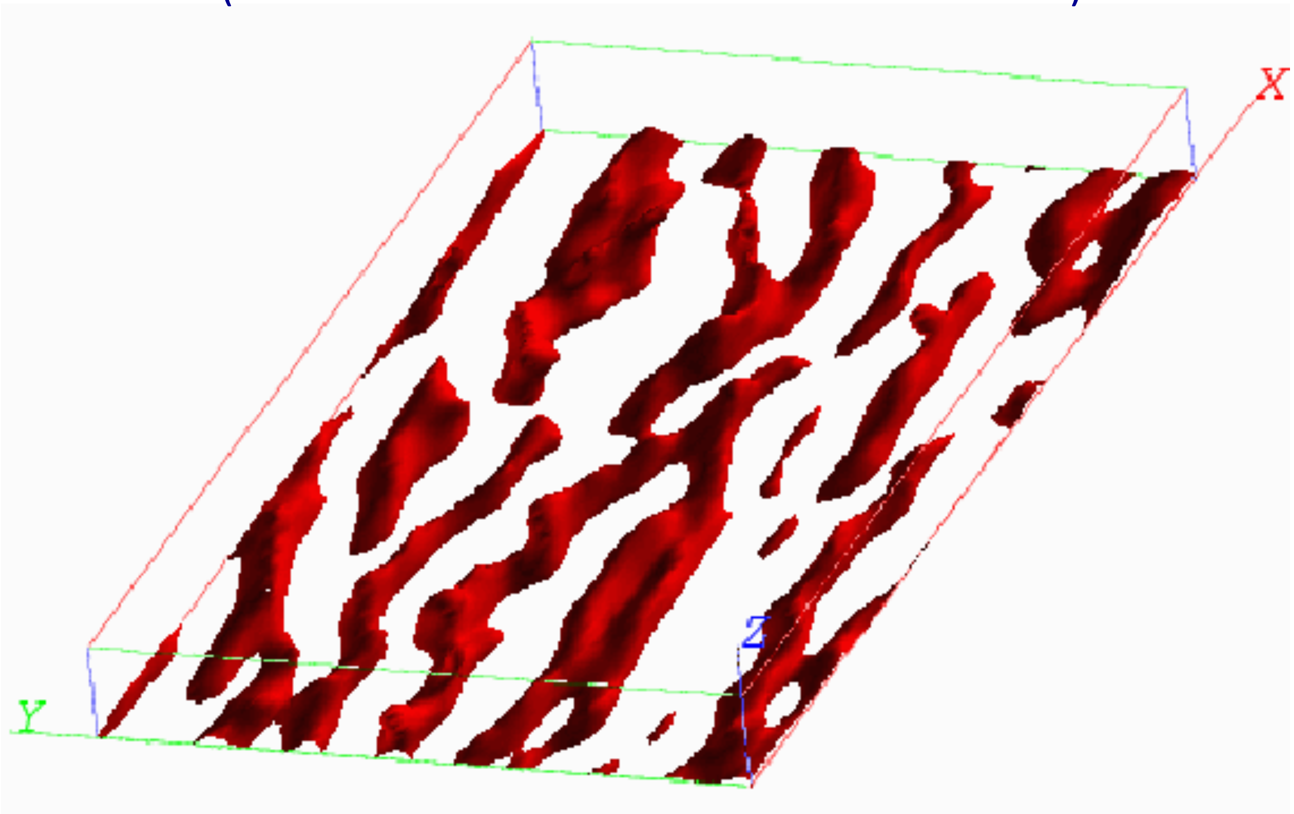


Example of turbulent coherent vortices in channel flow

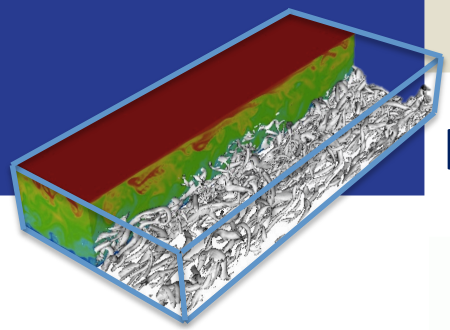


Interlude: Coherent structures in TBL

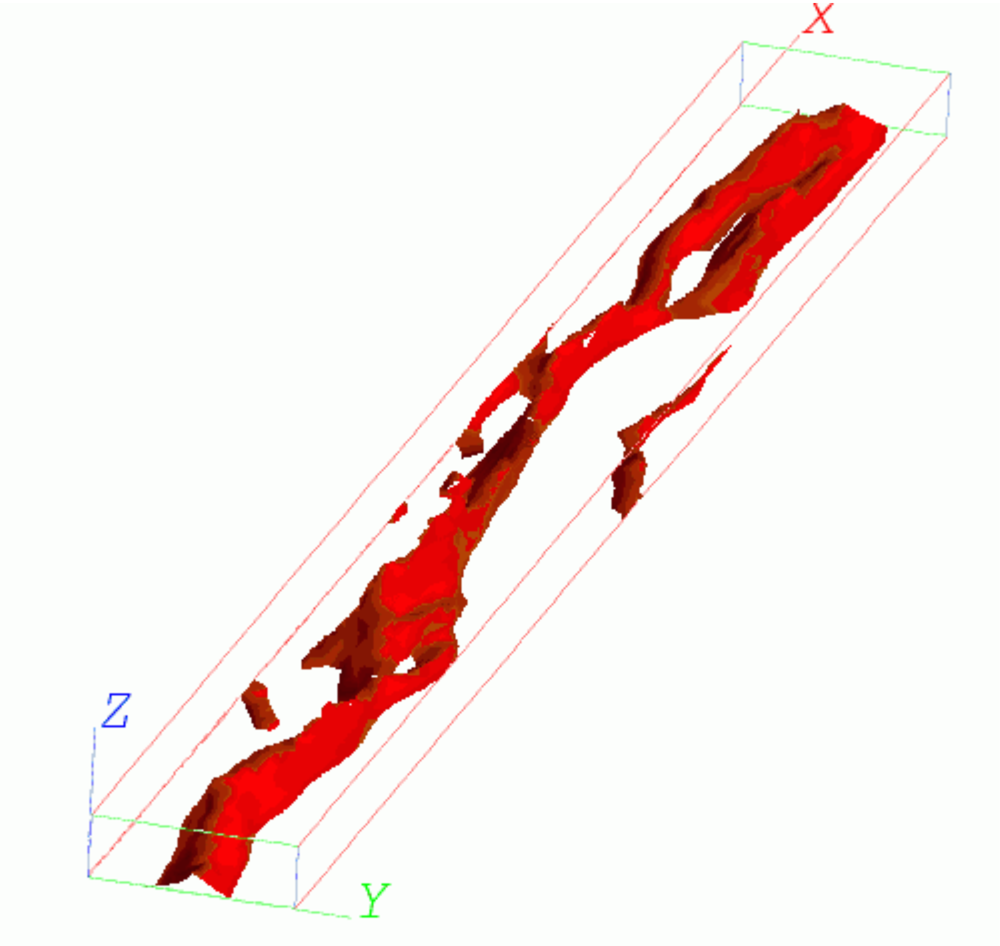
Observation: Structure of the fluid velocity fluctuations near the wall
(ref. Case: turbulent Poiseuille channel flow)



Red: Low-speed Streaks (near-wall regions with negative streamwise velocity fluctuations)



Interlude: Coherent structures in TBL



Red: Low-speed Streaks (near-wall regions with negative streamwise velocity fluctuations)

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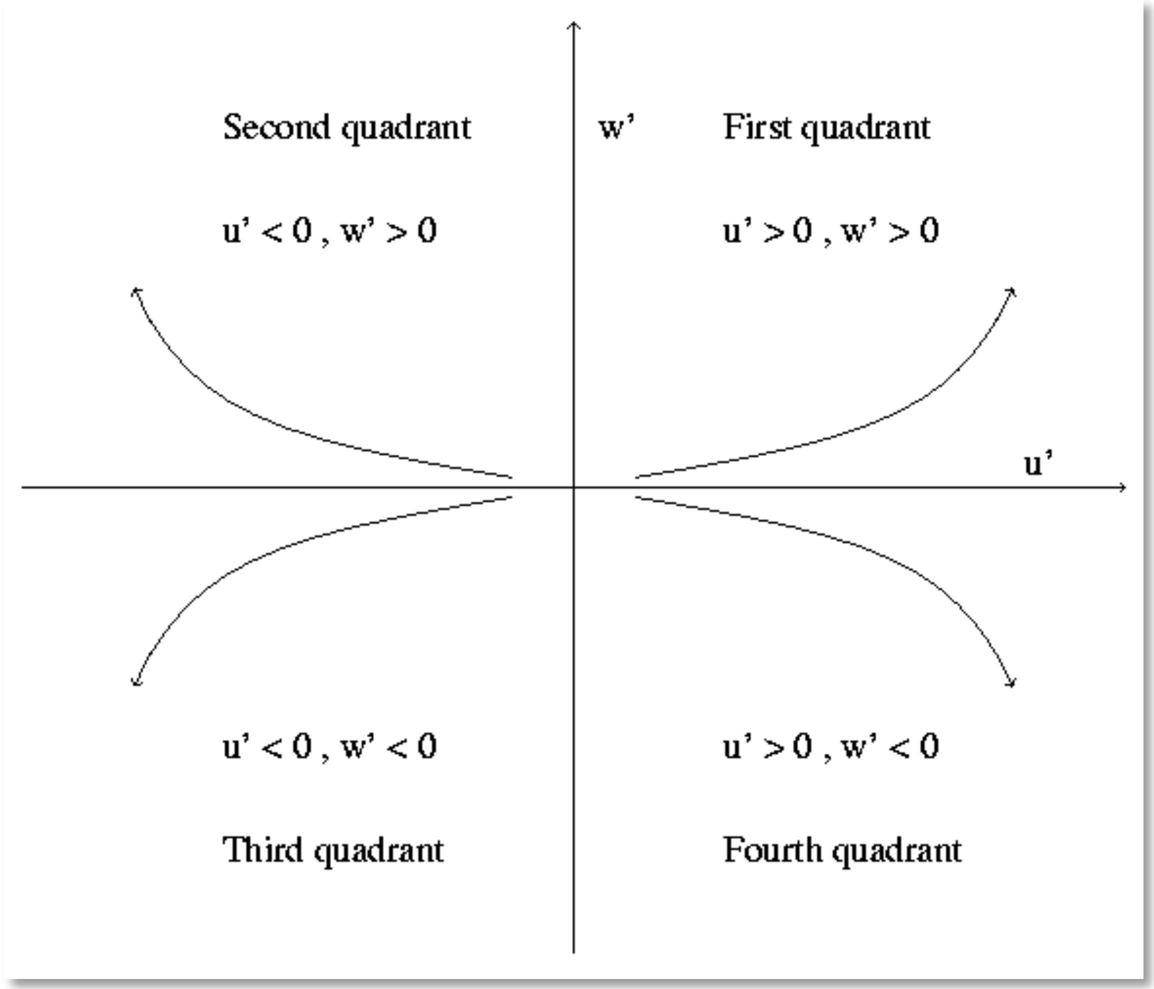
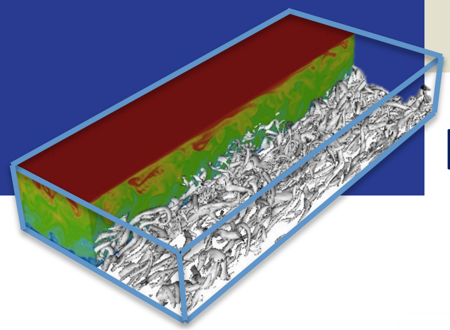
Interlude: Coherent structures in TBL

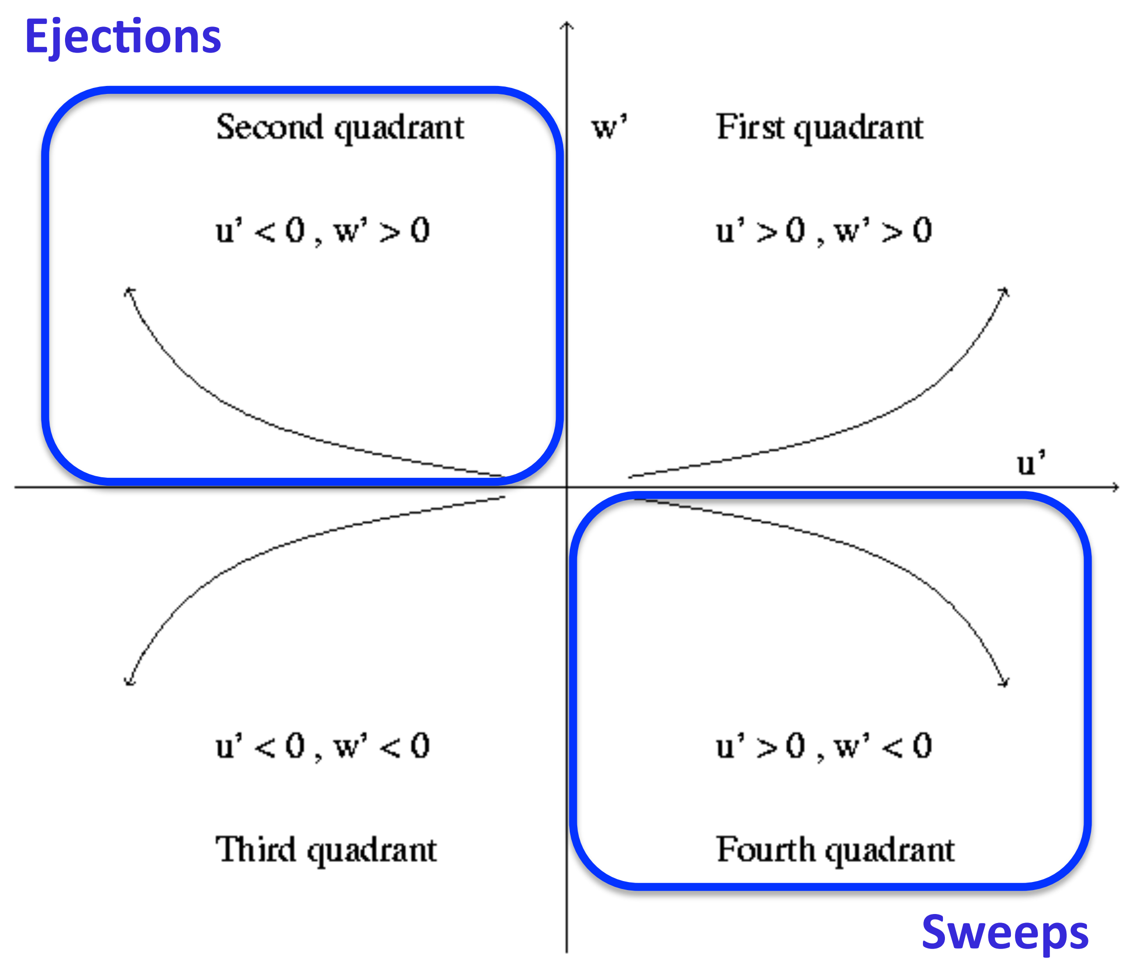
Turbulent transfer at the wall: Reynolds stresses

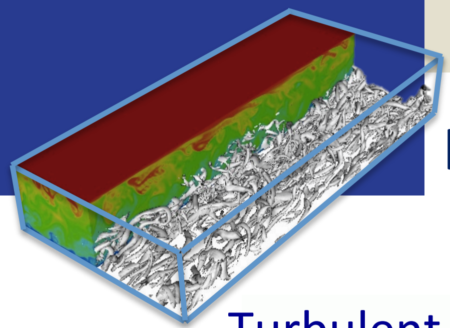




Interlude: Coherent structures in TBL

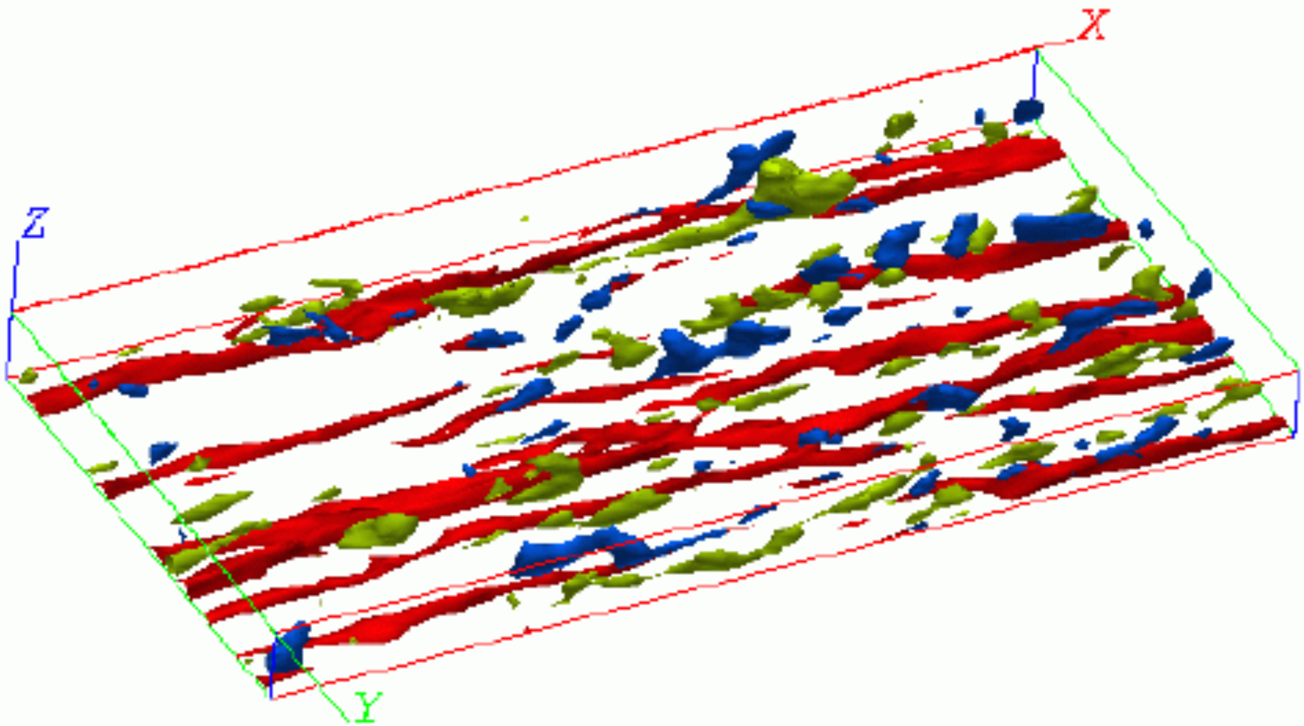
Turbulent transfer at the wall: Reynolds stresses





Interlude: Coherent structures in TBL

Turbulent transfer at the wall: Sweeps, ejections, low-speed streaks



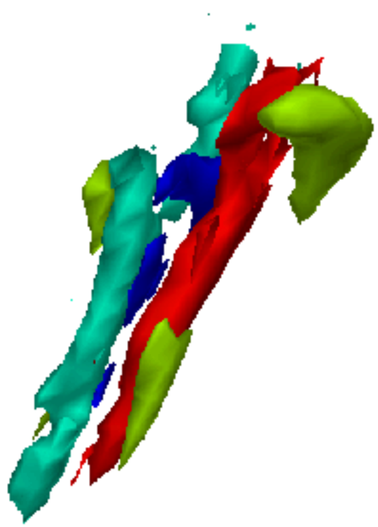
Red: Low-speed Streak

Blue: Ejection

Green: Sweep

Interlude: Coherent structures in TBL

Turbulent wall transfer: Sweeps, ejections, streamwise vortices

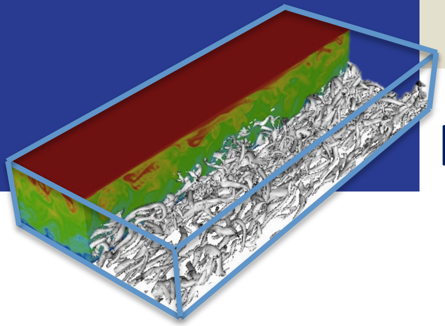


Red: Clockwise Streamwise Vortex

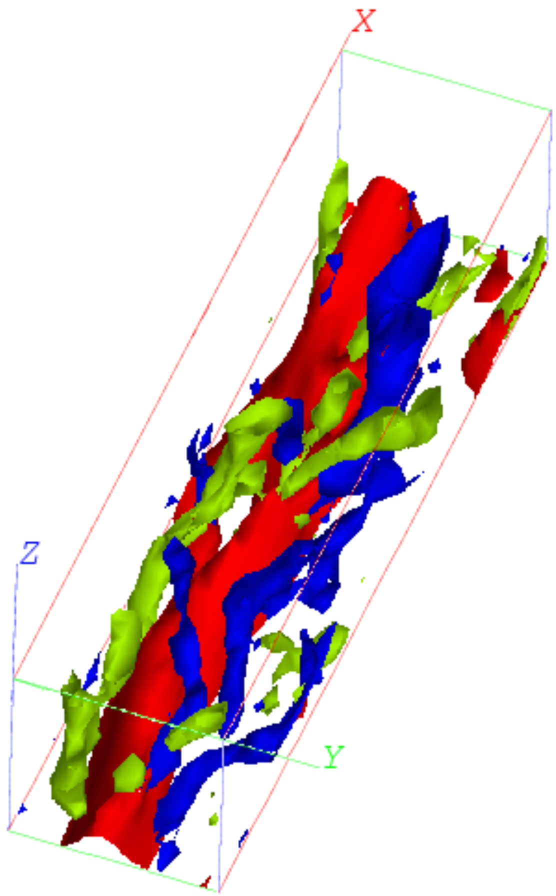
??????: Counter Clockwise Streamwise Vortex

Green: Sweep

Blue: Ejection



Interlude: Coherent structures in TBL

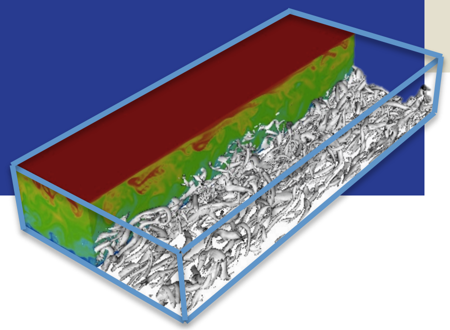


Red: Low Speed Streak

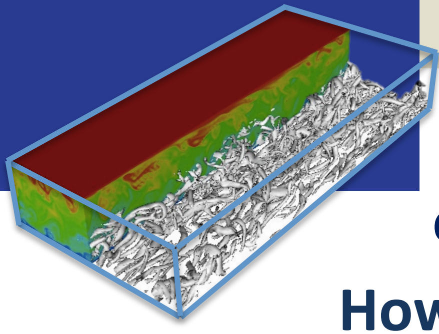
Blue: Clockwise Streamwise Vortex

Green: Counter- Clockwise Streamwise Vortex

Turbulence regeneration cycle: Physical explanation of the Reynolds stresses



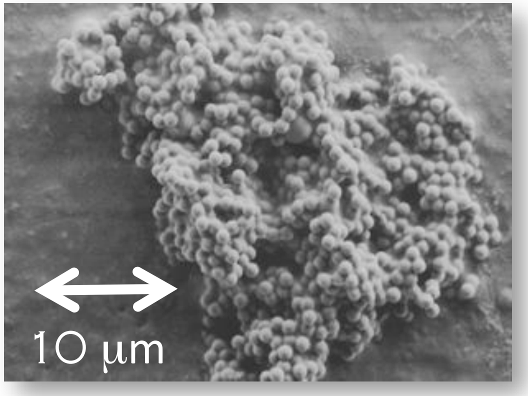
End of the interlude…



So far, we only considered inertial effects on preferential concentration…

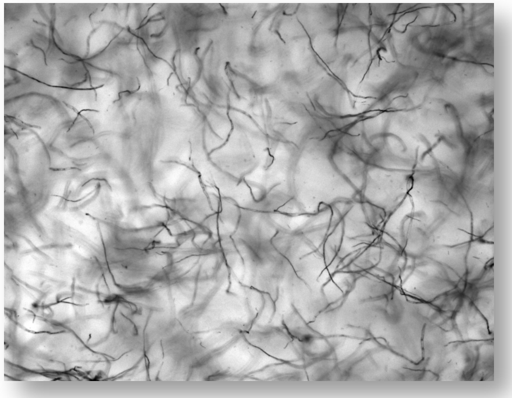
However, inertia is not the only source of bias!

- Non-sphericity

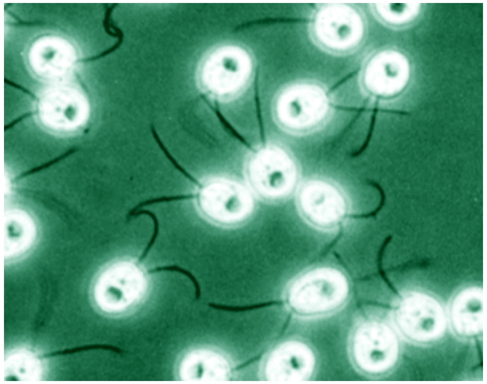


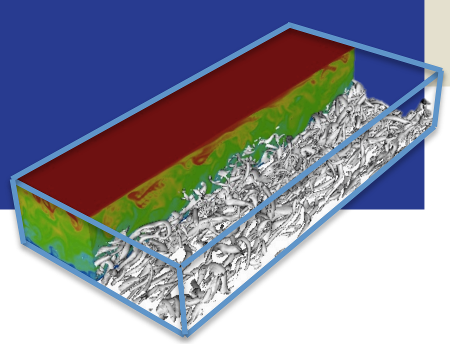
Complexity arises from { **Anisotropy of turbulence** + **Anisotropy of particles!** }

- Flexibility

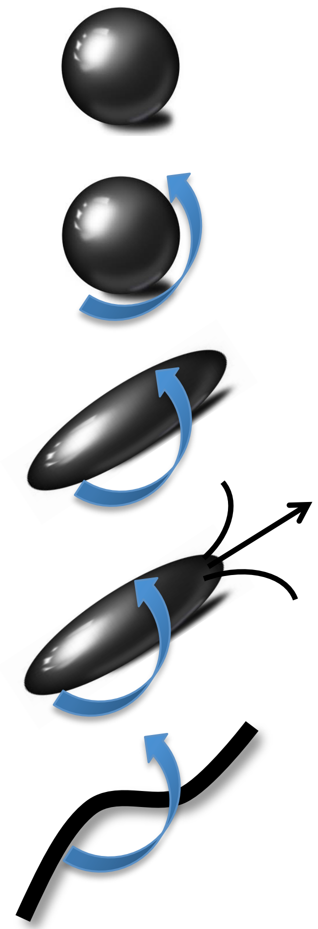


- Motility





Source of bias other than inertia require additional modelling



$\mathbf{x}(t), \mathbf{v}(\mathbf{x}(t),t)$

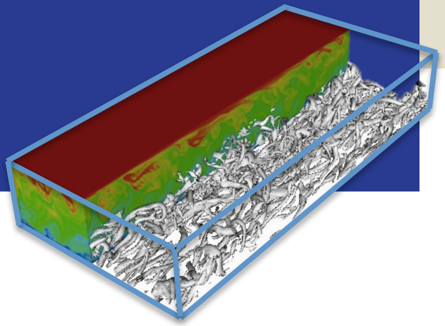
$\mathbf{x}(t), \mathbf{v}(\mathbf{x}(t),t), \omega(\mathbf{x}(t),t)$

$\mathbf{x}(t,\lambda), \mathbf{v}(\mathbf{x}(t,\lambda),t,\lambda), \omega(\mathbf{x}(t,\lambda),t,\lambda)$

$\mathbf{x}(t,\lambda), \mathbf{v}(\mathbf{x}(t,\lambda),t,\lambda), \omega(\mathbf{x}(t,\lambda),t,\lambda), \mathbf{o}(\mathbf{x}(t,\lambda),t,\lambda)$

$\mathbf{x}(t,\lambda), \mathbf{v}(\mathbf{x}(t,\lambda),t,\lambda), \omega(\mathbf{x}(t,\lambda),t,\lambda), \mathbf{o}(\mathbf{x}(t,\lambda),t,\lambda), \psi(\mathbf{x}(t,\lambda),t,\lambda)$

Additional particle functionalities must be modelled!

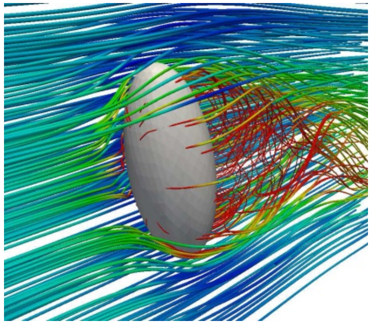


Complex particles in multiphase flows: (Some) modelling challenges

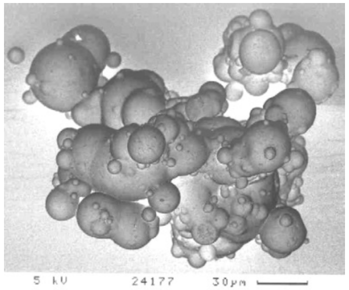
We need to model the effects of particle's

(I) shape

Elongation

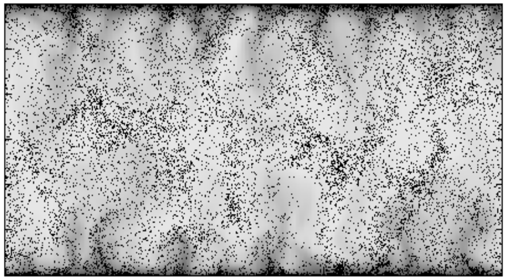


Non-sphericity

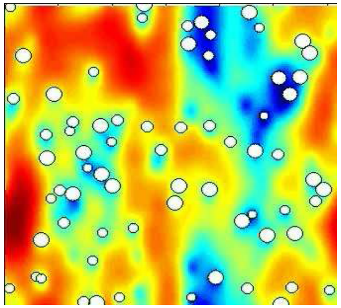


(II) size

Point-wise

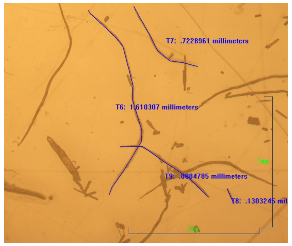


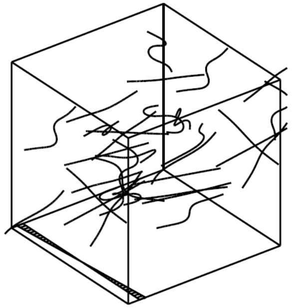
Fully-resolved



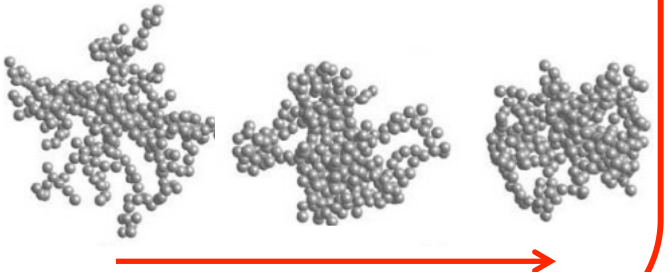
(III) deformability

Flexibility

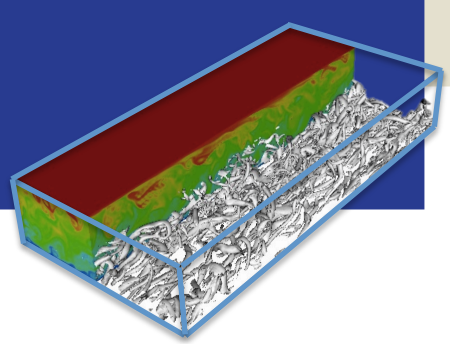




Restructuring

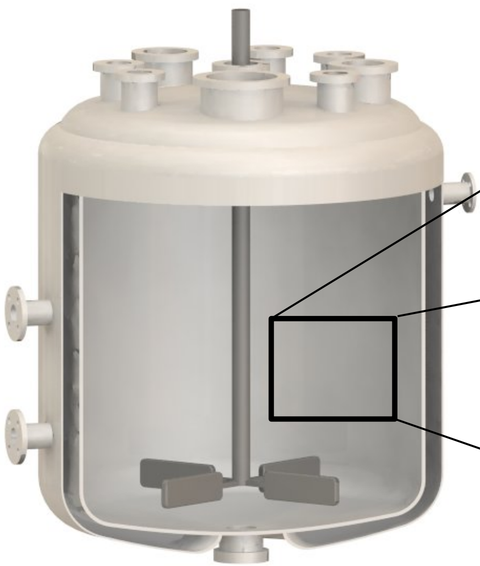


time

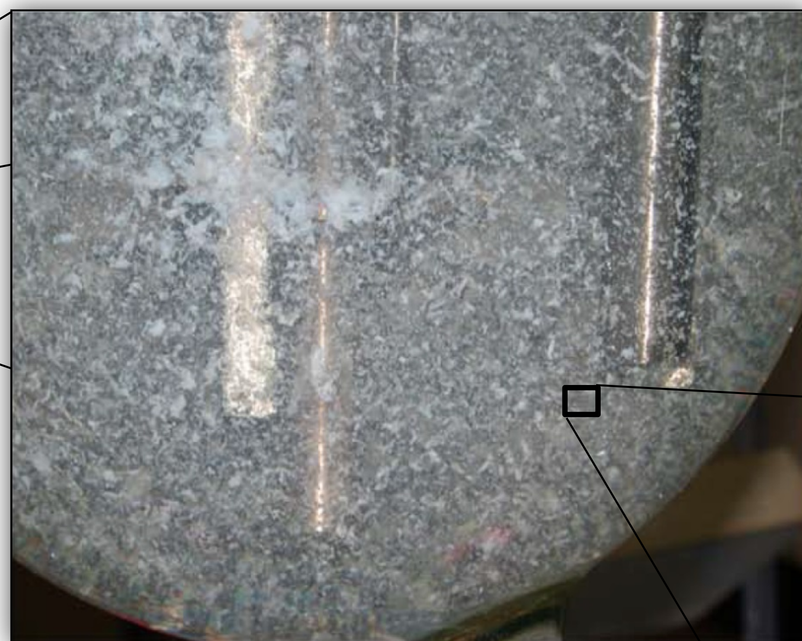


(I) Modelling shape effects: Deviations from sphericity

Colloidal suspension in continuous stirred tank



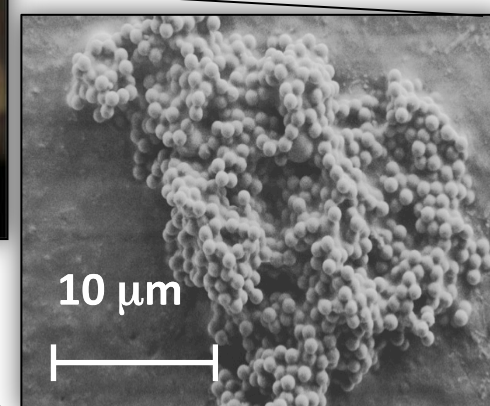
MACRO



MESO

Particles in the colloidal and micro-meter size range stick together and form aggregates.

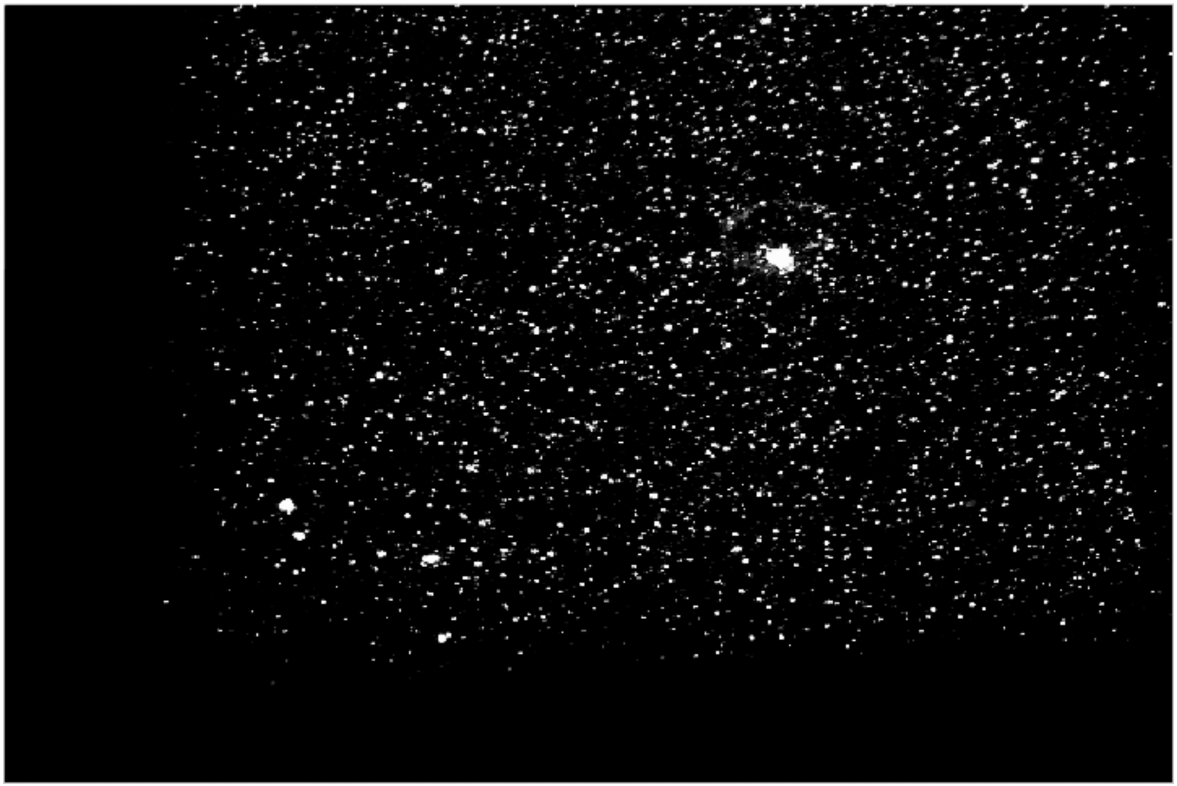
Fluid turbulence can produce shear-induced breakup of the aggregates.



MICRO

Pictures: M. Soos, D. Marchisio, J. Sefcik, *AIChE J.* (2013)
Soos, et al., *J. Colloid Interface Sci.* (2008)

(I) Modelling shape effects: Deviations from sphericity



Pictures: M. Soos, D. Marchisio, J. Sefcik, *AIChE J.* (2013)
Soos, et al., *J. Colloid Interface Sci.* (2008)

Polystyrene aggregate in homogeneous and isotropic turbulent flow (resolved by PTV).

$Re_\lambda \approx 70$

$\eta = 0.33\,\mathrm{mm}$

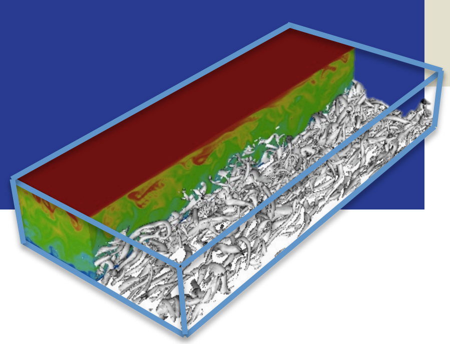
$\tau_\eta = 0.1\,\mathrm{s}$

$\langle \varepsilon \rangle \approx 0.9\,\mathrm{cm}^2\,\mathrm{s}^{-3}$

$L/\eta = 120$

$G = 10\,\mathrm{s}^{-1}$

The aggregate is subject to **fluctuating hydrodynamic stresses** that act along its trajectory…



Interlude: Energy dissipation rate

(From: S.B. Pope, Turbulent Flows)

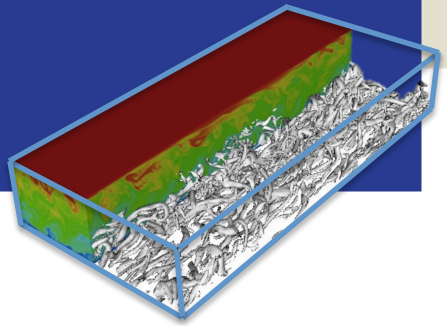
$$\boldsymbol{U}(\boldsymbol{x},t) = \langle \boldsymbol{U}(\boldsymbol{x},t)\rangle + \boldsymbol{u}(\boldsymbol{x},t)$$ Reynolds decomposition $\Rightarrow$ $$k \equiv \tfrac{1}{2}\langle \boldsymbol{u}\cdot\boldsymbol{u}\rangle = \tfrac{1}{2}\langle u_i u_i\rangle$$ TKE

From $$\frac{\bar{D}k}{\bar{D}t} + \nabla\cdot\boldsymbol{T}' = \mathcal{P} - \varepsilon,$$ with $$T_i' \equiv \tfrac{1}{2}\langle u_i u_j u_j\rangle + \langle u_i p'\rangle/\rho - 2\nu\langle u_j s_{ij}\rangle$$

$$\boxed{\varepsilon \equiv 2\nu\langle s_{ij}s_{ij}\rangle}$$

with $$s_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$ Fluctuating rate of strain

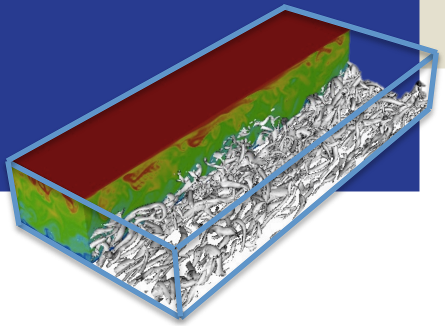
or simply *dissipation*. The fluctuating velocity gradients $(\partial u_i/\partial x_j)$ working against the fluctuating deviatoric stresses $(2\nu s_{ij})$ transform kinetic energy into internal energy. (As illustrated in Exercise 5.22, the resulting rise in



Interlude: Energy dissipation rate

It can be shown that:

$$\varepsilon \equiv \underbrace{\nu \left\langle \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} \right\rangle}_{\text{Pseudo-dissipation}} + \nu \frac{\partial^2 \langle u_i u_j \rangle}{\partial x_i \partial x_j}$$



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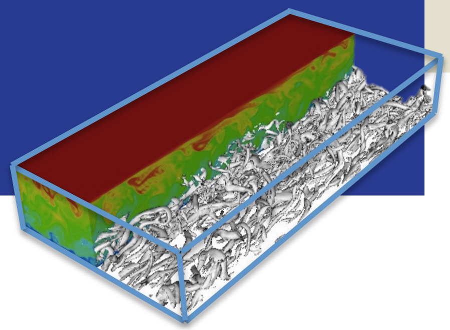


Interlude: Energy dissipation rate

It can be shown that:

$$\varepsilon \equiv \nu \underbrace{\left\langle \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} \right\rangle}_{\text{Pseudo-dissipation}} + \underbrace{\cancel{\nu \frac{\partial^2 \langle u_i u_j \rangle}{\partial x_i \partial x_j}}}_{\text{Typically small...}}$$

In homogeneous isotropic turbulence:

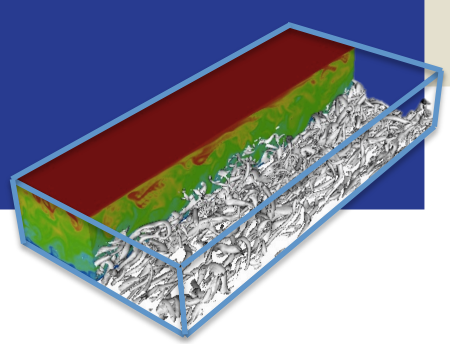
$$\varepsilon = \nu \left\langle \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} \right\rangle = \tfrac{15}{2} \nu \beta = 15\nu \underbrace{\left\langle \left(\frac{\partial u_1}{\partial x_1} \right)^2 \right\rangle}_{\text{1D surrogate}}$$

This comes from:

$$\left\langle \frac{\partial u_i}{\partial x_j} \frac{\partial u_k}{\partial x_\ell} \right\rangle = \alpha \delta_{ij} \delta_{k\ell} + \beta \delta_{ik} \delta_{j\ell} + \gamma \delta_{i\ell} \delta_{jk} \Longrightarrow \left\langle \frac{\partial u_i}{\partial x_j} \frac{\partial u_k}{\partial x_\ell} \right\rangle = \beta \left(\delta_{ik} \delta_{j\ell} - \tfrac{1}{4} \delta_{ij} \delta_{k\ell} - \tfrac{1}{4} \delta_{i\ell} \delta_{jk} \right)$$

$$\partial u_i / \partial x_i = 0 \quad \rightarrow \quad 3\alpha + \beta + \gamma = 0$$

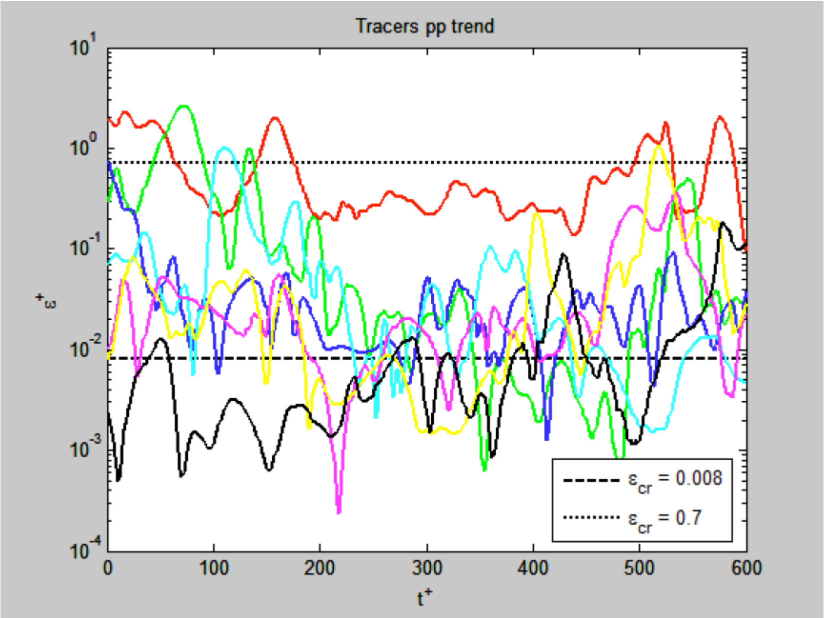
$$\left\langle \frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_\ell} \right\rangle = 0 \quad \rightarrow \quad \alpha + \beta + 3\gamma = 0$$



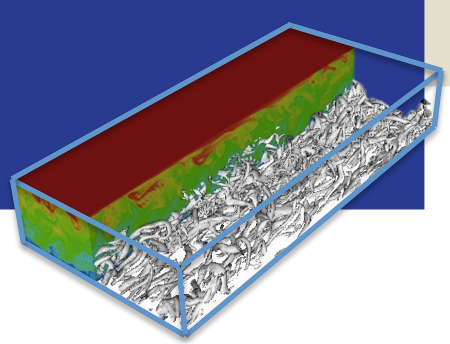
Interlude: Energy dissipation rate

Observations:

- Dissipation of kinetic energy by viscosity in fully-developed turbulence occurs primarily at the smallest flow scales
- Dissipation is highly intermittent: Local values of ε can be orders of magnitude larger than the mean
- This because of (1) large velocity gradients AND/OR (2) tiny shear layers across which velocity varies significantly

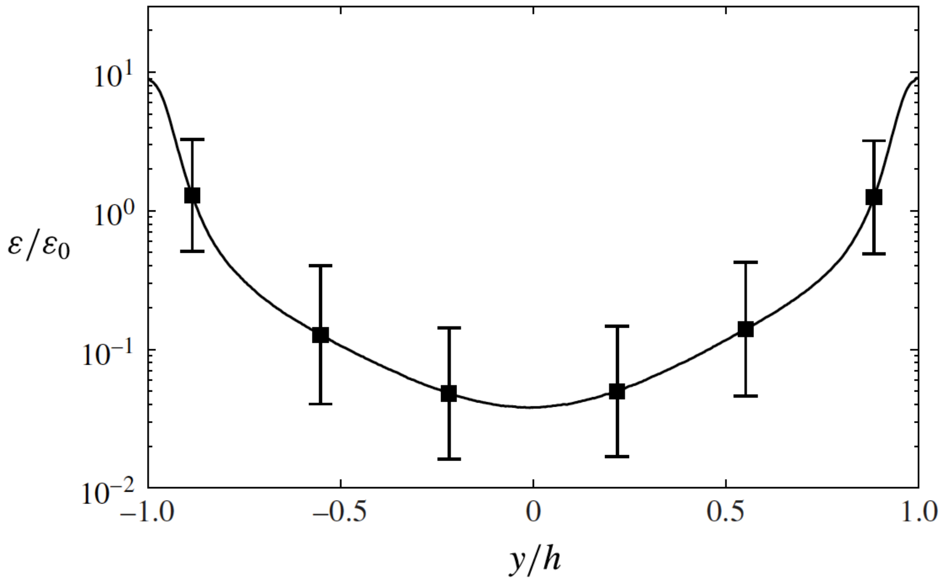


- Dissipation can be connected to a locally varying scale, $\eta(\mathbf{x},t)$, associated with the fluctuations in the velocity gradients field
- Dissipation occurs over a range of fluctuating scales η



Interlude: Energy dissipation rate

(From: Babler et al., JFM, vol. 766, 2012)

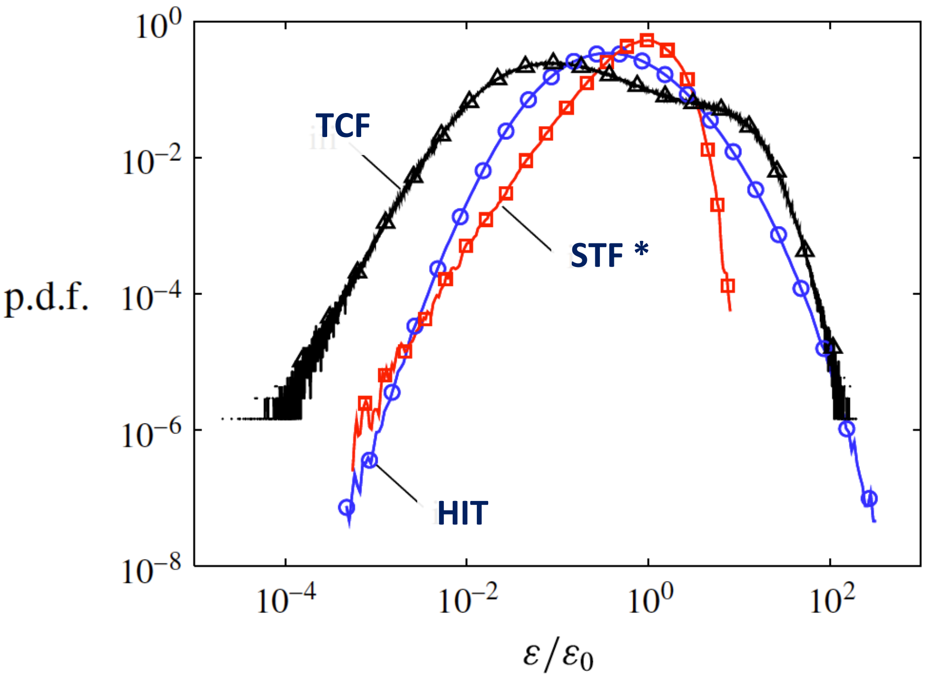


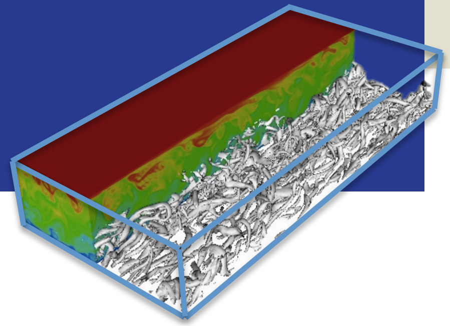
Mean energy dissipation along the wall-normal direction in turbulent channel flow (Babler et al., JFM, 2015)

Note: ε_o= volume-averaged mean dissipation

PDF of mean energy dissipation for different instances of turbulent flow (Babler et al., JFM, 2015)

$$* \quad \boldsymbol{u}(\boldsymbol{x},t) = \sum \hat{\boldsymbol{u}}'_k(t)\mathrm{e}^{ikx}$$



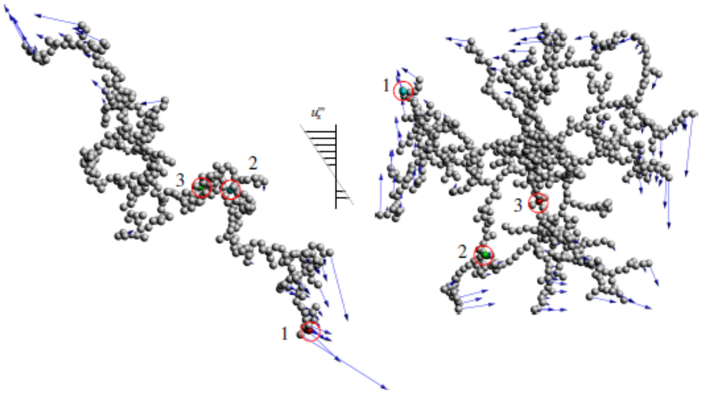


End of the interlude…

(I) Modelling shape effects: Deviations from sphericity

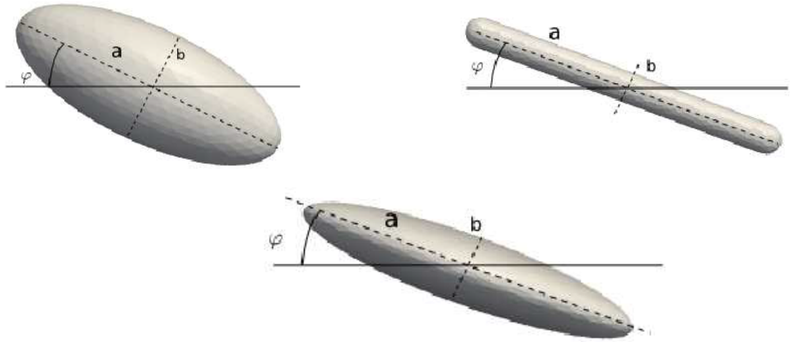
Non-spherical particles: translation and rotation are coupled!

- Irregular (e.g. aggregates, agglomerates)

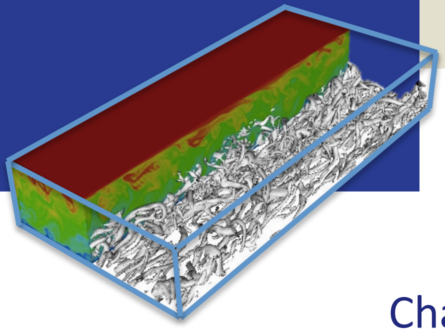


No mathematical model available!

- Regular (e.g. ellipsoids, rods or disks)



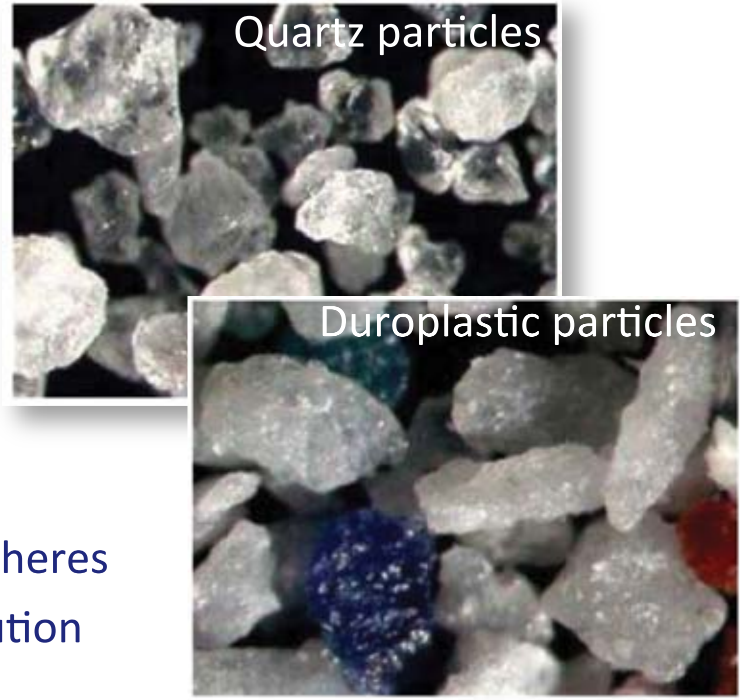
Equations of motion can be derived!
(e.g. slender body theory)



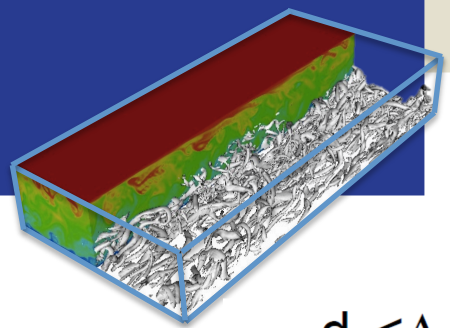
(I) Modelling shape effects: Deviations from sphericity

Challenges for non-spherical particles with irregular shape:

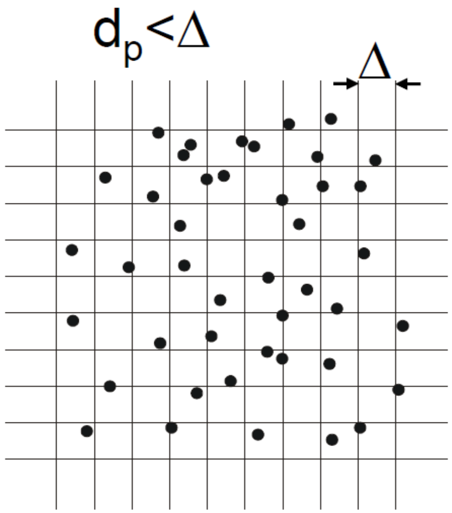
- Model all relevant forces acting on particles:
  - Correlations for aerodynamic coefficients currently based on statistical distributions
  - No measure available for shear-induced and rotation-induced lift



- Model wall-collision:
  - need to 'convert' particles into equivalent spheres
  - Need to obtain statistical measures of restitution and friction coefficients
- Heavily dependent on availability of accurate experimental measurements or particle-level direct simulations



(II) Modelling size effects: Pointwise vs Fully-resolved

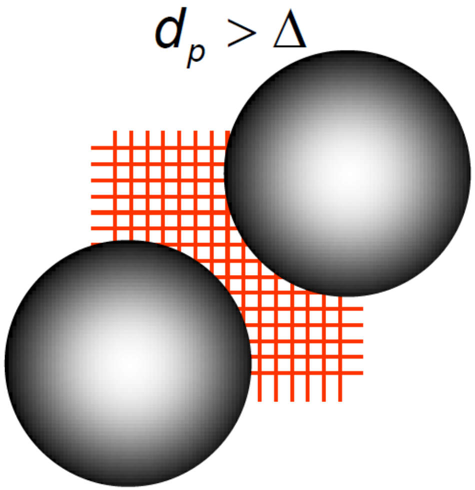


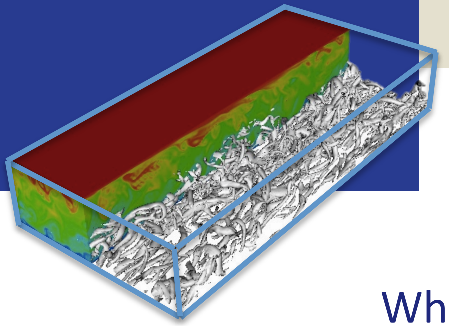
Point particles:

- Size << (DNS) grid spacing
- Flow around the particle not resolved
- Particles moved around by drag, lift, …
- Up to **O(10^8)** particles

Fully-resolved particles:

- Size > grid spacing
- Hydrodynamics and hydrodynamic forces resolved
- Direct coupling between particle motion and fluid flow
- Up to **O(10^4)** particles

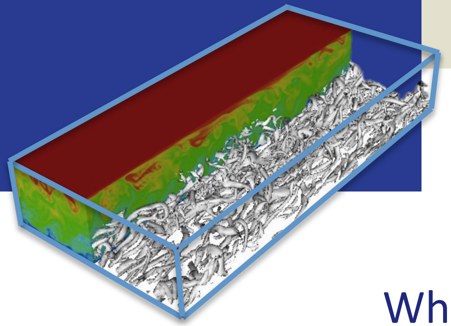




(II) Modelling size effects:
Pointwise vs Fully-resolved

What can we learn from fully-resolved particle simulations?

In the context of the Eulerian-Lagrangian approach:



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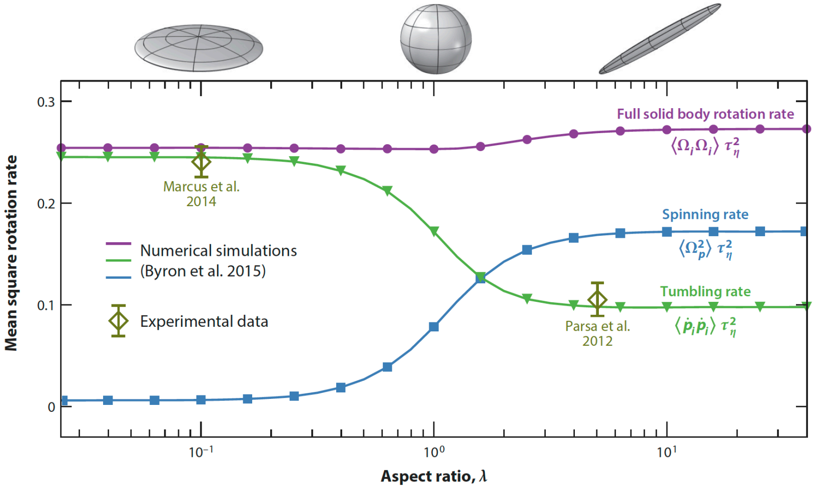
(II) Modelling size effects: Pointwise vs Fully-resolved

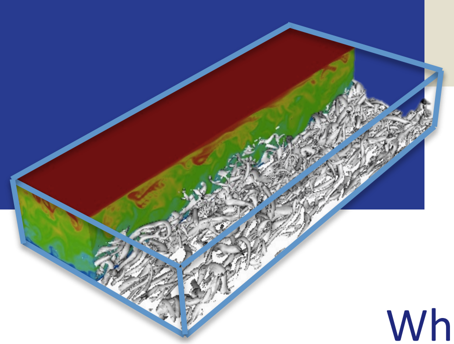
What can we learn from fully-resolved particle simulations?

In the context of the Eulerian-Lagrangian approach:

Rotation rate of rods/ellipsoids



Calculation of rotation rates provides access to statistics of the fluid velocity gradients



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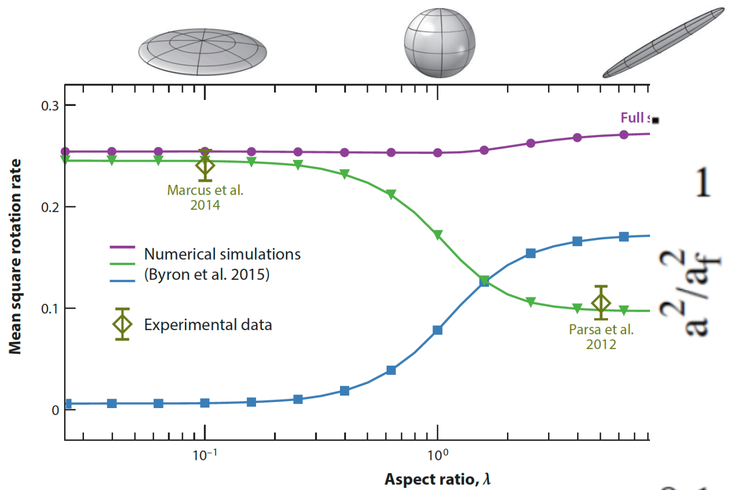
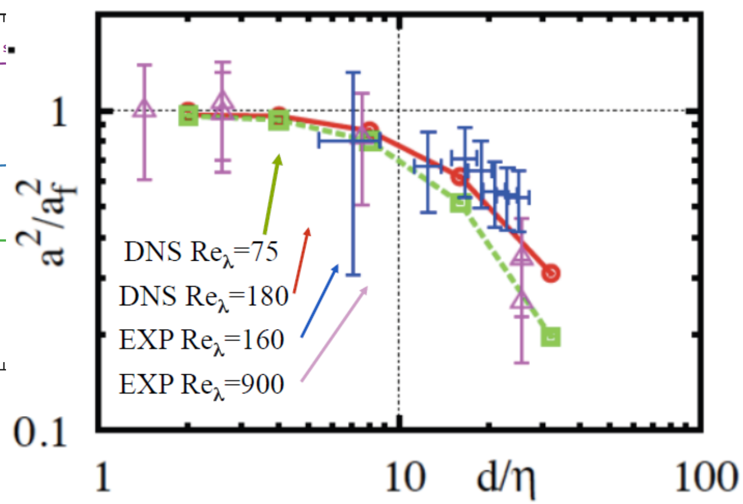
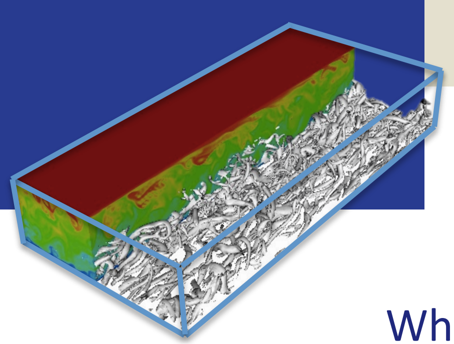


Calculation of rotation rates provides access to statistics of the fluid velocity gradients

Acceleration statistics



Acceleration variance of neutrally-buoyant particles in HIT (Calzavarini et al., JFM, 2014)



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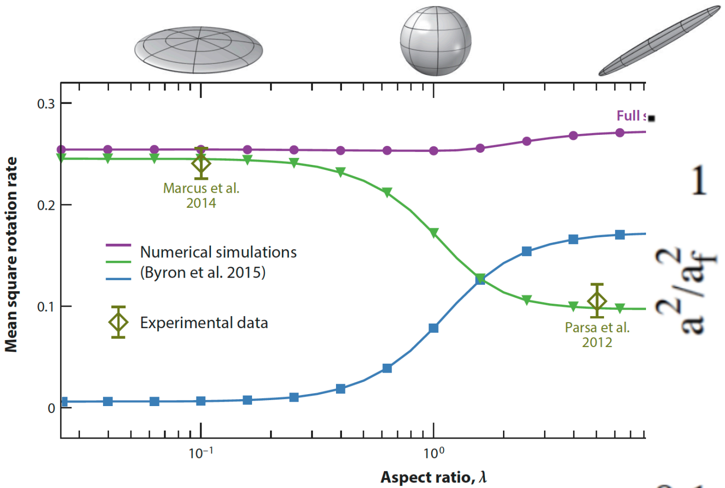

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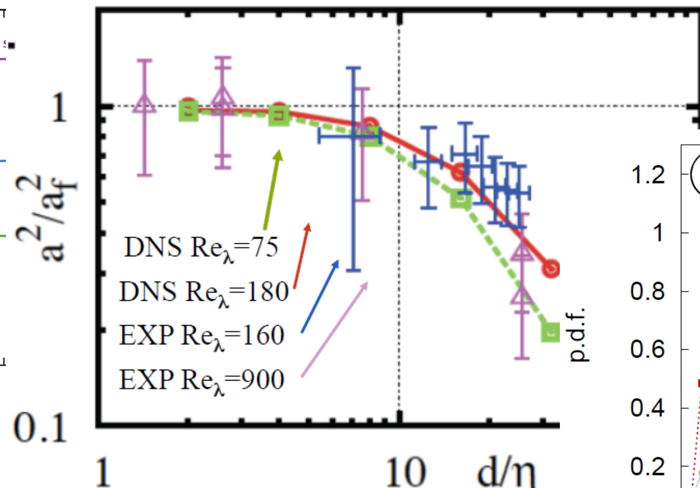
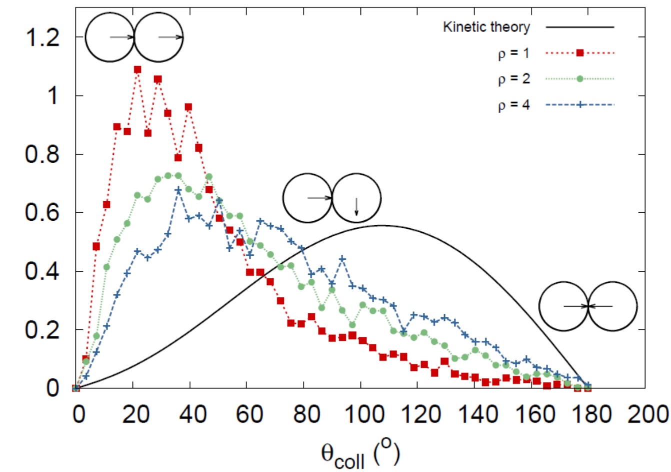
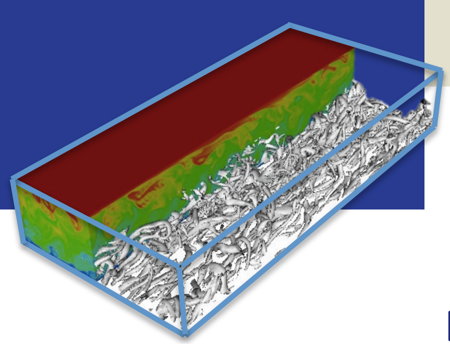


Acceleration variance of neutrally- particles in HIT (Calzavarini et al., J

Collision times & contact angles



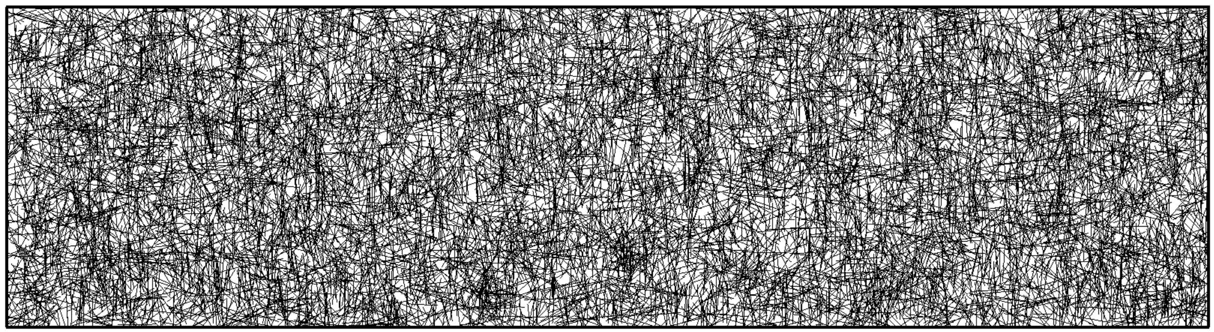
Pdf of contact angles of neutrally/slightly buoyant particles in HIT (Brandle de Motta et al., 2014)



(III) Modelling deformability: Rigid vs Flexible particles

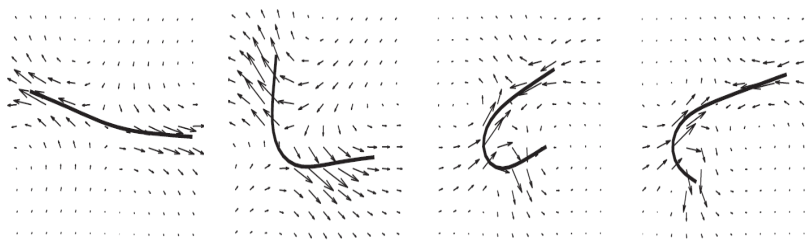
Either "simple" rigid fibers in "complex" turbulent flows…

Dispersion of rigid fibers in turbulent channel flow (Marchioli et al., 2010)

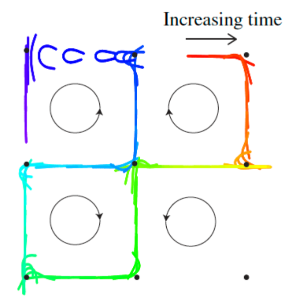


…or "complex" flexible fibers in "simple" shear flow

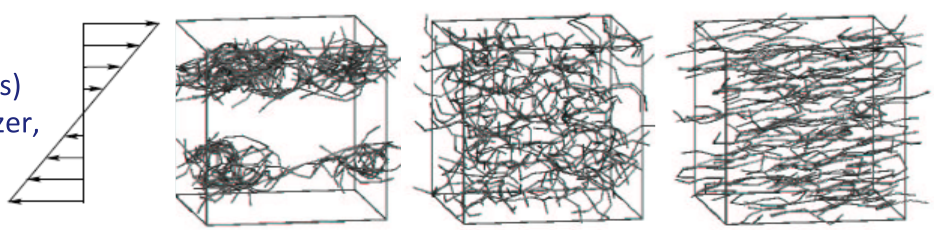
Isolated flexible fiber in unbounded shear flow (Lindstrom & Uesaka, Phys. Fluids, 2007)



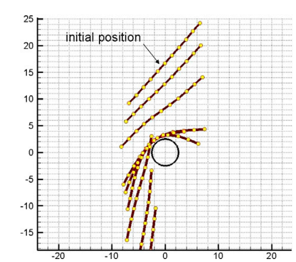
Elastic fiber in viscous cellular flow (Quennouz et al, JFM 2015)

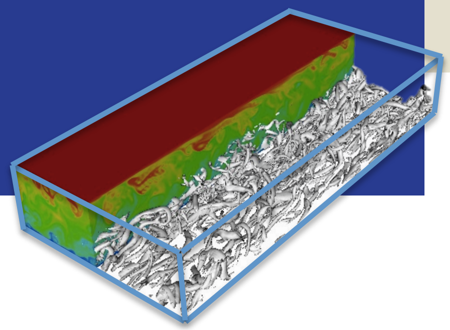


Flexible fibers (with different bending stiffness) in linear shear flow (Switzer, PhD thesis, 2002)

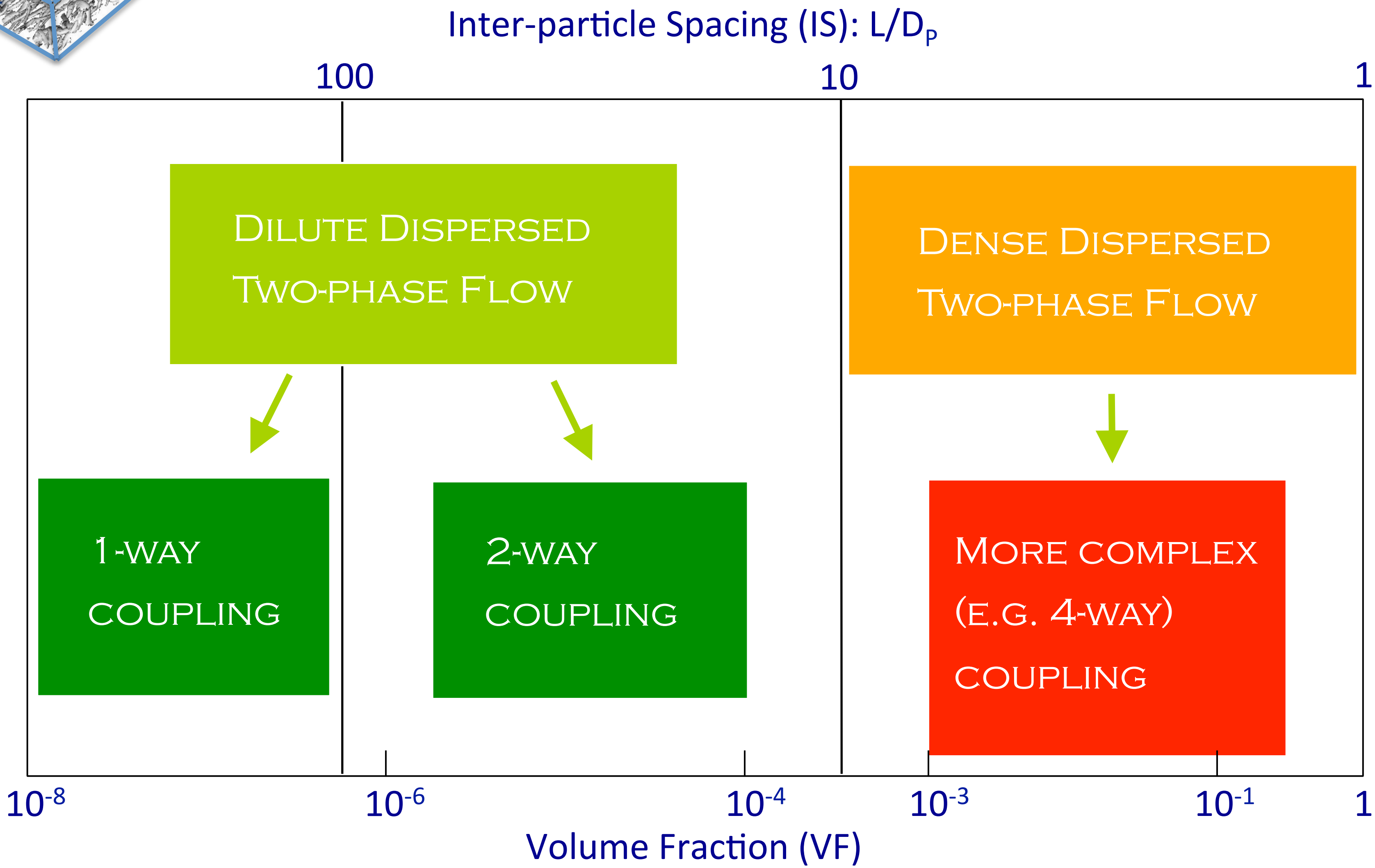


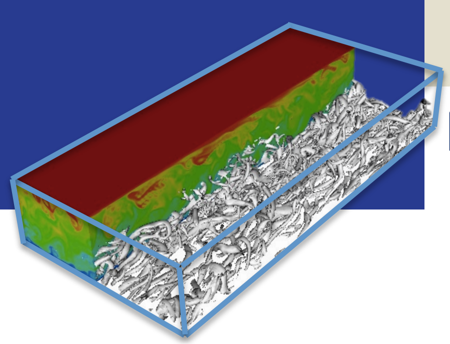
Flexible fiber motion in the flow field of a cylinder (Vakil & Green, IJMF, 2011)





Further modeling issues: Particle-fluid coupling (2-way coupling)





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Further modeling issues: Particle-fluid coupling (2-way coupling)

One-way coupling (VF<10^{-6} ; IS >100):

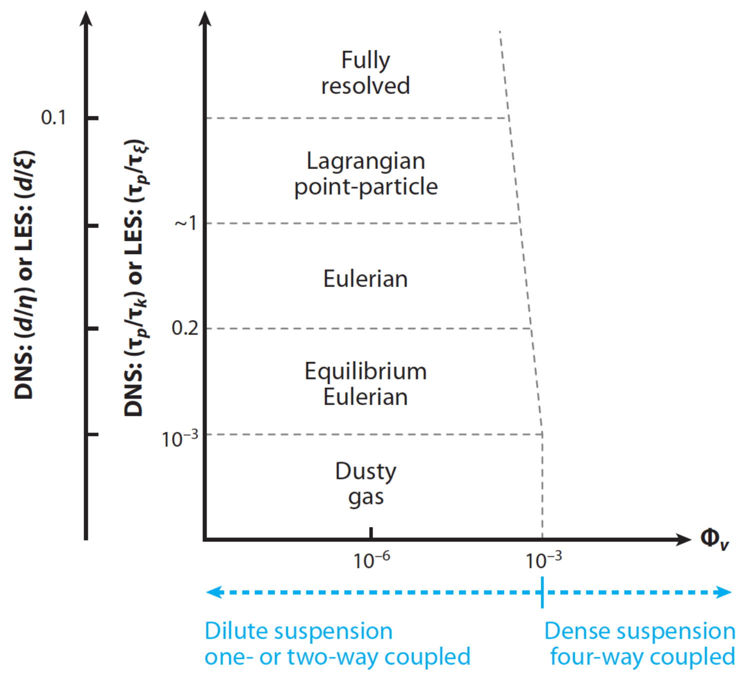
Particles do not influence significantly the flow field
→ Allows to investigate the effect of flow on particle motion/dispersion/distribution
→ Suffices to solve for particle momentum balance (cheap)

Two-way coupling (10^{-6} <VF<10^{-4}; 10<IS<100)

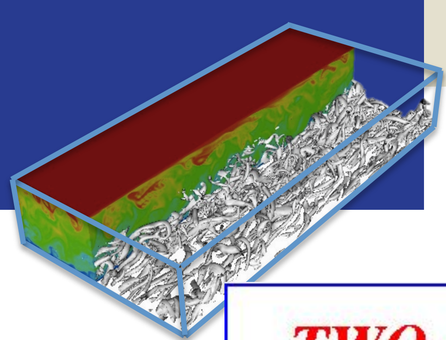
Particles influence the flow field dynamics
→ allows investigation of flow modulation by particles
→ Need to solve for particle AND fluid momentum balance (fair)

More complex coupling (10^{-3} <VF<1; 1< IS<10)

Particles influence the flow field dynamics
→ allows investigation of flow modulation by particles
→ Need to solve for particle AND fluid momentum & mass balance (expensive!)



(courtesy of Balachandar & Eaton, ARFM, 2010)



2-way coupling: The fluid *feels* particle momentum exchange

TWO–WAY EFFECT (point–force approximation)

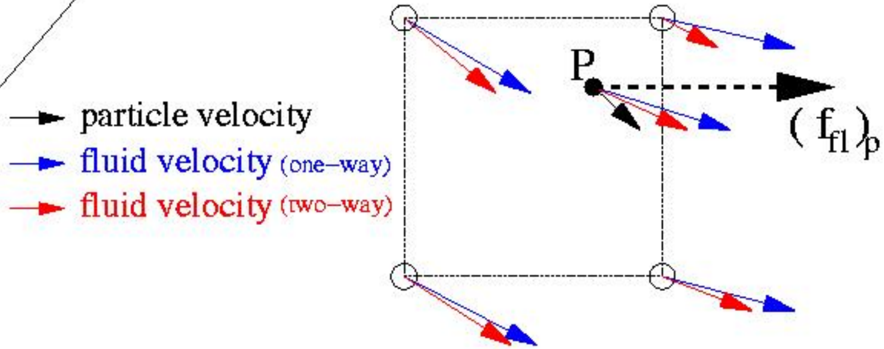
Fluid equations

$$\nabla \cdot \mathbf{v} = 0$$

$$\rho \frac{\partial \mathbf{v}}{\partial \theta} + \rho \mathbf{v} \cdot \nabla \mathbf{v} = \mu \nabla^2 \mathbf{v} - \nabla p + \tilde{\mathbf{f}}_{2w}$$

Drag force on particle

$$\left(\mathbf{f}_{fl}\right)_p = \frac{(\mathbf{v} - \mathbf{v}_p)}{\tau_p} f(Re_p)$$



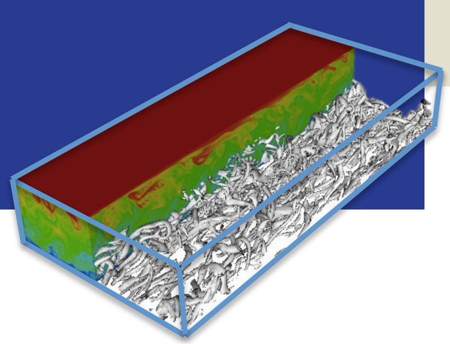
Particle tracking

$$m_p \frac{\partial \mathbf{v}_p}{\partial \theta} = \left(\mathbf{f}_{fl}\right)_p$$

$$\frac{\partial \mathbf{x}_p}{\partial \theta} = \mathbf{v}_p$$

Momentum exchange term

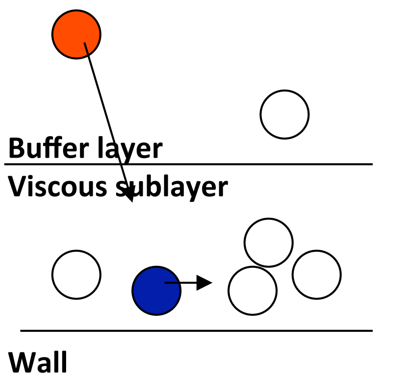
$$\tilde{\mathbf{f}}_{2w} = -\sum_{p=1}^{n_p} \left(\mathbf{f}_{fl}\right)_p \delta\left(\mathbf{x} - \mathbf{x}_p\right)$$

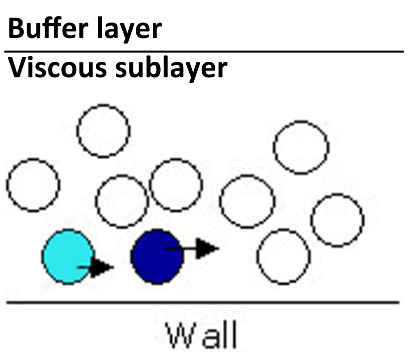


Further modeling issues: Particle-particle collisions (4-way coupling)

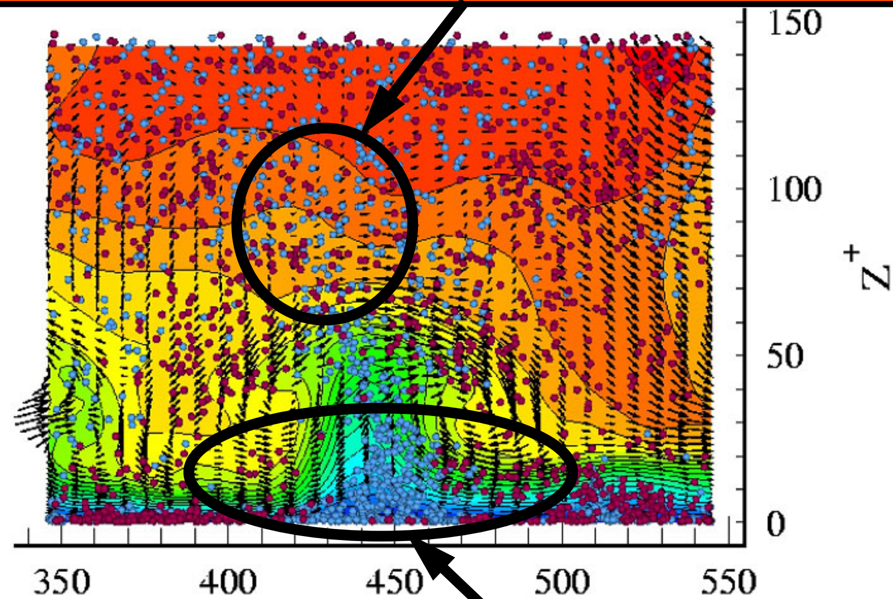
Physics learned from our simple model (in DNS):

Depending on relative velocity between colliding particles:



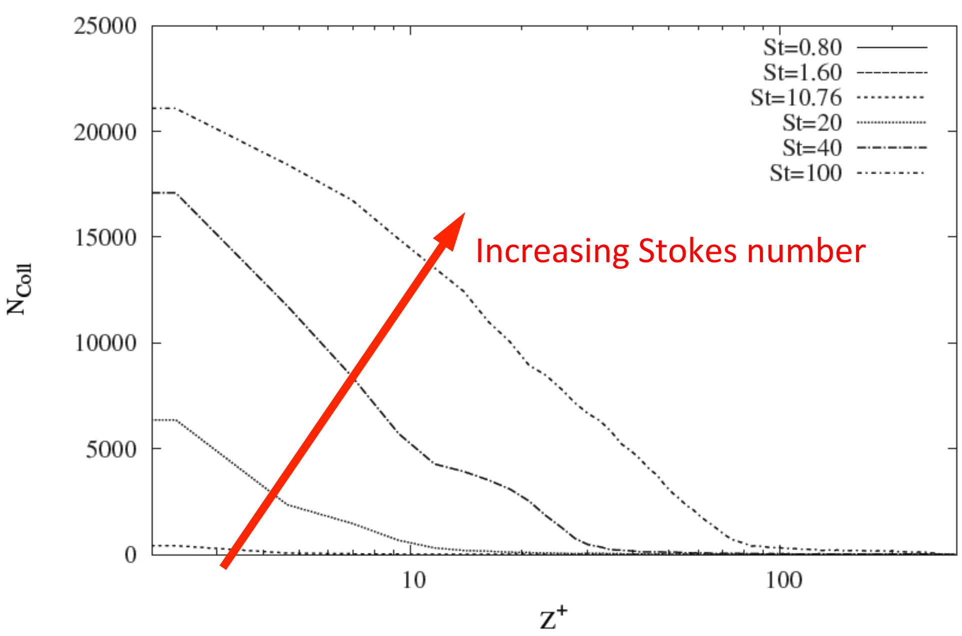


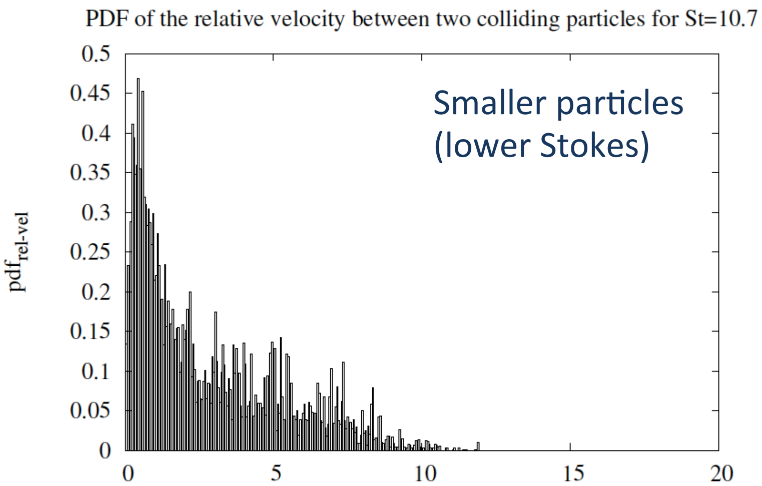
High energy collisions (characterized by possible particle resuspension)

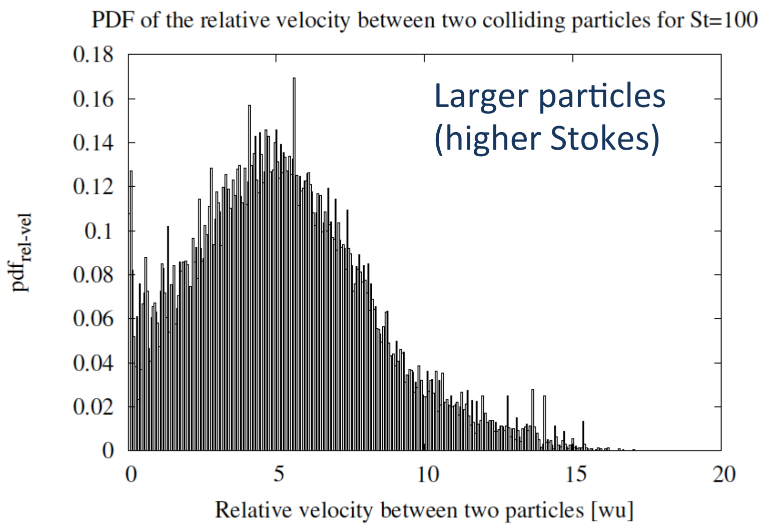


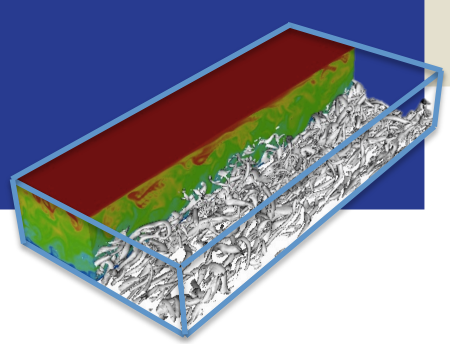
Low energy collisions (characterized by multiple collision events)

Further modeling issues: Particle-particle collisions (4-way coupling)









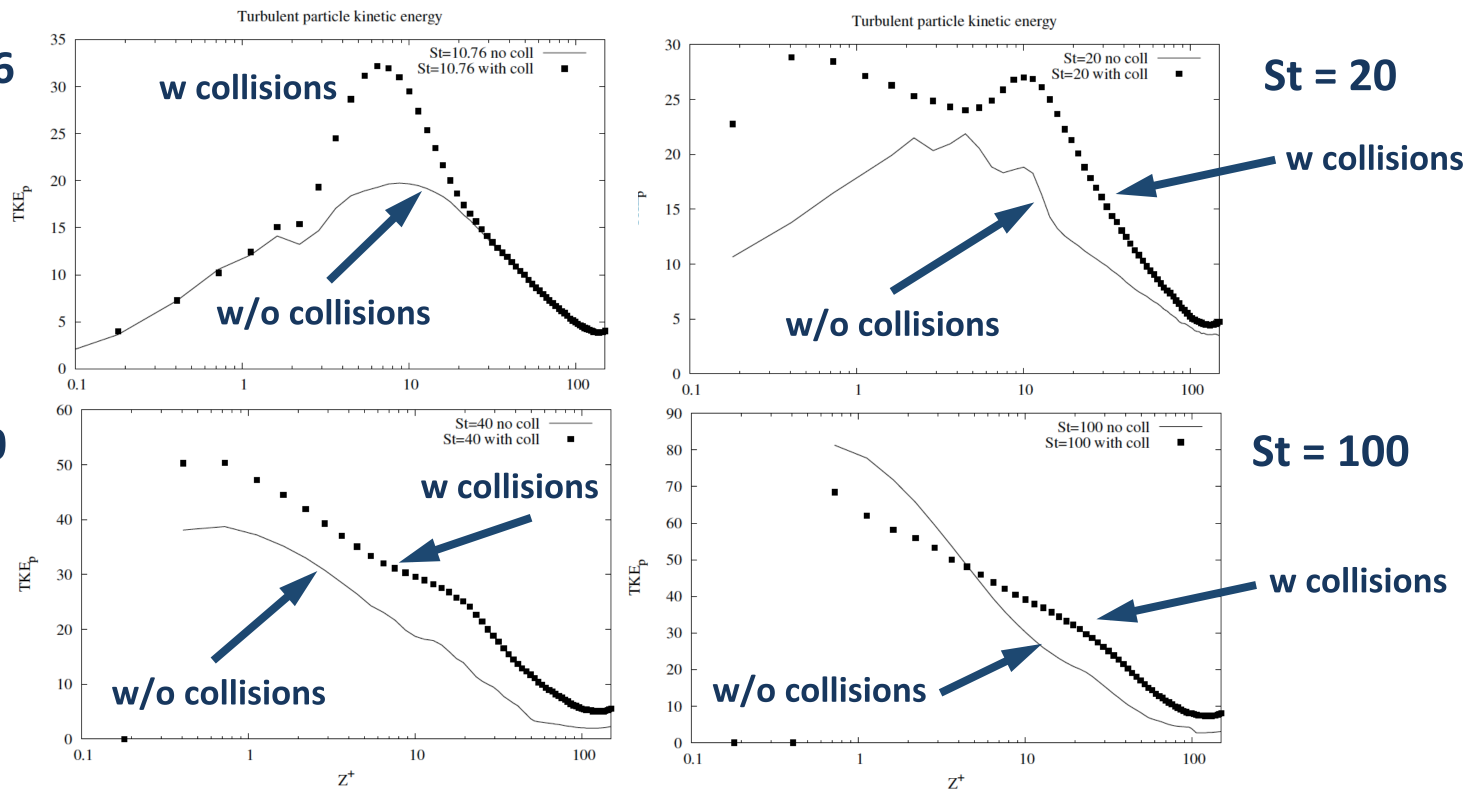
Further modeling issues: Particle-particle collisions (4-way coupling)

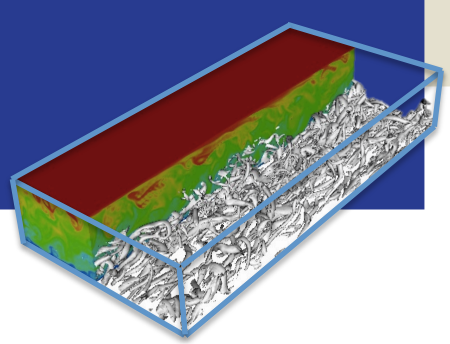
St = 10.76

St = 20

St = 40

St = 100





Multiphase Flow Laboratory
University of Udine

Modelling all relevant sources of bias
allows us to tackle important questions:

How do particles-turbulence interactions give rise to large-scale macroscopic patterns and dynamics?

What is the underlying physics behind this macroscopic behaviour?