Cannonballs in (dusty) turbulence

Drag, Accretion & Concentrations

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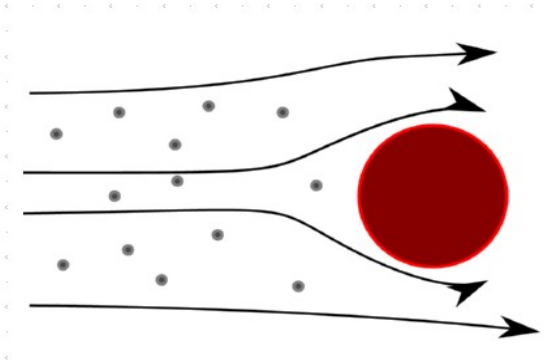
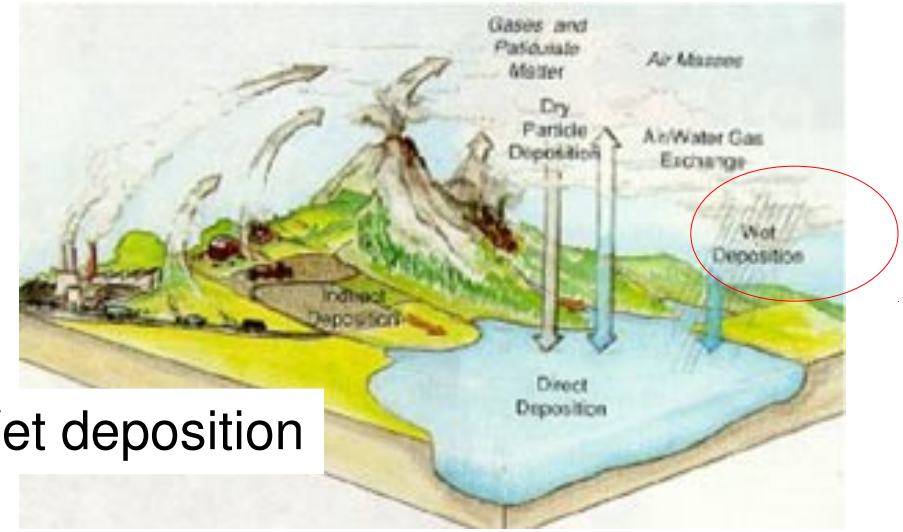
Motivation - Applications

CONTEXT: Large particle moving through a (turbulent) fluid seeded with small inertial particles:





Wet deposition

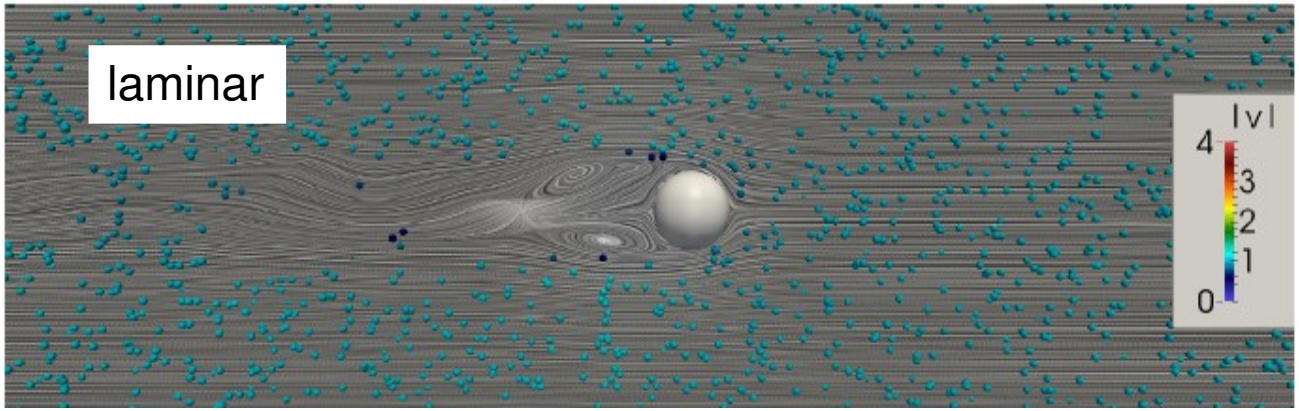
Sekiya and Takeda (2003)

Collision rates of small particles with big body

Motivation – Physical problem

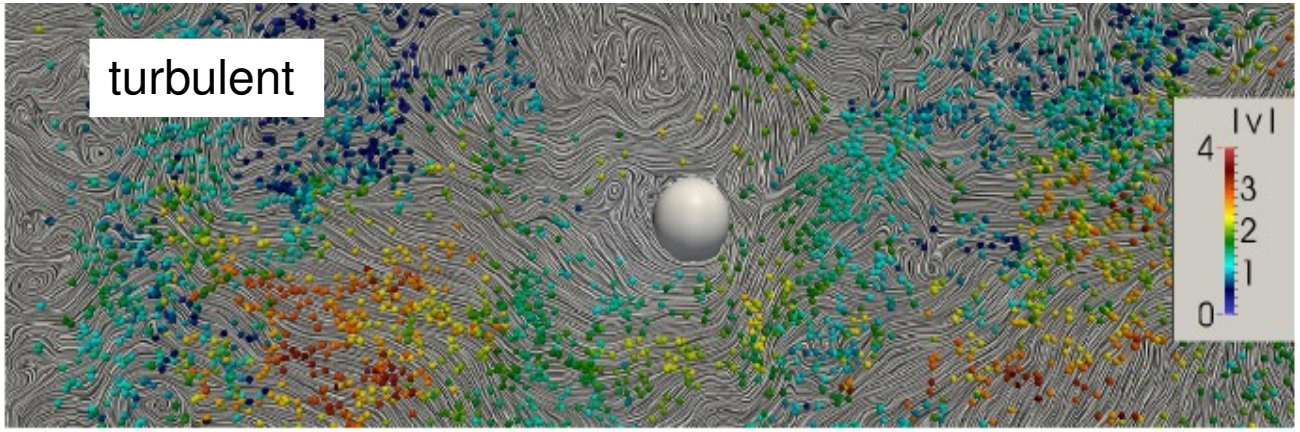
Interaction of big body with stream of small inertial particles

- Small particle collision rates
- Wake interactions

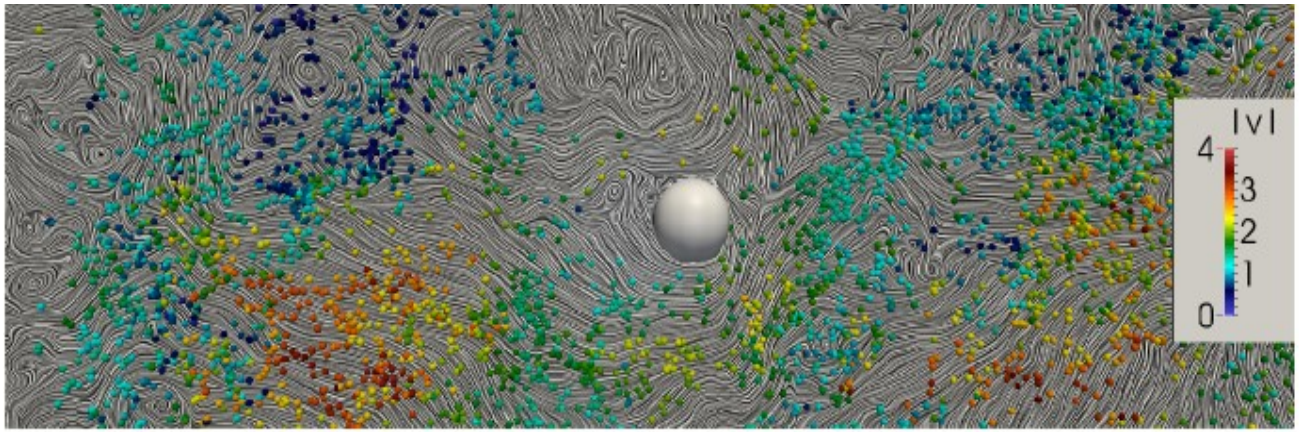


Influence of turbulent velocity fluctuations

- Drag force
- Wake modification
- Collision rates



Numerical challenges

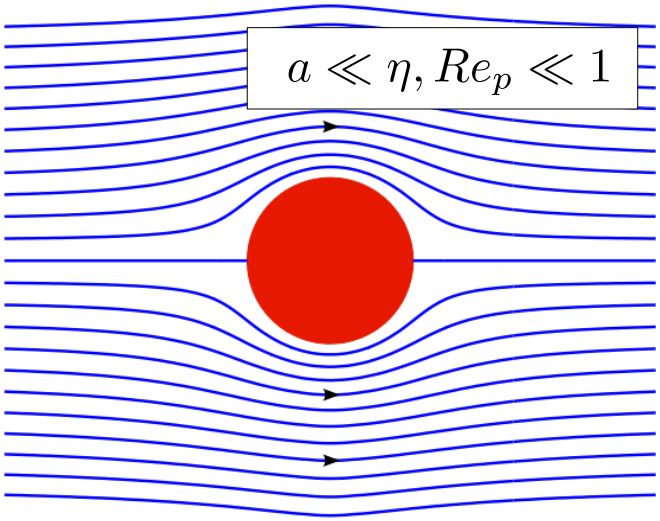


What does we need?

- Equations and solver for fluid motion
  No-slip boundary condition on big particle
  High Reynolds numbers

- Equations for small particle motion
  Integration of many trajectories for statistics

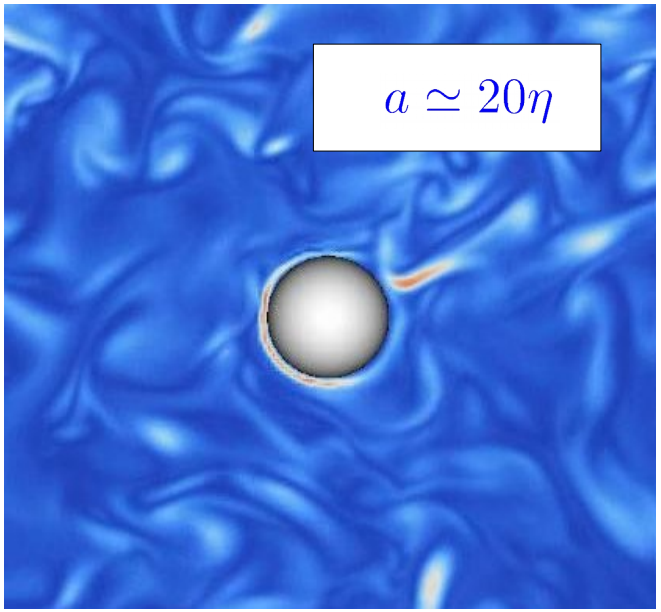
Small vs large particles



Analytically known drag force and flow structure

Stokes drag $\dfrac{d\boldsymbol{v}}{dt} = \dfrac{3\nu}{a^2}(\boldsymbol{u} - \boldsymbol{v})$

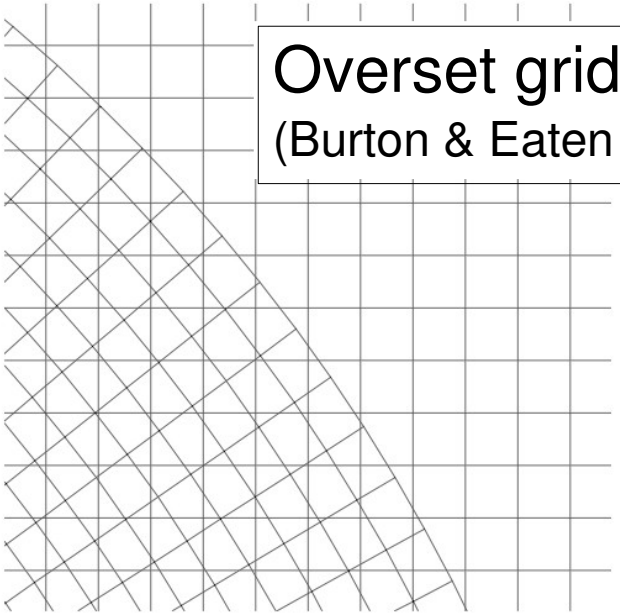
$\boldsymbol{u}$ known → ODE for small particle trajectories



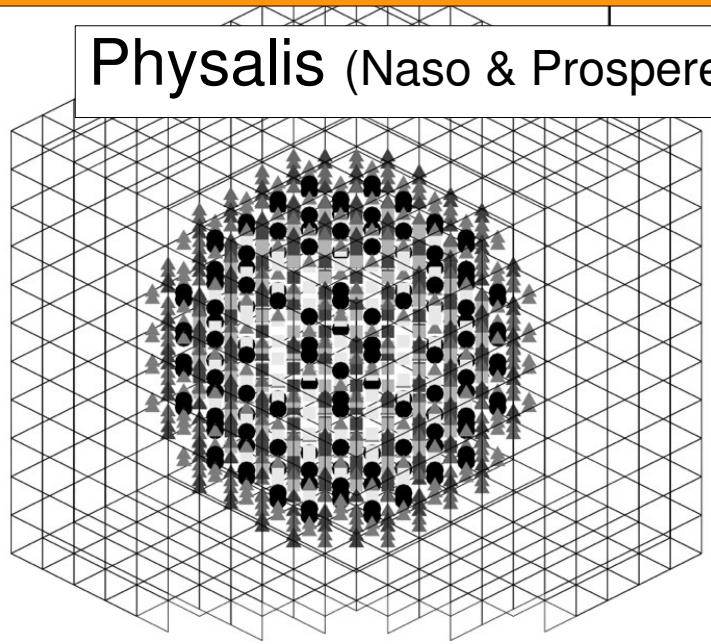
What if particle the particle is bigger?

→ handle the boundary layer!

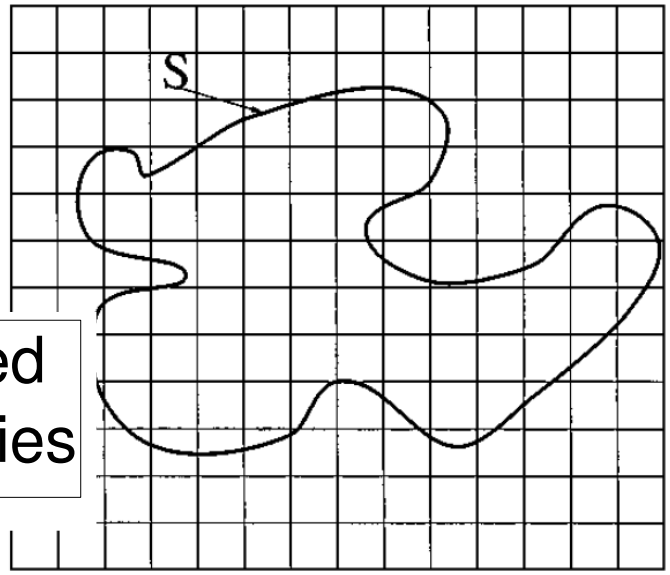
The numerical problem



Overset grid
(Burton & Eaten 2005)



Physalis (Naso & Prosperetti 2010)



Immersed boundaries

FIG. 1. Sketch of the immersed boundary.

- Solving dynamics on complete grid
- Imposing boundary conditions on S

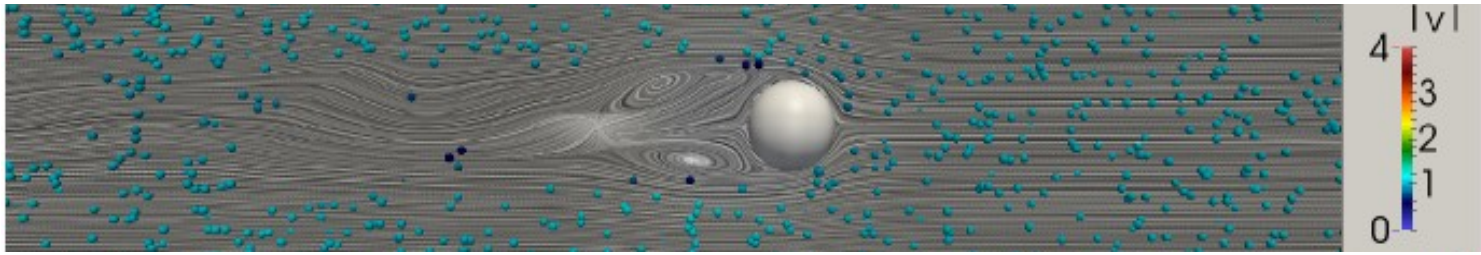
Advantages :

- Arbitrary shapes of S
- Easy to implement
- Compatible with Fourier-spectral codes

Shortcomings :

- Accuracy (order, boundary layer)

Numerical method



- Fluid: Navier-Stokes equations by pseudo-spectral method

$$\partial_t \boldsymbol{u} + \boldsymbol{u}\cdot\nabla\boldsymbol{u} = -\nabla p + \boldsymbol{f} + \nu\nabla^2\boldsymbol{u}, \quad \nabla\cdot\boldsymbol{u} = 0 \qquad \langle\boldsymbol{u}\rangle = U\boldsymbol{e}_x$$

$\boldsymbol{u}$: velocity field, ν: kinematic viscosity, $\boldsymbol{f} = \boldsymbol{f_e} + \boldsymbol{f_b}$: forcing (external + boundary)

- Small particles : heavy particles with low Re → Stokes drag

$$\ddot{\boldsymbol{X}} = \frac{1}{\tau}\left[\boldsymbol{u}(\boldsymbol{X},t) - \dot{\boldsymbol{X}}\right]$$

$\tau = 2\rho_\mathrm{p} a^2/(9\rho_\mathrm{f}\nu)$ particle response time

$\mathrm{St} = \tau/(d/U)$

Effect of inertia based on particle crossing time

- No-slip boundary conditions: penalty method (direct forcing, Fadlun et al. 2000) :

$$\boldsymbol{V} = \boldsymbol{u}|_{sphere} = 0$$

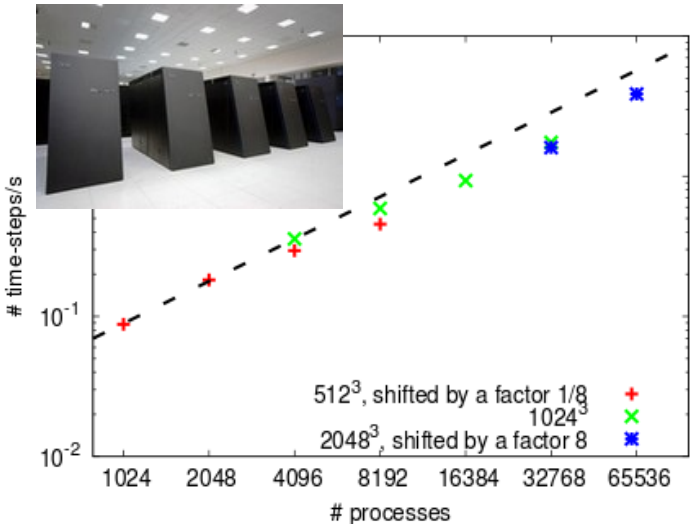
discretized Navier-Stokes equation : $\mathrm{u}^{n+1} - u^n = \Delta t(rhs^n + f_b^n)$

replacing $\mathrm{u}^{n+1} \to V^{n+1}$ yields force $\mathrm{f}_b^n = -rhs^n + (V^{n+1} - u^n)/\Delta t$

Numerical method – bounday conditions

Advantages:

- Standard Fourier-solver for incompressible turbulence
- Massive parallel codes
- Easy to implement



Difficulties:

- Truncated Fourier representation and discontinuities
- No-slip condition and divergence-freeness at the boundaries

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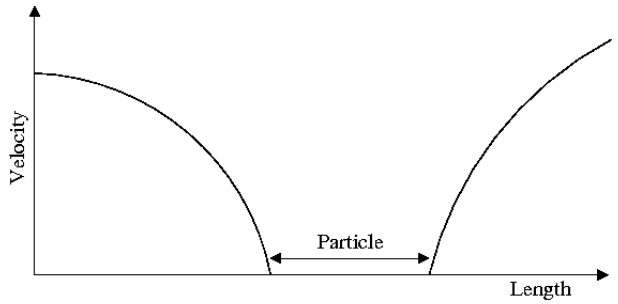
Discontinuities in the derivative of the velocity field

→ lost spectral accuracy (non-smooth)

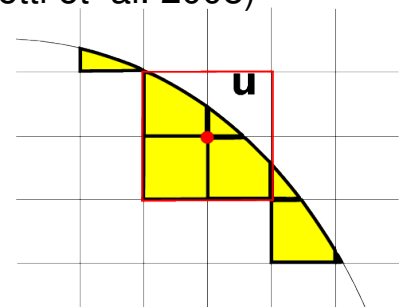
→ Gibbs oscillations at the discontinuities



Smoothed particle: volume-fraction scheme (Fadlun et al. 2000, Pasquetti et al. 2008)

- reduces Gibbs-oszillation
- allows for a moving particle
- in the spirit of a volumic forcing

$$\chi = \frac{1}{2h} \int_{(i-1)h}^{(i+1)h} \chi dx$$



Numerical method – no-slip & solenoidal

Main troubles :

- Operations boundary conditions (B) and divergence-freeness (P) do not commute !
- Fourier : poisson-equation for p with periodic boundary condtions

Solution : pressure predictor (Brown et al. 2001)

$$\tilde{u}^{n+1} = u^n + \Delta t\,[-(u^n \cdot \nabla)u^n - \nu \Delta u^n - \nabla p^n] \qquad \Delta p^n = \nabla \cdot [(u^n \cdot \nabla)u^n]$$

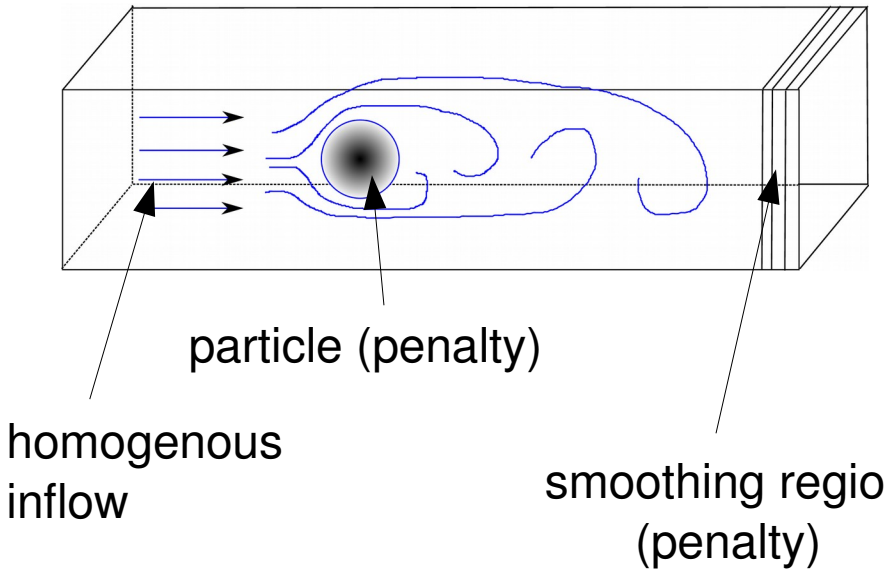
$$\tilde{\tilde{u}}^{n+1} = B(\tilde{u}^{n+1}) \equiv \tilde{u}^{n+1} + f_b^n$$

$$u^{n+1} = P(\tilde{\tilde{u}}^{n+1})$$

Usually no predictor ∇p – only projection

Benchmark-setup :

Numerical windtunnel



- regular grid with e.g. 256x256x1024 grid-points
- periodic boundary conditions at the surfaces
- penalty for particle and smoothing region

Numerical method – no-slip & solenoidal

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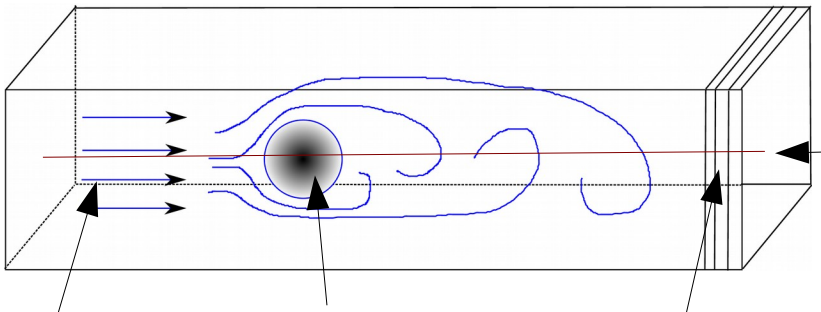
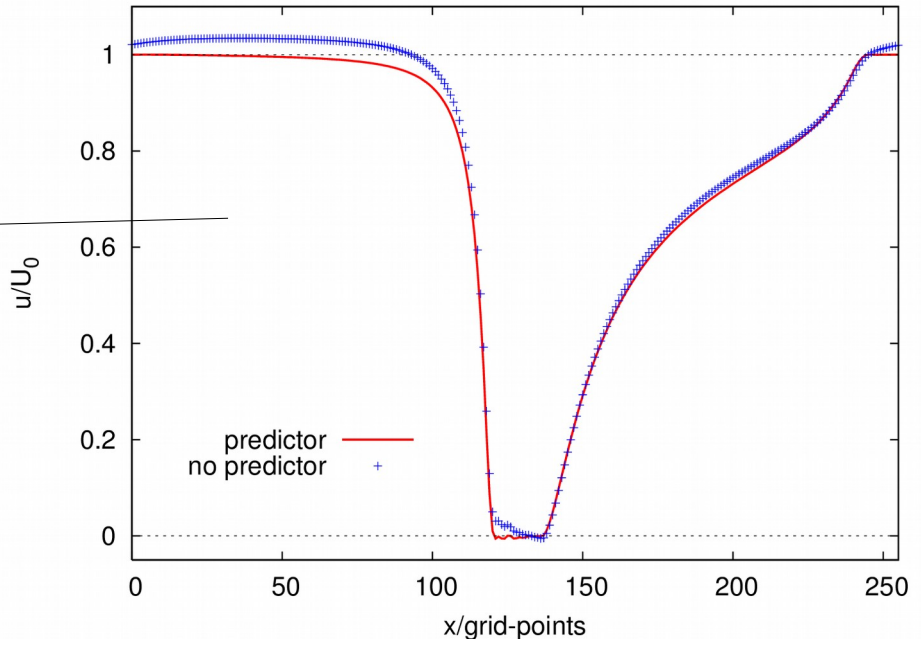


particle (penalty)

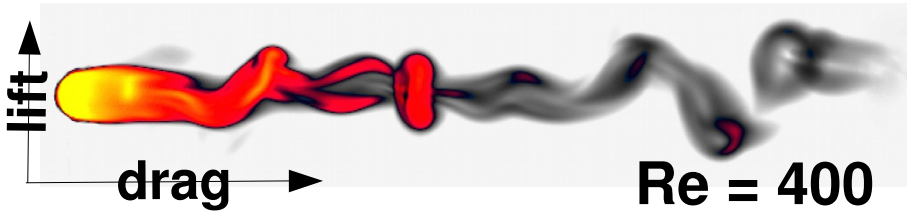
homogenous inflow

smoothing region (penalty)

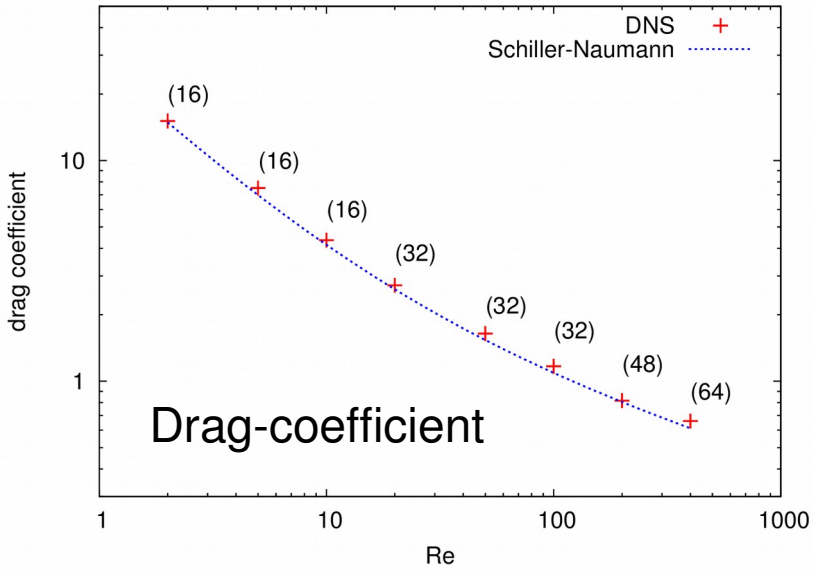


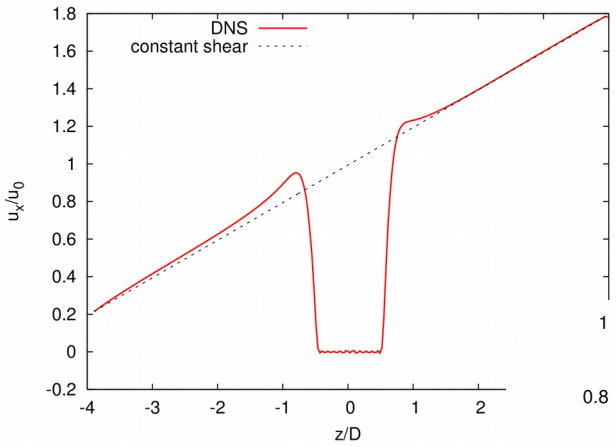
Numerical method - benchmarks

Forces on the particles



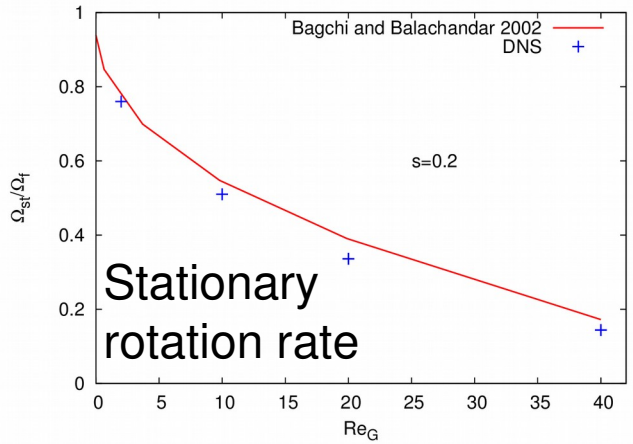
Drag-coefficient $C_D = F_D/(0.5\,U_\infty^2 \pi r^2)$

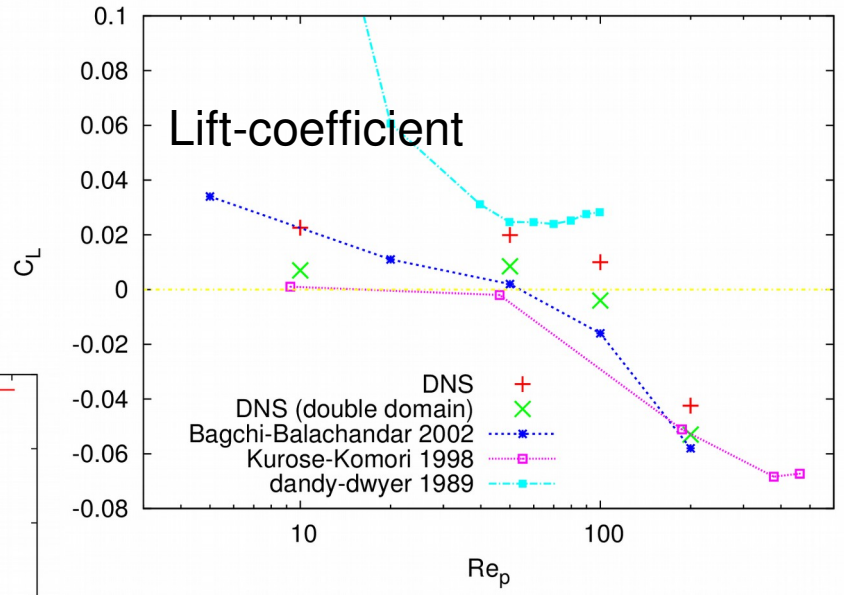




Constant shear:

$s = \nabla u\, D/u_\infty$





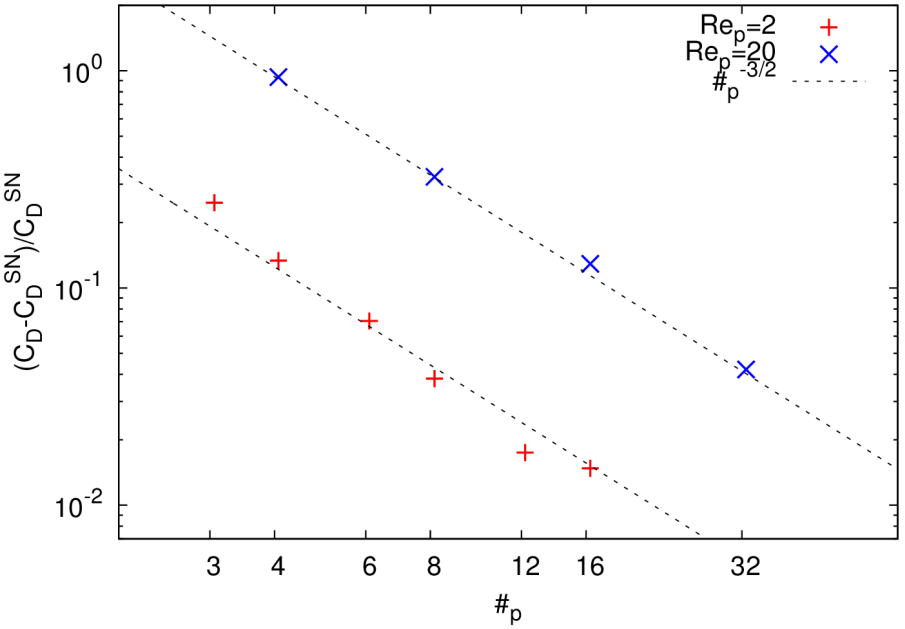
Numerical method - convergence

Convergence rate:

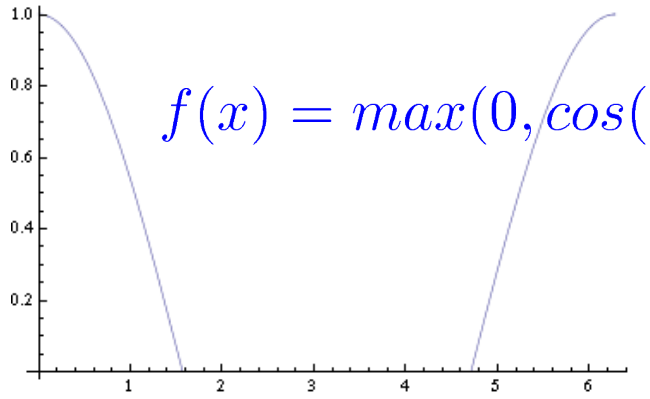
Boundary layer thickness $\delta_b \sim Re^{-1/2}$

Resolution : $D/\Delta_x \sim \delta_b/\Delta_x$

for $Re = const$

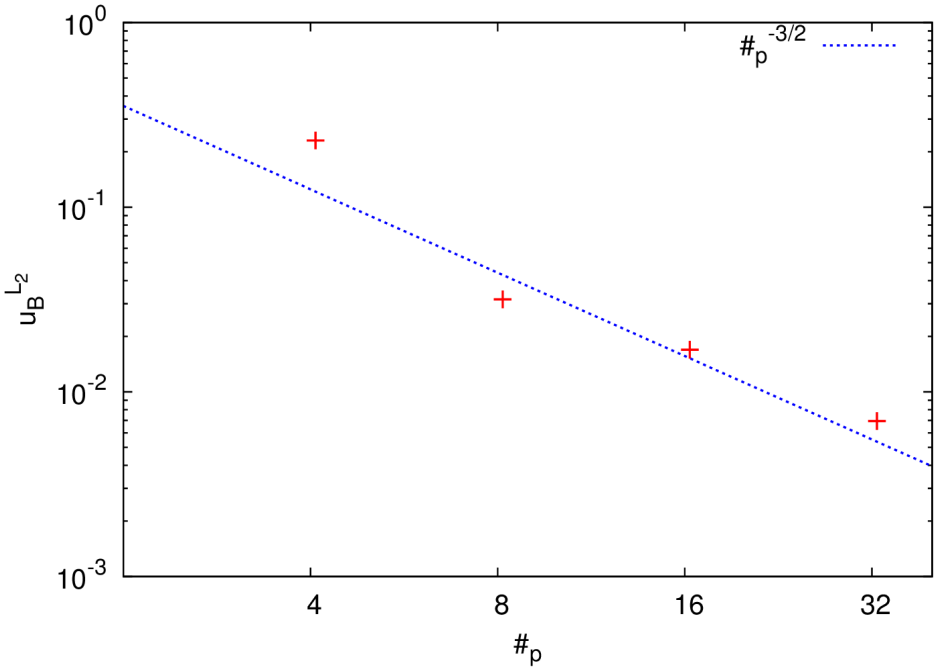


Why -3/2?

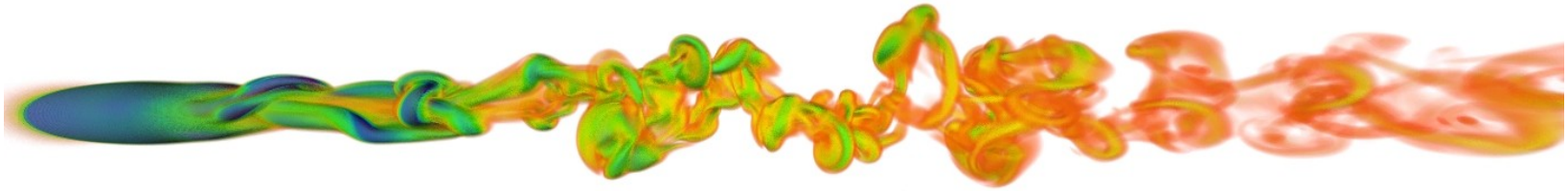


$$f(x) = max(0, cos(x))$$

L_2-Norm $\left(\int_B f_K(x)^2 dx\right)^{1/2} \sim K^{-3/2}$

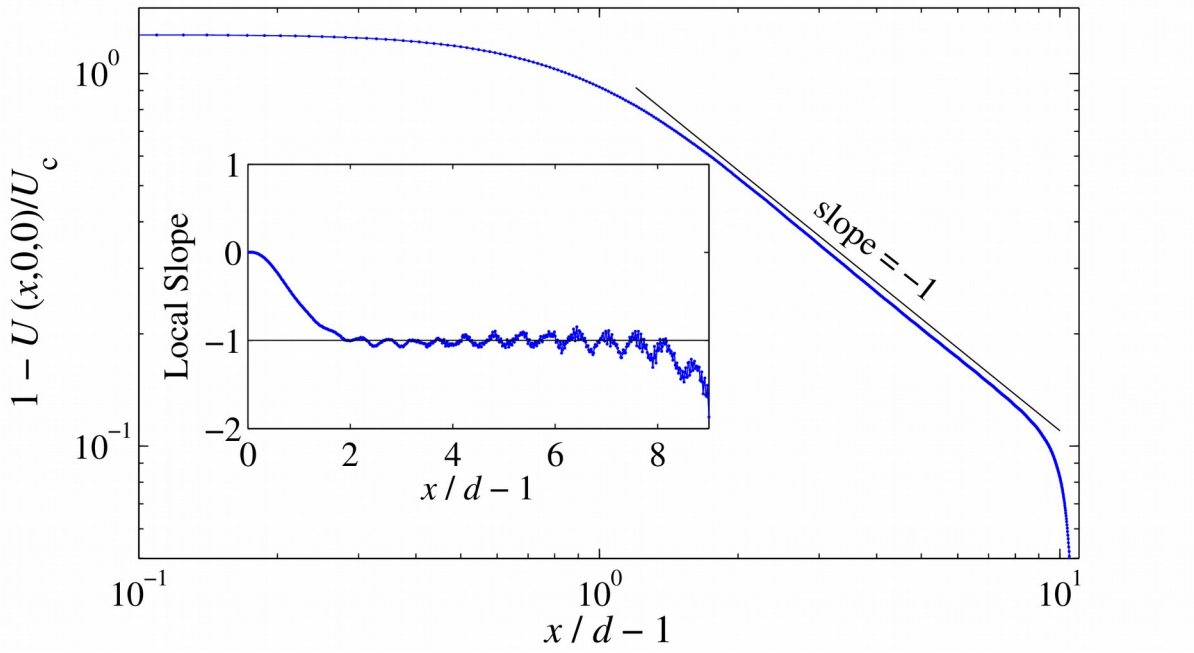


Benchmark - wake



Mean velocity deficit : $\Delta U = 1 - U(x,0,0)/U_c \sim x^{-1}$

(Wu & Faeth 1994, Bagchi & Balachandar 2004)



Results

1) Particle collision rates
2) Particle-wake interactions
3) Drag force

Small particle collision rates

Problem Parameters :

Particle Reynolds number

$$100 \leq Re_p = \frac{d\,U_c}{\nu} \leq 1000$$

Fluid Reynolds number

$$0 \leq Re = \frac{u_{rms}\,L}{\nu} \leq 3000$$

Turbulent intensity

$$0 \leq I = \frac{u_{rms}}{U_c} \leq 1.2$$

Dust Stokes number

$$0 \leq \tau \leq 80$$

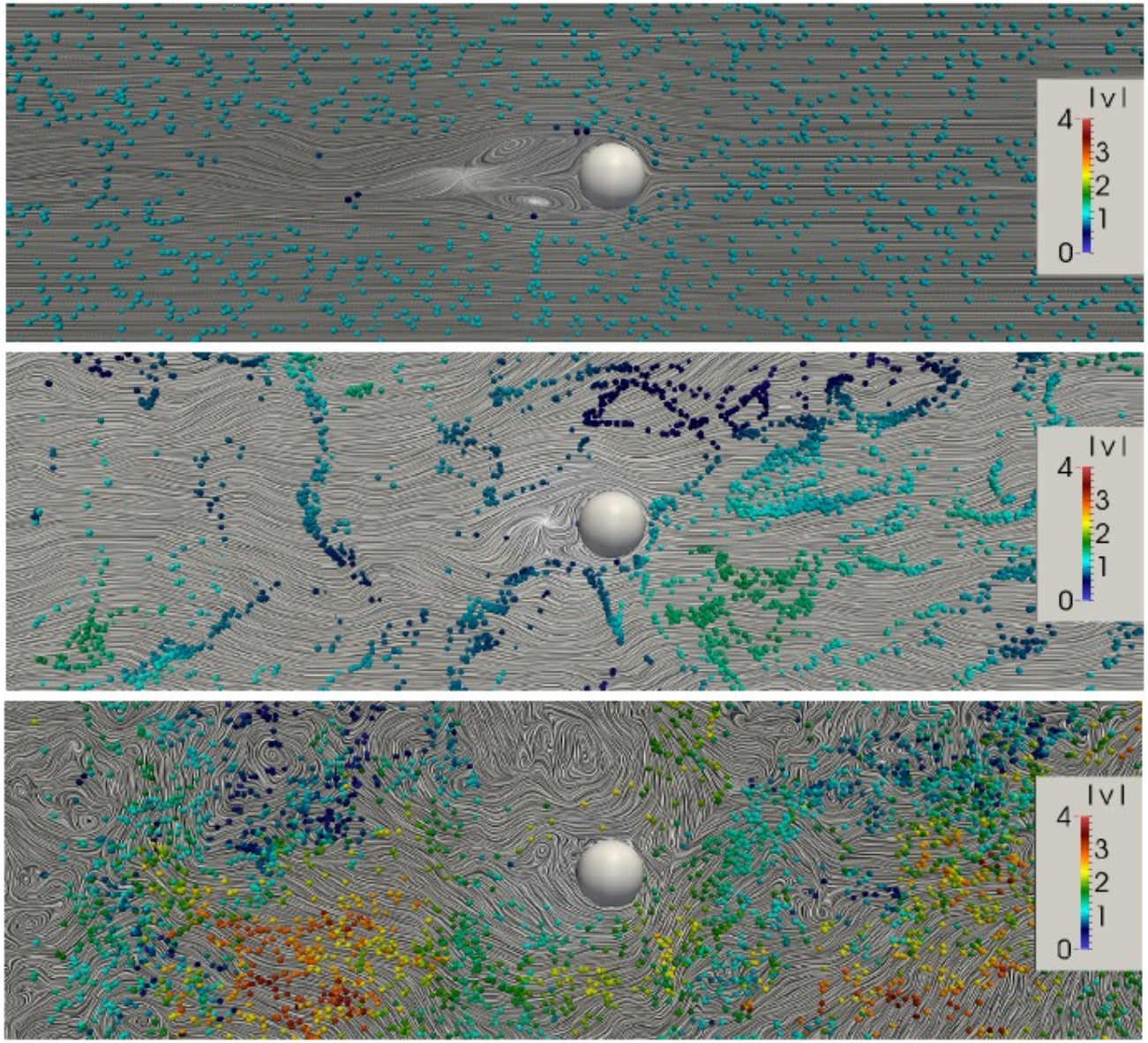
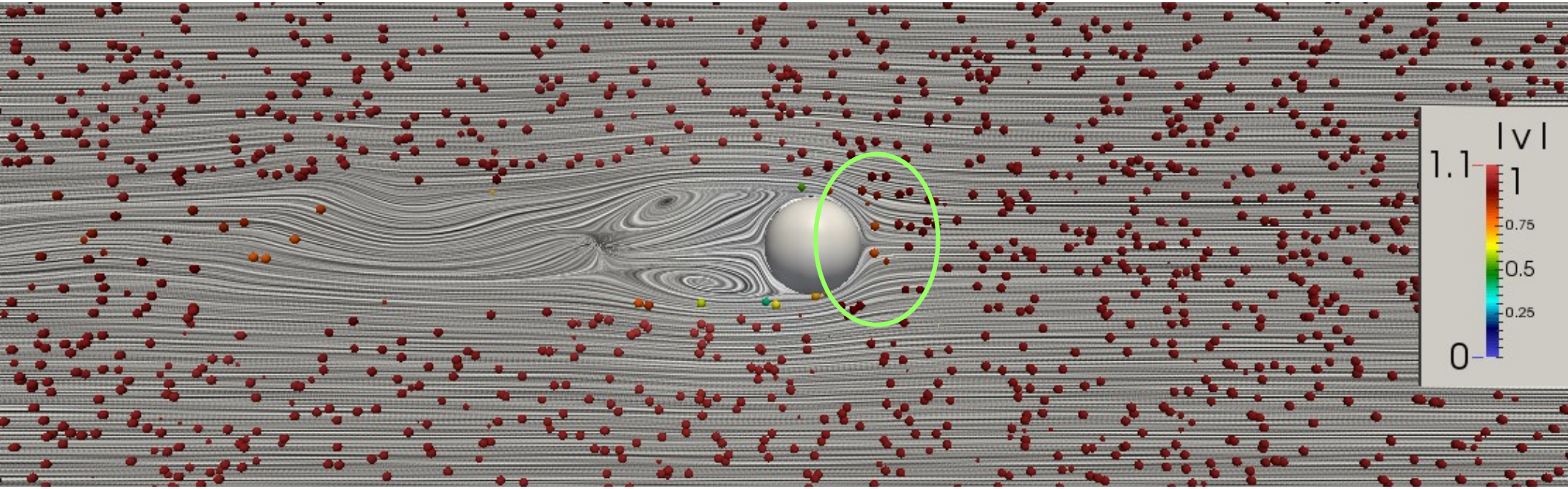


Fig. 1. Instantaneous streamlines of the gas flow and dust particles ($St = 0.8$) for I=0 (laminar), $I = 0.29$ (weakly turbulent), and $I = 1.18$ (strongly turbulent) from top to bottom. Note that while $St = 0.8$ for all shown cases, $St_\eta = 1.25$ for $I = 0.29$ and $St_\eta = 9.8$ for $I = 1.18$ so that the clustering properties of the shown particles change from one I to another.

Small particle collision rates

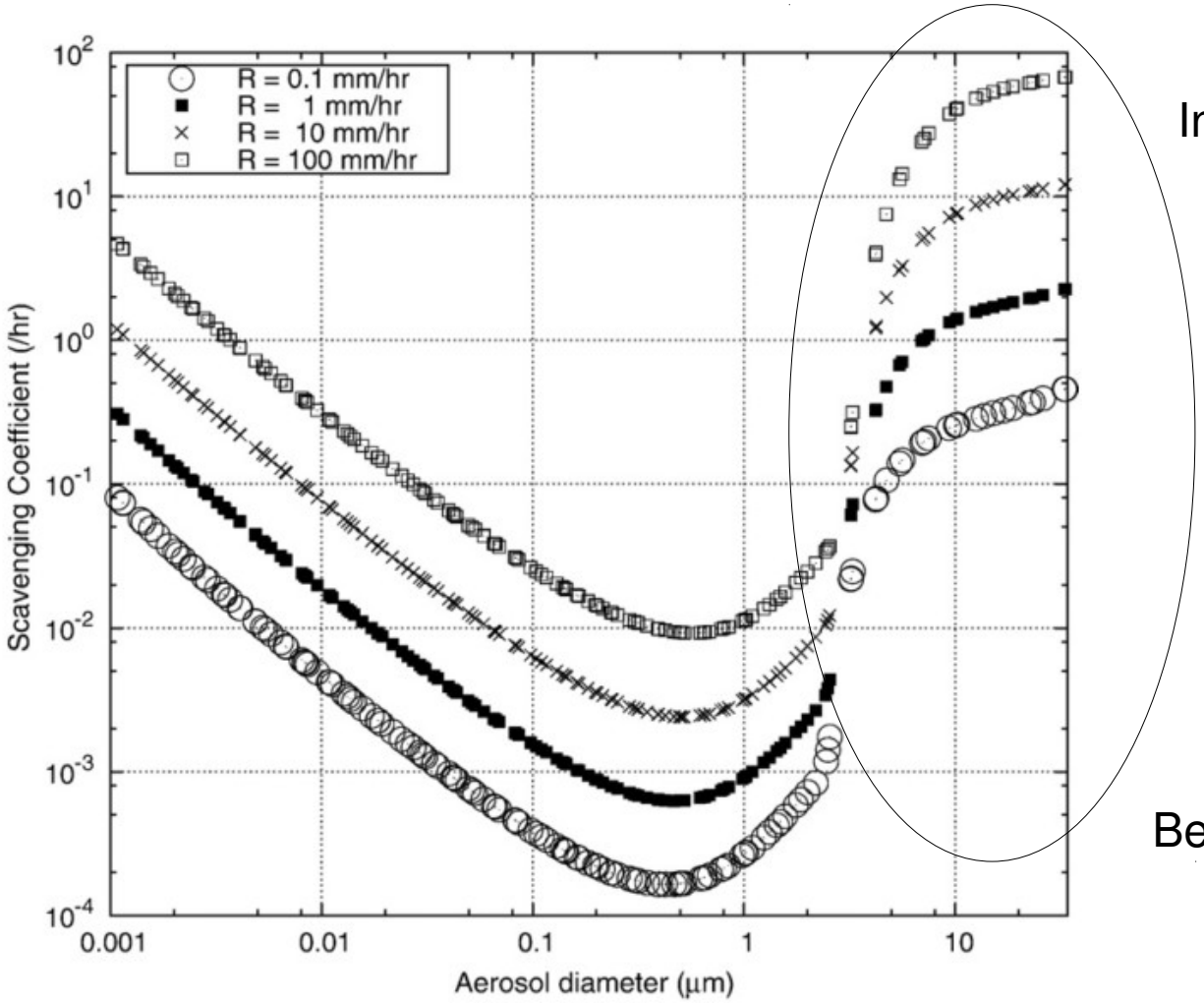
Laminar (uniform) inflow



Small particle collision rates

Application: Wet deposition of aerosols by falling raindrops

$$\gamma(d) = \int_0^\infty \pi/4\, U_t(D)\, E(d,D)\, n(D) dD$$

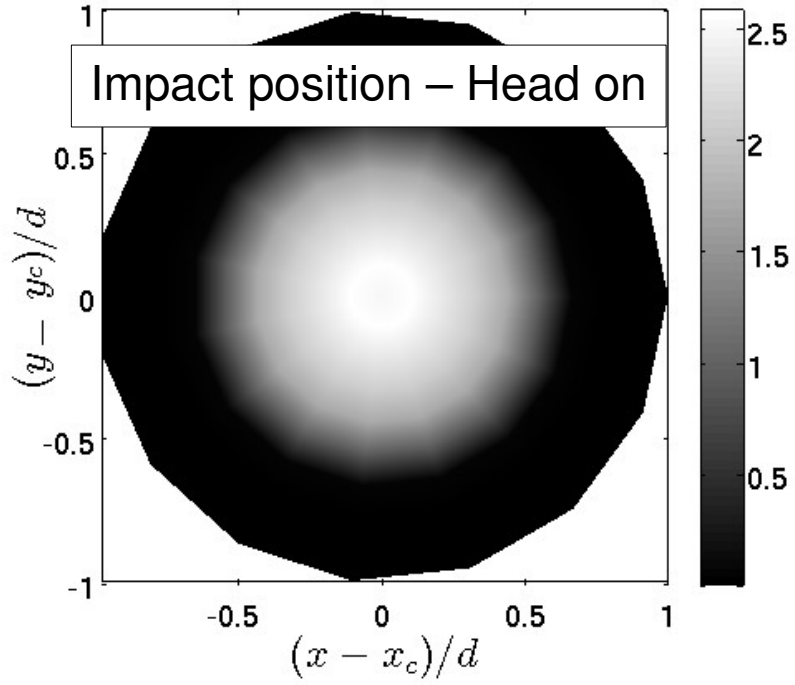


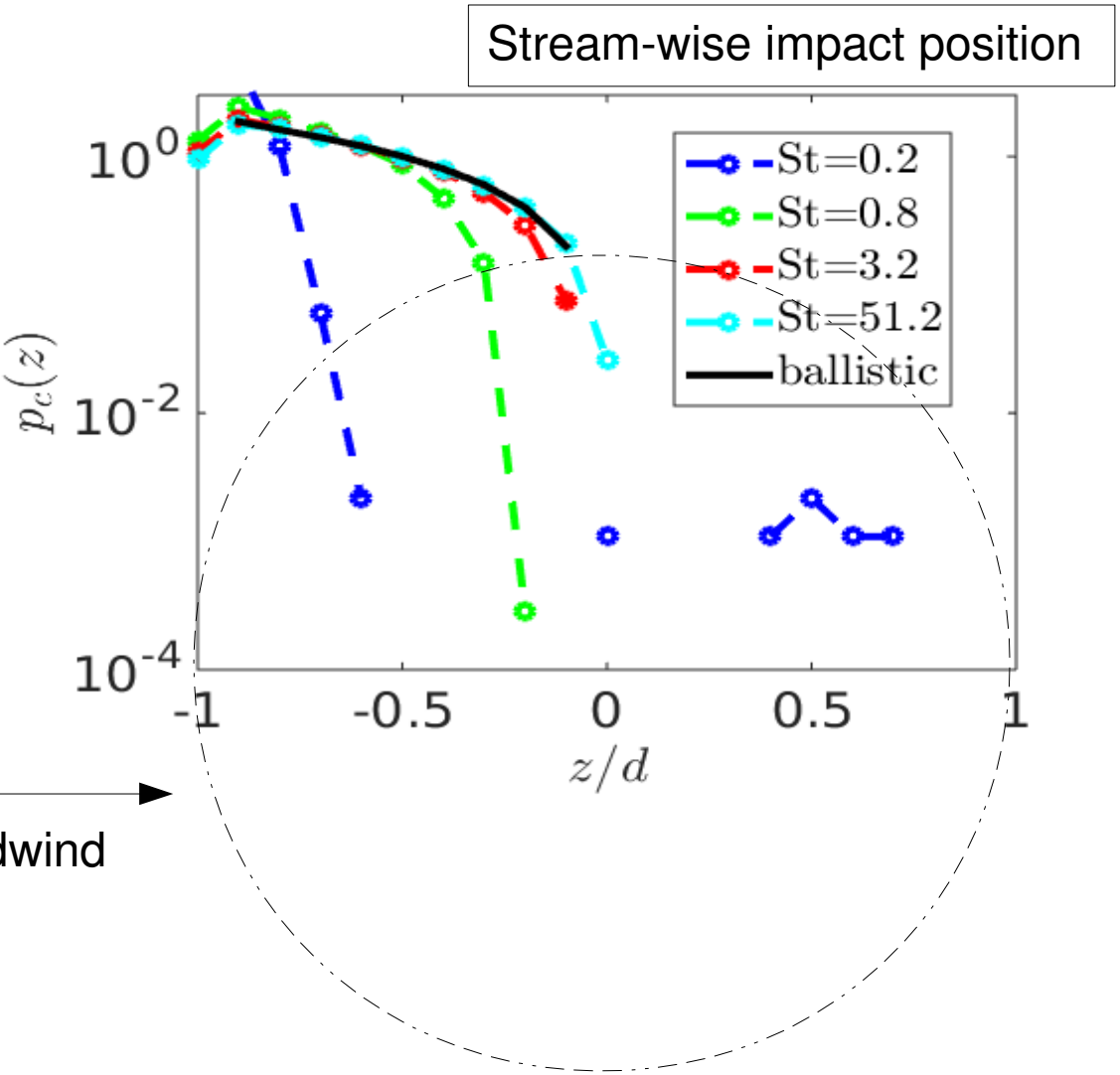
Inertial impaction

Berthet - Leriche et al. (2010)

LAMINAR collision statistics

Where do collisions happen ?

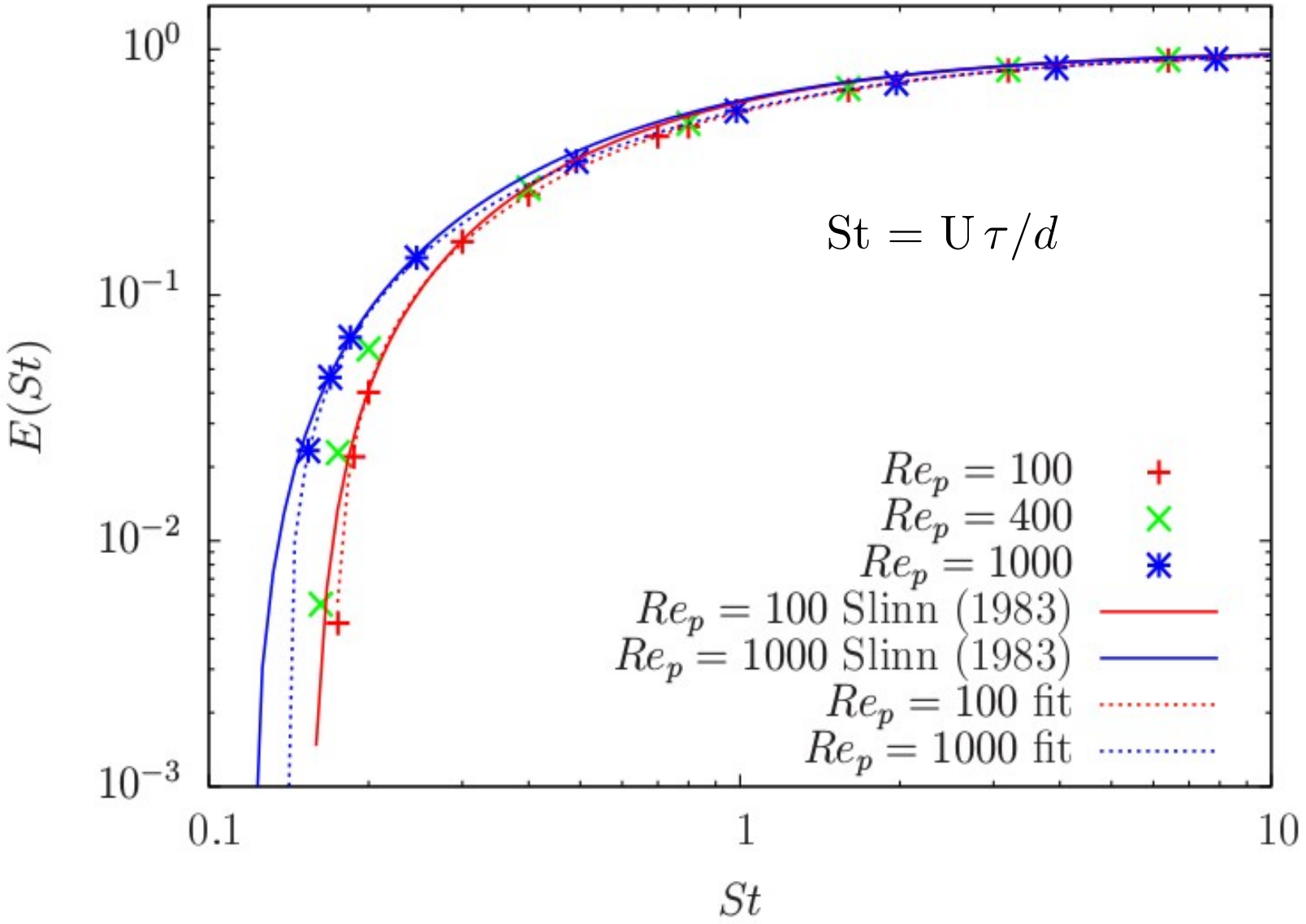




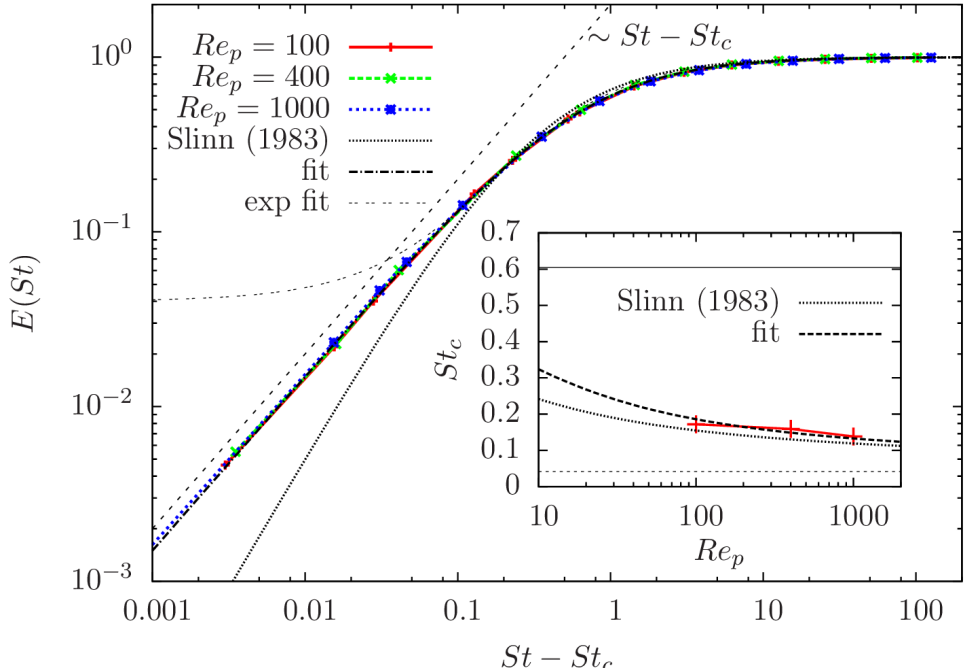
- Collisions are concentrated around the axis of symmetry
- Virtually no backward collision happen

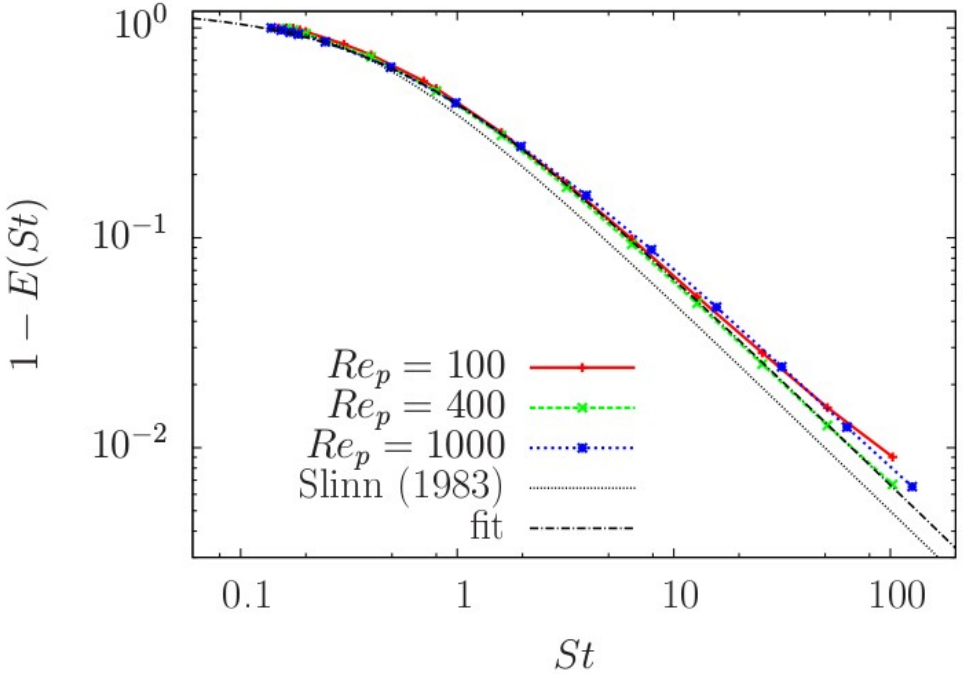
LAMINAR Collision statistics

Collision rate



LAMINAR Collision statistics





Small St limit :

- Critical Stokes number St_c
- Euler flow : $St_c = 1/24$
- Stokes flow : $St_c = 0.6$
- Re-collapse with linear slope

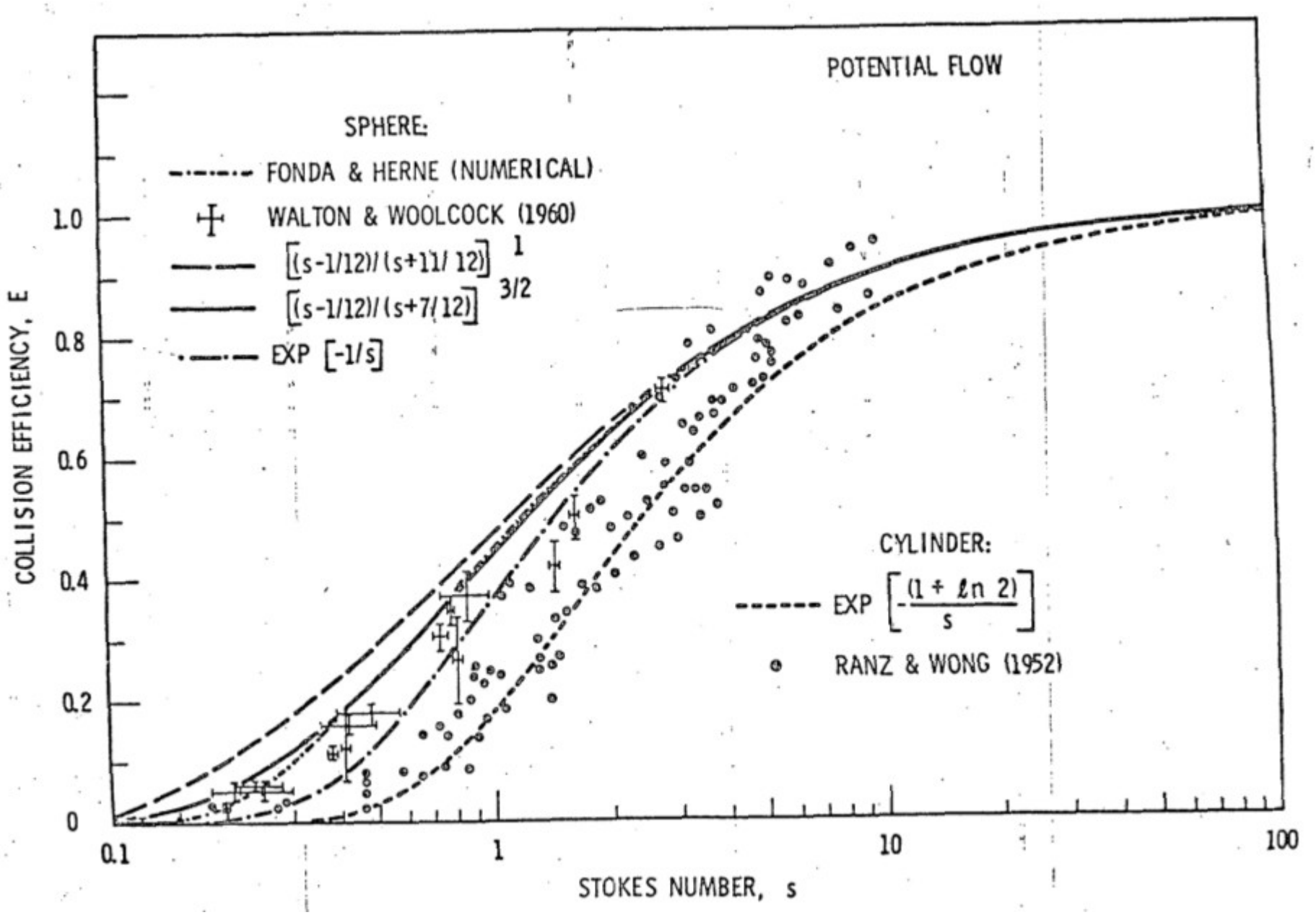
fit : $\frac{St-St_c}{St-St_c+2/3}$

Slinn : $\left(\frac{St-St_c}{St-St_c+2/3}\right)^{3/2}$

Large St limit :

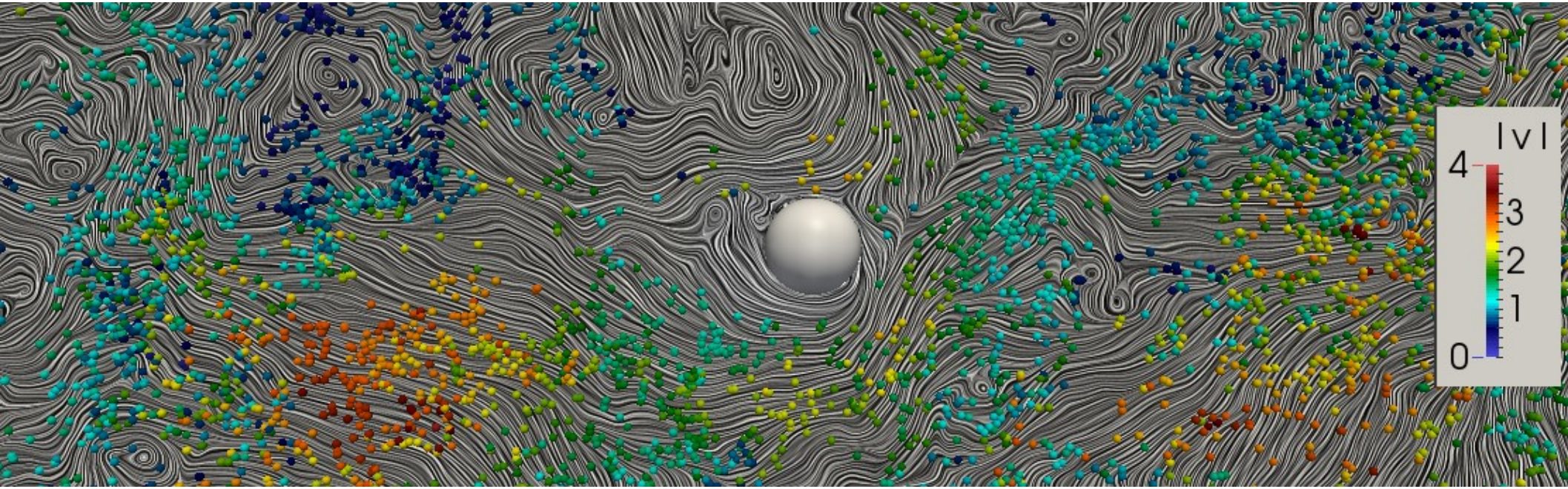
- Re-collapse with $\mathrm{E(St)} \sim 1 - 1/St$

Slinn's fit (1974)

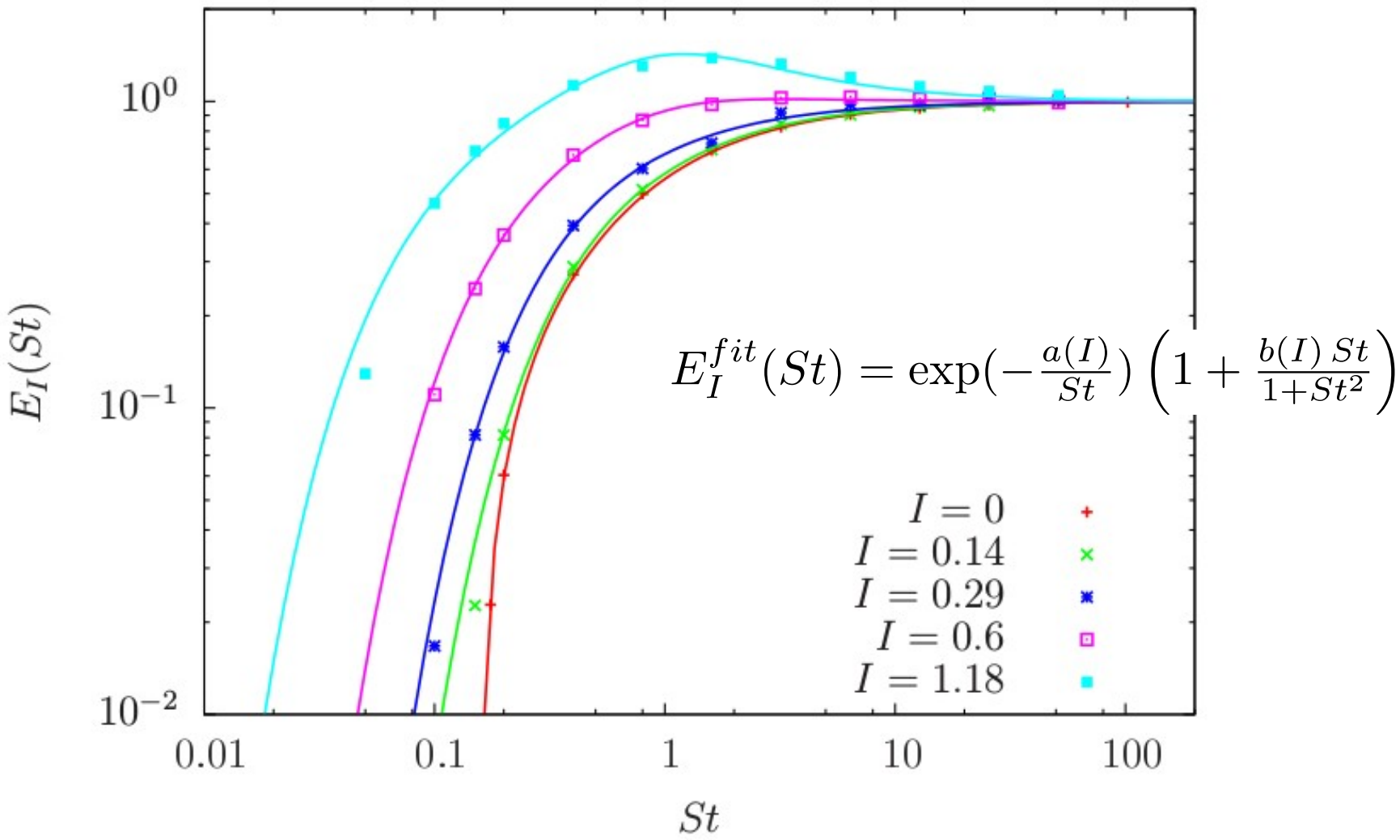


Small particle collision rates

Turbulent inflow



TURBULENT Collision Statistics



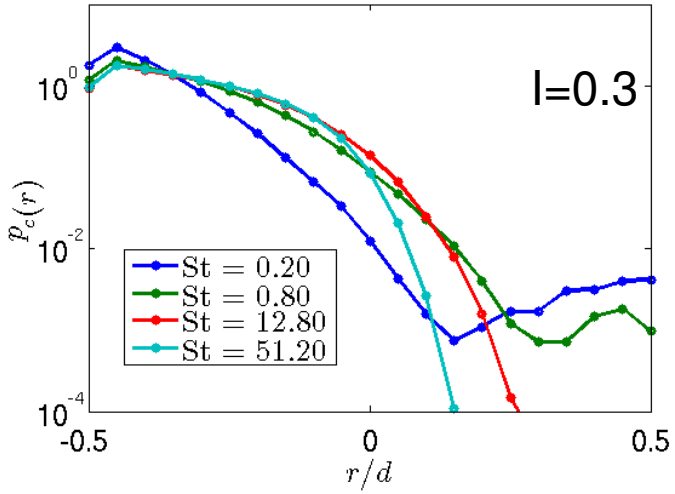
- Turbulence increases significantly the collision efficiency
- Collision efficiency can be larger than unity
- Probably no critical Stokes number

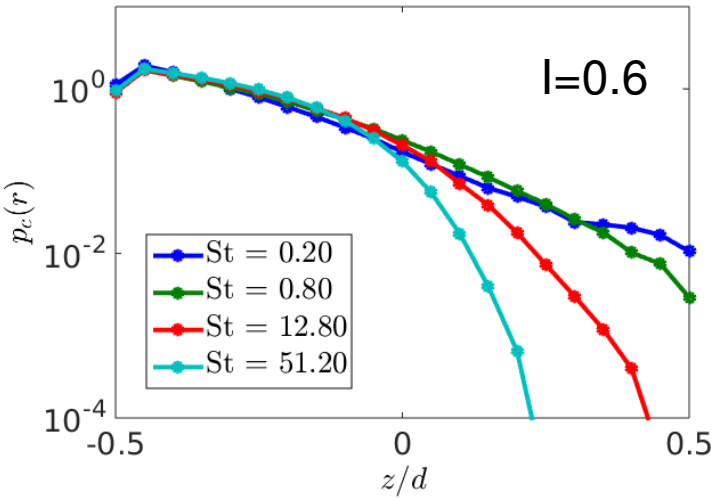
Turbulence effects on collision rate I

1) Fluctuating head wind

- Increase of collision rate (higher Re → higher collision rate)
- Velocity distribution → no critical Stokes number

2) Randomization of impact direction and position (→ backward collisions)



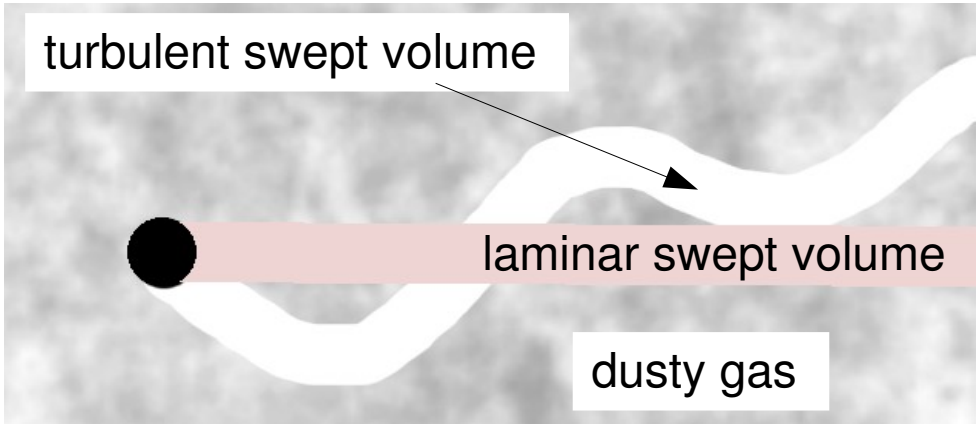


3) Increase of swept volume

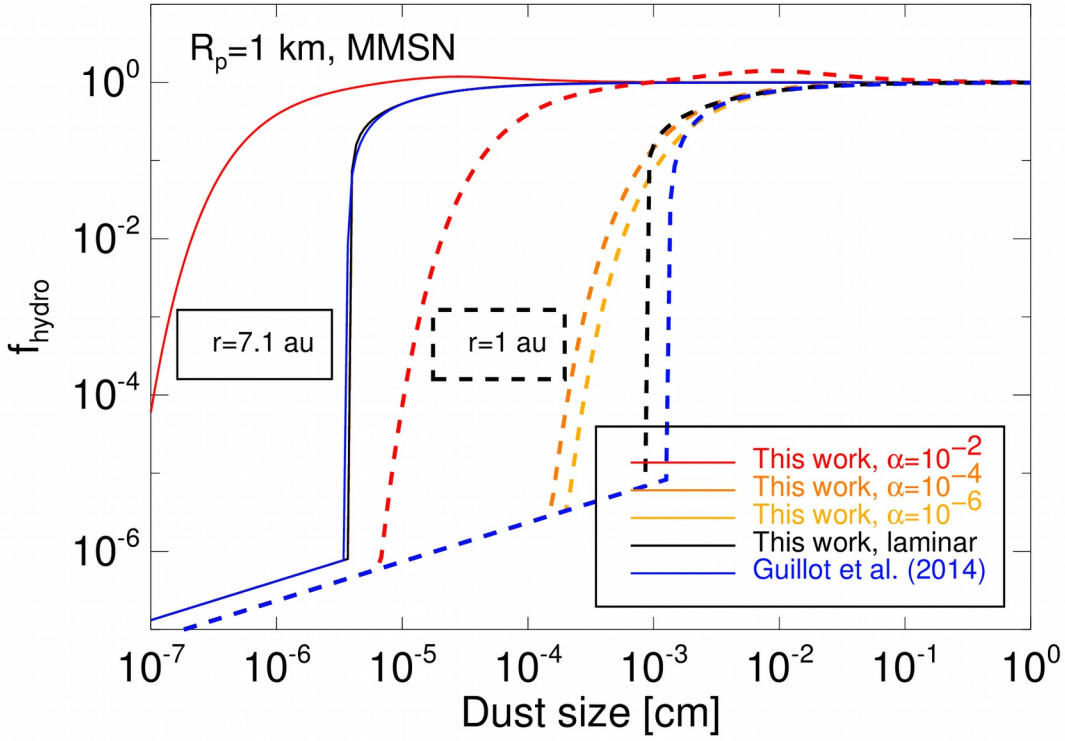
turbulent volume > laminar volume
simple computation for sinusoidal motion:

$$E_I(St) = E_0(St)(1 + \frac{I^2}{1+St^2})$$

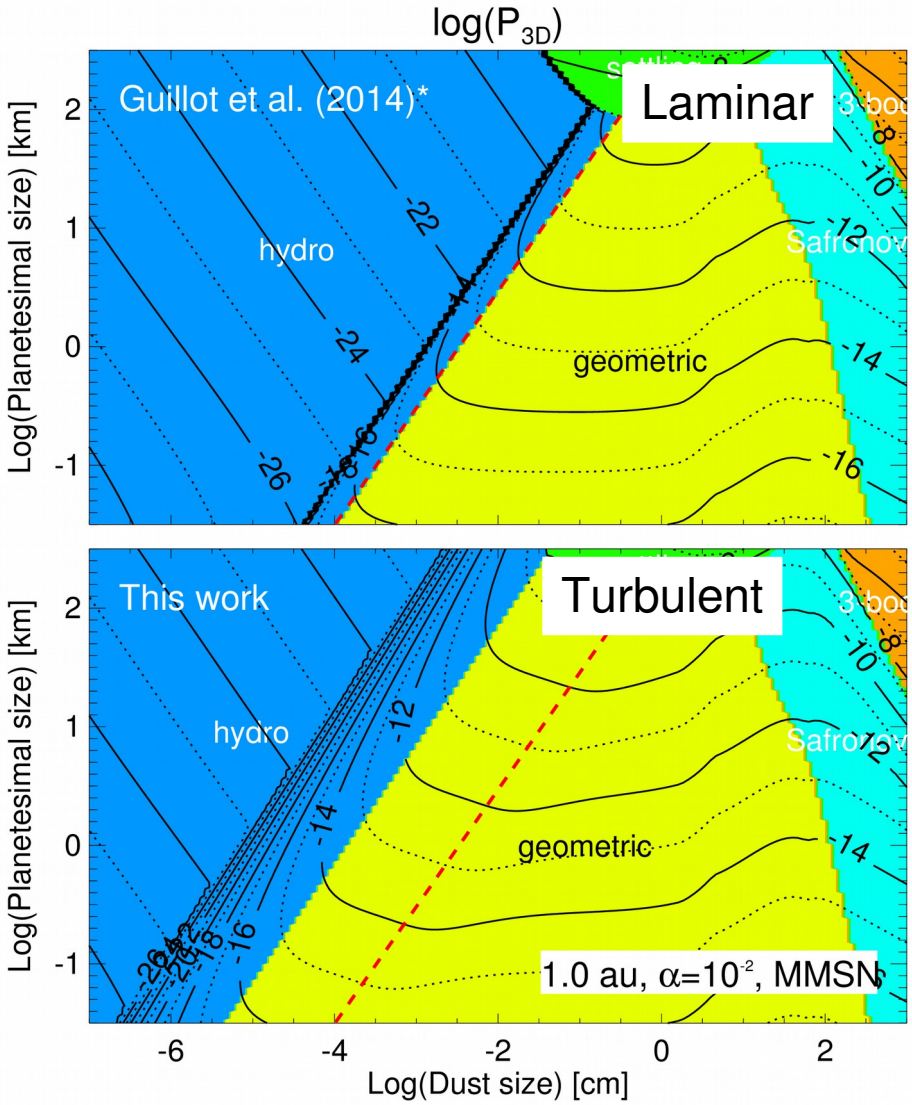
Allows for collision rate > 1!



Consequences for planet formation



Extension of the geometric regime to smaller dust sizes by turbulence



Collision efficiency for different orbital distances and turbulent intensities

alpha parameter: Turbulent eddy viscosity

$$\nu_t = \alpha\, c_s\, H$$

Importance of collision speeds

Different collision scenarios

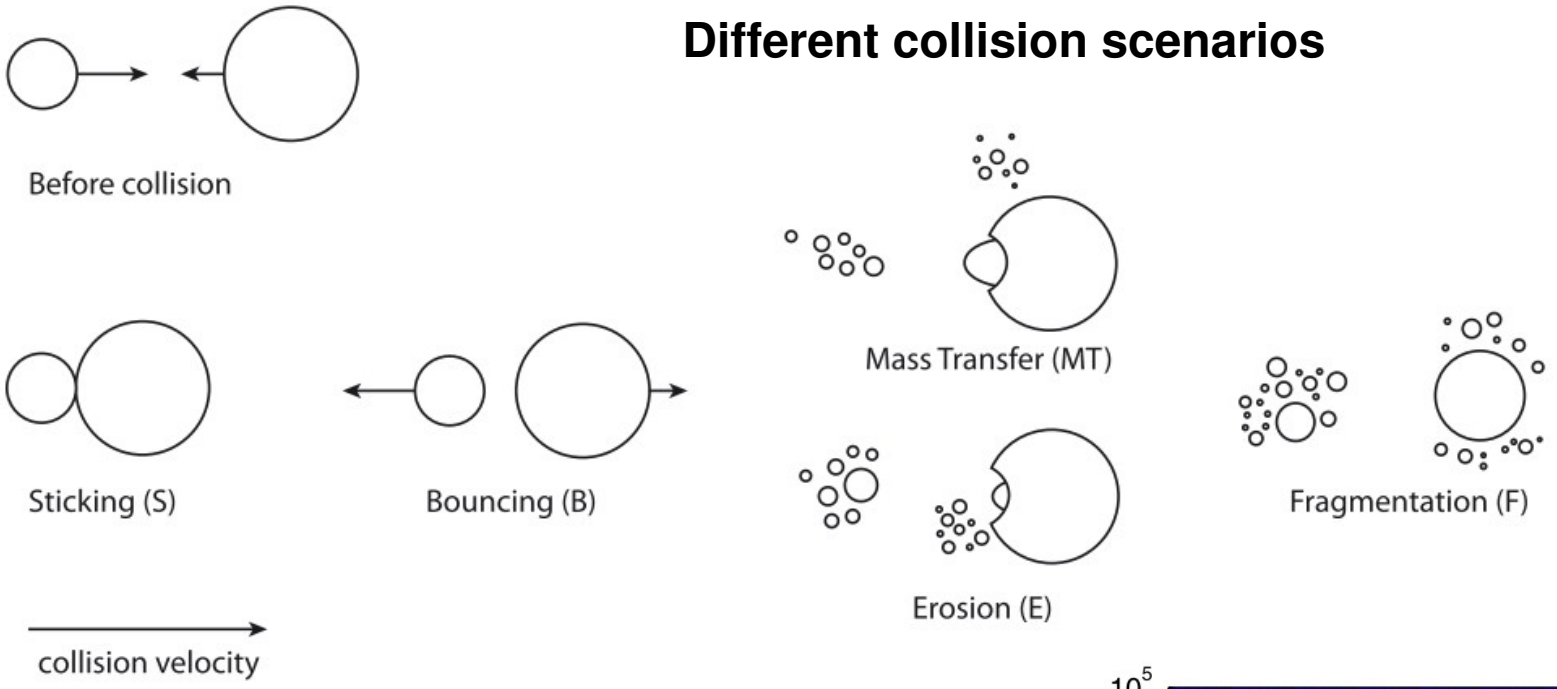
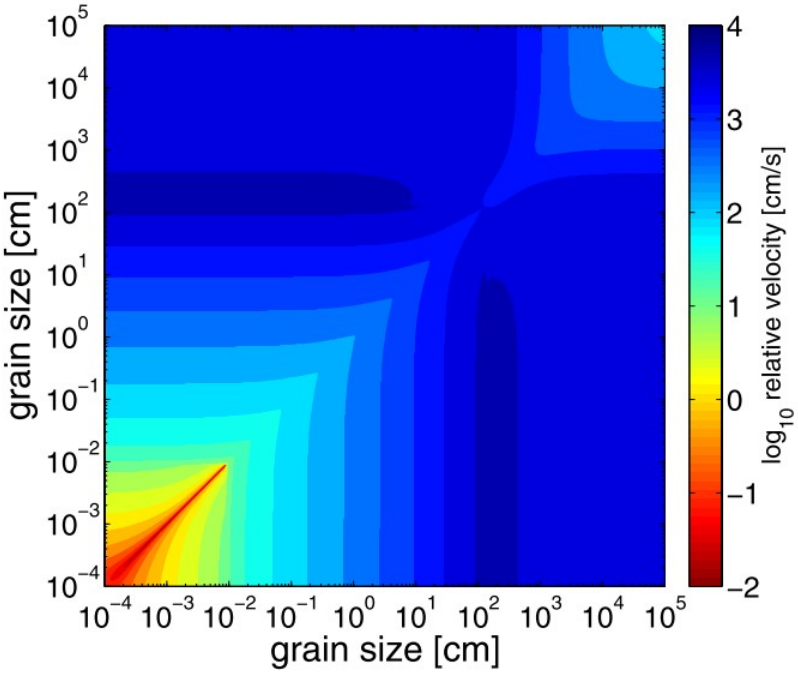


Fig. 2. Sketch of the five possible outcomes described in Sect. 3 sorted in rough order of collision
neously in a collision, and we define a mass transfer collision as leading to net growth for the tar
loss. This outcome is extremely dependent on the mass-ratio of the particles, thus adding a secon

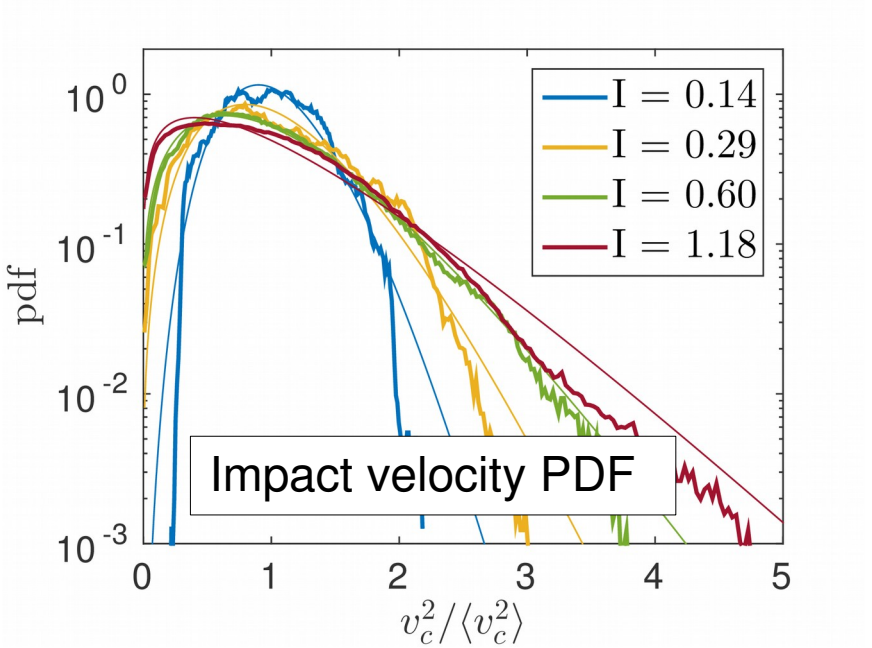
Population evolution models use velocity maps:

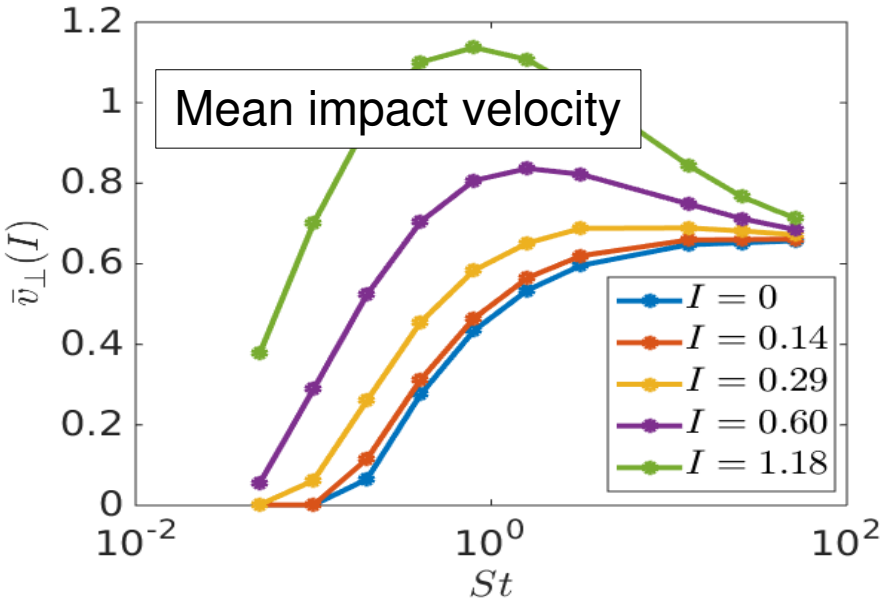
Windmark et al. (2012)

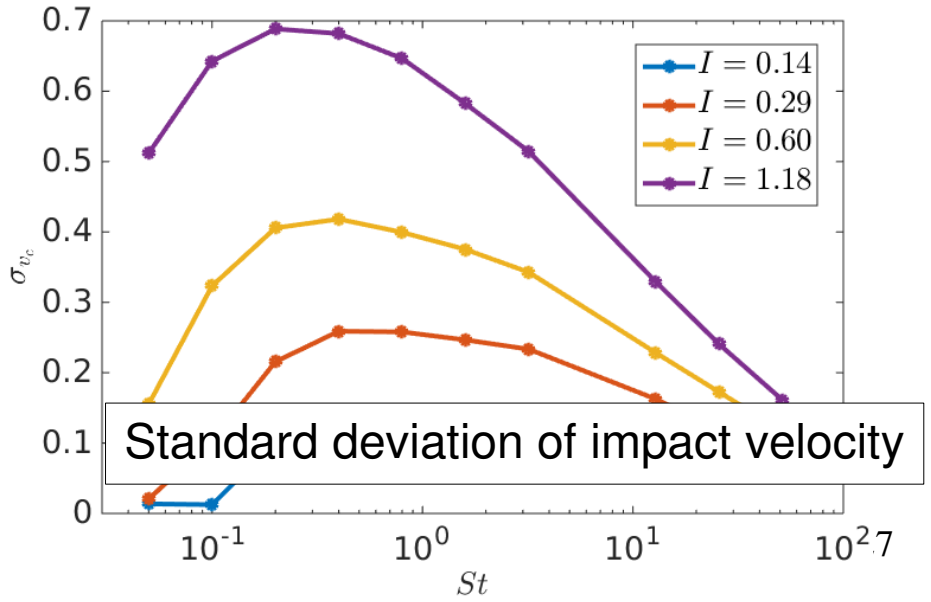


Measured collision speeds

- Turbulent fluctuations lead to velocity distribution
- Distribution fairly modeled by non-central chi-squared distribution
- Turbulence increases mean impact speed with maximum close to St=1
- Standard deviation approx. proportional to turbulence intensity

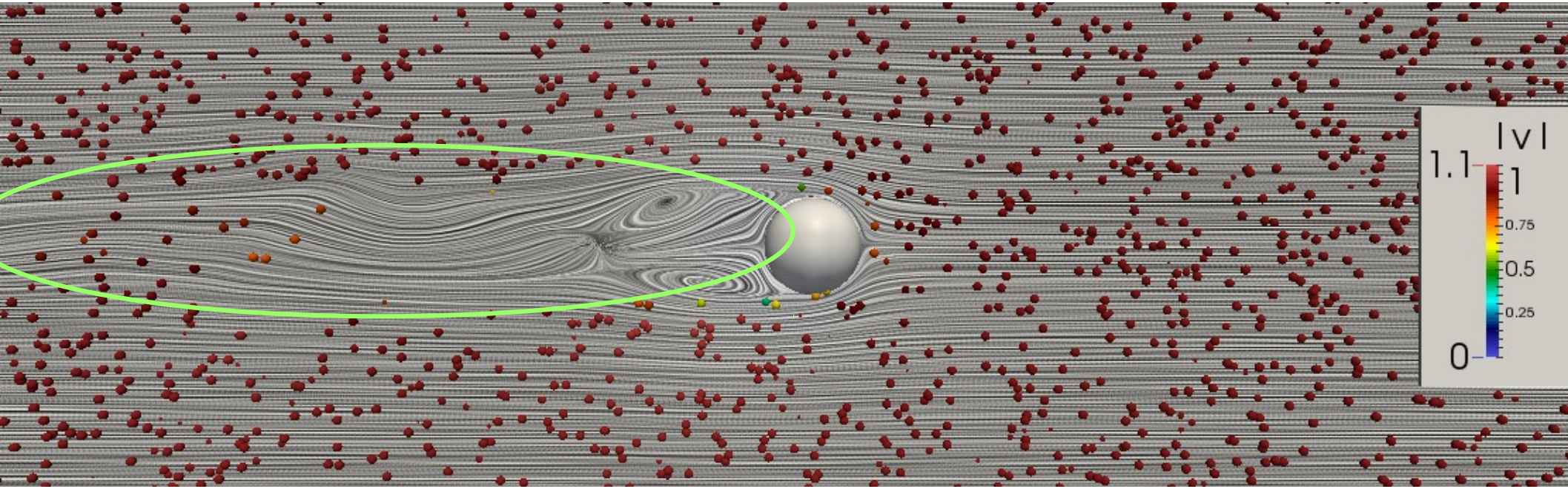






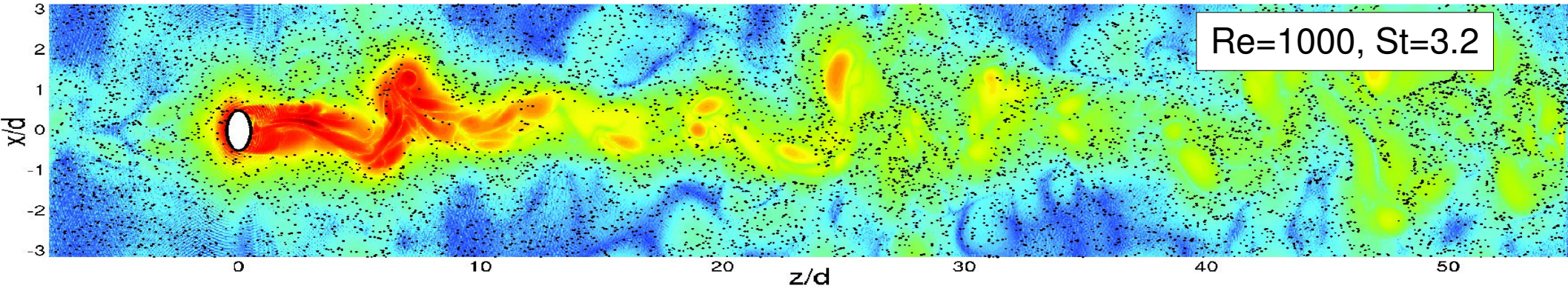
Small particle wake interactions

Laminar (uniform) inflow



Dust in the wake

What happens to particles that passed the sphere ?



Okubo-Weiss parameter

$$\Delta = \left(\frac{\det[\hat{\sigma}]}{2}\right)^2 - \left(\frac{\mathrm{tr}[\hat{\sigma}^2]}{6}\right)^3$$

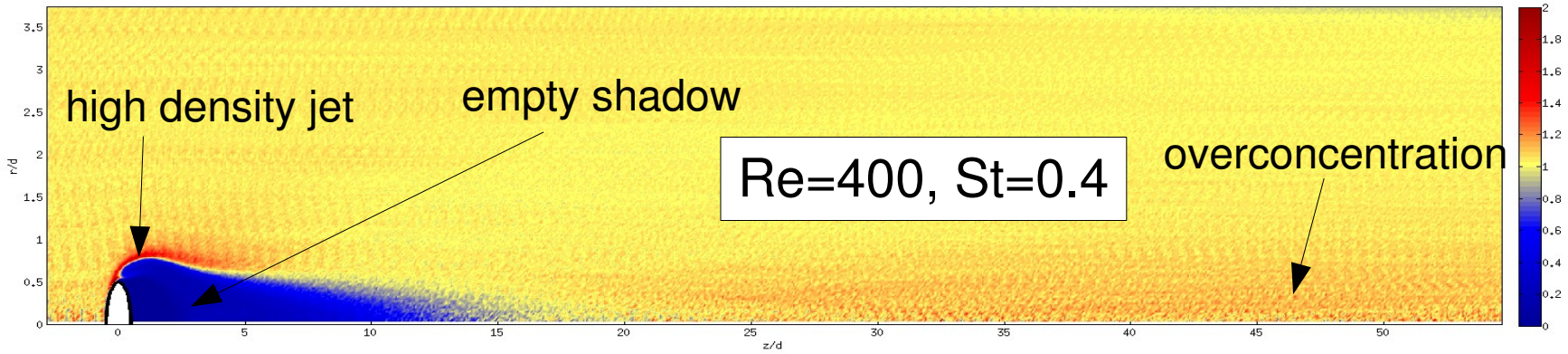
$\Delta < 0$ straining regions

$\Delta > 0$ rotational regions

$\hat{\sigma} = \partial_i u_j$ strain matrix

Particles interact with the shed structures – they are ejected

Mean particle densities



Experimental measurement (Jacober and Matteson 1990)

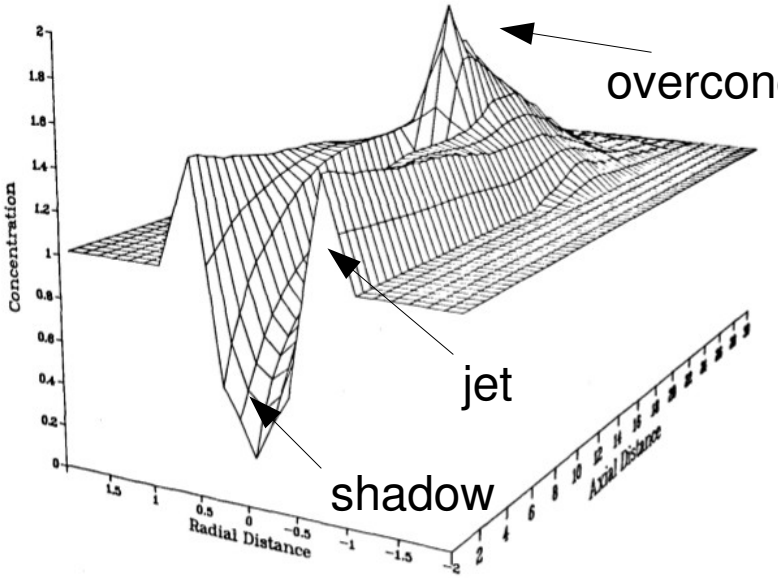
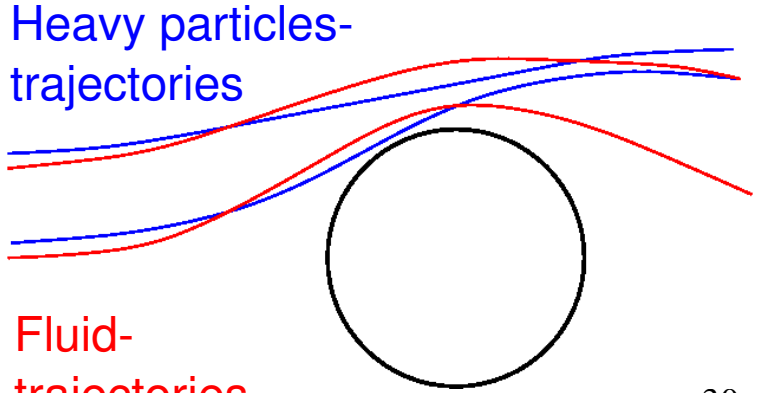
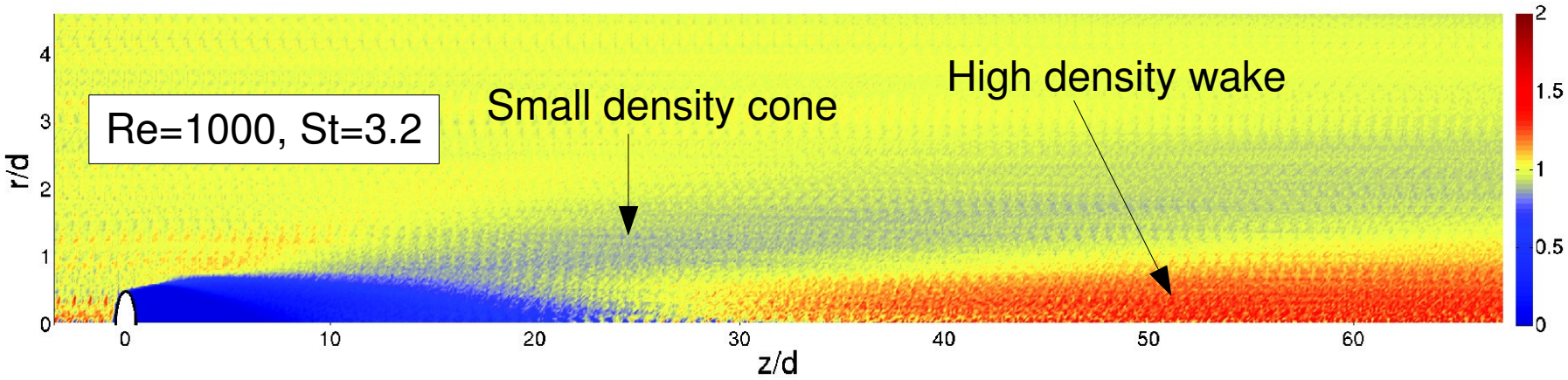


FIGURE 7. Axial and radial particle concentration distribution in the sphere wake for 10-μm particles and a free stream velocity of 6.1 m/s (radial and axial distances in radii).

Jet creation mechanism

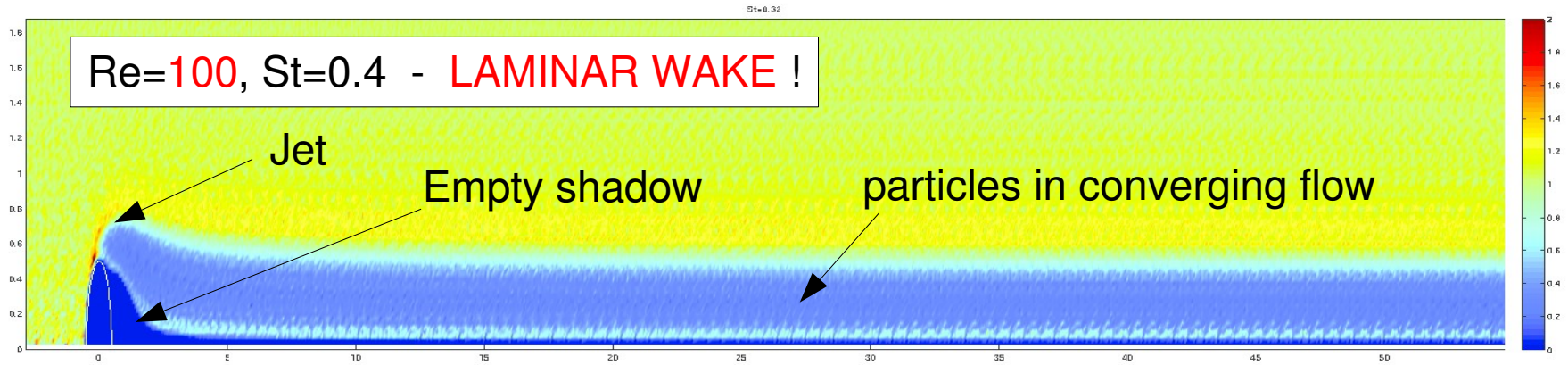


The wake : Mean particle densities



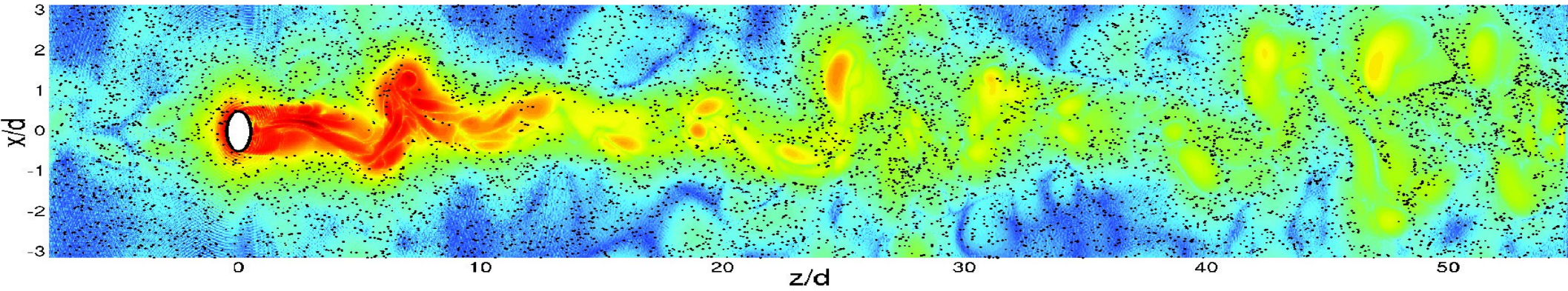
Jacober and Matteson : wake concentrations from collapsing jet

But: Concentrations only for turbulent wakes !

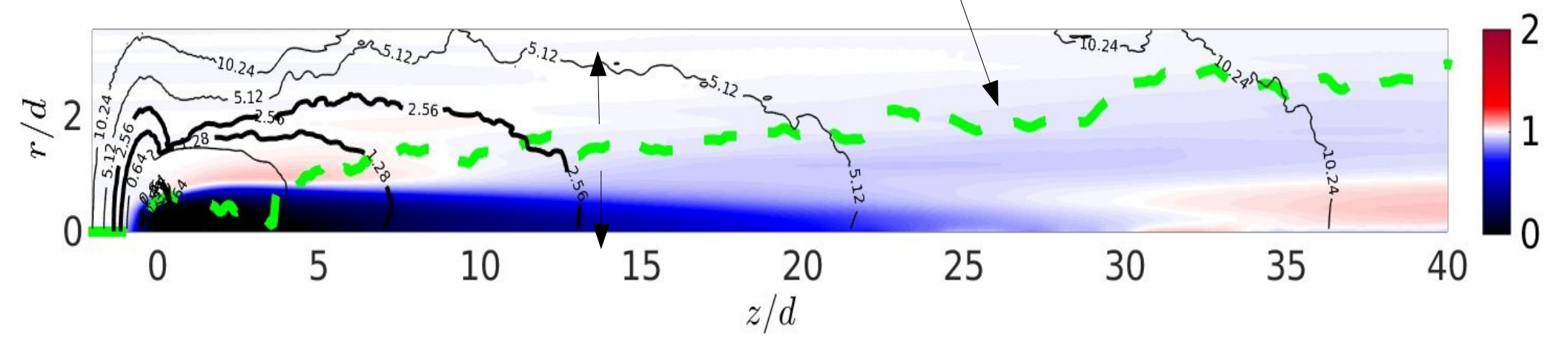


Concentration in the wake due to turbulent fluctuations

Wake concentration mecanism



Maximum of Δ depends on stream-wise position



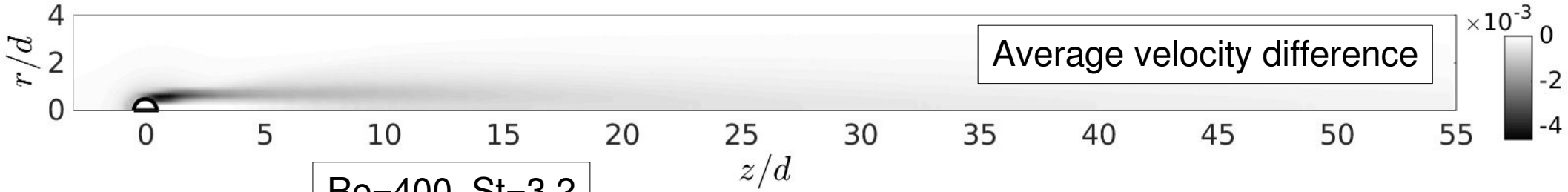
Resonant ($\mathrm{St} \simeq 1$) ejection from vortices determines starting point of overconcentration

Inter-particle collisions

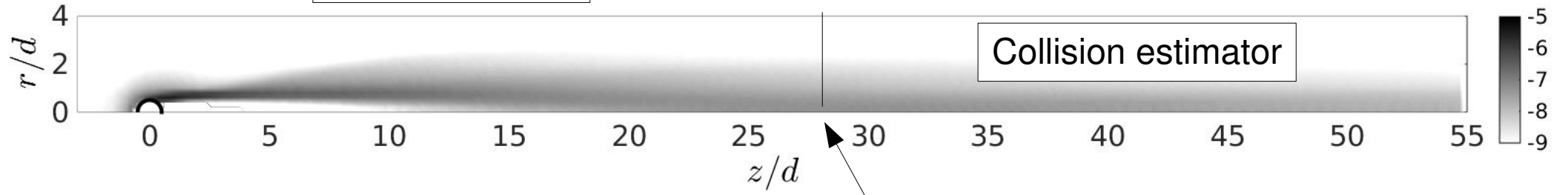
Rough collision estimator : $p_c(x) = -\langle n(x)^2 \rangle \langle w^-(x) \rangle$

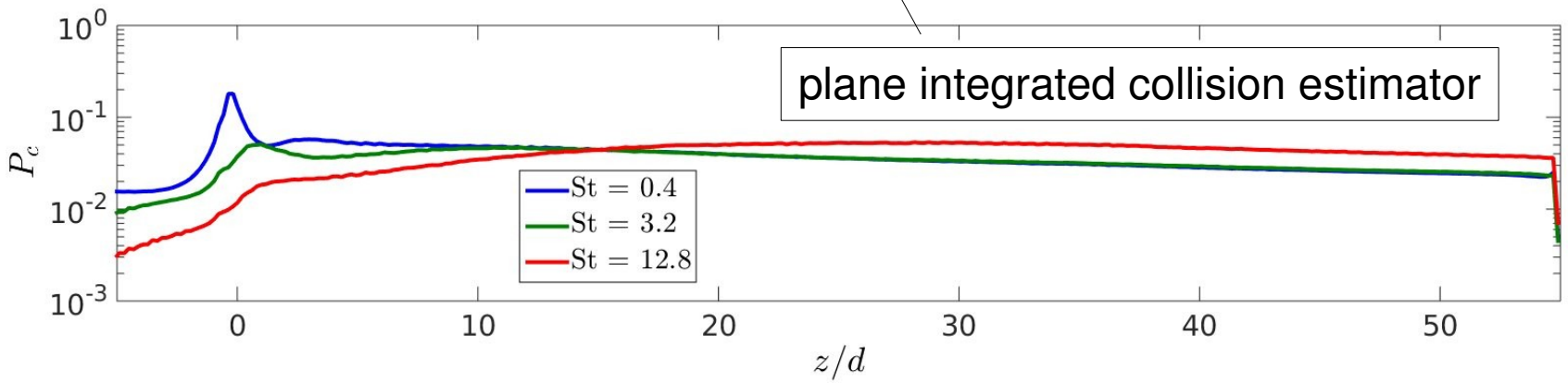
$n(x)^2$: number of particle pairs

approaching particles → $w^-(x)$ longitudinal velocity difference

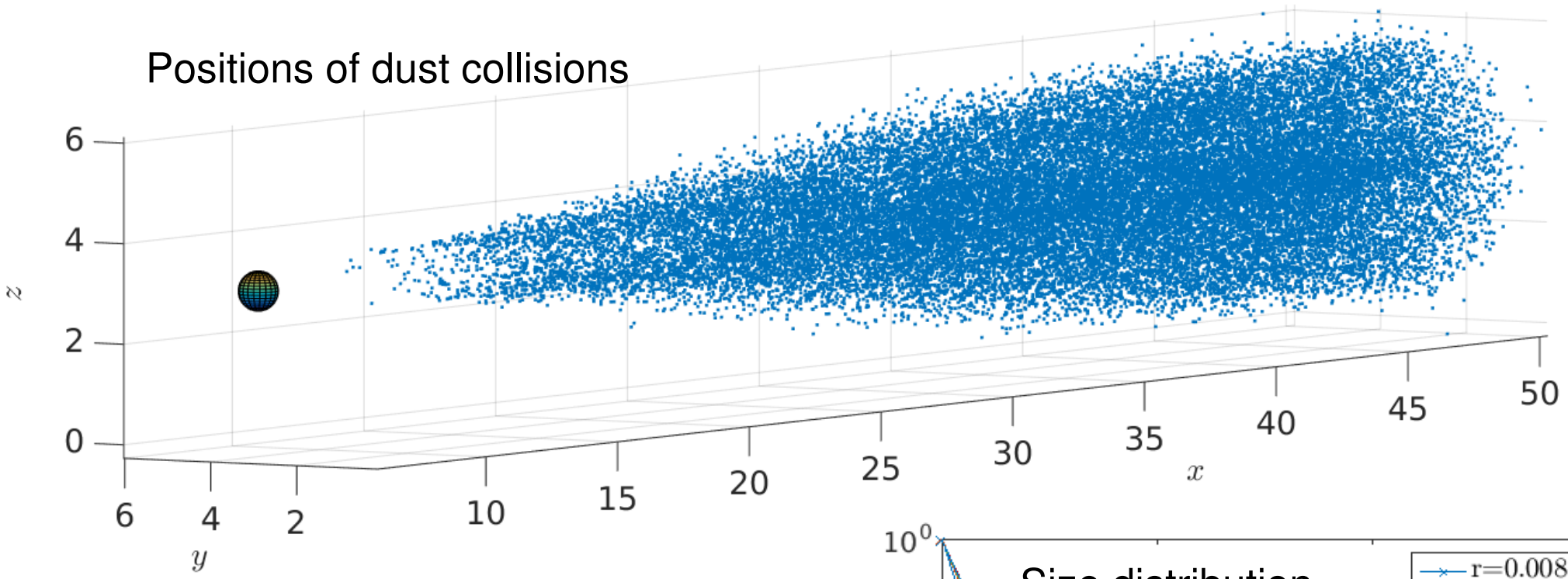


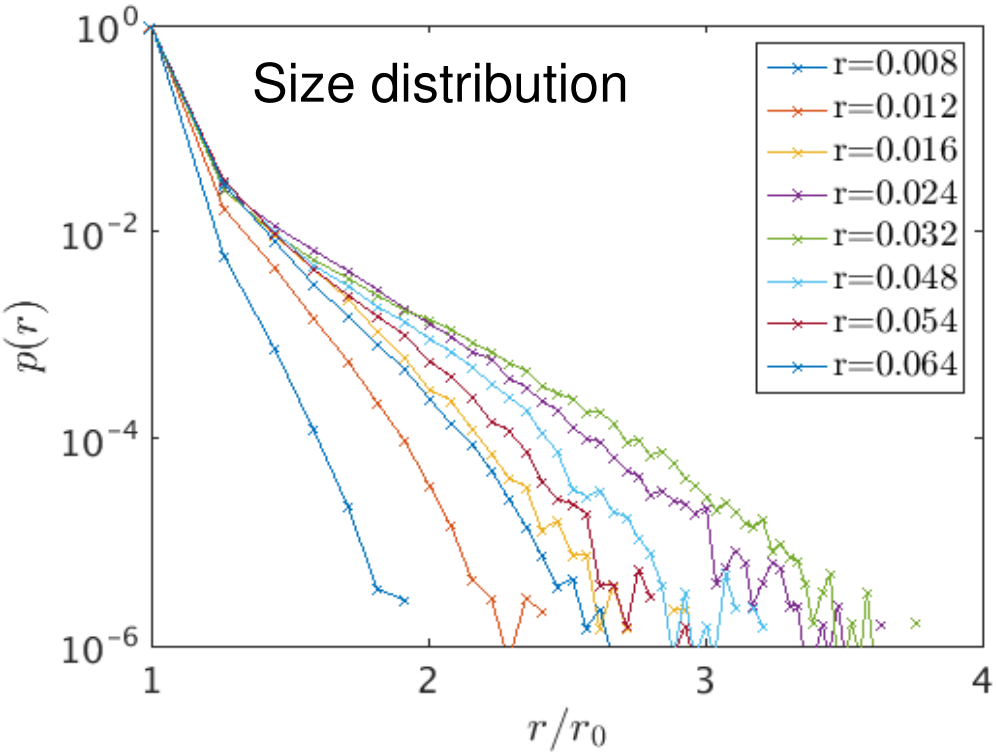
Re=400, St=3.2





Soon with “real” inter-dust collisions

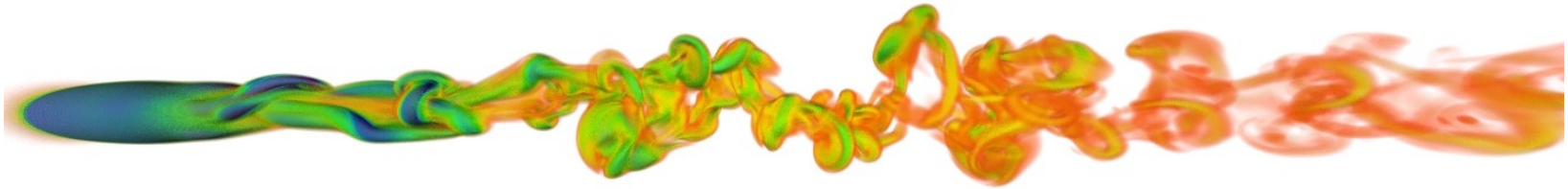




- Functional form of size-distribution
- Estimate processing efficiency of swarm of big particles (planetesimals)

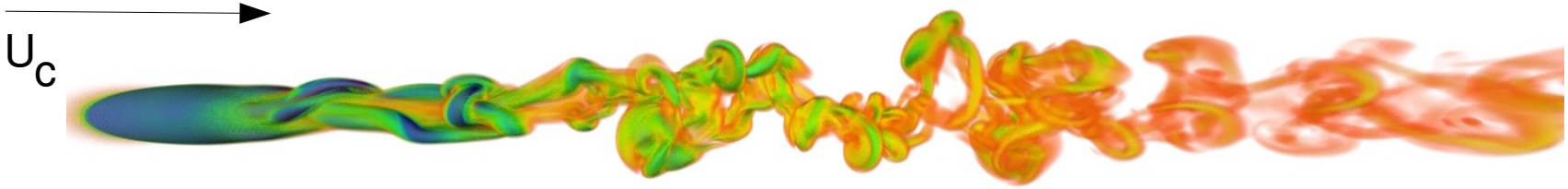
The drag force

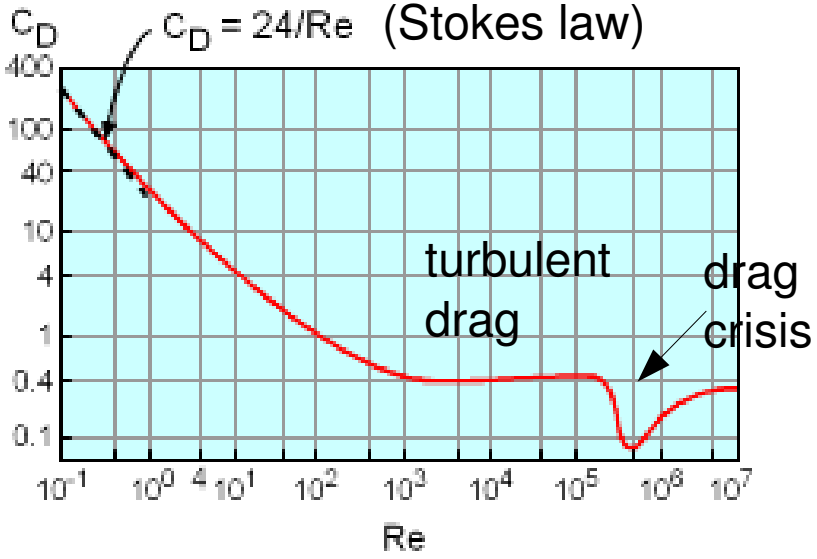
Particle in a laminar flow



Particle in a turbulent flow

The drag coefficient and flow profiles



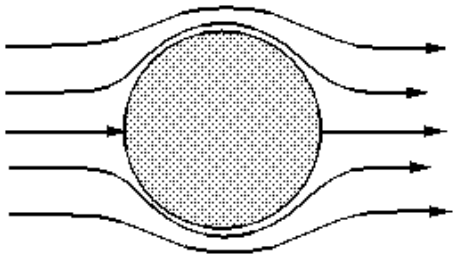


Drag-coefficient

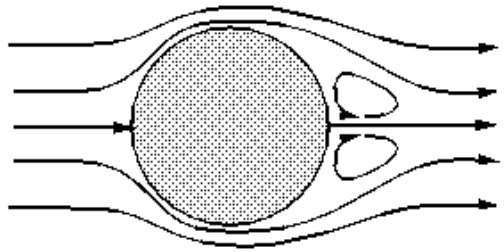
$$C_D = \frac{8\,F}{\rho\, U_c^2 \pi d^2}$$

$$Re_p = \frac{d\,U_c}{\nu}$$

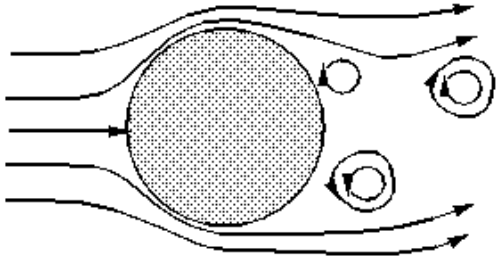
F	drag force
U_c	inflow speed
d	sphere diameter
ρ	fluid density
ν	fluid viscosity



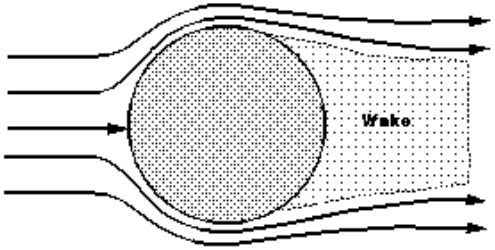
$Re_p \lesssim 23$



$23 \lesssim Re_p \lesssim 350$



$350 \lesssim Re_p \lesssim 10^5$



$Re_p \gtrsim 10^5$

Complicated drag force and boundary layer already for a constant inflow

The drag coefficient and flow profiles

NOW: Large sphere moving through turbulent fluid

- How does the drag force depend on turbulent fluctuations?
- How is the fluid affected?

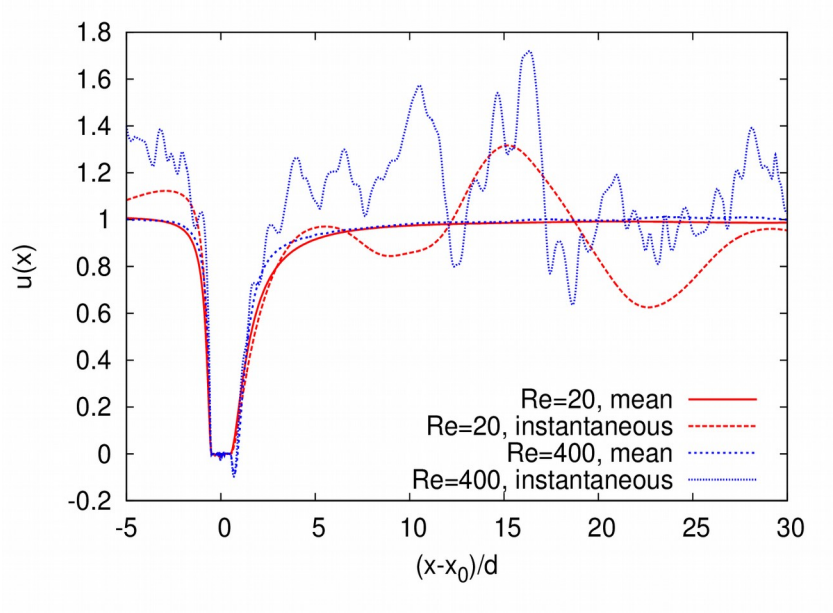
Dimensionless parameters :

- Particle Reynolds number $20 \leq Re_p = \frac{d\,U_c}{\nu} \leq 400$
- Fluid Reynolds number $0 \leq Re = \frac{u_{rms}\,L}{\nu} \leq 930$
- Turbulent intensity $0 \leq I = \frac{u_{rms}}{U_c} \leq 0.6$

Drag force from immersed boundary method: $\int_S \nabla \cdot \boldsymbol{T} dV = \int_S \boldsymbol{f_b} dV$

$\boldsymbol{T} = -p\boldsymbol{I}_3 + \nu(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)$ stress-tensor

Drag force – Large scale effects



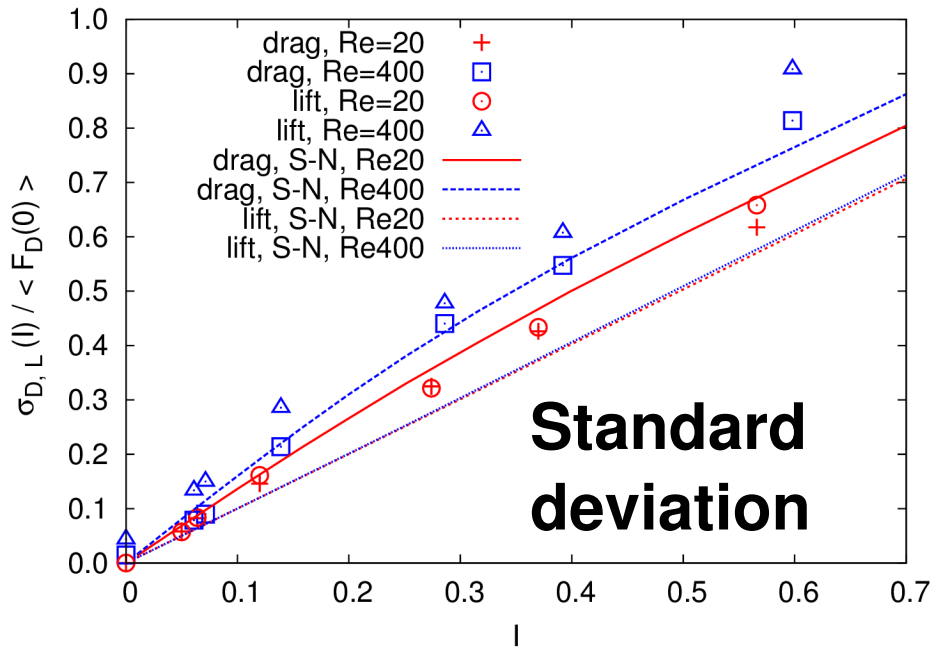
Drag is not linear

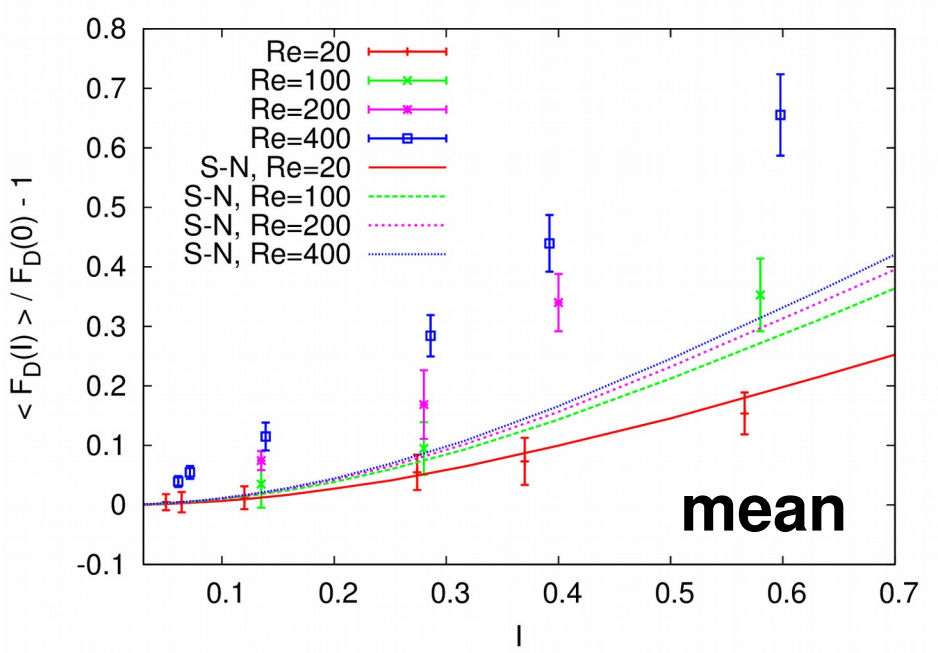
→ Effective drag force (Bagchi and Balachandar, 2003 & Kim and Balachandar, 2010)

Fitting formular of Schiller and Naumann (1933)

$$\boldsymbol{F} \approx \boldsymbol{F}^{\mathrm{SN}}(\boldsymbol{U}) = 3\pi\, d\, \nu \left[1 + 0.15 \left(\frac{|\boldsymbol{U}|\, d}{\nu}\right)^{0.687}\right] \boldsymbol{U}.$$

Test: $$\overline{\boldsymbol{F}}^{\mathrm{SN}}(I) = \frac{1}{\left(\sqrt{2\pi}\, u_{\mathrm{rms}}\right)^3} \int \boldsymbol{F}^{\mathrm{SN}}(\boldsymbol{U})\, \mathrm{e}^{-|\mathcal{U}|^2/(2u_{\mathrm{rms}}^2)}\, \mathrm{d}^3\mathcal{U}$$





Drag force – Small scale effects

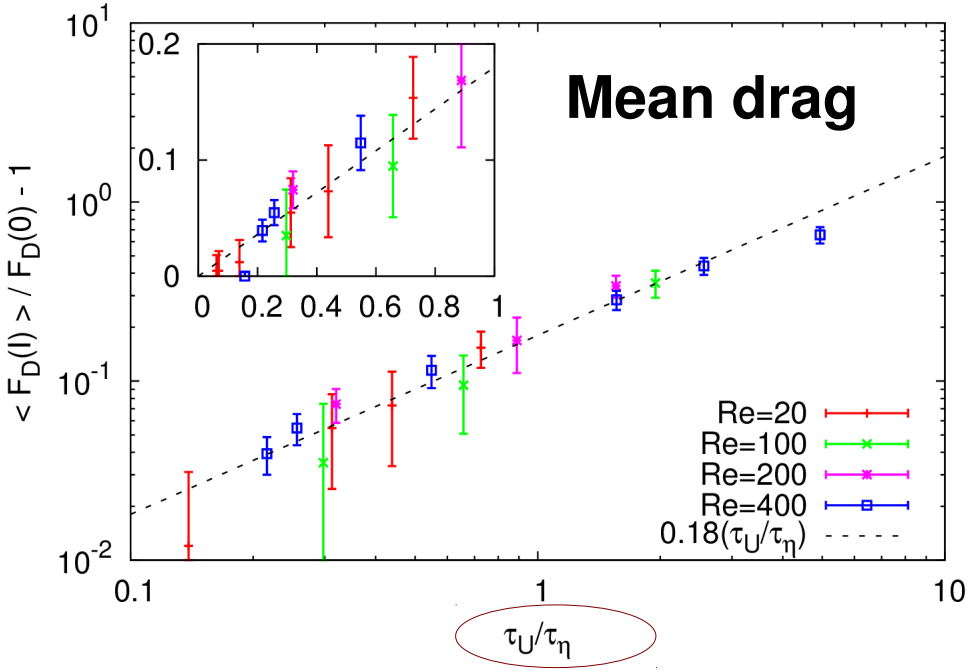
Another approach:
Drag increase by **modified velocity gradients** at the particle surface

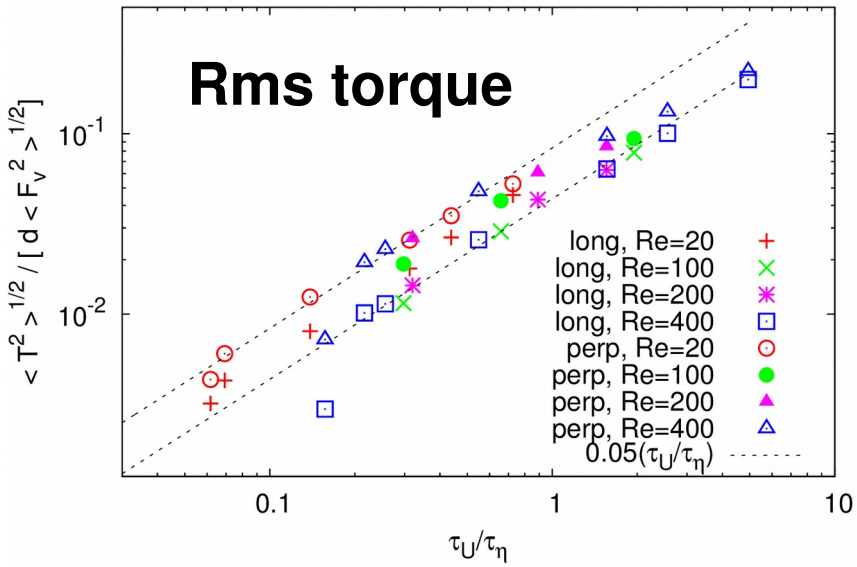
Laminar gradient $\sim U_c/d$

Turbulent gradient $u_\eta/\eta = \tau_\eta^{-1} = \nu^{-1/2}\varepsilon^{1/2}$

$\tau_\mathrm{U} = d/U_c$ Sweeping time

$\tau_\eta = (\nu/\varepsilon)^{1/2}$ Kolmogorov time scale

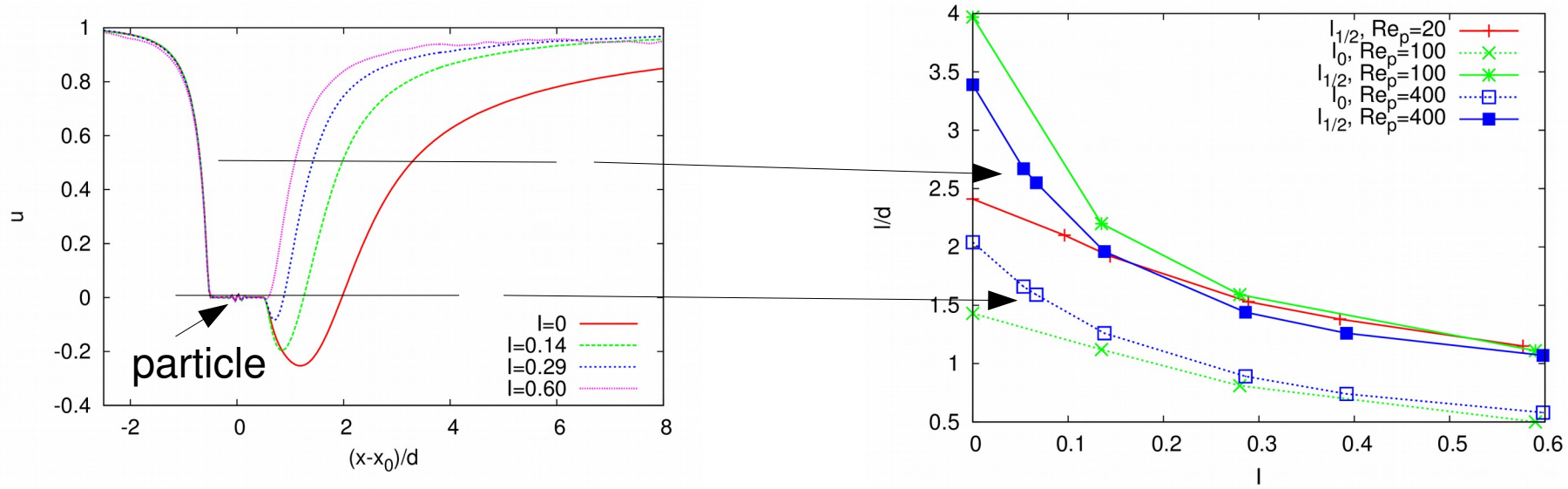




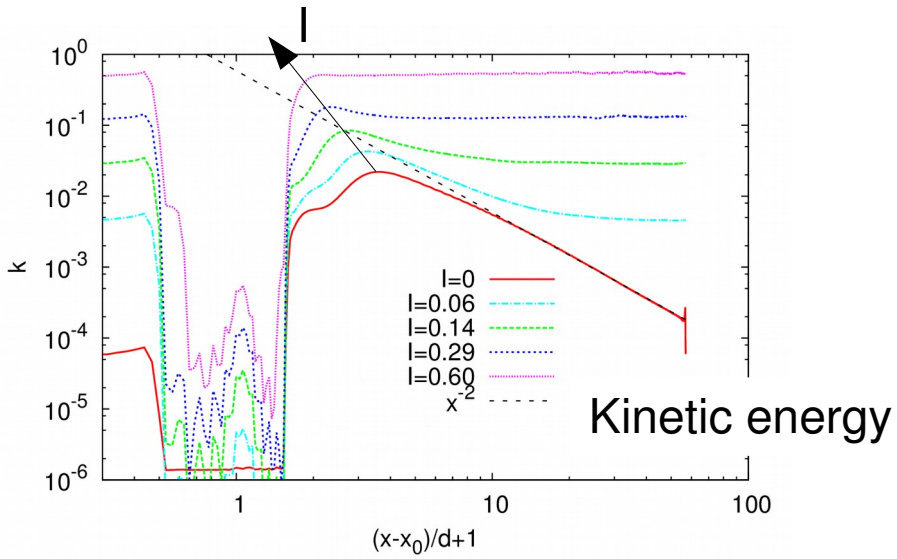
Small and large scales increase the drag on the particle

Shortening of the wake

Average velocity profile (Re=400)



Turbulent fluctuations significantely reduce wake length



Kinetic energy

- falls off quadratically
- maximum shifts to the particle surface

Conclusions

Outer turbulence leads to
- more dust – particle collisions
- higher dust impact speeds
- increased drag forces
- shortening of the wake

Turbulent wake leads to
- dust concentrations behind the sphere
- inter-dust collisions and heavy modification of the dust size distribution

Homann, Bec, Grauer (2013) JFM 721:155
Homann & Bec (2015) Phys. Fluids 27:053301
Homann, Guillot, Bec, Ormel, Ida, Tanga (2016) to appear in A&A

Perspectives
- Effect of rotation of sphere?
- Gravitational focusing?
- Effect of back-reaction of the particles?

Numerical implementation aspects

How to handle millions (or billions!) of particles in a numerical code?

Particle storage in HPC simulations

Array of Structure (AoS) vs Structure of Array (SoA)

```
struct Particle
{
  int id;

  double pos[3];
  double vel[3];

  float mass;
};

Particle particle;
particle.id = 1;

list<Particle> particleList;
particleList.push_back(Particle());
```

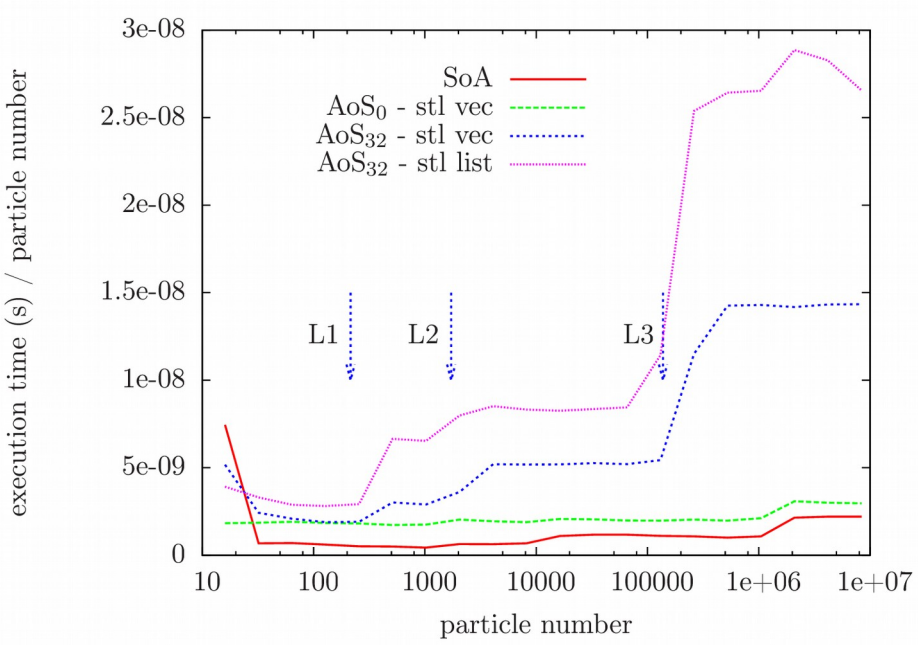
```
struct ParticleArray
{
  vector<int> id;

  vector<double> posX;
  vector<double> velX;

  vector<float> mass;

  void resize(int i) {
    id.resize(i);
    posX.resize(i);
    ...
  }

  void init() { ... }
  void output() { ... }
  ...
};
```

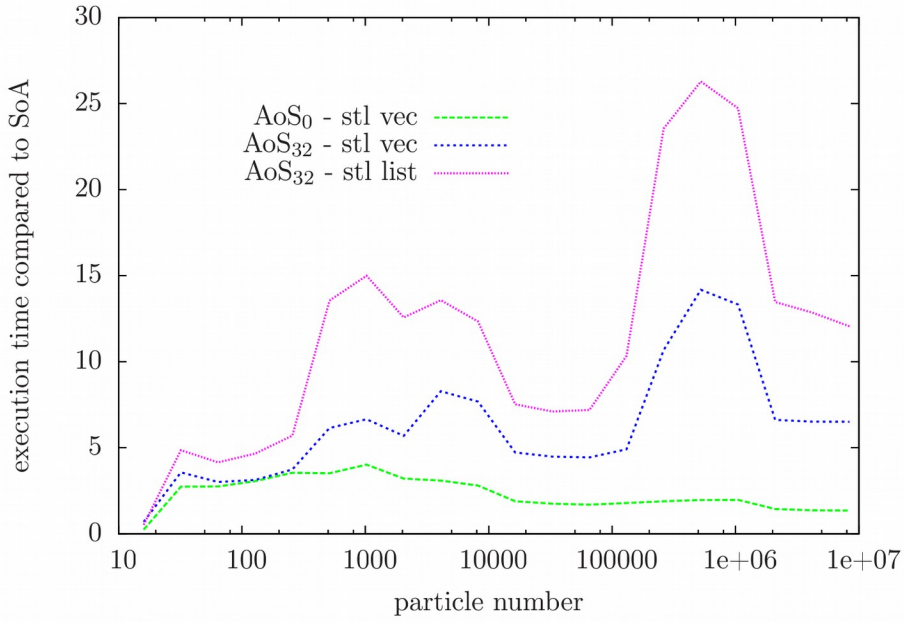
AoS (Particle = Object) is convenient:

- Modification of particle properties (charge, history)
- Creation/Deletion of particles
- I/O and MPI

Particle storage: Benchmark for CPUs

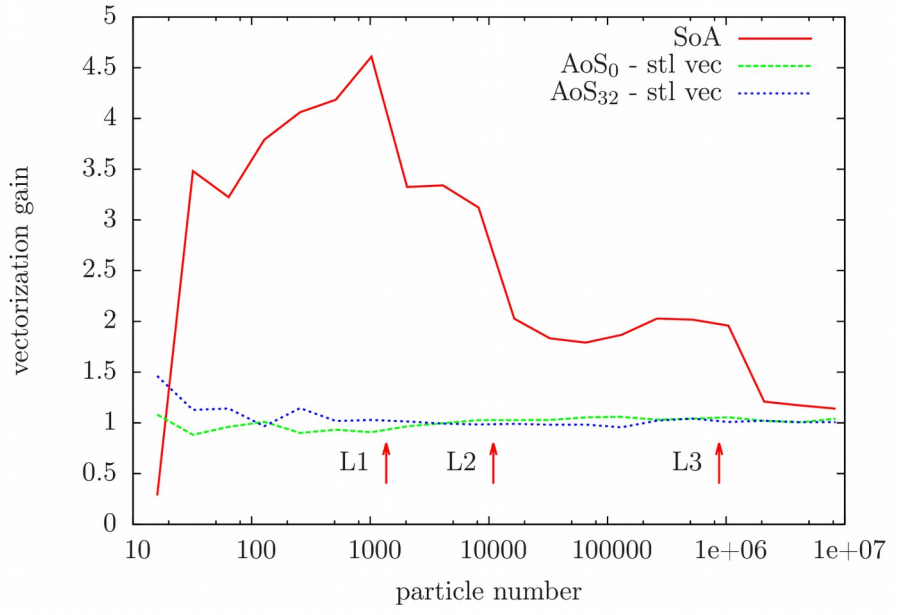
Euler-type for-loop over all particles: $\vec{x} += dt\,\vec{v}$





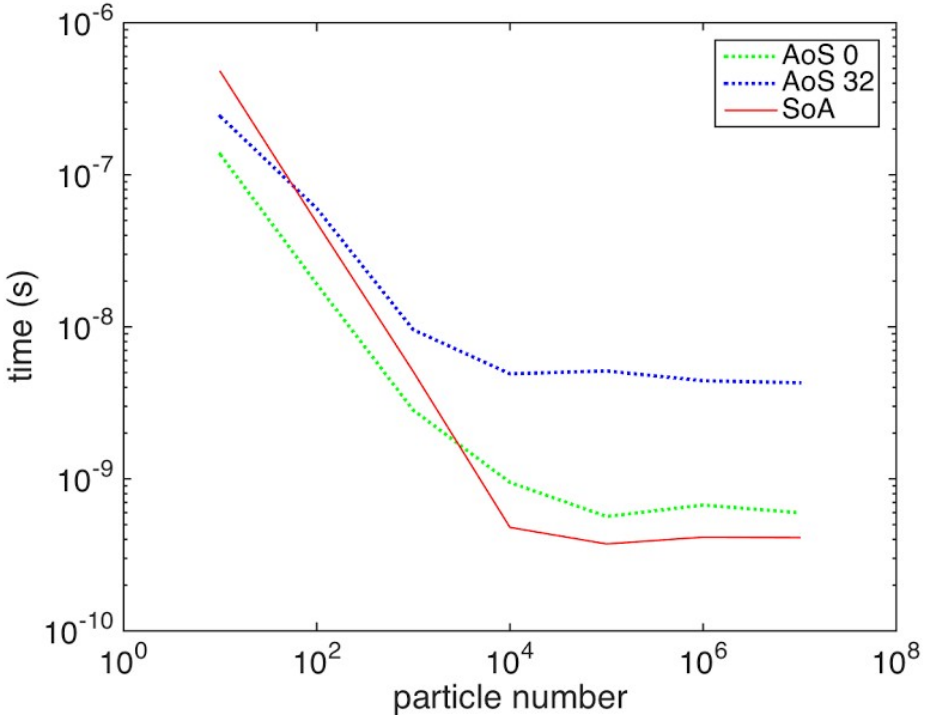
AoS are (much) slower than SoA!

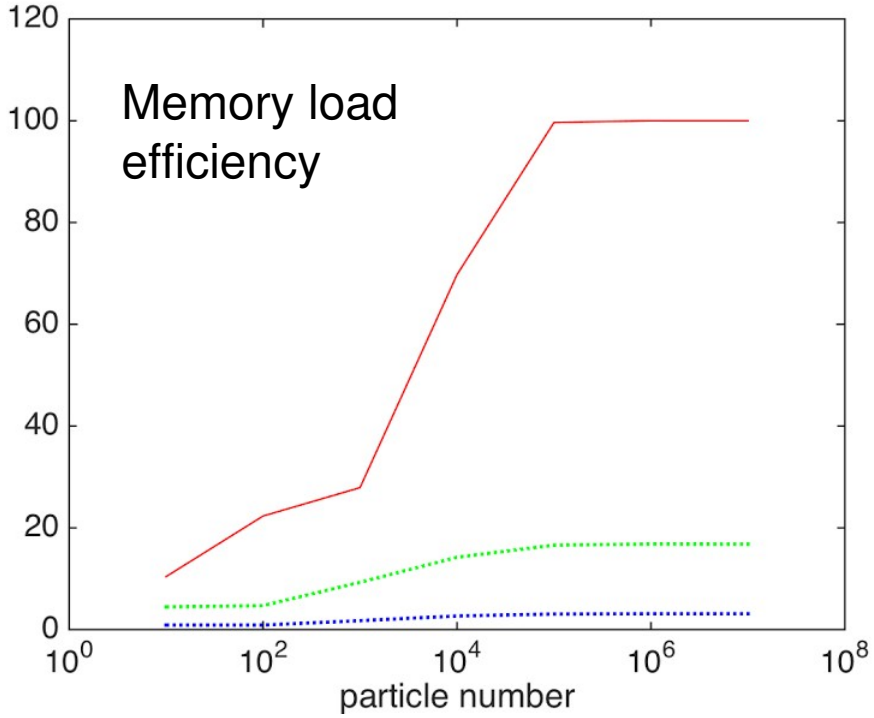
- Vectorization
  accelerating operations on cached data
- Cache
  Pollution from unused particle properties



Particle storage: Benchmark for **GPUs**

Euler-type for-loop over all particles: $\vec{x} += dt\,\vec{v}$





AoS are slower than SoA for large particle numbers

- Memory bandwidth: Pollution from unused particle properties
- Cache benefits at small particle numbers

A fast and flexible library (SoAX)

```
// Define attributes by SOAX macro
SOAX_ATTRIBUTE(id, 'N');        // identity (number)
SOAX_ATTRIBUTE(pos, 'P');       // position
SOAX_ATTRIBUTE(vel, 'V');       // velocity
SOAX_ATTRIBUTE(mass, 'M');      // mass

// std::tuple holding attributes
// of specified type and dimension
typedef std::tuple<id<int,1>,
                   pos<double,3>,
                   vel<double,3>,
                   mass<float,1>> Attributes;

// create structure of array for 42 particles
Soax<Attributes> soa(42);

// access attributes:
soa.id(0) = 0;           // set identity
soa.pos(i,0) = 100;      // set x-coordinate

// array-wise operations using
// expression templates (x = vy - vz)
soa.posArr(0) = soa.velArr(1) - soa.velArr(2);

// extract and treat a particle as an object
auto particle = soax.getElement(7);
particle.id() = 42;
particle.pos(0) = 3.14;
soax.push_back(particle);
```

- Optimal Performance (same as c-arrays)
- Handyness of Arrays of Structure (particle = object)

Implementation of SoAx

- Inheritance
- C++11
- **Template meta-programming**
  Simple example: Compute the factorial at compile time

```
template <int N>
struct Factorial
{
    enum { value = N * Factorial<N - 1>::value };
};

template <>
struct Factorial<0>
{
    enum { value = 1 };
};
```

`Factorial<11>::value` is a compile time constant

Implementation of SoAx

Template meta-programming

Second example: User provided function on arrays

Set all particle data to a given value (here 42):

Code to write by user:
+
Function object (SetToValue):
=
Code generated at compile time

```
p.apply<SetToValue>(42);
```

```
struct SetToValue
{
  template<class T, class Type>
  static void doIt(T& t, Type value) {
    auto tRef = *t;
    for(int i=0;i<t->size();i++)
    t[i] = value;
  }
};
```

Implementation of SoAx

Application of Functor (SetToValue) to all arrays by recursive instantiation:

```
template<class Tuple, std::size_t N, class DoItClass>
struct TupleDo {

  template<class... Args>
  static void doIt(Tuple& t, Args... args)
  {
    TupleDo<Tuple, N-1, DoItClass>::doIt(t,args...);
    DoItClass::doIt(std::get<N-1>(t),args...);
  }
};

template<class Tuple, class DoItClass>
struct TupleDo<Tuple, 1, DoItClass> {

  template<class... Args>
  static void doIt(Tuple& t, Args... args)
  {
     DoItClass::doIt(std::get<0>(t),args...);
  }
};
```

Conclusions

Use Structures of Arrays!

Homann & Laenen (2016) in preparation for Comp. Phys. Comm.

Thank you for your attention!