
Simulations of solid-liquid suspensions *from dilute to dense*

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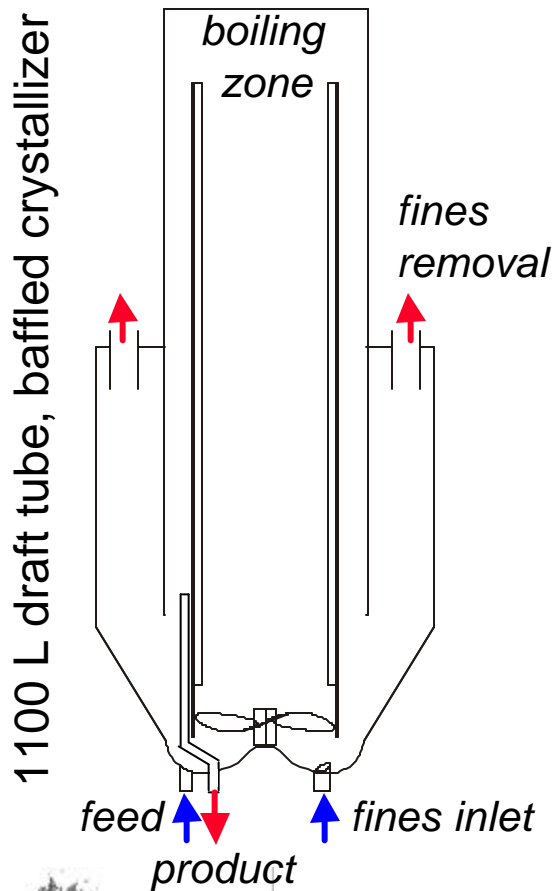


Outline

- Introduction
 - liquid-solid examples (why do we do this work?)
 - ® industrial crystallization, fluidization, ...
- Dilute systems
 - a point-particle approach **~1% solids vol.**
 - stirred suspensions
- DNS with solid-liquid interface resolution
 - methodology **~10% solids vol.**
 - particle-particle interactions in turbulent flow
- Liquid-solid fluidization
 - inhomogeneities **~50% solids vol.**
 - bulk viscosity in Euler/Euler closure
- Sheared suspensions



(G)LS example: industrial crystallization



TU Delft

Transport physics

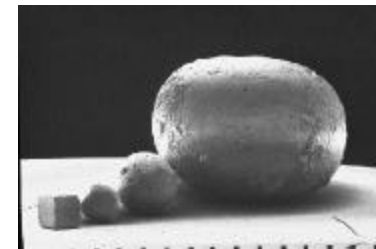
- turbulent flow
- multiphase (gas/liquid/solid) system
- heat and mass transfer

particle-turbulence interaction

Micro-scale physics

- primary nucleation
- growth
- agglomeration
- attrition (secondary nucleation)

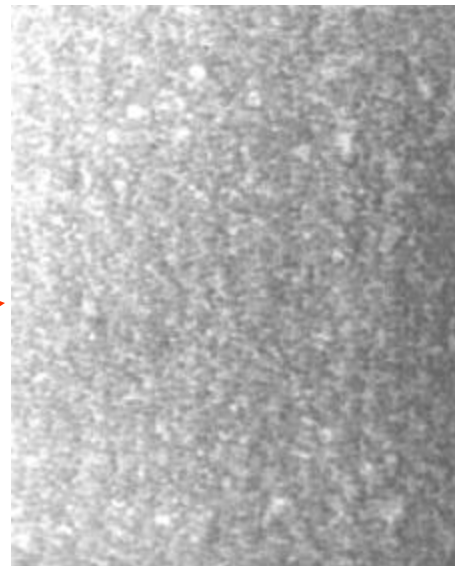
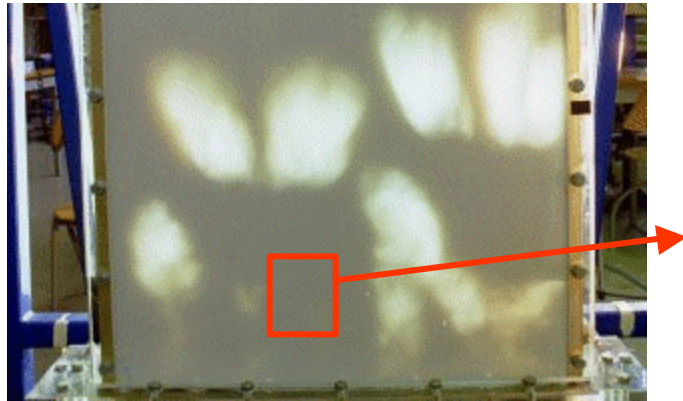
collisions (particle-particle and particle-impeller)



GS/LS example: fluidization

flat fluidized beds

air-polystyrene system $\frac{\rho_s}{\rho_f} \approx 1000$



water-steel $\frac{\rho_s}{\rho_f} \approx 8$



inhomogeneities

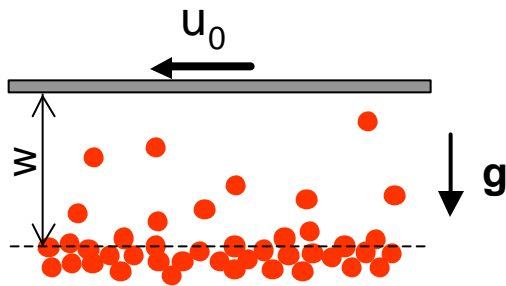
- mixing
- transfer processes

courtesy É. Guazelli
(IUSTI, CNRS-UMR)



LS example: sheared granular bed

glass beads in water $\frac{\rho_s}{\rho_f} \approx 2.5$



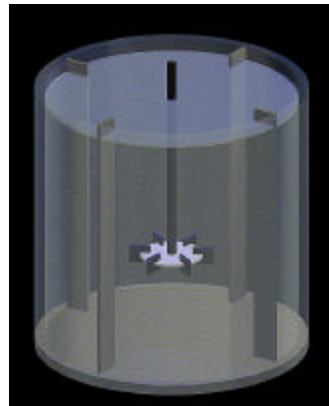
courtesy François Charru (IMFT)

sedimentation and resuspension

Agitated liquid-solid flow

Issues:

- attrition, formation of fines (role of collisions)
- power consumption
- scale-up
- ...



A starting point:

just-suspended experiments:
Zwietering (1958); Baldi *et al.* (1978)

$$N_{js} = s \frac{d_p^{0.2} \mu_L^{0.1} (g\Delta\rho)^{0.45} \phi_m^{0.13}}{\rho_L^{0.55} D^{0.85}}$$

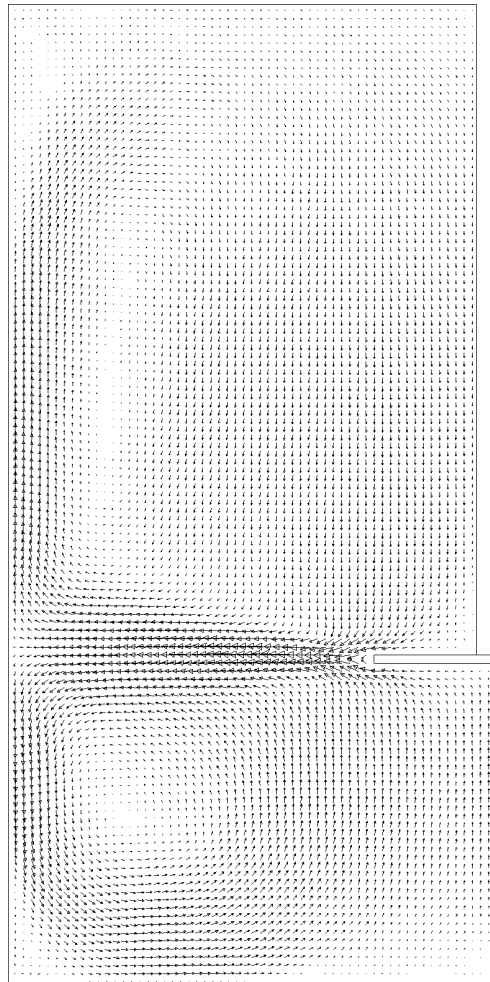
hydrodyn. interaction
collisions
2way coupling

with $s \approx 15$ for $\frac{T}{C} = \frac{T}{D} = 3$

(Rushton turbine in baffled tank)



Single-phase flow: LES

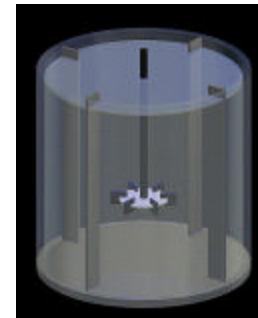


average flow



single realization

\vec{v}_{tip}

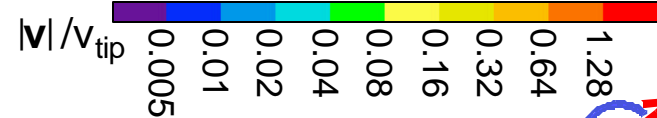
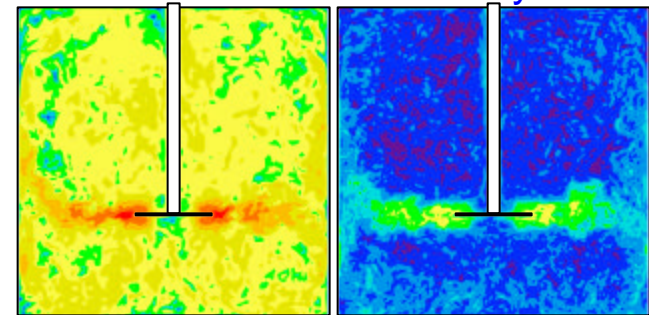


$$Re = \frac{ND^2}{\nu} = 10^5$$

Smagorinsky SGS model ($c_s=0.1$)

Lattice-Boltzmann discretization

single realization: magnitude of
GS and SGS velocity



Solid phase dynamics: Lagrangian

Equations of motion for the spherical particles

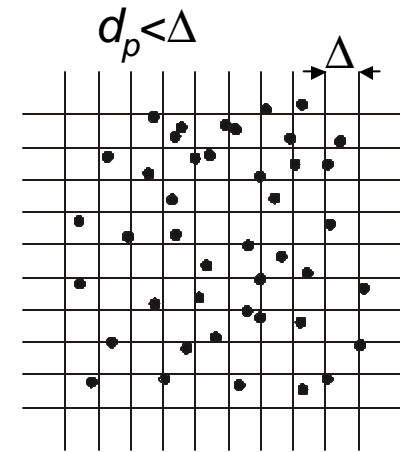
$$\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_p$$

$$(m_p + m_a) \frac{d\mathbf{v}_p}{dt} = \sum \mathbf{F}_p$$

$$I \frac{d\boldsymbol{\omega}_p}{dt} = \sum \mathbf{T}_p$$

added mass
 forces: gravity, drag, lift, stress gradients
 particle rotation: Magnus force, rotational slip velocities

from *single-particle* correlations



Collisions:

- hard-sphere particle-particle and particle-wall collisions
- 2 parameters: restitution coefficient e (=1 mostly)
friction coefficient μ_f (=0 mostly)



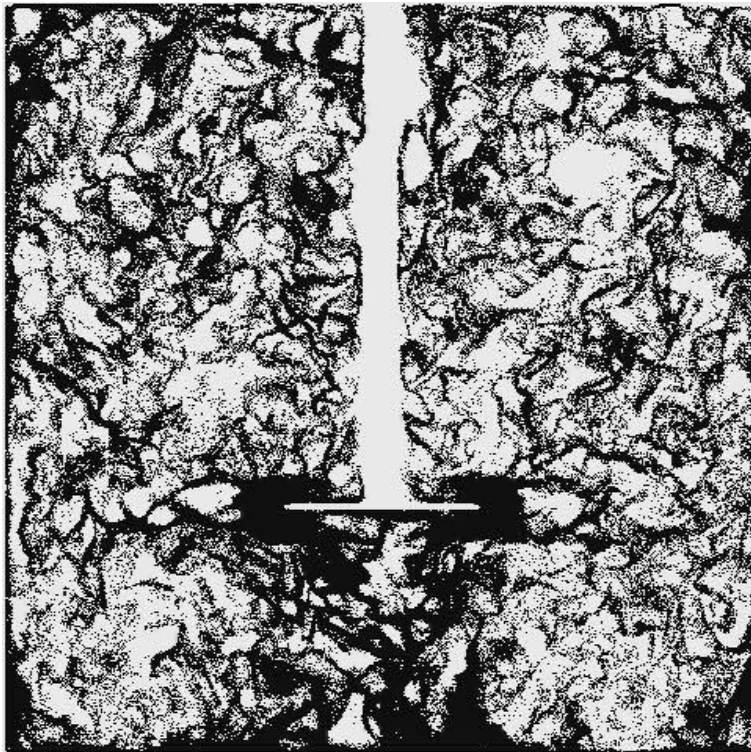


Results: impressions

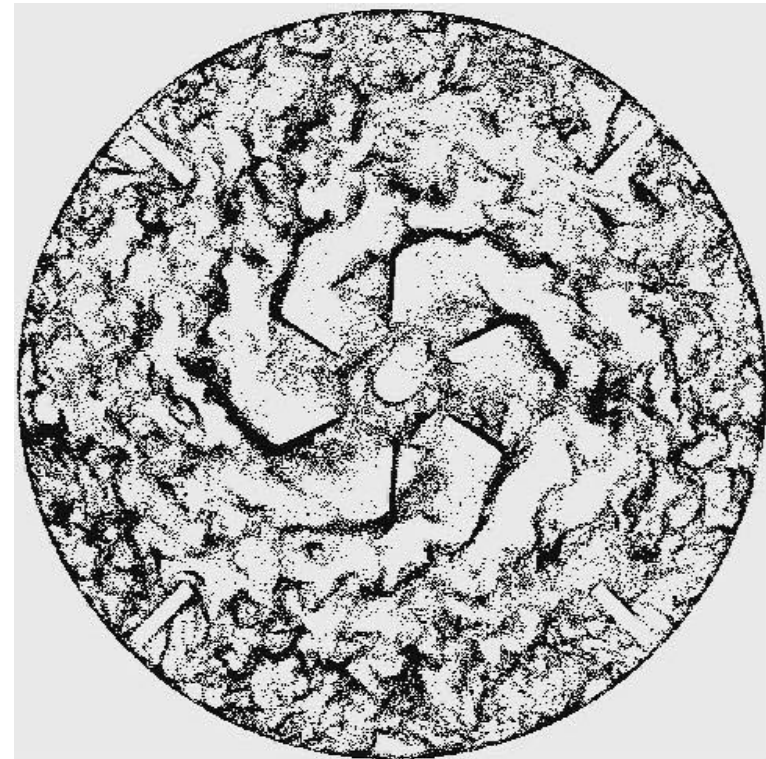
10 liter vessel, $d_p=0.3$ mm,
 $\rho_{\text{part}}/\rho_{\text{liq}}=2.5$, $\phi_V=3.6\%$, $n_p=2.4 \cdot 10^7$

$$Re = \frac{ND^2}{\nu} = 10^5$$

$$St = \frac{\rho_{\text{part}}}{\rho_{\text{liq}}} \frac{d_p^2 6N}{18\nu} = O(1)$$



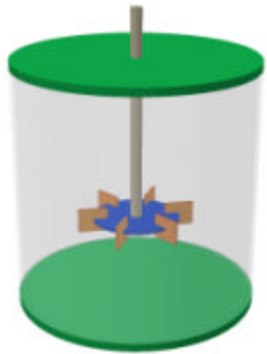
vertical cross section



horizontal cross section



Intermezzo: unbaffled tank



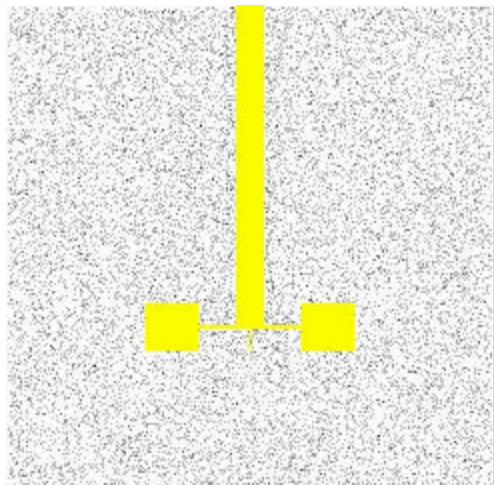
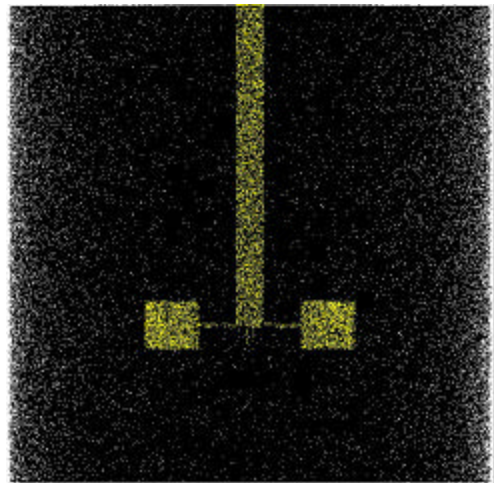
side view

5.4 liter

$d_p = 0.5$ mm

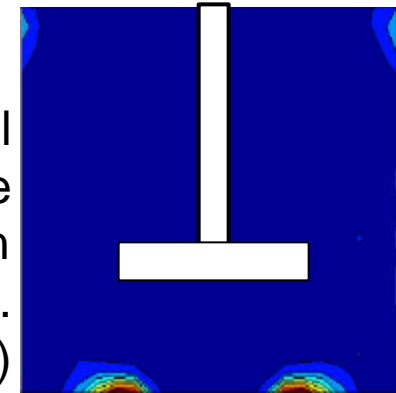
$\rho_{\text{part}}/\rho_{\text{liq}} = 2.5$

cross section



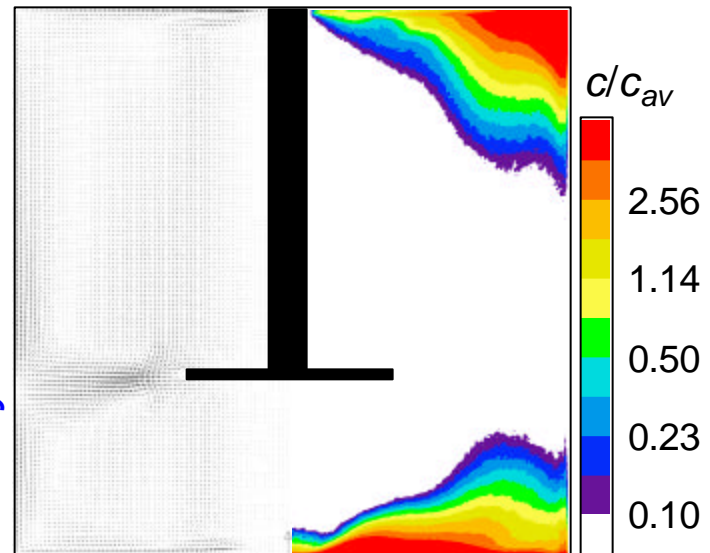
time averages

experimental
particle
concentration
(thanks to A.
Brucato)



simulation

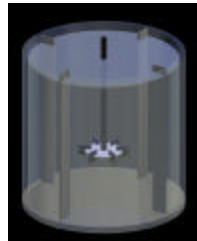
velocity vectors



c/c_{av}
2.56
1.14
0.50
0.23
0.10
p-concentration (log-scale)



The quest for (just) suspended



$N=16.5$ rev/s
 $N_{js}=13.5$ rev/s

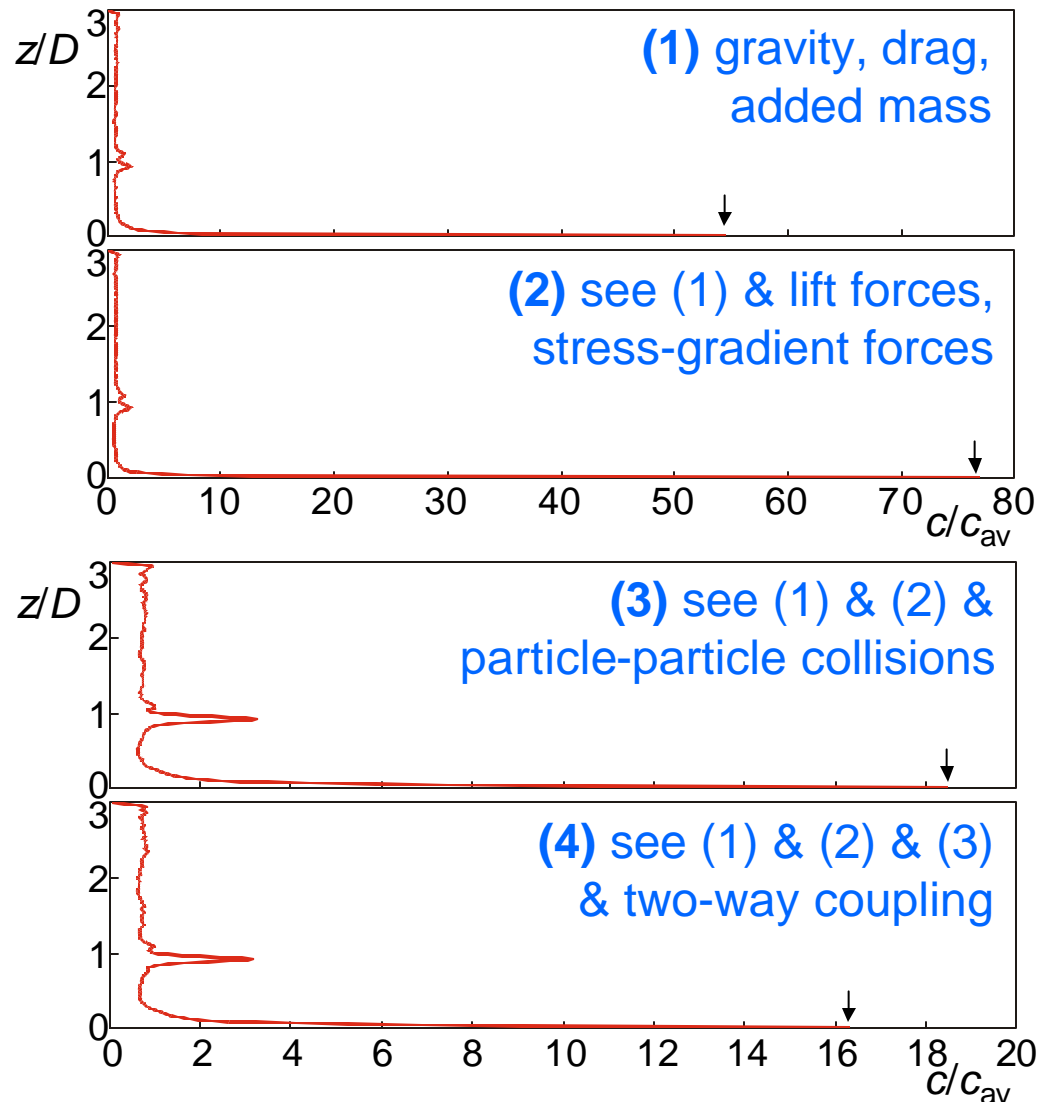
vertical concentration profiles at $2r/T=0.45$

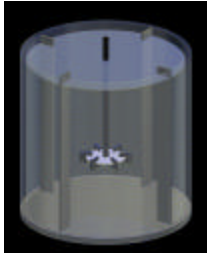
closest packing of spheres:
 $c_{cp}/c_{av}=78$

ratio drag and lift force

$$\frac{F_{lift}}{F_{drag}} \approx 0.1 \sqrt{\frac{d_p^2 \omega}{\nu}}$$

e.g. if $\omega=10N$: $F_{lift} \gg 0.5F_{drag}$

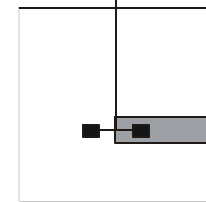




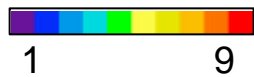
Particle-particle collisions

$d_p=0.3$ mm,
 $\phi_V=0.95\%$

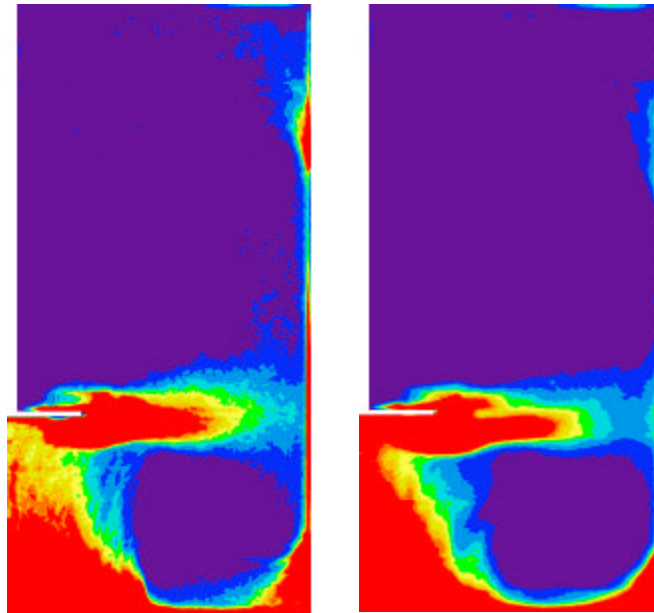
$d_p=0.47$ mm,
 $\phi_V=3.6\%$



collision frequencies
(color scale according to Von Smulochowski)

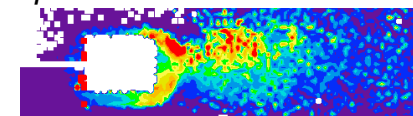


$r_{col}/r_{col,Sm}$

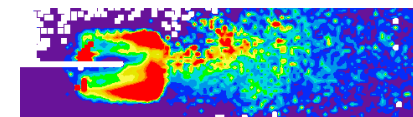


collision intensities

$d_p=0.3$ mm, $\phi_V=0.95\%$

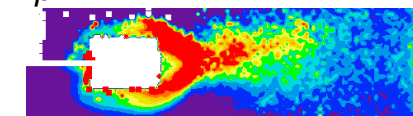


0°

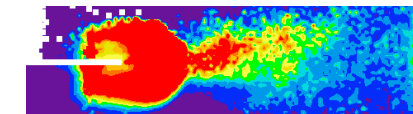


55°

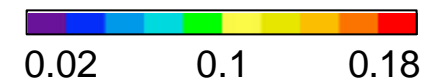
$d_p=0.47$ mm, $\phi_V=3.6\%$



0°



55°

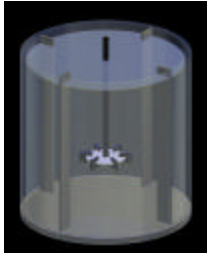


v_{rel}^2/v_{tip}^2

refer collision rates to Von Smulochowski:

$$r_{col,Sm} = \frac{4}{3} \dot{\gamma} d_p^3 M^2 \quad \dot{\gamma} = \sqrt{\frac{\bar{\epsilon}}{\nu}}$$



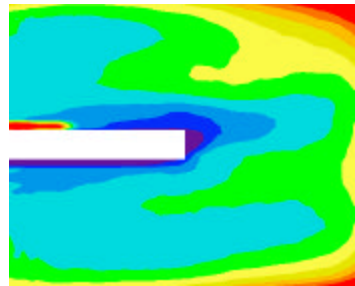


Particle-impeller collisions

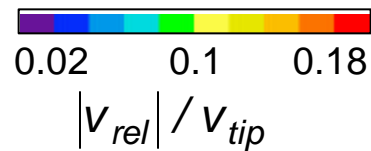
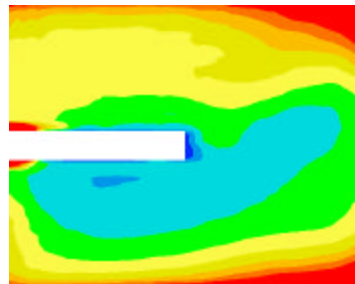
collision intensities

*front surface of
impeller blade*

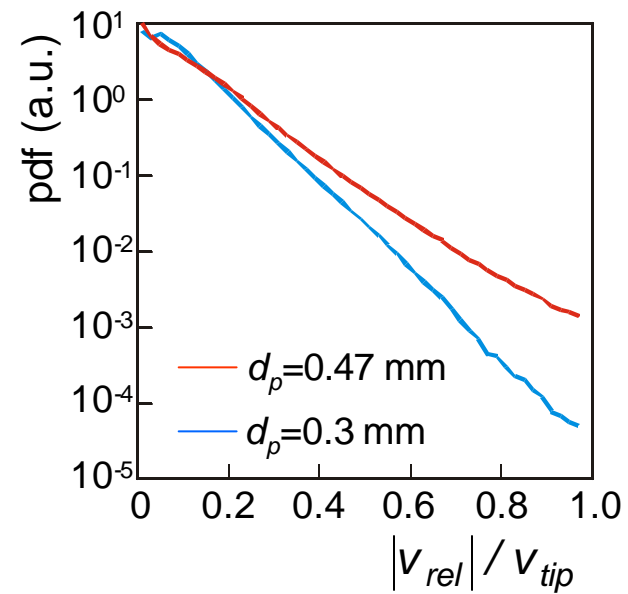
$d_p=0.3$ mm,
 $\phi_V=0.95\%$



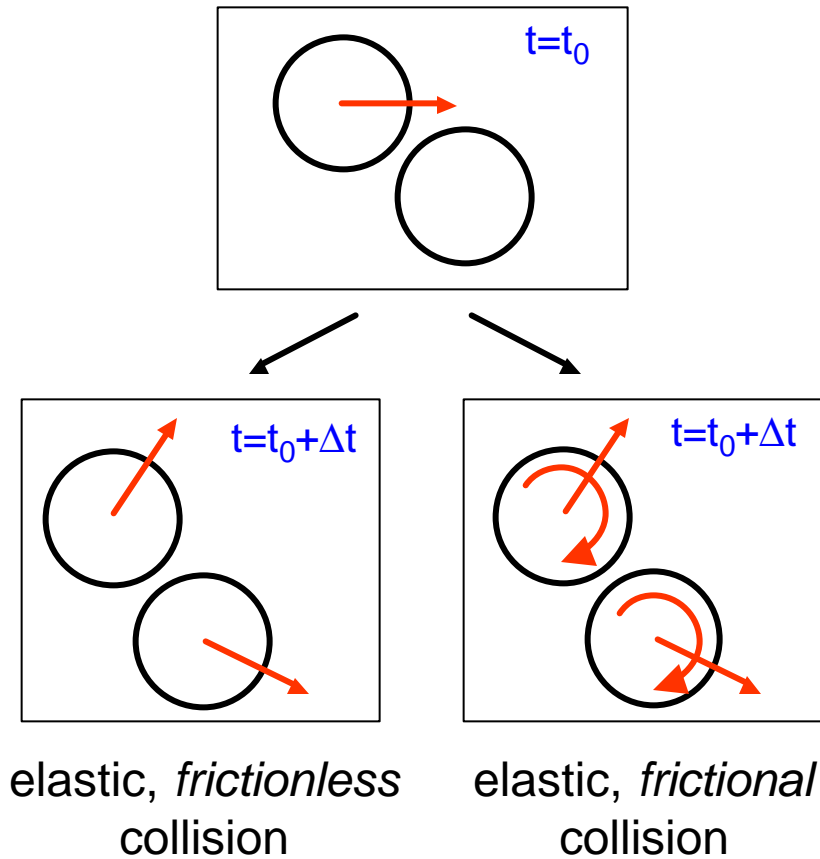
$d_p=0.47$ mm,
 $\phi_V=3.6\%$



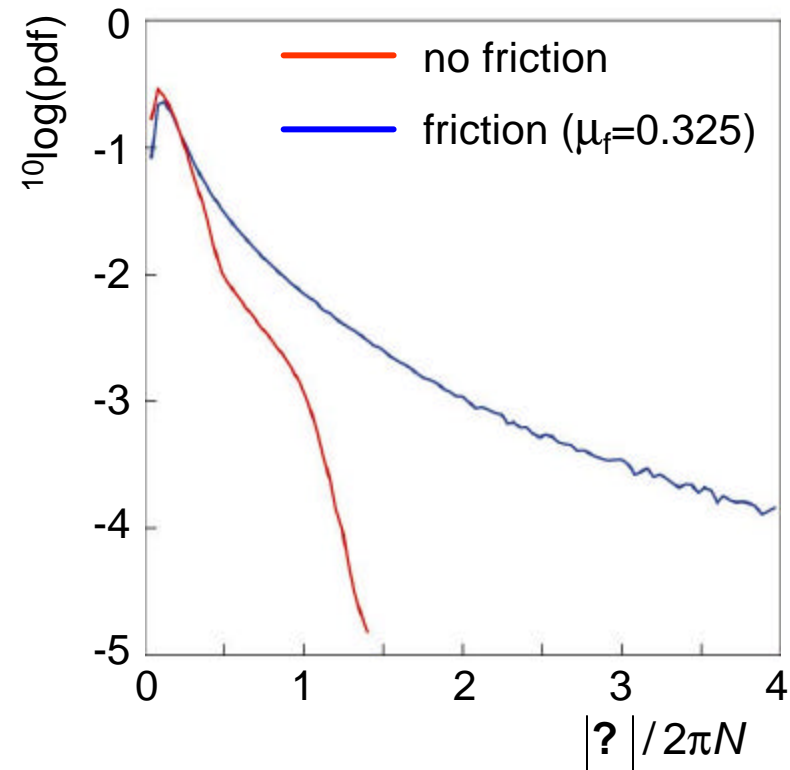
*probability density function
(pdf) of particle-impeller
collision velocities*



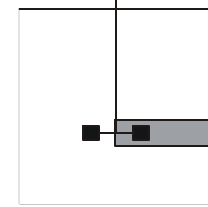
Collision mechanics



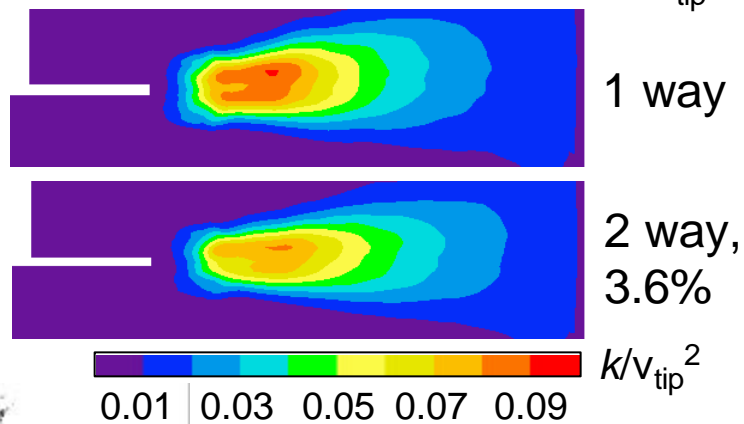
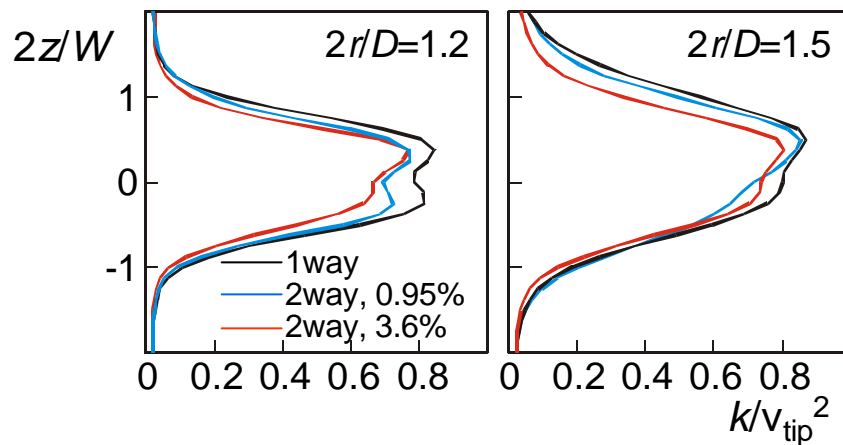
pdf of the particle's angular velocity
(single realization, entire vessel)



One- and two-way coupling

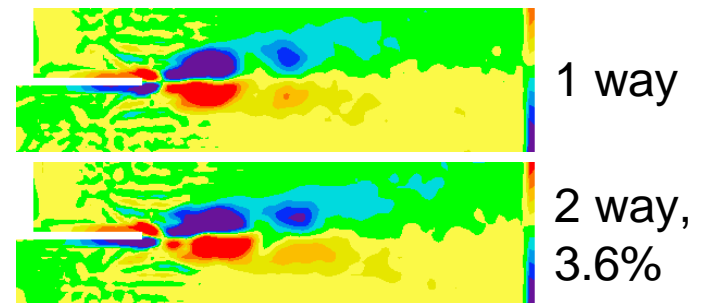


phase-averaged turbulent kinetic energy in the impeller outstream

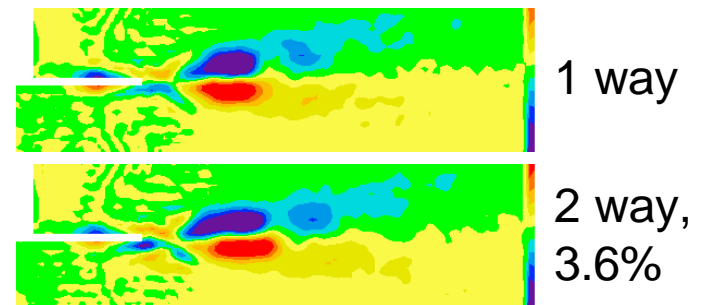


trailing vortex system

30°

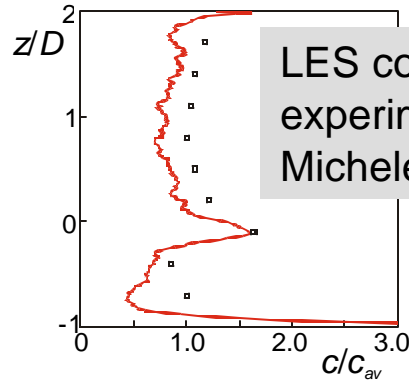


45°

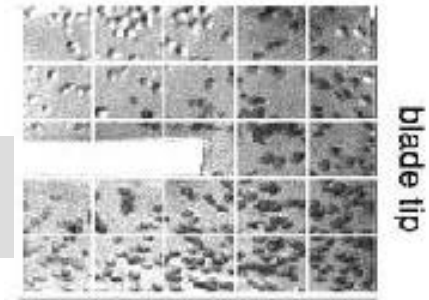
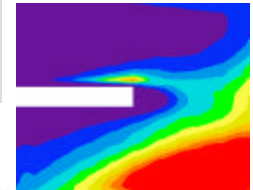


How to proceed?

Experimental validation
 particle concentration profiles
 particle-impeller collisions



LES compared to experimental data of Micheletti et al. 2003

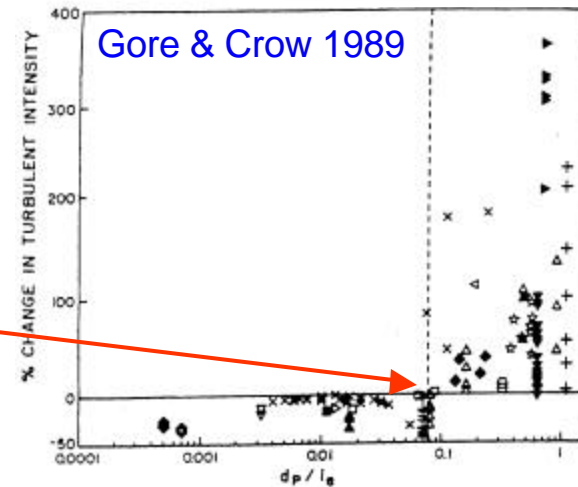


impact tests Kee & Rielly 2004

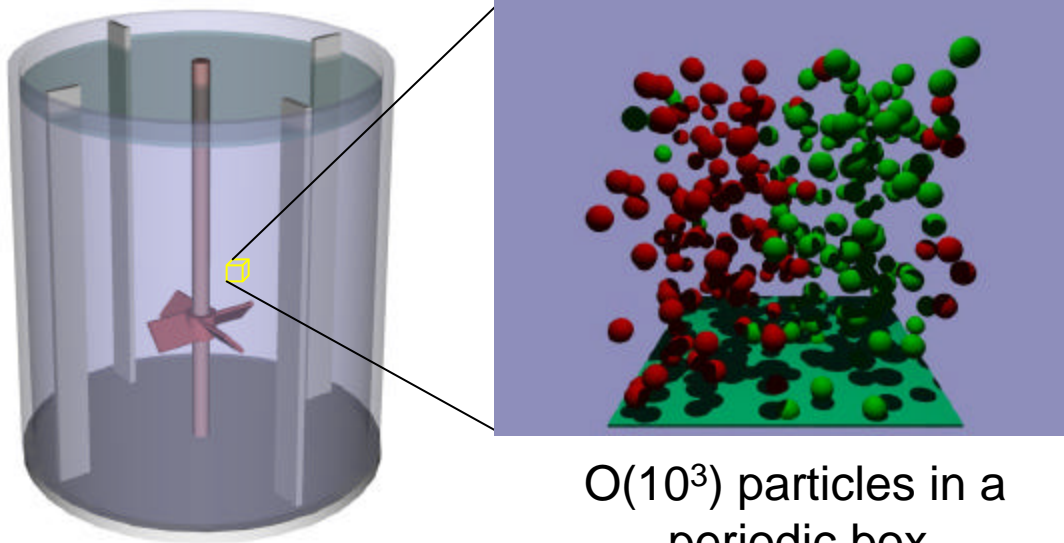
Solid-liquid system with density ratio ≈ 2.5
 many concepts borrowed from solid-gas systems

- point particles
- neglect history force
- neglect lubrication
- simple two-way coupling

We need to investigate finite-particle-size effects



DNS with interface resolution¹



$O(10^3)$ particles in a
periodic box

Particles:

Lattice-Boltzmann simulation
Fully resolved particles

Turbulence:

Fluctuating bodyforce²

Particle interactions:

Through LB fluid
Lubrication forces
Hard-sphere p-p collisions

- Particle – turbulence interaction
- Collision statistics

¹ Ten Cate et al. *JFM* 2004

² Alvelius *PoF* 1999



Lattice-Boltzmann (LB) discretization

Particles move from one lattice site to the other and collide:

$$N_i(\mathbf{x} + \mathbf{c}_i, t + 1) = N_i(\mathbf{x}, t) + \Gamma_i(\mathbf{N})$$

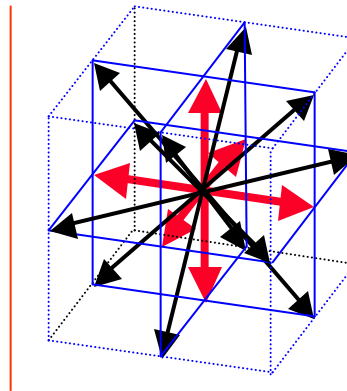
$$\rho u_\alpha = \sum_i c_{i\alpha} N_i$$

2nd order (space and time) representation of a Navier-Stokes-like equation, e.g.:

$$\frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial}{\partial x_\beta} \rho u_\alpha u_\beta = -\frac{1}{3} \frac{\partial \rho}{\partial x_\alpha} + \nu \frac{\partial}{\partial x_\beta} \left(\frac{\partial \rho u_\beta}{\partial x_\alpha} + \frac{\partial \rho u_\alpha}{\partial x_\beta} \right) + f_\alpha$$

this is incompressible Navier-Stokes if $|\mathbf{u}^2| \ll c_{\text{sound}}^2$

$$p = \frac{\rho}{3} \rightarrow c_{\text{sound}} = \sqrt{\frac{1}{3}}$$



Space, time, and velocity are discretized:

local operations:
good parallel efficiency
uniform, cubic lattice

velocity/
physical time-step
constraint

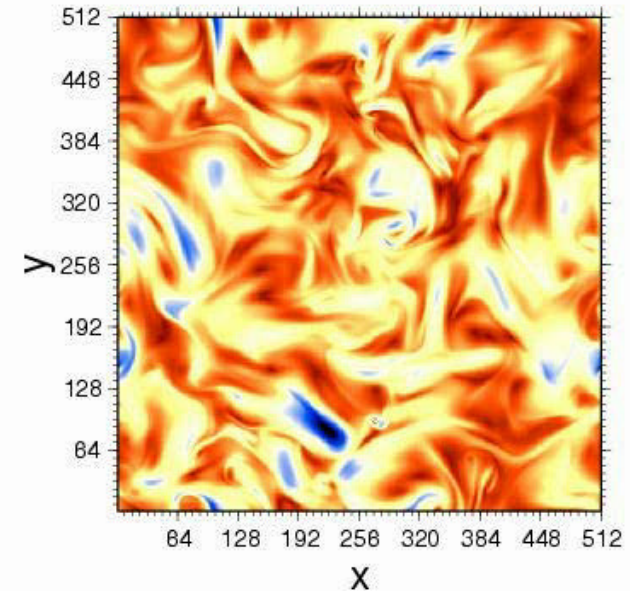
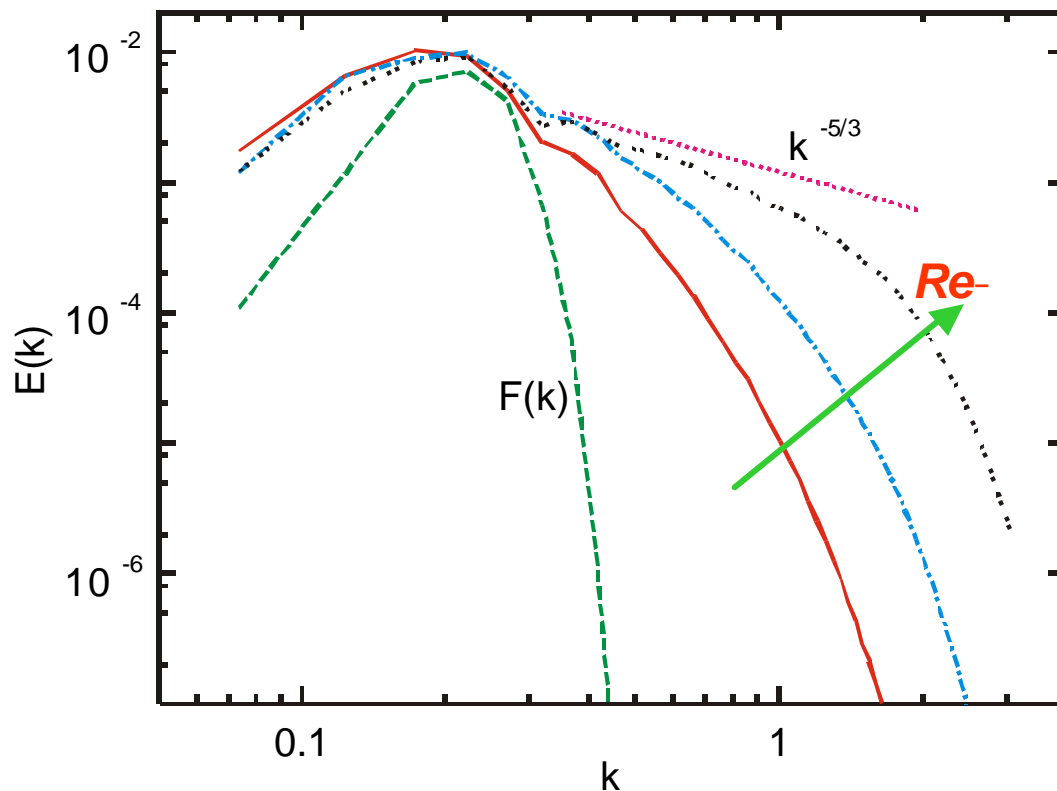


Forced turbulence within LB

single-phase flow

$$Re_{forcing} = \frac{u^* l^*}{\nu} = 18,000$$

$$\eta_K = 0.5 \Delta \quad 512^3 \text{ cubic grid}$$



colors: velocity magnitude

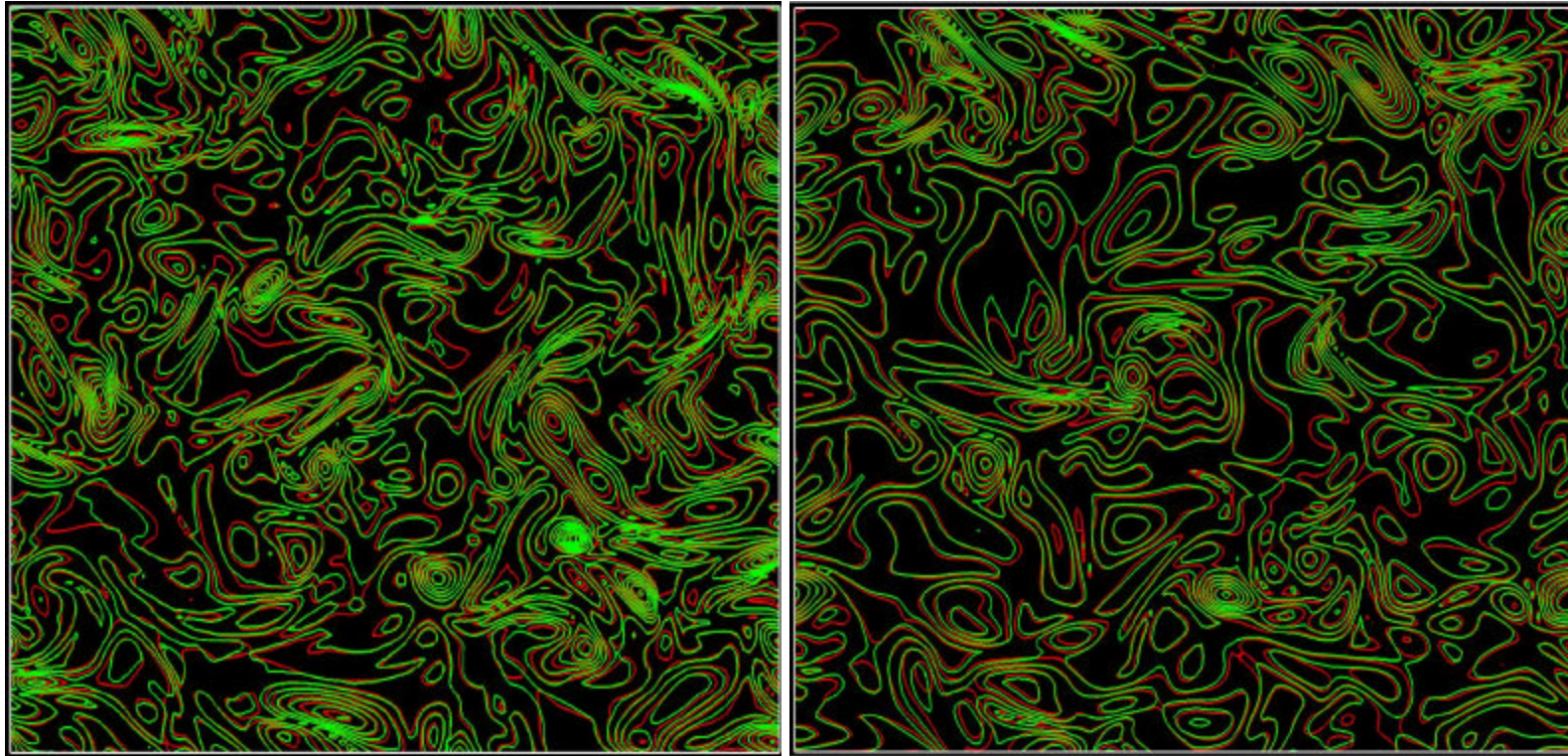


DNS of decaying homogeneous, isotropic turbulence

$$Re_\lambda = \sqrt{\frac{3K(t=0)}{2}} \frac{\lambda}{\nu} = 35$$

— spectral
— LB

LB is a competitive tool for (single-phase) turbulence simulations

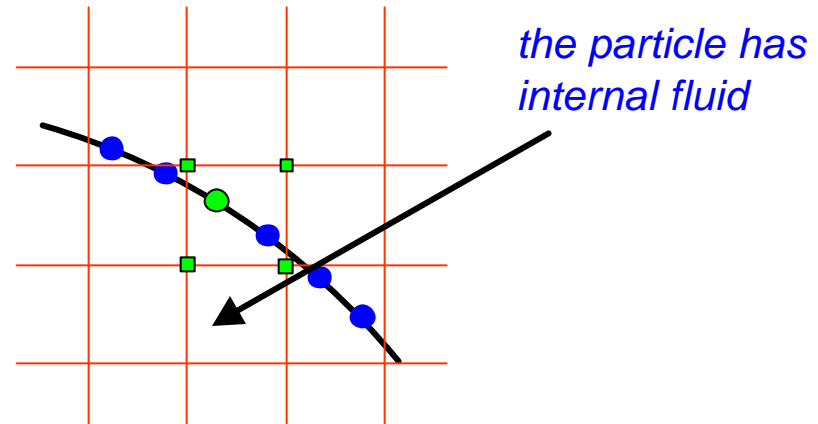
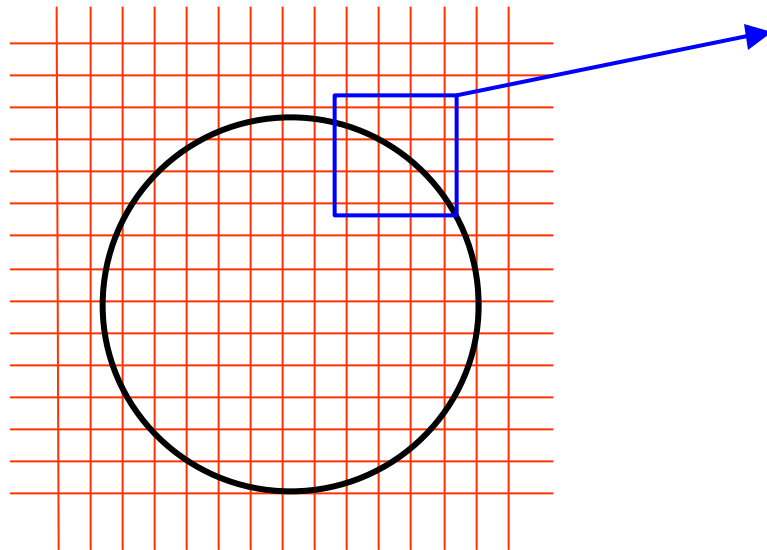


$|\nabla \times \mathbf{u}|$ contours at 2 moments in time started from same initial condition



Boundary conditions: forcing method^(1,2)

no-slip at the surface of the moving, spherical particles



at ● determine the fluid local velocity by interpolation from ■

$$\mathbf{?u} = \mathbf{u}_{\text{fluid}} - (\mathbf{u}_{\text{particle}} + \mathbf{?}_{\text{particle}} \times \mathbf{r})$$

$$\mathbf{F}^{i+1} = \alpha \mathbf{F}^i - \beta \mathbf{?u} \quad \alpha=0.95; \beta=1.8$$

distribute \mathbf{F}^{i+1} at ● to the lattice-nodes ■

$-\Sigma \mathbf{F}$ is the fluid to particle force

(1) Goldstein et al., *J. Comp. Phys.* **105** (1993)

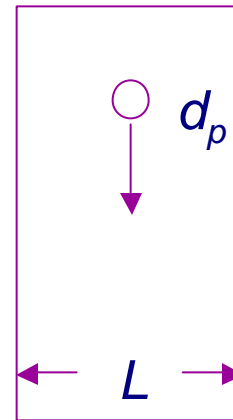
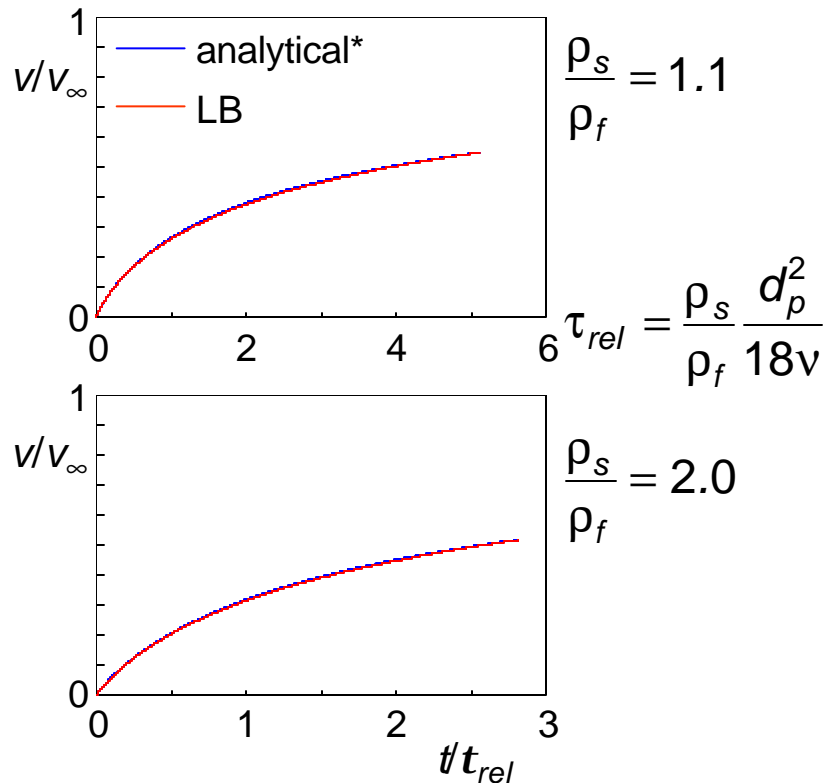
applied within spectral method

(2) Ten Cate et al., *Phys. Fluids* **14** (2002)

applied within LB method

Single-particle tests

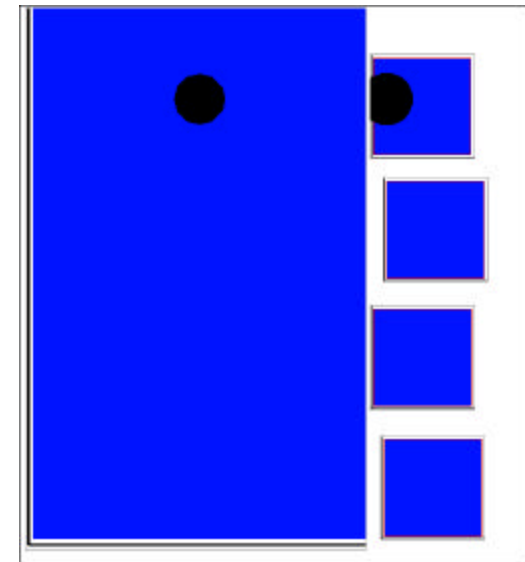
Start-up of a sphere falling under gravity ($Re_p < 1$)



PIV experiment of a falling sphere in a closed box*

$$Re_p = \frac{U_{p,\infty} d_p}{\nu} = 1.5 \dots 32$$

$$\frac{d_p}{L} = 0.15$$



$Re_p = 32$

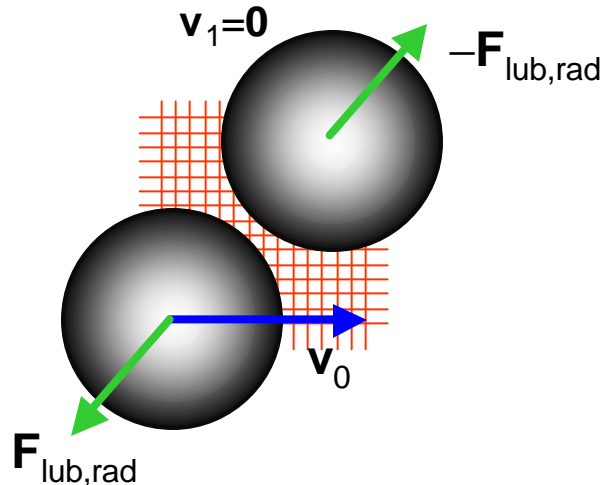
LB simulation PIV exp



Lubrication forces (and torques)*

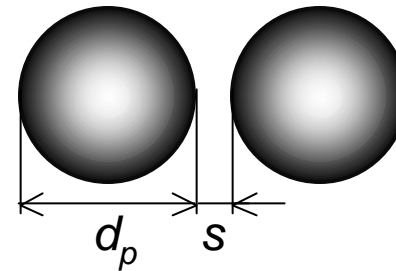
For particles in close proximity to another particle or a wall

Example:
radial lubrication force



$$\text{radial lubrication force} \propto \frac{d}{s}$$

$$\text{tangential lubrication force} \propto \ln\left(\frac{d}{s}\right)$$



lubrication switched on once $s \leq \delta$
with $\delta = 0.1 d_p$ ($\approx \Delta$)

$$F_{\text{lub,rad}} \propto \frac{d_p}{s} - \frac{d_p}{\delta}$$

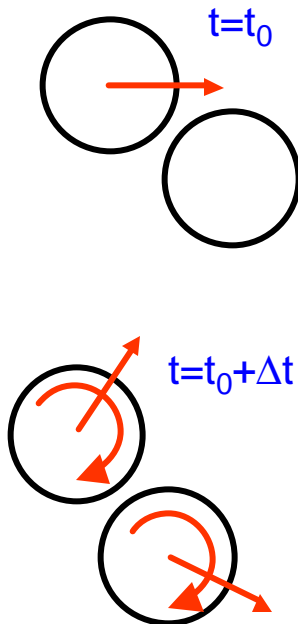
$$F_{\text{lub,tang}} \propto \ln\left(\frac{d_p}{s}\right) - \ln\left(\frac{d_p}{\delta}\right)$$

limit the lubrication force if $s \leq \varepsilon$
with $\varepsilon = 10^{-4} d_p$
(surface roughness)

* Kim & Karrila: *Microhydrodynamics* (1991)
Nguyen & Ladd, *Phys. Rev. E*, **66** (2002)



Hard-sphere collisions



A two parameter model*

- restitution coefficient e
- Coulomb friction coefficient μ_f

default settings: $e=1$, $\mu_f=0$

no overlap between particles is allowed:

event-driven simulation of particle motion

* Yamamoto et al., *JFM*, **442** (2001)



Settings for solid-liquid simulations

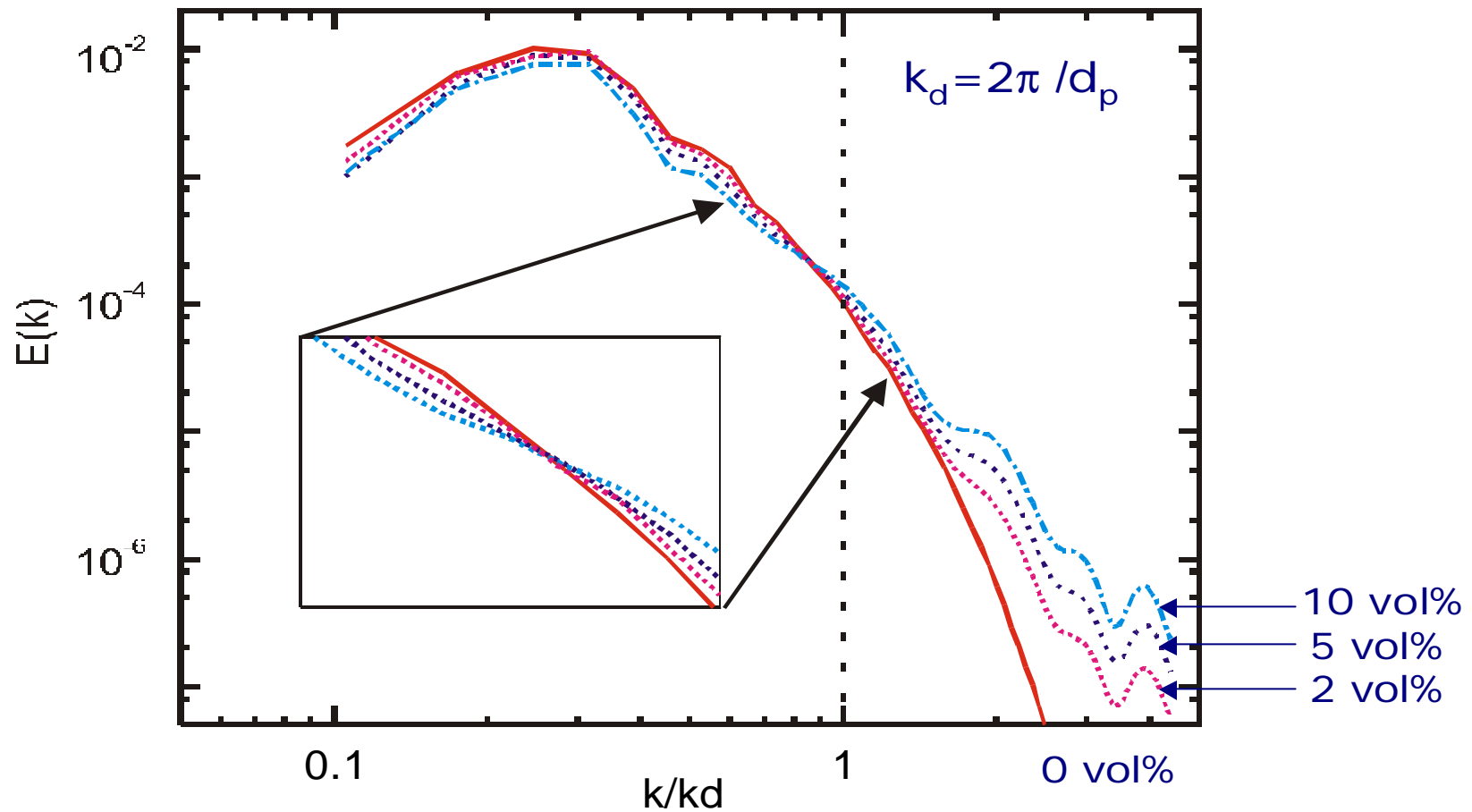
Particle diameter in grid units: 8

Kolmogorov scale in grid units: 1.2

| Vol % | ρ_p / ρ_f | N_p |
|-------|-------------------|-------|
| 2 | 1.414 | 773 |
| 5 | 1.414 | 2200 |
| 10 | 1.414 | 3868 |
| 5 | 1.146 | 2200 |
| 5 | 1.728 | 2200 |

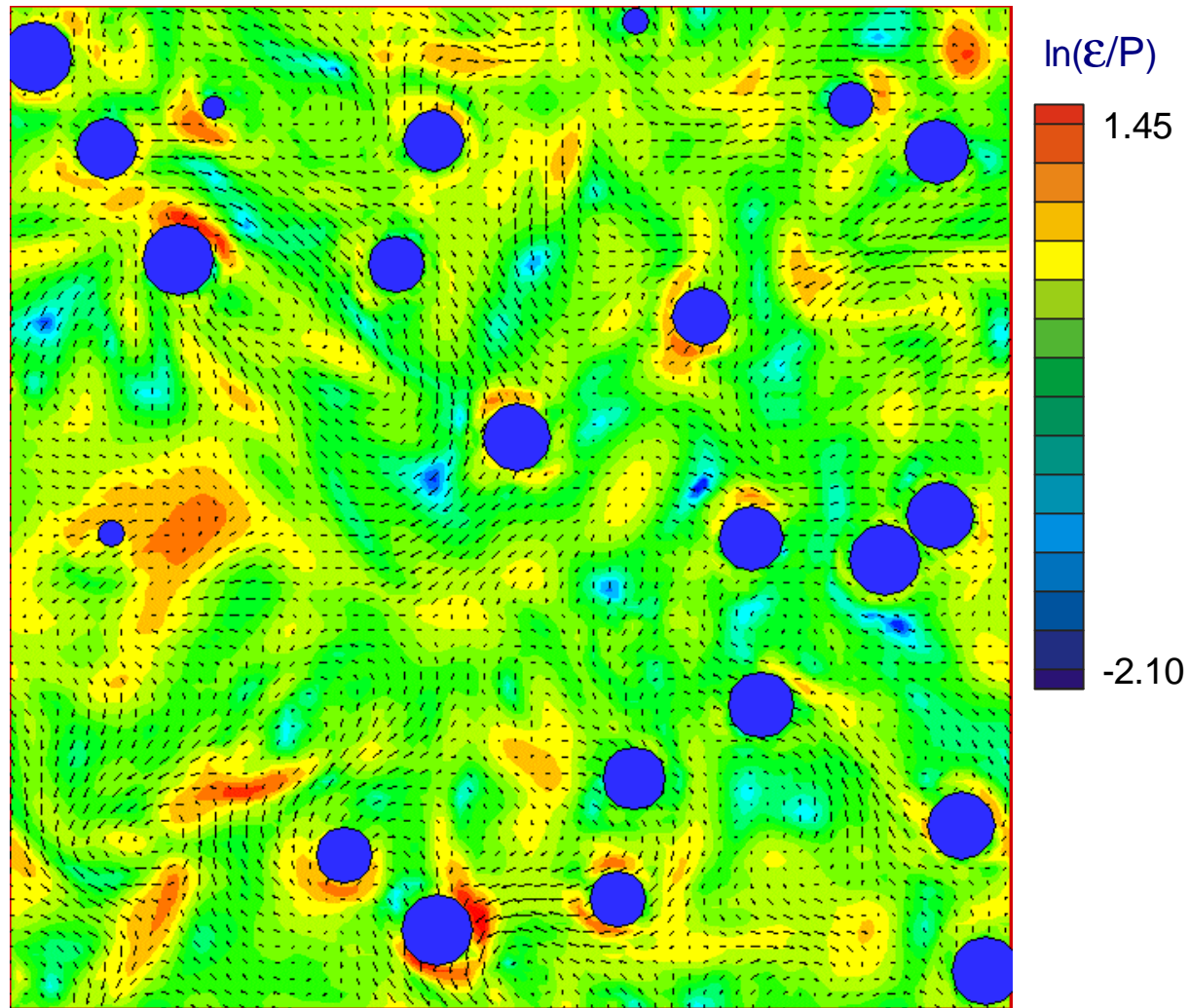


Particle-turbulence interaction

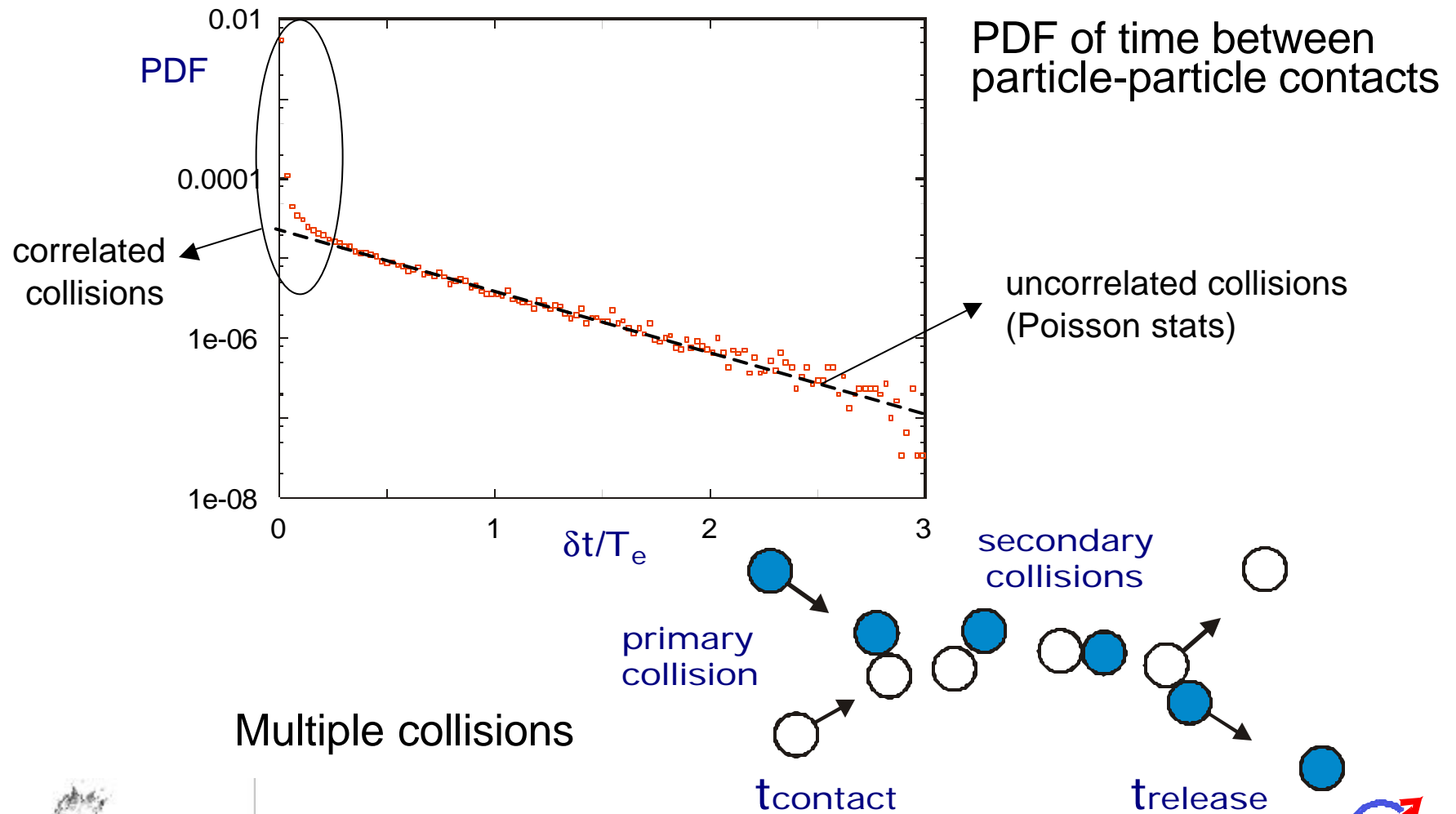


Energy dissipation rate

Flow field cross section



Short range interactions

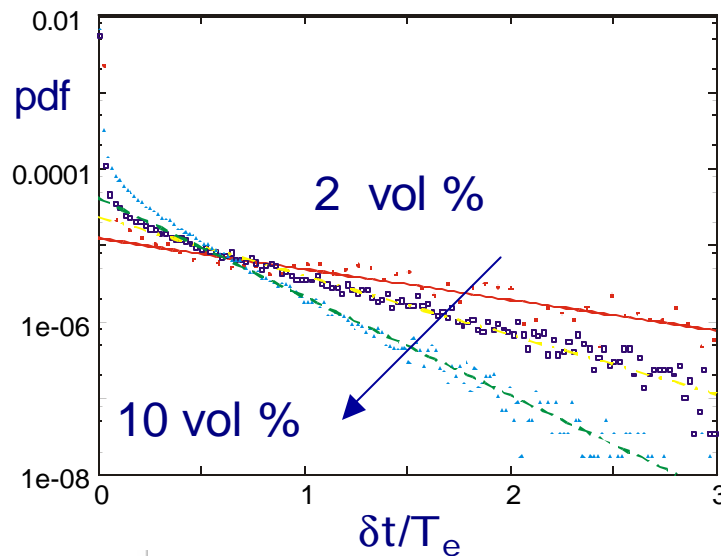


Short range interactions (2)

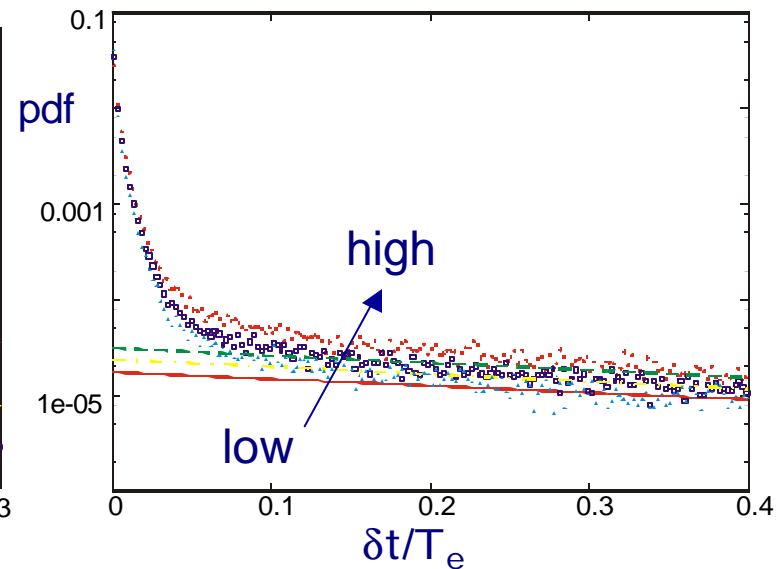
primary collisions:

exponential behavior of the PDF (Poisson-process)

effect of number density



effect of solids density



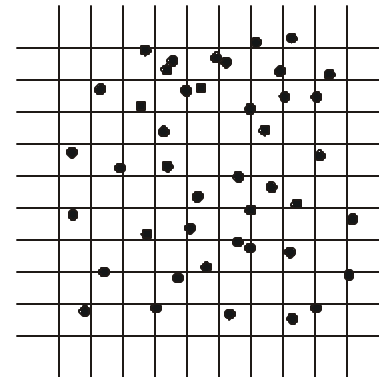
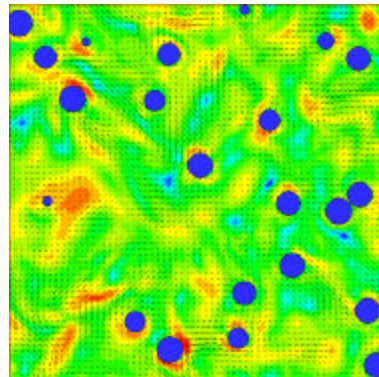
What did we learn?

- Turbulence modulation by particles
- Primary and secondary collision mechanism demonstrated
- Collision time depends on volume fraction
Primary/Secondary collision ratio depends on particle inertia

To do

compare point-particle LES/DNS and full DNS on periodic domains
relative particle velocities
collisions statistics

....



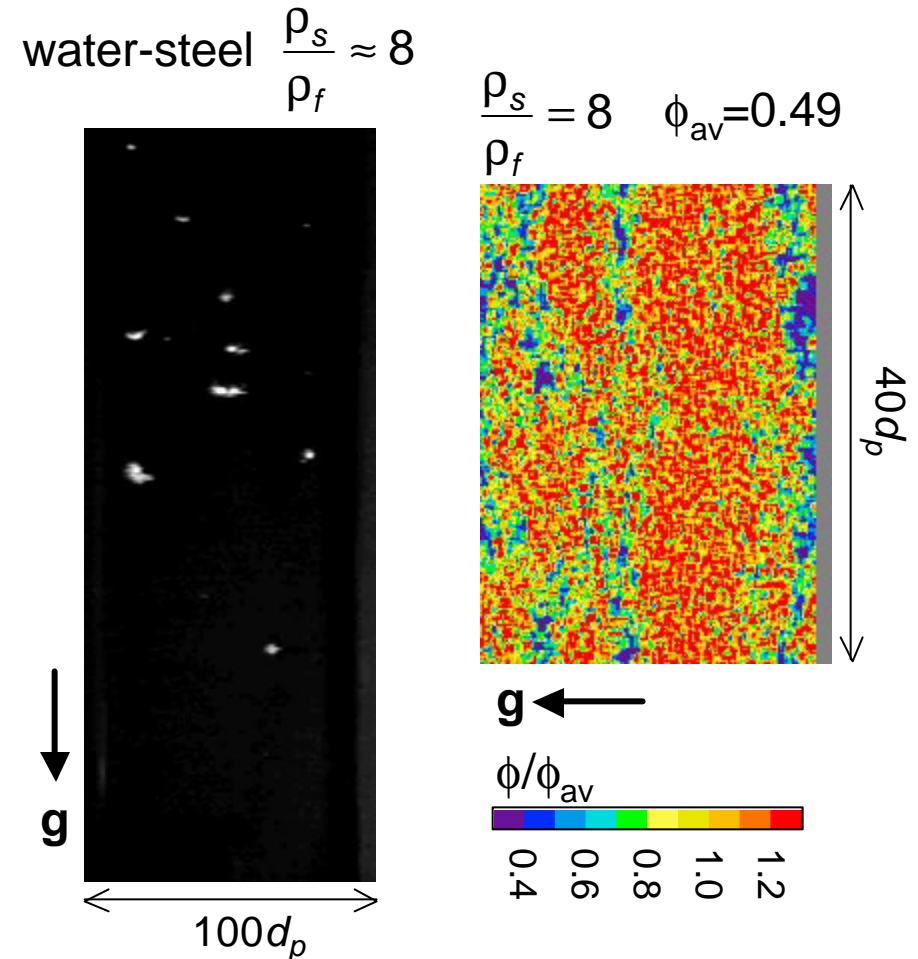
Much denser systems: liquid-solid fluidization

$\phi_s \approx 0.5$
no turbulence

Same methodology as for
turbulent suspension
Lattice-Boltzmann method for the
fluid flow
with immersed boundary
technique for no-slip at solid-
liquid interface

Hard-sphere collision algorithm

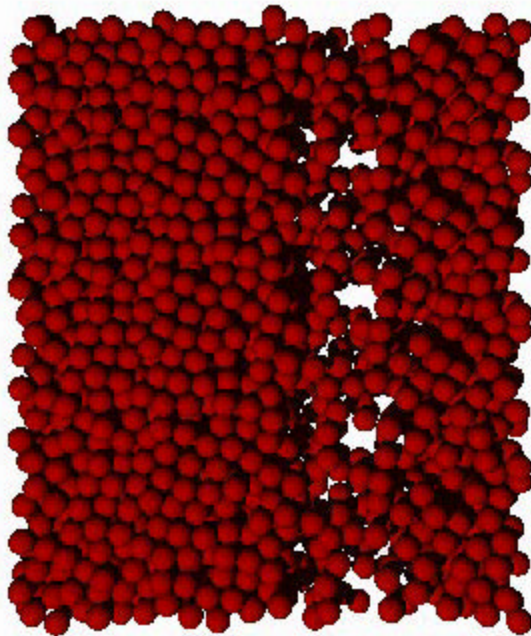
Lubrication forces



Detailed view of void formation

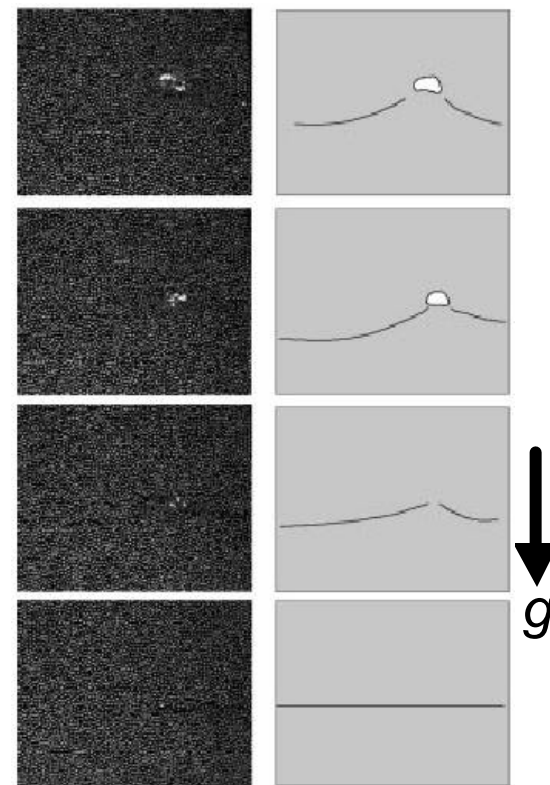
Onset of 2D instabilities in a flat bed

3D domain: $20d_p \times 24d_p \times 6d_p$ $\phi_{av}=0.505$ $\frac{\rho_s}{\rho_f} = 16$



$g \leftarrow e=1, \mu_f=0$
TU Delft

Compare to the scenario as measured by Duru & Guazzelli*



* *JFM* 470 (2002)

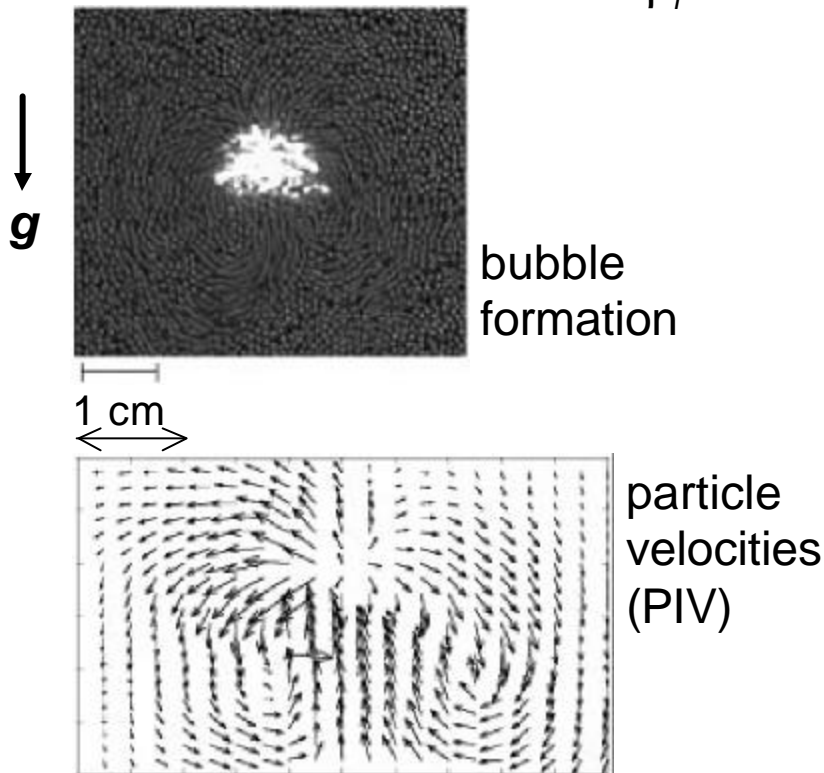
1 cm ($d_p=1$ mm)



Voids in flat beds (ctd)

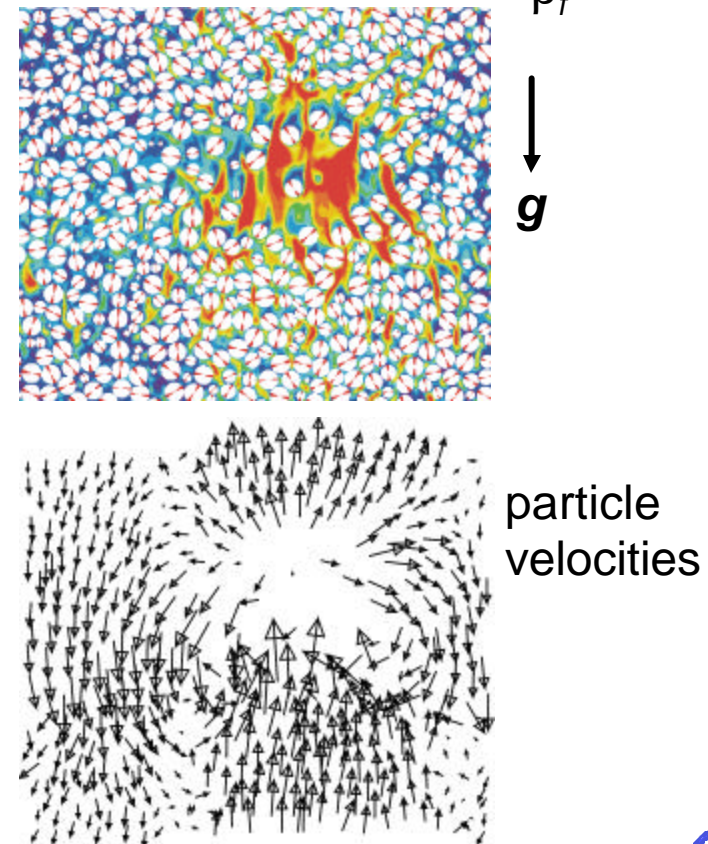
Experiments*

1 mm steel beads in water $\frac{\rho_s}{\rho_f} = 8$



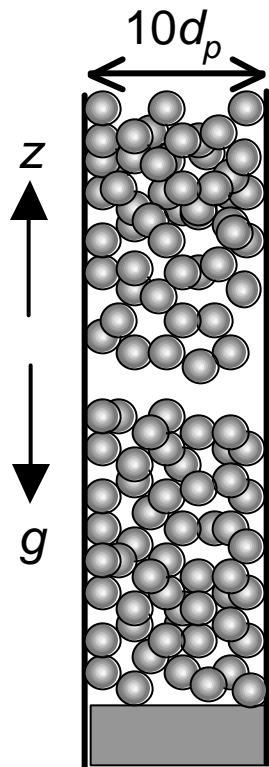
Simulations

0.7 mm beads in water $\frac{\rho_s}{\rho_f} = 16$



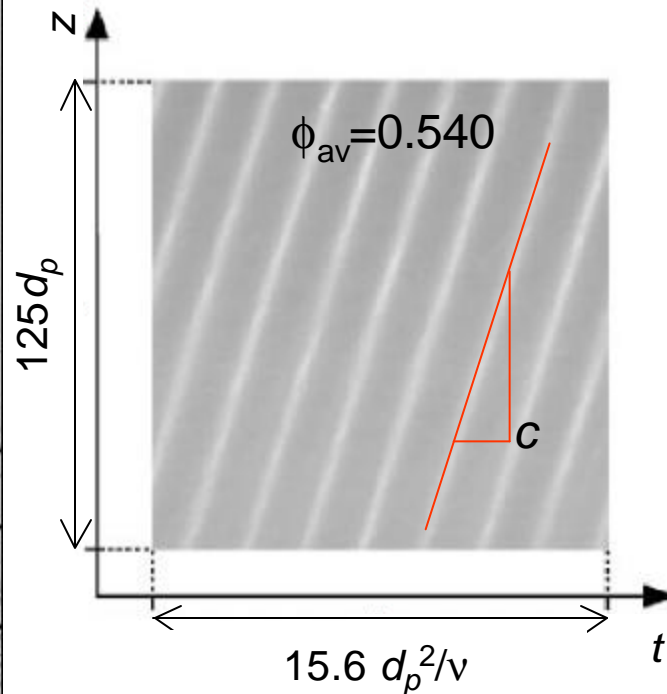
One step simpler: 1D (narrow) beds

typically 1 mm glass beads in water.



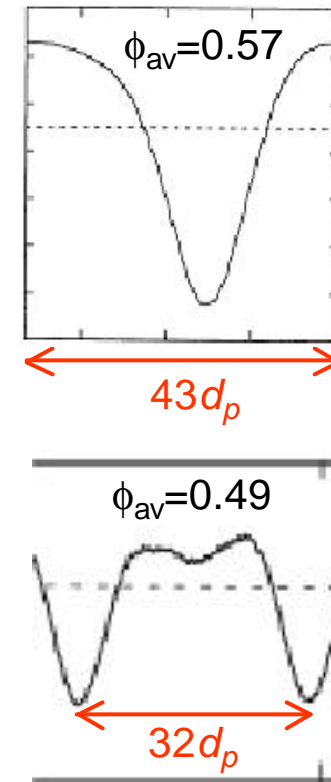
liquid flow

Experimental result*: planar wave instability



space-time plot of ϕ_s

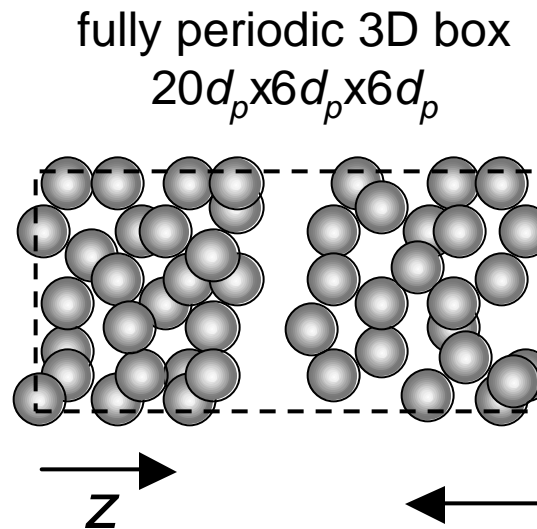
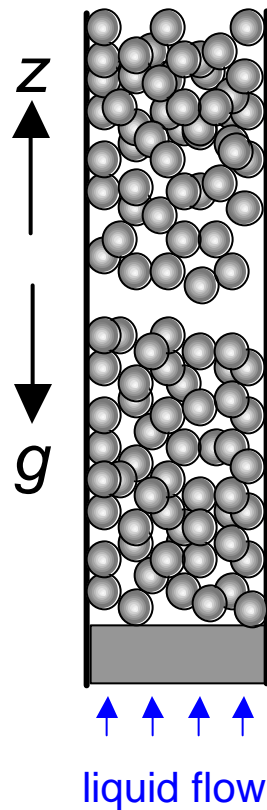
ϕ_s -wave shapes



* Duru et al., *JFM* 452 (2002)



Modeling step



$$\mathbf{f}_p = -(\rho_s - \rho_{mixture}) g \mathbf{e}_z$$

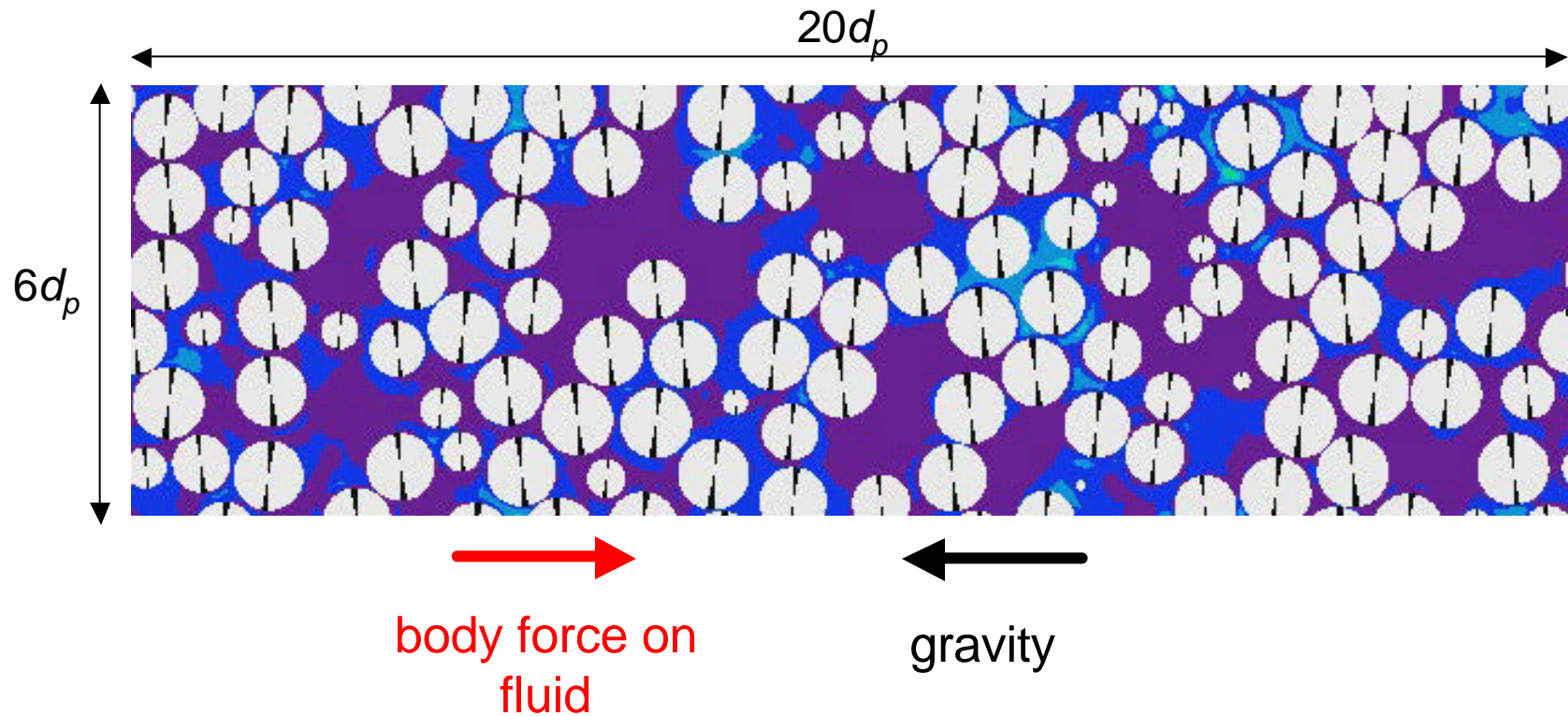
$$\mathbf{f}_f = (\rho_{mixture} - \rho_f) g \mathbf{e}_z$$

$$\rho_{mixture} = \phi_s \rho_s + (1 - \phi_s) \rho_f$$



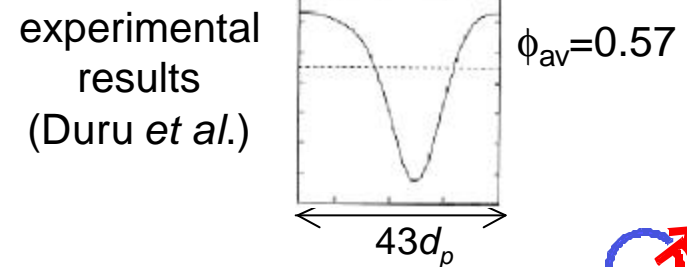
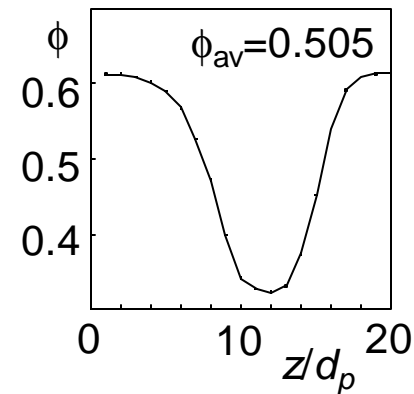
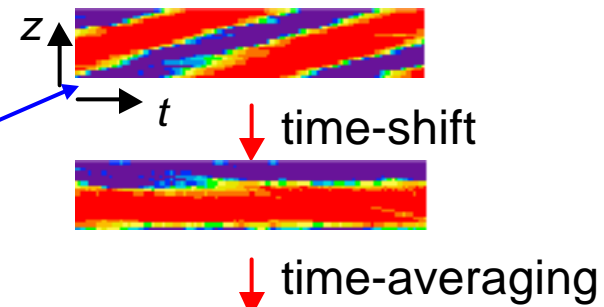
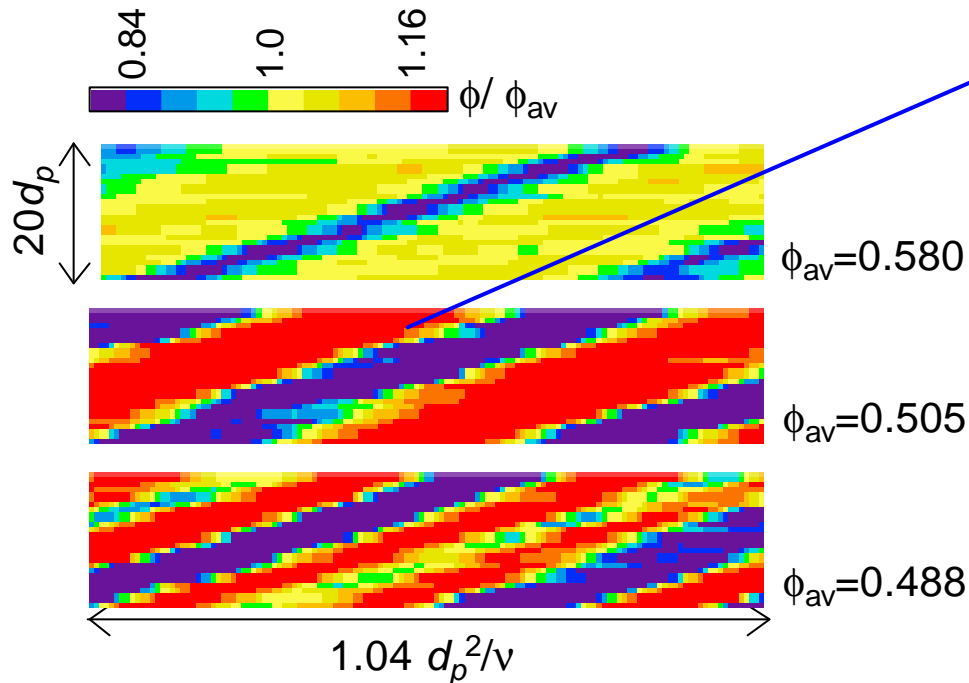
Simulation of L-S fluidization

$\phi_{av}=0.505$ $\frac{\rho_s}{\rho_f} = 4.1$ Cross-section from fully periodic, 3D domain



Wave-speed and wave-shape

Simulated space-time plots



Wave speeds

$$\left(\frac{c d_p}{v}\right)_{exp} = 29 \pm 1 \quad \left(\frac{c d_p}{v}\right)_{num} = 33 \pm 2$$

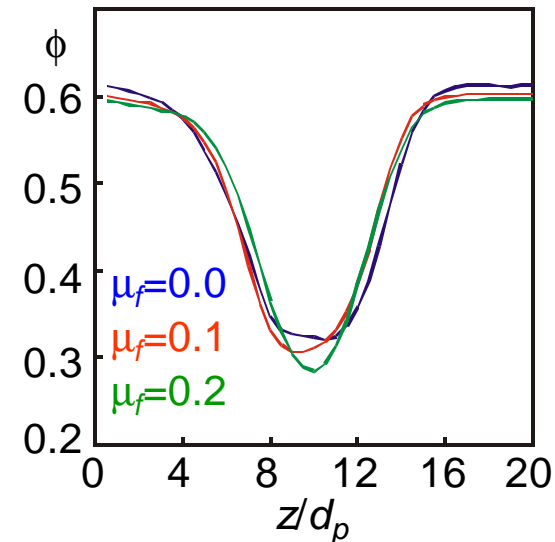
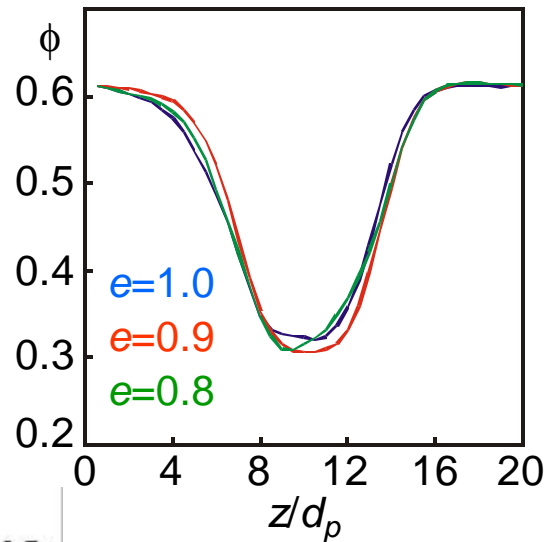
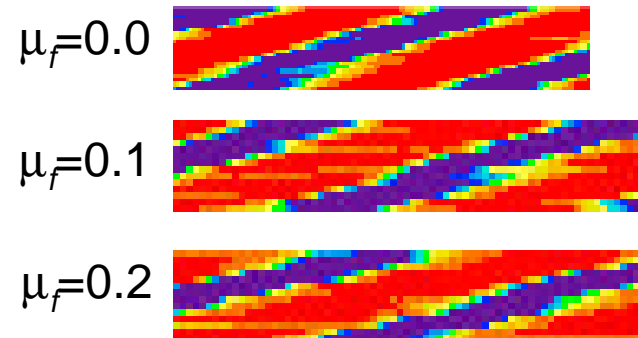
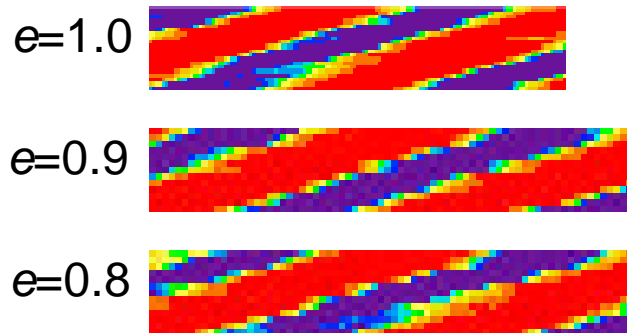
TU Delft



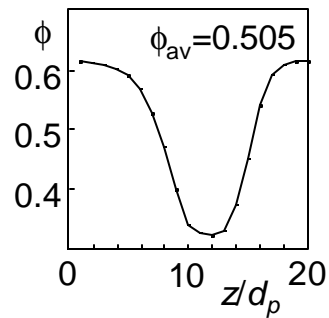
Collision parameters ($\phi_{av}=0.505$)

frictionless collisions ($\mu_f=0.0$)

elastic collisions ($e=1.0$)



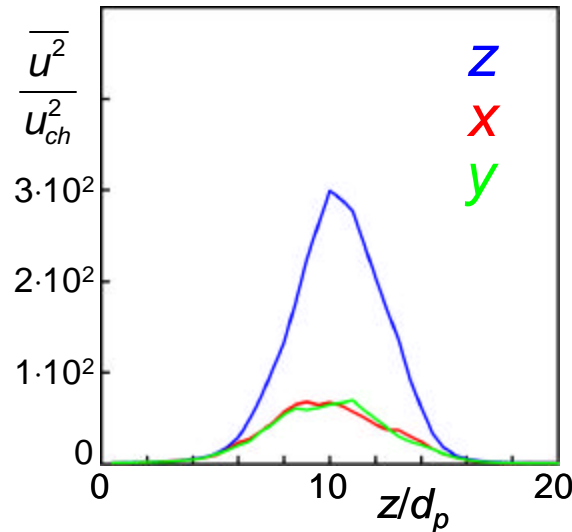
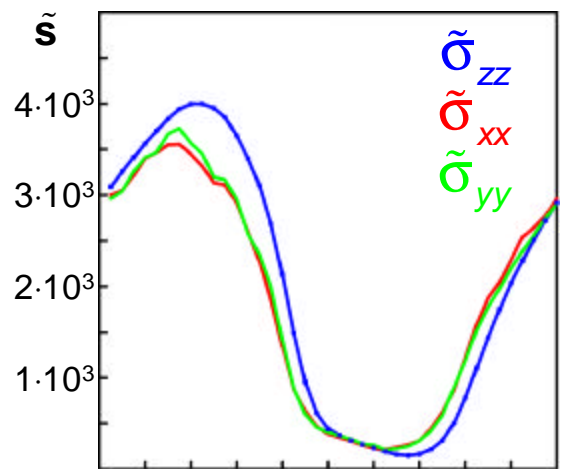
Momentum transfer (stress)



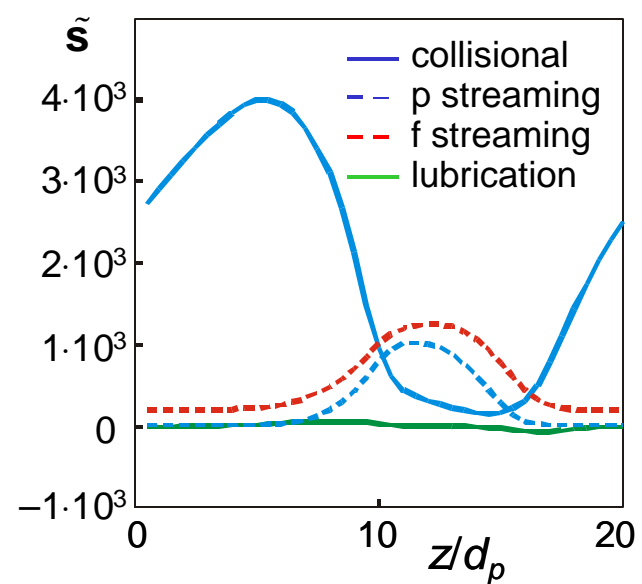
$$\tilde{\mathbf{s}} = \frac{\mathbf{s}}{\rho_f u_{ch}^2}$$

$$u_{ch} = \frac{v}{d_p}$$

(an)isotropy

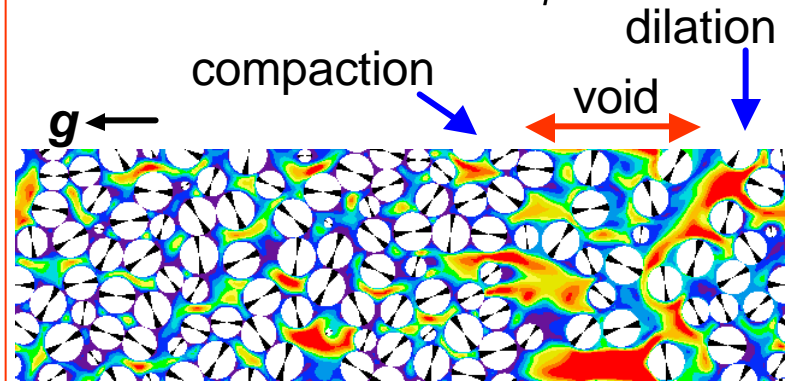


relative magnitude of zz stresses



collisional stress

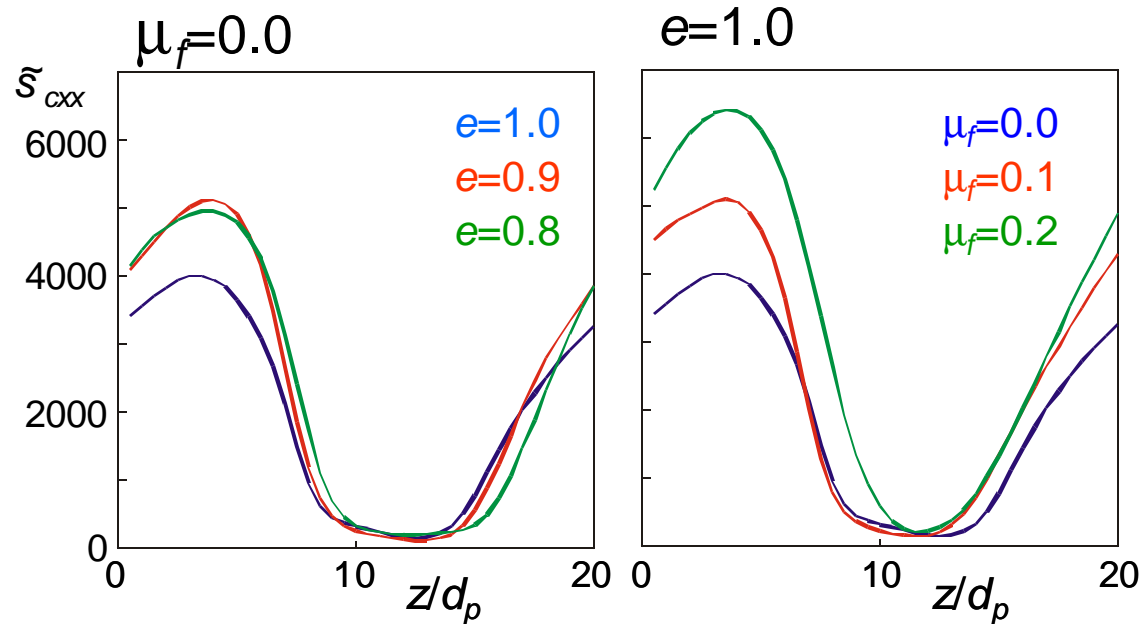
p-streaming stress



Momentum transfer (stress) (2)

influence of collision parameters on σ_{czz}

$$\tilde{\mathbf{s}} = \frac{\mathbf{s}}{\rho_f u_{ch}^2}$$
$$u_{ch} = \frac{v}{d_p}$$



Collisional pressure ($\phi_{av}=0.505$)

$$p_c = \frac{1}{3}(\sigma_{c,xx} + \sigma_{c,yy} + \sigma_{c,zz})$$

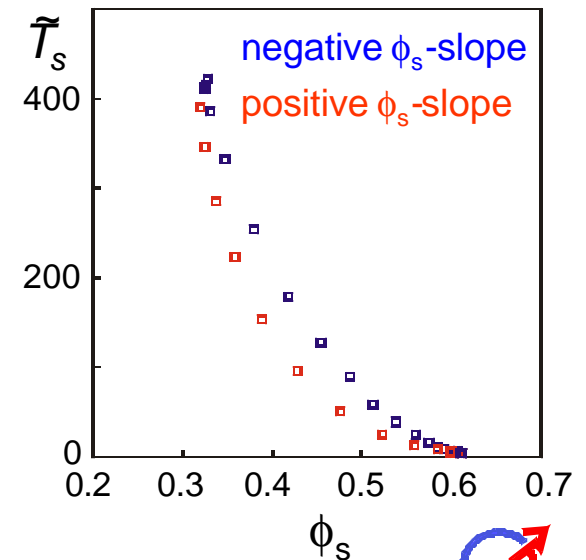
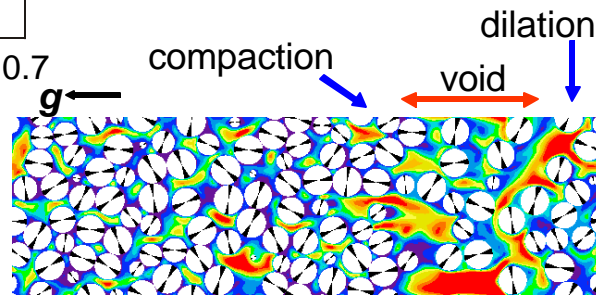
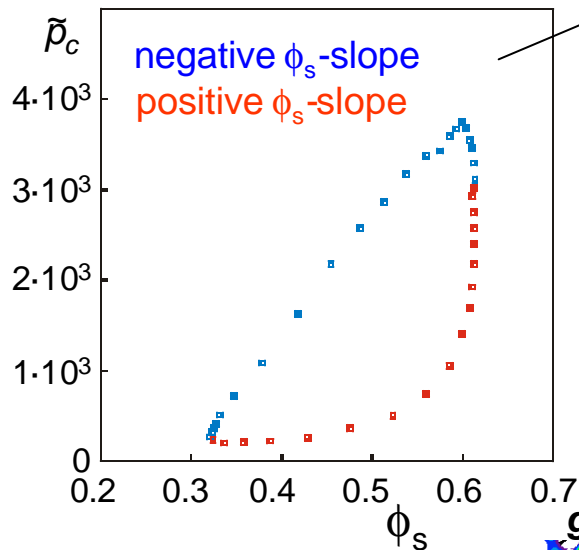
negative ϕ_s -slope: compaction
positive ϕ_s -slope: dilation

$$\bar{p}_c = \frac{p_c}{\rho_f U_{ch}^2}$$

p_c not a unique function of ϕ_s

result of granular temperature?
(cannot be the only reason)

$$\tilde{T}_s = \frac{T_s}{U_{ch}^2}$$

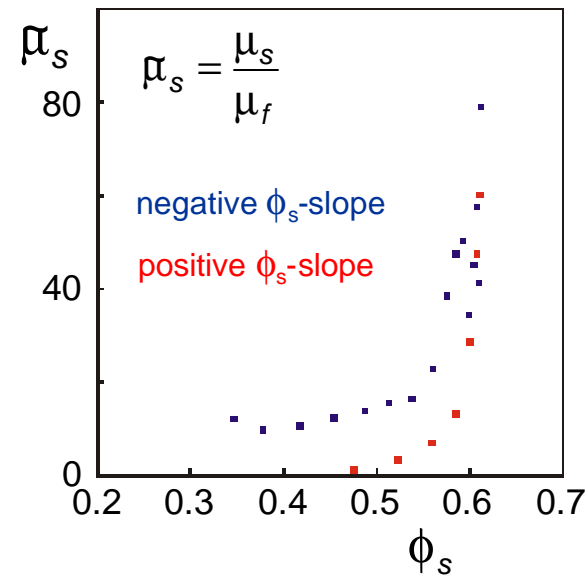


Solids-phase viscosity ($\phi_{av}=0.505$)

$$\tau_{zz} = \frac{4}{3} \mu_s \frac{du_{z,p}}{dz}$$

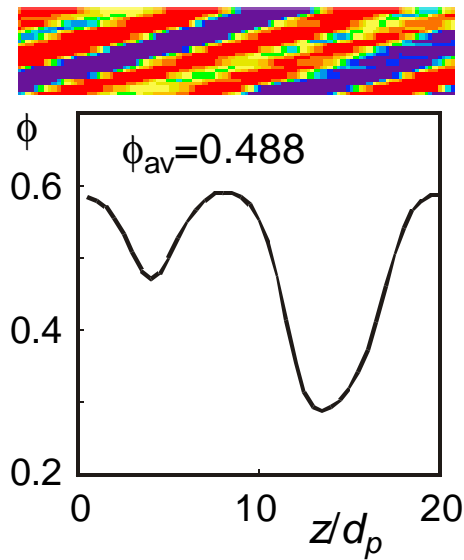
τ_{zz} : deviatoric solids-phase stress

(sum of collisional and p-streaming stress)

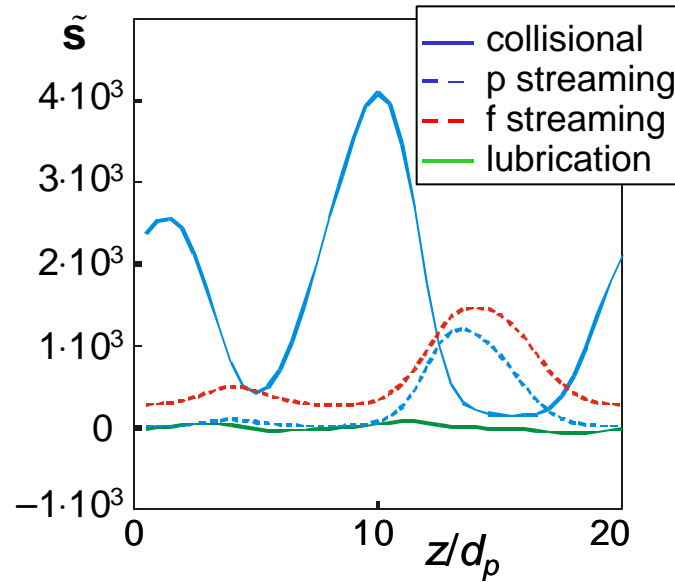


$$\phi_{av} = 0.488$$

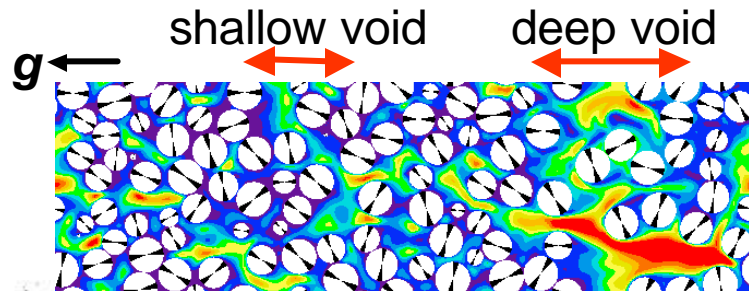
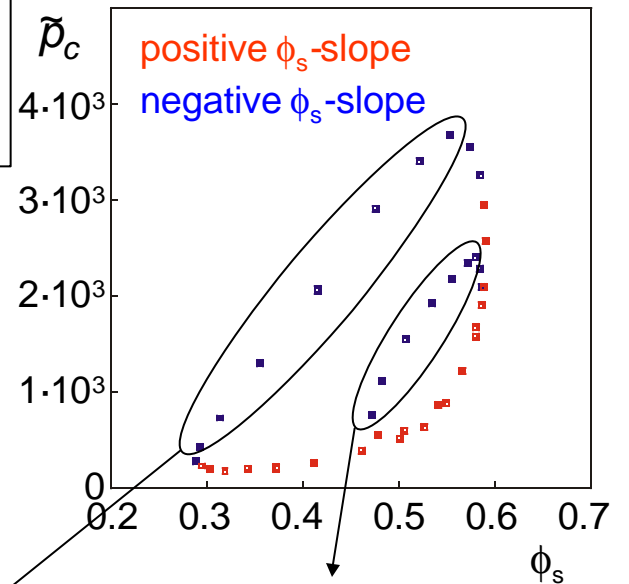
double hump wave



relative magnitude of stresses



collisional pressure



deep void

shallow void

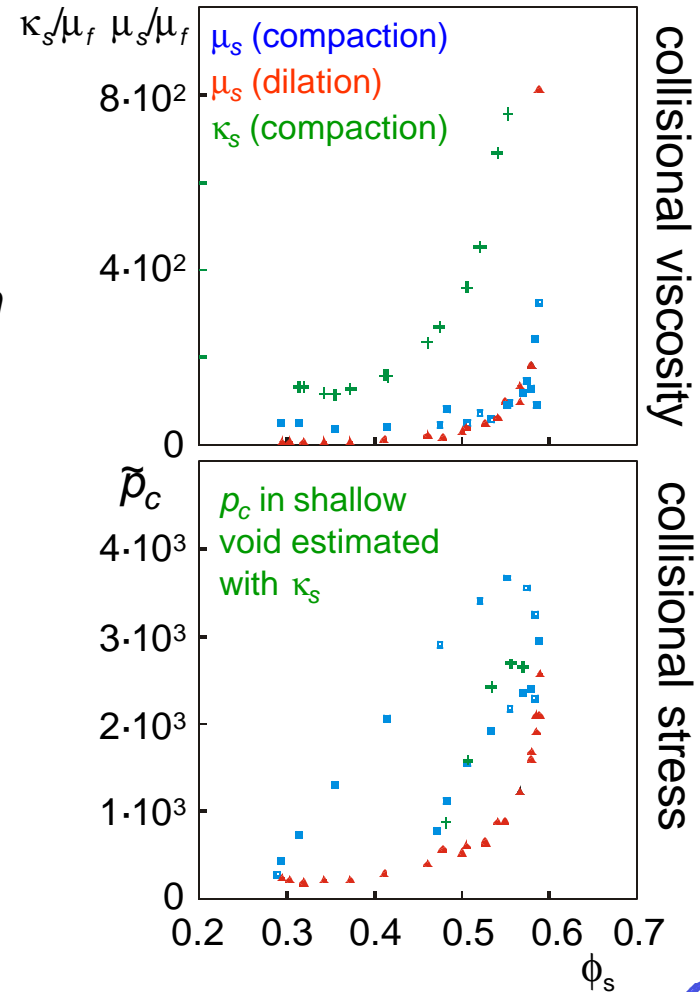
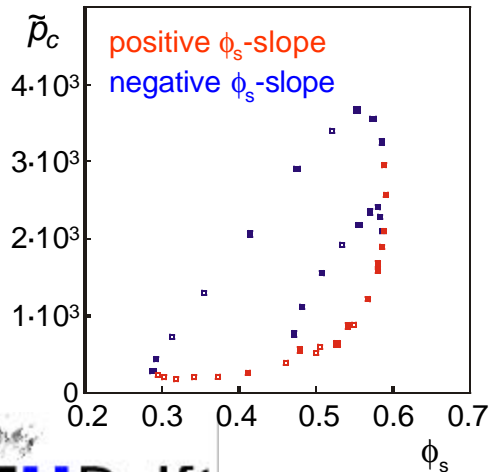
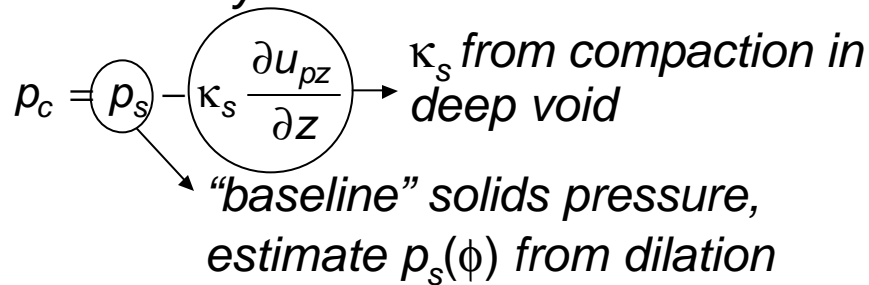
$$\tilde{p}_c = \frac{p_c}{\rho_f U_{ch}^2}$$



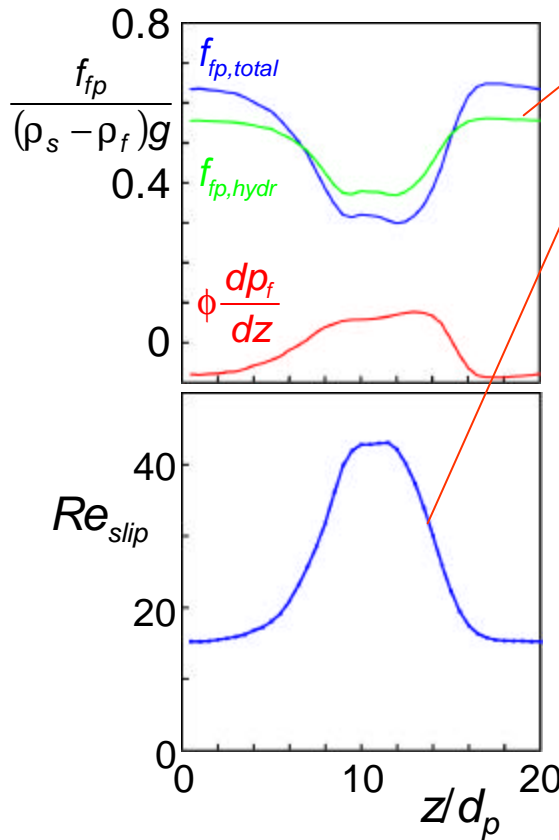
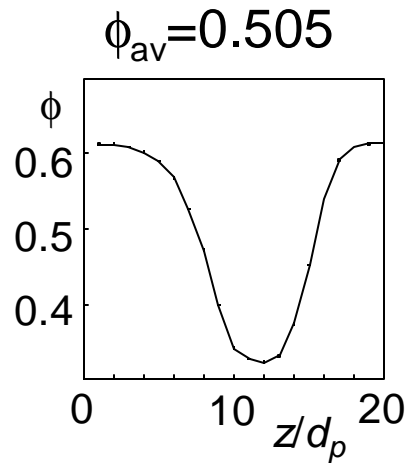
Role of bulk viscosity

collisional pressure under compaction
much higher than under dilation

interpret this in terms of the solids-phase
bulk viscosity

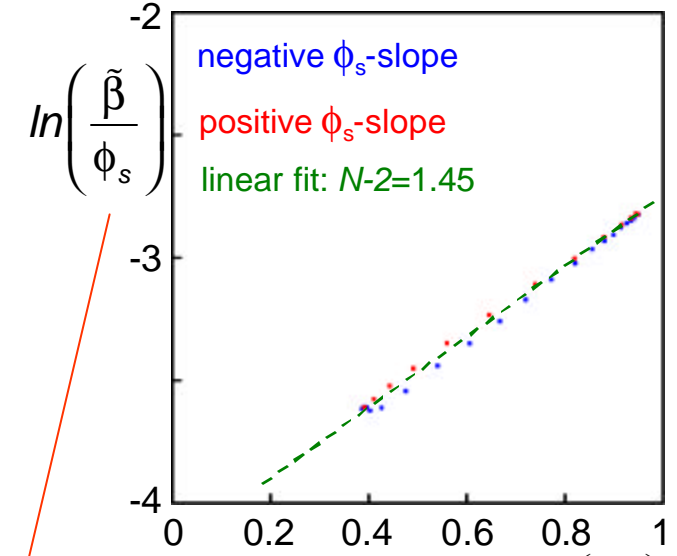


Hydrodynamic forces



$$\beta = \frac{f_{fp,hydr}}{u_{slip}} \quad v_{sed} = v_{p\infty} (1 - \phi_s)^N$$

$$\beta \frac{v}{\phi_s (\rho_s - \rho_f) d_p g} \propto \phi_f^{-(N-2)} \left(\frac{v}{d_p u_{p\infty}} \right)$$

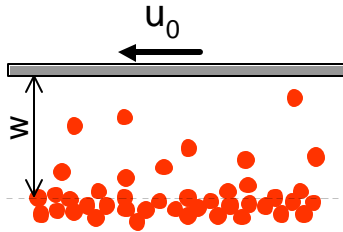


$$\tilde{\beta} = \beta \frac{u_{ch}}{g(\rho_s - \rho_f)}$$

$$\ln \left(\frac{1}{\phi_f} \right)$$



Sheared granular beds



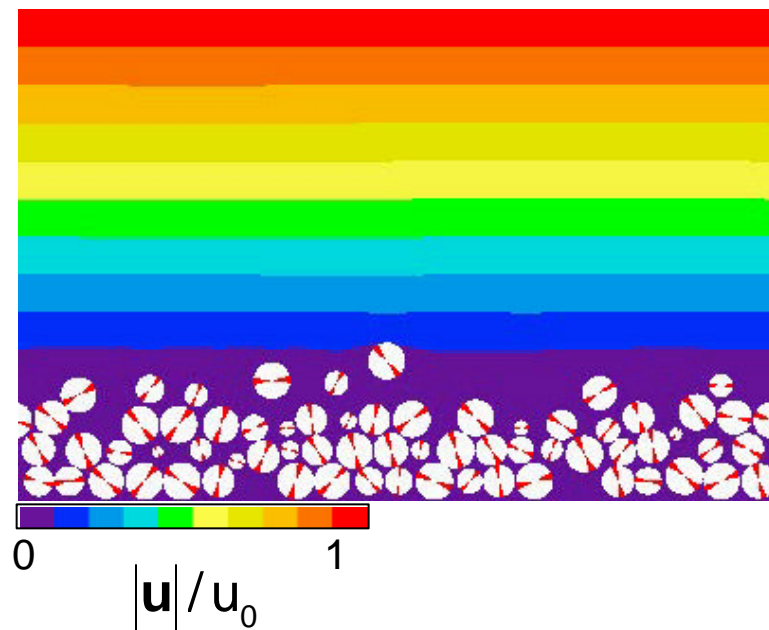
$$Re_{\text{part}} = \frac{d_p^2 \bar{\dot{\gamma}}}{\nu} = 0.2 \quad \left(\bar{\dot{\gamma}} \equiv \frac{u_0}{w} \right) \quad \frac{\rho_s}{\rho_f} = 1.14$$

Experiment (Charru *et al.*)



http://www.imft.fr/recherche/interface/english/theme7/op_2.html

Simulation



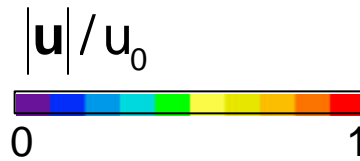
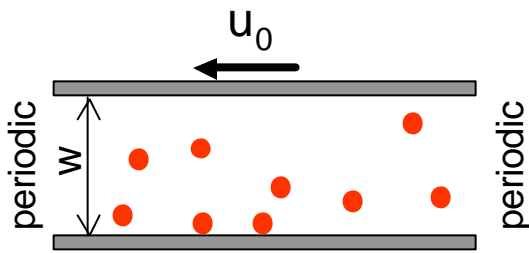
Increase Re_{part} : resuspension in turbulent flow

sedimentation and resuspension:

description of particle-wall interaction is critical

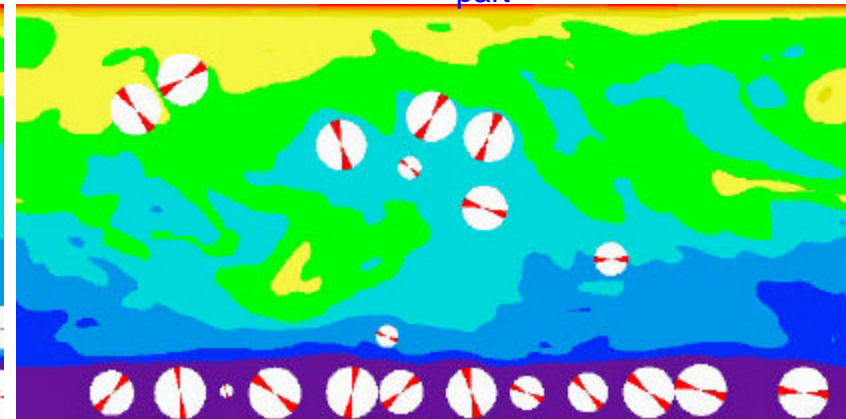
$$Re_{\text{part}} = \frac{d_p^2 \bar{\dot{\gamma}}}{\nu} \quad \left(\bar{\dot{\gamma}} \equiv \frac{u_0}{w} \right)$$

$$\frac{\rho_{\text{part}}}{\rho_{\text{fluid}}} = 2 \quad \phi_{V,\text{solid}} = 10\%$$



$Re_{\text{part}} = 625$

$Re_{\text{part}} = 1250 \rightarrow 2500$



Sheared suspensions

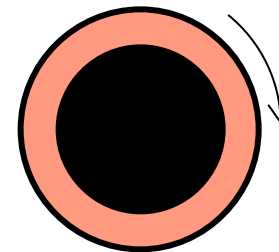
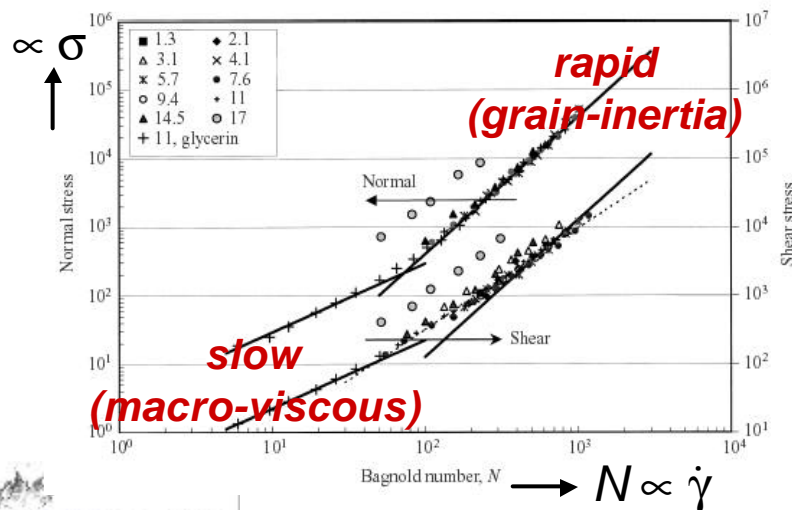
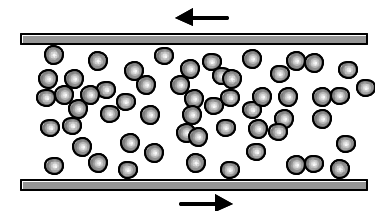
Momentum transfer in granular-fluid flows

The elementary picture in simple shear due to Bagnold (1954):

“slow” flows: viscous effects dominate: $\sigma \propto \dot{\gamma} \nu_{fluid}$

“rapid” flows: collisional stress dominates:

$$\sigma \propto \dot{\gamma} \nu_{eff} \rightarrow \nu_{eff} \propto l^2 \dot{\gamma} \rightarrow \sigma \propto \dot{\gamma}^2$$



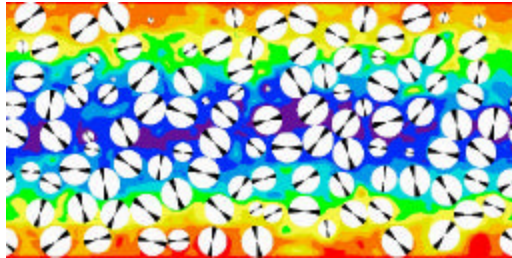
Bagnold's experiment:
Couette device

measurement of shear
and normal stress

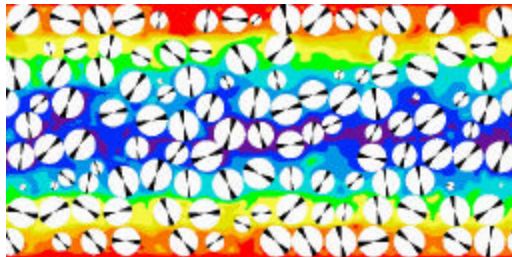


Qualitative observations

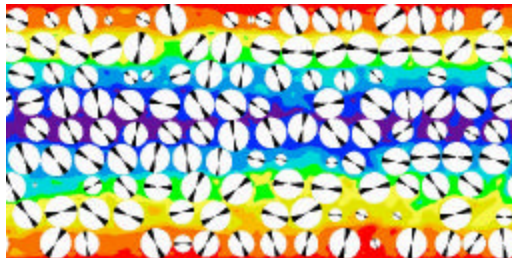
$\phi_{\text{solid}}=0.46$



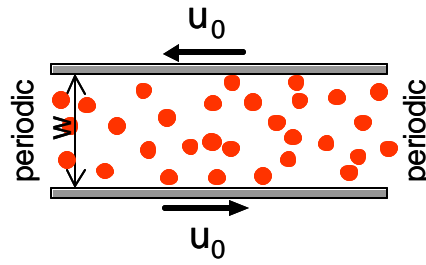
$\phi_{\text{solid}}=0.50$



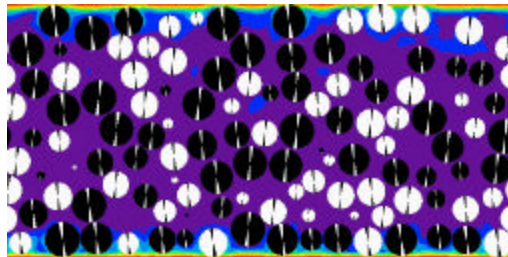
$\phi_{\text{solid}}=0.55$



monodisperse systems

$\phi_{\text{solid}}=0.50$

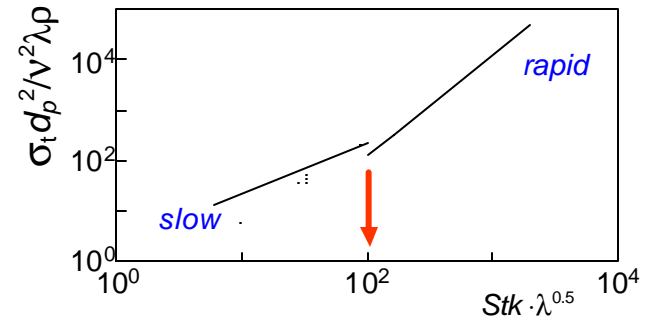


bi-disperse system

$$d_{p,black} = 1.2 d_{p,white}$$



$$N = St \cdot \lambda^{0.5} \approx 100$$



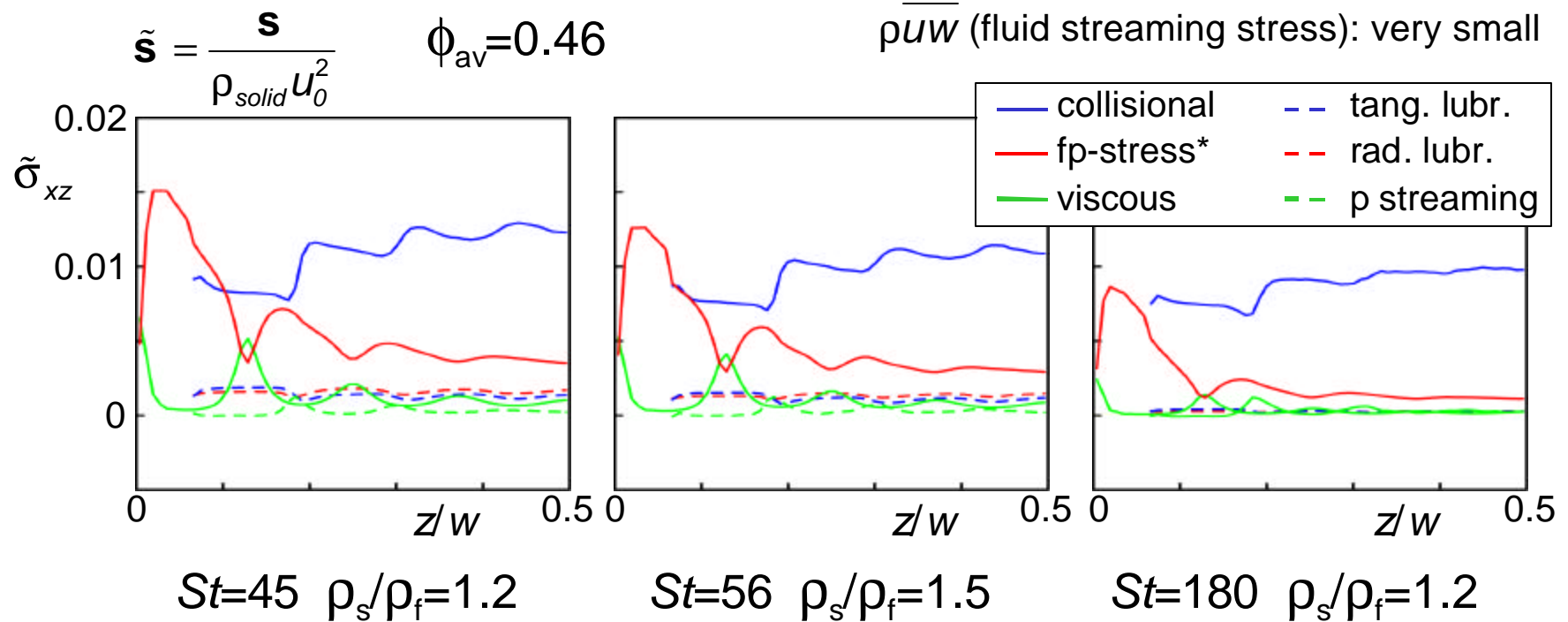
these are cross-sections
of 3D simulations:
spherical particles move
in en out of the plane

Shear-induced ordering

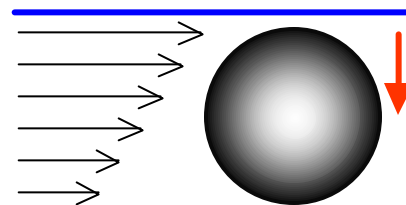
- consequences for stresses
- polydispersity opposes ordering



Shear stresses



In Bagnold's grain-inertia scaling the dimensionless stresses would be independent of St



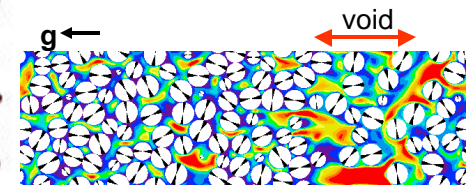
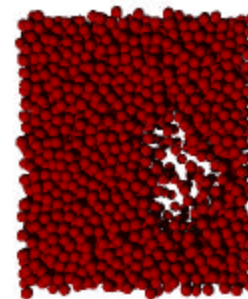
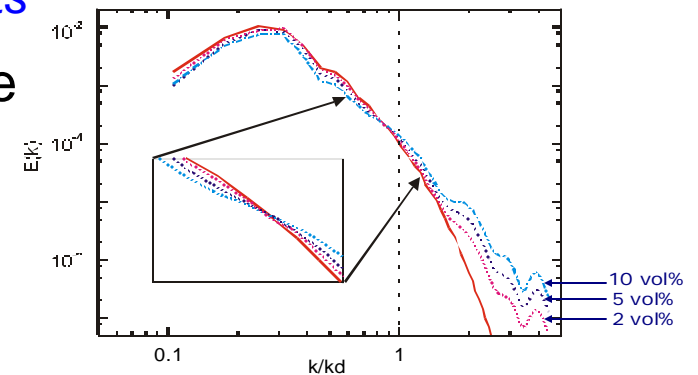
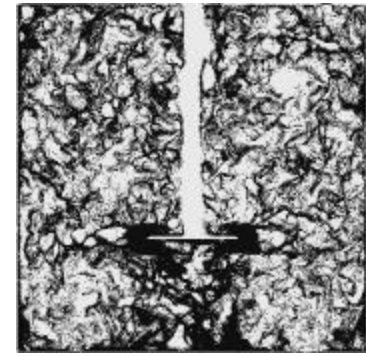
* **fp-stress:**
momentum transfer in z-direction due to traction at particle surface: *finite-size effect*

* Jackson, *Chem. Eng. Sc.* **52** (1997)



Summary

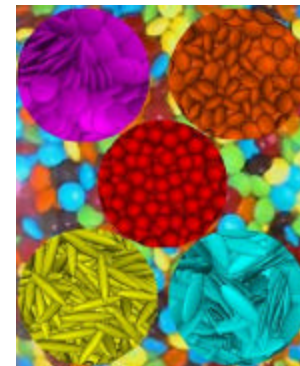
- Point particle approach in turbulent liquid-solid systems: possibilities and limitations
 - detailed information on particle motion and collisions in complex flows
 - the physics of two-way coupling and turbulent scales versus particle size → *finite size effects*
- Lattice-Boltzmann-based methodology for the *dynamics* of (dense) suspensions
- Turbulent suspensions
 - turbulence modification
 - collision dynamics: primary and secondary collisions
- Dense suspensions, fluidization
 - collisional stress dominates in the bulk
 - dilation and compaction behave differently in terms of stresses



Simulation tool for complex fluids

Non-spherical particles

fibrous materials
concrete (high Stokes numbers)



Donev et al., *Physical Rev. Lett.* 92 (2004)

Colloidal systems

self organization



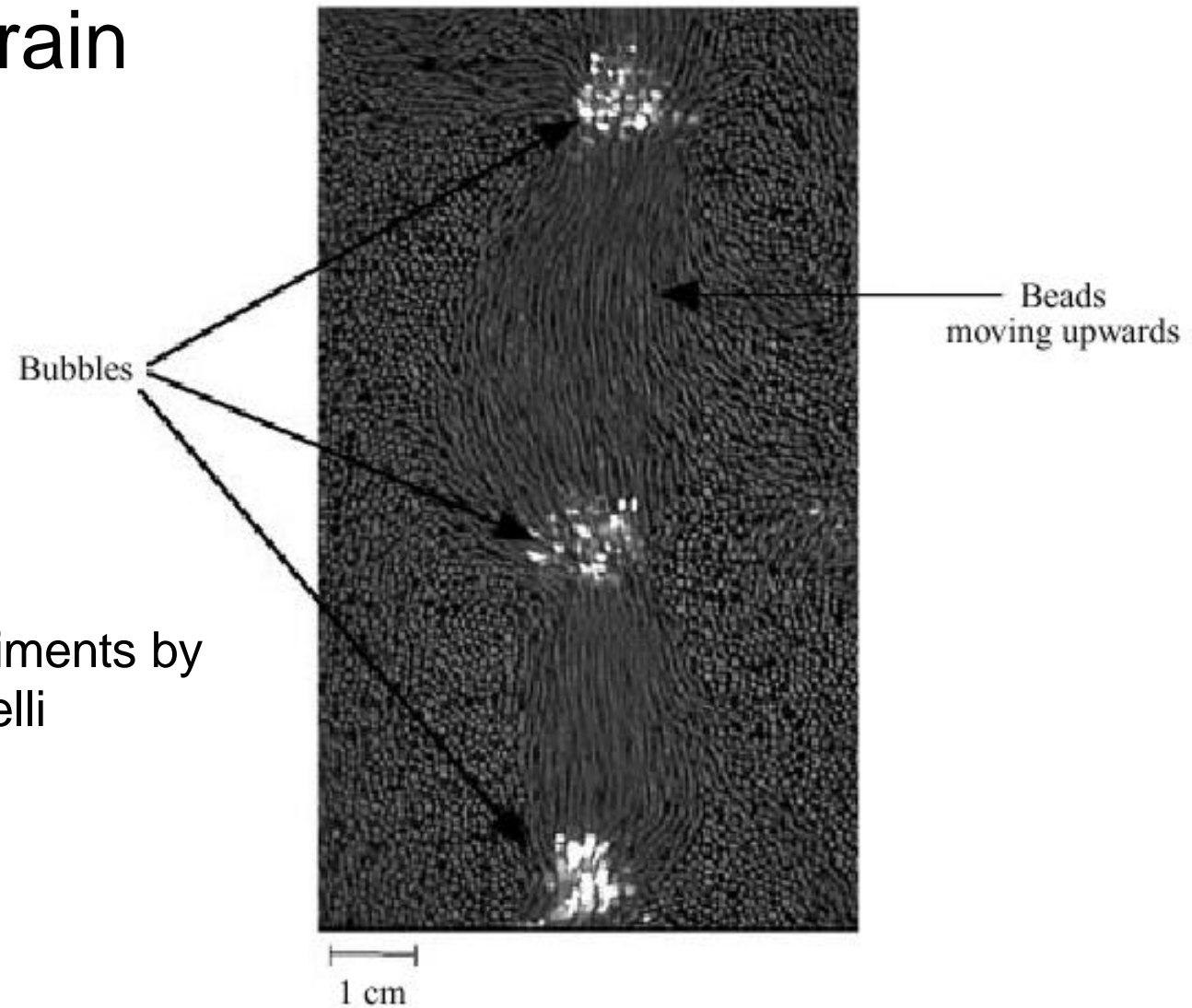
Reservoir engineering

oil recovery by displacement with water



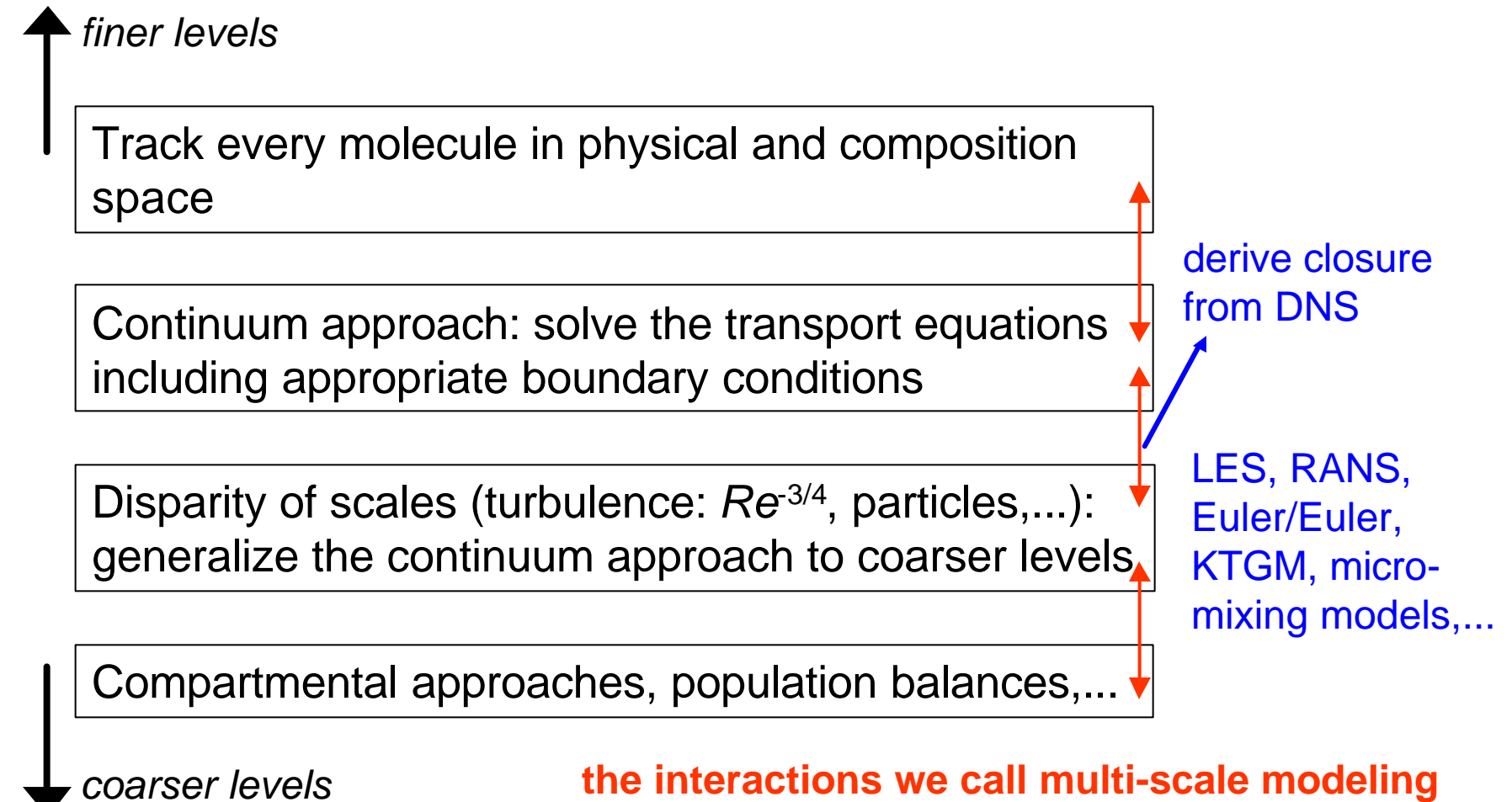


Bubble train



from the experiments by
Duru & Guazzelli
JFM **470** (2002)

Levels in process simulation



3D view

