Dense suspensions
the richness of solid-liquid interactions at the particle scale

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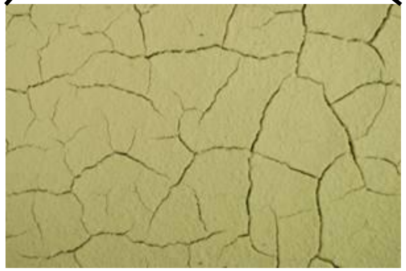
Alberta: oil sands

mining

tailings

Non-Newtonian liquids with solid particles



clay suspension

reclaimed land

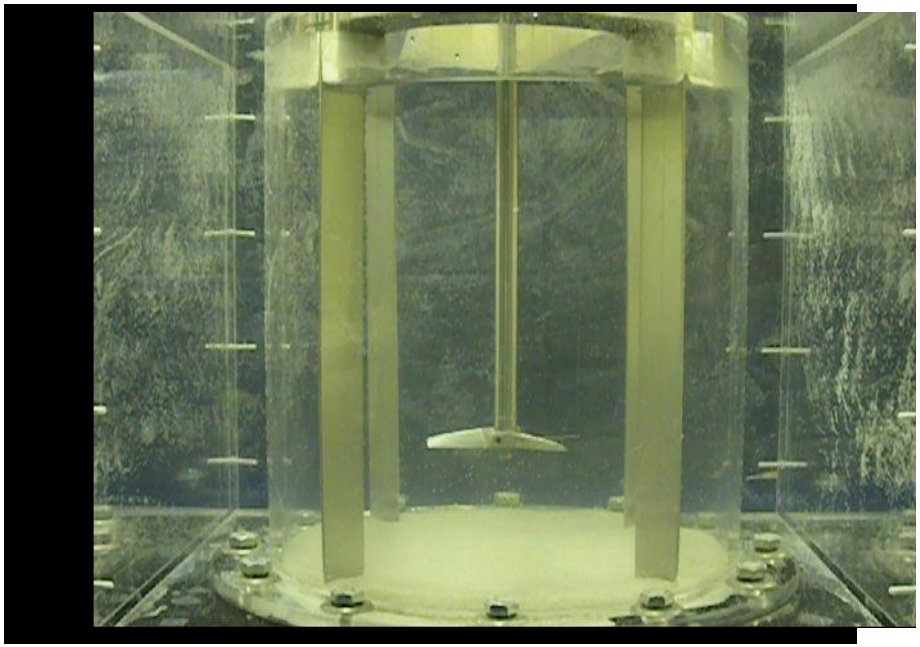
Oil sands processing – e.g.: “Hydro-transport”

Slurry pipeline with oilsands, water, air

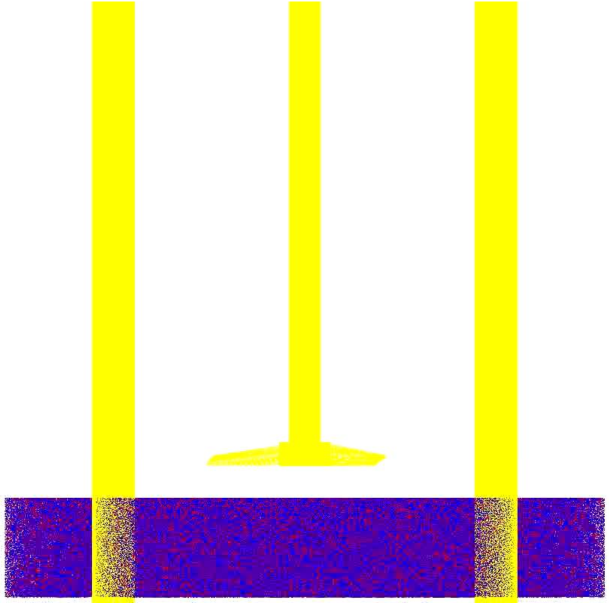
- wildly turbulent flow
- very wide particle size distribution: from bricks to clay platelets (‘nano particles’)
- inhomogeneous multiphase flow
- pipe-wall erosion and sedimentation (formation of stagnant layers) are issues

Solid particles in (turbulent) flow

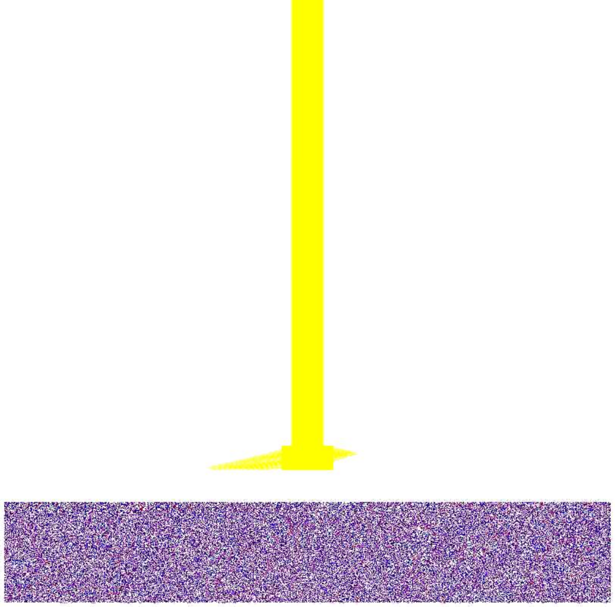
experiment



simulation – side view



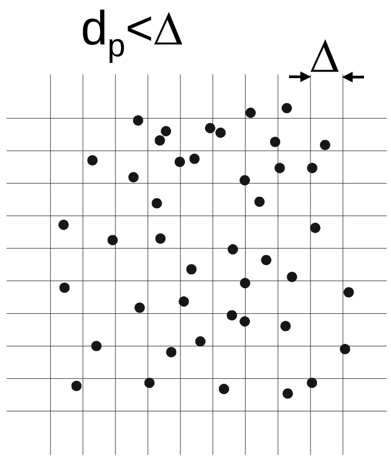
simulation – cross section



the good thing about simulations:
easy to look inside

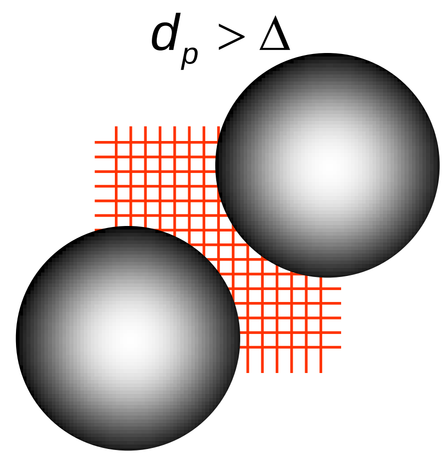
Lagrangian solid-liquid simulations

unresolved particles versus resolved particles



particle size < grid spacing
$\rightarrow$flow around particles is not resolved
particle are moved around by drag forces & more exotic forces
particles collide

up to 10^8 particles



particle size > grid spacing
hydrodynamics and hydrodynamic forces are fully resolved
direct coupling between particle motion and liquid flow

up to 10^4 particles

My typical SL parameter space

solids volume fraction ϕ	> 0.1
solid over liquid density ratio	$2 < \frac{\rho_p}{\rho} < 10$
Stokes number $St = \frac{\text{particle time scale}}{\text{flow time scale}}$	O(1)
Reynolds number (based on particle size)	anywhere, mostly $Re \geq 1$

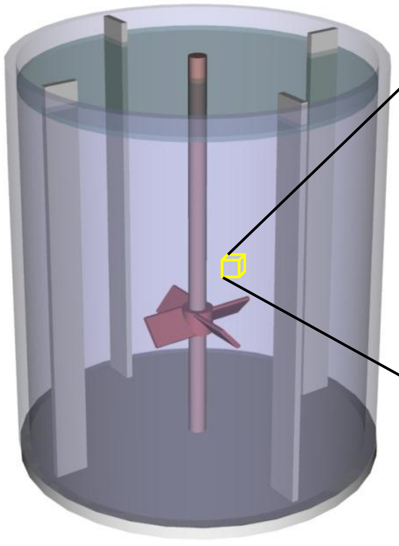
We do not get away with

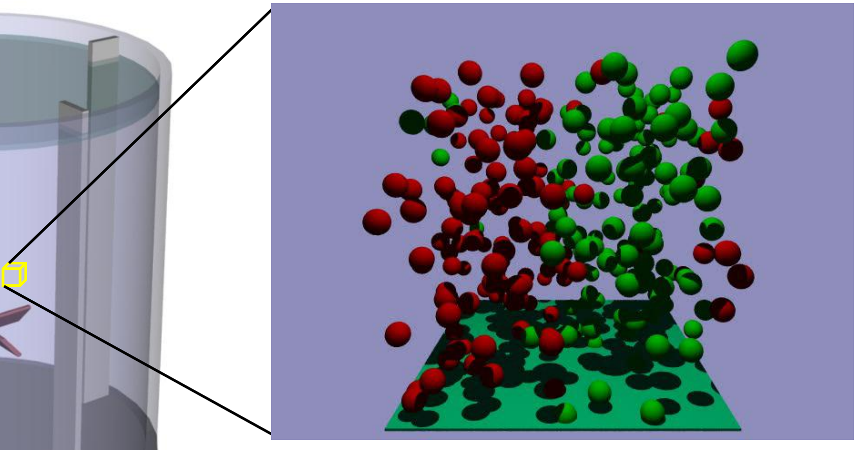
- one-way coupling
- drag-only
- no collisions

On the positive side

- non-Brownian particles

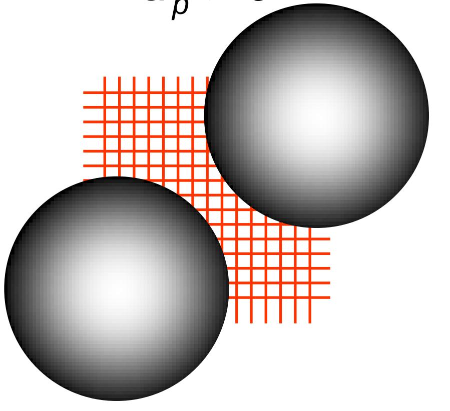
Meso-scale simulations





O(10^3) particles in a 3D periodic domain

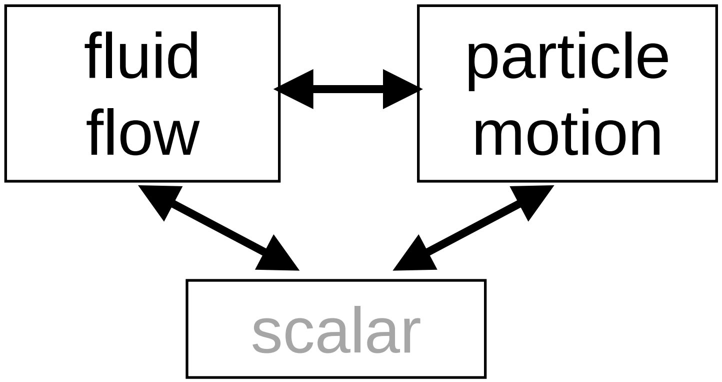
$d_p > \delta$

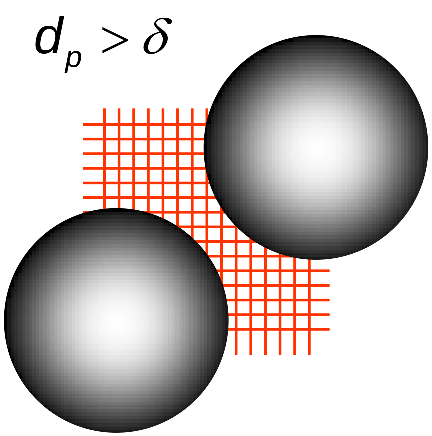


direct simulations resolving the solid-liquid interfaces

Our interests
- *see what happens* at the meso-scale
- feed back meso-scale insights as (subgrid) models to the macro-scale

A few words on modeling & numerics





Lattice-Boltzmann method for solving the flow of interstitial fluid

- 3D, time-dependent

Explicitly resolve the solid-liquid interface: *immersed boundary method*

- particle diameter typically 12 grid-spacings

Solve equations of linear and rotational motion for each sphere

- forces & torques:
  - directly (and fully) coupled to hydrodynamics
  - plus gravity
- hard-sphere collisions

NB: in this talk: particles are spheres

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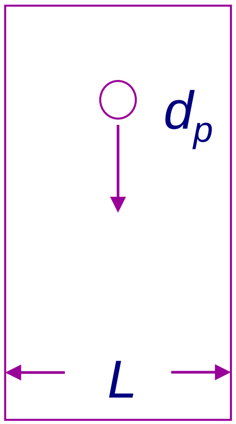
Some validation material

single particle validation

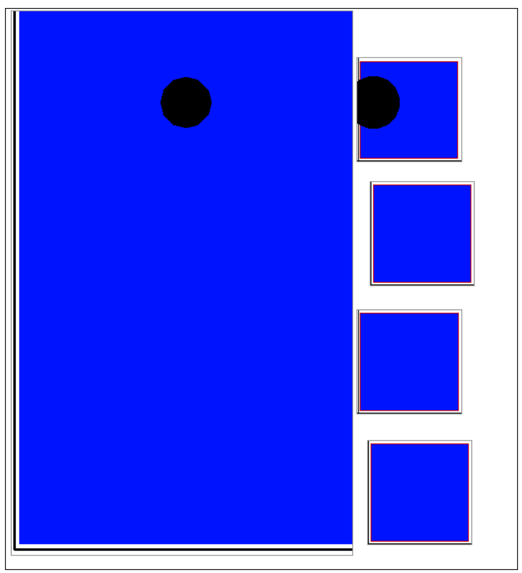


PIV experiment of a falling sphere in a closed box*

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

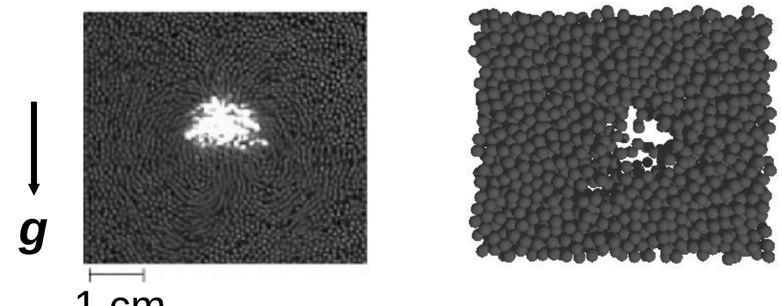
$$\frac{d_p}{L} = 0.15$$

$Re_p = 32$

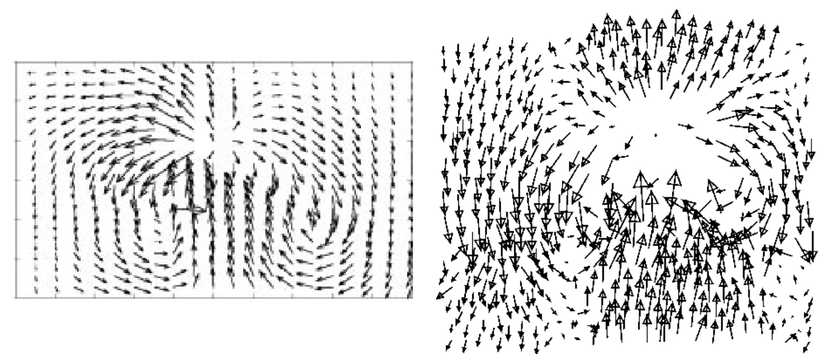


LB simulation PIV exp

multiple particle validation: liquid-solid fluidization



void formation



particle velocities

experiment** simulation***

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

** Duru & Guazzelli *JFM* (2002)

*** Derksen & Sundaresan *JFM* (2007)

Rest of this talk: sample applications

what to learn from meso-scale simulations?

erosion & sedimentation

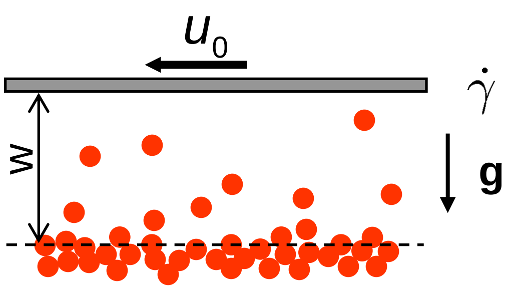
aggregation / flocculation

Hydro-transport

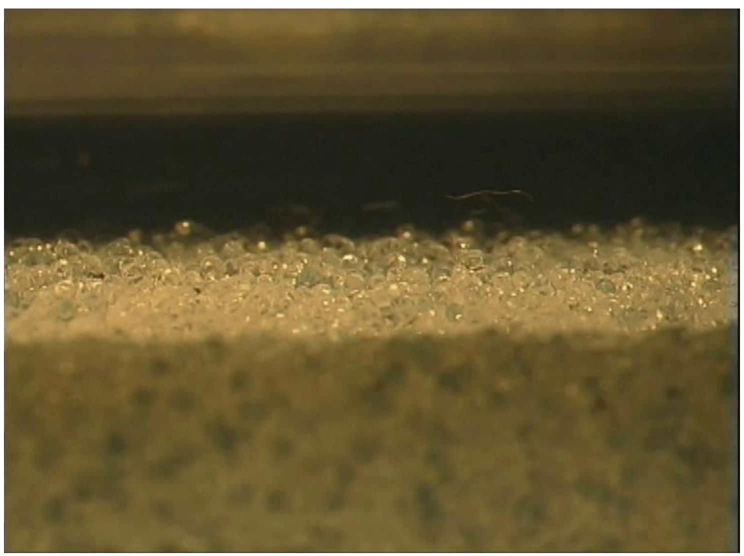
Back to the slurry pipeline

Erosion & sedimentation

Start simple: laminar flow, spherical particles, monosized



$$\dot{\gamma} = \frac{u_0}{W}$$



Movie: courtesy François Charru (IMFT)

Shields number

shear stress over net gravity

$$\theta = \frac{\rho \nu \dot{\gamma}}{g \;\; \rho_p - \rho \;\; 2a}$$

Reynolds number

$$\mathrm{Re} = \frac{\dot{\gamma} a^2}{\nu}$$

Density ratio

minor role for if Re is modest

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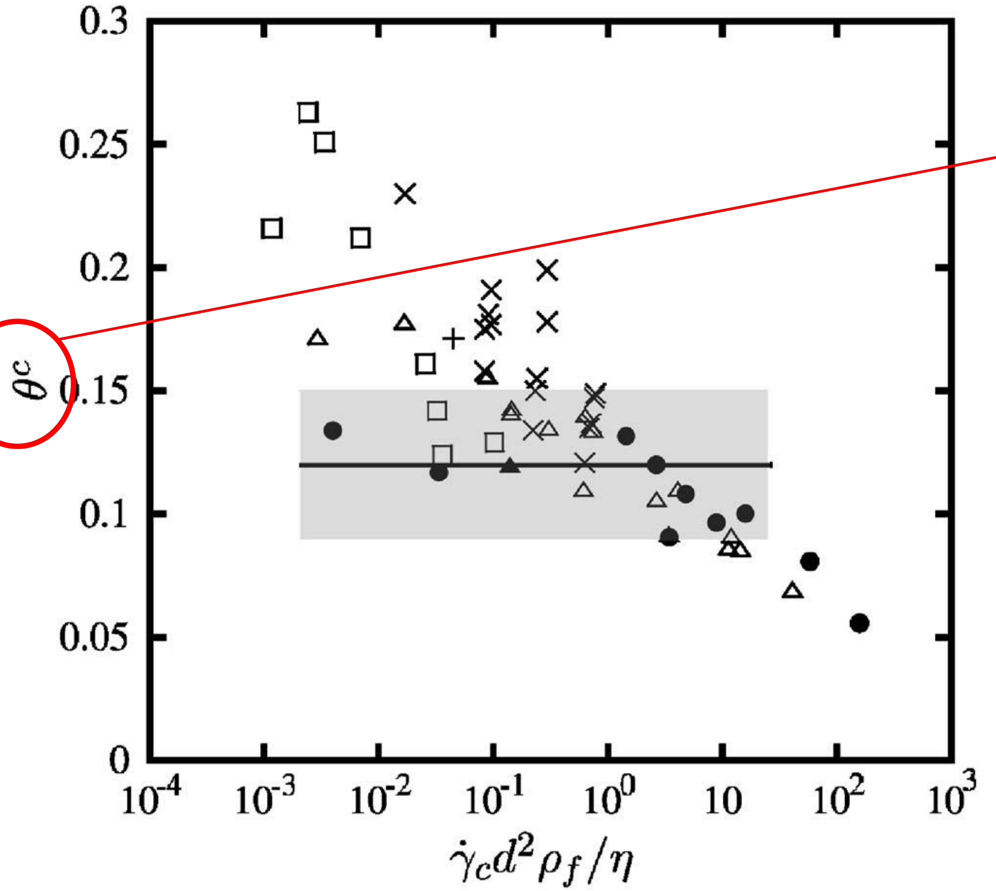
Experimental data



θ^c

critical Shields number

onset of bed erosion

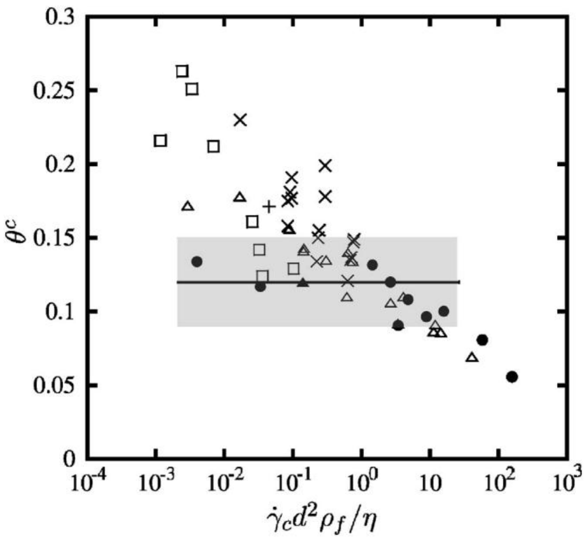
Quite some scatter

systems are hard to control at the particle-scale

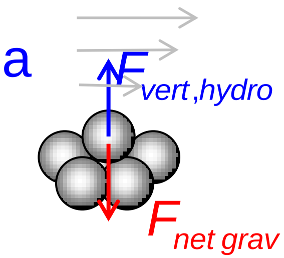
- non-sphericity
- friction coeffs
- short-range interactions

Ouriemi et al., *PoF* **19** (2007)

Back-of-envelope analysis for low Re



for the bed to start moving we need a vertical hydrodynamic force that overcomes net gravity $\rightarrow$ at θ^c



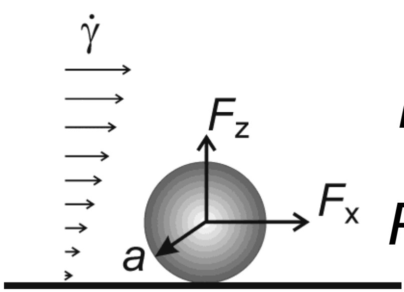
$$F_{vert,hydro} = \frac{4\pi}{3} a^3 g \ \ \rho_p - \rho \ \ = \frac{4\pi}{3} a^2 \frac{1}{\theta_c} \rho \nu \dot{\gamma}$$

$$\theta = \frac{\rho \nu \dot{\gamma}}{g \ \ \rho_p - \rho \ \ 2a}$$

θ^c independent of Re

$$\rightarrow F_{vert,hydro} \propto a^2 \rho \nu \dot{\gamma}$$

$$\boxed{\mathrm{Re} = \frac{\dot{\gamma} a^2}{\nu}}$$



$$F_x = 32.1 \rho \nu \dot{\gamma} a^2 \ (*)$$

$$F_z = 9.22 \dot{\gamma}^2 a^4 \ (**)$$

OK,
except for the fact that F_x is *horizontal*

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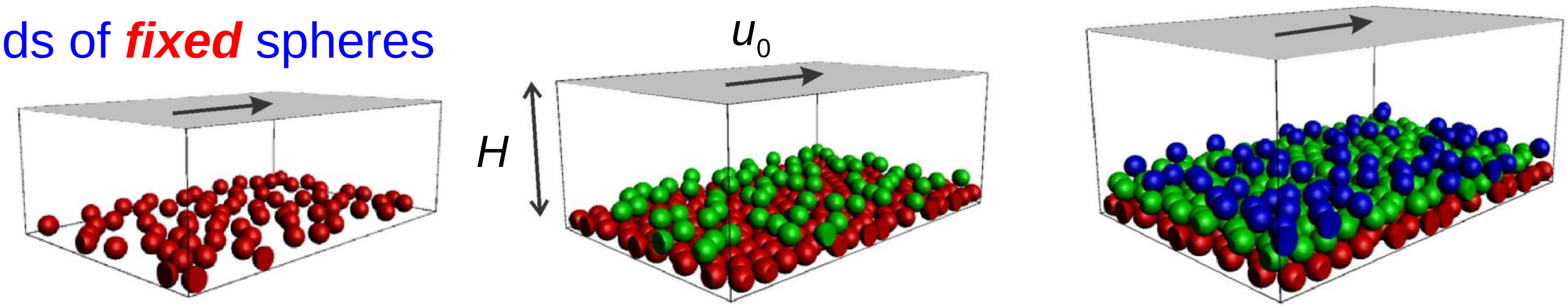
(*) O'Neill, *CES* **23** (1968) (**) Leighton & Acrivos, *ZAMP* **36** (1985)

A single-sphere may be too simple

*to understand the critical Shields number**

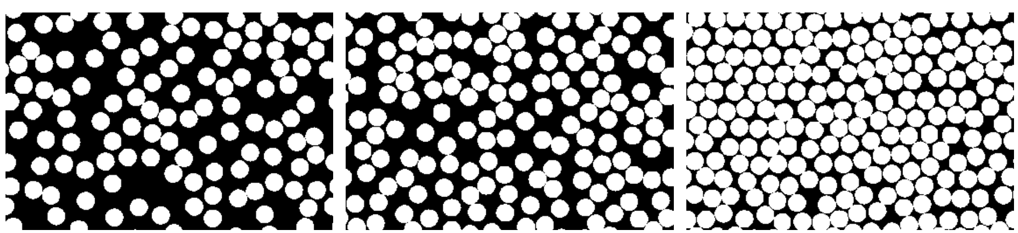
beds of ***fixed*** spheres



monolayers double layers triple layers

Surface occupancy σ monolayers

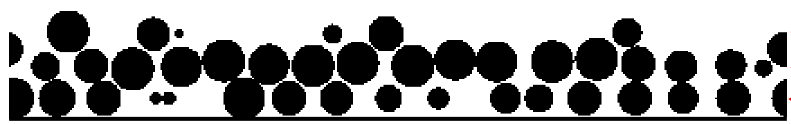
$\sigma = n\pi a^2 = 0.4$ 0.5 0.7



$$\mathrm{Re} = \frac{\dot{\gamma} a^2}{\nu}$$

$$\dot{\gamma} = \frac{u_0}{H}$$

cross section through typical triple layer bed



$\sigma_3 = 0.40$

$\sigma_2 = 0.70$

$\sigma_1 = 0.70$

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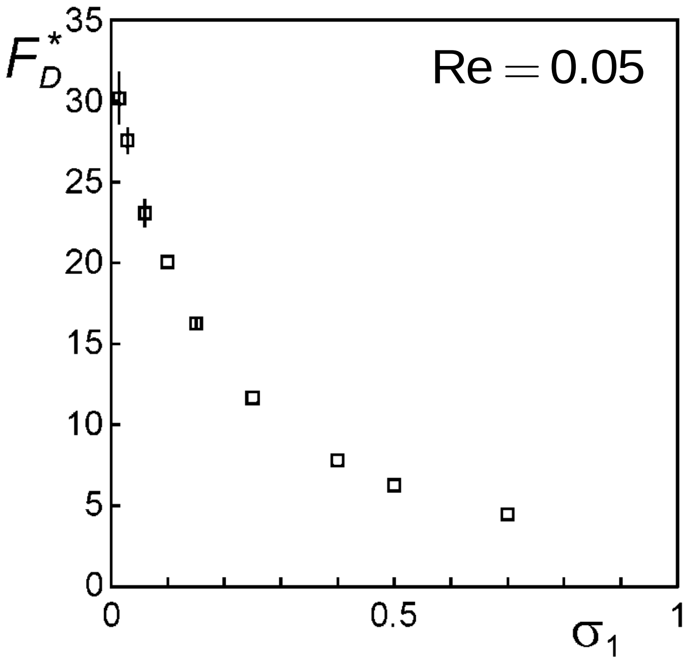
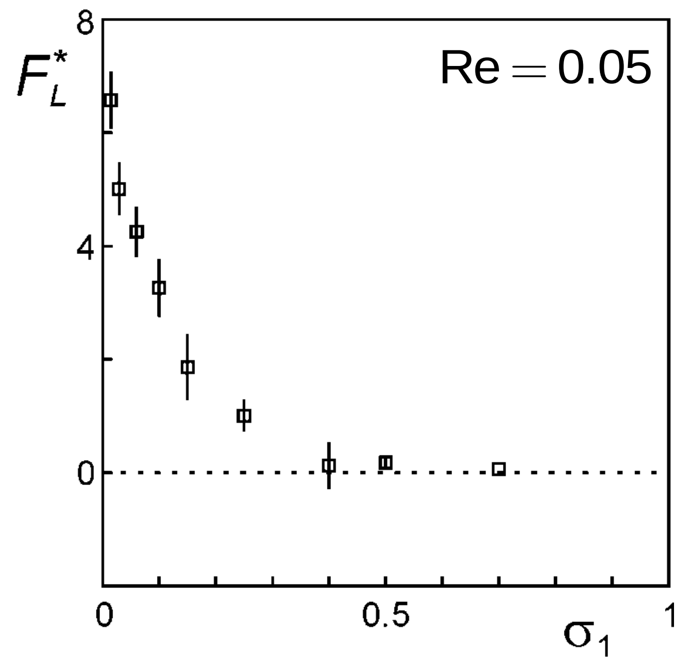
* Derksen & Larsen, *JFM* **673** (2011)

Average drag and lift - Monolayers





$$F_D^* \equiv \frac{F_D}{\rho \nu \dot{\gamma} a^2}$$

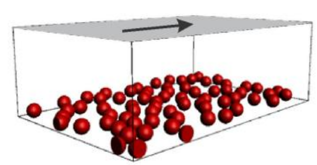
$$F_L^* \equiv \frac{F_L}{\rho \dot{\gamma}^2 a^4}$$

remember,
single sphere

$$F_D^* = 32.1$$

$$F_L^* = 9.22$$

color: velocity magnitude



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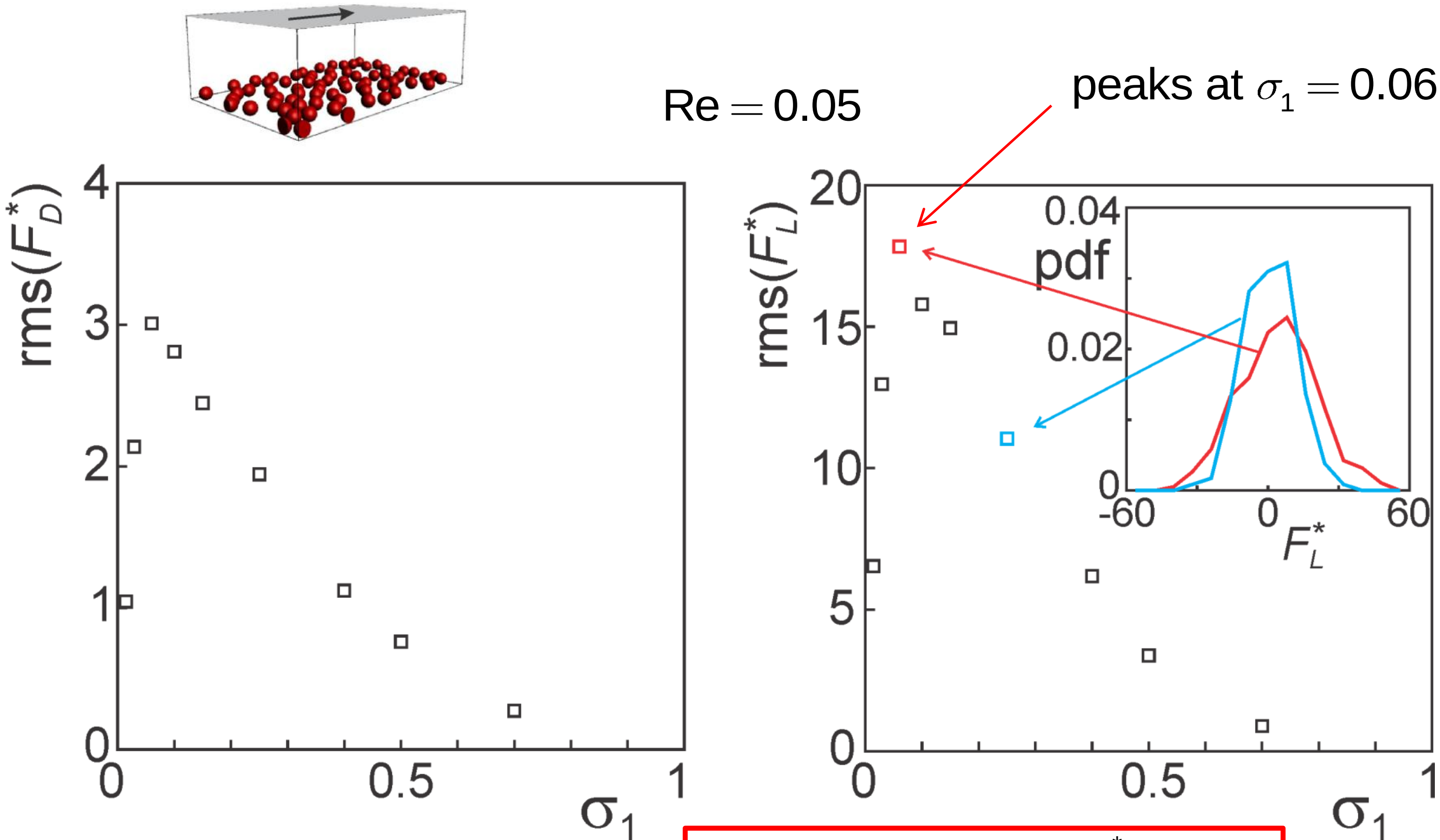
Sphere-to-sphere force variation - Mono



single sphere

$F_D^* = 32.1$

$F_L^* = 9.22$

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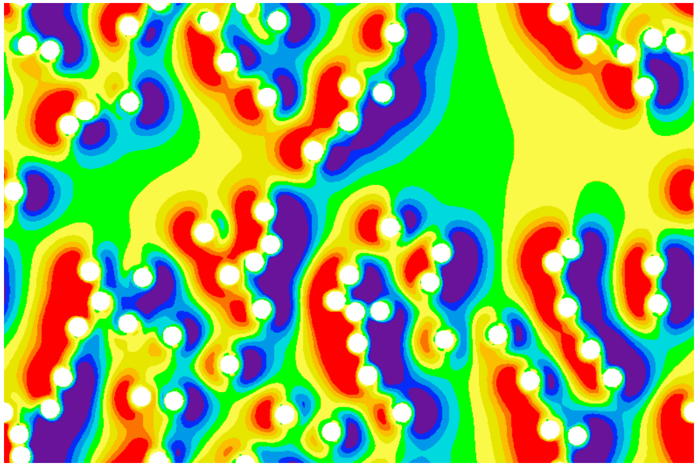
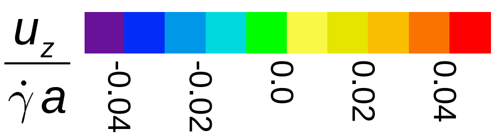
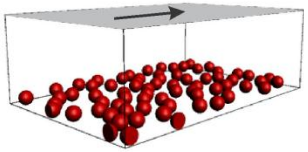
Lift turns into vertical viscous drag

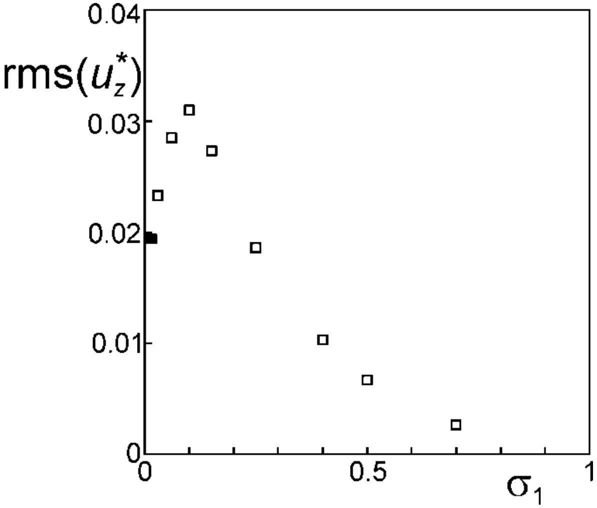
vertical velocity one radius (a) above the wall



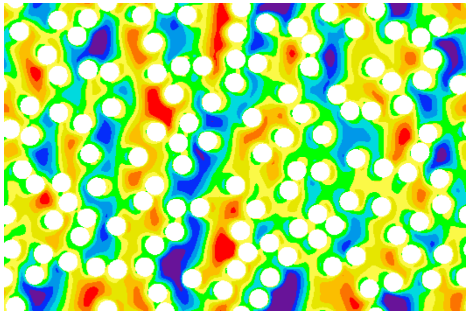
$\sigma_1 = 0.06$



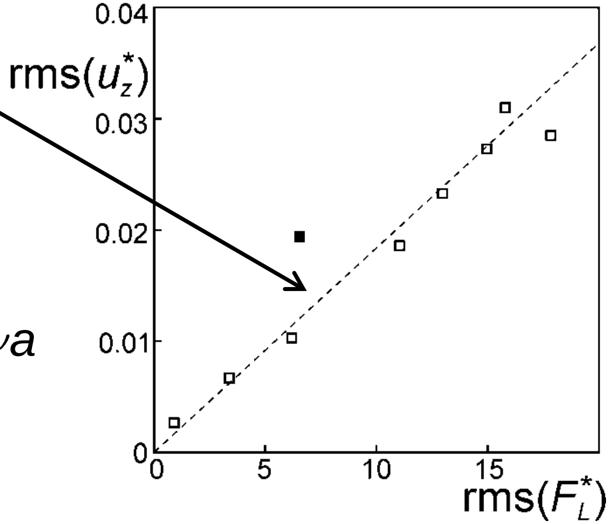




$\sigma_1 = 0.25$



linear trend



$$\text{rms } F_L^* = \beta \text{ rms } u_z^*$$

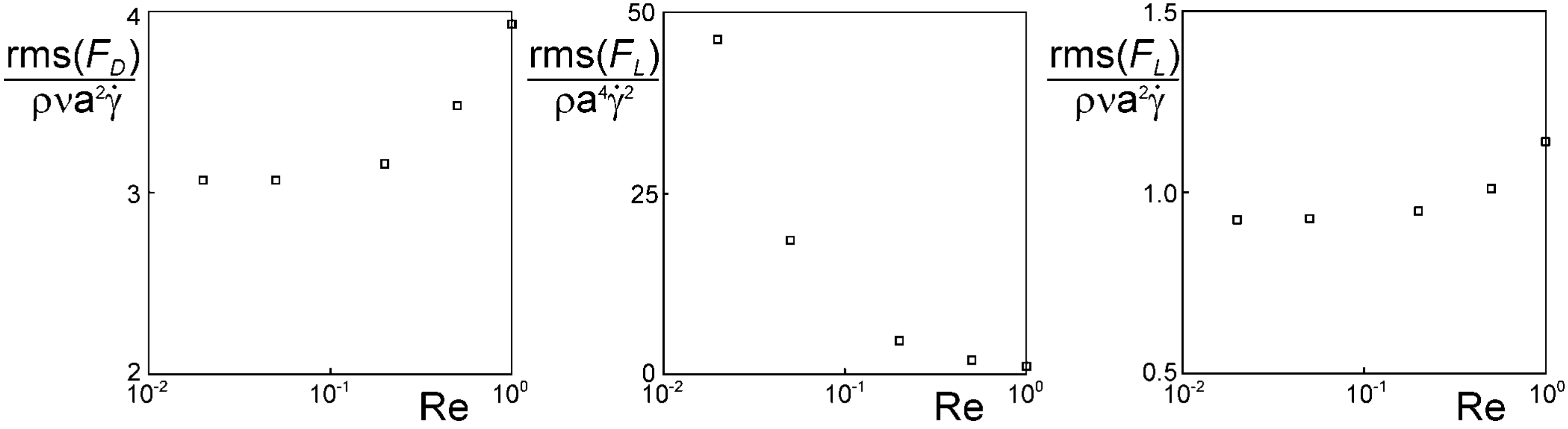
$$\beta \approx 550$$

$$\text{if rms } F_L = \text{rms } u_z \;\; 6\pi\rho\nu a$$

$$\text{then } \beta = \frac{6\pi}{\text{Re}} \approx 380$$

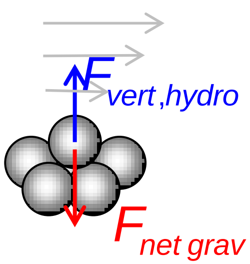
Lift as vertical viscous drag - Monolayers

rms-drag, viscous scaling | rms-lift, inertial scaling | rms-lift, viscous scaling



for the critical Shields number to be independent of Re we needed a vertical force that scales like

$$\rightarrow F_{vert,hydro} \propto a^2 \rho \nu \dot{\gamma}$$

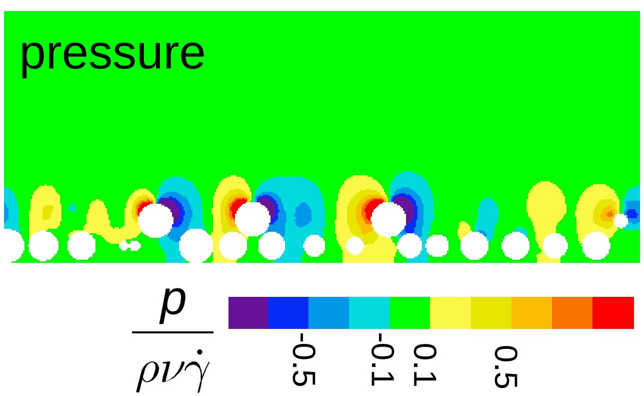


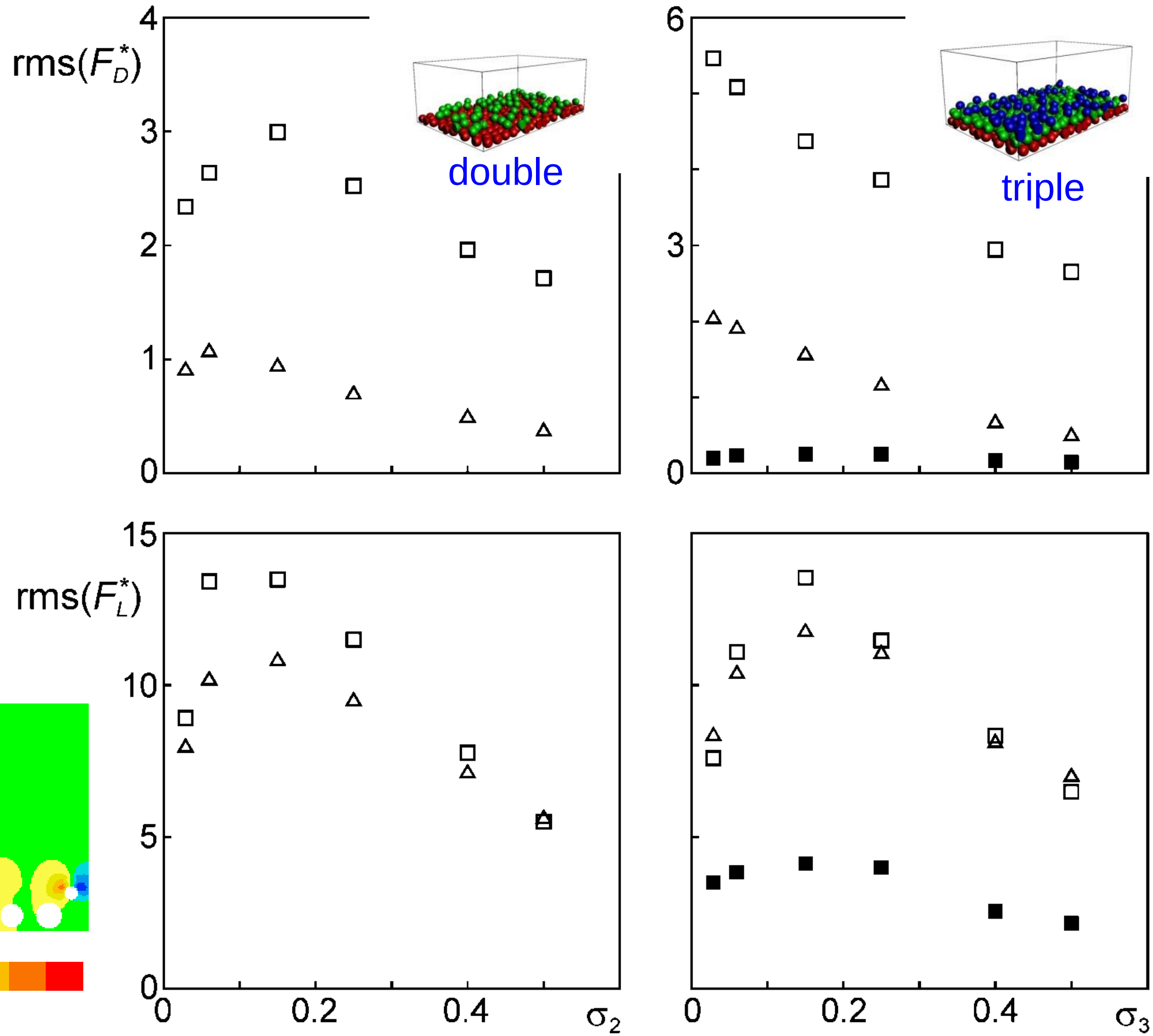
here you have it in terms of an rms vertical *force level*

RMS of drag and lift forces

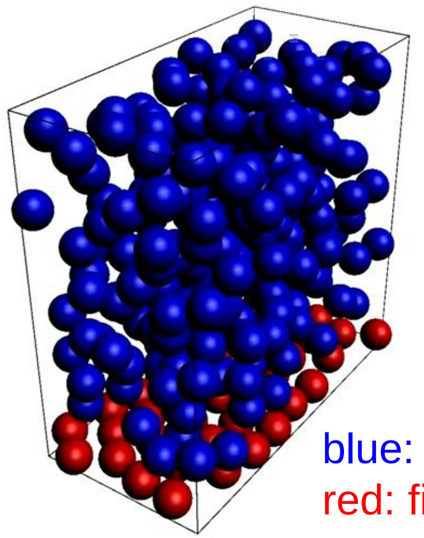
double & triple layers

as a function of σ of the top layer





Let’s try moving spheres



blue: mobile
red: fixed

initialization: create a granular bed of equally sized spheres

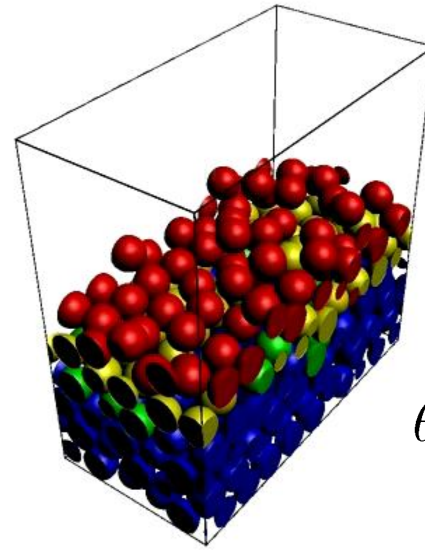
add liquid and then shear the liquid above the bed

● $\frac{u_p}{a\dot{\gamma}} > 0.1$

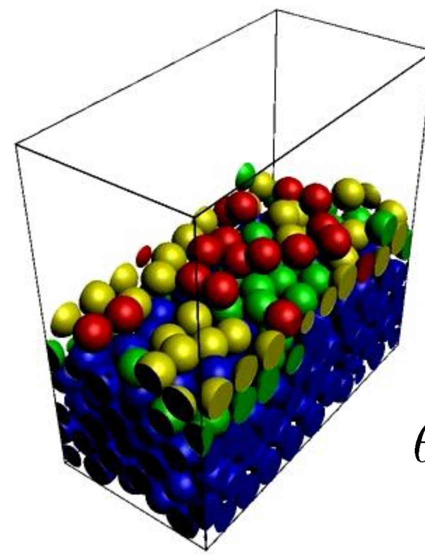
● $0.1 \geq \frac{u_p}{a\dot{\gamma}} > 0.05$

● $0.05 \geq \frac{u_p}{a\dot{\gamma}} > 0.025$

● $0.025 \geq \frac{u_p}{a\dot{\gamma}}$



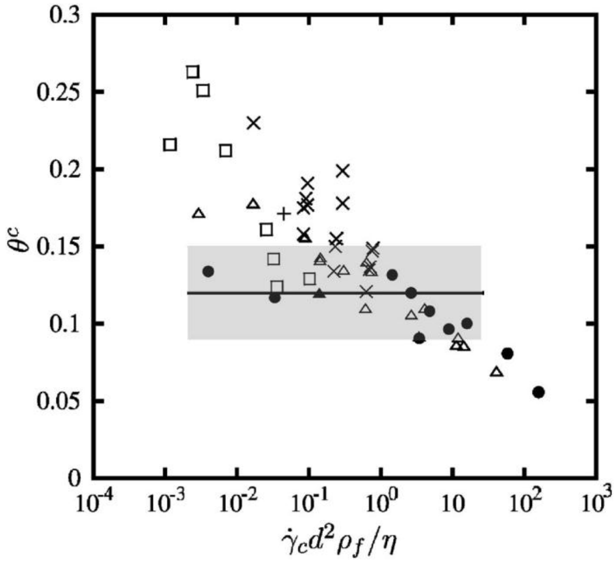
$\theta = 0.80$



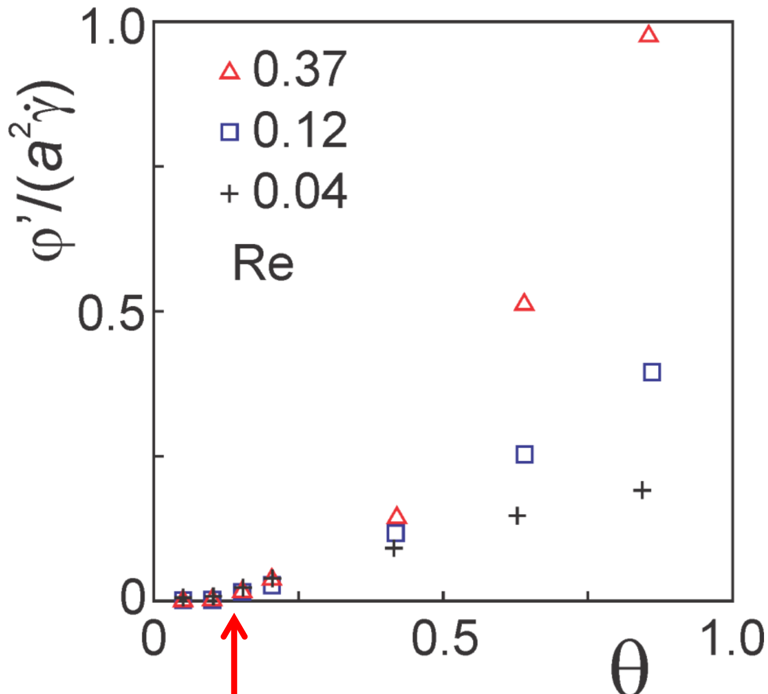
$\theta = 0.40$

the Shields number $$\theta = \frac{\rho \nu \dot{\gamma}}{g \;\; \rho_p - \rho \;\; 2a}$$

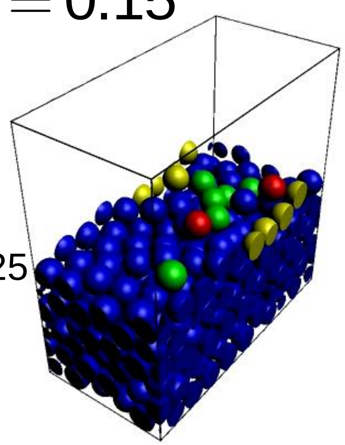
Critical Shields number?



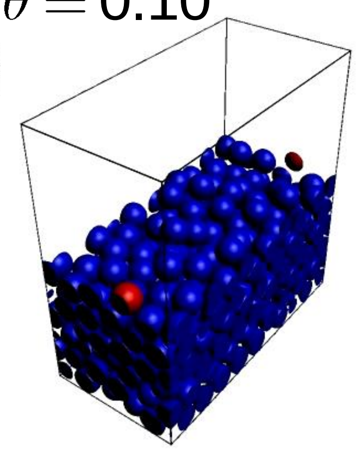
average solids flux per unit width



$\theta = 0.15$



$\theta = 0.10$



● $\frac{u_p}{a\dot\gamma} > 0.1$

● $0.1 \geq \frac{u_p}{a\dot\gamma} > 0.05$

● $0.05 \geq \frac{u_p}{a\dot\gamma} > 0.025$

● $0.025 \geq \frac{u_p}{a\dot\gamma}$

lo and behold: $0.1 < \theta^c < 0.15$

critical features: lubrication forces & friction coefficient in p-p collisions

Sample applications

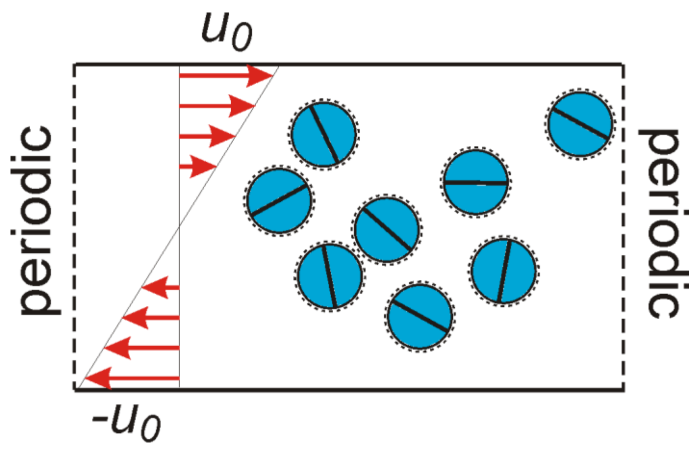
what to learn from meso-scale simulations?

erosion & sedimentation

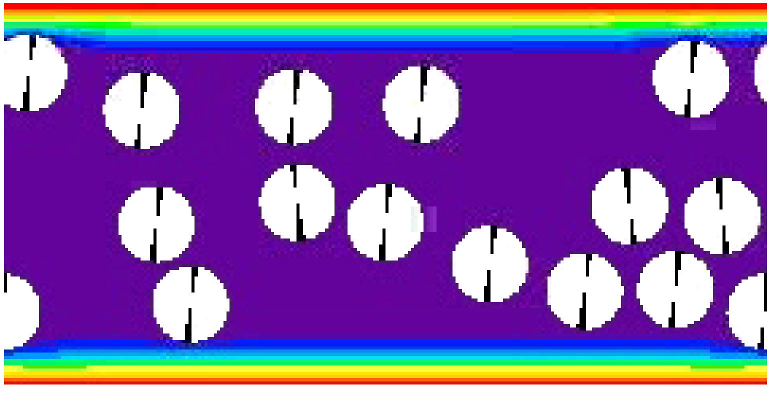
aggregation / flocculation ←

Aggregation at the meso-scale

a little bit of recent work

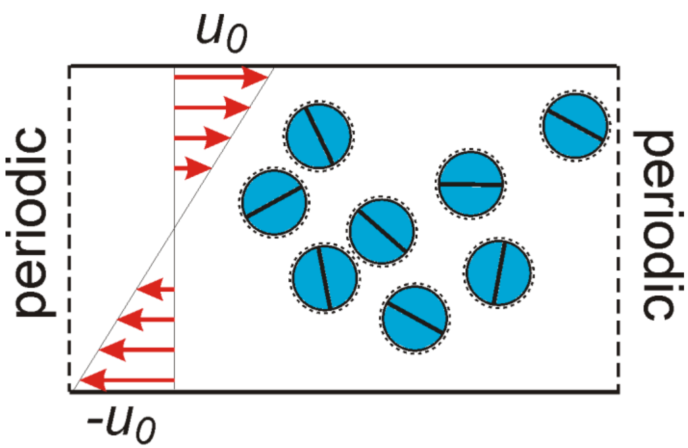


sticky particles in shear flow



A closer look at aggregation

at the meso-scale



attractive interaction between particles defined by a

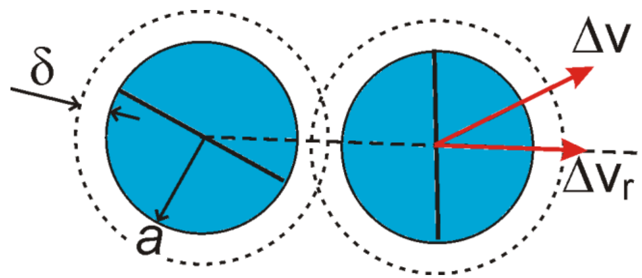
square-well-potential

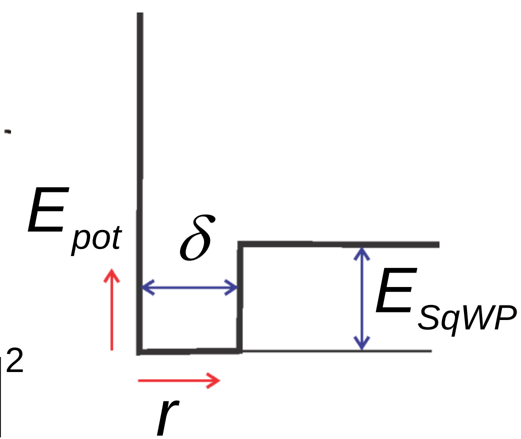
two parameters: δ and Δv_c

if $\Delta v_r < \Delta v_c$ particles stick

dimensionless numbers

$$\frac{\Delta v_c}{a\dot{\gamma}} \qquad \frac{\delta}{a}$$





in energy terms: $$E_{SqWP} = \frac{1}{2} m_p \left[\Delta v_c\right]^2$$

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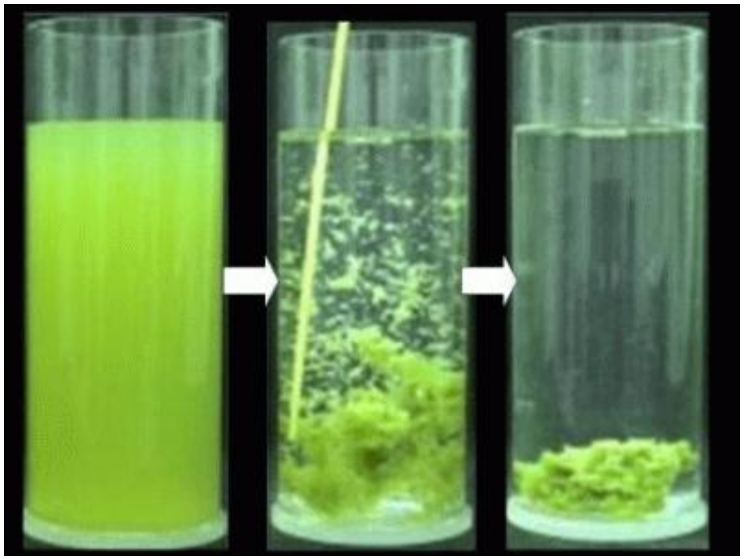
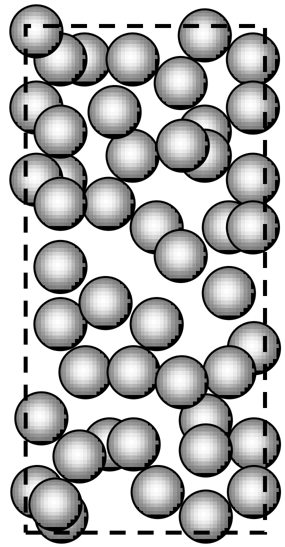
Flocculation

aggregation enhanced settling



Flocculation, Global Poly-Glu Co., Ltd ©

computational approach



solid, sticky spheres in a 3D periodic domain

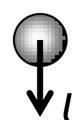
$$\downarrow \mathbf{f}_{\mathbf{p}} = -\left(\rho_p - \rho_m\right) g\mathbf{e}_{\mathbf{z}}$$

$$\uparrow \mathbf{f}_{\mathbf{f}} = \left(\rho_m - \rho\right) g\mathbf{e}_{\mathbf{z}}$$

$$\rho_m = \phi\rho_p + \left(1-\phi\right)\rho$$

the main dimensionless variables are

SqWP

ϕ (solids volume fraction)	$\mathrm{Re}_\infty \equiv \dfrac{2aU_\infty}{\nu}$  $\downarrow U_\infty$	$\dfrac{\Delta v_c}{U_\infty}$	$\dfrac{\delta}{a}$
0.12 – 0.32	6 – 72	0.005 – 0.03	0.025

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Computational flocculation

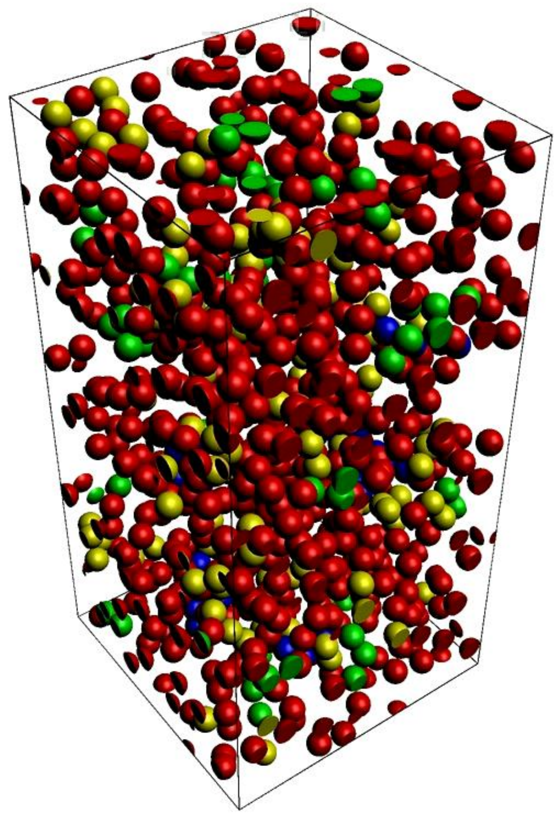
$\phi = 0.12$

$$\frac{\Delta v_c}{U_\infty} = 0.025$$

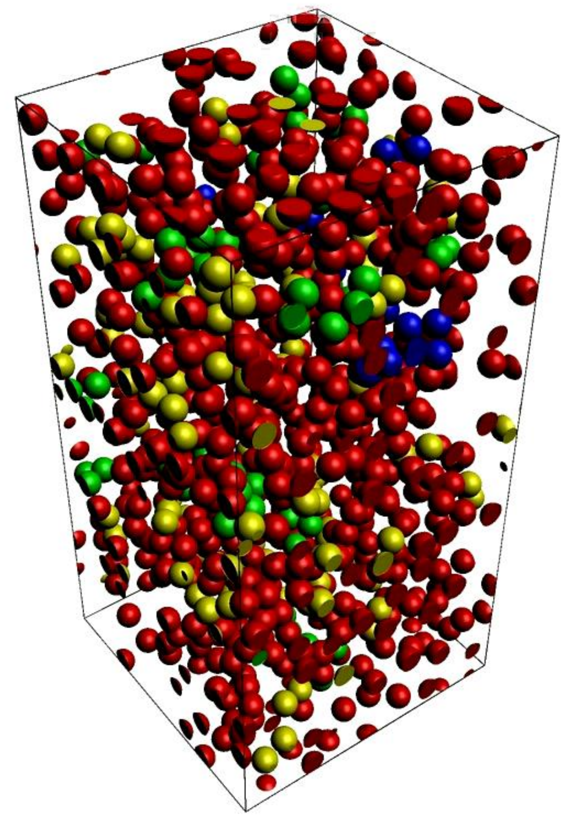
color: flock size

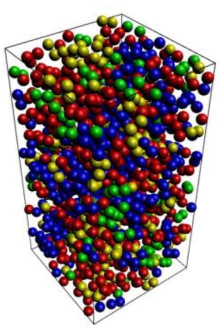
- $n_{agg} = 1$
- $n_{agg} = 2$
- $n_{agg} = 3$
- $n_{agg} \geq 4$

$Re_\infty = 24$



$Re_\infty = 6$





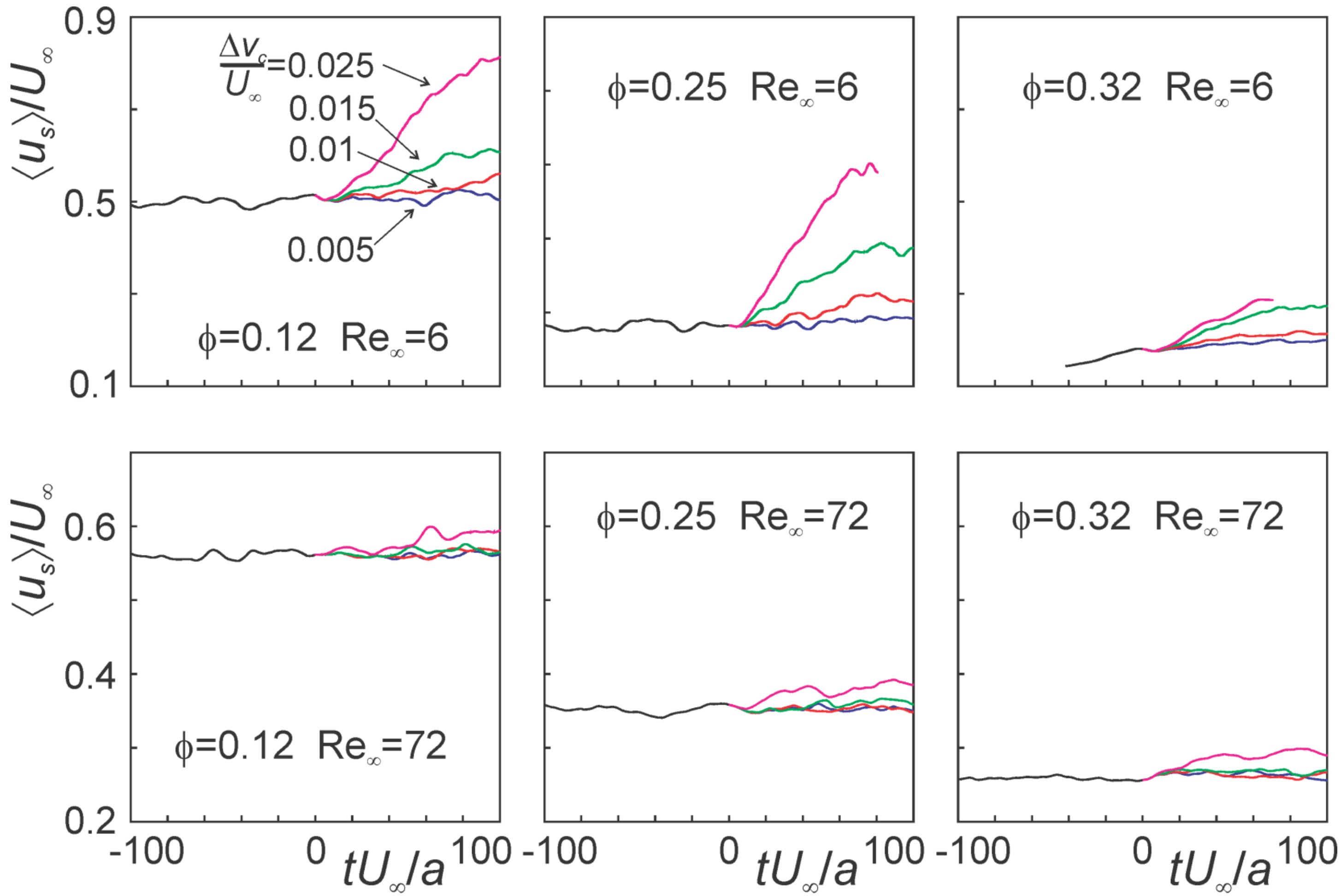
$\phi = 0.2$

for reference

Settling velocities

average settling velocity as a function of time

at t=0 we switch on the SqWP



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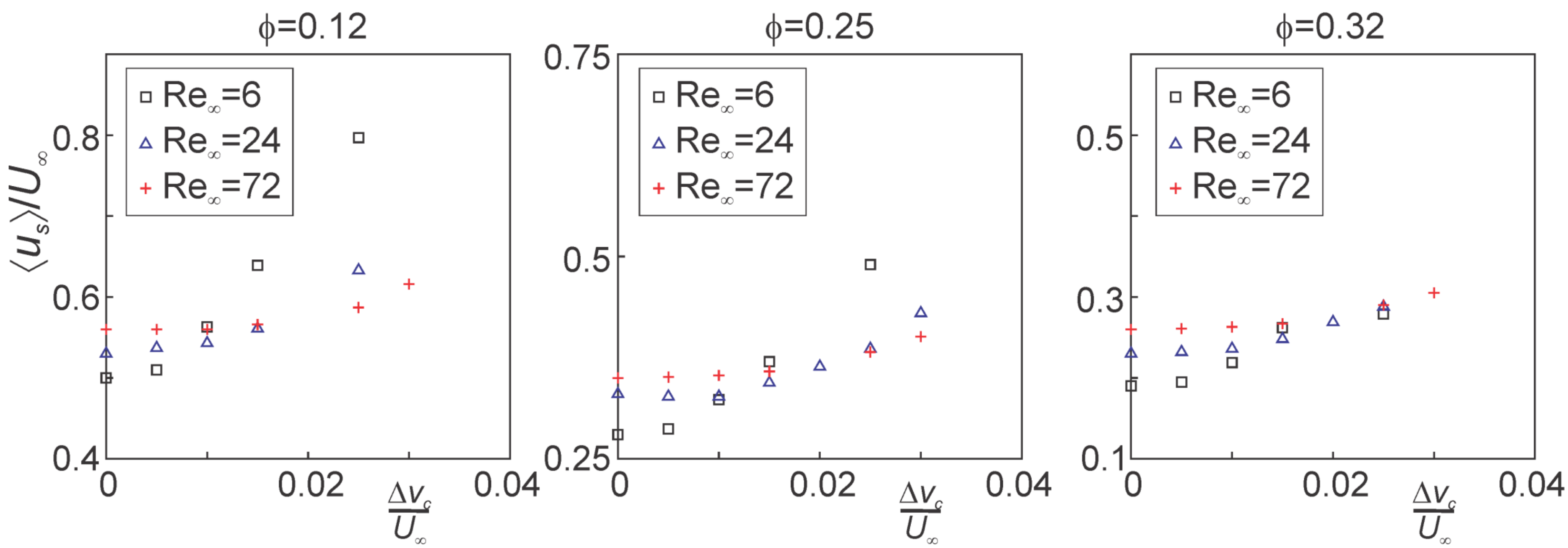
Average settling velocities

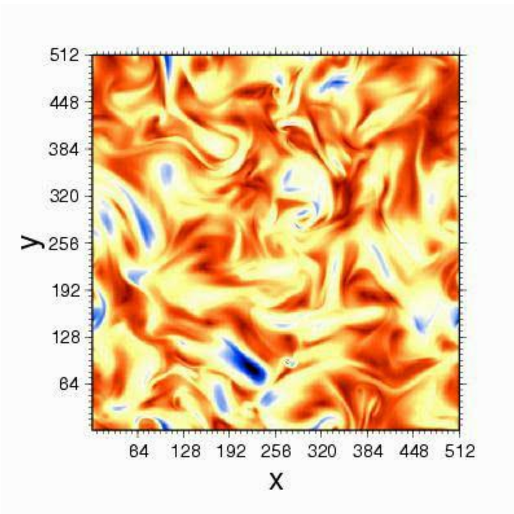
as a function of the strength of the SqWP



(more data points coming – simulations running as we speak)

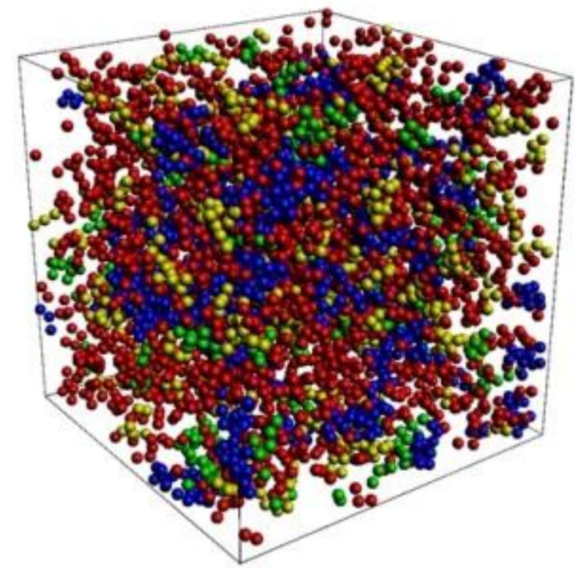
Sticky particles in turbulence

flocculation is now called aggregation



generate homogeneous isotropic turbulence in (again) a fully periodic, 3D domain – *through linear forcing**

& add solid, spherical sticky particles



key dimensionless variables

ϕ : solids volume fraction

$\frac{\eta_K}{a}$: Kolmogorov scale over sphere radius ~0.15 - atypical

$\frac{\Delta v_c}{\upsilon_K}$: SqWP depth over Kolmogorov velocity scale ~0.3

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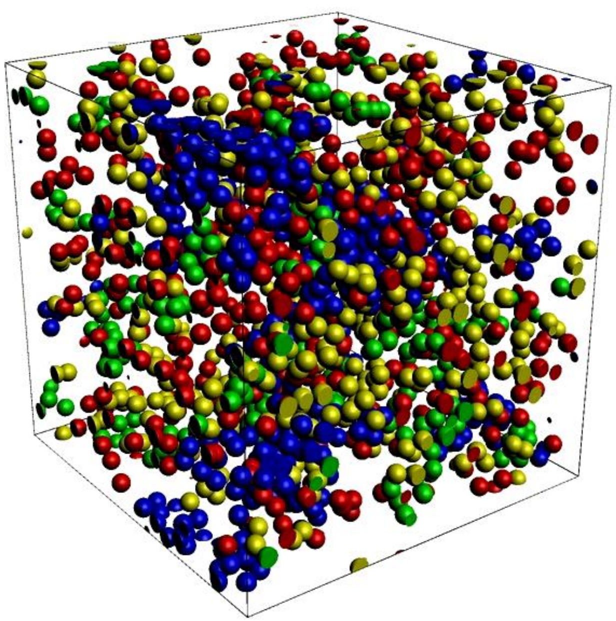
* Rosales & Meneveau, *PoF* **17** (2005)

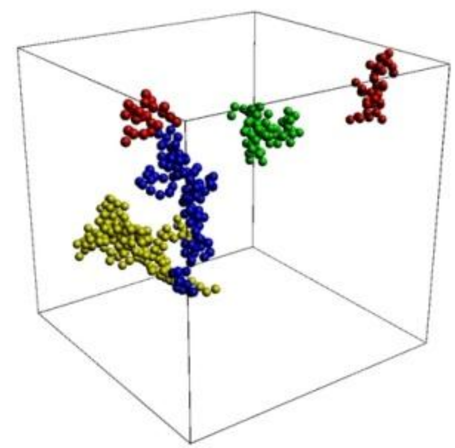
Aggregation in turbulence

$$\phi = 0.08 \quad \frac{\eta_K}{a} = 0.13 \quad \frac{\Delta v_c}{\upsilon_K} = 0.3$$



color: aggregate size

- primary sphere
- $2 \le n_{agg} < 5$
- $5 \le n_{agg} < 8$
- $n_{agg} \ge 8$

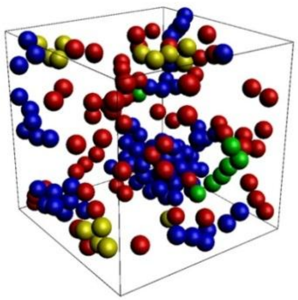


the 4 largest aggregates at some moment

Domain size quickly becomes an issue

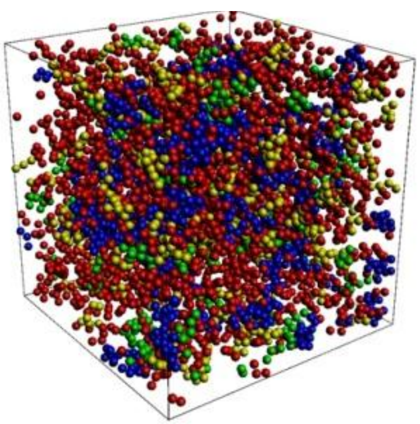
- for representative aggregate size distributions
- to create well-developed turbulence

$(20a)^3$



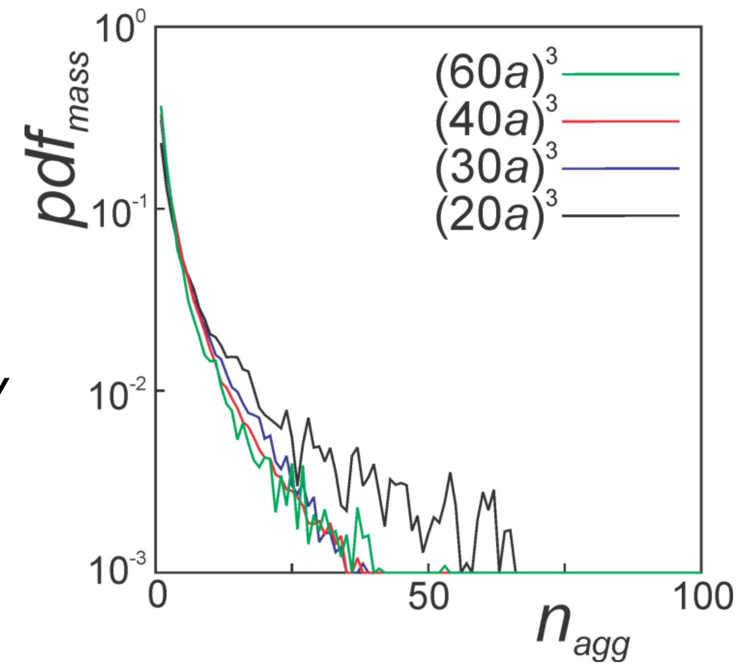
too small

$(60a)^3$



gets computationally challenging

aggregate size distributions

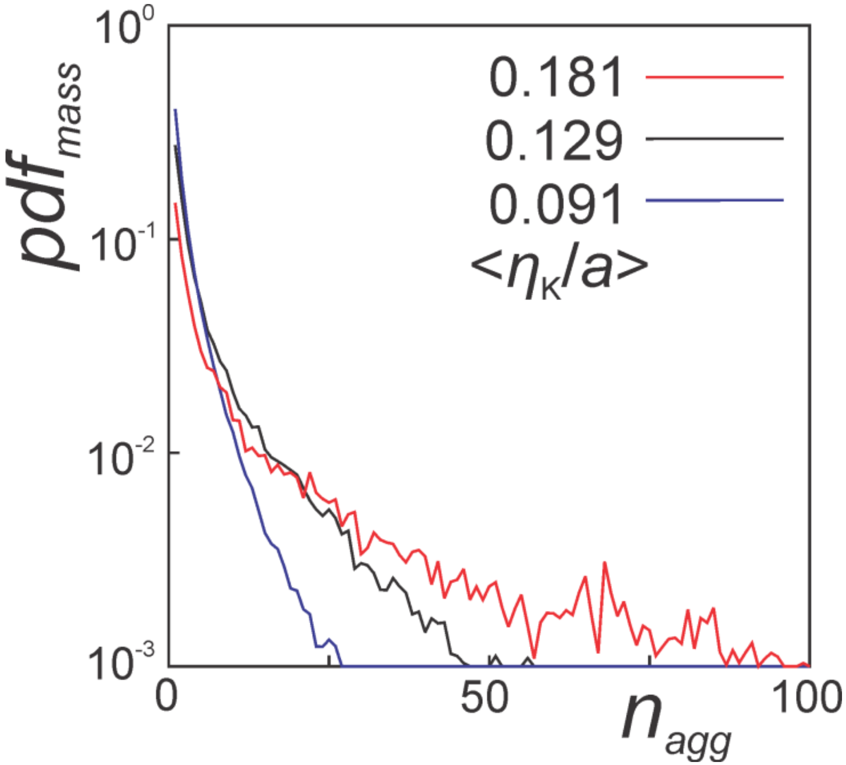


Some preliminary results

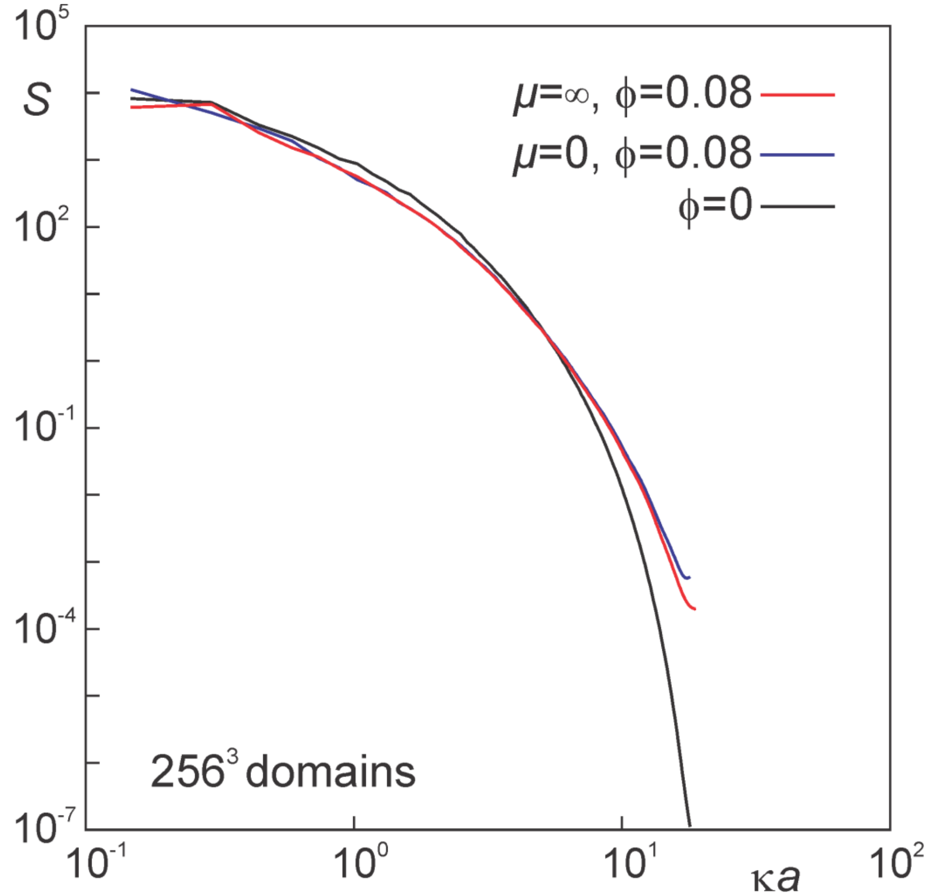
aggregate size distributions

effect of η_K

(the smaller η_K, the more power input)



turbulence modulation by the solids



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Summary & Perspective

- Dense SL systems, lots of SL interactions
- Computational approach
  - *minimal modeling*
  - *small (meso-scale) systems*
- Erosion & sedimentation
  - *lift & drag $\leftrightarrow$ critical Shields number*
- Aggregation / flocculation
  - *effect of flocculants depends on Reynolds number*

Perspective

More complexity

non-spherical particles

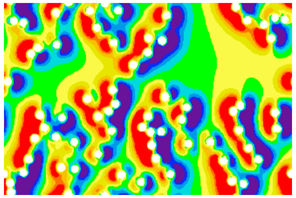
soft (deformable) particles

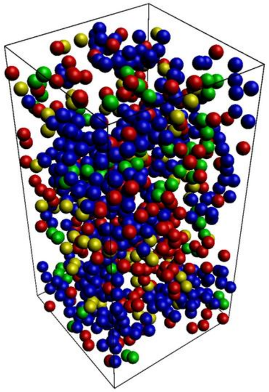
Erosion

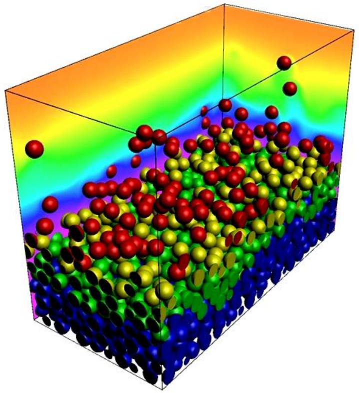
*towards turbulence**

Aggregation

what happens if $\dfrac{\eta_K}{a} \leq 1-$*ish*



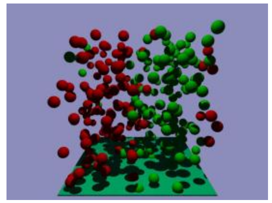




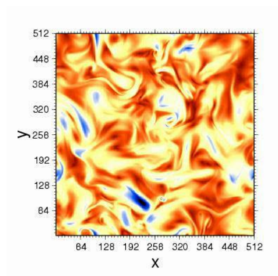
Acknowledgements

(former) students

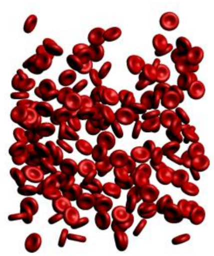
Andreas ten Cate



Eelco van Vliet



Orest Shardt



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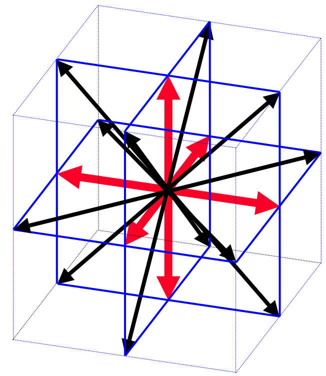
Lattice-Boltzmann method

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

$$f_i(\mathbf{x}+\mathbf{e}_i, t+1) = f_i(\mathbf{x}, t) + \Omega_i(f(\mathbf{x}, t))$$

$$\rho = \sum_i f_i \qquad \rho\mathbf{u} = \sum_i f_i \mathbf{e}_i$$



Space, time, *and velocity* are discretized:

local operations: good parallel efficiency

uniform, cubic lattice

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

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

velocity/ physical time-step constraint

this is incompressible Navier-Stokes if $\left|\mathbf{u}^2\right| << c_{sound}{}^2$

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

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