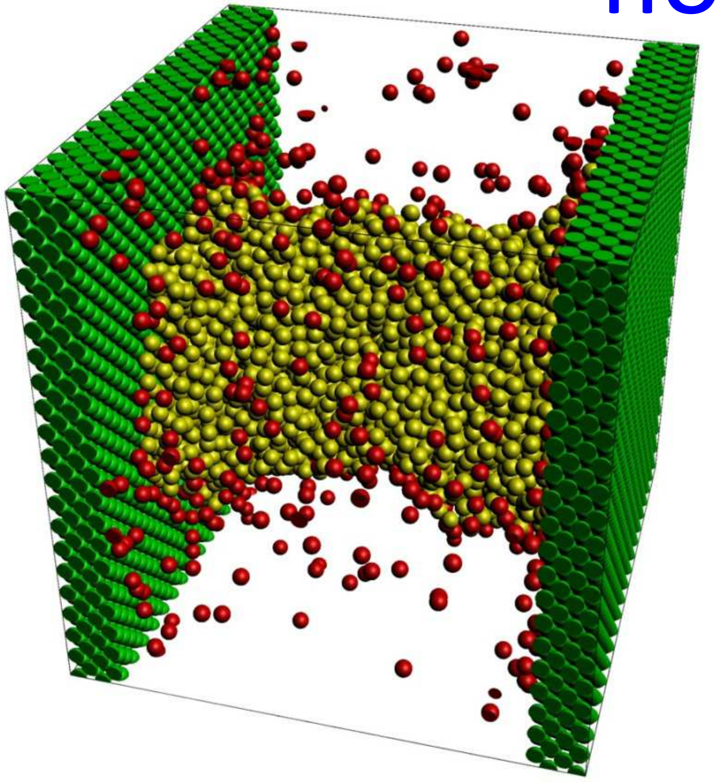
Simulations of dispersed multiphase flow at the particle level



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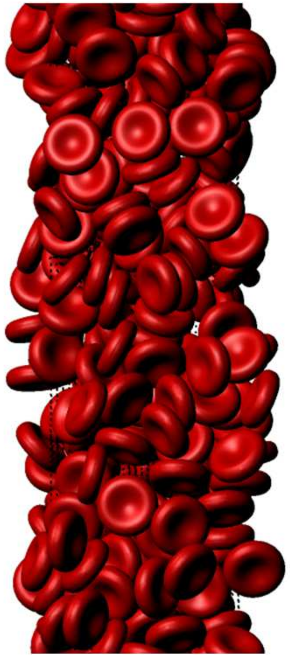
http://homepage.tudelft.nl/s0j2f/

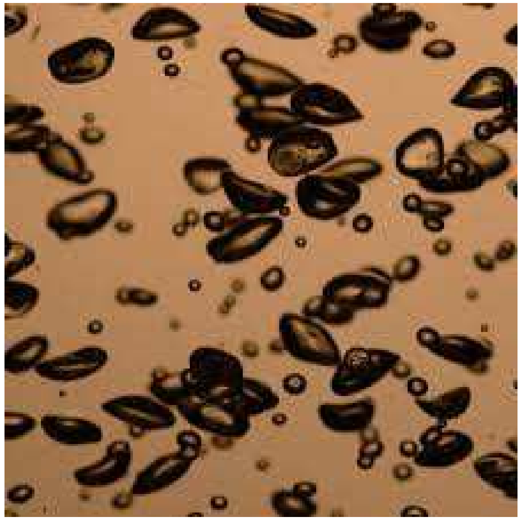
Multiphase flow

collective behavior ↔ particle-scale processes

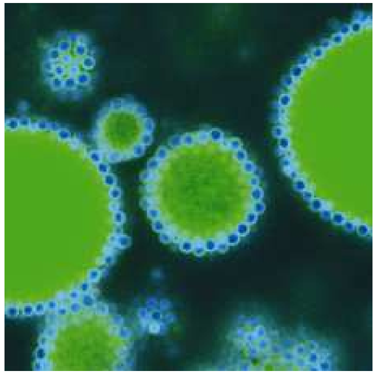


blood

sediment transport



bubbly flow



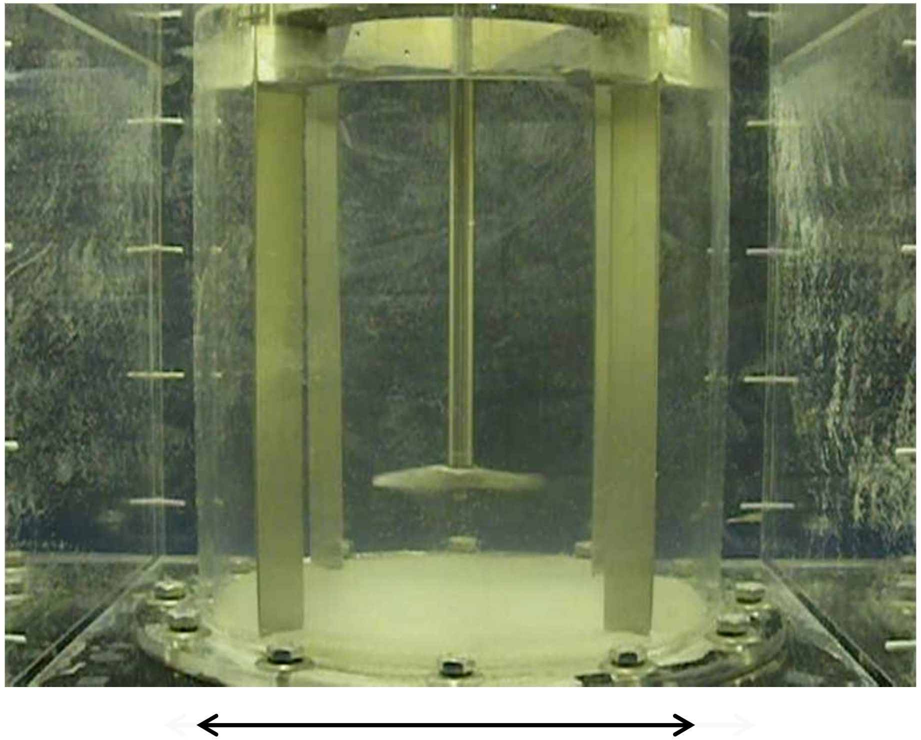
(Pickering) emulsion

predictive modeling & simulation

- flow dynamics
- mass transfer & mixing
- interface dynamics

@ the particle scale ("*meso-scale*")

Macroscopic multiphase transport



~ 30 cm

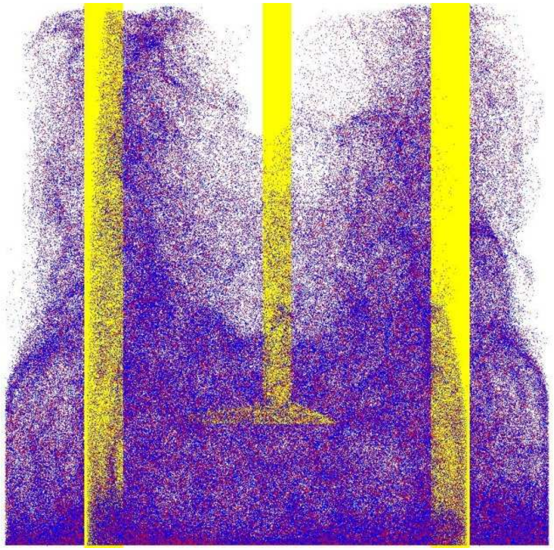
$$\mathrm{Re} = \frac{ND^2}{\nu} \approx 10^5$$

turbulent flow

"inertial" particles

wide spectrum of (length) scales

particle size, tank size,
turbulence scales

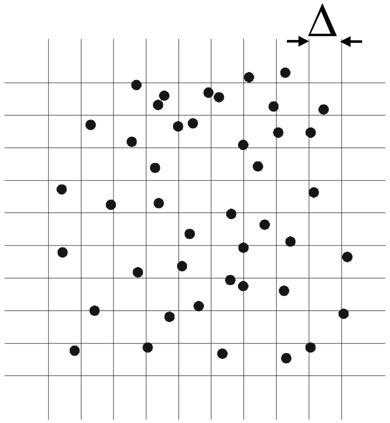


$n_p \approx 10^6$

Ayranci et al *CES* 2012

Unresolved vs resolved particles

$$2a = d_p < \Delta$$

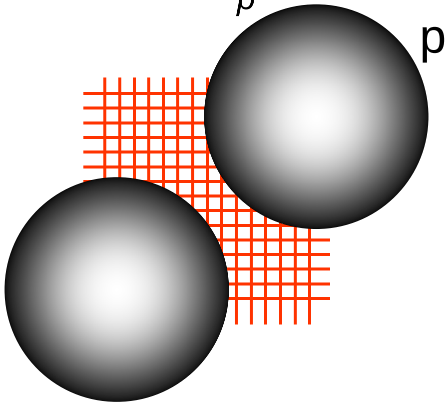


particle size < fluid grid spacing

particle dynamics based on empirical force correlations

up to **10^8** particles

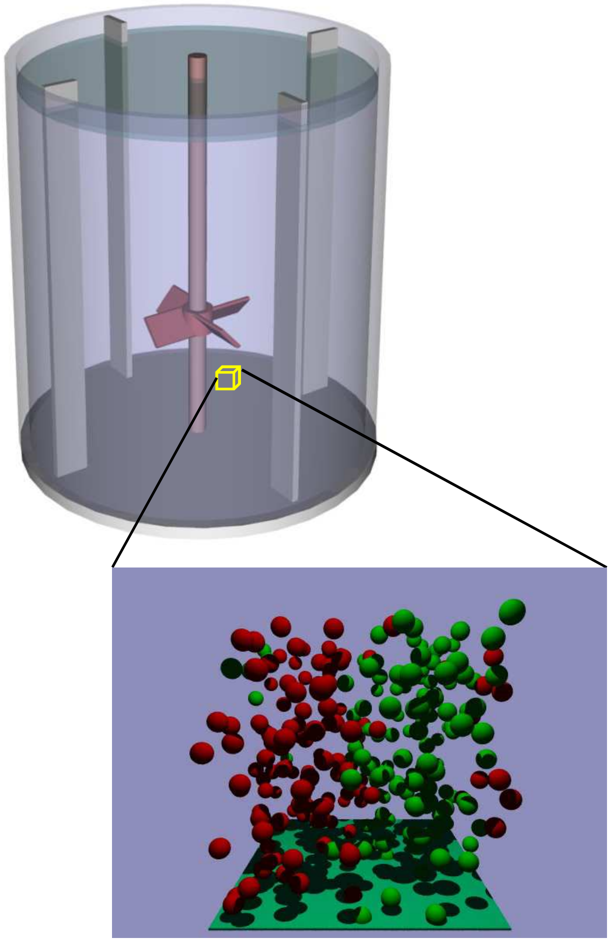
$$2a = d_p > \Delta$$



particle size > grid spacing

no need for empiricism*

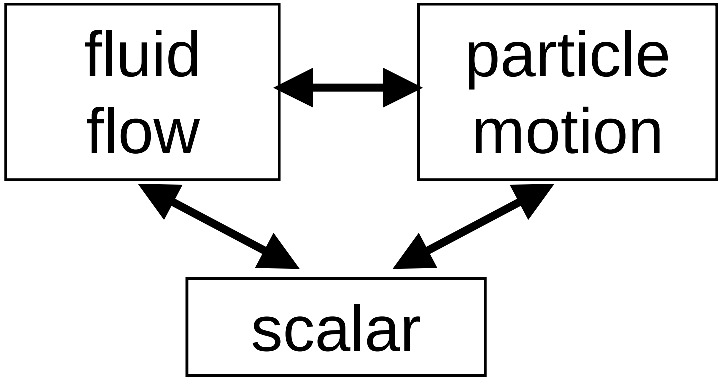
up to **10^4** particles

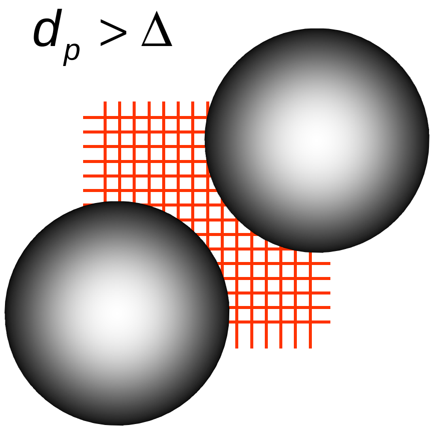


“multi-scale”

*fine print

Quick overview of numerics*





Lattice-Boltzmann method for solving the flow of interstitial fluid

- 3D, time-dependent

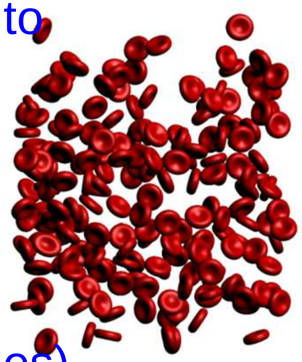
Explicitly resolve the solid-liquid interface: ***immersed boundary method***

- particle size typically 12 grid-spacings

Solve equations of linear and rotational motion for each sphere

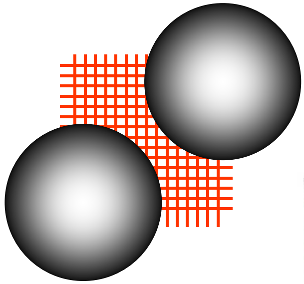
- forces & torques:
  - directly (and fully) coupled to hydrodynamics
  - plus gravity

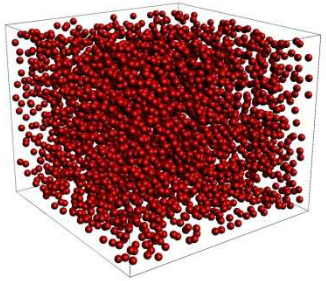
- hard-sphere collisions or soft interactions (mostly for non-spherical particles)



*Derksen & Sundaresan, *JFM* **587** (2007)

A miniature mixing tank

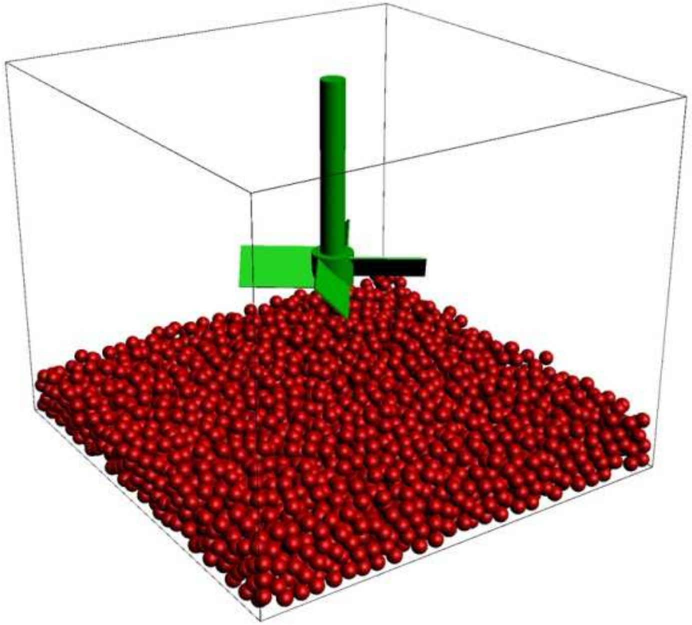




$$\mathrm{Re} = \frac{ND^2}{\nu} \approx 2{,}000$$

$\phi \approx$ 0.08 (3,600 spheres)

$\frac{\rho_p}{\rho} = 2.5$ (glass beads in water)



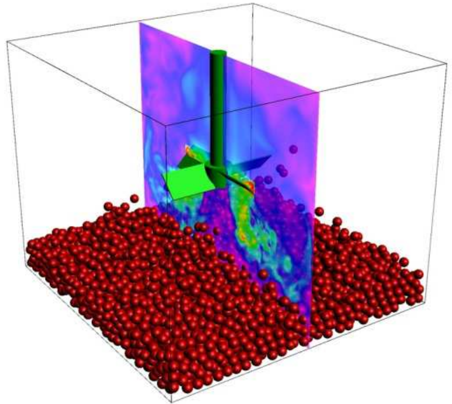
initial state
zero velocity for solid & liquid
all particles on the bottom

$$\theta = \frac{\rho N^2 D^2}{g\left(\rho_p - \rho\right) 2a} = 6 \ldots 96$$

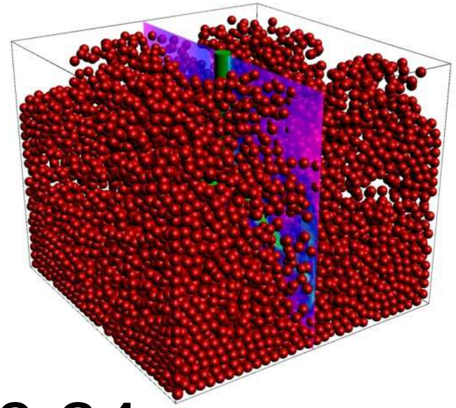
a modified Shields number

Derksen *AIChEJ* 2012

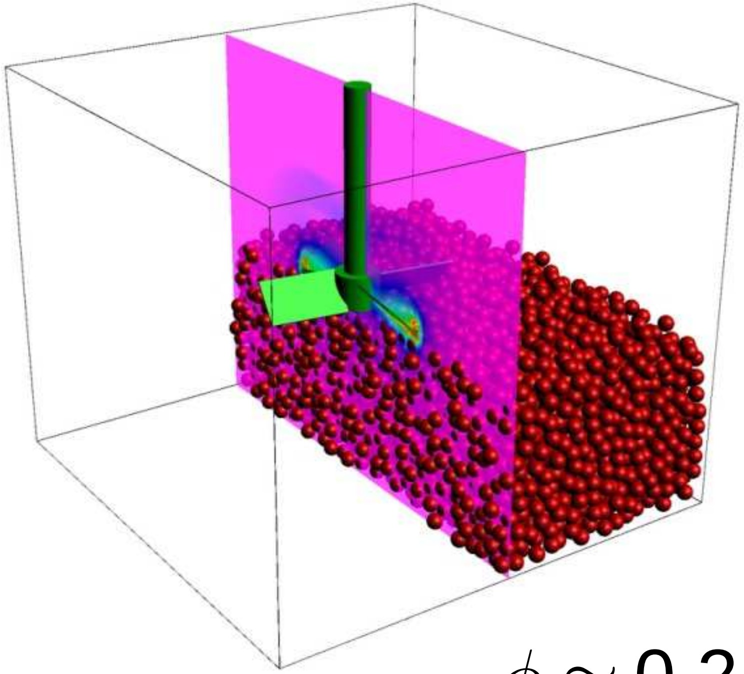
Start-up of suspension process



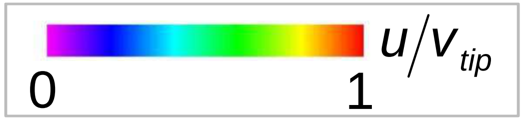
$\phi \approx 0.08$



$\phi \approx 0.24$

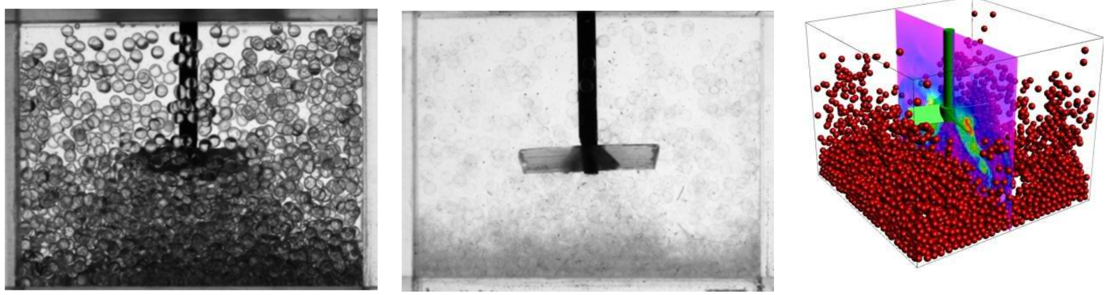


$\phi \approx 0.24$



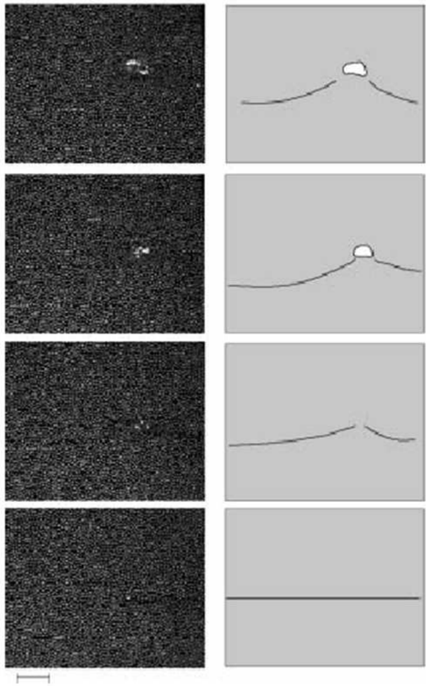
Experimental validation

@ Institut de Mécanique des Fluides de Toulouse

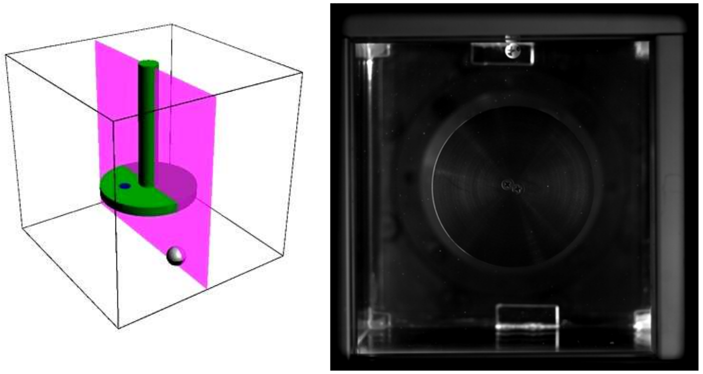


refractive index matching for optical access

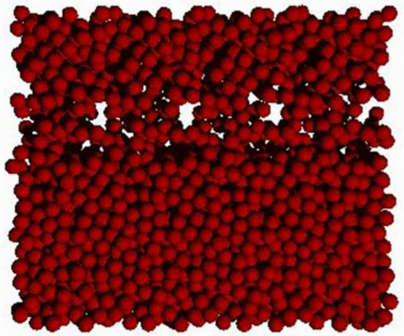
a liquid fluidization experiment..*



@ Beijing University of Chemical Technology†



*..& our simulation***



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†Mo et al *AIChEJ* 2015

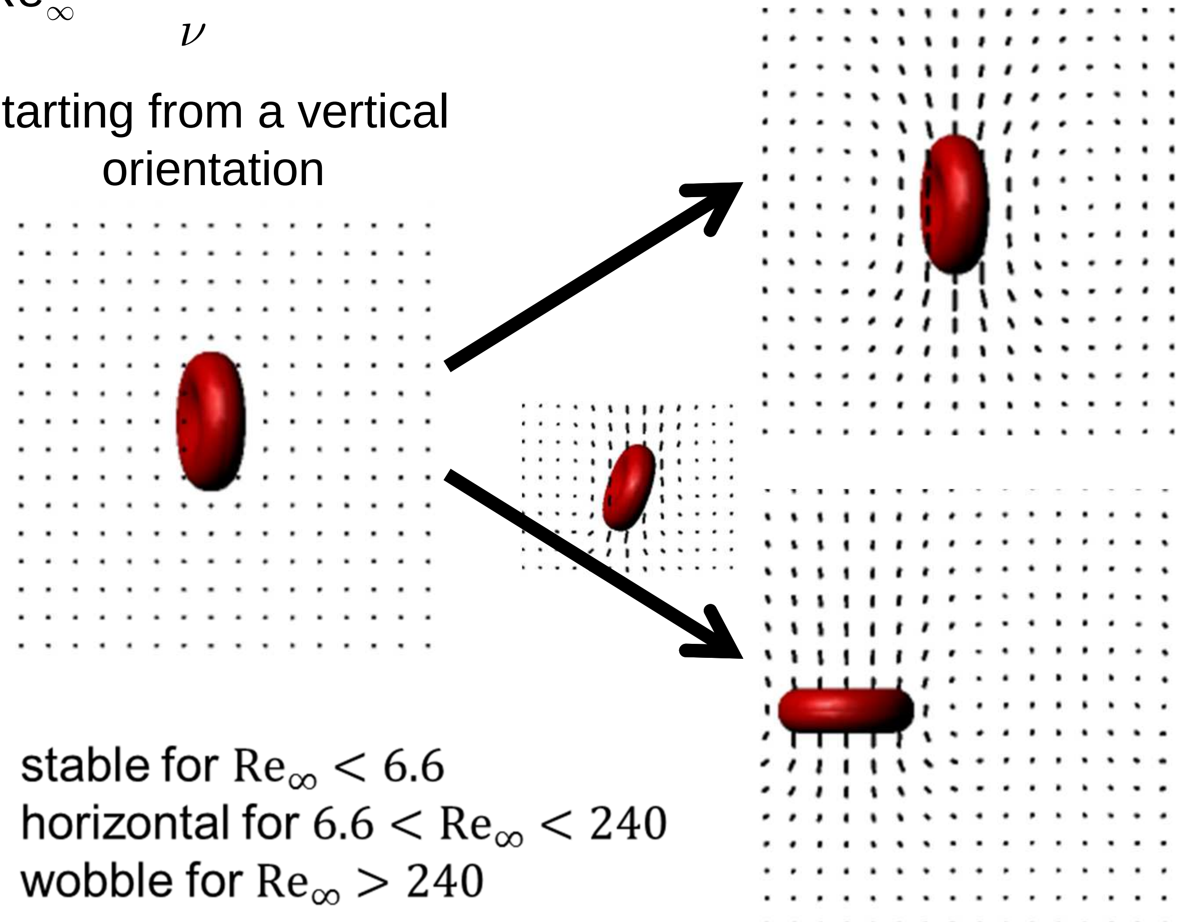
*Duru, Guazelli *JFM* 2002
**Derksen, Sundaresan *JFM* 2007

More experimental validation

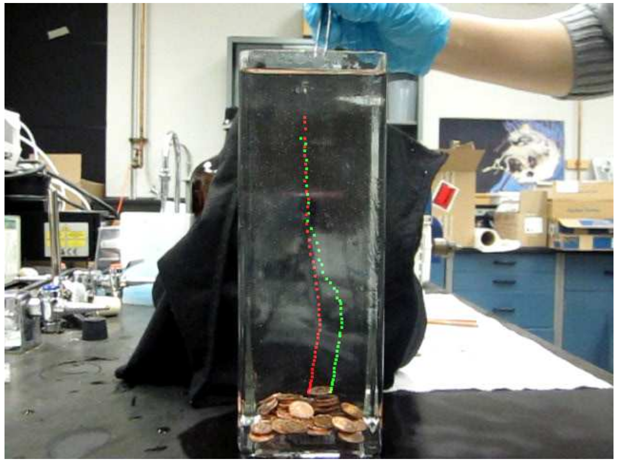
very simple experiments

$$\mathrm{Re}_\infty = \frac{u_\infty D}{\nu}$$

starting from a vertical orientation



remains vertical for $\mathrm{Re}_\infty = 1.2$



a High School experiment

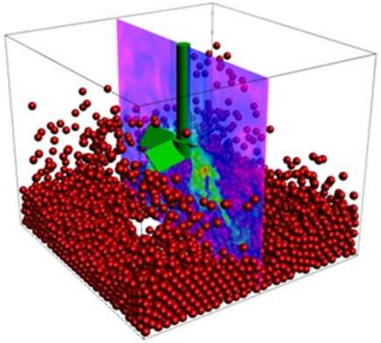
flips to horizontal for $\mathrm{Re}_\infty = 7.3$

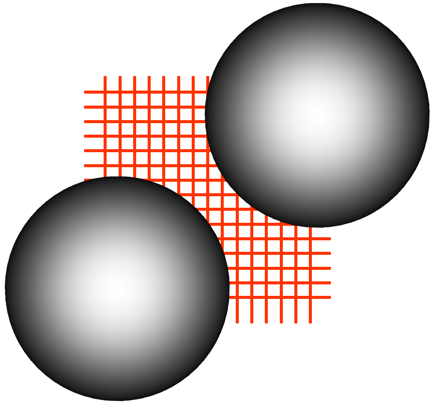
- stable for $\mathrm{Re}_\infty < 6.6$
- horizontal for $6.6 < \mathrm{Re}_\infty < 240$
- wobble for $\mathrm{Re}_\infty > 240$

Becker *Can. J. Chem. Eng* 1959

Mass transfer

- start with zero concentration in the liquid
- apply a c=1 boundary condition at the particle surface
- solve a convection-diffusion equation in c

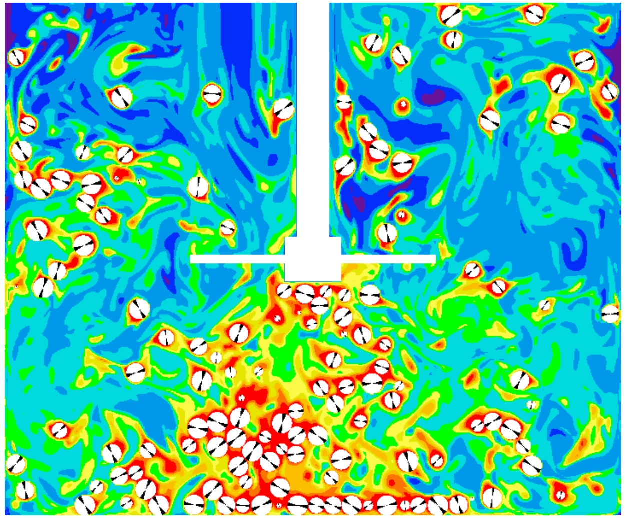




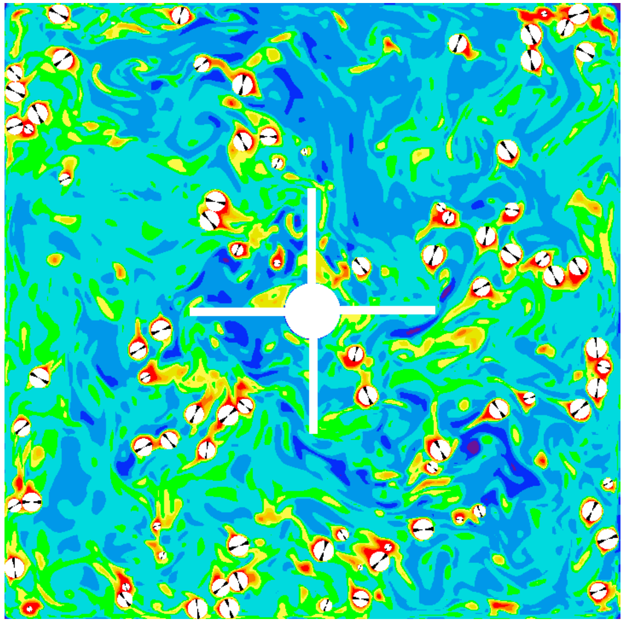
hydrodynamic resolution
$2a = d_p = 16\Delta$

Liquid systems: resolution is a **serious** concern given high Schmidt numbers

$$\mathrm{Sc} \equiv \frac{\nu}{\Gamma} = O\left(10^3\right)$$

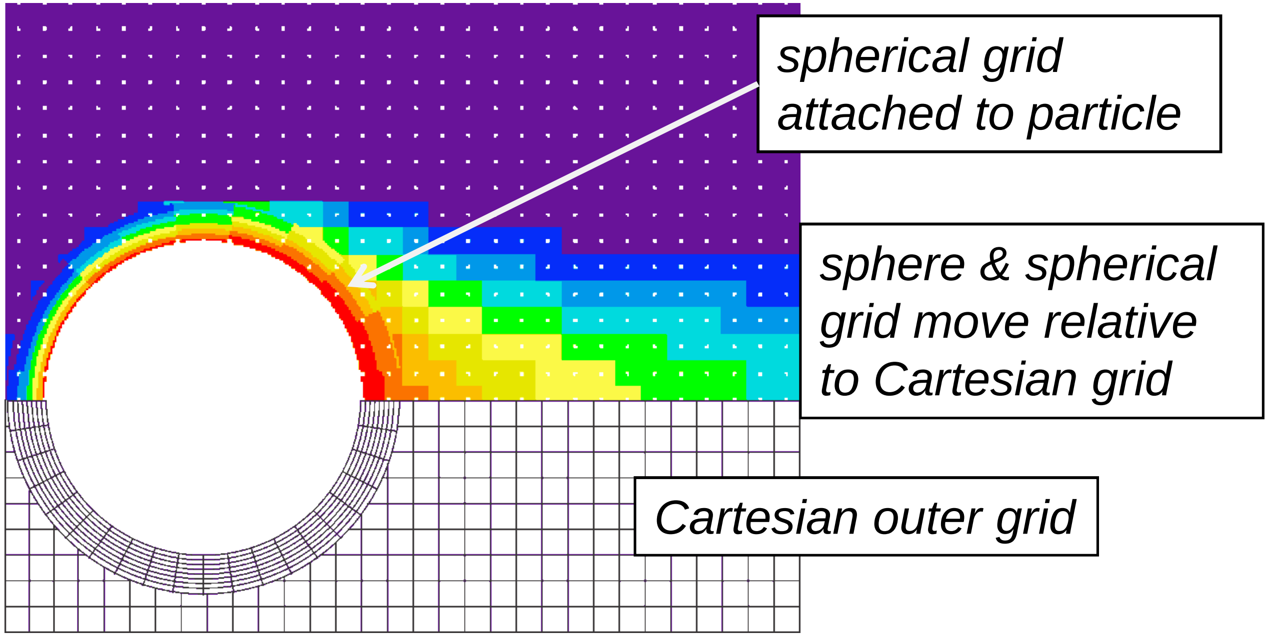


vertical cross section



horizontal cross section

Coupled overlapping domains*


spherical grid attached to particle

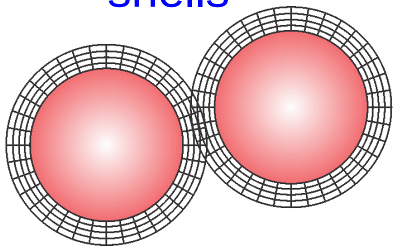
sphere & spherical grid move relative to Cartesian grid

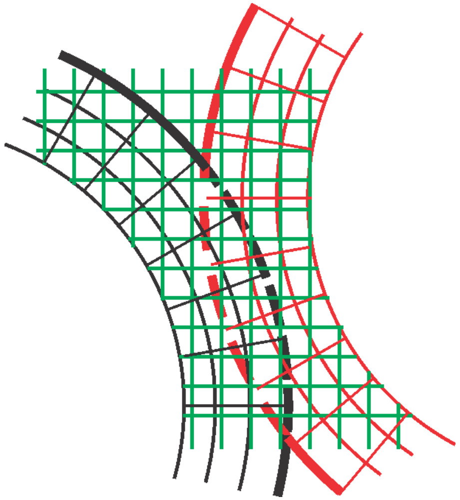
Cartesian outer grid

Communication between the grids:
linear interpolation

- velocity on the spherical grid is imposed from the outer grid
- concentration fields are two-way coupled between the grids

multiple particles will have overlapping shells**





...mixing rules…

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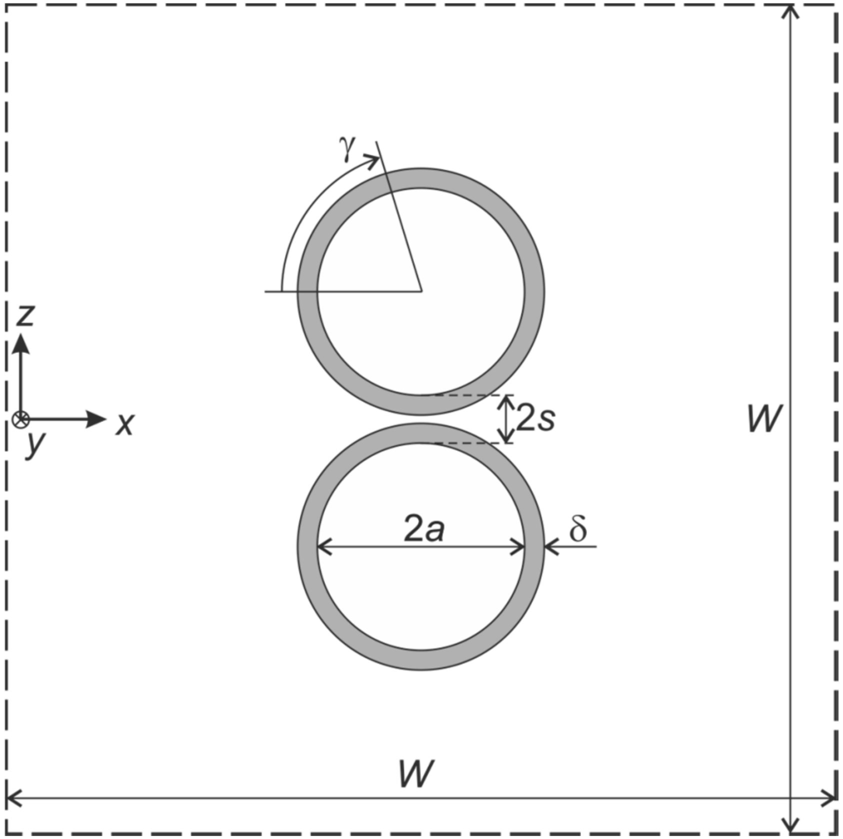
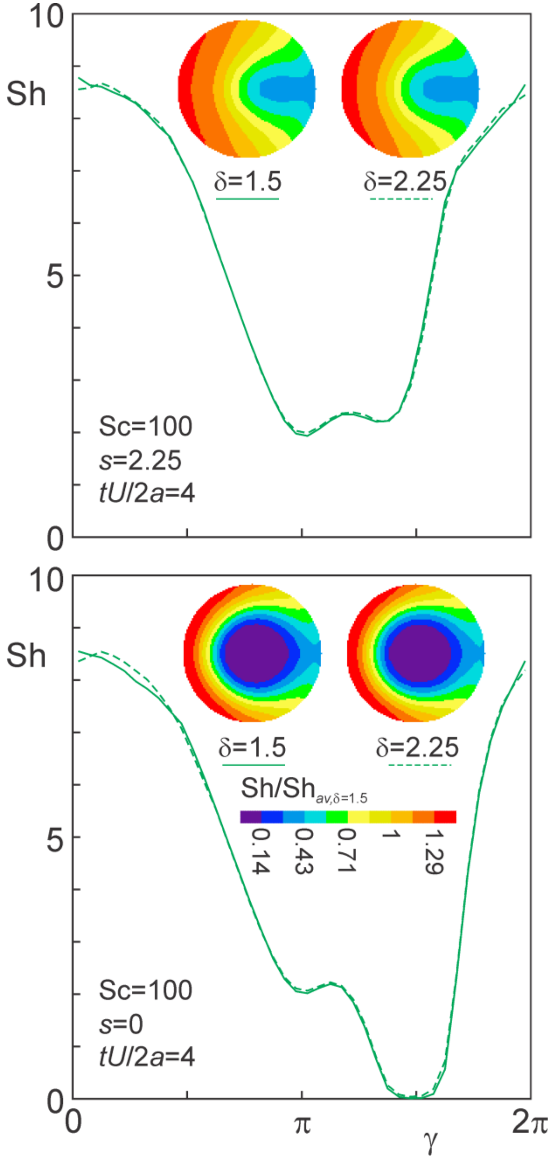
* Derksen *AIChEJ* 2014
** Derksen *CEJ* 2014

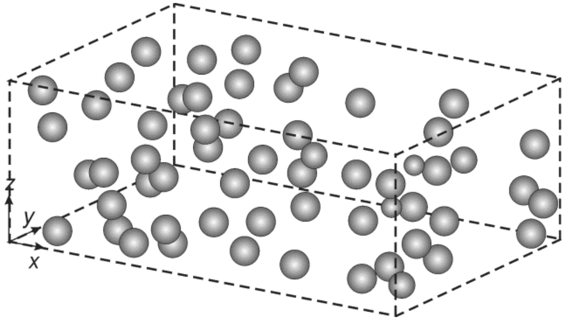
Two-sphere benchmark

overall flow in *x*-direction





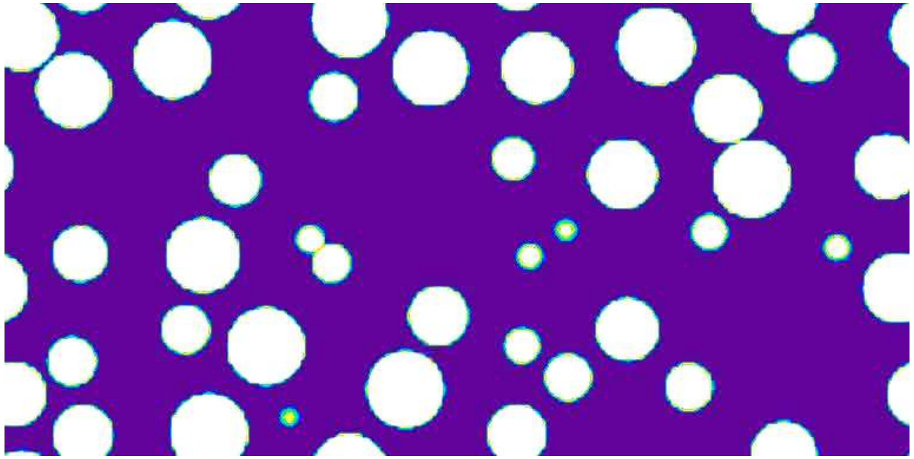
Fixed beds versus moving spheres

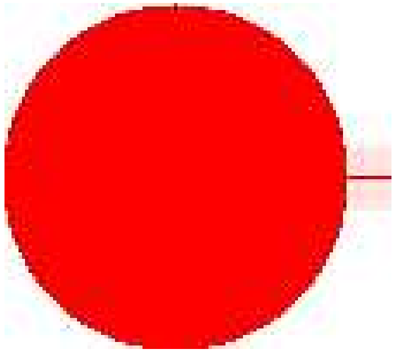


$$\mathrm{Re} = \frac{\langle u \rangle 2a}{\nu} = 1$$

$$\phi = 0.2$$

$$\mathrm{Sc} = 10^3$$





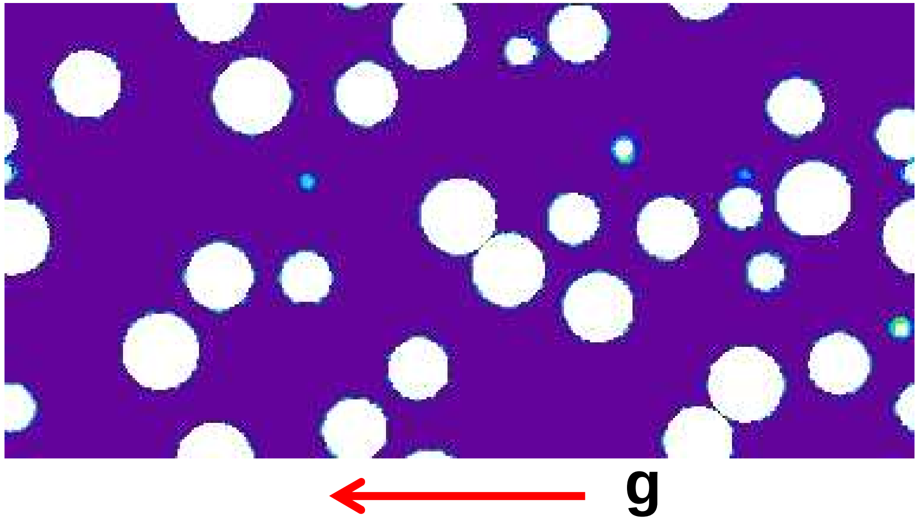
$$\mathrm{Re} = \frac{\langle u - v_p \rangle 2a}{\nu} = 1$$

$$\phi = 0.2$$

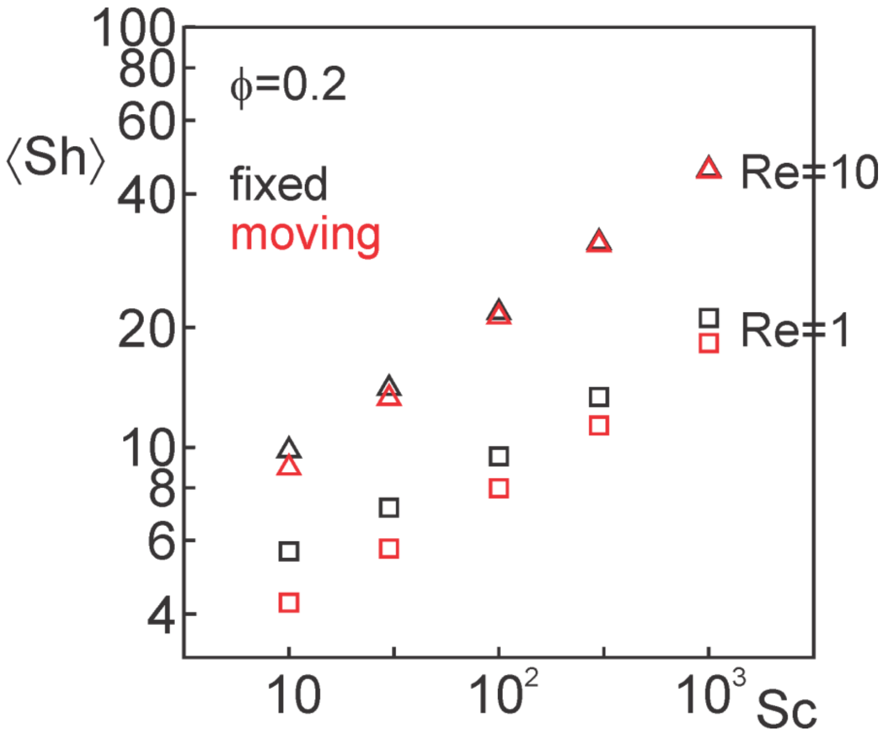
$$\mathrm{Sc} = 10^3$$

$$\rho_p / \rho_\ell = 4$$

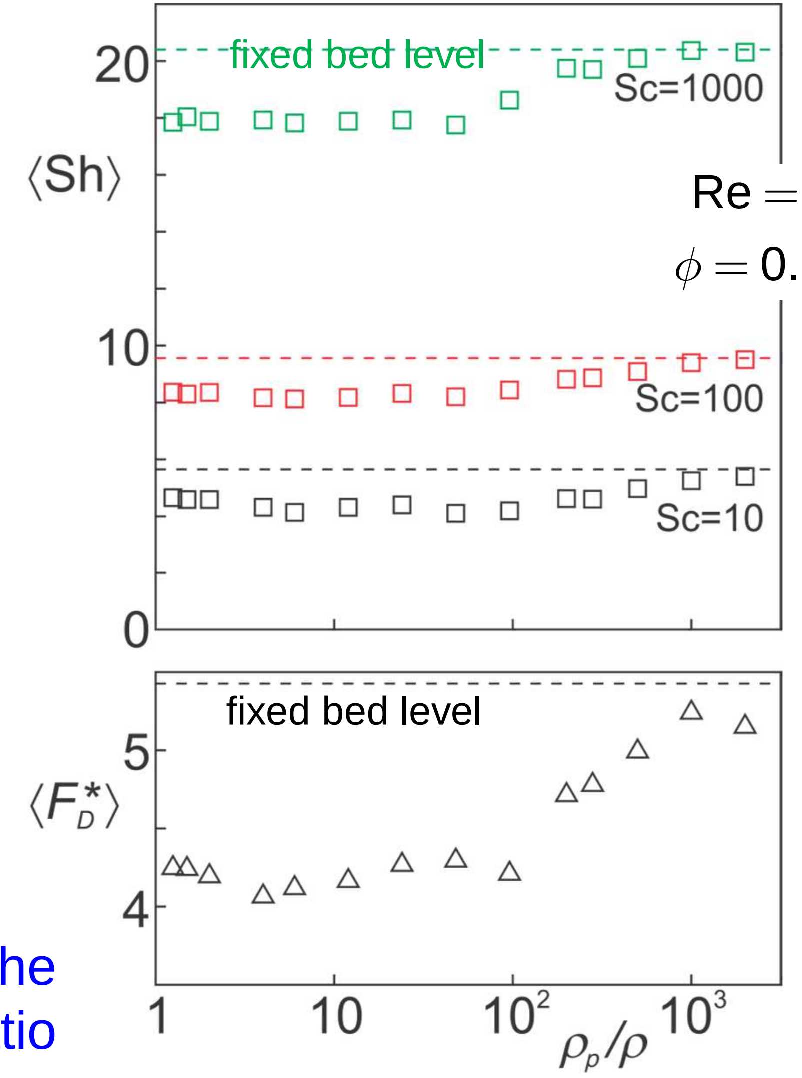
sedimenting
spheres



Compare Sherwood numbers



$$\rho_p / \rho_\ell = 4$$



$\mathrm{Re} = 1$

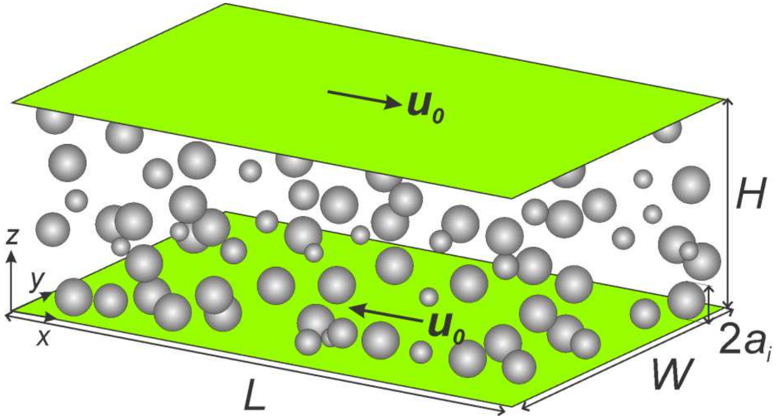
$\phi = 0.2$

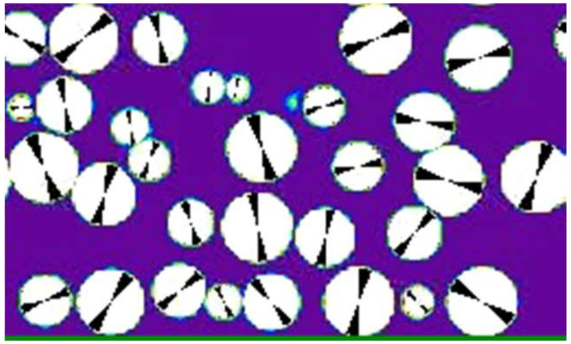
the role of the density ratio

Some more mass transfer

“industrial” applications

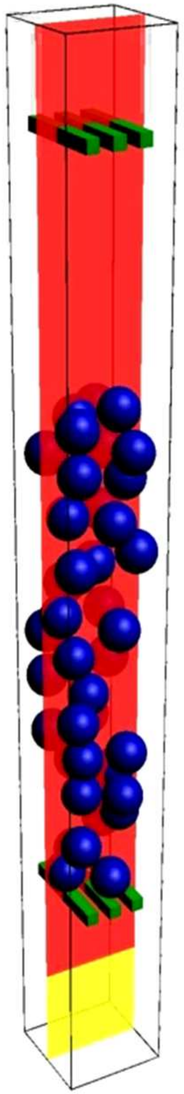
hot melt extrusion*





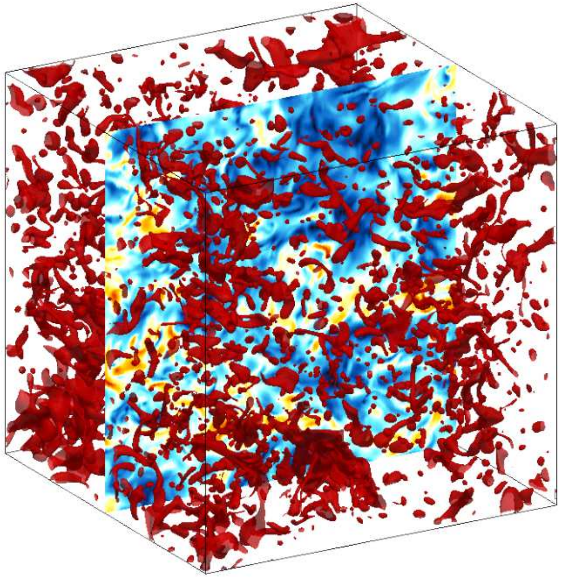
breakthrough in a
micro reactor**

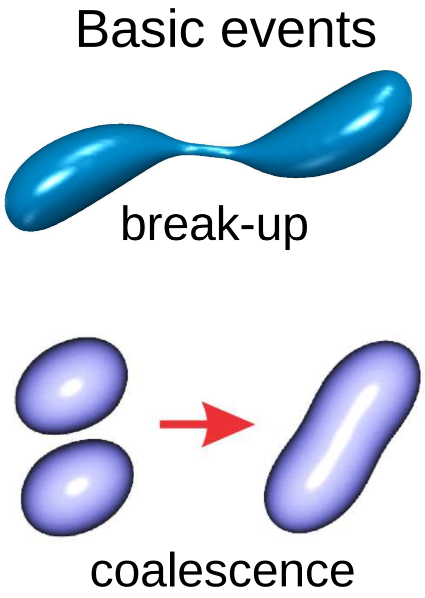
most of the yellow agent
adsorbs on the particles



*Derksen et al *ChERD* 2015
**Derksen *Micro Nano Fluidics* 2014

Liquid-liquid dispersions (emulsions)



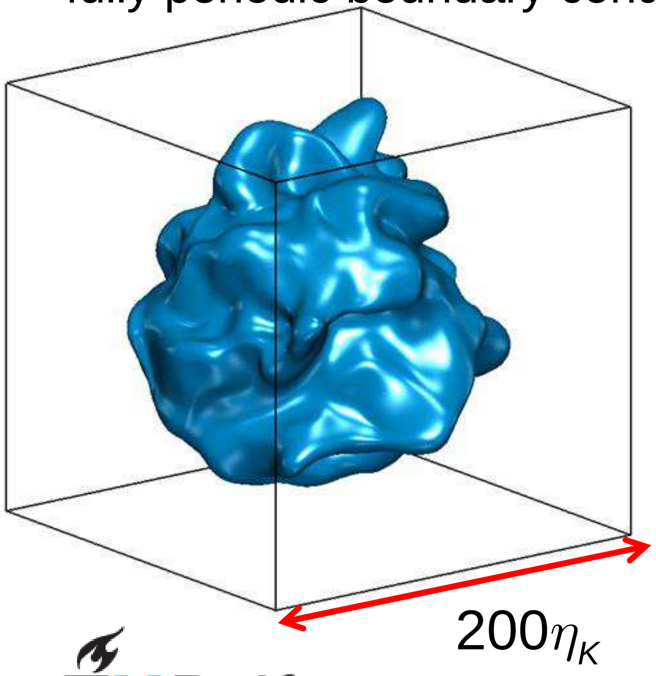


flow dynamics ↔ drop size distribution ↔ interfacial area ↔ inter-phase mass transfer ↔ apparent rheology ↔ stability ↔ product formulation

Turbulent emulsions

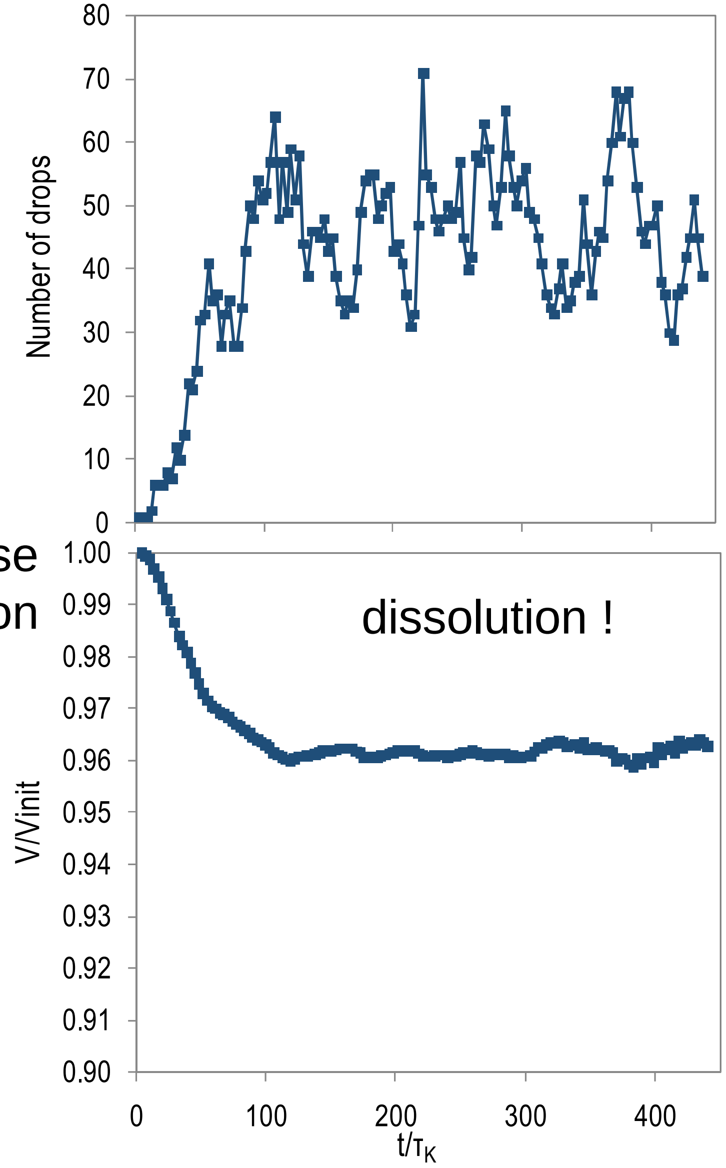
two immiscible liquids in homogeneous, isotropic turbulence*

same viscosity
same density
fully periodic boundary conditions



disperse phase volume fraction

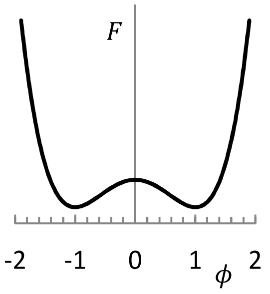
φ=0.20



* Komrakova et al *AIChEJ* 2015

A methods slide: binary liquids

ϕ: order parameter controls composition



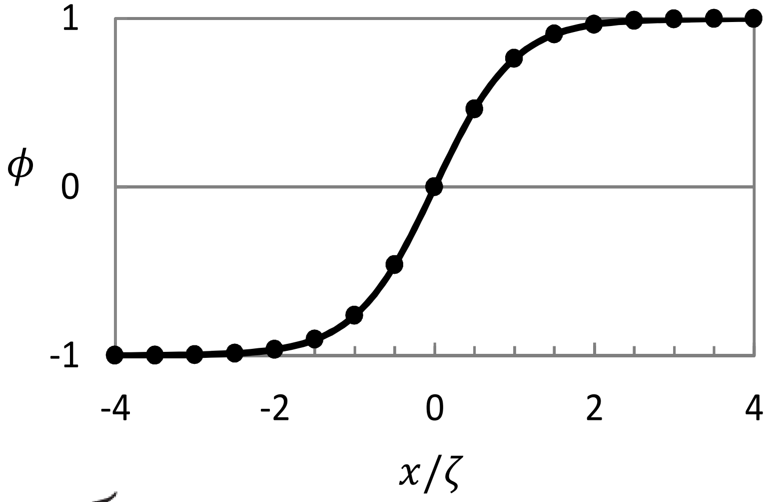
advection-diffusion

$$\frac{\partial\phi}{\partial t}+\nabla\cdot(\phi\vec{u})=M\nabla^2\mu$$

chemical potential

$$\mu=\frac{\delta F}{\delta\phi}=A\phi(\phi^2-1)-\kappa\nabla^2\phi$$

coupled with hydrodynamics through body force $\vec{b}=-\phi\nabla\mu$



a "diffuse" interface

interface thickness

$$\zeta=\sqrt{2\frac{\kappa}{A}}$$

surface tension

$$\sigma=\frac{2\sqrt{2}}{3}\sqrt{\kappa A}$$

proper interface is resolution: $\zeta\approx 1-2$

Briant, Yeomans *Phys Rev E* 2004

Make the flow simpler: breakup in shear

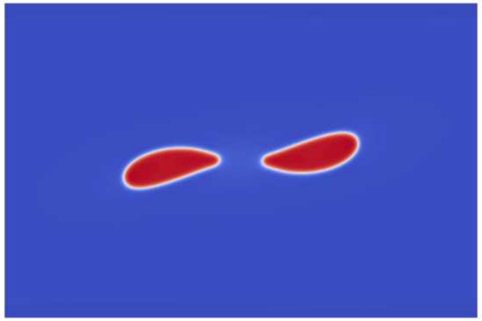
$$\mathrm{Ca} = \frac{\mu_m a \dot{\gamma}}{\sigma}$$ Capillary number

starting point:
spherical drop with
radius *a*

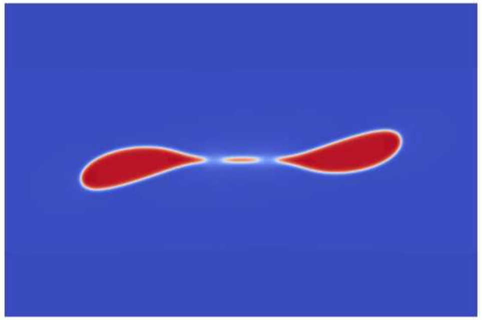
Ca=0.42 $\quad \mathrm{Re} = 0.06 \quad \lambda = 1$

just above Ca_c (Ca-critical)

The good news:
breakage / non-breakage
is largely independent of
resolution

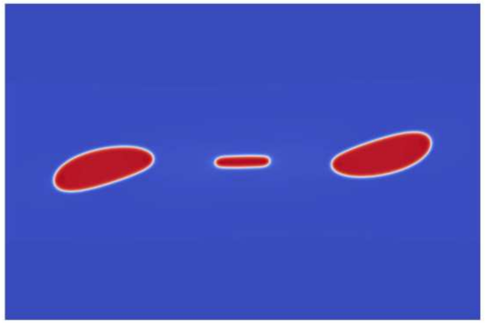


resolution: *a*=20



a=25

quick
dissolution

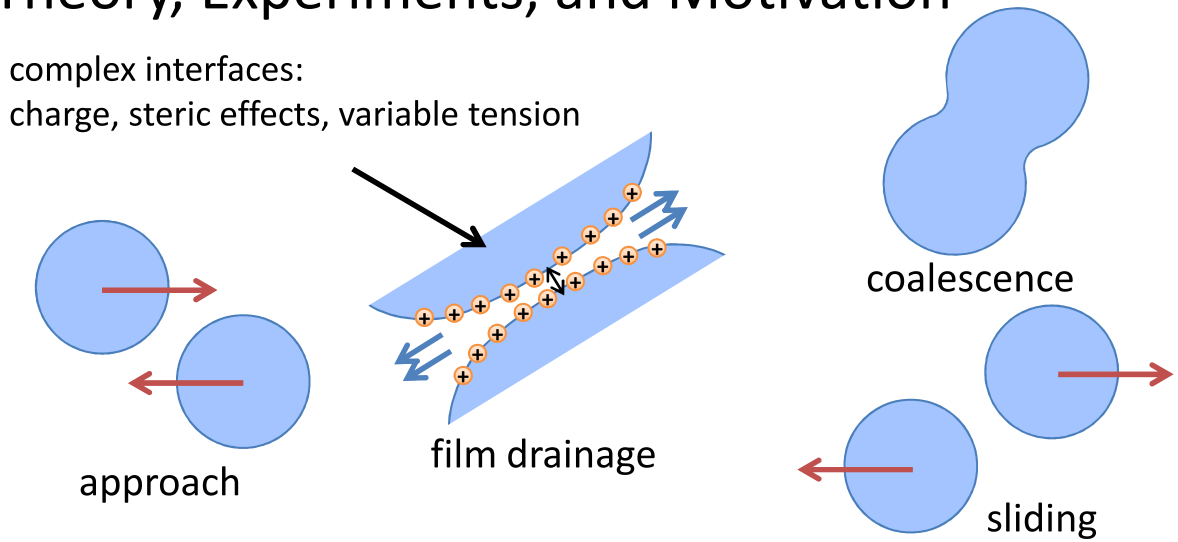


a=30

Komrakova et al *IJMF* 2014

Coalescence in shear

Theory, Experiments, and Motivation

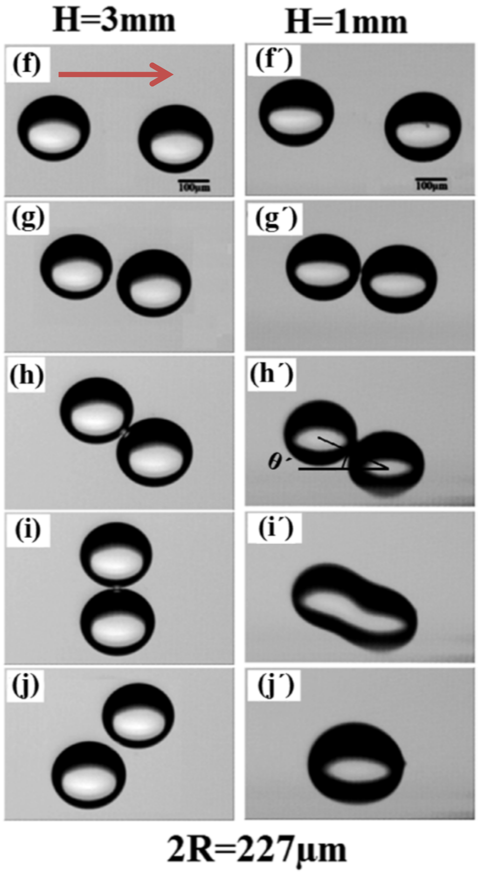

complex interfaces:
charge, steric effects, variable tension

approach

film drainage

coalescence

sliding



Chen et al. *Langmuir* 2009

simulations at critical conditions are challenging

- topological change; 30 nm film vs. 100 µm drops

clean polymer systems

- hydrodynamics, surface tension, van der Waals forces

charged surfaces and electrolytes

- additional electrostatic interactions

Uncharged drops

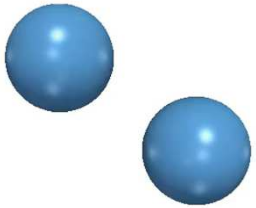
capillary number determines
outcome of collision

$$\mathrm{Ca} = \frac{\rho \nu R \dot{\gamma}}{\sigma}$$

$\Delta Y / 2R = \mathbf{0.86}$

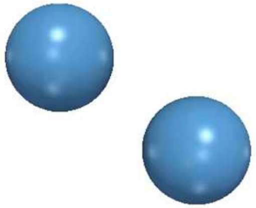
Ca = 0.095

sliding



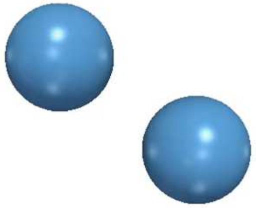
Ca = 0.085

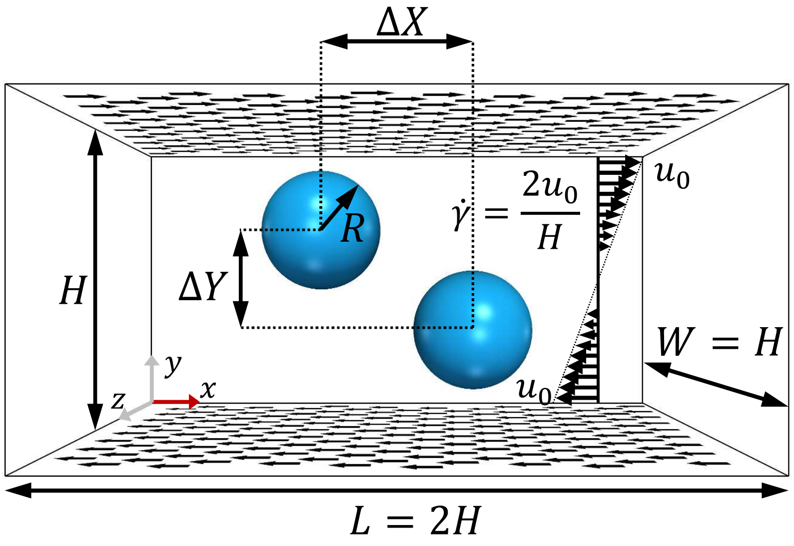
temporary bridge



Ca = 0.080

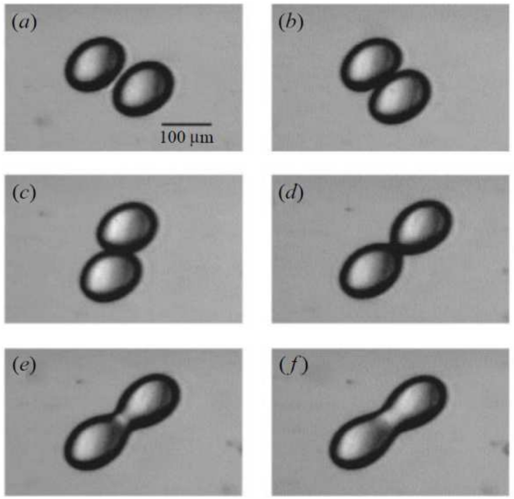
coalescence





uniform density & viscosity

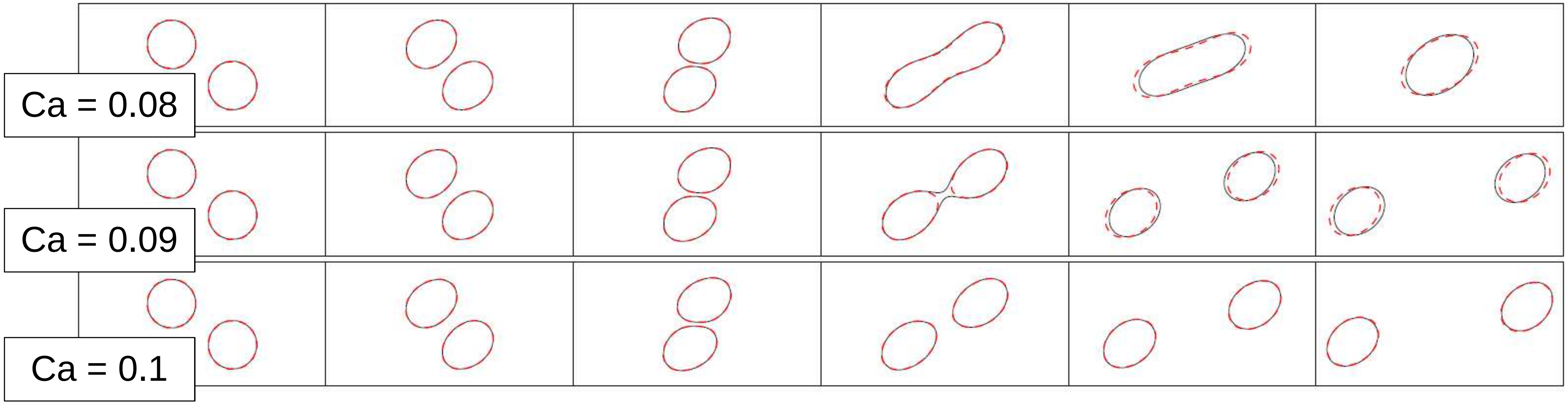
Guido, Simeone *J Fluid Mech* (1998)



Shardt, Derksen, Mitra *Langmuir* 2013

We are (fairly) grid independent

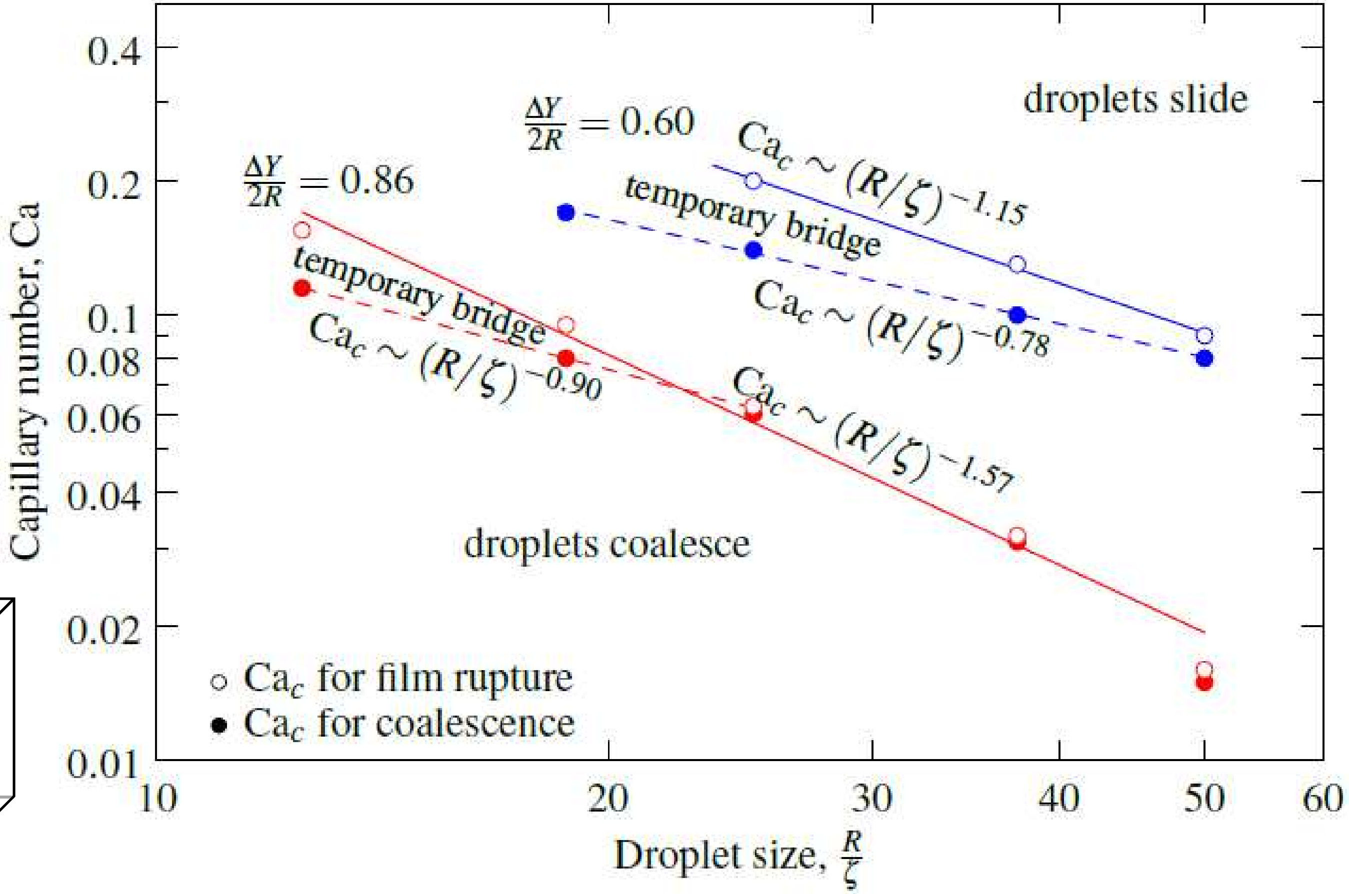
Solid black: $R = 75, \zeta = 4$ Dashed red: $R = 37.5, \zeta = 2$

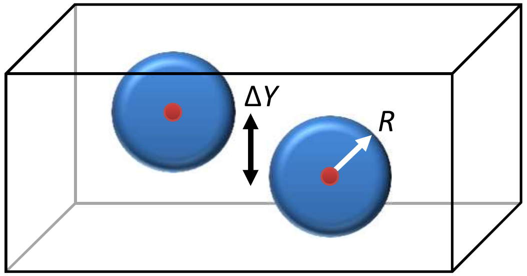


Doubling interface resolution does not change outcome.
$\therefore$ adequately resolved with $\zeta = 2$

Critical capillary numbers

$$\text{Ca} = \frac{\rho \nu R \dot{\gamma}}{\sigma}$$





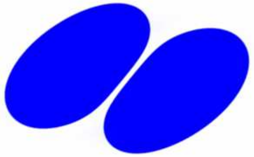
….towards lower $\Delta Y/2R$ to compare with experiments

…need higher resolution

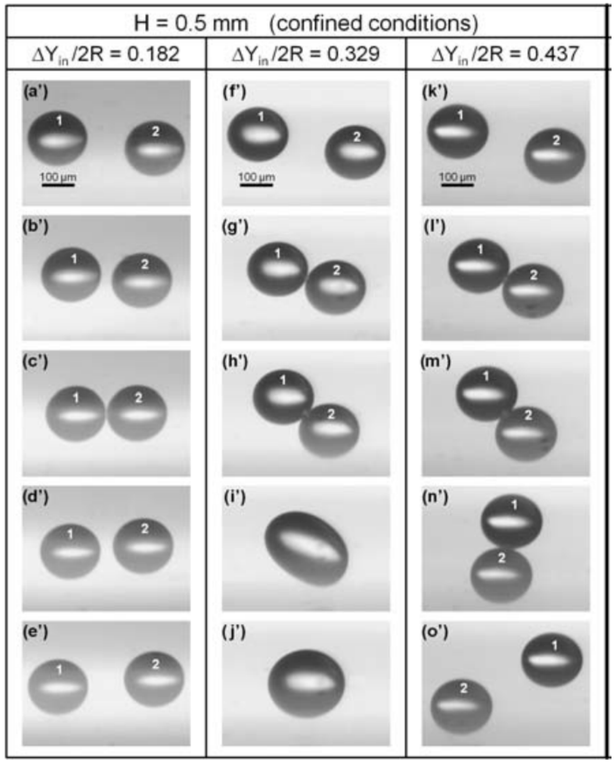
$\Delta Y/2R = 0.2 \quad R = 200\ lattice\ units$

Ca = 0.1

Ca = 0.2



Ca = 0.25

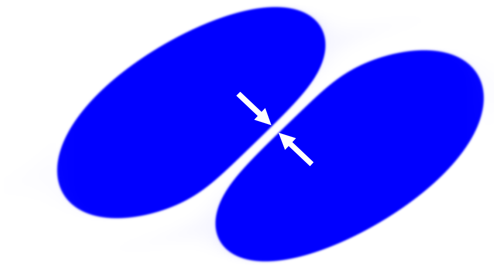


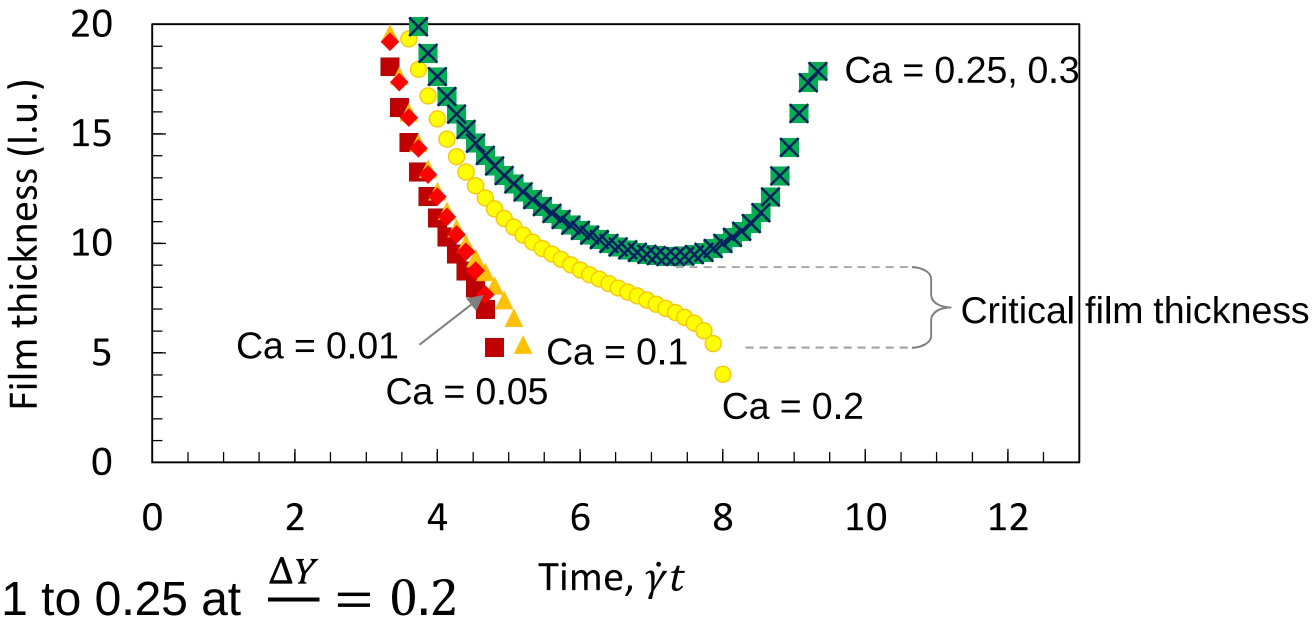
De Bruyn et al. *JCIS* 2013

$$\mathrm{Ca} = \frac{\rho\nu R\dot{\gamma}}{\sigma}$$

Shardt, Mitra, Derksen *Langmuir* 2014

Evolution of film thickness





critical capillary number 0.1 to 0.25 at $\frac{\Delta Y}{2R} = 0.2$

a **good question** would be: how big are these drops actually?

an estimate can be based on minimum film thickness

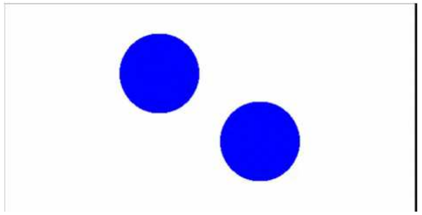
minimum film thickness 5 – 10 l.u. ~ 30 nm

$\Rightarrow R = 200\text{: } 0.6 - 1.2\ \mu m$

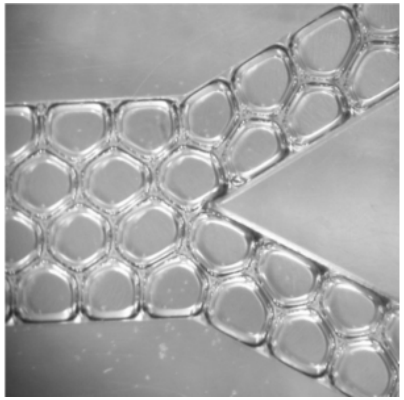
imagine simulating coalescence of 1 mm drops

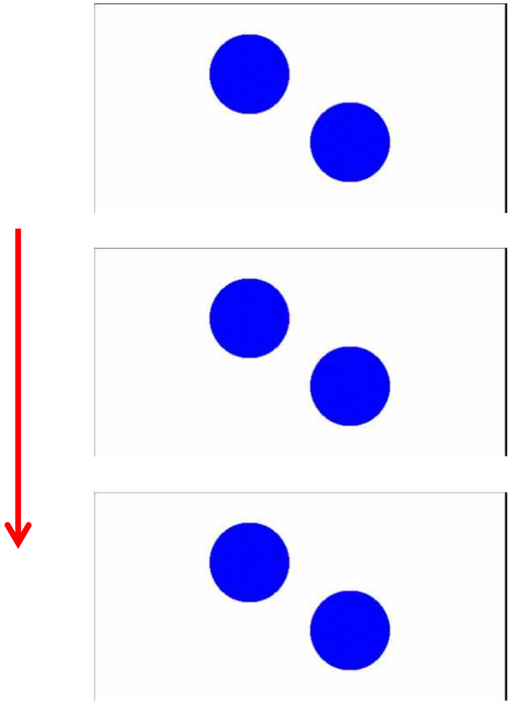
Charged drops

$$\mathrm{Ca} = \frac{\rho \nu a \dot{\gamma}}{\sigma} = 0.06$$



uncharged





charged with
Debye length

$$\kappa^{-1} = 0.2a$$

increasing electric
field strength

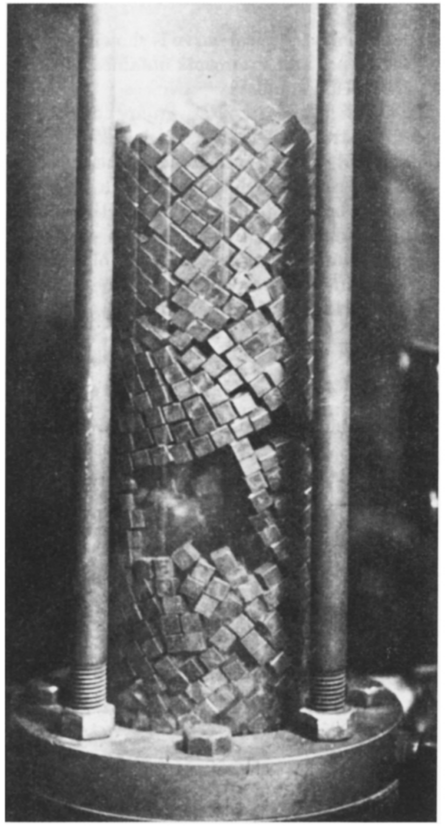
factor 10 each time

Sedimentation/fluidization

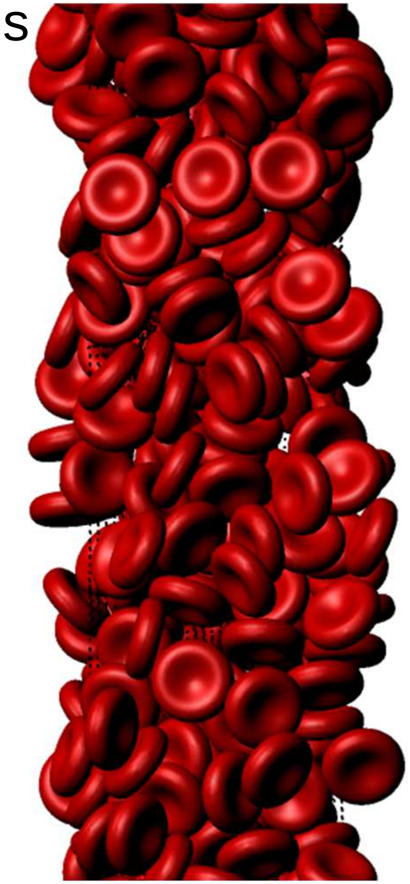
with an emphasis on non-spherical particles

“coker”

steel cubes in fluidization

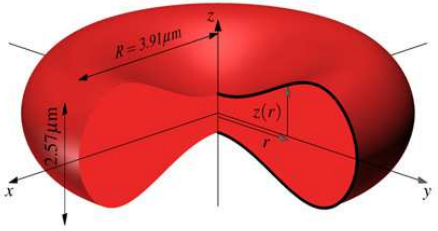


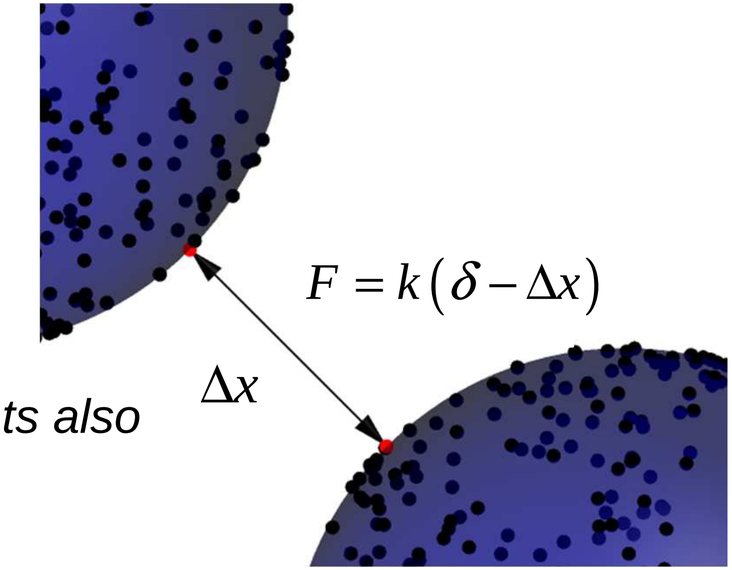
sedimenting red blood cells



*Richardson and Zaki *Trans. Inst. Chem. Eng.* **32** (1954)

RBC’s as sample non-spherical particles





$$F = k(\delta - \Delta x)$$

Specific challenges*

- collision handling

    repulsive spring force between surface points also used for immersed boundary

- low density ratio $\rho_p / \rho = 1.07$

    use modified finite difference method for stability

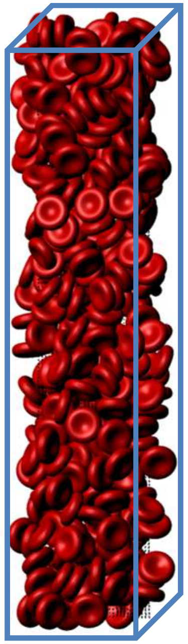
- high solids volume fraction (~0.45)
    - *compaction procedure for initialization*
    - *frequent collisions*

---

* Shardt & Derksen, *IJ Multiphase Flow* **47** (2012)

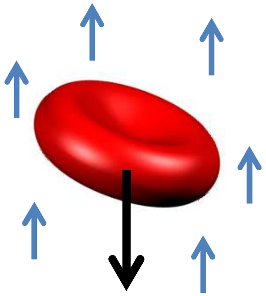
Settling of a dense suspension

all boundaries
are periodic



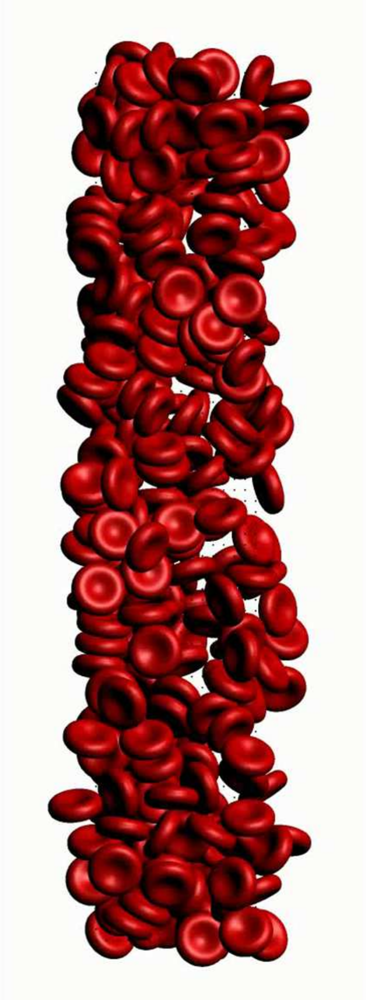
291 particles
$\phi = 0.35$

body force on fluid



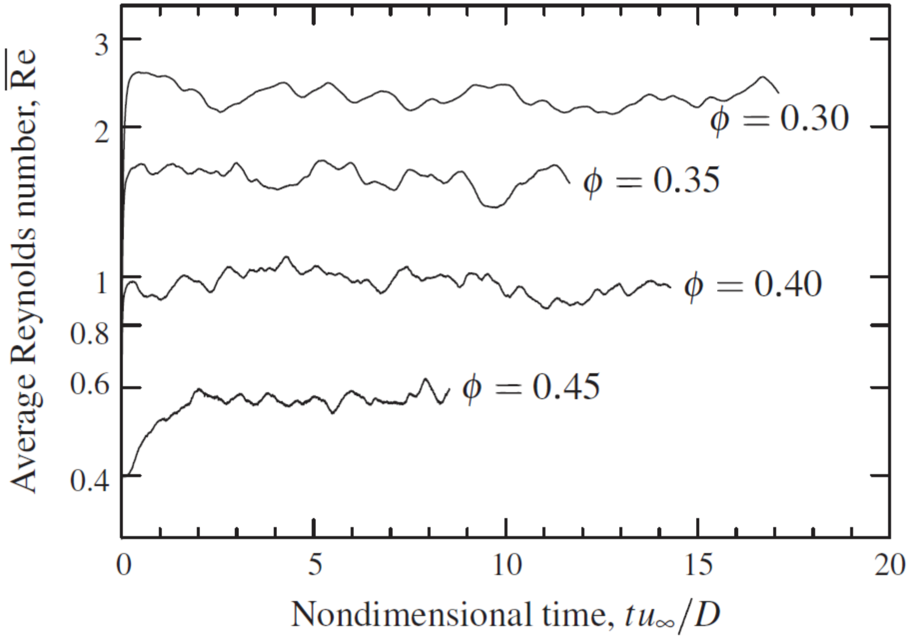
balances gravity

resolution
D = 20 nodes

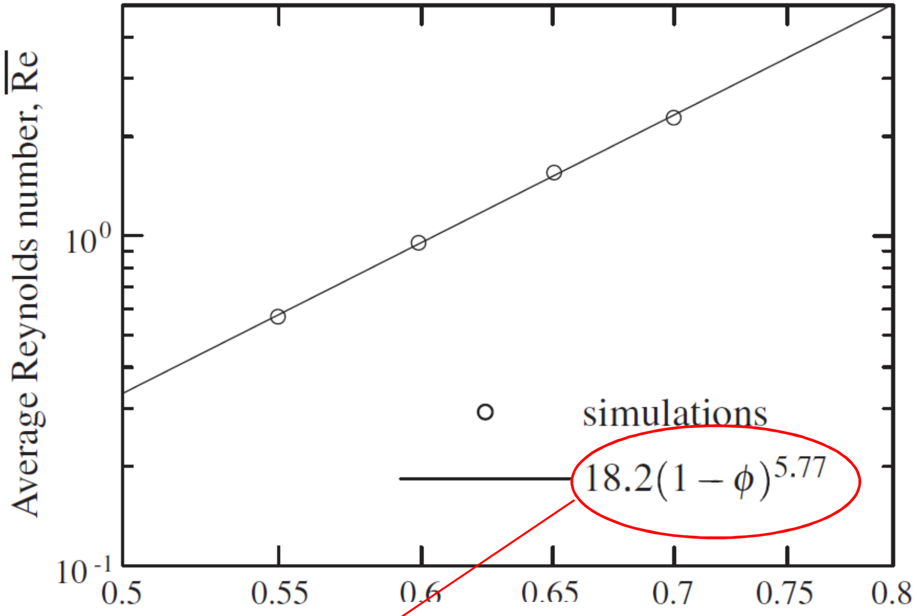


removing
particles
reveals flow
cross-
section

Hindered settling



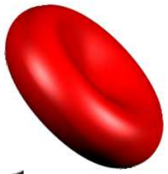
$$\overline{\mathrm{Re}} = \frac{\bar{u}_{\mathrm{slip}} D}{\nu}$$



$1-\phi$

void fraction

The RZ fit suggests $\mathrm{Re}_\infty = 18.2$

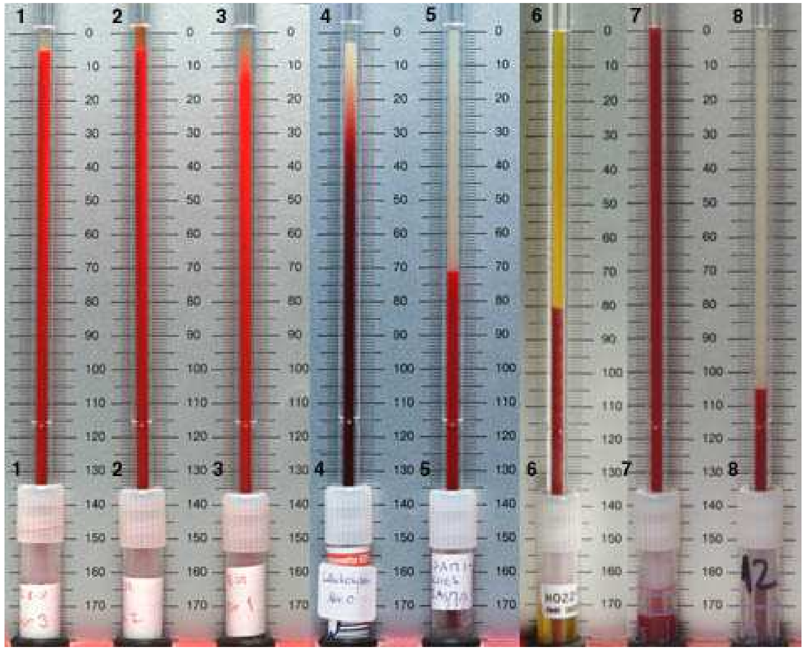


→ an - on average - inclined RBC

Richardson-Zaki (RZ) $\frac{\overline{u}_{slip}}{u_\infty} = (1-\phi)^n$

Human erythrocyte sedimentation rate

U. Woermann
edu.cpln.ch/hemosurf/data/Lab-Images/all_ESRs.jpg



ESR blood tests

Typical human ESR is 3 – 9 mm/h

@ $\phi = 0.35$

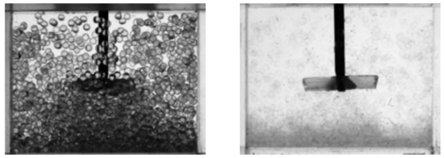
Simulations: 0.18 mm/h

surface forces between RBCs and proteins in blood cause agglomeration

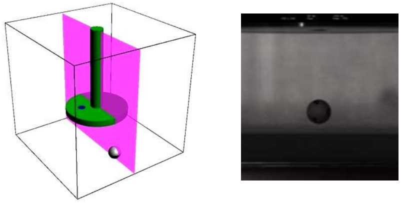
Acknowledgements

Collaborators & students

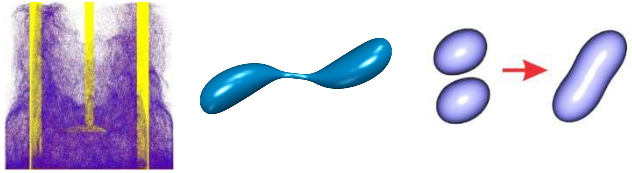
Gaopan Kong & Eric Climent in Toulouse



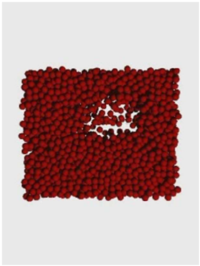
Junyan Mo, Zhipeng Li & Bruce Gao in Beijing



Alexandra Komrakova, Inci Ayranci, Suzanne Kresta, Orest Shardt & Jue Wang in Edmonton



Sankaran Sundaresan in Princeton



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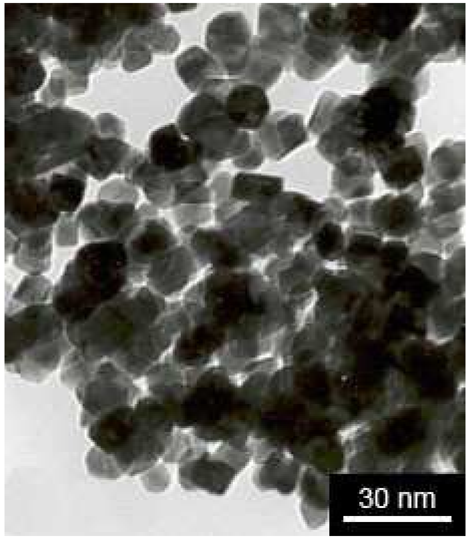
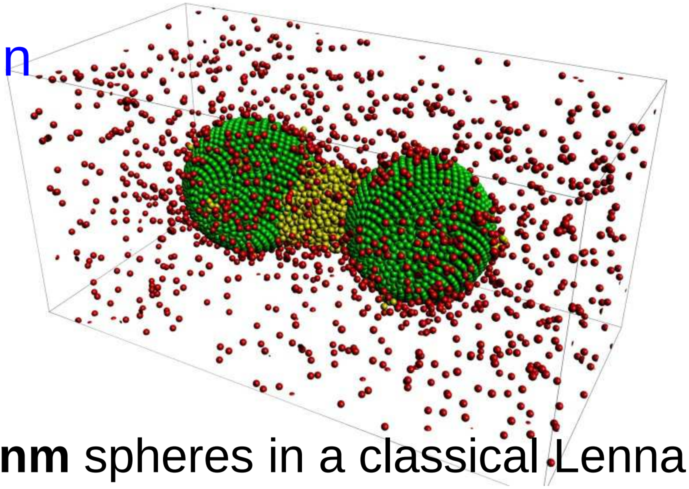
Beyond continuum modeling



example: aggregation of nanoparticles
&
liquid bridges

Molecular Dynamics

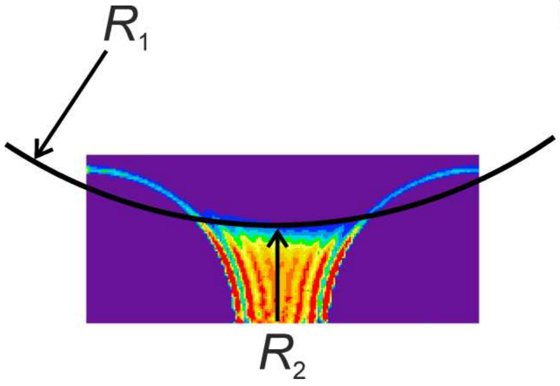
TiO_2 nanoparticles

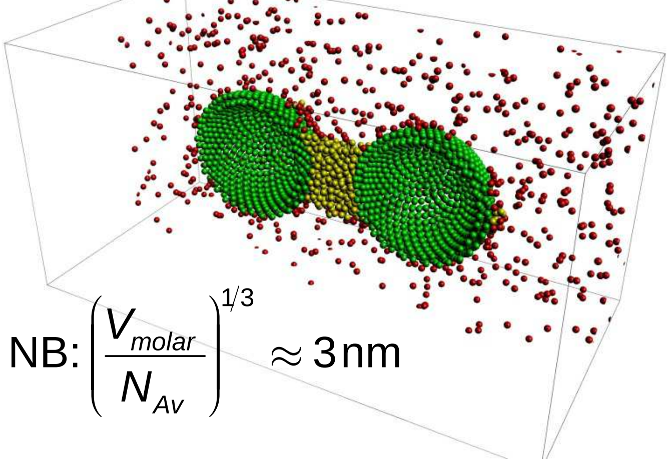


8 nm spheres in a classical Lennard-Jones fluid
(red=vapor; yellow=liquid; green=solid)

$$f = \sigma \pi R_2 \left(1 - \frac{R_2}{R_1} \right)$$

(+ is attractive)





NB: $\left(\frac{V_{molar}}{N_{Av}} \right)^{1/3} \approx 3\,\mathrm{nm}$

Liquid bridge (molecular) dynamics