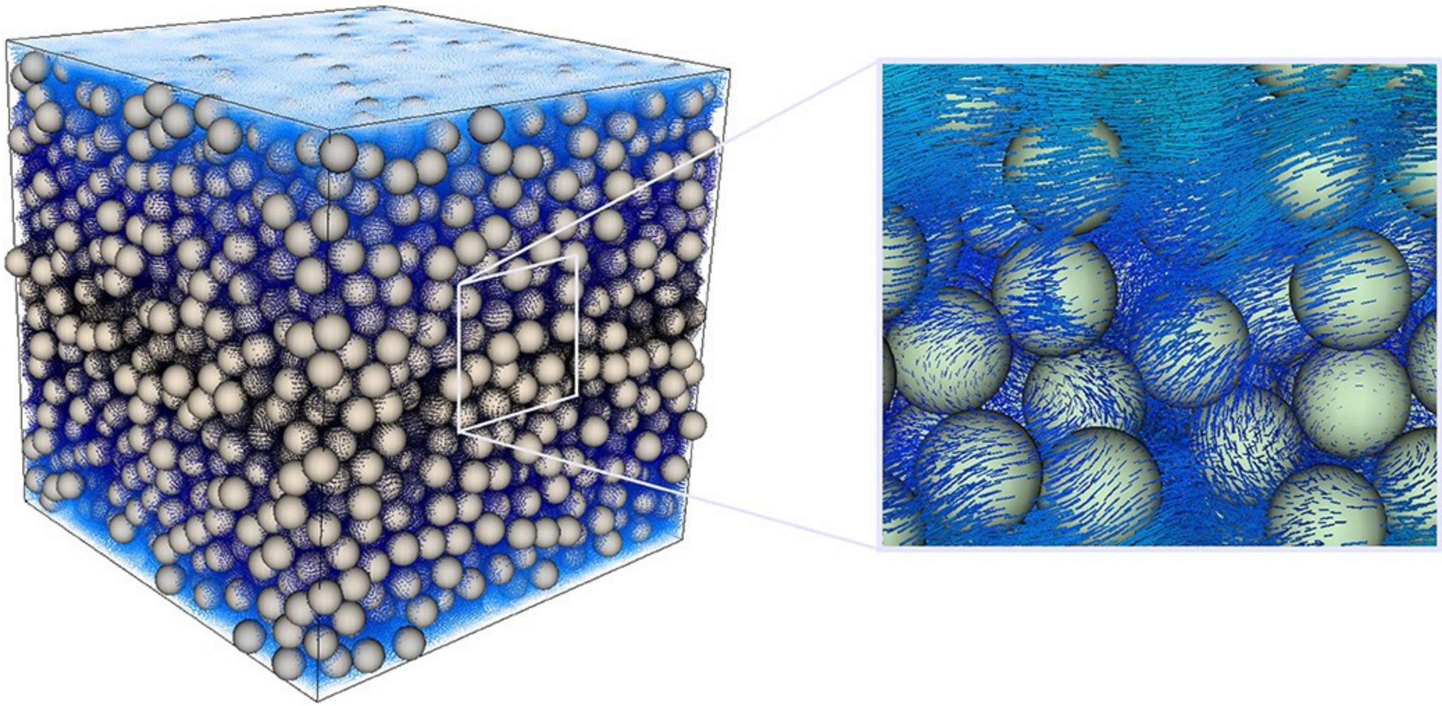
Particle methods for complex particulate systems



Marco Ellero

Zienkiewicz Centre for Computational Engineering
Swansea University, UK

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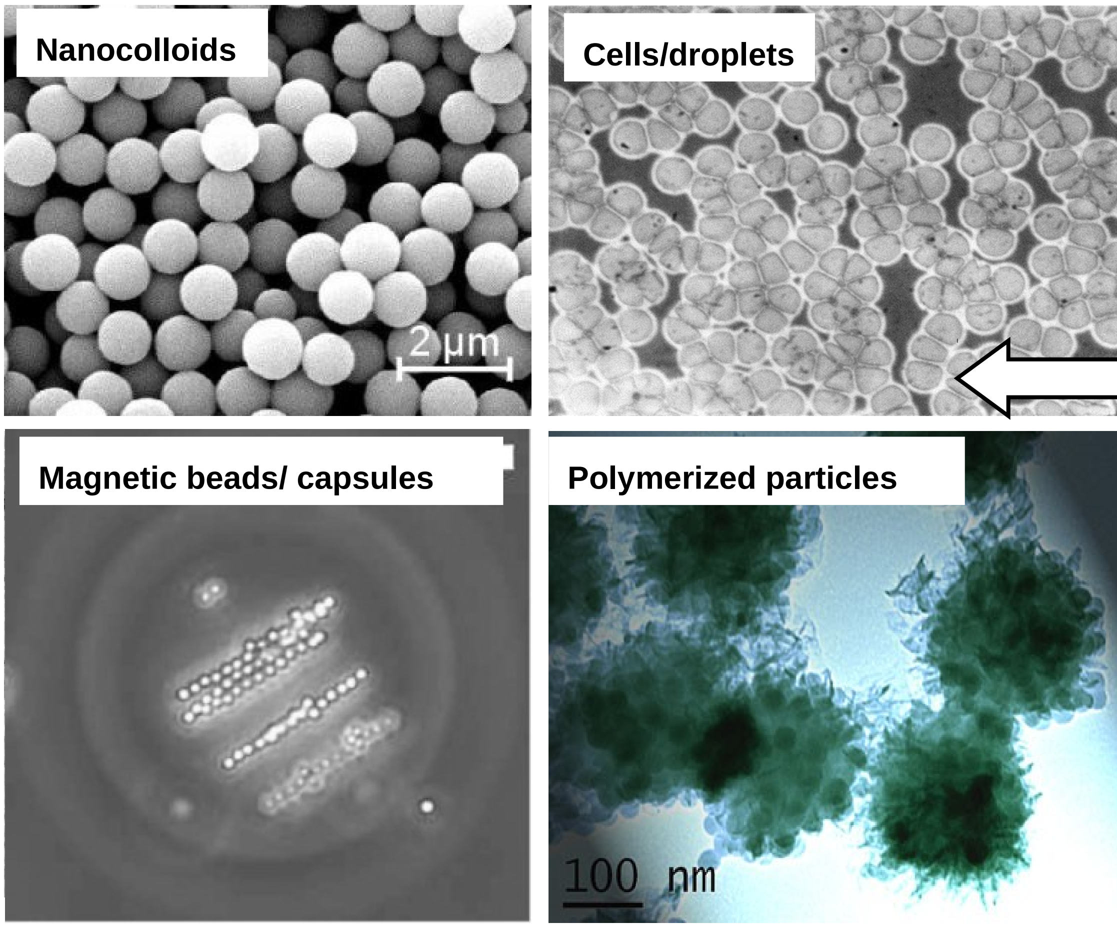
Prifysgol Abertawe

Motivations: particulate systems

Microstructure

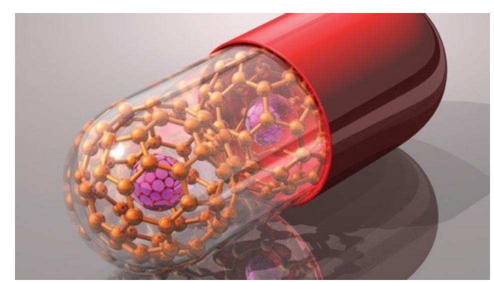


Cosmetics, creams

Chemicals paints

Industrial products, biological liquids

Personalized healthcare - nanomedicine



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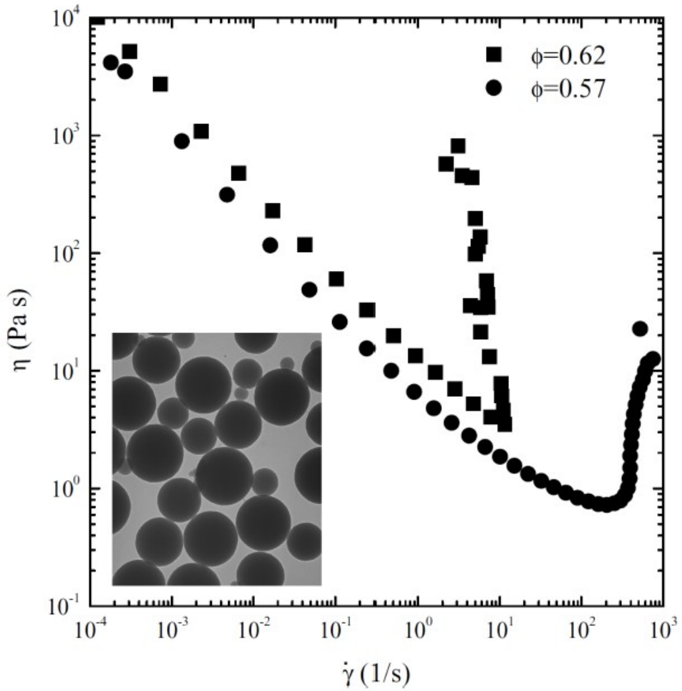
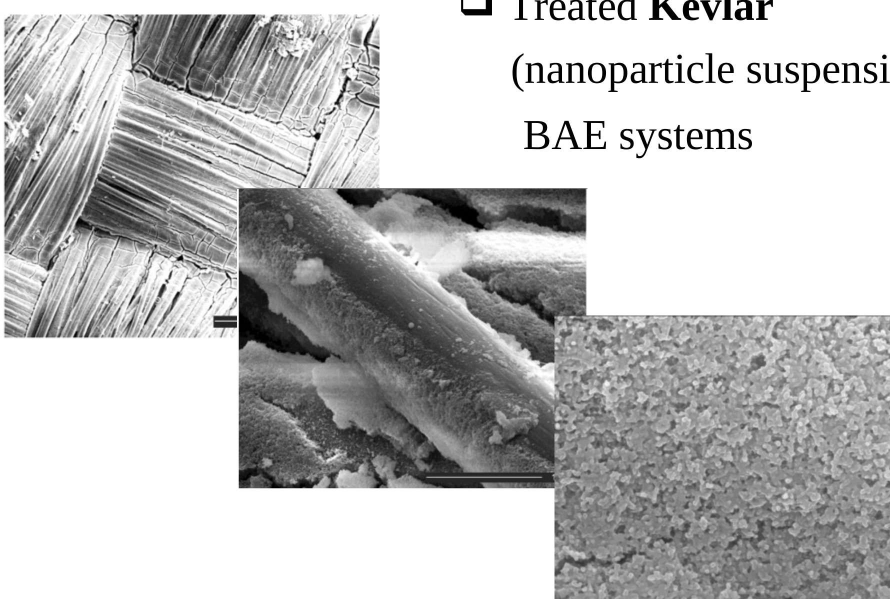
Example I: smart materials – liquid body armours





- Treated **Kevlar**
  (nanoparticle suspension)
  BAE systems

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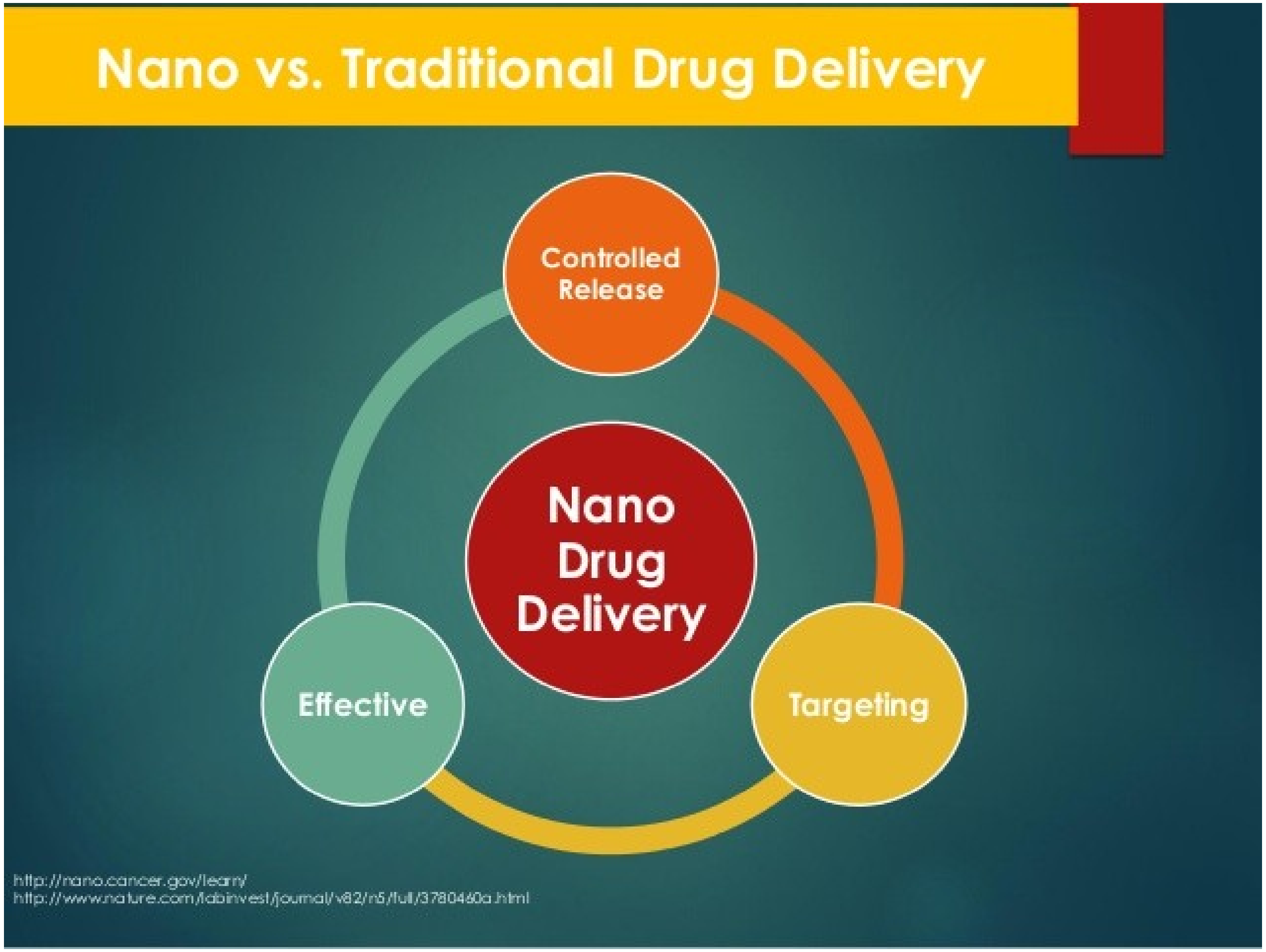
Example II: magnetic nanoparticles – drug delivery



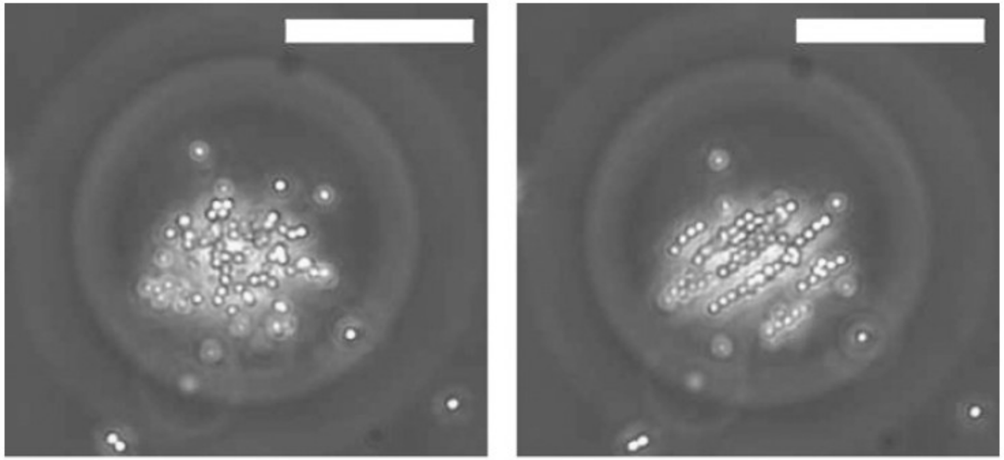
Example II: magnetic nanoparticles – drug delivery

PAPER www.rsc.org/loc | Lab on a Chip

Magneto-mechanical mixing and manipulation of picoliter volumes in vesicles†

Thomas Franke,[*ab] Lothar Schmid,[a] David A. Weitz[b] and Achim Wixforth[a]

Lab Chip, 2009, **9**, 2831–2835 | 2831



(a) before switch-on of magnetic field   (b) 3s after switch-on

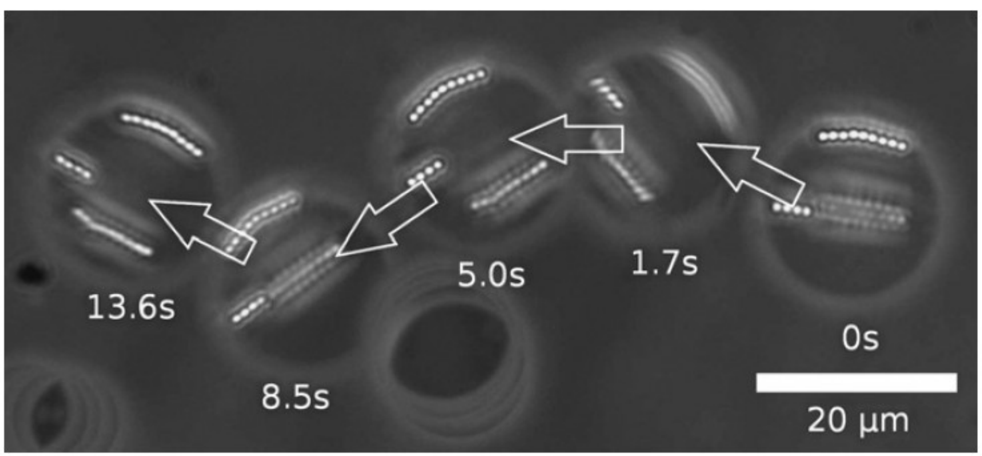
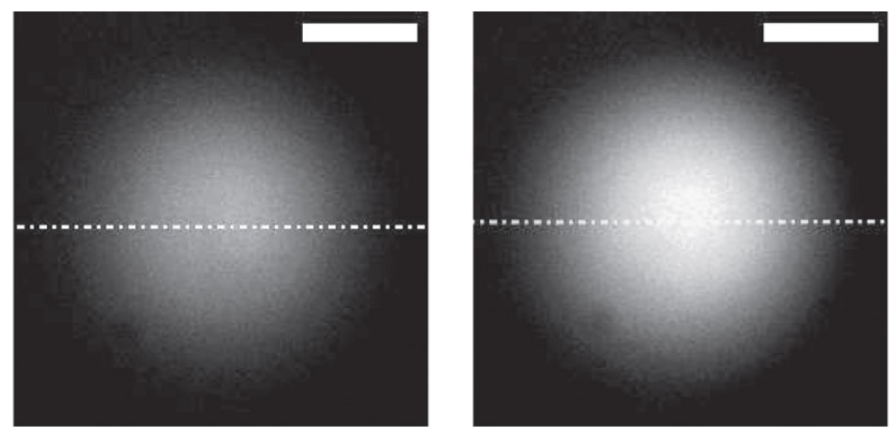


Fig. 2 Micrograph of a vesicle which includes about 20 super-paramagnetic beads being chained up. We control the magnetic field gradient to direct the vesicle along a designated path. Th

- ❑ Large unilamellar vesicle/capsule (100-500nm)
- ❑ magnetic nano-particle (1-10nm)

- ❑ external magnetic field: particle chaining
- ❑ magnetic field gradient → **motion**
- ❑ rotating field: actuate internal fluid promoting **mixing** and/or **reaction**

- ❑ drug delivery: capsule positioning-targeting
- ❑ drug mixing-release by diffusion



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Outline

- **Multiscale particle methods**:
  towards thermodynamic-consistent discretization of PDEs
- **Particulate systems modelling**
- **Rheology of concentrated suspensions**
- **Paramagnetic nanoparticle suspensions**
- **Further applications and conclusions**

Outline

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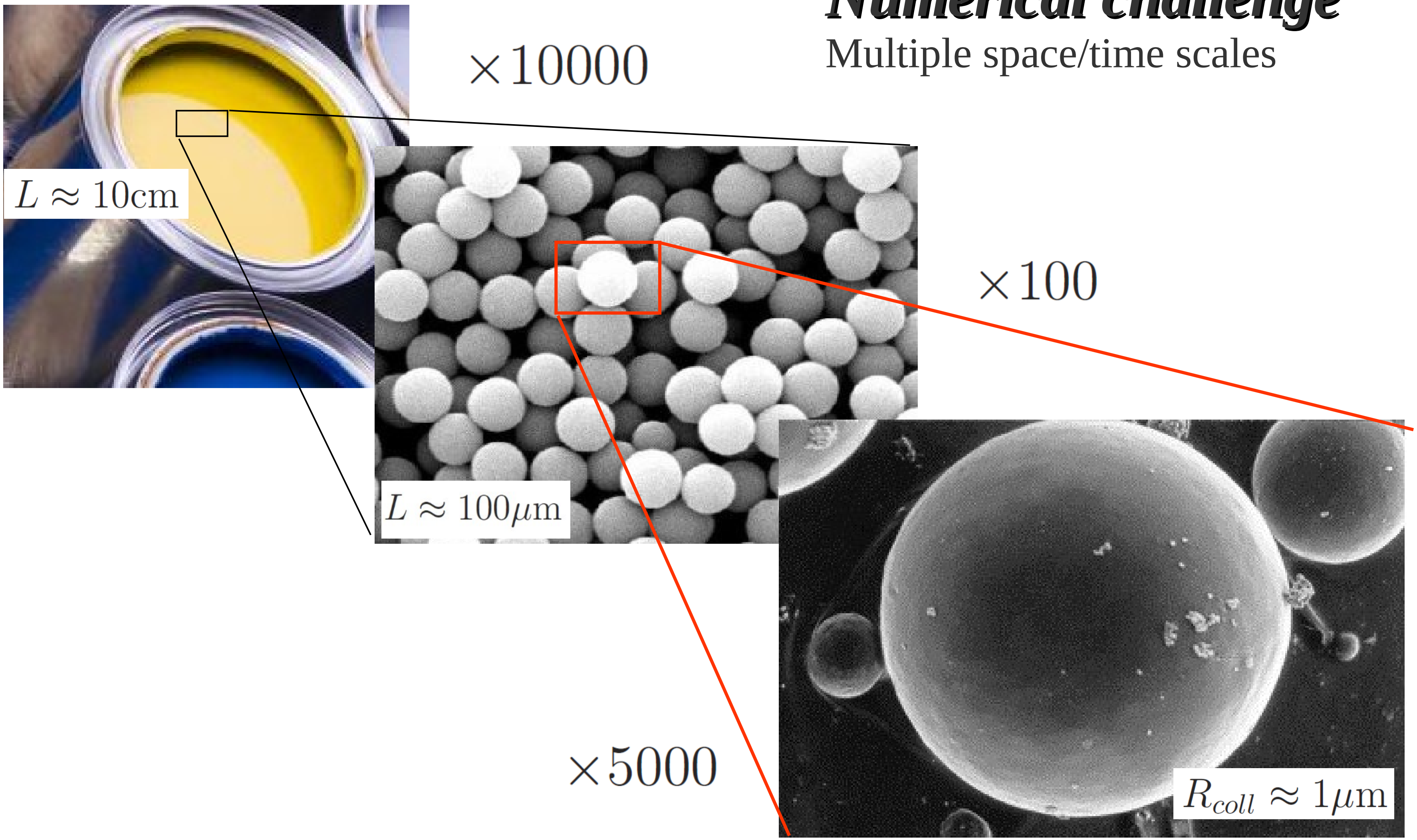
Motivations: particulate systems modelling

Numerical challenge

Multiple space/time scales



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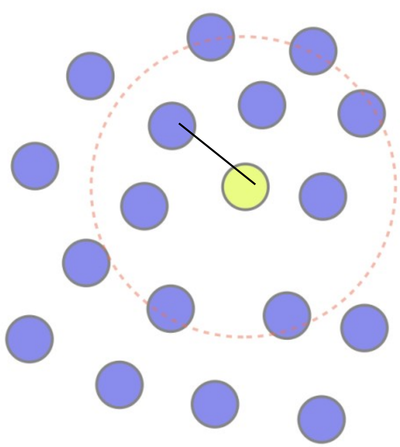
Multiscale particle methods

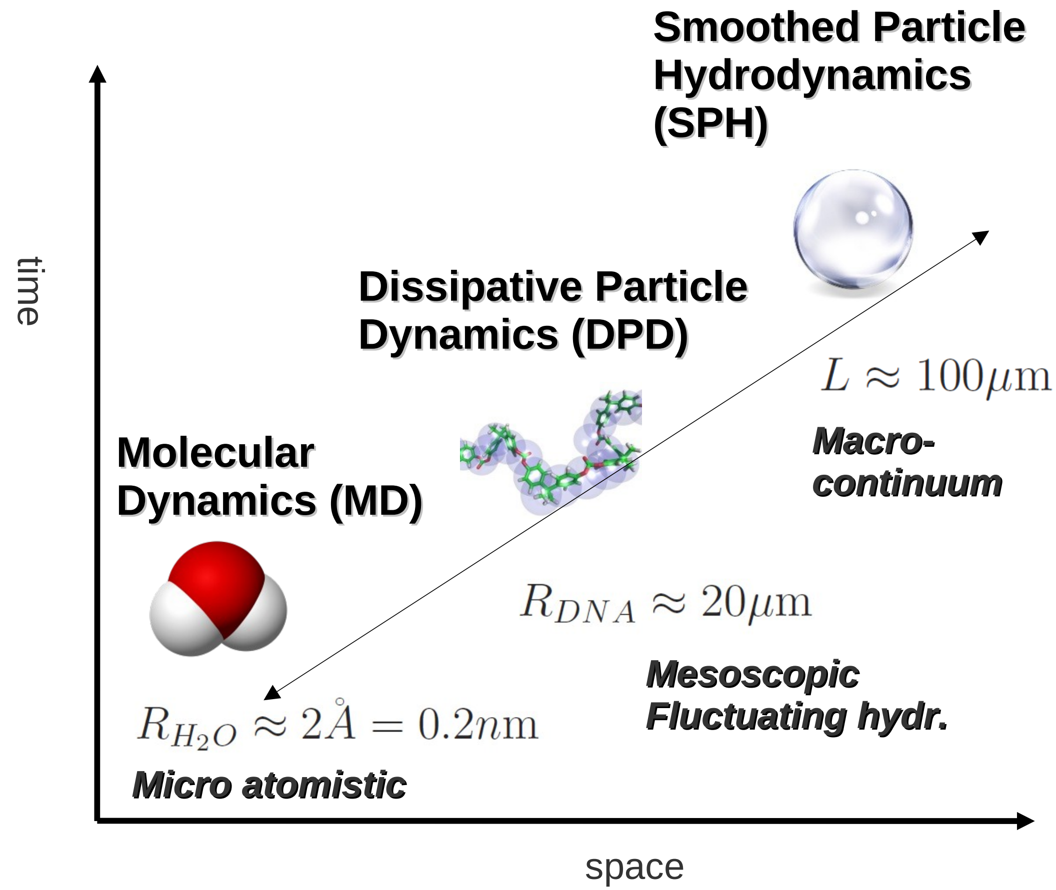
- Specific choice of inter-particle forces defines implicitly the particle-realization and set the method.

- set of ODEs

$$\begin{aligned}\dot{\mathbf{r}}_i &= \mathbf{v}_i\\ \dot{\mathbf{v}}_i &= \sum_j \mathbf{F}_{ij}\end{aligned}$$

Local interactions





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Multiscale particle methods

- Specific choice of inter-particle forces defines implicitly the particle-realization and set the method.

- set of ODEs

$$
\begin{aligned}
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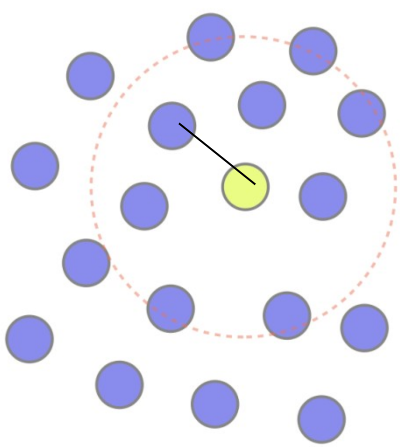
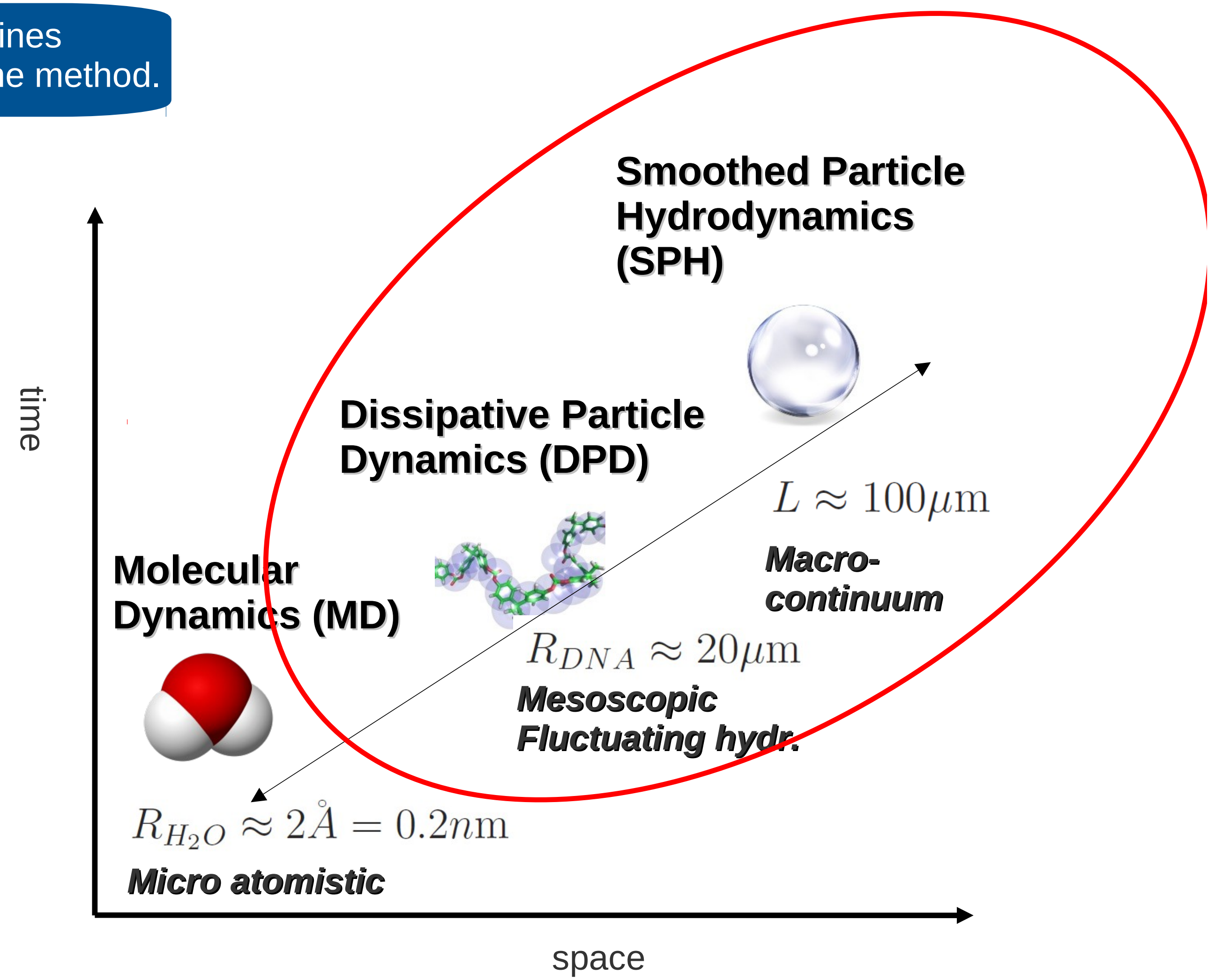
\end{aligned}
$$

Local interactions





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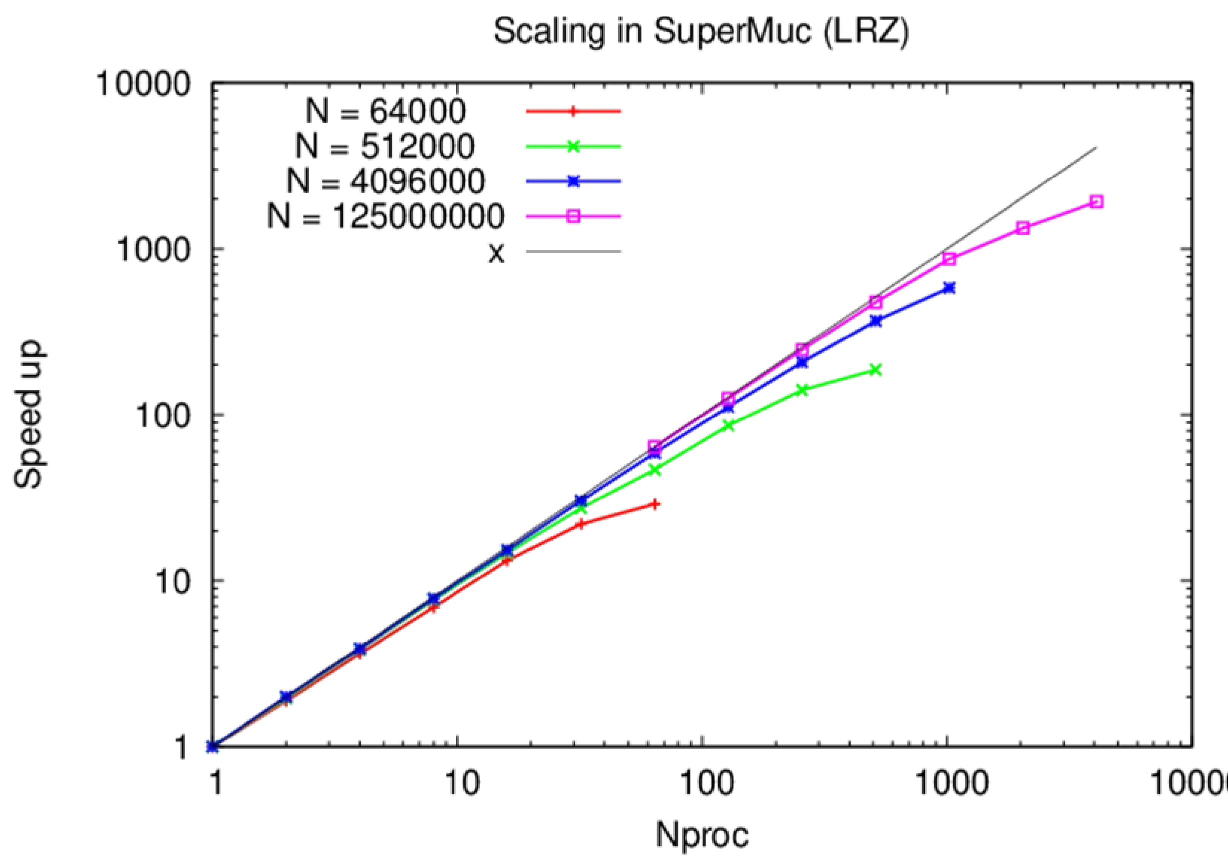
Multiscale particle methods: HPC

Parallel Particle Mesh library (PPM)

PPM is a software layer between the Message Passing Interface (MPI) and codes for simulations of physical systems using hybrid particle-mesh methods. The library is developed at the Institute of Computational Science (ETH) and is based on a unifying formulation for the simulations of discrete and continuous systems using particles (I. Sbalzarini, P. Koumoutsakos)



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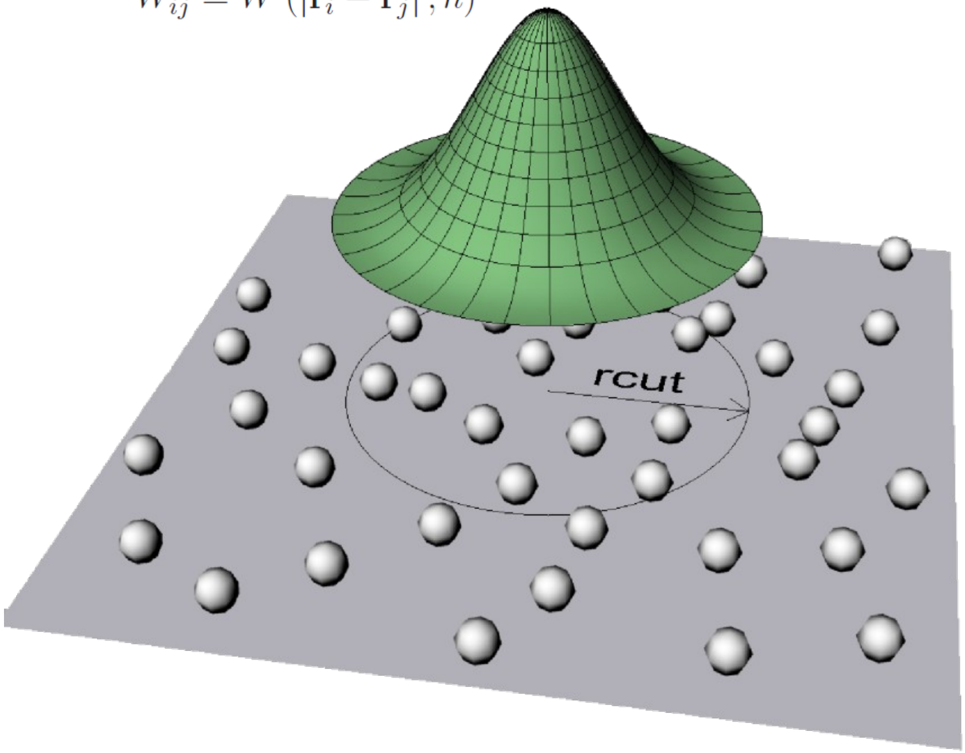
Smoothed Particle Hydrodynamics

$W_{ij} = W\left(\left|\mathbf{r}_i - \mathbf{r}_j\right|, h\right)$



J. J Monaghan. Smoothed particle hydrodynamics. *Rep. Prog. Phys.*, 68(8):1703–1759, 2005.

SPH volume $\mathcal{V}_i$

$$\frac{1}{\mathcal{V}_i} = d_i = \sum_{j=1}^{N_F} W\left(\left|\boldsymbol{r}_i - \boldsymbol{r}_j\right|\right)$$

$$f(\mathbf{x}) = \int_\Omega f(\mathbf{x}')\delta(\mathbf{x} - \mathbf{x}')\, d\mathbf{x}'$$

$\Downarrow$ mollification

$$\langle f(\mathbf{x})\rangle = \int_\Omega f(\mathbf{x}')W(\mathbf{x} - \mathbf{x}', h)\, d\mathbf{x}'$$

$\Downarrow$ quadrature

$\int \to \sum$

$$\langle f(\boldsymbol{x})\rangle \simeq \sum_j \frac{m_j}{\rho_j} f_j\, W(|\boldsymbol{x} - \boldsymbol{x}_j|, h)$$

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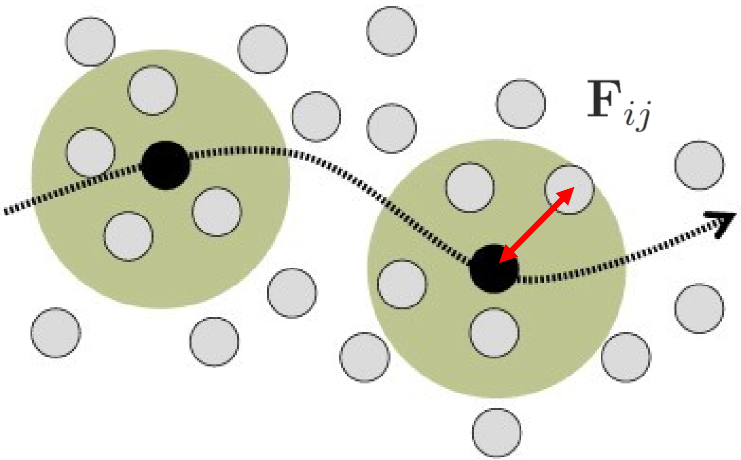
Smoothed Particle Hydrodynamics

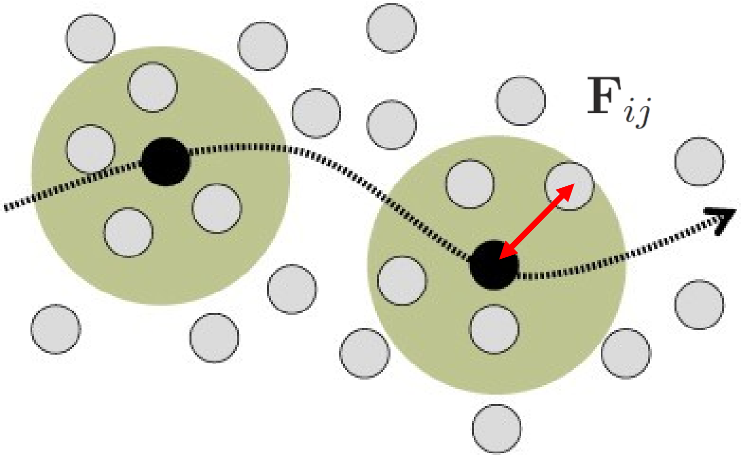
$$\dot{\mathbf{r}}_i = \mathbf{v}_i$$

$$m\dot{\mathbf{v}}_i = \underbrace{-\sum_j \left(\frac{P_i}{d_i^2} + \frac{P_j}{d_j^2}\right) W'_{ij}\mathbf{e}_{ij}}_{\mathbf{F}_{ij}^C} + \underbrace{\frac{5\eta}{3}\sum_j \frac{W'_{ij}}{d_i d_j r_{ij}}\left[\mathbf{v}_{ij} + (\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})\,\mathbf{e}_{ij}\right]}_{\mathbf{F}_{ij}^D} \cdot$$



Smoothed Particle Hydrodynamics

$$
\begin{aligned}
\dot{\mathbf{r}}_i &= \mathbf{v}_i \\
m\dot{\mathbf{v}}_i &= \underbrace{-\sum_j \left(\frac{P_i}{d_i^2} + \frac{P_j}{d_j^2}\right) W'_{ij}\mathbf{e}_{ij}}_{(\nabla p/\rho)_i} + \underbrace{\frac{5\eta}{3}\sum_j \frac{W'_{ij}}{d_i d_j r_{ij}}\left[\mathbf{v}_{ij} + (\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})\,\mathbf{e}_{ij}\right]}_{\eta\nabla^2\mathbf{v}_i + (\eta/3)\ \nabla(\nabla\cdot\mathbf{v}_i)}
\end{aligned}
$$



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Smoothed Particle Hydrodynamics

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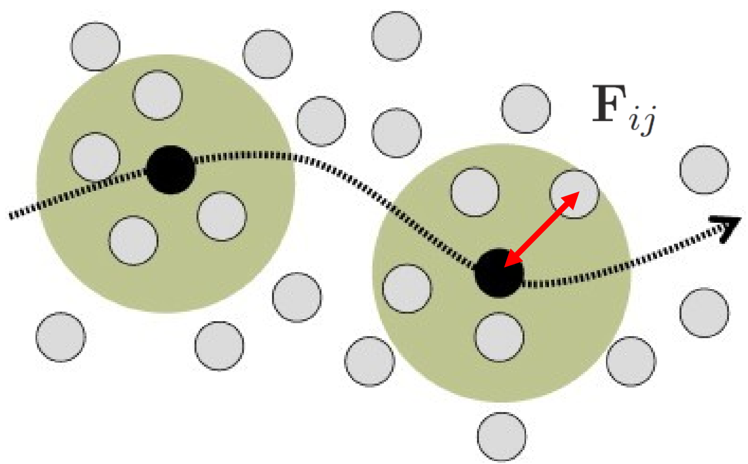
$$T_i\dot{S}_i = \underbrace{-\frac{5\eta}{6}\sum_j \frac{W'_{ij}}{d_i d_j r_{ij}}\left[\mathbf{v}_{ij}^2 + (\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})^2\right]}_{\phi_i=\eta(\nabla\mathbf{v}:\nabla\mathbf{v})_i} + \underbrace{2\kappa\sum_j \frac{W'_{ij}}{d_i d_j r_{ij}} T_{ij}}_{\kappa\nabla^2 T_i}$$



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Smoothed Particle Hydrodynamics

$$\dot{\mathbf{r}}_i = \mathbf{v}_i$$

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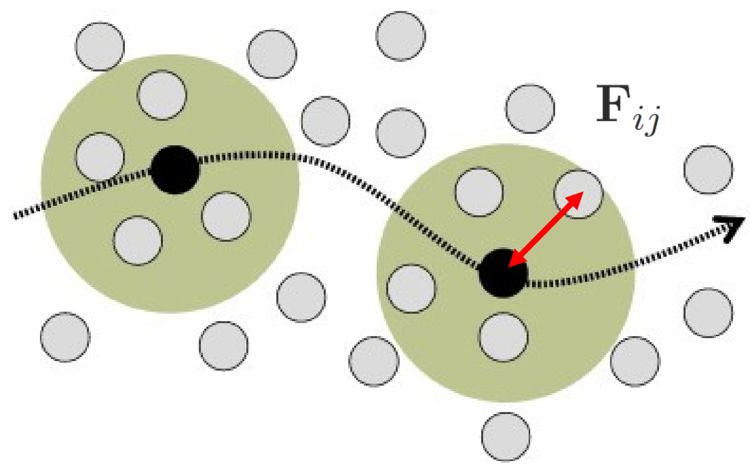
- **Lagrangian meshless discretization**
  (non)isothermal Navier-Stokes equations



How to introduce (Brownian) thermal fluctuations?

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Smoothed Dissipative Particle Dynamics

Espanol, Revenga, *Phys Rev E* (2003)
Vazquez, Ellero, Espanol : *J. Chem. Phys.* (2009)

$$\begin{aligned} \dot{\mathbf{r}}_i &= \mathbf{v}_i \\ m\dot{\mathbf{v}}_i &= \underbrace{-\sum_j \left(\frac{P_i}{d_i^2}+\frac{P_j}{d_j^2}\right) W'_{ij}\mathbf{e}_{ij}}_{\mathbf{F}_{ij}^C} + \underbrace{\frac{5\eta}{3}\sum_j \frac{W'_{ij}}{d_i d_j r_{ij}}\left[\mathbf{v}_{ij} + (\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})\,\mathbf{e}_{ij}\right]}_{\mathbf{F}_{ij}^D} + \sum_j \underbrace{A_{ij}\frac{d\bar{\boldsymbol{\xi}}_{ij}}{dt}\cdot\mathbf{e}_{ij}}_{\mathbf{F}_{ij}^R} \end{aligned}$$

$$d\bar{\boldsymbol{\xi}}_{ij} = \frac{1}{2}\left(d\boldsymbol{\xi}_{ij} + d\boldsymbol{\xi}_{ij}^T\right)$$

symmetric independent matrix Wiener process

$$\begin{aligned} \langle d\xi_{ij}^{\alpha\beta}\rangle &= 0 \\ \langle \xi_{ij}^{\alpha\alpha'}\xi_{i'j'}^{\beta\beta'}(t')\rangle &= (\delta_{ii'}\delta_{jj'} + \delta_{ij'}\delta_{ji'})\,\delta^{\alpha\beta}\delta^{\alpha'\beta'}dt \end{aligned}$$

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Smoothed Dissipative Particle Dynamics

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$$\begin{aligned} \dot{\mathbf{r}}_i &= \mathbf{v}_i \\ m\dot{\mathbf{v}}_i &= -\sum_j \left(\frac{P_i}{d_i^2}+\frac{P_j}{d_j^2}\right) W'_{ij}\mathbf{e}_{ij} + \frac{5\eta}{3}\sum_j \frac{W'_{ij}}{d_i d_j r_{ij}}\left[\mathbf{v}_{ij} + \left(\mathbf{e}_{ij}\cdot\mathbf{v}_{ij}\right)\mathbf{e}_{ij}\right] + \sum_j A_{ij}\frac{d\bar{\boldsymbol{\xi}}_{ij}}{dt}\cdot\mathbf{e}_{ij} \end{aligned}$$

Fluctuation Dissipation Theorem (FDT)

$$d\tilde{\mathbf{x}}\,d\tilde{\mathbf{x}}^T = 2k_B\mathbf{M}\,dt$$

$$d\bar{\boldsymbol{\xi}}_{ij} = \frac{1}{2}\left(d\boldsymbol{\xi}_{ij} + d\boldsymbol{\xi}_{ij}^T\right)$$

symmetric independent matrix Wiener process

$$\begin{aligned} \langle d\xi_{ij}^{\alpha\beta}\rangle &= 0 \\ \langle \xi_{ij}^{\alpha\alpha'}\xi_{i'j'}^{\beta\beta'}(t')\rangle &= \left(\delta_{ii'}\delta_{jj'} + \delta_{ij'}\delta_{ji'}\right)\delta^{\alpha\beta}\delta^{\alpha'\beta'}dt \end{aligned}$$

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Smoothed Dissipative Particle Dynamics

Non-isothermal case

Espanol, Revenga, *Phys Rev E* (2003)
Vazquez, Ellero, Espanol : *J. Chem. Phys*. (2009)

$$\dot{\mathbf{r}}_i = \mathbf{v}_i$$

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Smoothed Dissipative Particle Dynamics

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Vazquez, Ellero, Espanol : *J. Chem. Phys.* (2009)

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T_i\dot{S}_i &= -\frac{5\eta}{6}\sum_j \frac{W'_{ij}}{d_i d_j r_{ij}}\left[\mathbf{v}_{ij}^2 + (\mathbf{e}_{ij}\cdot\mathbf{v}_{ij})^2\right] + 2\kappa\sum_j \frac{W'_{ij}}{d_i d_j r_{ij}}T_{ij} + T_i d\tilde{S}_i
\end{aligned}$$

Thermodynamically-consistent (TC) Lagrangian discretization of stochastic Navier-Stokes equations. Thermodynamics Laws satisfied discretely by design (not only in the continuum limit).

$d\tilde{\mathbf{x}}d\tilde{\mathbf{x}}^T = 2k_B\mathbf{M}dt$	Fluctuation-Dissipation Theorem
$\dot{E} = \sum_i \dot{E}_i = 0$	Energy conservation (1st Law)
$\dot{S} = \sum_i \dot{S}_i = \sum_i \frac{\phi_i}{T_i} + \kappa\sum_{ij}\frac{-W'_{ij}}{d_i d_j r_{ij} T_i T_j}T_{ij}^2 \geq 0$	Entropy increase (2nd Law)

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SDPD: towards TC discretizations of arbitrary PDEs

TC incorporation of thermal fluctuations can be done systematically and rigorosuly in particle methods for any known PDEs.

Generalization of PDEs down to mesoscopic scales where Brownian motion is important.

PHYSICAL REVIEW E **79**, 056707 (2009)

Smoothed particle hydrodynamic model for viscoelastic fluids with thermal fluctuations

Adolfo Vázquez-Quesada,[1] Marco Ellero,[1,2] and Pep Español[1,3]

Microfluid Nanofluid (2012) 13:249–260
DOI 10.1007/s10404-012-0954-2

RESEARCH PAPER

A SPH-based particle model for computational microrheology

Adolfo Vázquez-Quesada · Marco Ellero · Pep Español

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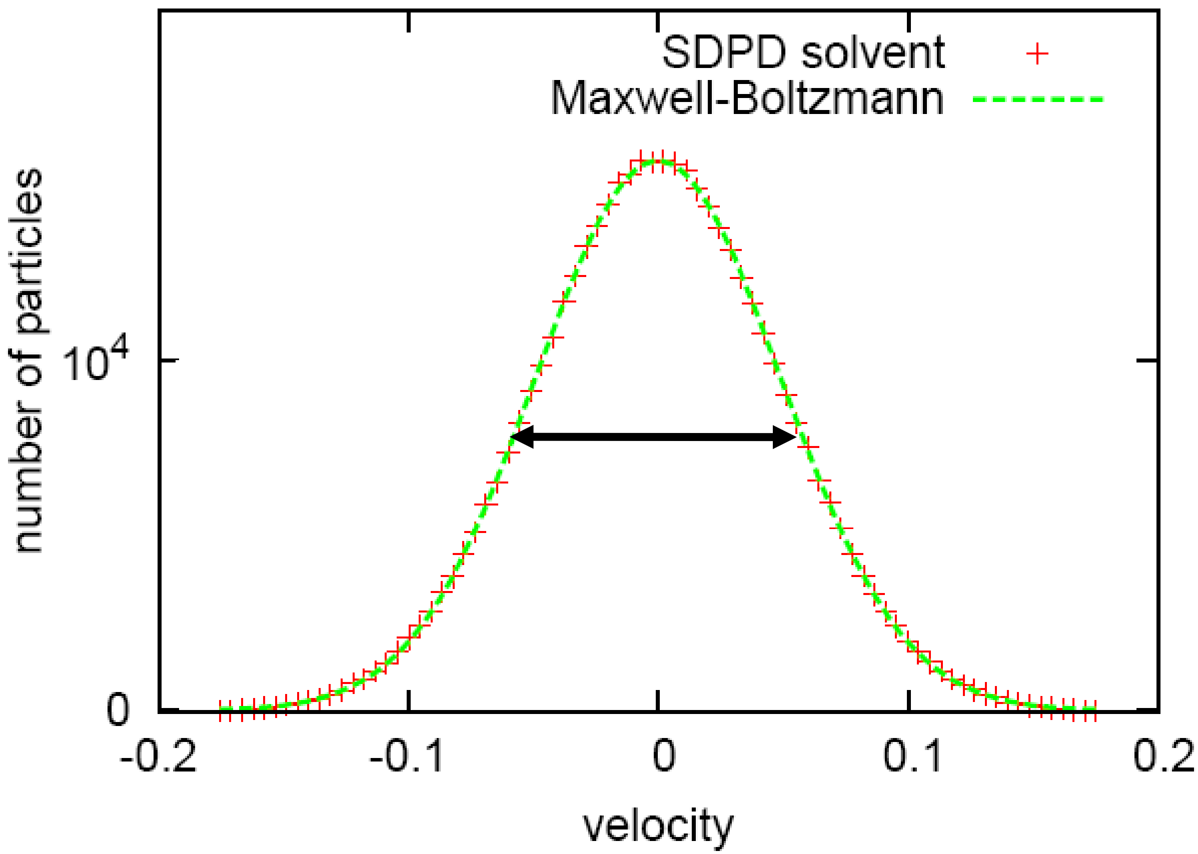
Smoothed Dissipative Particle Dynamics

Thermal fluctuations: Brownian motion



- particle volume-dependent thermal fluctuations

$$\langle \mathbf{v}_i^2 \rangle = D \frac{k_B T}{\rho_0} \frac{1}{\mathcal{V}}$$

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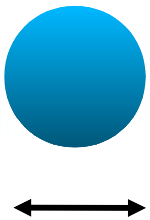
Smoothed Dissipative Particle Dynamics

Scaling of thermal fluctuations

Vazquez, et al. : *J. Chem. Phys*. 130 (2009) 034901

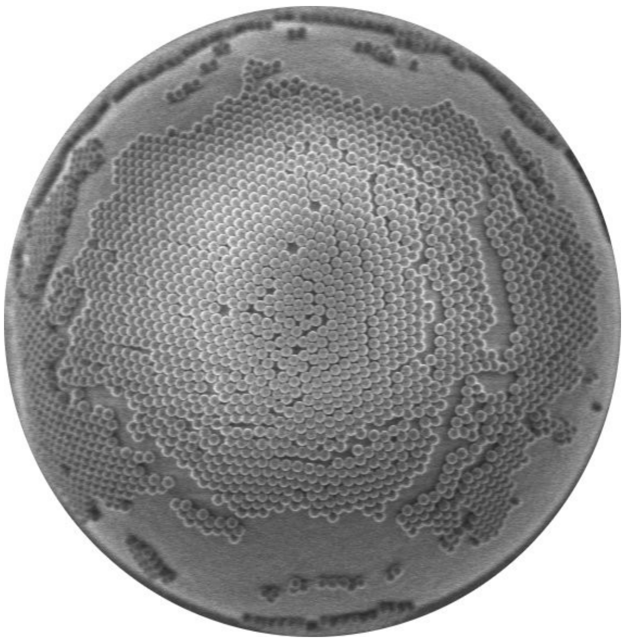


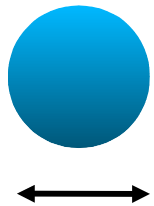
$l = 3cm$

$L = 30cm$

$$\langle v_i^2 \rangle = D \frac{k_B T}{\rho_0} \frac{1}{V} \approx 0$$

(SPH)





$l = 1\mu\text{m}$

$L = 10\,\mu m$

$$\langle v_i^2 \rangle = D \frac{k_B T}{\rho_0} \frac{1}{V} \neq 0$$

(SDPD)

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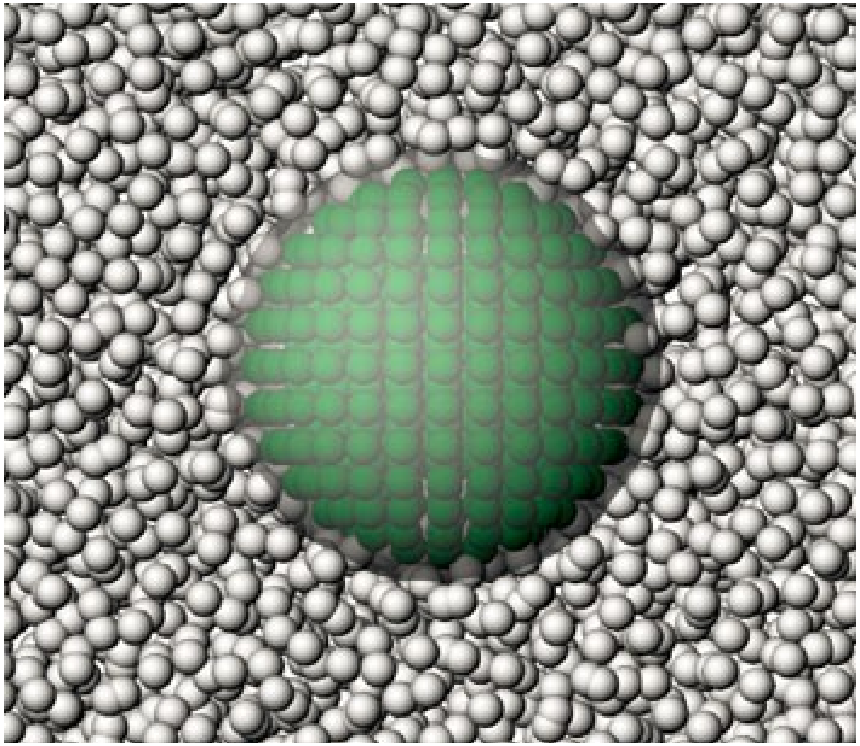
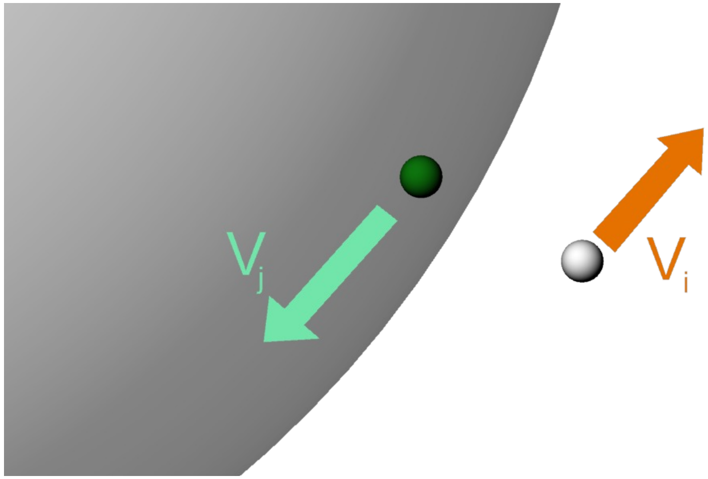
Suspended solid particles





No slip $\longrightarrow$ Morris boundary conditions

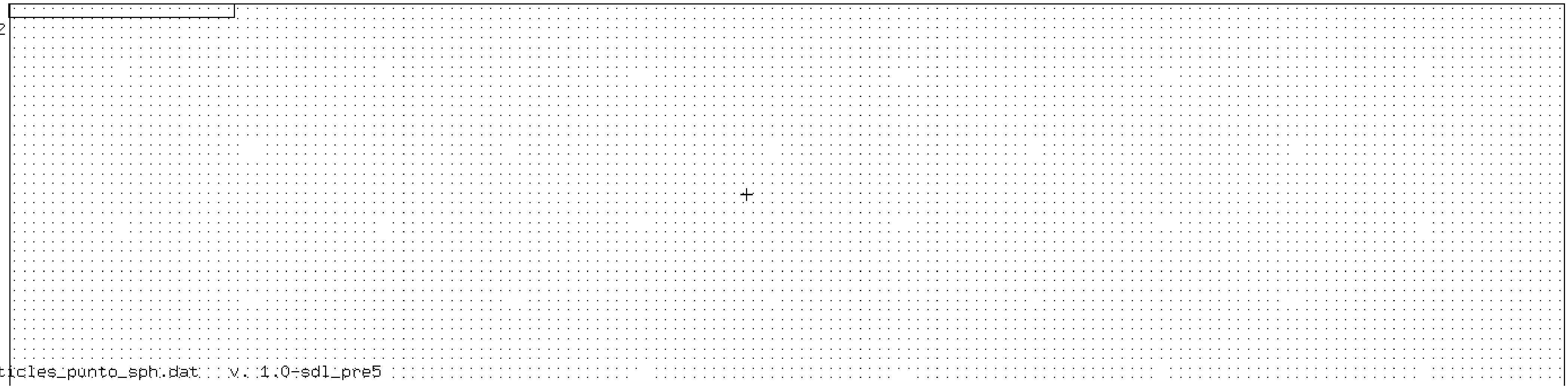
$$\boldsymbol{F}_\alpha^{\mathrm{sph}} = \sum_{j\in\alpha} \boldsymbol{F}_j$$

$$\boldsymbol{T}_\alpha^{\mathrm{sph}} = \sum_{j\in\alpha} (\boldsymbol{r_j} - \boldsymbol{R}_\alpha) \times \boldsymbol{F}_j$$

J P. Morris, P. J. Fox, and Y. Zhu. Modeling low reynolds number incompressible flows using sph. *J. Comput. Phys.*, 136(1):214–226, 1997.

X. Bian, S. Litvinov, R. Qian, M. Ellero, N.A. Adams, Physics of Fluids **24**(1), 012002 (2012)

Suspended solid particles



Beside formal thermodynamic consistency, also some technical advantages: SPH/SDPD

Fluid particles act as flowing discretization volumes.

Lagrangian description: no need of an underlying grid/remeshing

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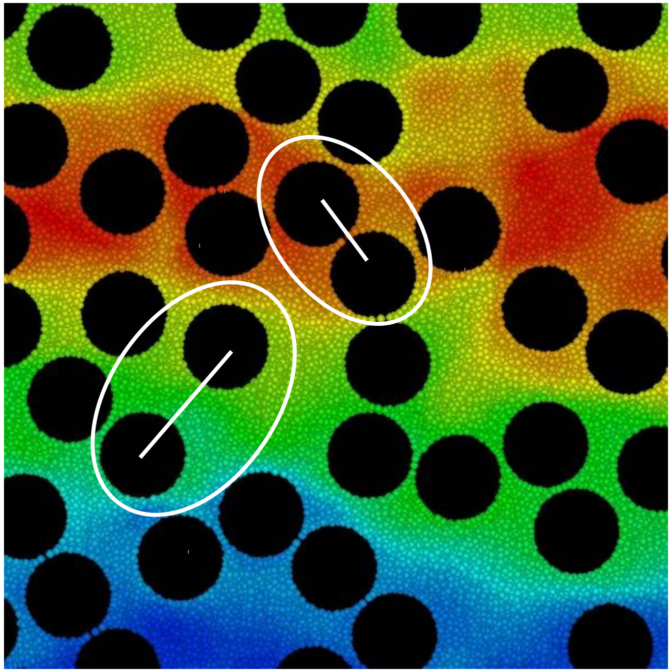
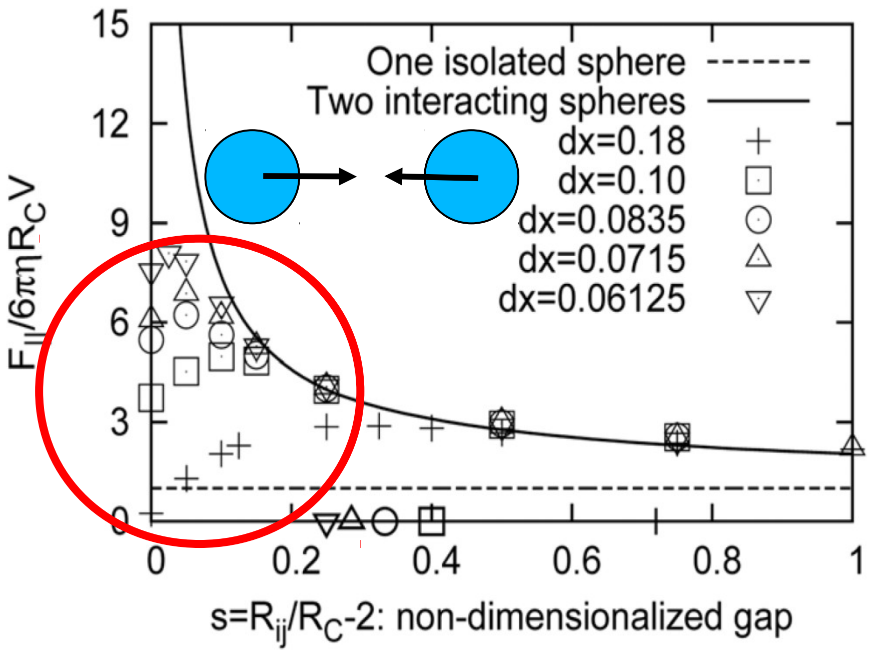
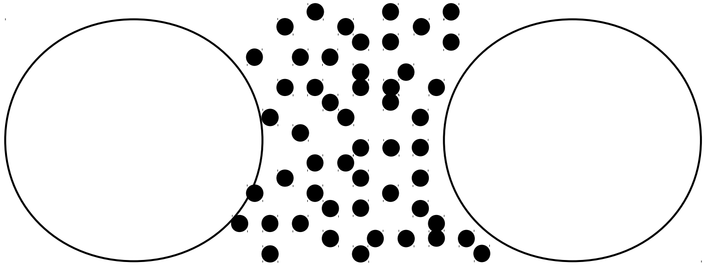
Suspended solid particles: lubrication

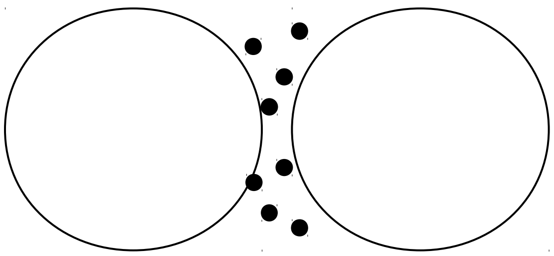




- Enough particles to resolve the fluid in the gap long-range hydrodynamic interactions → ok



- When the solid particles are too close…?



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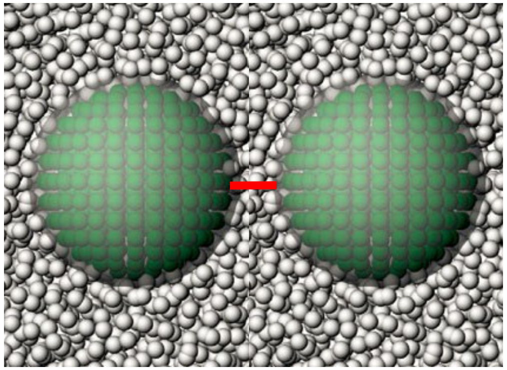
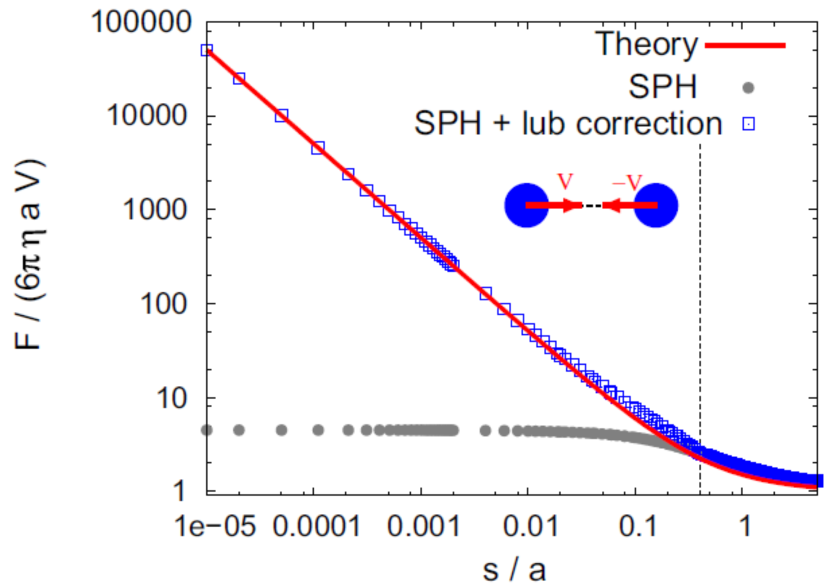
Suspended solid particles: lubrication



$$\mathbf{F}_{\alpha} = \mathbf{F}_{\alpha}^{\mathrm{SPH}} + \sum_{\beta \neq \alpha} \mathbf{F}_{\alpha\beta}^{lub\_cor}$$



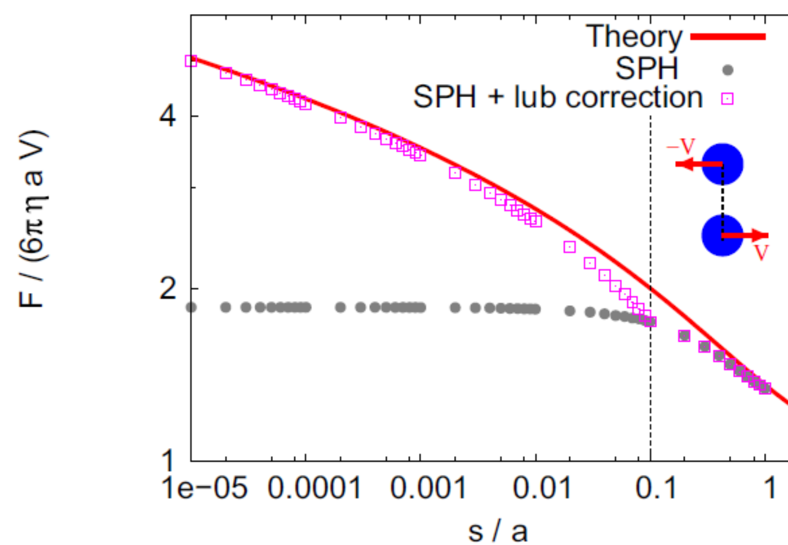
Normal/tangential lubrication

$$\boldsymbol{F}^{n}_{\alpha\beta}(s) = f_{\alpha\beta}(s)\boldsymbol{V}_{\alpha\beta} \cdot \boldsymbol{e}_{\alpha\beta}\boldsymbol{e}_{\alpha\beta}$$

$$\boldsymbol{F}^{t}_{\alpha\beta}(s) = g_{\alpha\beta}(s)\boldsymbol{V}_{\alpha\beta} \cdot (\mathbf{1} - \boldsymbol{e}_{\alpha\beta}\boldsymbol{e}_{\alpha\beta})$$

Vazquez, Ellero JNNFM (2016) in press

- Lubrication interaction singular
- Explicit inegrators numerically unstable
- **Implicit splitting schemes lubrication dynamics**
- Bian Ellero, *Comp. Phys. Comm.* 2014



S. Kim, S.J. Karrila, *Microhydrodynamics: principles and selected applications* (1991)

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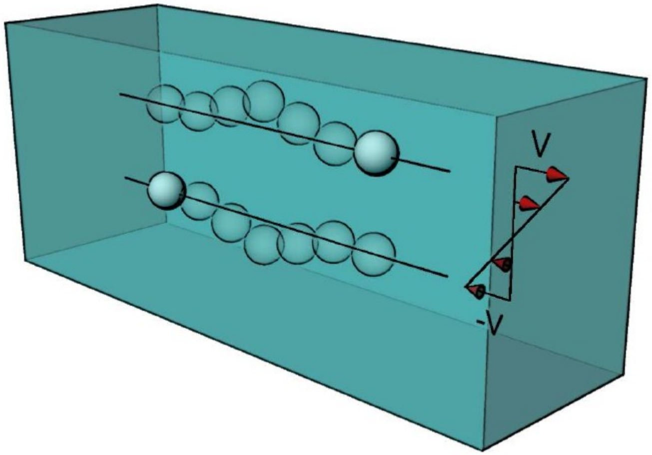
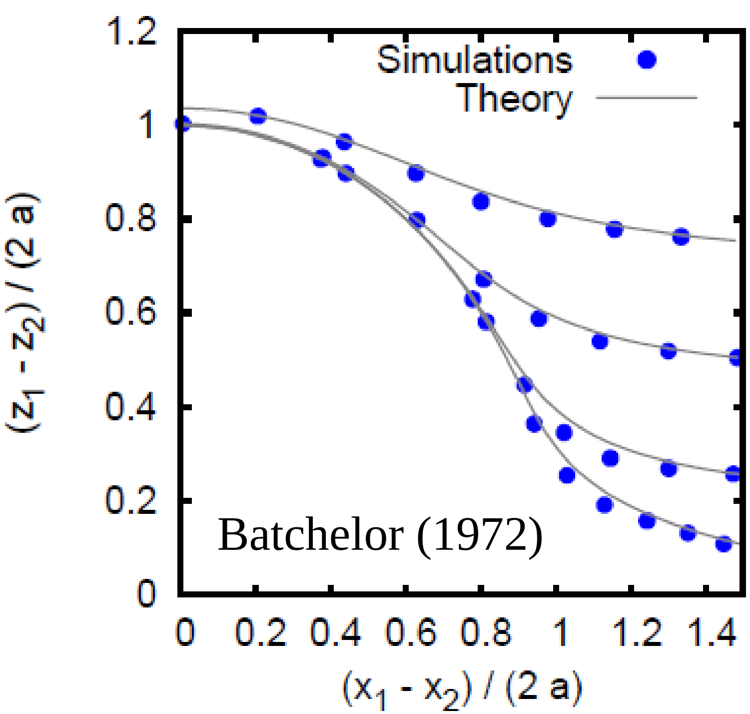
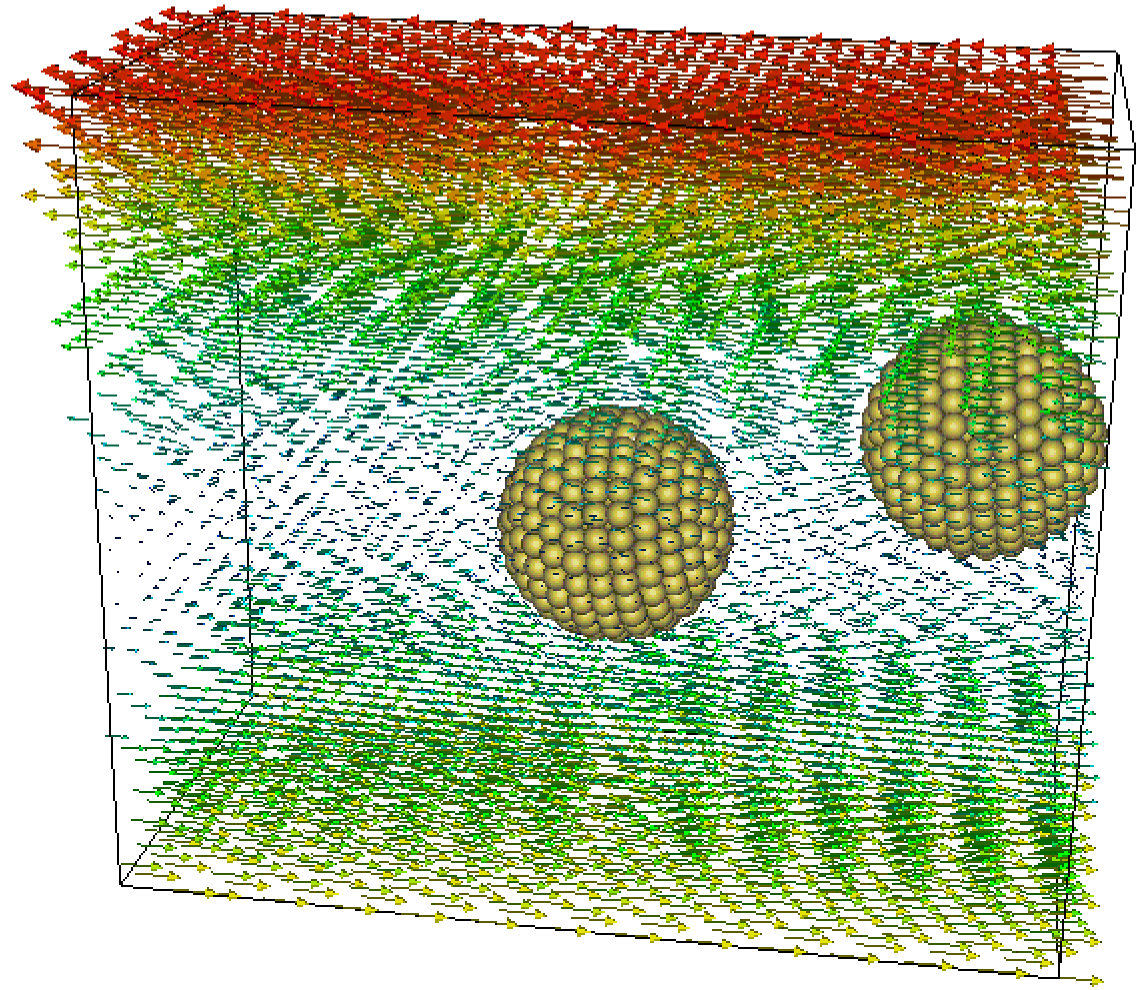
Suspended solid particles: dynamics in shear flow







Vazquez, Ellero. : *J. Non-Newt Fluid Mech* (2016)

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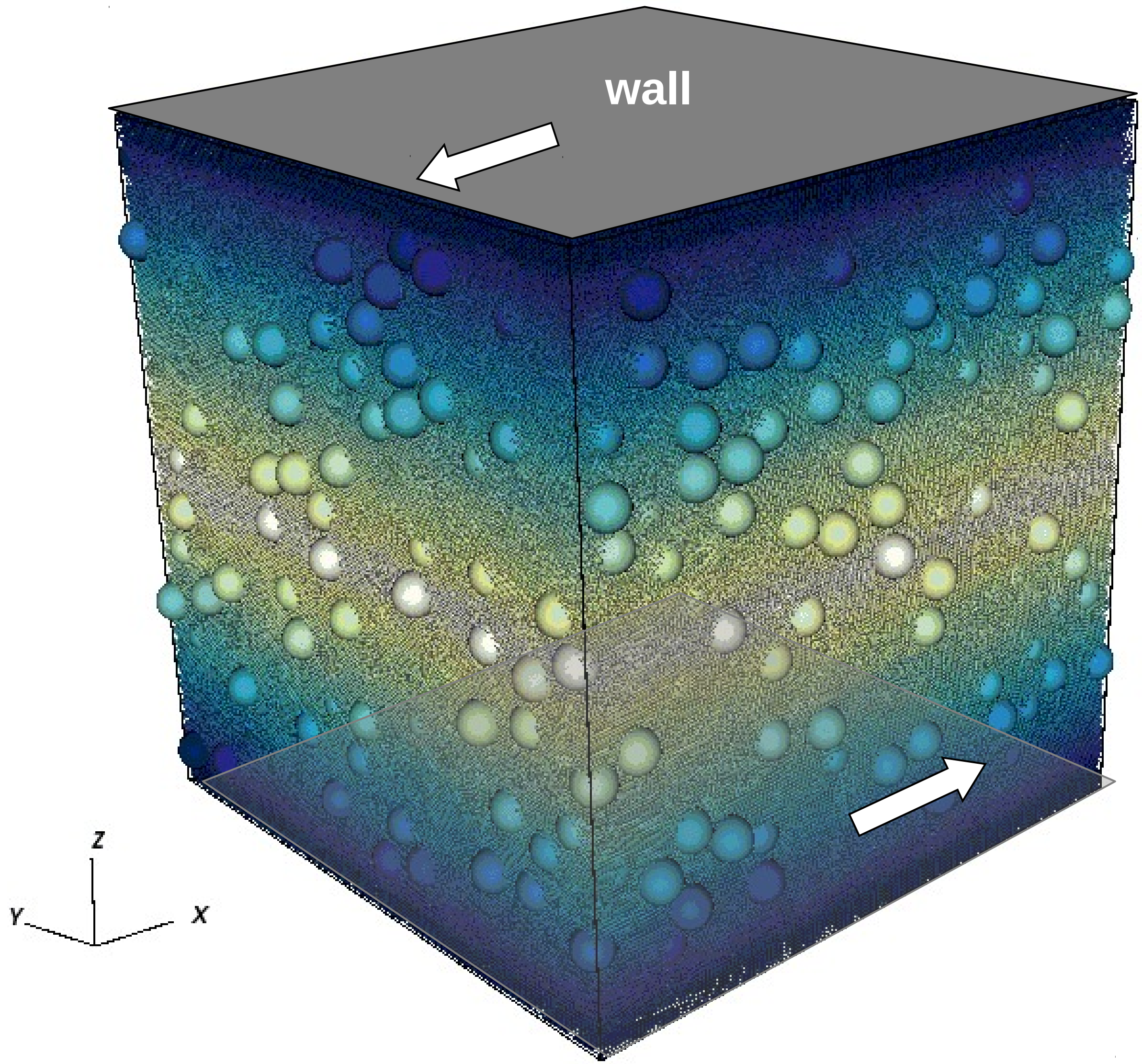
Particulate system: rheology



- $\pm V_w$
- $\dot{\gamma}^{in} = 2V_w/L_z$
- $\eta = \dfrac{\sigma_{xz}}{\dot{\gamma}} = \dfrac{F_x}{L_x L_y \dot{\gamma}}$
- *Φ*= 0-0.5
- *a*=1, *L*=32, Re_p=0.006
- N=4.000.000 particles
- Nc≈4000 (*Φ*= 0.4)

of a simulation corresponding to solid con-
4, and box size $L_x = 32a, L_y = 32a, L_z =$
ımber of solid particles was $N_c = 3129$ and
s $N \approx 4.3 \times 10^6$. Solid and fluid particles
with grey and blue colors respectively. In
es correspond to velocity vectors associated
to SPH fluid particles. For clarity, upper/lower walls have
not been drawn. To rule out finite size effects on rheology,
simulations were conducted up to gap size $H = 64a$.

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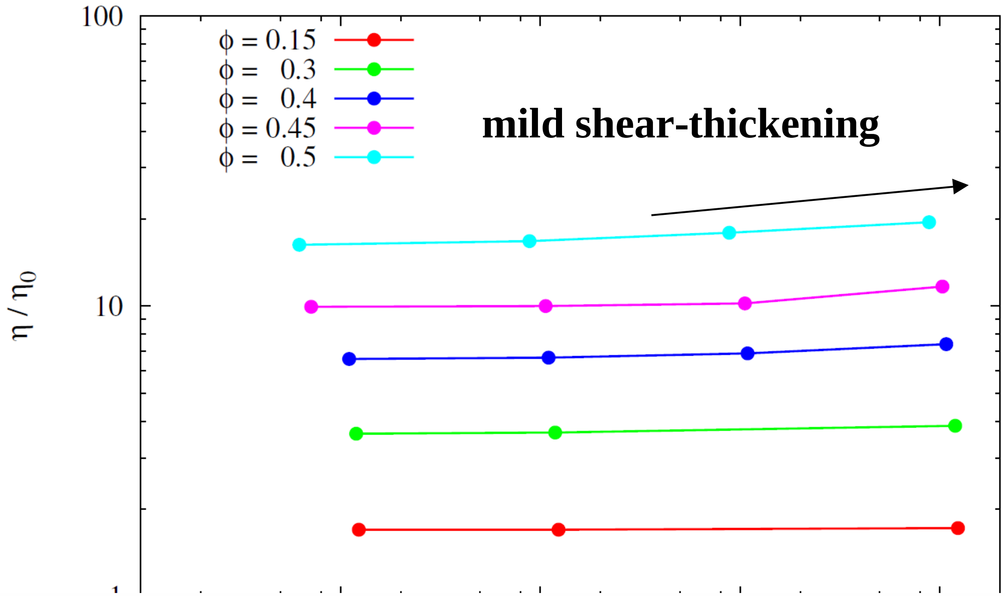
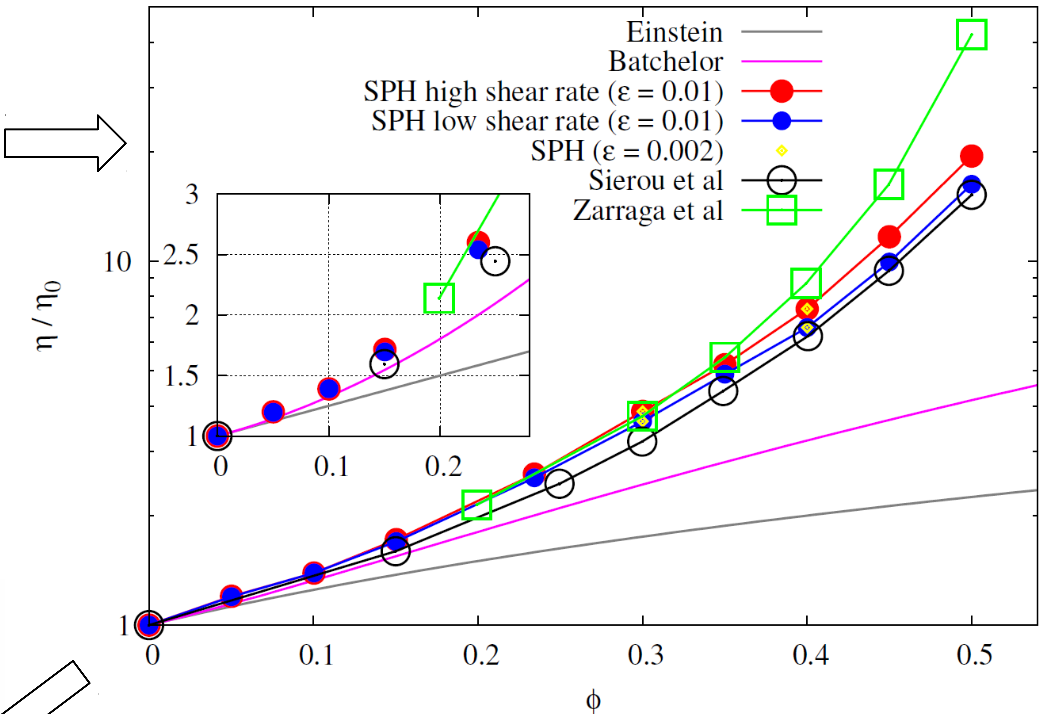
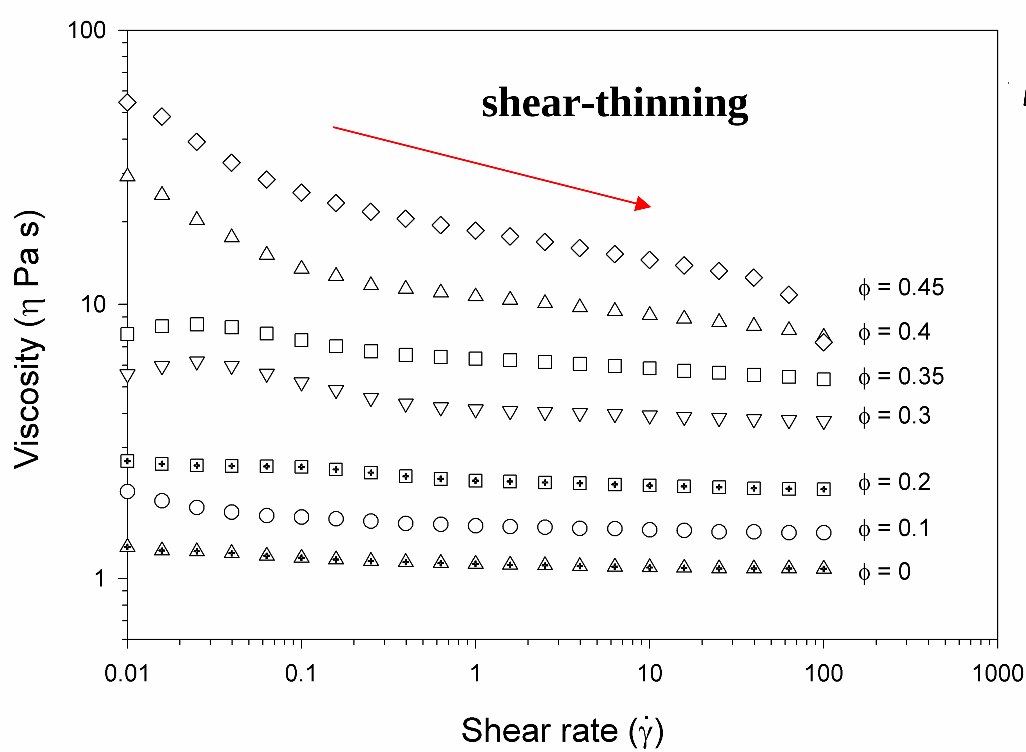
Particulate system: rheology

Vazquez, Ellero JNNFM (2016) in press







- ❑ Rheology Newtonian suspension
- ❑ Experimental
  (Acrivos 1980, Zarraga 2001, Tanner 2013)

No current explanation: > 30yrs problem

Tanner JOR (2013)

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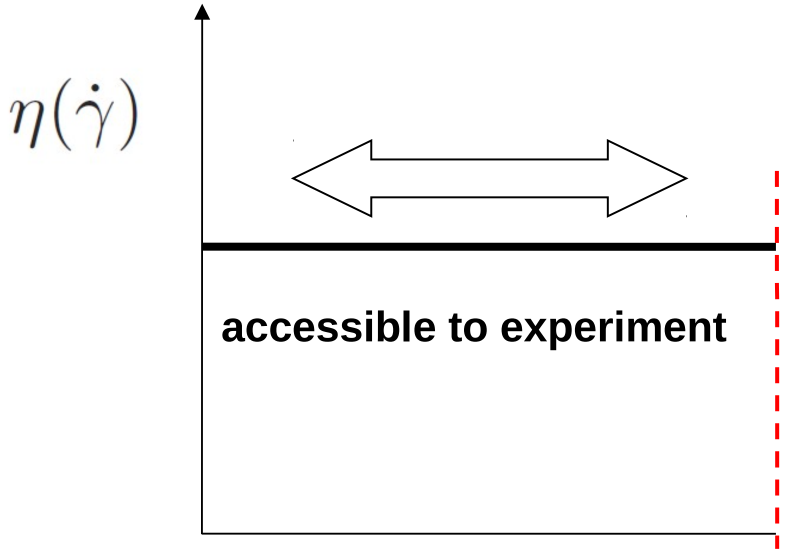
„Hidden“ shear-rate non-Newtonian effects

- Suspending fluids are *nominally* Newtonian according to experimentalists.

Vazquez, Tanner, Ellero Phys Rev Lett (under review)

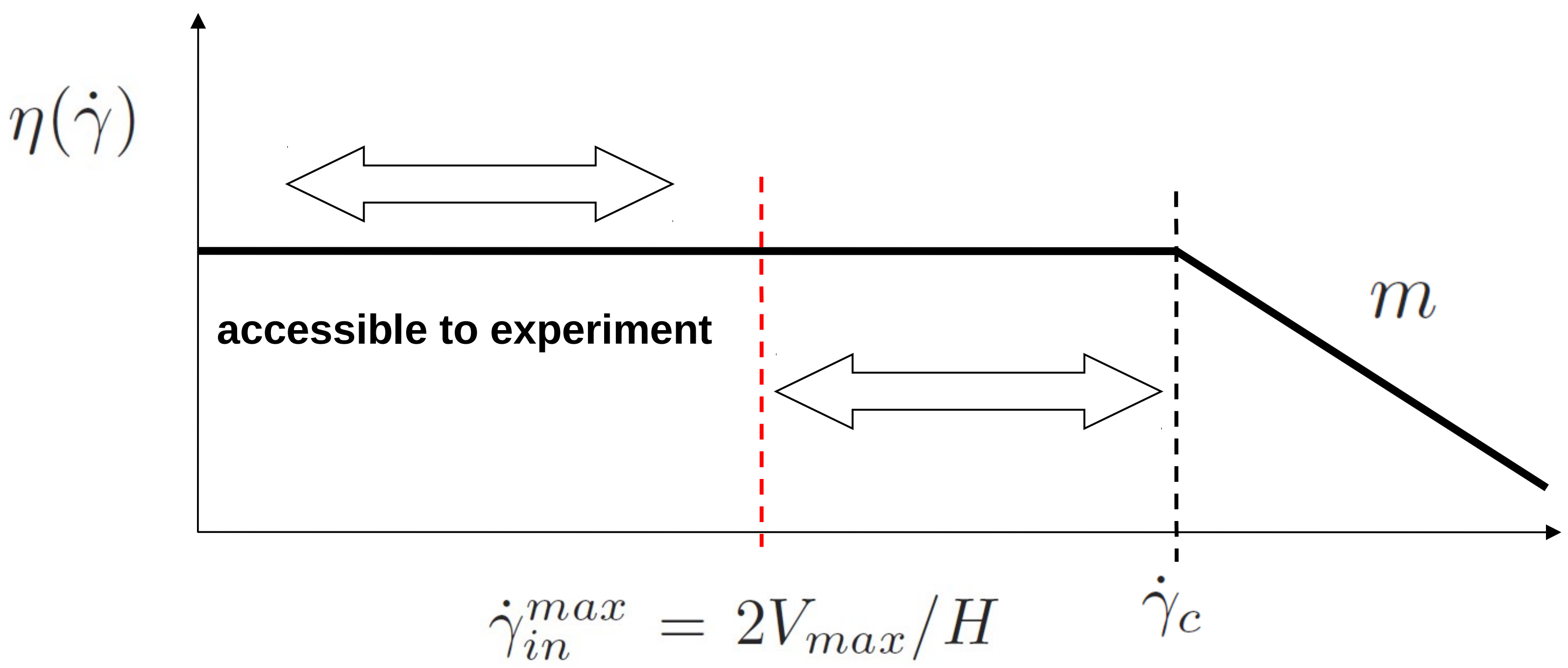


$$\dot{\gamma}_{in}^{max} = 2V_{max}/H$$

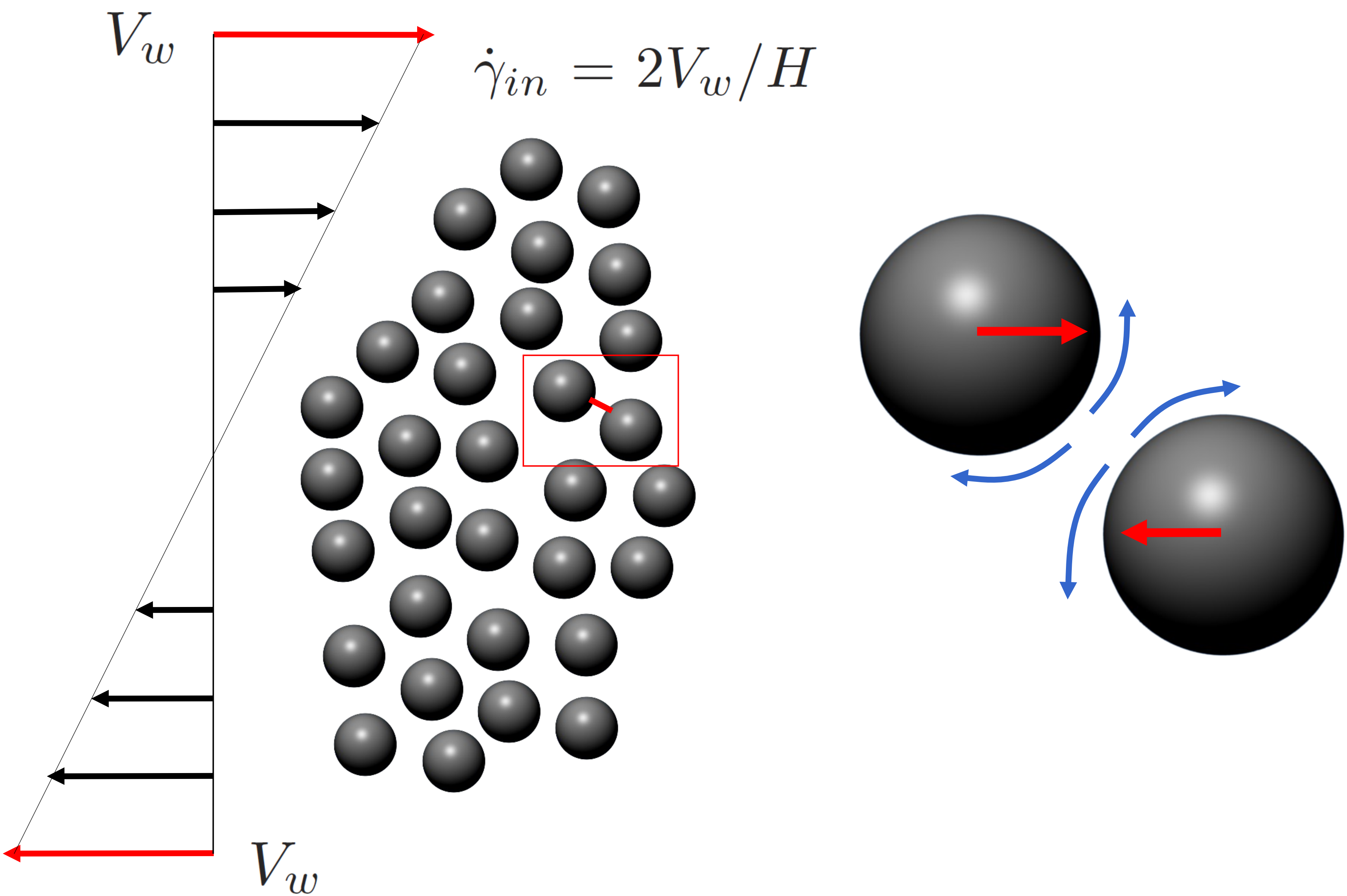
„*Hidden*“ shear-rate non-Newtonian effects

- Suspending fluids are *nominally* Newtonian according to experimentalists.

Vazquez, Tanner, Ellero Phys Rev Lett (under review)



„Hidden" shear-rate non-Newtonian effects



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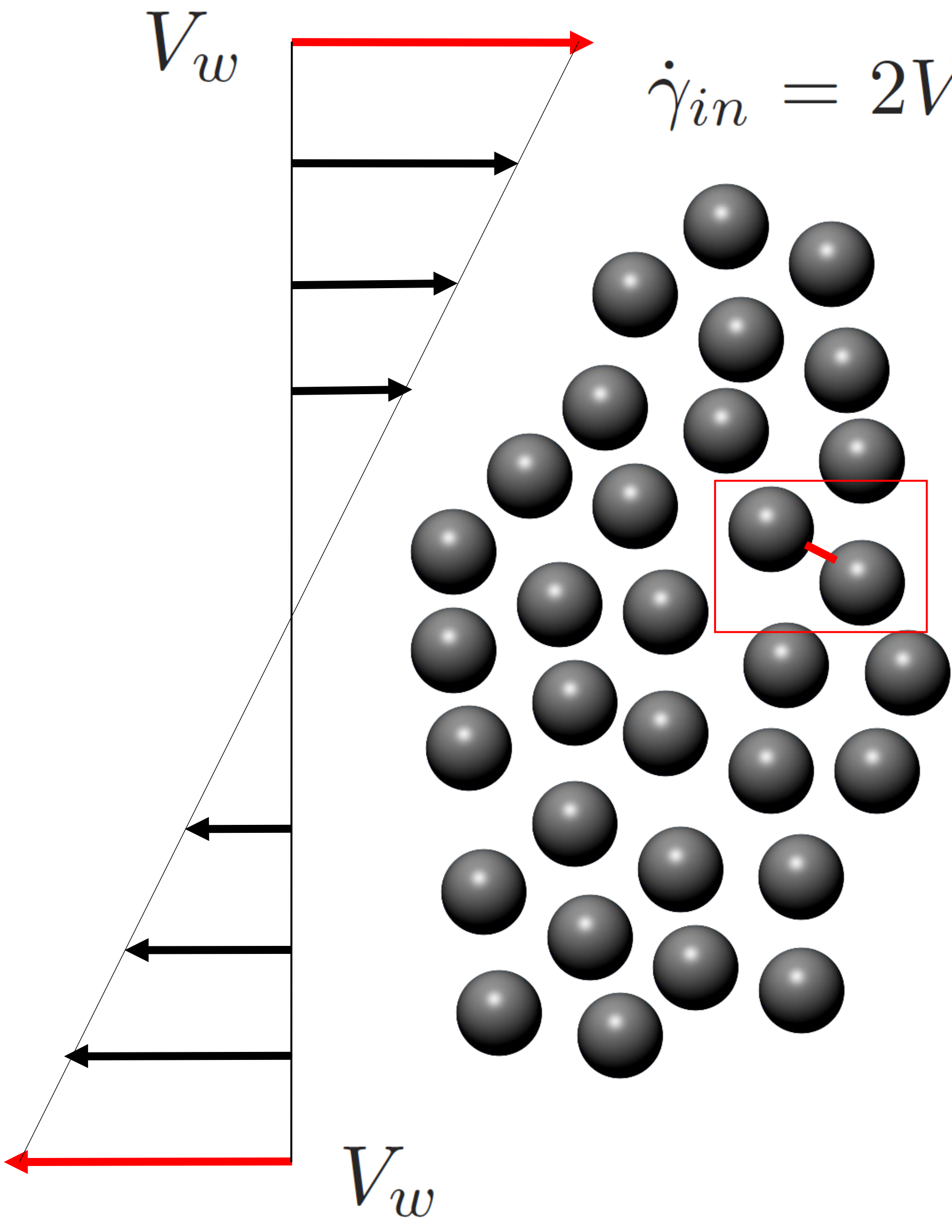
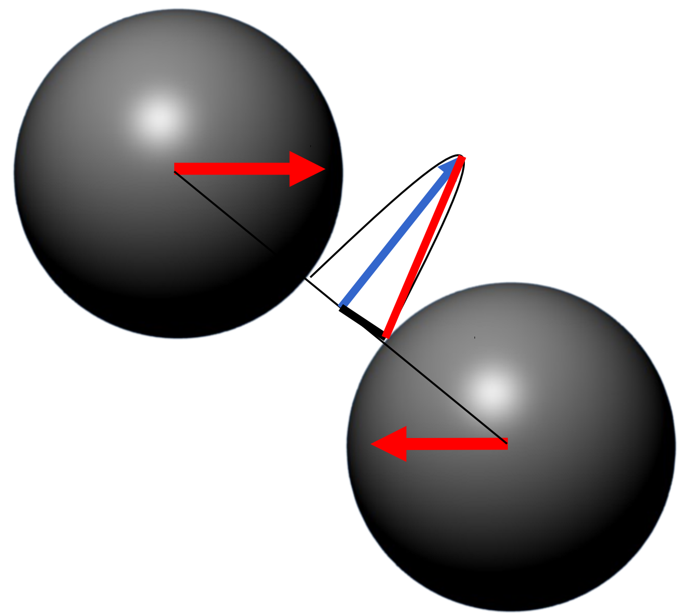
„*Hidden*“ shear-rate non-Newtonian effects



$$\dot{\gamma}_{in} = 2V_w/H$$



$$\dot{\gamma}_{loc} \;=\; 9\|\boldsymbol{V}_{\alpha\beta}\|/(16s)\sqrt{3a/s}$$

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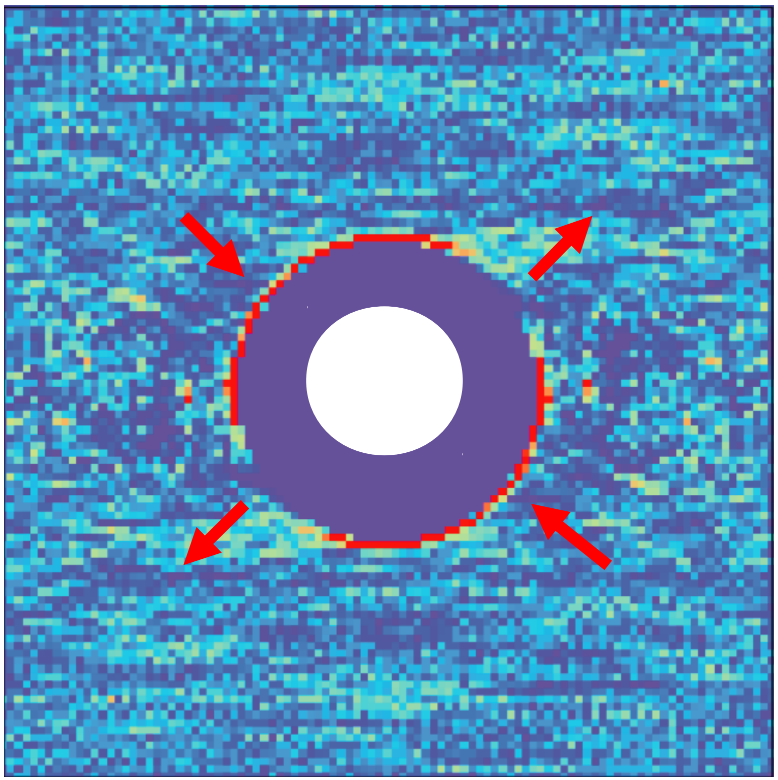
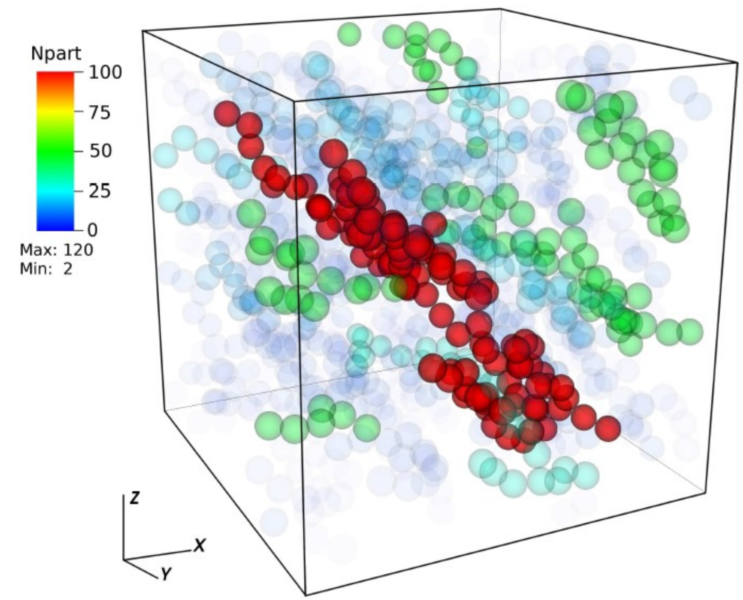
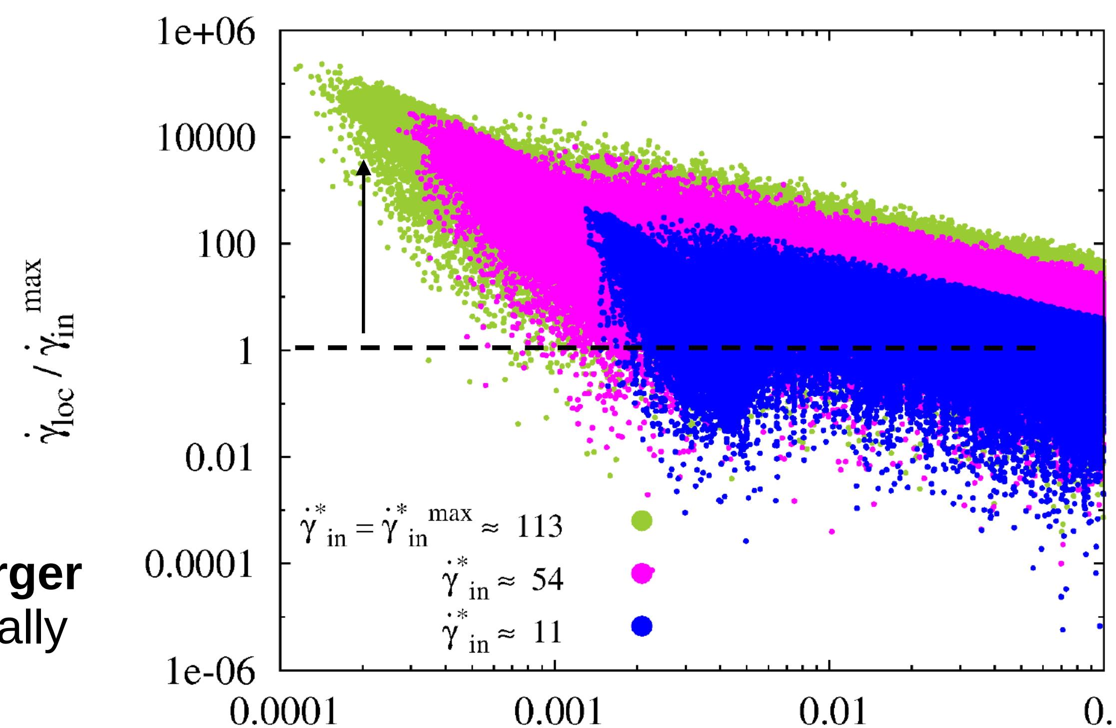
„Hidden“ shear-rate non-Newtonian effects

- radial distribution function (x-z)

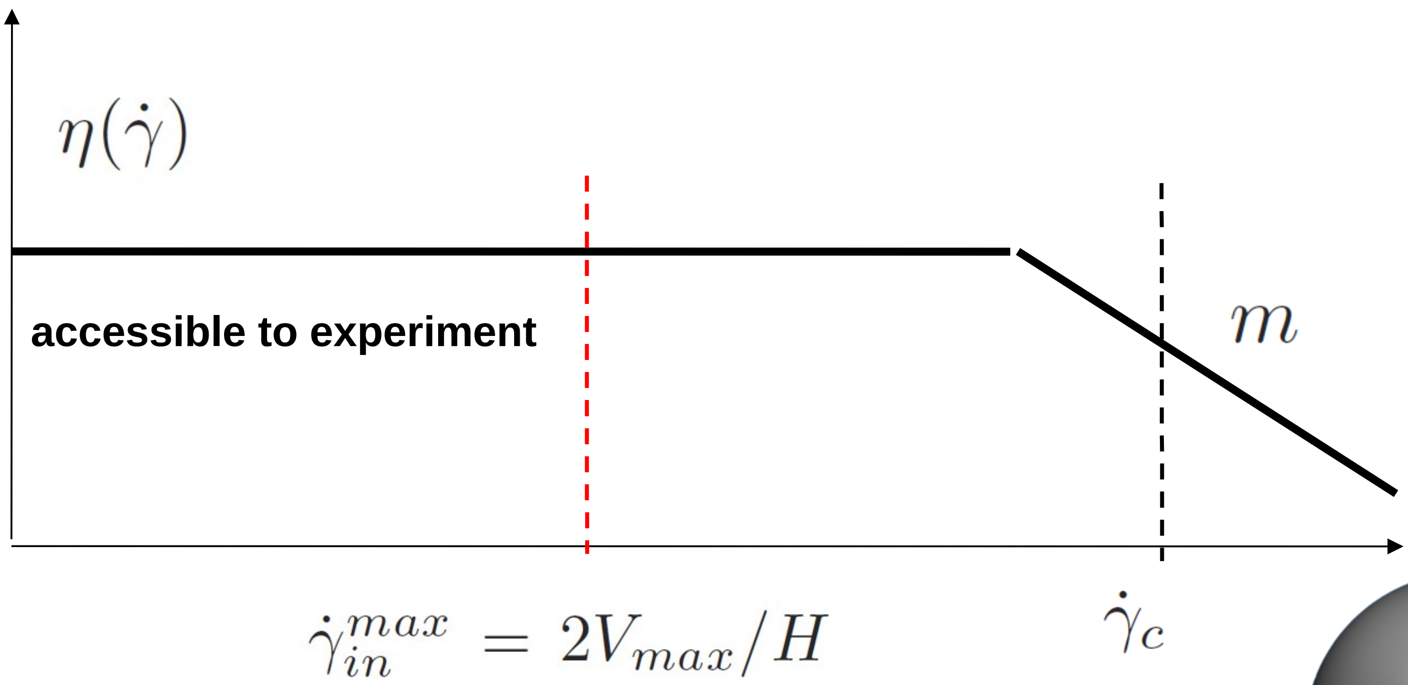




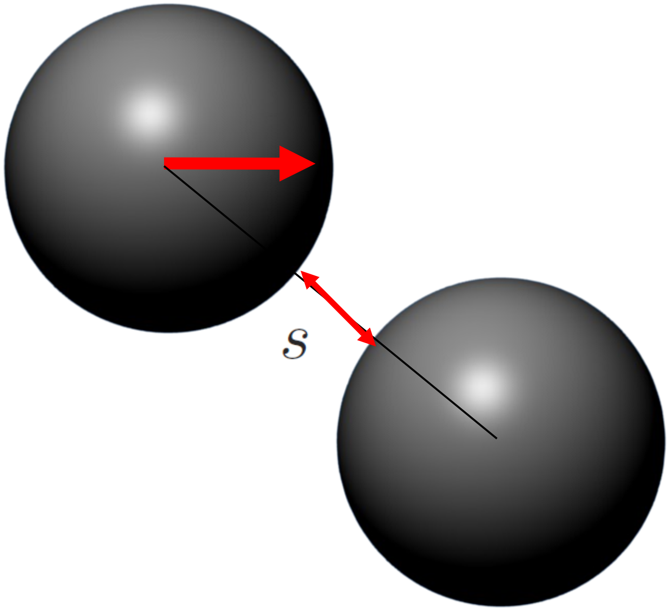


Local shear rates in the interstitial fluid domain can be **orders of magnitude larger** than the shear rate applied macroscopically

„*Hidden*“ shear-rate non-Newtonian effects



$$\boxed{\eta(\dot\gamma) = \eta_0 \begin{cases} 1, & \dot\gamma < \dot\gamma_c \\ \left(\frac{\dot\gamma}{\dot\gamma_c}\right)^m, & \dot\gamma \geq \dot\gamma_c \end{cases}}$$



$$\boldsymbol{F}^{\mathrm{lub}}_{\alpha\beta}(s) = -6\pi\eta_0 \left(\frac{a_\alpha a_\beta}{a_\alpha + a_\beta}\right)^2 \frac{1}{s} \left(\boldsymbol{V}_{\alpha\beta} \cdot \boldsymbol{e}_{\alpha\beta}\right) \boldsymbol{e}_{\alpha\beta}$$

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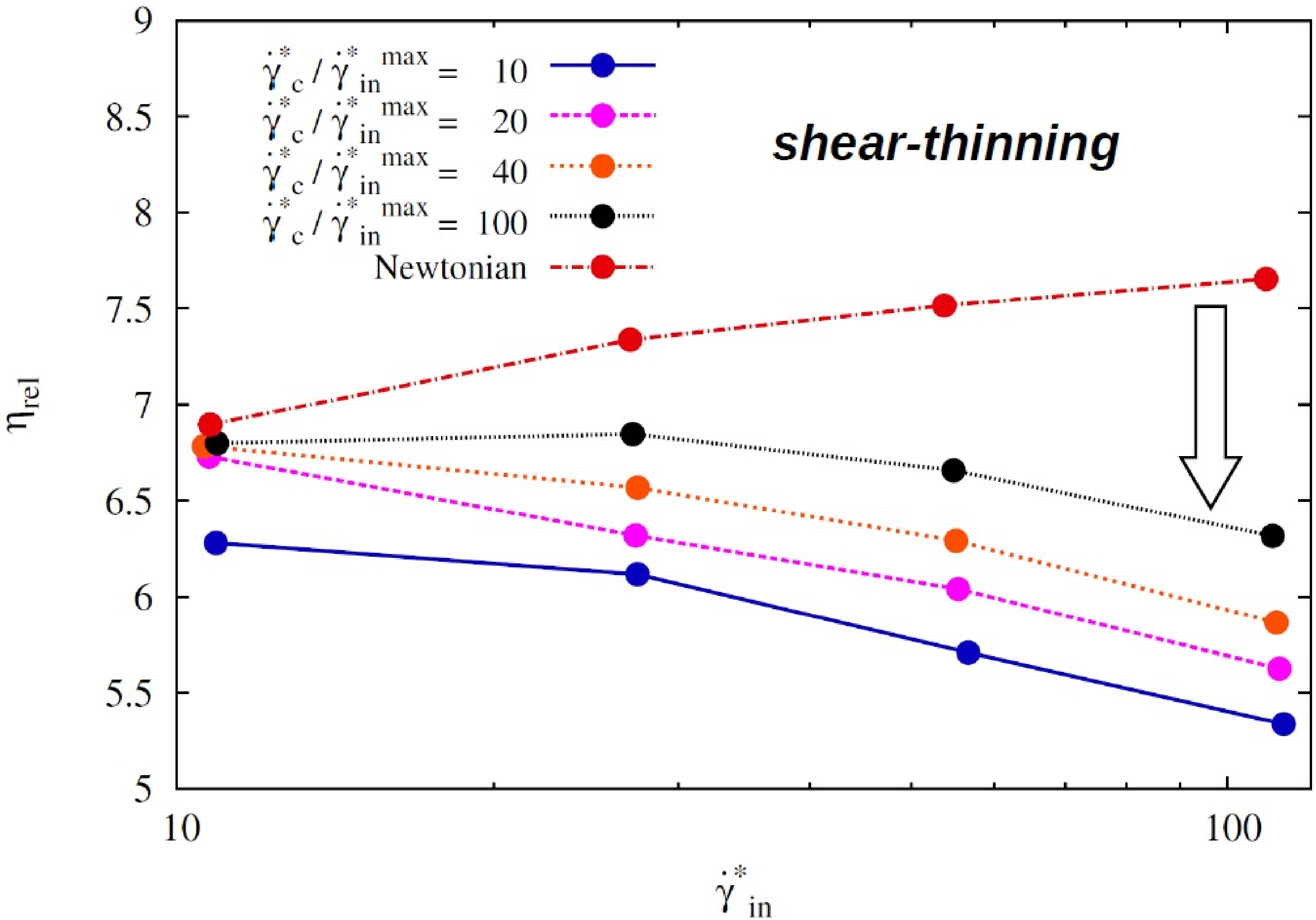
„*Hidden*“ shear-rate non-Newtonian effects

- Qualitative agreement



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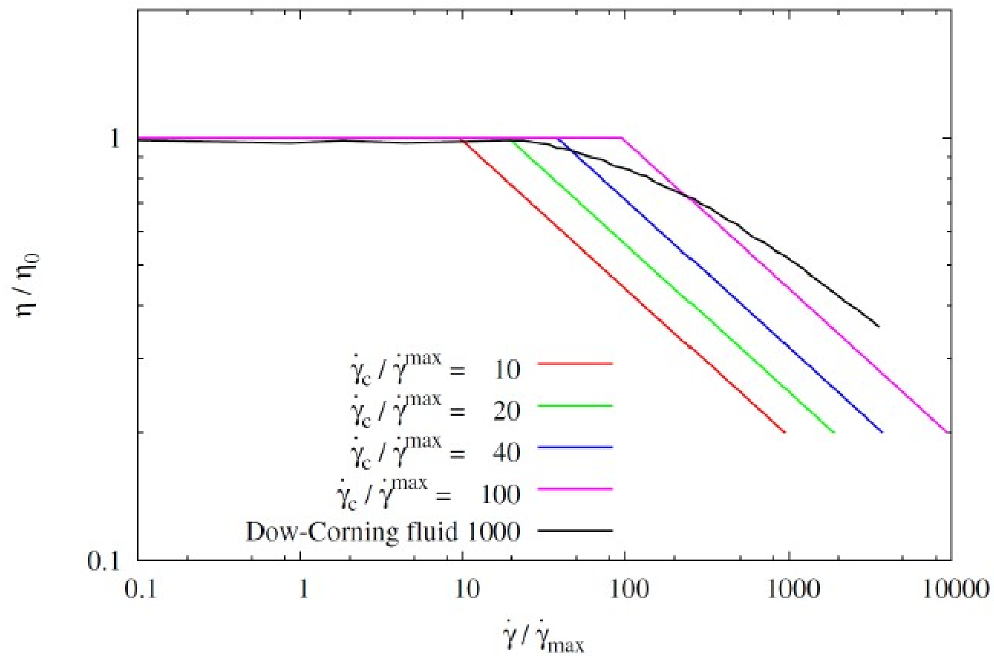
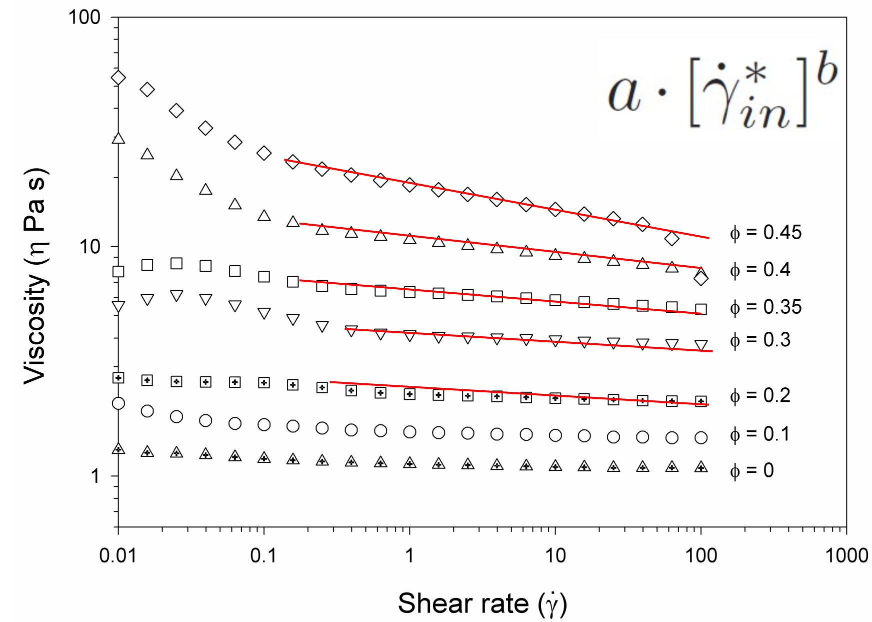
„Hidden“ shear-rate non-Newtonian effects

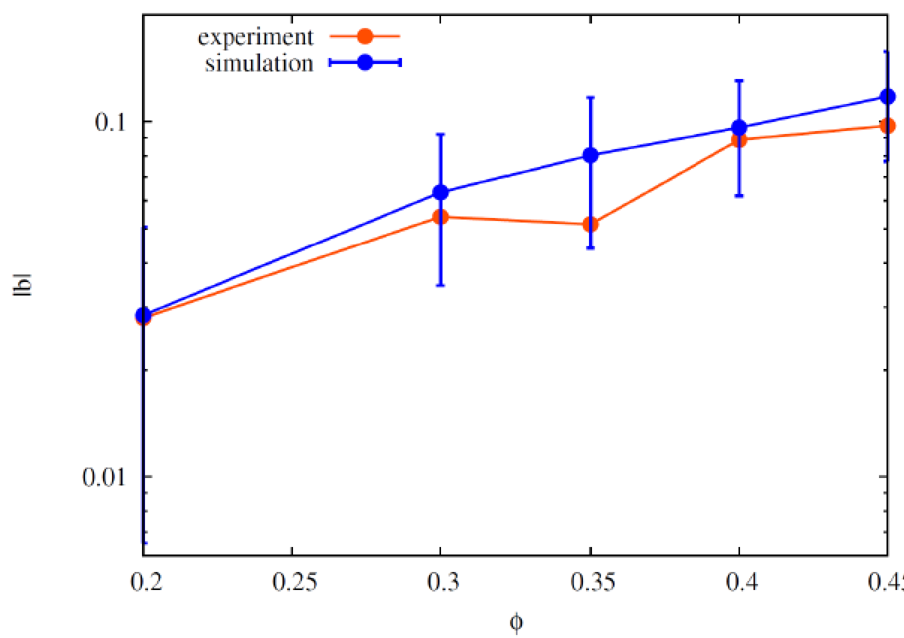
- Matching exact “hidden” high-shear rate properties of silicon fluids





Flow Behavior of Narrow-Distribution Polydimethylsiloxane

C. L. LEE, K. E. POLMANTEER, and E. G. KING, *Dow Corning Corporation, Midland, Michigan, 48640*



- Quantitative agreement

Outline

- **Multiscale particle methods:** towards thermodynamics- consistent discretization of PDEs
- **Particulate systems modelling**
- **Rheology of concentrated suspensions**
- **Paramagnetic nanoparticle suspensions**
- **Further applications and conclusions**

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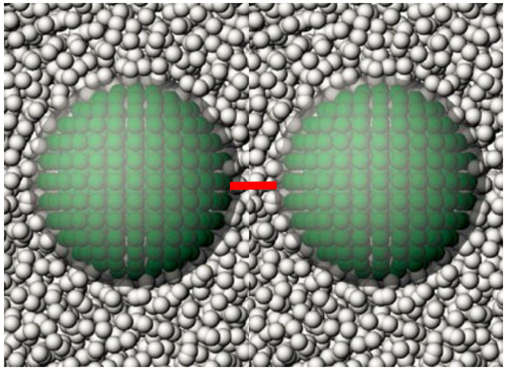
Paramagnetic nanoparticles



- external magnetic field $\boldsymbol{B}$
- magnetic dipole $\boldsymbol{m}_i = \frac{V_c \Delta\chi}{\mu_0} \boldsymbol{B}$
- magnetic force

$$\boldsymbol{F}_B^{ij} = \frac{3\mu_0}{4\pi r_{ij}^4} \left[(\boldsymbol{m}_i \cdot \boldsymbol{e}_{ij})\, \boldsymbol{m}_j + (\boldsymbol{m}_j \cdot \boldsymbol{e}_{ij})\, \boldsymbol{m}_i - \right.$$
$$\left. (5\, (\boldsymbol{m}_j \cdot \boldsymbol{e}_{ij})\, (\boldsymbol{m}_i \cdot \boldsymbol{e}_{ij}) - (\boldsymbol{m}_i \cdot \boldsymbol{m}_j))\, \boldsymbol{e}_{ij} \right]$$

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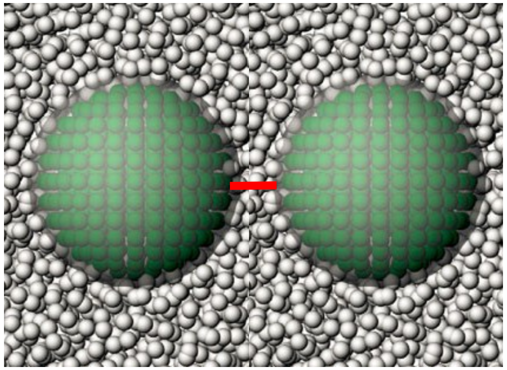
Paramagnetic nanoparticles



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- constant ***B***

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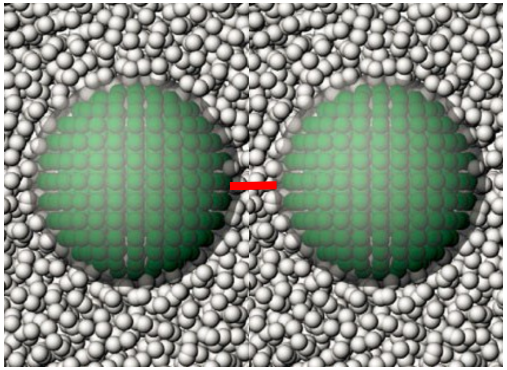
Paramagnetic nanoparticles



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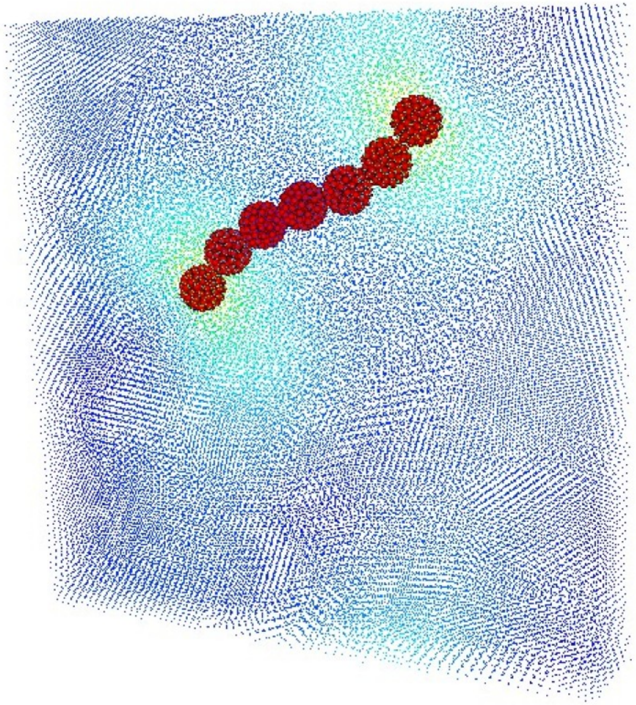
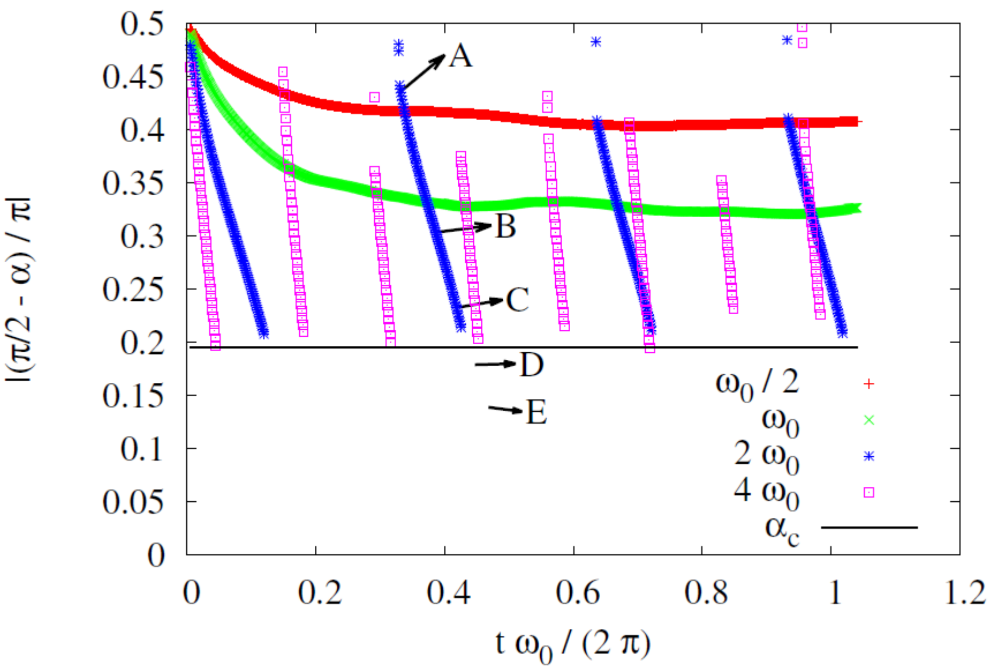
$$\left. (5\, (\boldsymbol{m}_j \cdot \boldsymbol{e}_{ij})\, (\boldsymbol{m}_i \cdot \boldsymbol{e}_{ij}) - (\boldsymbol{m}_i \cdot \boldsymbol{m}_j))\, \boldsymbol{e}_{ij} \right]$$

- constant ***B***

- rotating $\boldsymbol{B} = B_0(\cos(\omega t), \sin(\omega t), 0)$



Paramagnetic nanoparticles: S-shape and breakup



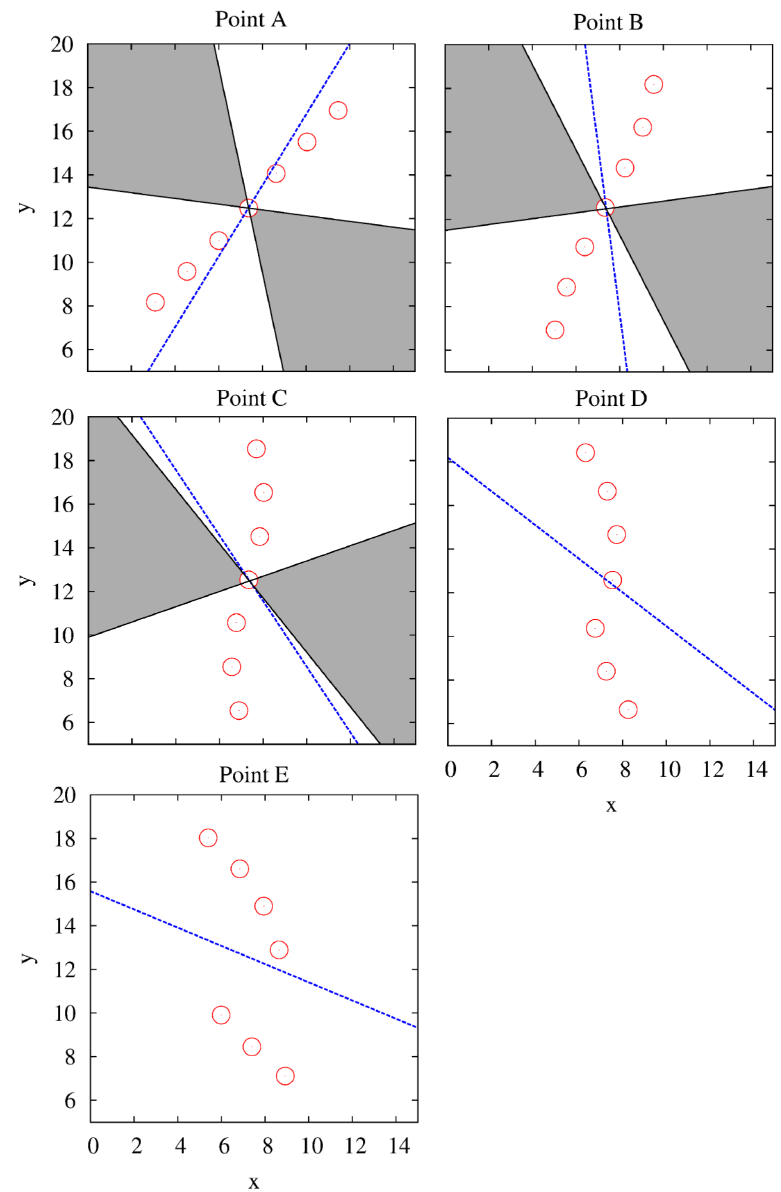
- chains try to follow rotating B
- Small ω: rigid rods (no delay)
- Moderate ω:: deformation S-shape (delay)
- High ω: significant S-shape deformation

$$\boldsymbol{F}_B^{ij}|_{\boldsymbol{e}_{ij}} = \frac{F_0}{r_{ij}^4}\left[1 - 3\left(\overline{\boldsymbol{m}} \cdot \boldsymbol{e}_{ij}\right)^2\right]\boldsymbol{e}_{ij}$$

- largest angle between m-B at the center chain

$$\arccos\left(\frac{1}{\sqrt{3}}\right) < \alpha$$

magnetic normal repulsion → breakup



Exp comparison
Under work

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Outline

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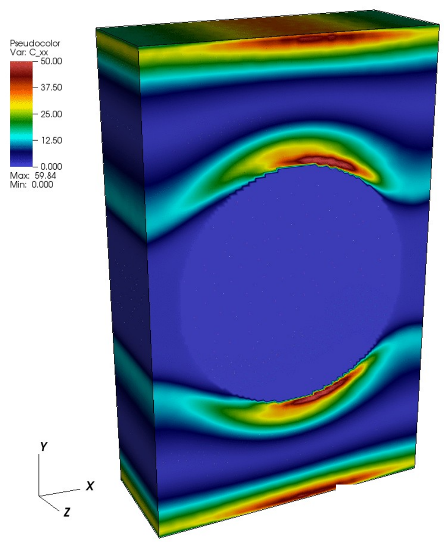
Other fields of applications

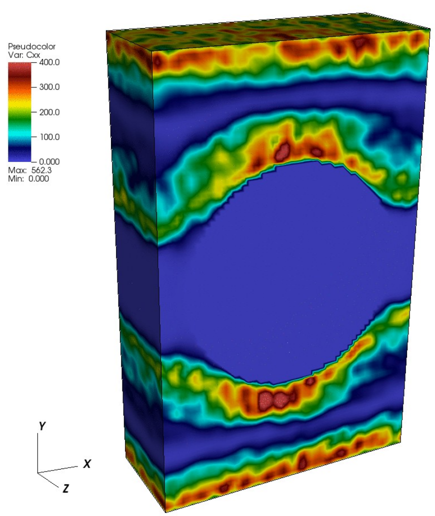
- **Elastic turbulence**: zero Reynolds number (polymeric fluids)

Weissenberg number

$$\mathrm{We} = \frac{\lambda V}{R}$$



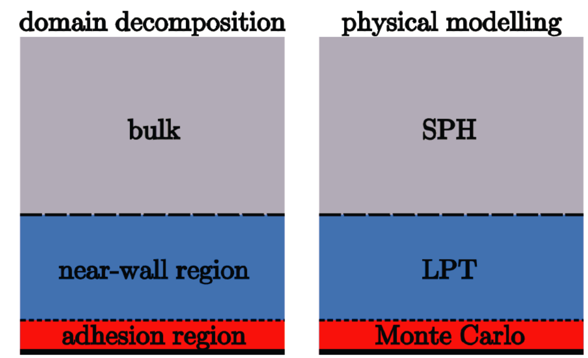
$$\mathrm{We} \ll 1$$

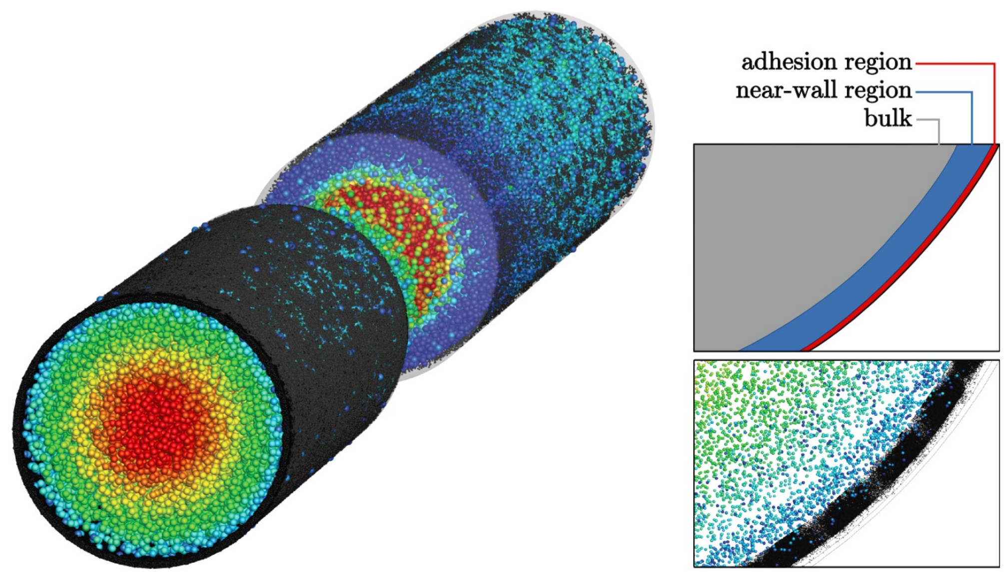


$$\mathrm{We} \gg 1$$

Grilli, Vazquez, Ellero, Phys Rev Lett (2013)

- Multiscale modelling blood near-wall leukocyte dynamics





Gholami, Comerford Ellero, Int J. Num. Meth Biomed Eng (2014)
Gholami, Comerford Ellero, Jbiomech. Model Mechanobiol. (2015)

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