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軟らかな粒子の慣性サスペンションのレオロジー

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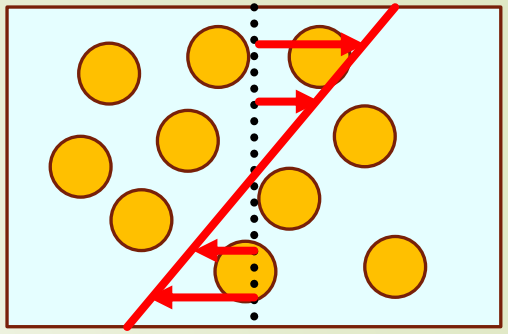
Introduction

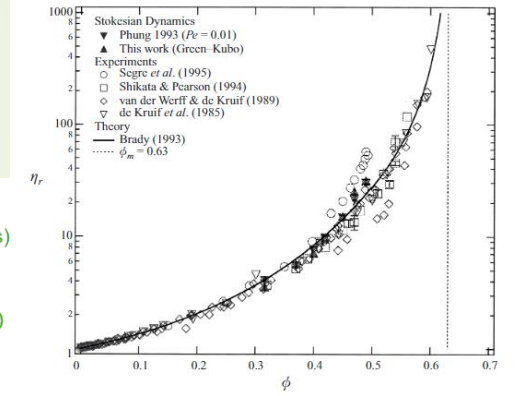


Solvent viscosity: η_0
Shear rate: $\dot{\gamma}$

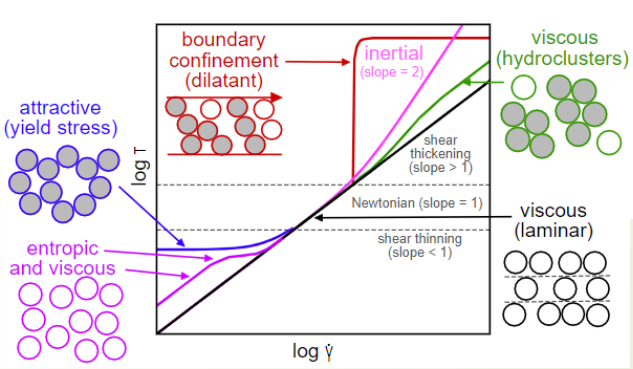
- Viscosity $\eta(\varphi) \equiv \frac{\sigma(\varphi)}{\dot{\gamma}}$: characterizes noneq. transport

  Dilute case (Einstein, 1906): $\frac{\eta_s(\varphi)}{\eta_0} = 1 + \frac{5}{2}\varphi \quad (\varphi \leq 0.03)$

  Dense case (near jamming): $\frac{\eta_s(\varphi)}{\eta_0} = \left(1 - \frac{\varphi}{\varphi_m}\right)^{-2}$ (empirical)

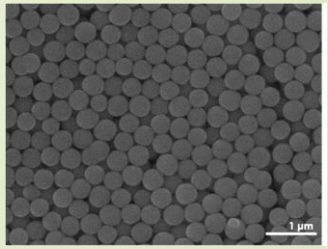


- Shear rate dependent viscosity
  - Shear thickening (thinning): Viscosity becomes large (small) as $\dot{\gamma}$ increases.



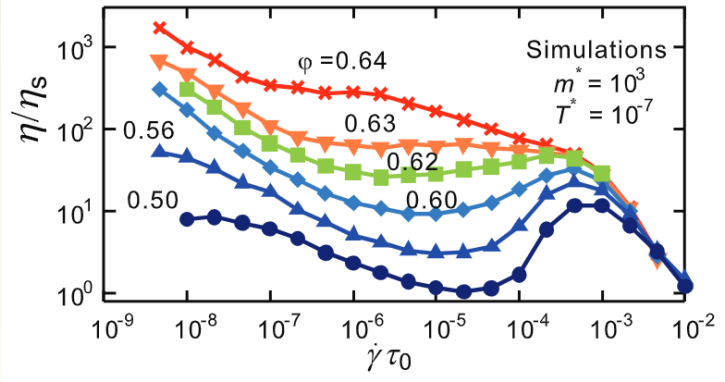
  - "Inertial effect" is often ignored. (overdamped) If this is not ignored, system is called as "inertial suspensions" (a model of aerosols or colloid)

COVID-19

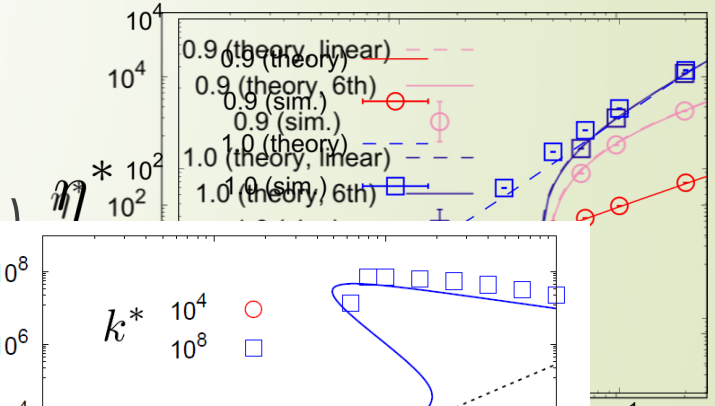


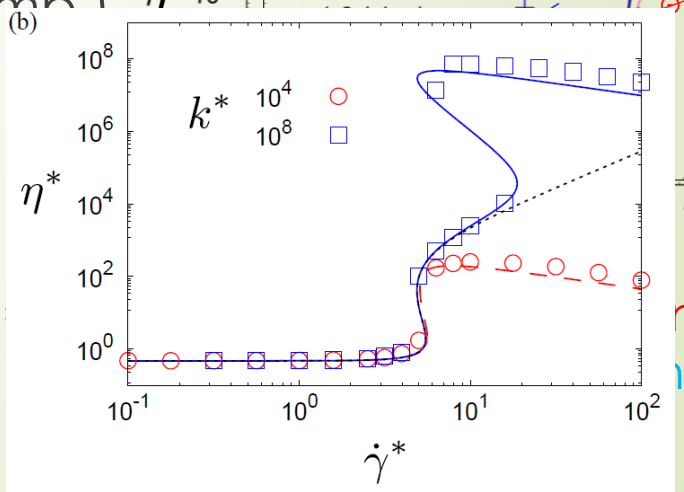
Previous studies of inertial suspension

System: frictionless, Stokes' drag



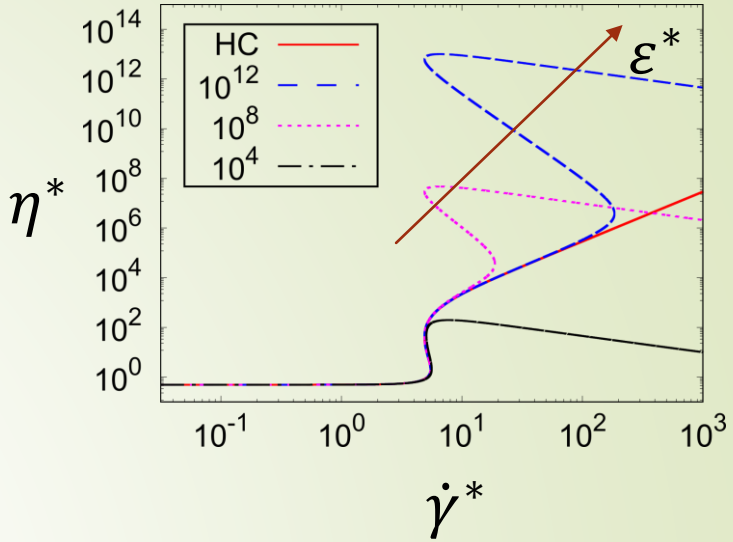
- Dense suspension (soft-core particles)
  - Kawasaki, Ikeda, & Berthier, EPL (2014)
  - Thinning → thickening → thinning for $\varphi \lesssim 0.60$
  - No thickening for $\varphi \gtrsim 0.63$
  - ※ Only contact contribution
- Dilute to moderately dense inertial suspension (**hard-core**)
  - Hayakawa & Takada, PTEP (2019), Takada, Hayakawa, Santos, & Garzó, PRE (2020)
  - DST-like behavior for dilute systems (≅ ignited-quenched transition of the kinetic temp.)
  - Change to CST-like behavior at $\varphi \simeq 0.0176$
  - Agreement for $\varphi \lesssim 0.5$
- Dilute inertial suspension (**soft-core**)
  - Sugimoto & Takada, JPSJ (2020)
  - DST-like behavior can occur twice.





DST
CST

- Dilute inertial suspension (**soft-core**), Second DST-like behavior
  ⇐ Softness of particles
  "Does this behavior survive even in denser situations?"



		Hard-core	Soft-core
Theory & Sim.	Dilute	Hayakawa & Takada PTEP (2019)	Sugimoto & Takada JPSJ (2020)
Theory & Sim.	Moderately dense	Hayakawa, Takada, & Garzó PRE (2017), Takada, Hayakawa, Santos, & Garzó PRE (2020)	This study
Sim.	Dense		Kawasaki, Ikeda, & Berthier EPL (2014)

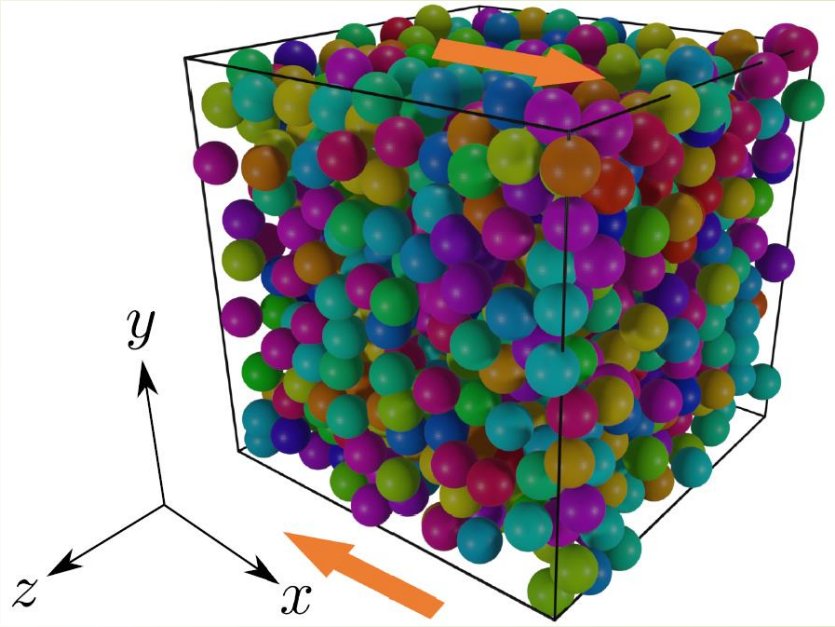
Our question:
Is it possible to observe DST-like behaviors for simple systems, esp, frictionless soft-core systems?

Approach:
- Langevin simulation
- (Kinetic theory of inertial suspension)

Model and setup

- System = Particle + Solvent
- Particle:
  monodisperse (mass m, diameter d)

$$\frac{d\boldsymbol{r}_i}{dt} = \frac{\boldsymbol{p}_i}{m} + \dot{\gamma} y_i \hat{\boldsymbol{e}}_x$$
$$\frac{d\boldsymbol{p}_i}{dt} = \sum_{j \neq i} \boldsymbol{F}_{ij}^{(\mathrm{el})} + \boldsymbol{F}_i^{\mathrm{H}} - \dot{\gamma} p_{i,y} \hat{\boldsymbol{e}}_x + \boldsymbol{\xi}_i(t)$$



Shear (shear rate: $\dot{\gamma}$)

Interparticle interaction = harmonic potential

$$\boldsymbol{F}_{ij}^{(\mathrm{el})} = -\frac{\partial U(r_{ij})}{\partial \boldsymbol{r}_i}, U(r_{ij}) = \frac{\varepsilon}{2}\left(1 - \frac{r_{ij}}{d}\right)^2 \Theta\left(1 - \frac{r_{ij}}{d}\right)$$

Hydrodynamic interaction
(Solvent: viscosity: η_0, temperature T_{env})

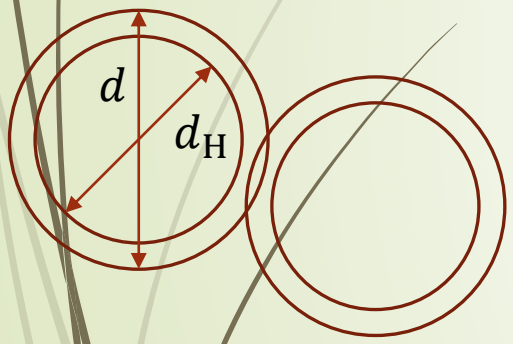
Noise term
(satisfies fluctuation-dissipation theorem)

- Solvent: viscosity η_0, temperature T_{env}

- We consider two cases for hydrodynamic interaction:

1. **Scalar resistance model**: $\boldsymbol{F}_i^{\mathrm{H}} = -\zeta \boldsymbol{p}_i$
   Only Stokes' drag ($\zeta = 3\pi d\eta_0/m$)
   Theoretical treatment is available.
   ☞ Enskog kinetic equation for the inertial suspension

2. **Stokes' + lubrication model**: $\boldsymbol{F}_i^{\mathrm{H}} = -\sum_j \overleftrightarrow{\zeta_{ij}}\, \boldsymbol{p}_j$
   $\overleftrightarrow{\zeta_{ij}}$ has nondiagonal components
   Introduction of roughness parameter (dimple)
   d: collision diameter, d_{H}: lubrication diameter
   $\delta \equiv \frac{d-d_{\mathrm{H}}}{d_{\mathrm{H}}} \sim 1\sim 10\%$: Magnitude of dimple
   (☞ Mari *et al.*, J. Rheol. **58**, 1693 (2014);
   Pradipto & Hayakawa, Soft Matter **16**, 945 (2020), etc.)



$$\zeta_{ij,\alpha\beta} = \begin{cases} \frac{3\pi d\eta_0}{m}\delta_{\alpha\beta} + \sum_{k\neq i}\frac{1}{m}A^{(1,1)}_{ik,\alpha\beta}\Theta(r_{\mathrm{c}} - r_{ik}) & (i=j) \\ -\frac{1}{m}A^{(1,1)}_{ij,\alpha\beta}\Theta(r_{\mathrm{c}} - r_{ij}) & (i\neq j) \end{cases}$$

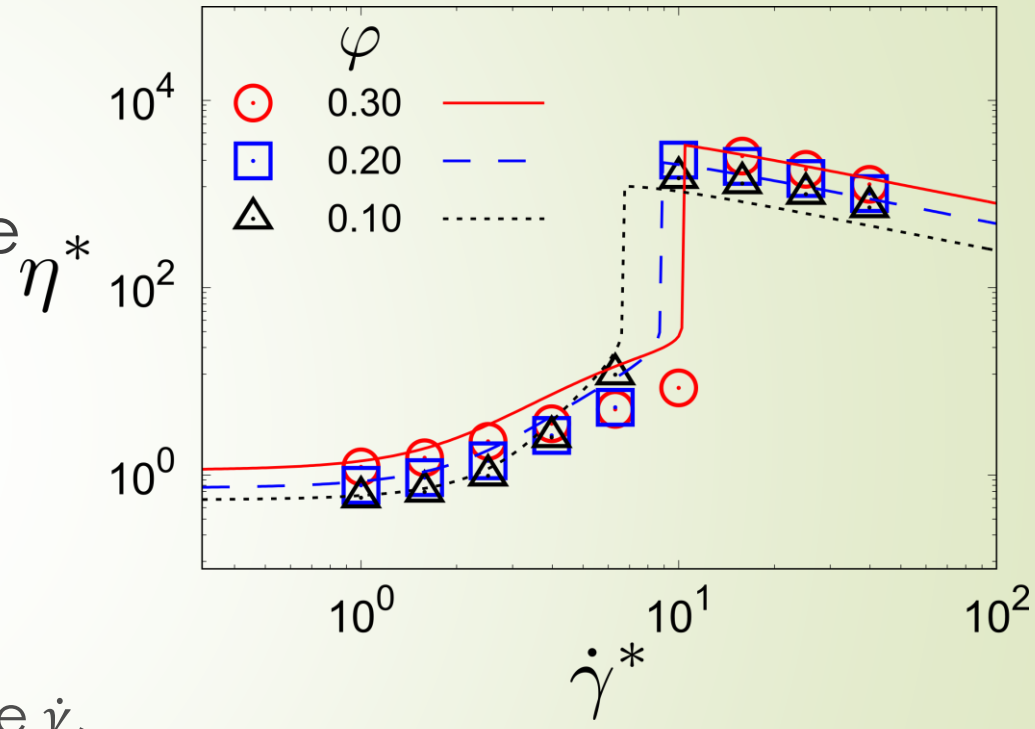
$A^{(1,1)}_{ij,\alpha\beta}$: function of $\hat{\boldsymbol{k}} \equiv \boldsymbol{r}_{ij}/|\boldsymbol{r}_{ij}|$ ($\boldsymbol{r}_{ij} \equiv \boldsymbol{r}_j - \boldsymbol{r}_i$)
(☞ Kim & Karrila, "Microhydrodynamics")
$r_{\mathrm{c}} \equiv d_{\mathrm{H}} + \lambda$: cutoff length ($\lambda = 0.25d$)

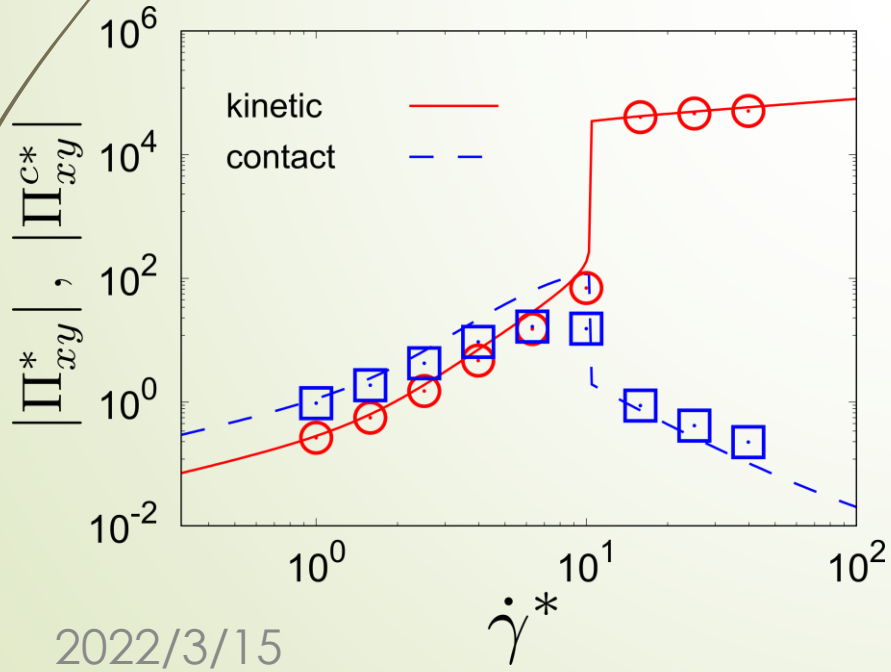
<u>(Dimensionless) control parameters</u>:
① Packing fraction: φ ② Shear rate: $\dot{\gamma}^* \equiv \dot{\gamma}/\zeta$
③ Particle softness: $\varepsilon^* \equiv \frac{\varepsilon}{m\sigma^2\zeta^2}$ ④ Env. temp.: $\xi_{\mathrm{env}} \equiv \sqrt{\frac{T_{\mathrm{env}}}{m}}\frac{1}{\zeta\sigma}$
⑤ Magnitude of dimple: δ (only for 2nd case)

Results ①: Scalar model

Parameters:
$\varphi = 0.10, 0.20, 0.30$
$\varepsilon^* = 10^4, \xi_{\mathrm{env}} = 1.0$

- **DST-like behavior survives** even for finite density.
  (⇔ CST-like for hard-core system)
- **Shear thinning** in high shear regime
- Kinetic theory reproduces the sim. results.





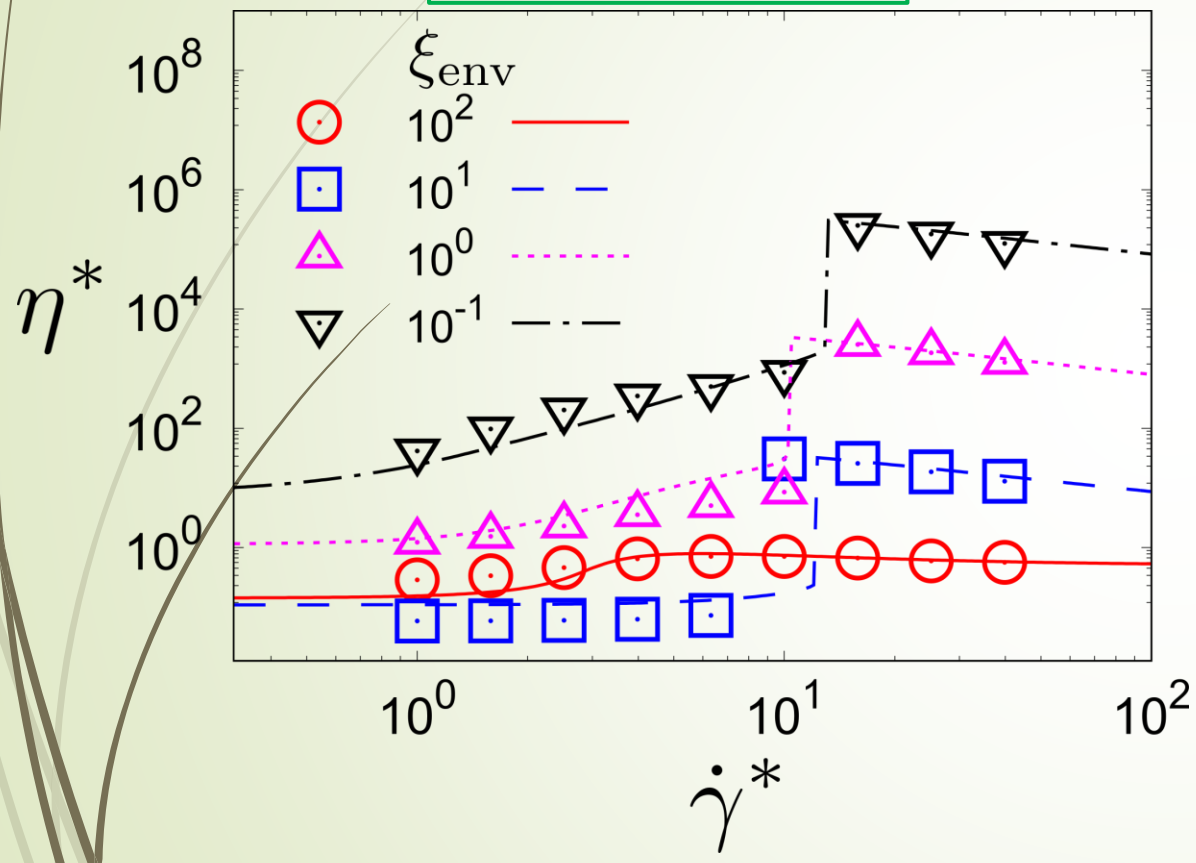
For large $\dot{\gamma}$,
Kinetic contribution ≫ Contact contribution

$$\left(P^k_{xy} = \frac{1}{V}\sum_i m v_{i,x} v_{i,y} \gg P^c_{xy} = \frac{1}{V}\sum_i \sum_{j \neq i} x_{ij} f_{ij,y} \right)$$

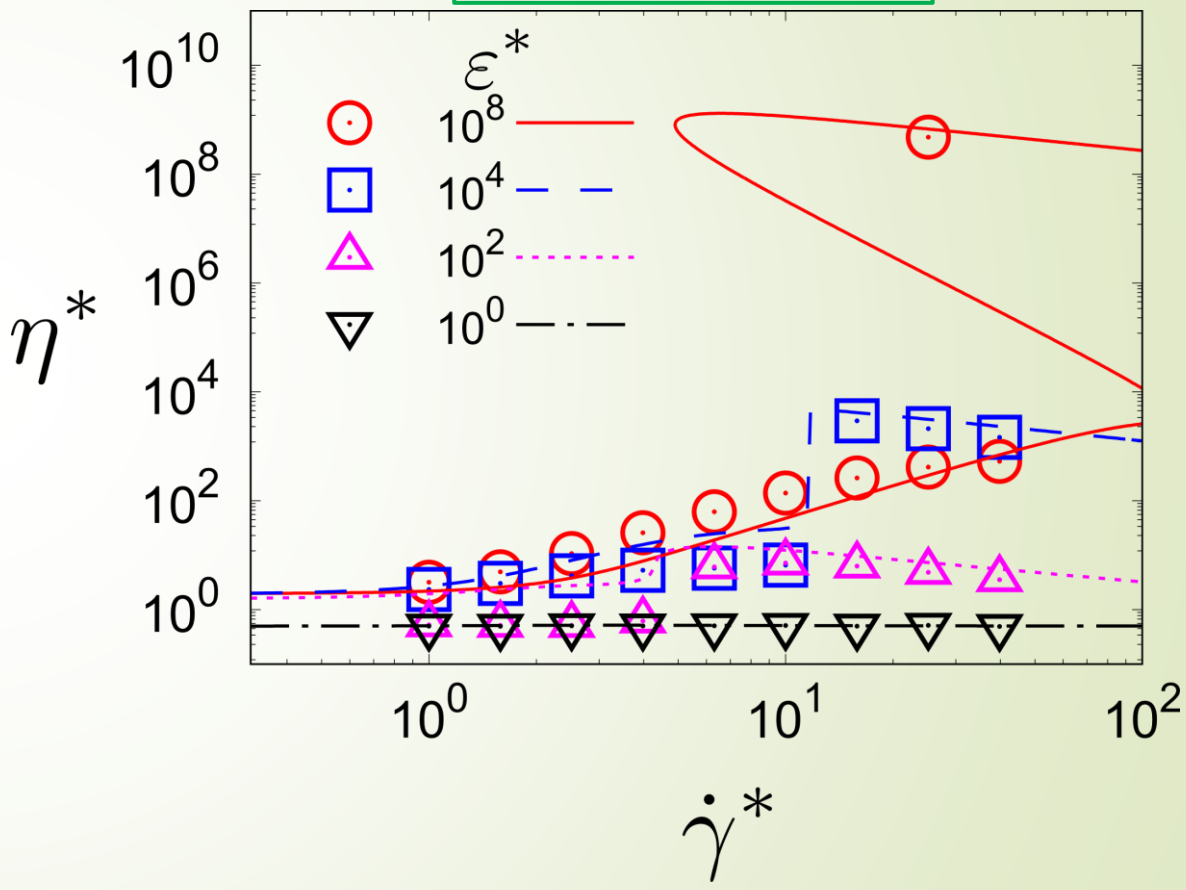
⇒ Inertia plays a role in this DST-like behavior.
(= cannot be ignored)

- Viscosity vs shear rate for various sets of parameters

Parameters:
$\varphi = 0.30, \varepsilon^* = 10^4$



Parameters:
$\varphi = 0.40, \xi_{\mathrm{env}} = 1.0$



Results ②: Stokes' + lubrication model

- Scaled viscosity $\tilde{\eta} \equiv \eta/\eta_1$ against the Peclet number $\mathrm{Pe} \equiv \frac{3\pi\eta_0 d^3}{4T_{\mathrm{env}}}\dot{\gamma}$

  $\eta \equiv P_{xy}/\dot{\gamma}, \eta_1 = \eta_0\left(1 + \frac{5}{2}\varphi + 4\varphi^2 + 42\varphi^3\right)$:

  η_1: Empirical expression of the apparent viscosity in the low shear limit

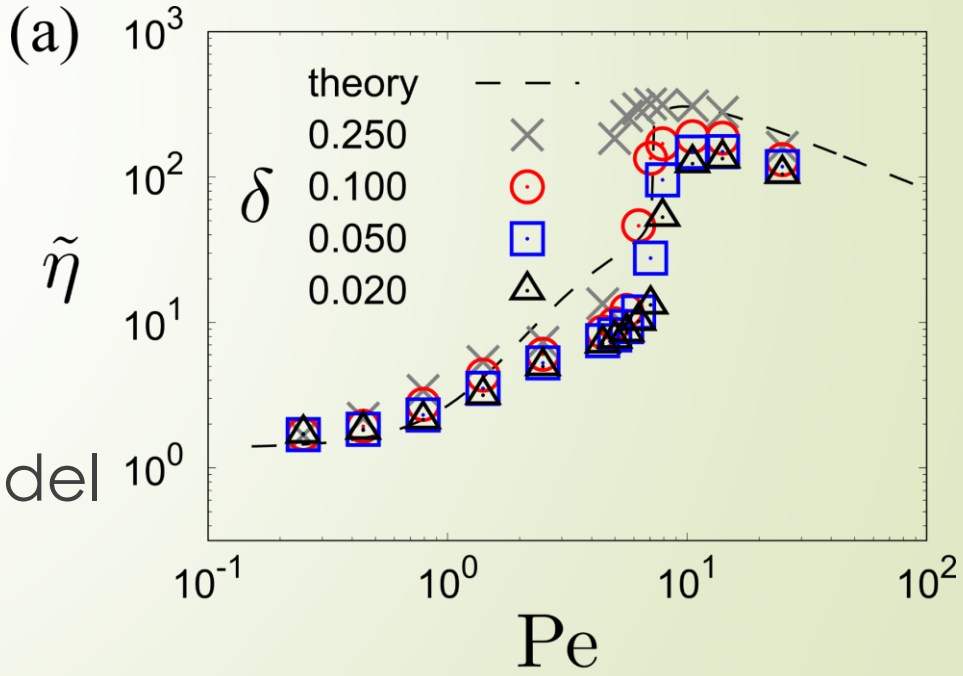
Parameters:
$\varphi = 0.30$
$\varepsilon^* = 10^4, \xi_{\mathrm{env}} = 1.0$

- Even for small δ (small dimple), **DST** occurs at $\mathrm{Pe} \simeq 10$.

  ⇔ DST occurs at $\mathrm{Pe} \simeq 20$ for frictional Brownian suspension

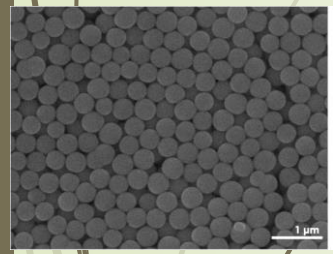
  ☞ Mari *et al.*, PNAS **112**, 15326 (2015)

- For larger δ, tends to the previous model



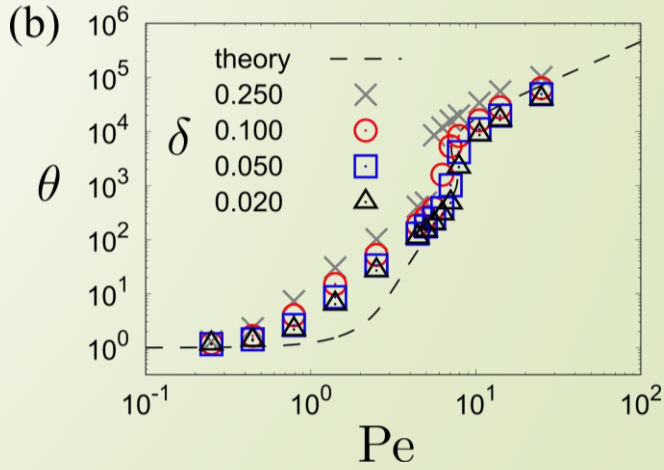
Discussion: Estimation of quantities

- Aerosol
  $d \sim 10^{-5}\ \mathrm{m}, \rho \sim 1\ \mathrm{g/cm^3}, E \sim 10\ \mathrm{GPa} \Rightarrow m \sim 10^{-12}\ \mathrm{kg}$
  Viscosity of air: $\eta_0 \sim 10^{-5}\ \mathrm{Pa \cdot s}$
  DST takes place at $\dot{\gamma}_\mathrm{c} \sim 10^3\ 1/\mathrm{s} \Rightarrow$ shear speed $10\ \mathrm{m/s}$ if $L = 1\ \mathrm{cm}$



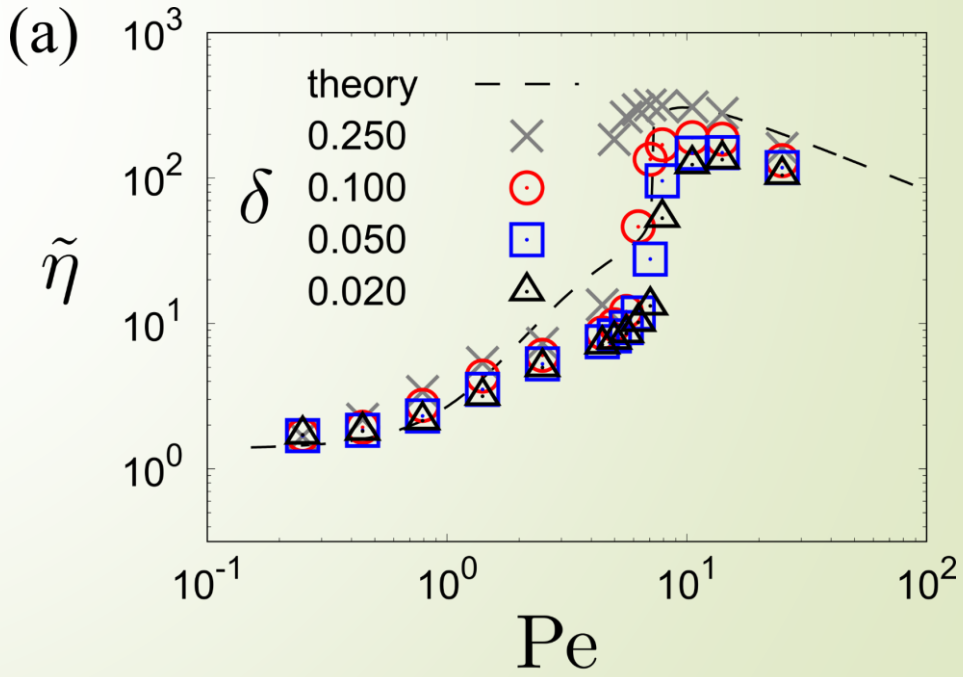
- Colloid
  $d \sim 10^{-6}\ \mathrm{m}, \rho \sim 1\ \mathrm{g/cm^3}, E \sim 1\ \mathrm{GPa} \Rightarrow m \sim 10^{-14}\ \mathrm{kg}$
  Viscosity of water: $\eta_0 \sim 10^{-3}\ \mathrm{Pa \cdot s}$
  DST takes place at $\dot{\gamma}_\mathrm{c} \sim 10^4\ 1/\mathrm{s} \Rightarrow$ shear speed $10^4\ \mathrm{m/s}$ if $L = 1\ \mathrm{cm}$

- Kinetic temperature becomes 10^2 times larger.
  Is it possible to achieve this?
  ⇒ This will open for all researchers.



Summary

- Softness induced DST-like behaviors for frictionless system
- Scalar model
  DST-like behaviors
  Good agreement between sim. and theory.
- Lubrication model
  DST-like behaviors survive
  even for small δ



Future work

- Long range interaction
  (inclusion of Lotne-Prager tensor)
- Verifiability in experiments