TUAT Mechanical Systems Engineering

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Discontinuous shear thickening of a moderately dense inertial suspension of hydrodynamically interacting frictionless soft particles

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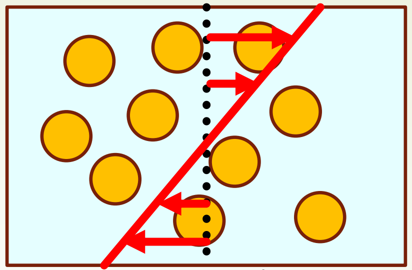
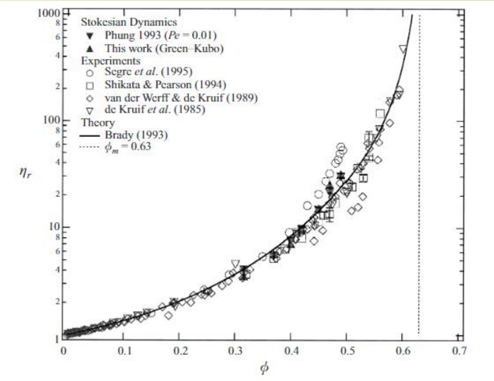
T4-08B-05, STATPHYS28,
August 8th, 2023 (Univ. Tokyo)

☞ S. Takada, K. Hara, & H. Hayakawa, arXiv:2207.05752
S. Takada, K. Hara, & H. Hayakawa, arXiv:2207.05348

Introduction





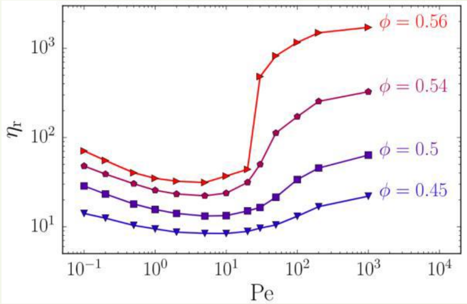
- Viscosity $\eta(\varphi) \equiv \sigma(\varphi)/\dot{\gamma}$: characterizes noneq. transport

  Dilute case (Einstein, 1906): $\eta_s(\varphi)/\eta_0 = 1 + (5/2)\varphi \quad (\varphi \le 0.03)$

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

solvent viscosity: η_0
shear rate: $\dot{\gamma}$

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

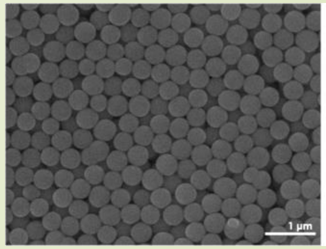


  - Discontinuous shear thickening (DST)
    can occur. (many mechanisms are proposed.)

"Inertial effect" is often IGNORED.
(Overdamped is assumed.)

  - If "ineria" is not ignored, system is called as
    "inertial suspensions"
    (a model of aerosols or colloid)

COVID-19

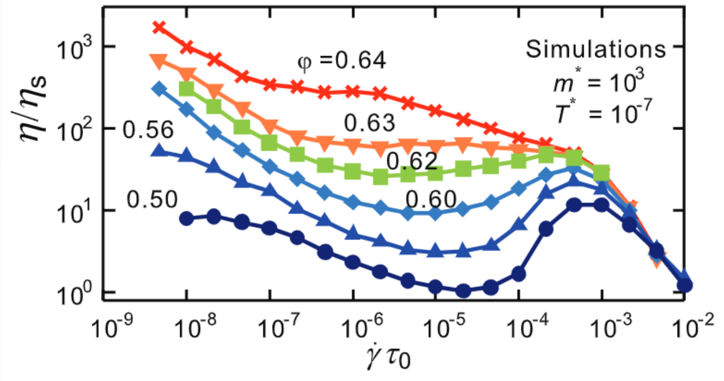


Previous studies on inertial suspension

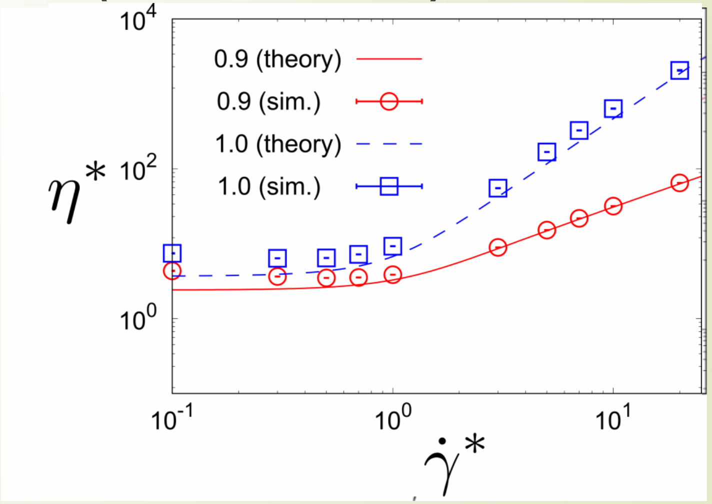
System: frictionless, Stokes' drag

- 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 is considered.



- 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)
  - Change to CST-like behavior at $\varphi \simeq 0.0176$
  - Agreement for $\varphi \lesssim 0.5$
  - Mpemba effect (hotter can become colder)
    ☞Prof. Santos's talk)

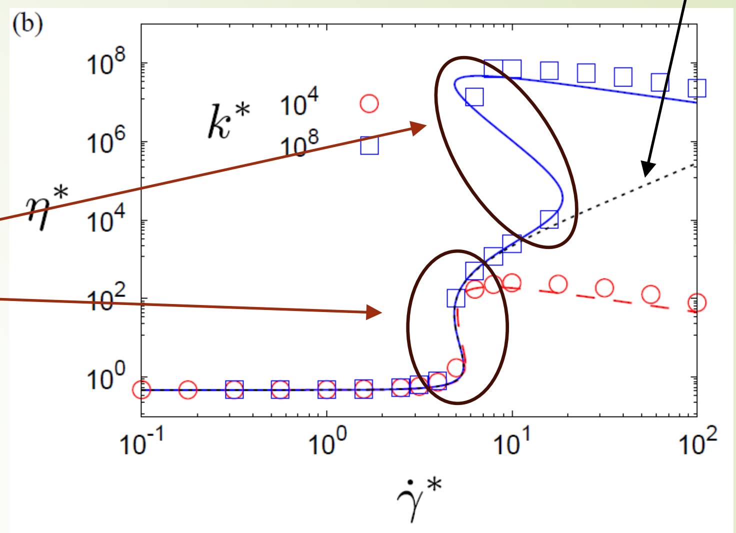


DST = Discontinuous Shear Thickening
CST = Continuous Shear Thickening

Previous studies on inertial suspension

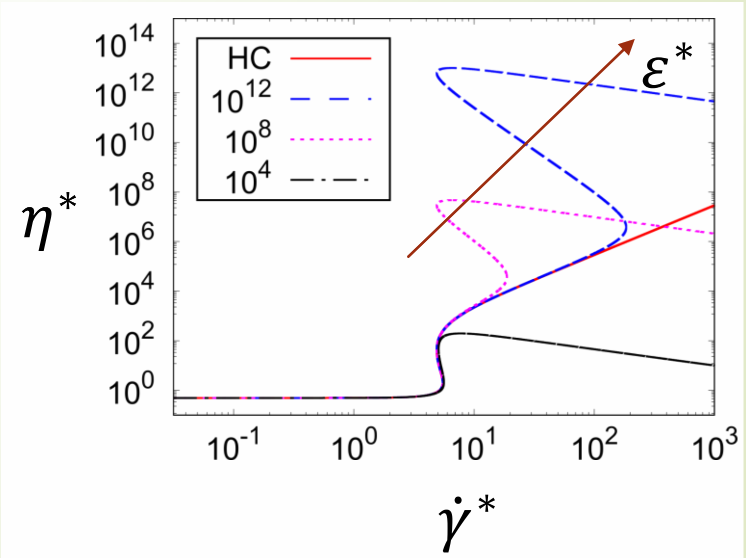
Hard-core system

- Dilute inertial suspension (**soft-core**)
  ☞ Sugimoto & Takada, JPSJ (2020)
  - DST-like behaviors can occur **TWICE**!!
  - Kinetic theory is also developed. (Good agreement with simulations.)



Origin of two DSTs:

- 1^{st} DST: occurs at the same $\dot{\gamma}^*$ as hard-core (same mechanism) ⇒ disappears as φ: ↗
- 2^{nd} DST: occurs depending on the softness of particles ⇒ **Softness (hardness) induced DST**



Motivation of this study

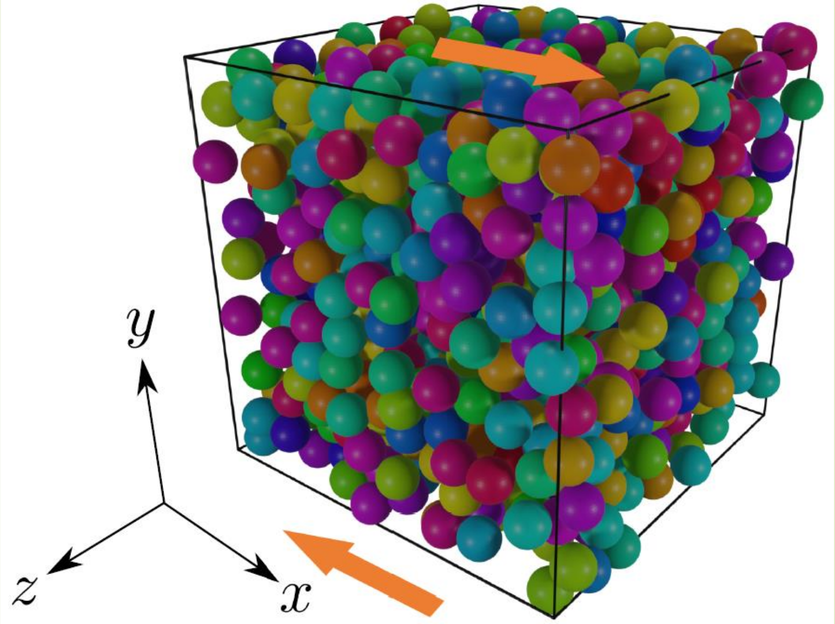
Our question:
Does the second DST in dilute systems survive for dense systems?

Approach:
Both numerical to theoretical
- Numerical:
  Langevin simulation
- Theoretical (for ①):
  (Kinetic theory of inertial suspension)

		Only Stokes' drag		Hydro.
		Hard-core	Soft-core	
Theory & Sim.	Dilute	Hayakawa & Takada, PTEP (2019)	Sugimoto & Takada, JPSJ (2020)	
Theory & Sim.	Mod. dense	Hayakawa, Takada, & Garzó, PRE (2017), Takada, Hayakawa, Santos, & Garzó, PRE (2020)	Our study ①	Our Study ②
Sim.	Dense		Kawasaki, Ikeda, & Berthier, EPL (2014)	Mari *et al.*, PNAS (2015)

Model and setup

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



$$\frac{d\boldsymbol{r}_i}{dt} = \frac{\boldsymbol{p}_i}{m} + \dot{\gamma} y_i \hat{\boldsymbol{e}}_x$$

$$\frac{d\boldsymbol{p}_i}{dt} = \sum_{j \neq i} \boldsymbol{F}_{ij}^{(\mathrm{el})} + \boldsymbol{F}_i^{\mathrm{H}} + \boldsymbol{\xi}_i(t)$$

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
from the solvent: **two models**

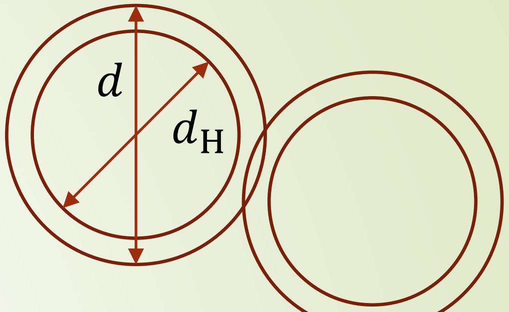
Noise term
(satisfies fluctuation-dissipation theorem)

- **Solvent (fluid)**: viscosity η_0, temperature T_{env} are kept constant.

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**: $\boldsymbol{F}_i^{\mathrm{H}} = -\sum_j \overleftrightarrow{\zeta}_{ij} \boldsymbol{p}_j$
   $\overleftrightarrow{\zeta}_{ij}$: non-diagonal, diverge at $r \to d$
   "Roughness parameter" (dimple) is introduced.
   $\delta \equiv \frac{d - d_{\mathrm{H}}}{d_{\mathrm{H}}} \sim 1$~$10\%$: Magnitude of dimple
   (☞ Mari *et al.*, J. Rheol. **58**, 1693 (2014);
   Pradipto & Hayakawa, Soft Matter **16**, 945 (2020), etc.)



d: collision diameter
d_{H}: lubrication diameter

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

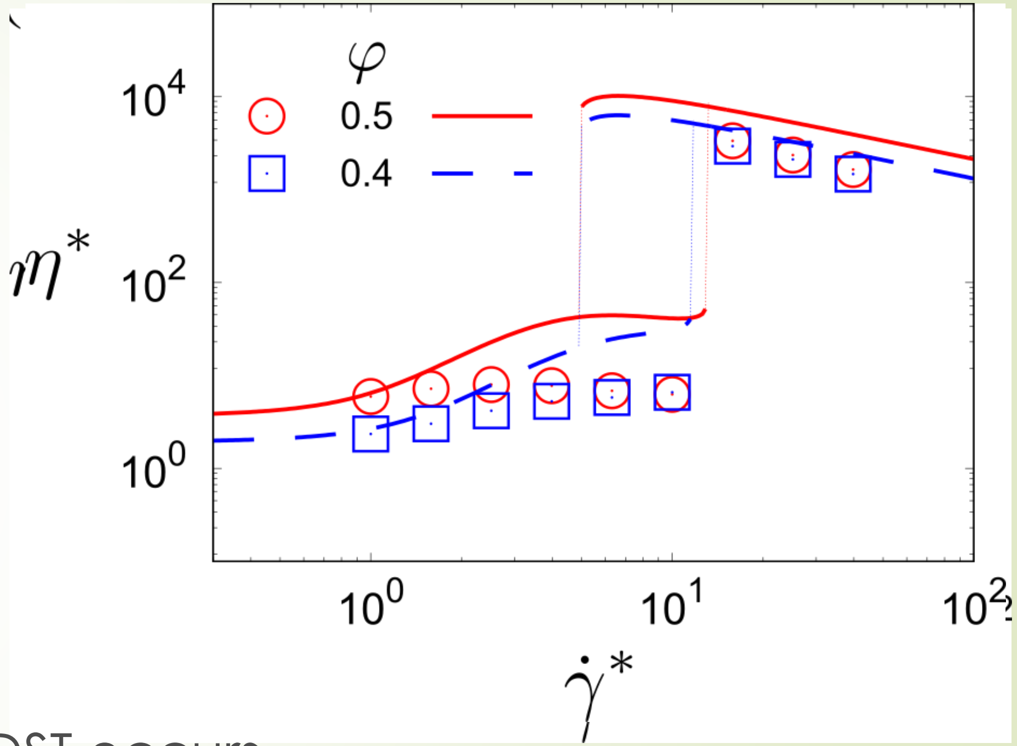
$A^{(1,1)}_{ij,\alpha\beta}$: function of $\hat{\boldsymbol{k}} \equiv \boldsymbol{r}_{ij}/|\boldsymbol{r}_{ij}|$
(☞ Kim & Karrila, "Microhydrodynamics")
$r_{\mathrm{c}} \equiv d_{\mathrm{H}} + \lambda$: cutoff length ($\lambda = 0.25d$)

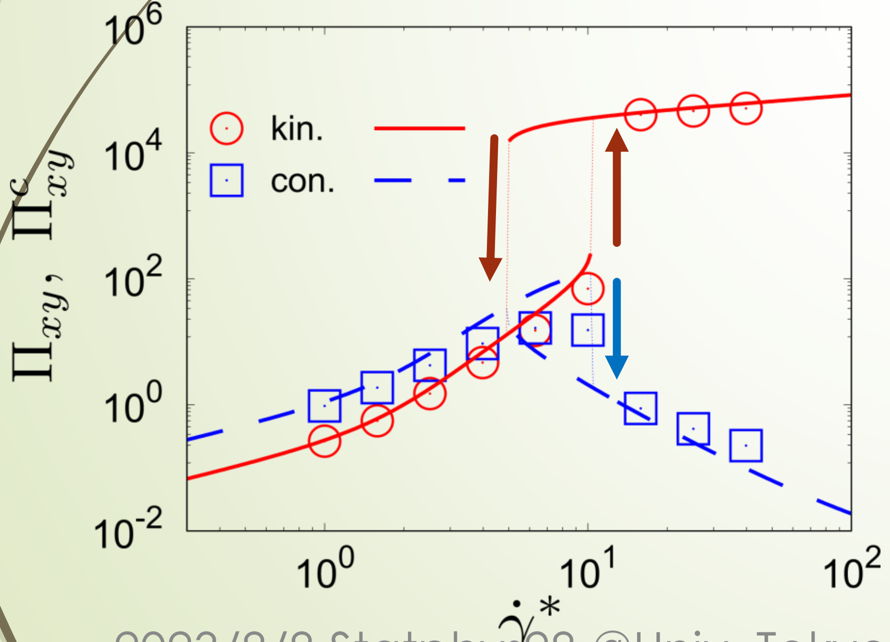
<u>(Dimensionless) control parameters</u>:
① Packing fraction: φ ② Shear rate: $\dot{\gamma}^* \equiv \dot{\gamma}/\zeta$
③ Particle hardness: $\varepsilon^* \equiv \frac{\varepsilon}{m\sigma^2\zeta^2}$ ④ Envir. temp.: $\xi_{\mathrm{env}} \equiv \sqrt{\frac{T_{\mathrm{env}}}{m}\frac{1}{\zeta\sigma}}$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

Results ①: Scalar model

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

- **(2nd) DST-like behavior survives** even for finite density φ. (⇔ CST-like for hard-core system)
- **Shear thinning** in high shear regime
- (Kinetic theory reproduces the sim. results.)





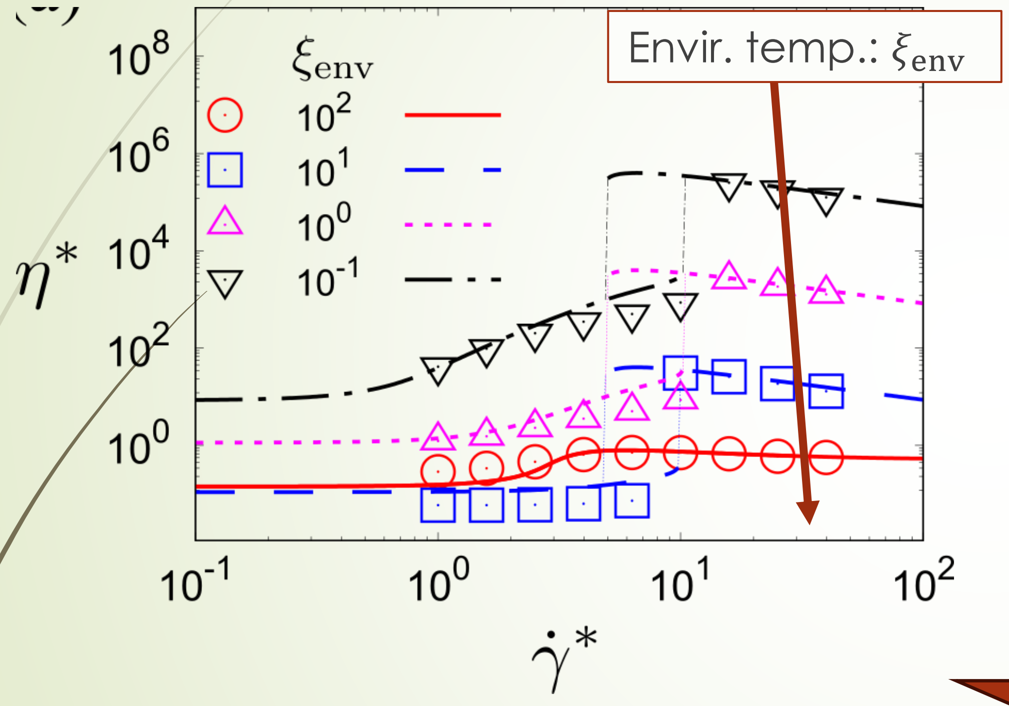
After the DST occurs,
Kinetic contribution ≫ Contact contribution

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

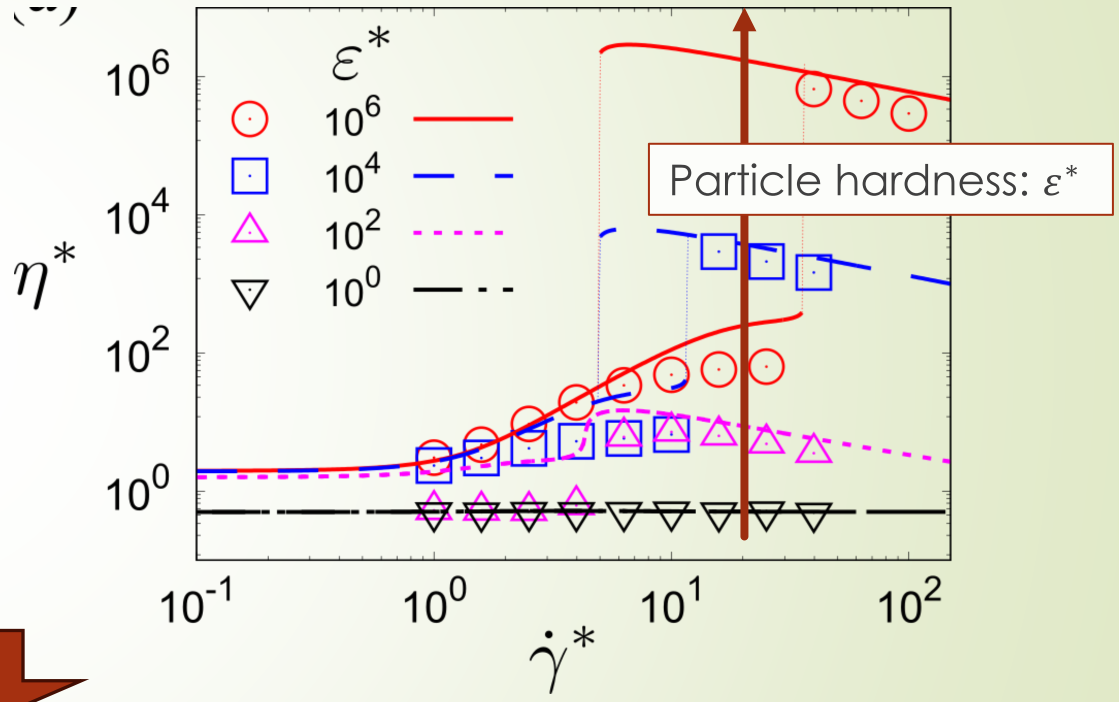
⇒ Inertia plays a crucial role for DST!!
(= cannot be ignored)

- Viscosity vs. shear rate for various sets of parameters

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



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



We can evaluate the parameters' space where the DST occurs.

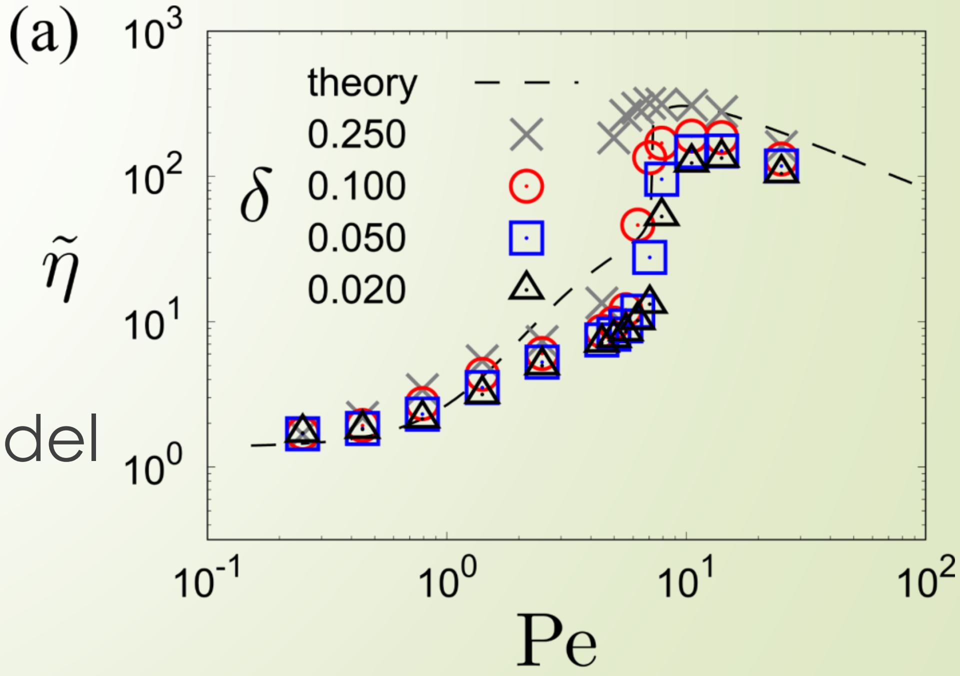
<u>Question</u>:
Does this DST survive when the lubrication forces exist?

Results ②: Stokes' + lubrication model

- Answer is Yes.
  Scaled viscosity $\tilde{\eta} \equiv \eta/\eta_1$ against the Peclet number $\mathrm{Pe} \equiv \frac{3\pi\eta_0 d^3}{4T_{\mathrm{env}}}\dot{\gamma}$ shows DST-like behavior.
  $\eta \equiv P_{xy}/\dot{\gamma}, \eta_1 = \eta_0(1 + 2.5\varphi + 4\varphi^2 + 42\varphi^3)$:
  η_1: Empirical expression of the apparent viscosity in the low shear limit

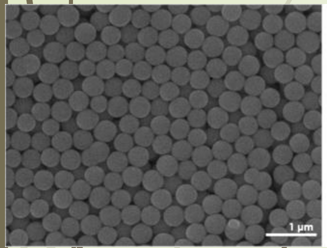
Parameters:
$\varphi = 0.30$
$\varepsilon^* = 10^4, \xi_{\mathrm{env}} = 1.0$

- 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



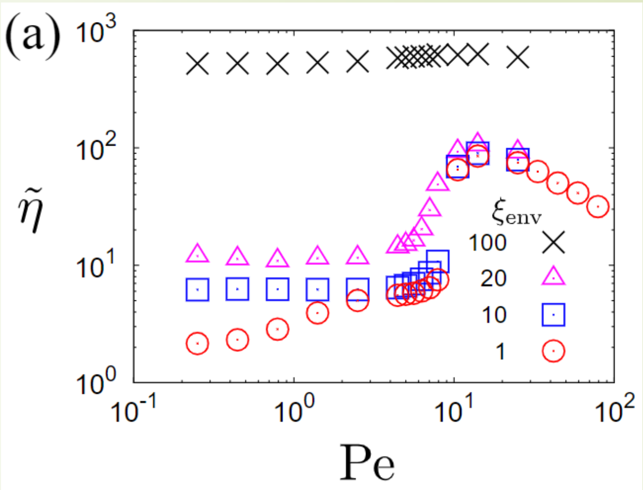
Disc.: Estimation of quantities for model ②

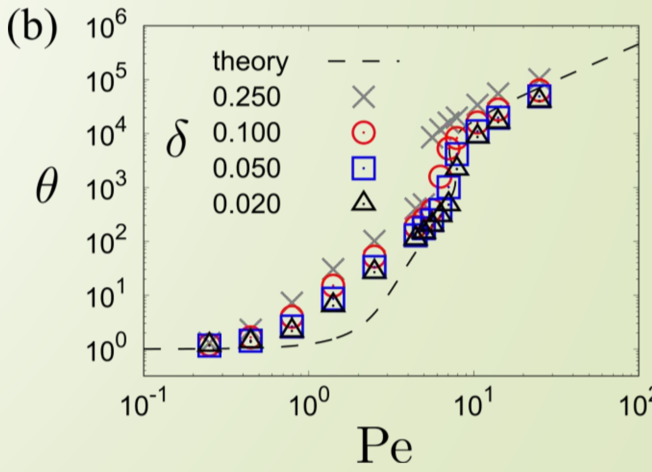
- Aerosol
  $d \sim 10^{-6}$ m, $\rho \sim 1$ g/cm^3, $E \sim 10$ GPa $\Rightarrow m \sim 10^{-14}$ kg
  Viscosity of air: $\eta_0 \sim 10^{-5}$ Pa · s
  DST takes place at $\dot{\gamma}_c \sim 10^4$ 1/s
  ⇒ shear speed 10^2 m/s if $L = 1$ cm



- Colloid
  $d \sim 2 \times 10^{-6}$ m, $\rho \sim 1$ g/cm^3, $E \sim 1$ GPa
  $\Rightarrow m \sim 10^{-15}$ kg
  Viscosity of water: $\eta_0 \sim 10^{-3}$ Pa · s
  Room temperature (300K): $\xi_{\mathrm{env}} \sim 2 \times 10^{-4}$

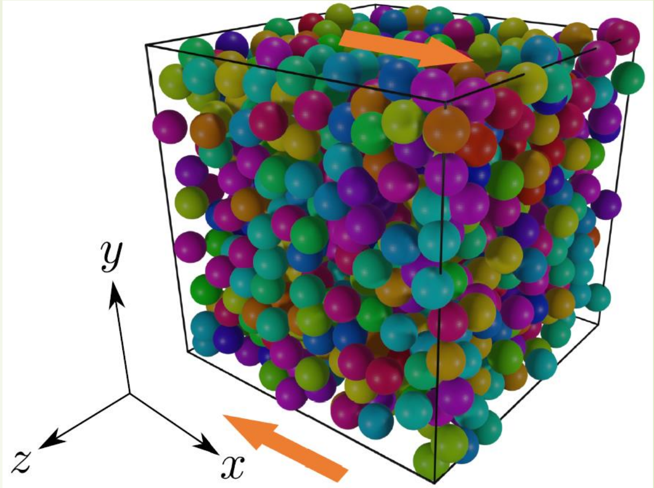
- Kinetic temperature becomes 10^2 times larger.
  Is it possible to achieve this?
  ⇒ This will open for discussion.

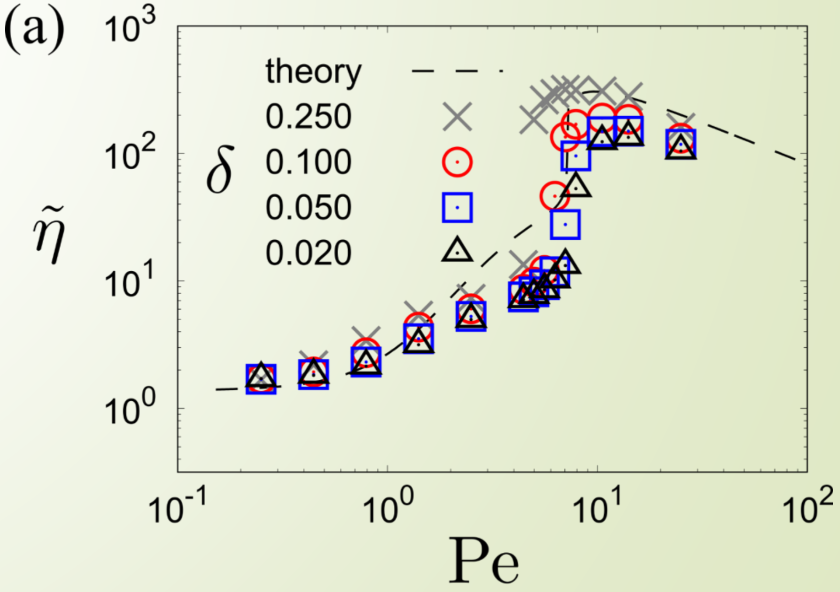




Summary

- Softness induced DST-like behaviors can exist for frictionless system.
- This DST survives even for finite densities.
- Scalar model
  DST-like behaviors
  Good agreement between sim. and theory.
- Lubrication model
  DST-like behaviors survive
  even for small roughness parameter





Future work

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