Kinetic theory of shear thickening for inertial suspensions

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collaboration with Satoshi Takada (Univ. Tokyo),
& Vicente Gárzo (Univ. Estremadura)

Rheolgy of disordered particles- suspensions, glassy and granular particles, June 18th-29th, 2018 (talk is held on June 21^{st}).

Refs: HH and S. Takada, arXiv:1611.07295, HH et al, PRE**96**, 042903 (2017).

Contents

- Introduction of shear thickening
- Kinetic model
- Kinetic theory of discontinuous shear thickening (DST) for dilute suspensions
- From DST to continuous shear thickening (CST) at finite density
- Application to binary mixtures
- Discussions
- Conclusions

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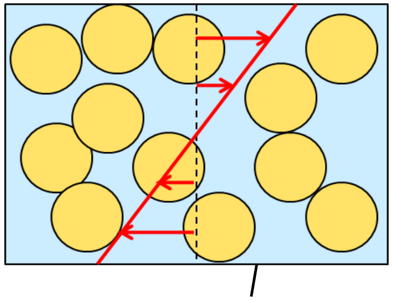
Shear thickening

- Shear thickening is the increment of the viscosity $\eta_s(\varphi) = \sigma(\varphi)/\dot{\gamma}$ against shear rate $\dot{\gamma}$.
- In particular, the discontinuous shear thickening (DST) has a drastic increase of the viscosity.
- Industrial applications to protective vest and traction control (break suspension)

$\dot{\gamma}=\partial v_x/\partial y$



solvent
(viscosity η_0)

http://youtube-video-download.info/video/EhdgkziFhrY

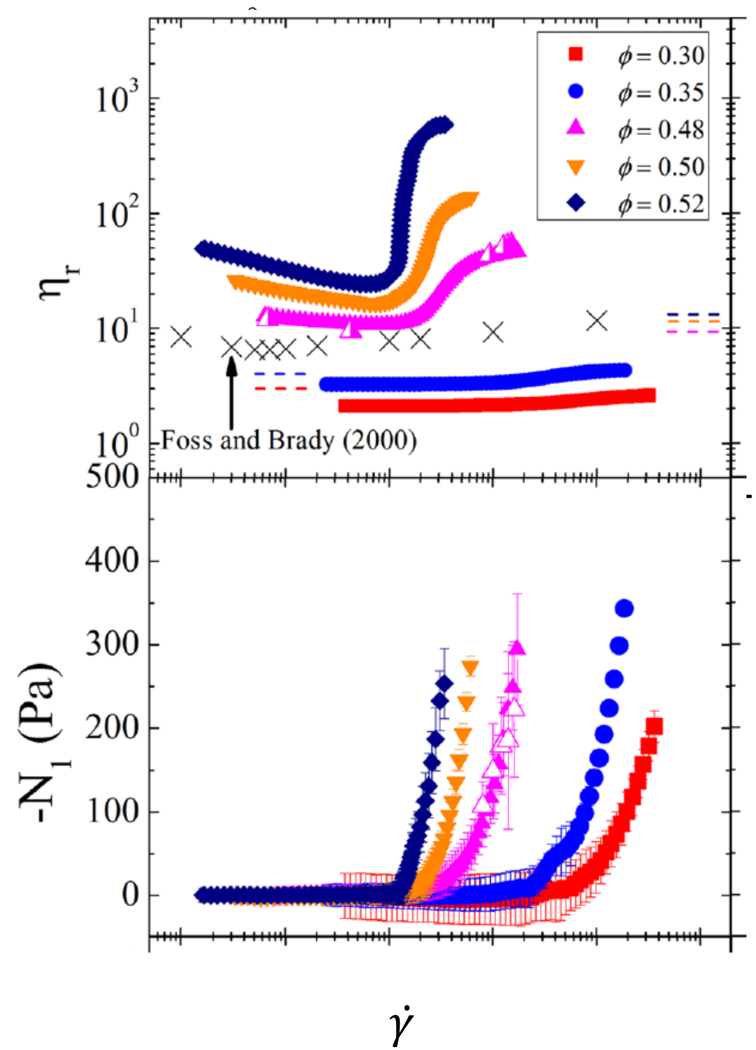
Discontinuous shear thickening (DST)

YITP
YUKAWA INSTITUTE FOR THEORETICAL PHYSICS

DST attracts much attention from physicists.

For DST in dense systems

- Mutual friction to stabilize percolaition is important
  M.Otsuki & H. Hayakawa, PRE **83**, 051301 (2011)
  R. Seto et al., PRL **111**, 218301 (2013).



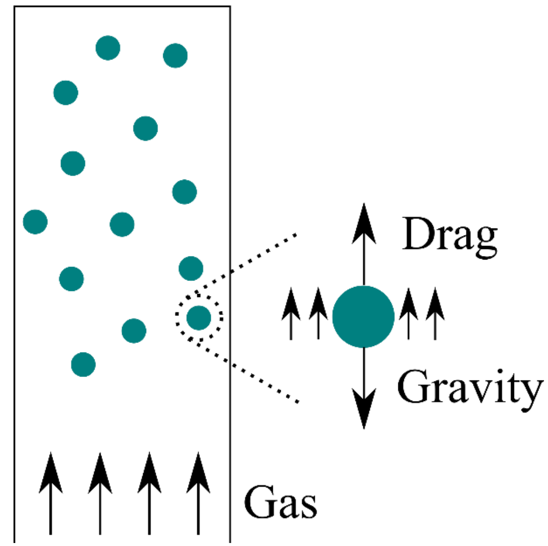
.3).

DST in experiments

- Normal stress difference is important.
  C. D. Cwalina & N.J. Wagner, J. Rheol. 58, 949 (2014)

Gas-solid suspensions

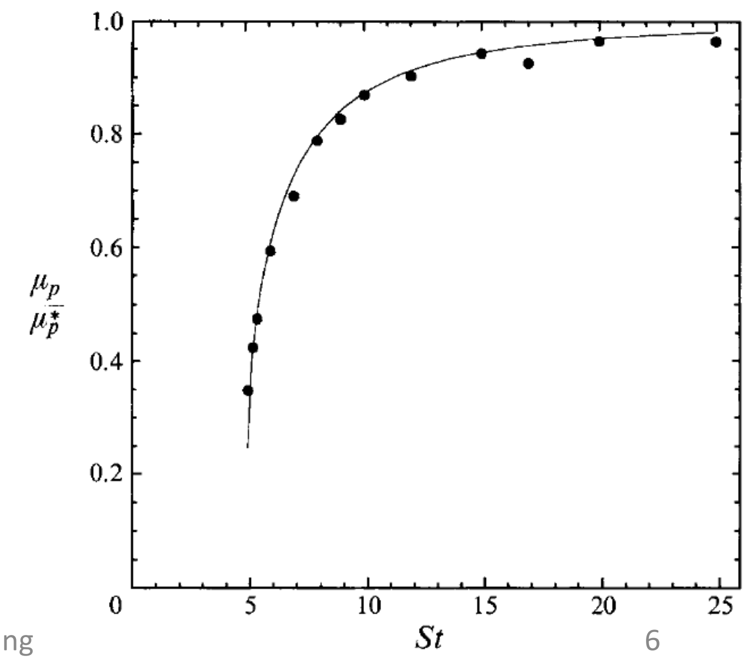
- Inertial suspensions
- Homogenous state is relialized by the balance between injecting gas flow & gravity.
- Relatively dilute system (theoretical treatment is available) without percolation picture



Previous (theoretical) study

Tsao and Koch, JFM **296**, 211 (1995) analyzed dilute gas-solid suspensions without thermal noise.

- Quenched-Ignited transition (DST-like transition for temperature but not for viscosity)



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Langevin model

- Suspensions are influenced by collisions and dag as well as thermal activation:

$$\frac{d\boldsymbol{p}_i}{dt} = -\zeta \boldsymbol{p}_i + \boldsymbol{F}_i^{(\mathrm{imp})} + m\boldsymbol{\xi}_i,$$

- where the noise satisfies

$$\langle \boldsymbol{\xi}_i(t) \rangle = 0, \quad \langle \xi_{i,\alpha}(t)\xi_{j,\beta}(t') \rangle = 2\zeta T_{\mathrm{ex}}\delta_{ij}\delta_{\alpha\beta}\delta(t-t').$$

- Here, we have introduced the peculiar momentum $\boldsymbol{p}_i \equiv m(\boldsymbol{v}_i - \dot{\gamma} y \boldsymbol{e}_x) = m\boldsymbol{V}_i$

the impulsive force $\boldsymbol{F}_i^{(\mathrm{imp})}$

Assumptions behind the Langevin model

- We assume that the drag force from the fluid is proportional to the fluid velocity.
  - Stokesian flow is assumed for relatively small grains.
- The drag coefficient is only determined by the average density of suspensions.
  - This is a mean field model $\zeta = \zeta_0 R(\varphi)$.
- Noise plays an important role for low shear regime to recover a thermal equilibrium state.

Simulation of Langevin equation

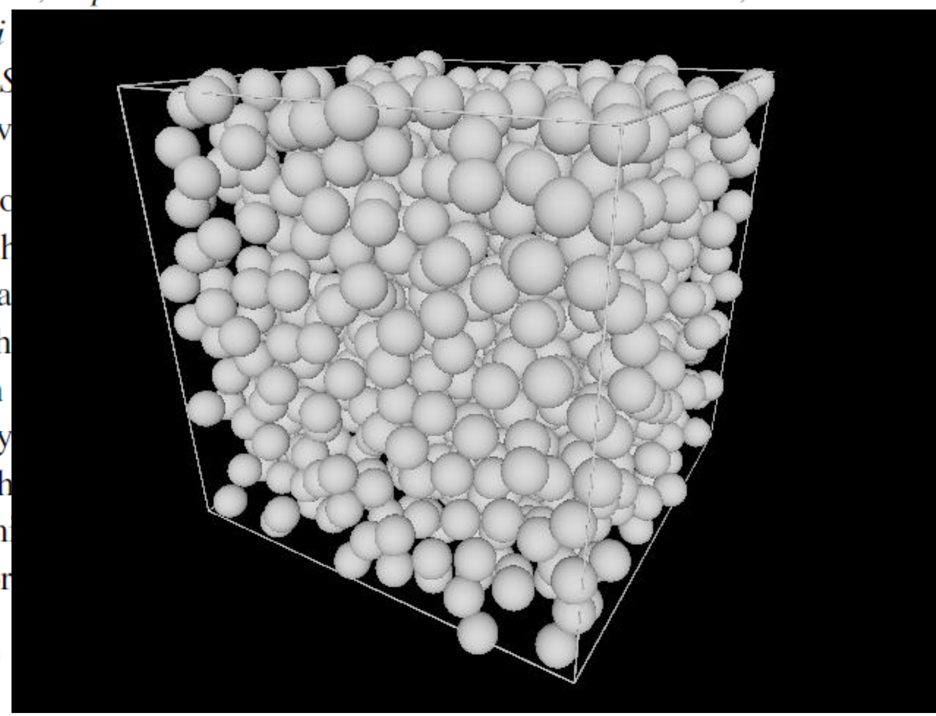
PHYSICAL REVIEW E **86**, 026709 (2012)

Event-driven Langevin simulations of hard spheres

A. Scala
ISC-CNR Dipartimento di Fisica, Sapienza Università di Roma Piazzale Moro 5, 00185 Roma, Italy,
IMT Alti Studi …
London Institute of Mathematical S … *Kingdom*

(Received 8 March 2012; rev … 12)

The blossoming of interest in coll … f hard-body systems. In particular, hard spheres h … is therefore necessary to study the complex dyna … lrodynamic interactions, the simplest model is th … numerical integration of the Langevin equation … n time step. This is not the case for hard-body sy … elation time of the noise and the time scale of th … nk operator associated with the Langevin dynami … unction, we introduce and test two algorithms for …



DOI: 10.1103/PhysRevE.86.026709 … g, 05.40.Jc

Boltzmann-Enskog equation

- Langevin model is equivalent to the kinetic equation (moderately dense case)

shear

collision integral

$$\left(\frac{\partial}{\partial t} - \boxed{\dot{\gamma} V_y \frac{\partial}{\partial V_x}}\right) f(\boldsymbol{r}, \boldsymbol{V}, t) = \boxed{\zeta \frac{\partial}{\partial \boldsymbol{V}} \cdot \left(\left\{ \boldsymbol{V} + \frac{T_{\rm ex}}{m} \frac{\partial}{\partial \boldsymbol{V}} \right\} f(\boldsymbol{r}, \boldsymbol{V}, t) \right)} + J_E(\boldsymbol{r}, \boldsymbol{V} | f),$$

friction
from back ground

- We adopt Boltzmann-Enskog equation

$$J_E(\boldsymbol{r}, \boldsymbol{V}_1 | f^{(2)}) = \sigma^{d-1} \int d\boldsymbol{v}_2 \int d\hat{\boldsymbol{\sigma}} \Theta(\boldsymbol{v}_{12} \cdot \hat{\boldsymbol{\sigma}})(\boldsymbol{v}_{12} \cdot \hat{\boldsymbol{\sigma}}) \left\{ \frac{f^{(2)}(\boldsymbol{r}, \boldsymbol{r} - \boldsymbol{\sigma}, \boldsymbol{v}_1^{**}, \boldsymbol{v}_2^{**}; t)}{e^2} - f^{(2)}(\boldsymbol{r}, \boldsymbol{r} + \boldsymbol{\sigma}, \boldsymbol{v}_1, \boldsymbol{v}_2; t) \right\},$$

$$= \sigma^{d-1} \chi \int d\boldsymbol{v}_2 \int d\hat{\boldsymbol{\sigma}} \Theta(\boldsymbol{v}_{12} \cdot \hat{\boldsymbol{\sigma}})(\boldsymbol{v}_{12} \cdot \hat{\boldsymbol{\sigma}}) \left[\frac{f(\boldsymbol{V}_1^{**}, t) f(\boldsymbol{V}_2^{**} + \dot{\gamma} \sigma \hat{\sigma}_y \boldsymbol{e}_x, t)}{e^2} - f(\boldsymbol{V}_1, t) f(\boldsymbol{V}_2 - \dot{\gamma} \hat{\sigma}_y \boldsymbol{e}_x, t) \right],$$

Decoupling (Enskog equation)

The coefficient of restitution

$$f^{(2)}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{v}_1, \boldsymbol{v}_2; t) = \chi(\boldsymbol{r}_1, \boldsymbol{r}_2 | n(t)) f(\boldsymbol{r}_1, \boldsymbol{v}_1, t) f(\boldsymbol{r}_2, \boldsymbol{v}_2, t),$$

Contents

Stress equation for dilute suspensions

$$\boxed{\frac{\partial}{\partial t}P^k_{\alpha\beta} + \dot\gamma(\delta_{\alpha x}P^k_{y\beta} + \delta_{\beta x}P^k_{y\alpha}) = -2\zeta(P^k_{\alpha\beta} - nT_{\rm ex}\delta_{\alpha\beta}) - \Lambda^E_{\alpha\beta},}$$

$$P^k_{\alpha\beta}(\boldsymbol{r},t) = m\int d\boldsymbol{v}V_\alpha V_\beta f(\boldsymbol{V},t), \quad \Lambda^E_{\alpha\beta} \equiv -m\int d\boldsymbol{V}V_\alpha V_\beta J_E(\boldsymbol{V}|f,f).$$

To get a closure we adopt Grad's 13 moment method

$$\boxed{f(\boldsymbol{V}) = f_{\rm eq}(\boldsymbol{V})\left[1 + \frac{m}{2T}\Pi_{\alpha\beta}V_\alpha V_\beta\right]}$$

$$f_{\rm eq}(\boldsymbol{V}) = n\left(\frac{m}{2nT}\right)^{d/2}\exp\left(-\frac{mV^2}{2T}\right); \quad \Pi_{\alpha\beta} \equiv \frac{P^k_{\alpha\beta}}{nT} - \delta_{\alpha\beta}$$

$$T = \frac{1}{dn}\int d\boldsymbol{V}\boldsymbol{V}^2 f(\boldsymbol{V})$$

A set of dynamic equations: dilute gases

$$\begin{aligned}
\frac{\partial}{\partial t}T &= -\frac{2\dot\gamma}{dn}P_{xy} - \gamma T + 2\zeta(T_{\rm ex} - T),\\
\frac{\partial}{\partial t}\Delta T &= -\frac{2}{n}\dot\gamma P_{xy} - (\nu + 2\zeta)\Delta T,\\
\frac{\partial}{\partial t}P_{xy} &= \dot\gamma n\left(\frac{\Delta T}{d} - T\right) - (\nu+2\zeta)P_{xy},
\end{aligned}$$

Kinetic temperature $P = P_{\alpha\alpha}/d = nT$

$P^k{}_{xy} = P_{xy}$

Anisotropy of the temperature $\Delta T = \frac{P^k_{xx} - P^k_{yy}}{n}$

Some relations in the steady state (dilute case)

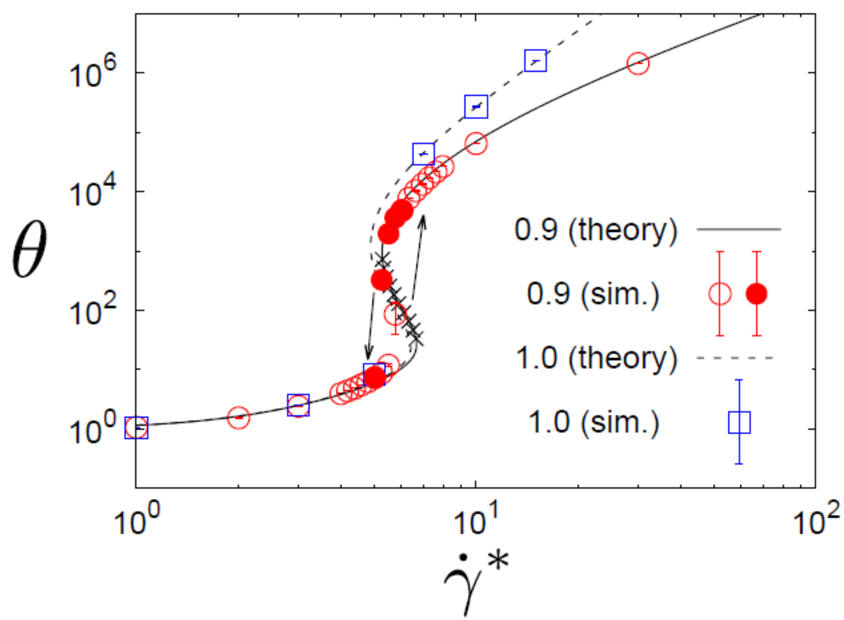
- Temperature ratio (normal stress difference) $$\frac{\Delta T}{T}=\frac{d(\gamma^*\sqrt{\theta}+2(1-\theta^{-1})}{\nu^*\sqrt{\theta}+2}$$
- Stress $$P_{xy}^*=-\frac{d\theta}{2\dot{\gamma}^*}\left\{\gamma^*\sqrt{\theta}+2(1-\theta^{-1})\right\}$$
- Shear rate $$\dot{\gamma}^*=(\nu^*\sqrt{\theta}+2)\sqrt{\frac{d[\gamma^*\sqrt{\theta}+2(1-\theta^{-1})]}{2[(\nu^*-\gamma^*)\sqrt{\theta}+2\theta^{-1}]}}$$
- Viscosity $$\eta^*=\frac{\theta\{(\nu^*-\gamma^*)\sqrt{\theta}+2\theta^{-1}\}}{(\nu^*\sqrt{\theta}+2)^2}$$

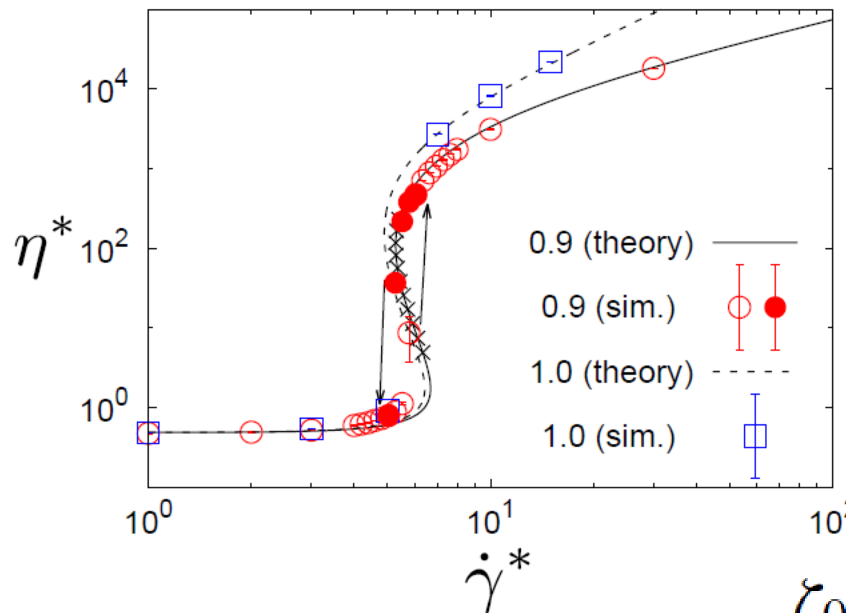
$$\theta\equiv T/T_{\rm ex}\qquad \nu^*=\frac{\nu}{\sqrt{T_{\rm ex}}\zeta_0},\quad \gamma^*=\frac{\gamma}{\sqrt{T_{\rm ex}}\zeta_0},\quad \dot{\gamma}^*=\frac{\dot{\gamma}}{\zeta_0\sqrt{T_{\rm ex}}}$$

DST in dilute suspensions

Flow curves for various restitution constant

=>Perfect agreement between the theory & simulation





$\theta \equiv T/T_{\rm ex}$ $\quad \varphi \approx 0.0052$ $\quad \dot{\gamma}^* = \dot{\gamma}/\zeta_0$ $\quad \eta^* \equiv \dfrac{\zeta_0 \eta}{n T_{\rm ex}}$

The lines are the analytic expressions of steady equations and the data are obtained from the Langevin simulation.

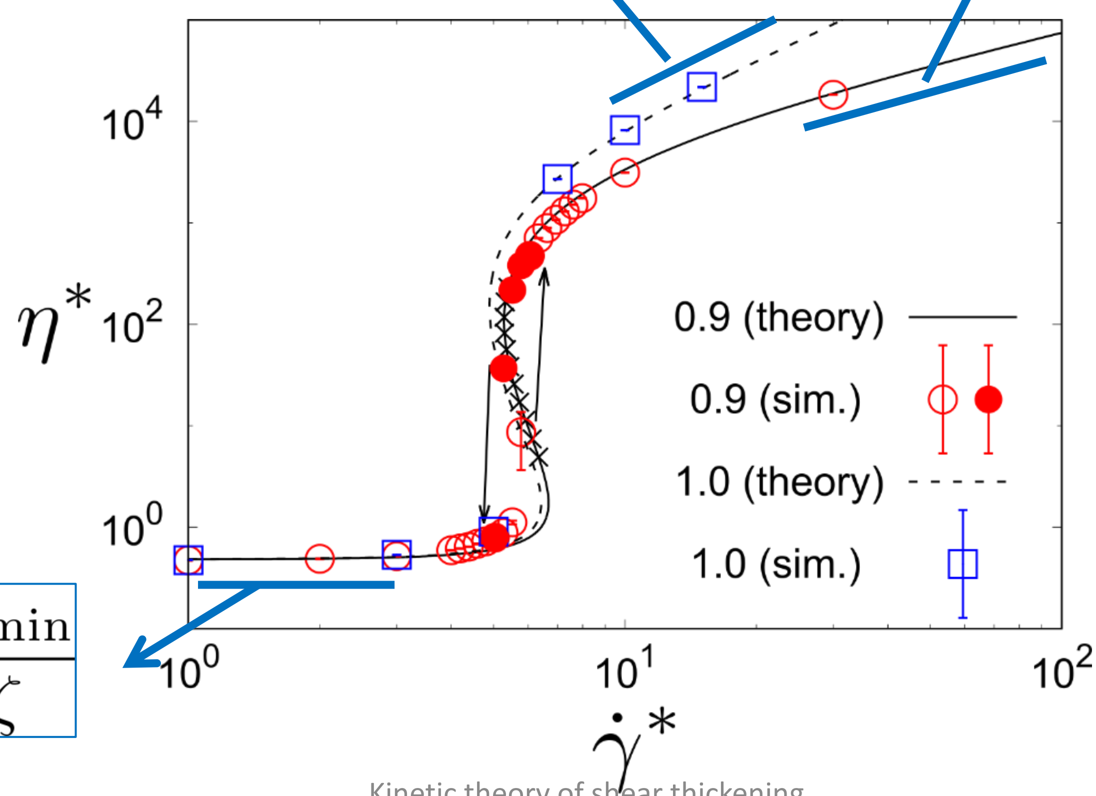
High and low shear limits

(e<1)

$$\eta \to \frac{\sqrt{2}(\nu_0-(1-e^2)\lambda_0)^{3/2}}{\sqrt{(1-e^2)d\lambda_0\nu_0^3 n}}\dot\gamma, \quad T \to \frac{2(\nu_0-(1-e^2)\lambda_0)}{(1-e^2)d\nu_0^2\lambda_0 n^2}\dot\gamma^2$$

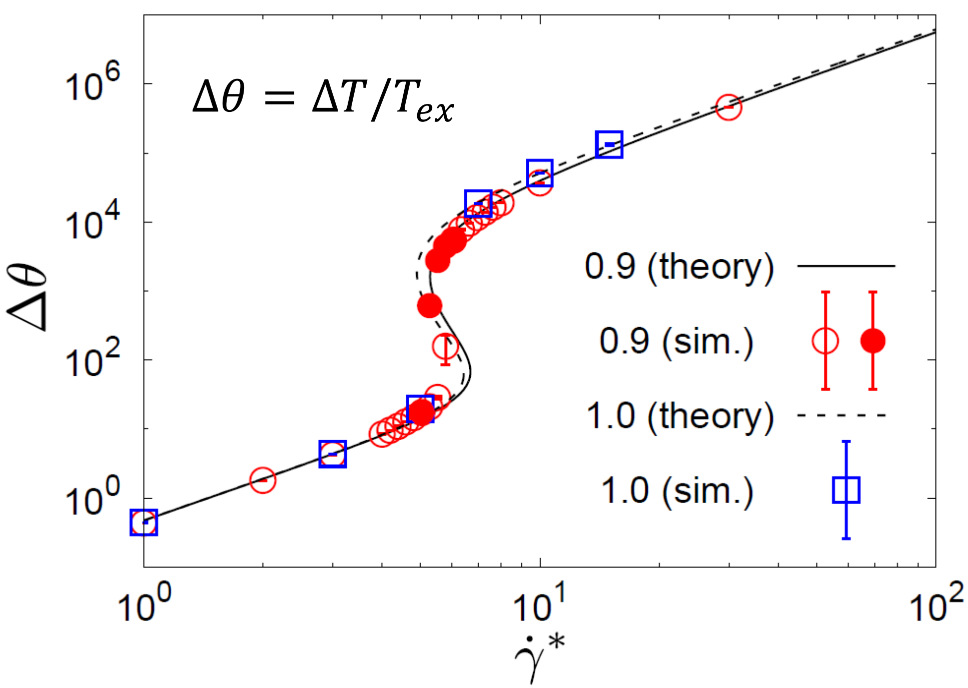
$$\eta \to \frac{1}{\zeta d\nu_0^2 n}\dot\gamma^2, \quad T \to \frac{1}{\zeta^2 d\nu_0^2 n^2}\dot\gamma^4$$

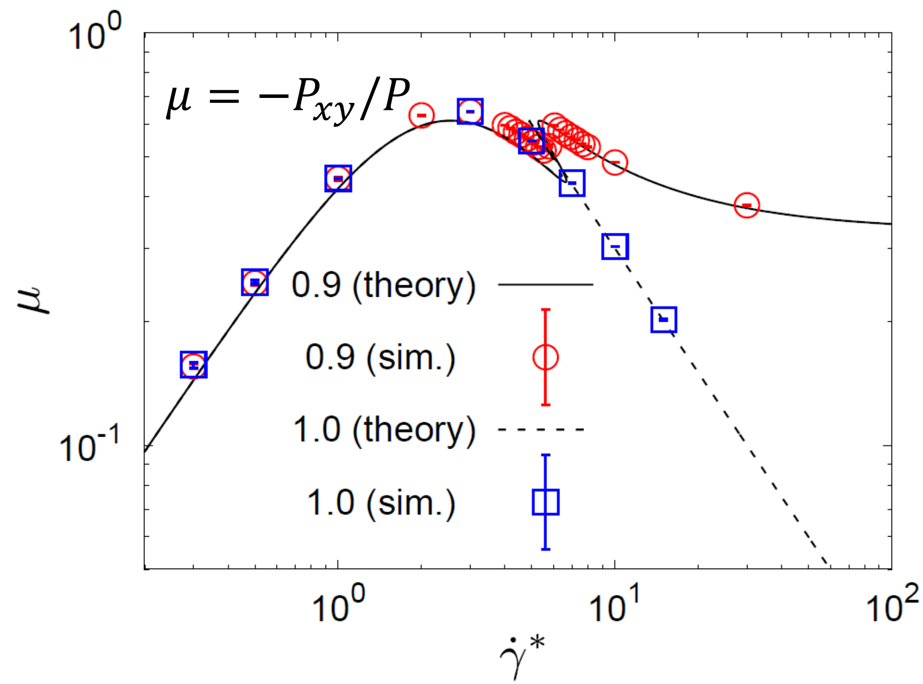
(e=1)



$$\eta \to \frac{nT_{\min}}{2\zeta}$$

Normal stress difference and shear ratio





$$\mu \to \sqrt{d/2}\gamma^*/\{\nu^*\sqrt{\nu^* - \gamma^*}\} \text{ for } e < 1$$

$$\mu \to d/\dot{\gamma}^* \text{ for } e = 1.$$

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Extension to finite density

- We can apply Grad's method to moderately dense suspensions.
- The collisional stress involves an additional contribution.
  - It is known that Enskog theory gives precise results for $\varphi < 0.5$.
- The treatment of the shear rate in the collisional stress is difficult.

=> This does not appear in Chapman-Enskog theory.

Stress equation for moderately dense gas

$$\boxed{\frac{\partial}{\partial t}P^k_{\alpha\beta}+\dot\gamma(\delta_{\alpha x}P_{y\beta}+\delta_{\beta x}P_{y\alpha})=-2\zeta(P^k_{\alpha\beta}-nT_{\rm ex}\delta_{\alpha\beta})-\overline{\Lambda}^E_{\alpha\beta}}$$

$$\overline{\Lambda}^E_{\alpha\beta}=\frac{1+e}{4}m\sigma^{d-1}\int d\boldsymbol{v}_1\int d\boldsymbol{v}_2\int d\hat{\boldsymbol{\sigma}}\Theta(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{v}_{12})(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{v}_{12})^2\{(v_{12,\alpha}\hat\sigma_\beta+\hat\sigma_\alpha v_{12,\beta})f_2(\boldsymbol{r},\boldsymbol{v}_1,\boldsymbol{r}+\boldsymbol{\sigma},\boldsymbol{v}_2;t)$$

$$-(1+e)(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{v}_{12})\hat\sigma_\alpha\hat\sigma_\beta f_2(\boldsymbol{r},\boldsymbol{v}_1,\boldsymbol{r}+\boldsymbol{\sigma},\boldsymbol{v}_2;t)\}$$

$$=g_0nT\{\nu\Pi^k_{\alpha\beta}+\gamma\delta_{\alpha\beta}$$
$$-\dot\gamma A_d(e,\varphi)[b_d(e)(\delta_{\alpha x}\delta_{\beta y}+\delta_{\alpha y}\delta_{\beta x})+c_d(e)(\Pi^k_{\alpha x}\delta_{\beta y}+\Pi^k_{\alpha y}\delta_{\beta x}+\Pi^k_{\beta x}\delta_{\alpha y}+\Pi^k_{\beta y}\delta_{\alpha x})-6(1+e)\delta_{\alpha\beta}\Pi^k_{xy}]\}$$

$$\nu=\frac{\sqrt{2}\pi^{(d-1)/2}n\sigma^{d-1}v_T(1+e)(2d+3-3e)}{d(d+2)\Gamma(\frac{d}{2})},$$

$$\gamma=\frac{\sqrt{2}\pi^{(d-1)/2}n\sigma^{d-1}v_T(1-e^2)}{d\Gamma(\frac{d}{2})}$$

$$A_d(e,\varphi)=\frac{2^{d-2}}{(d+2)(d+4)}\varphi(1+e),\quad b_d(e)=(d+4)(1-3e),\quad c_d(e)=2(d+1-3e).$$

Stress equations under Grad's approximation

$$\frac{d}{dt}T = -\frac{2\dot\gamma}{dn}\mathcal{C}_d(e,\phi)P_{xy}^k - \frac{2\dot\gamma}{dn}P_{xy}^c + 2\zeta(T_{\rm ex}-T) - \chi\gamma T,$$

$$\frac{d}{dt}\Delta T = -\frac{2}{n}\dot\gamma P_{xy} - (\nu\chi + 2\zeta)\Delta T,$$

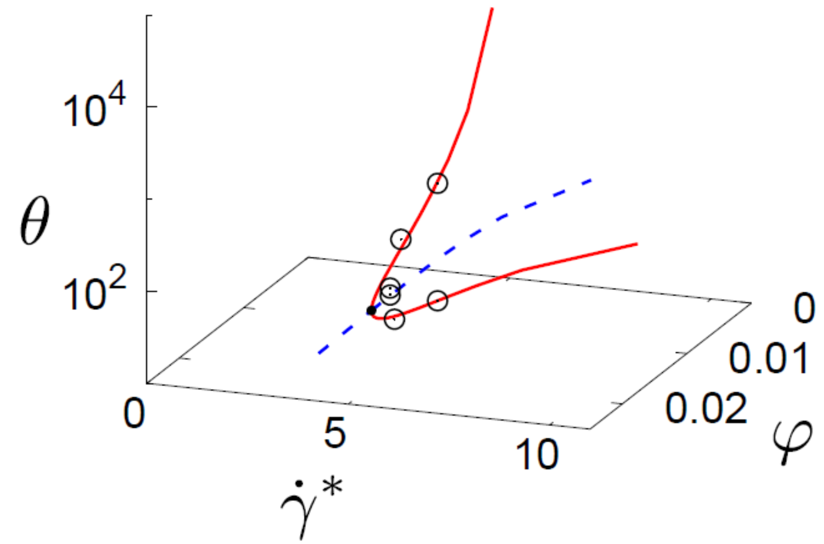
$$\frac{d}{dt}\delta T = \quad -\frac{2}{n}\dot\gamma(\mathcal{E}_d(e,\phi)P_{xy}^k + P_{xy}^c) - (\nu\chi + 2\zeta)\delta T,$$

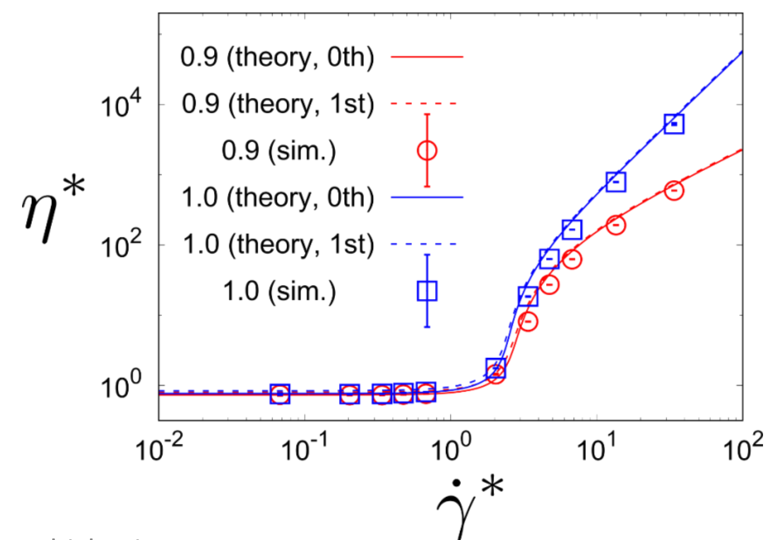
$$\frac{d}{dt}P_{xy}^k = \dot\gamma n\left(\frac{d-1}{d}\mathcal{D}_d(e,\phi)\Delta T - \frac{d-2}{d}\mathcal{E}_d(e,\phi)\delta T - \mathcal{C}_d(e,\phi)T\right) - \dot\gamma P_{yy}^c - (\nu\chi + 2\zeta)P_{xy}^k,$$

$$\Delta T \equiv \frac{P_{xx}^k - P_{yy}^k}{n}, \qquad \delta T \equiv \frac{P_{xx}^k - P_{zz}^k}{n} \qquad P_{xy} = {P_{xy}}^k + {P_{xy}}^c$$

From DST to CST

- DST becomes CST if the density becomes finite.
- We plot the line of $\partial\dot{\gamma}/\partial\theta = 0$, where the red one is $\partial^2\dot{\gamma}/\partial\theta^2 > 0$.
- It is analogous to the first order transition.

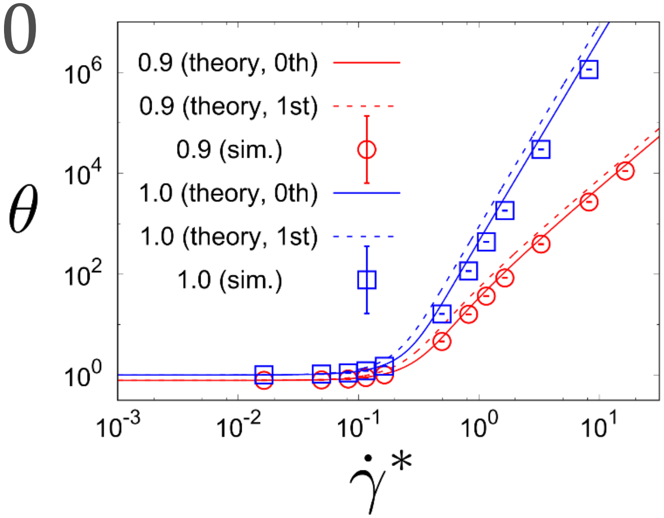


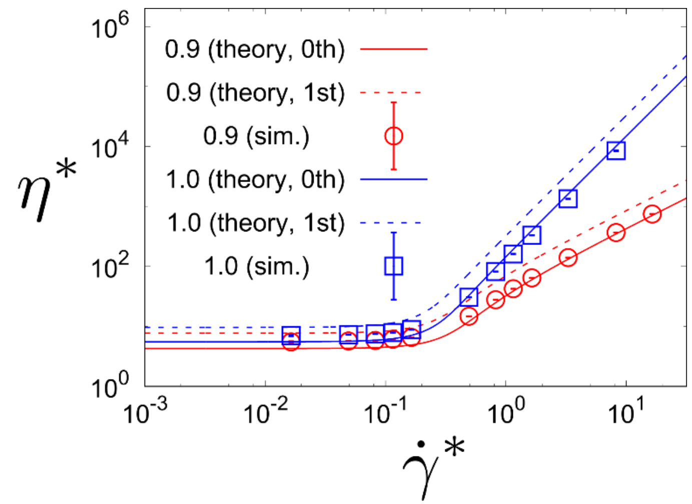


$\varphi = 0.05$

Moderately dense cases

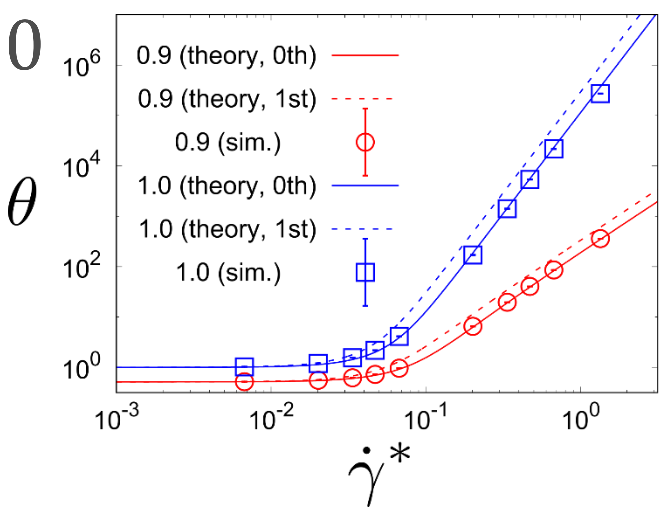
$\varphi = 0.30$

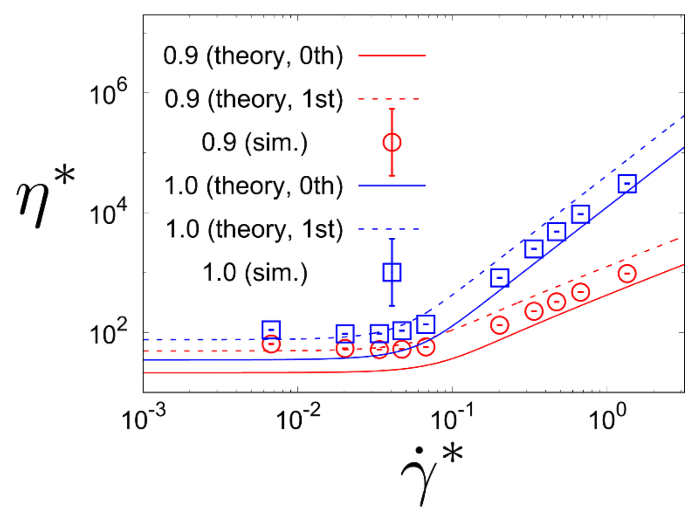




Temperature & Viscosity ⇒ good agreement

$\varphi = 0.50$

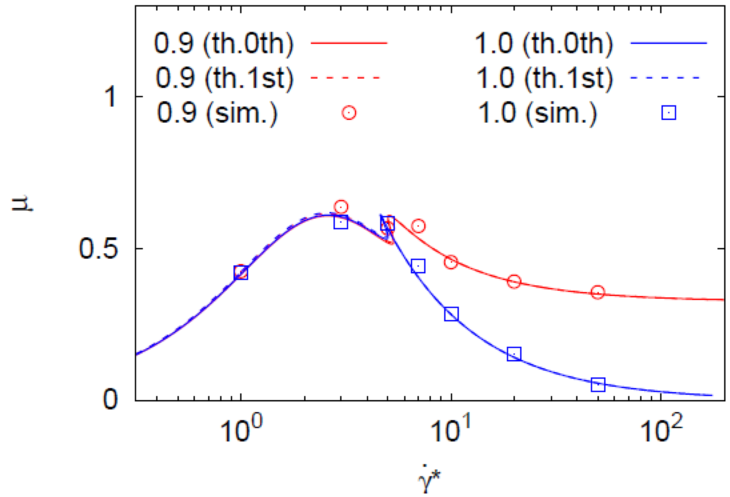


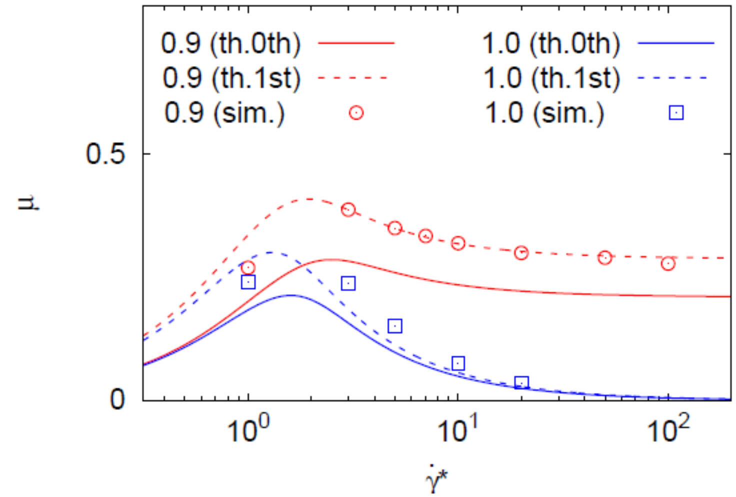


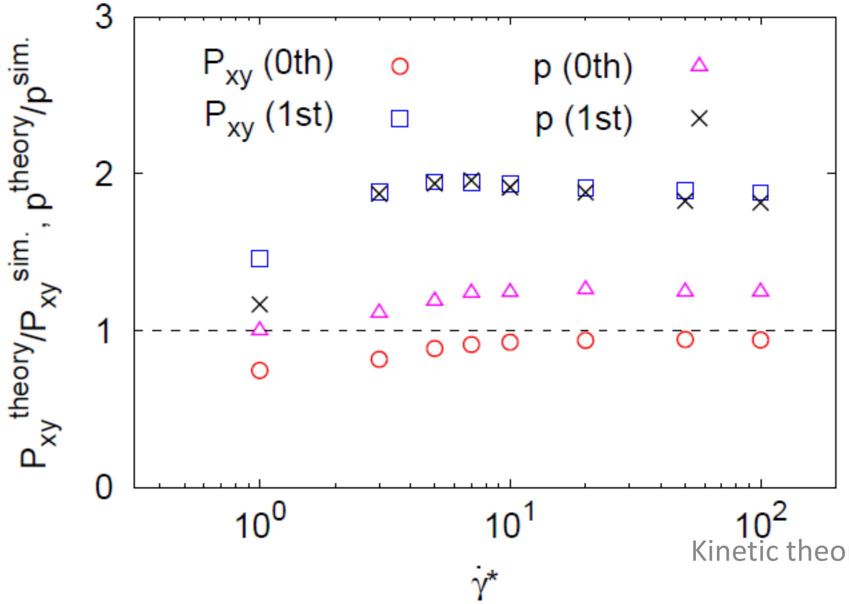
Temperature ⇒ good

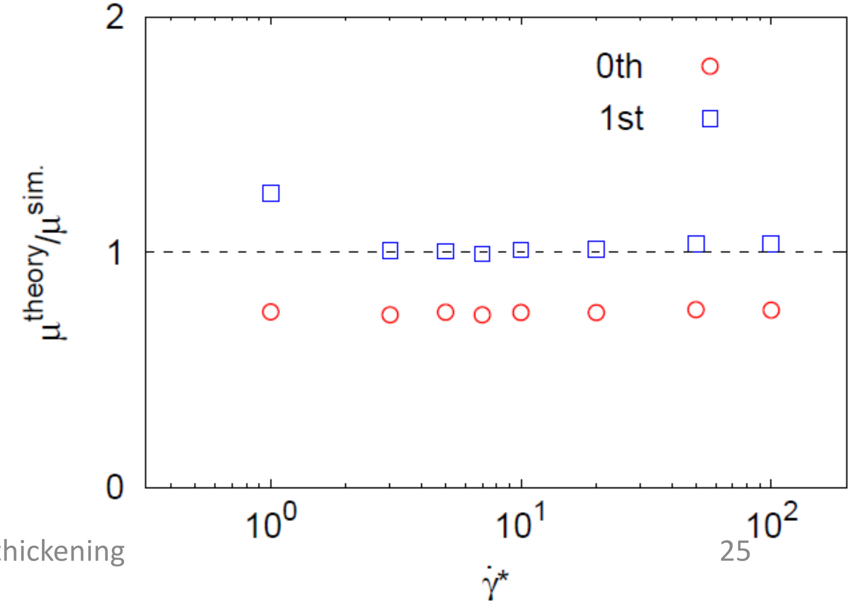
Viscosity ⇒ fare

Stress ratio

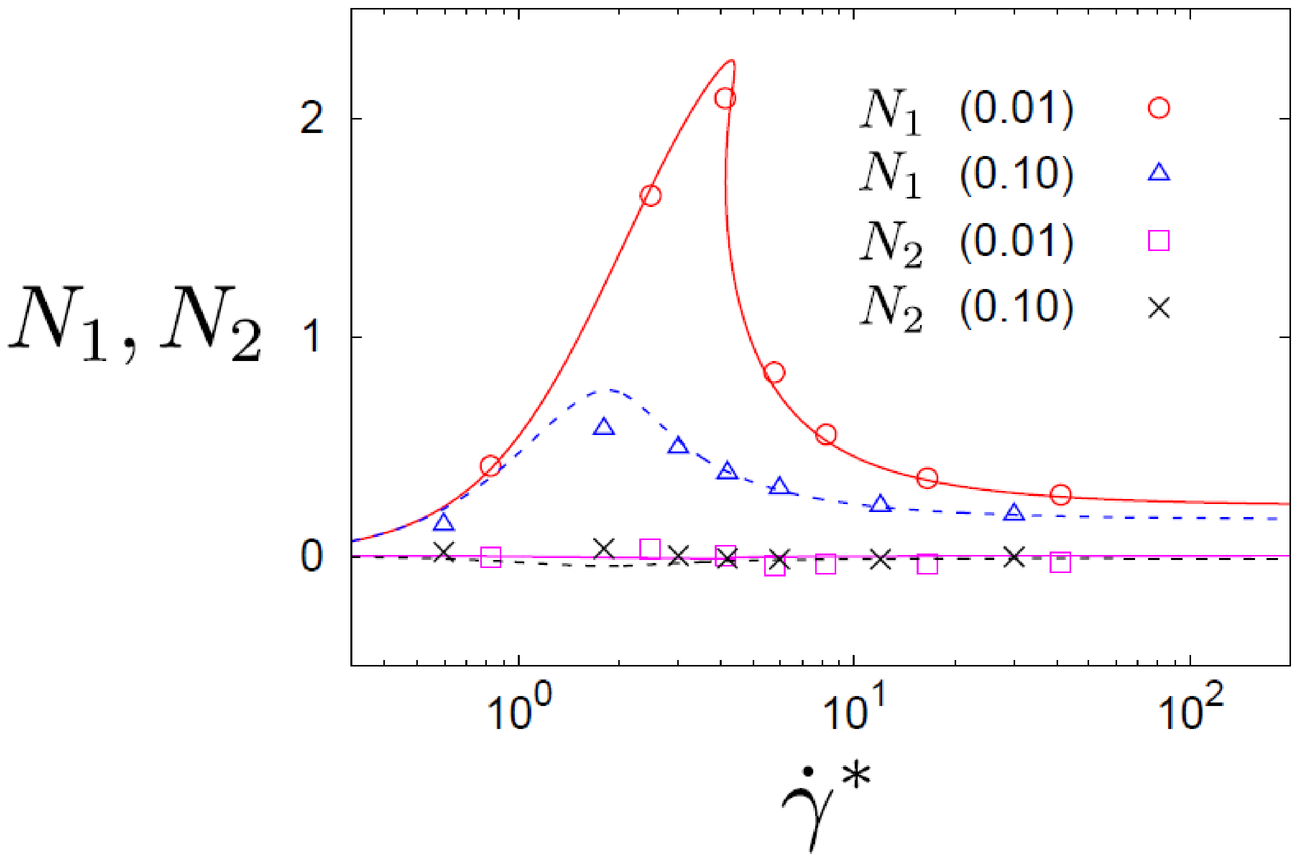








Normal stress differences



$$N_1 \equiv (P_{xx} - P_{yy})/P \qquad N_2 \equiv (P_{yy} - P_{zz})/P$$

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Motivation for study of binary mixtures

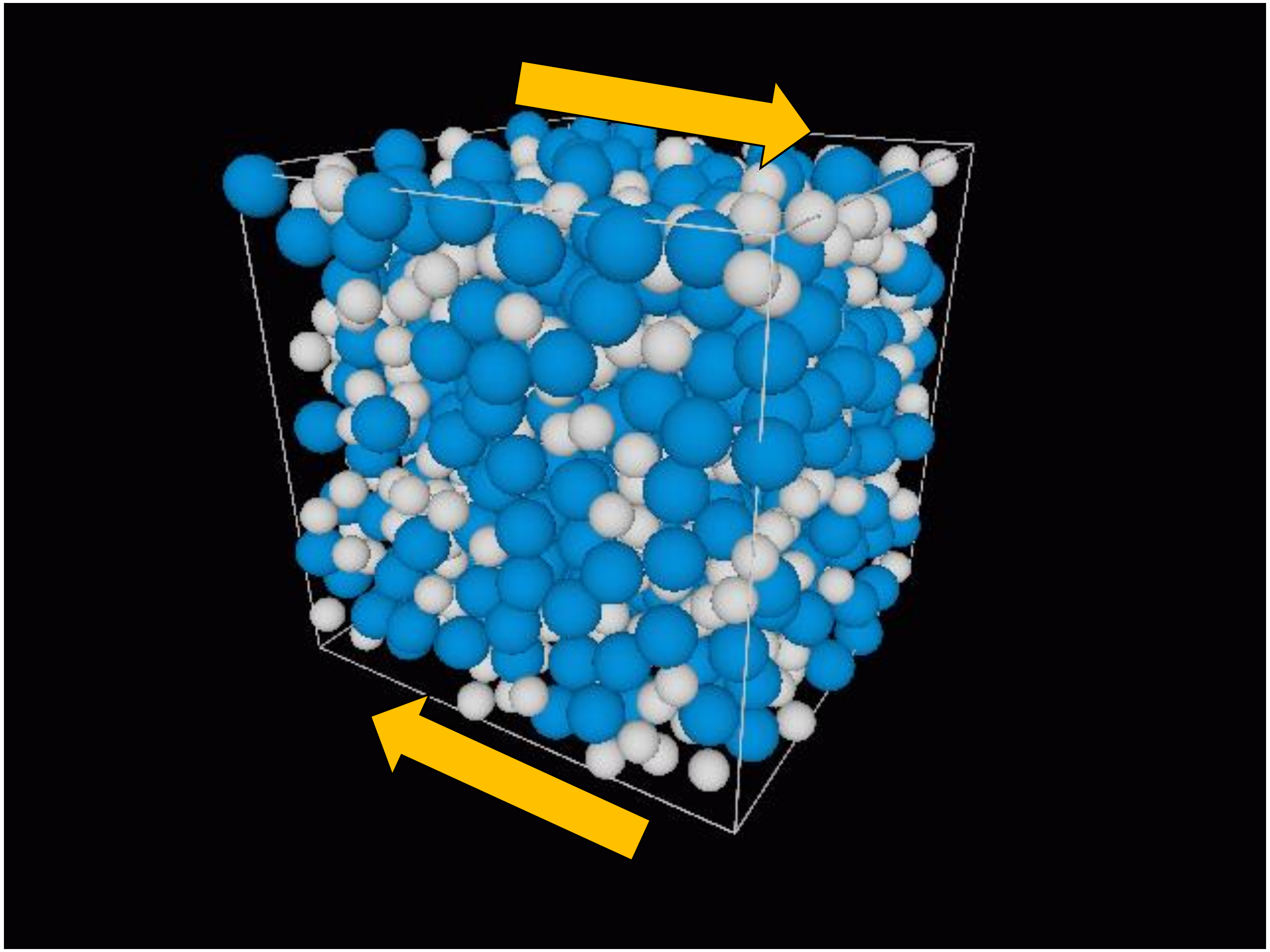
- To avoid crystallization for dense systems
- To discuss shear thinning for low shear regime
- To clarify the role of mutual diffusion between two spieces
- To extend the simple kinetic theory for mono-disperse systems to the complicated(?) kinetic theory for binary mixtures

Some examples of simulation for moderately dense systems

- Bidisperse system
- Number of particles:
$$N = N_1 + N_2, N_1 = N_2 = 500$$
- Diameter:
$$d_1 : d_2 = 1 : 1.4, d_1 = d, d_2 = 1.4d$$
- Restitution coefficient:
$$e_{11} = e_{22} = e_{12} \equiv e$$

The notations are same as those in our previous paper.
(All quantities are nondimensionalized in terms of m, d, ζ.)

Simulation movie ($\varphi = 0.4, e = 0.9$)



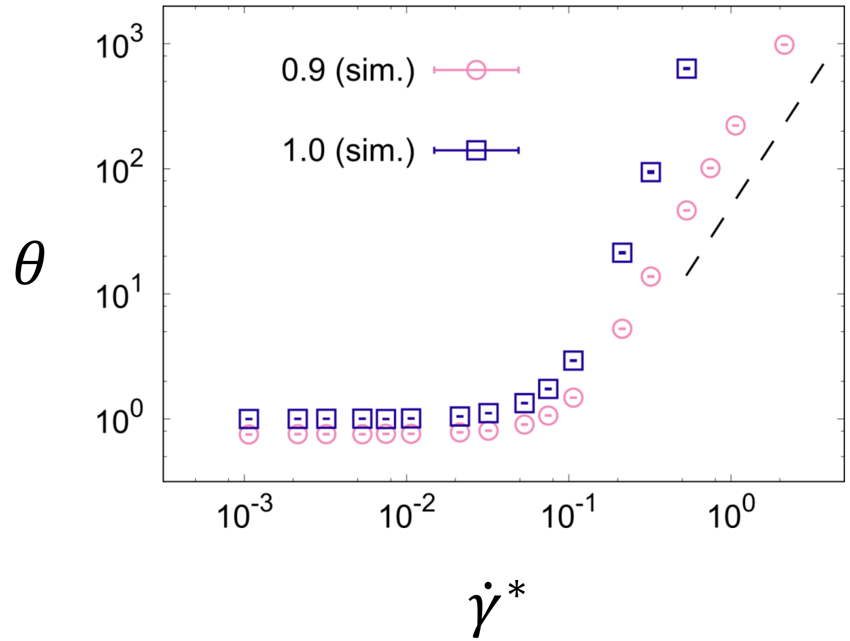
Simulation works!

Small particles: gray
Large particles: blue

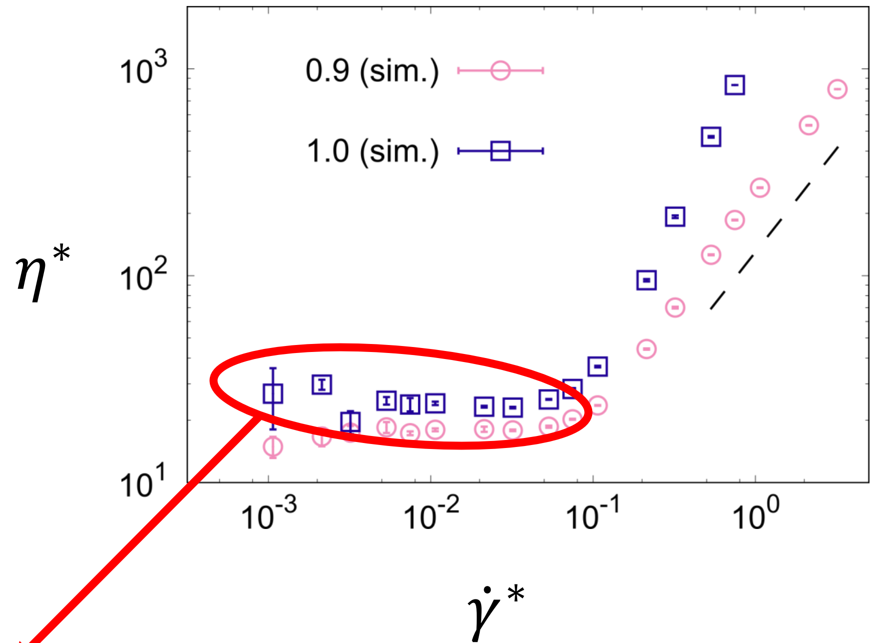
Results: moderately dense case

$$\varphi = 0.40$$

Temperature ratio



Shear viscosity



Shear thinning appears for $e = 1$!
But plateau for $e < 1$.

Some simulation for dilute cases

- Bidisperse system
- Number of particles:

$$N = N_1 + N_2, N_1 = N_2 = 500$$

- Diameter: 1:1.1, 1:1.4, 1:2, and 1:3
  ex.) $d_1 : d_2 = 1 : 1.4 \Longrightarrow d_1 = d, d_2 = 1.4d$

$$\text{mass ratio: } \frac{m_2}{m_1} = \left(\frac{d_2}{d_1}\right)^3$$

- Restitution coefficient:

$$e_{11} = e_{22} = e_{12} \equiv e = 0.9$$

- System size:
  $L = 39.4d\ (d_2 = 1.1d)$,
  $L = 46.1d\ (d_2 = 1.4d)$,
  $L = 61.8d\ (d_2 = 2d)$,
  $L = 90.2d\ (d_2 = 3d)$.

- Packing fraction

$$\varphi = \frac{N_1 \frac{\pi}{6} d_1^3 + N_2 \frac{\pi}{6} d_2^3}{L^3} = 0.01$$

Dimensionless parameters

- All quantities are nondimensionalized by mass $m = m_1$, diameter $d = d_1$, and drag coefficient ζ

$$T_{\rm ex} = 0.01 m d^2 \zeta^2$$

Shear rate: $\dot{\gamma}^* = \frac{\dot{\gamma}}{\zeta}$

Temperature: $\theta_i = \frac{T_i}{T_{\rm ex}}$

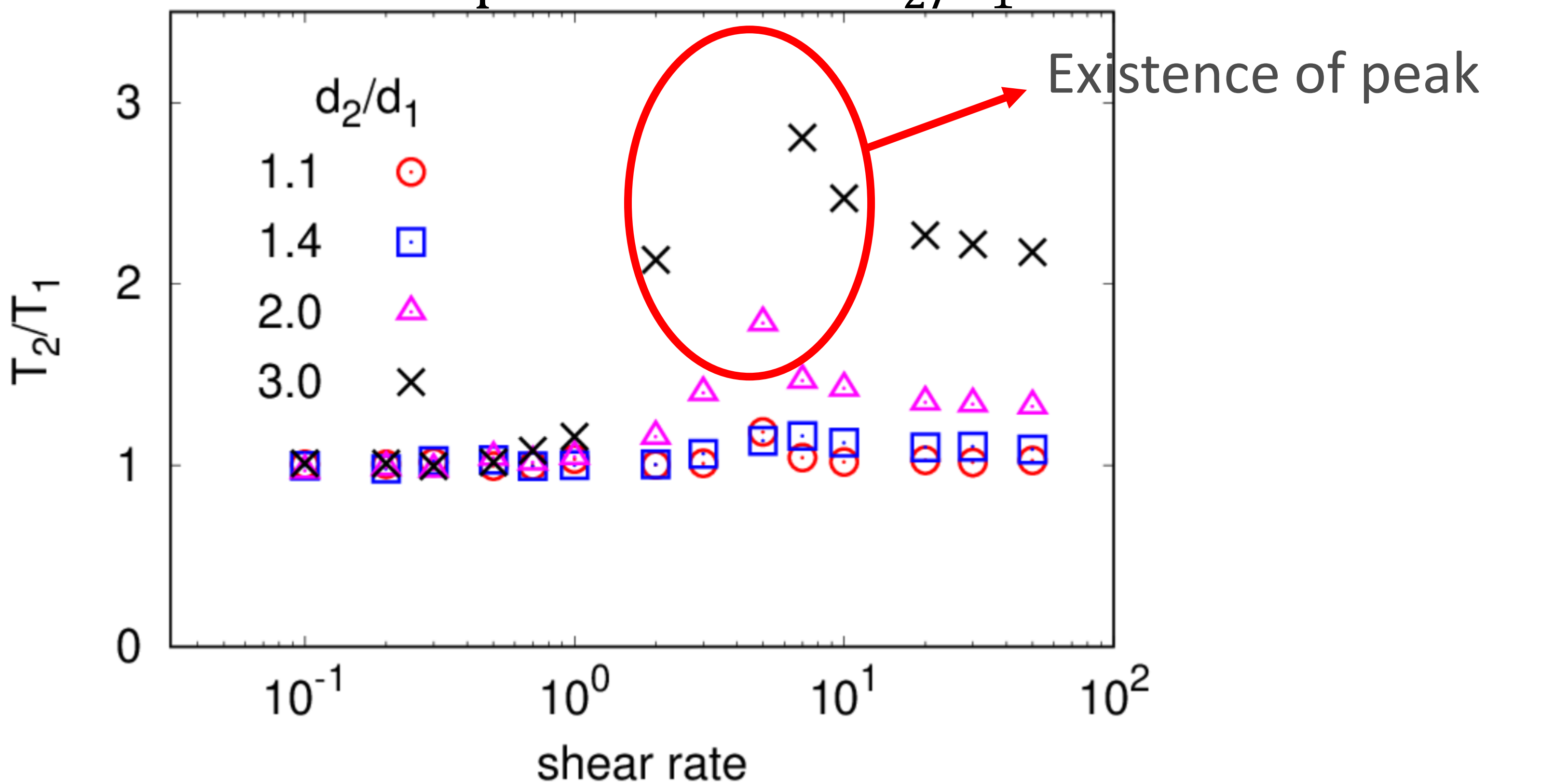
Stress tensor: $P^{k*} = \frac{P}{nT_{\rm ex}}$

Viscosity: $\eta^* = \frac{\eta\zeta}{nT_{\rm ex}}$

Same as
H. Hayakawa and S. Takada, arXiv:1611.07295
and
H. Hayakawa, S. Takada, and V. Garzó, Phys. Rev. E **96**, 042903 (2017)

Partial temperature ratio

Partial temperature ratio T_2/T_1



Low shear limit: $T_2/T_1 \to 1$

High shear limit:

$$T_2/T_1 \to 1.1\ (d_2/d_1 = 1.4), 1.3\ (d_2/d_1 = 2.0)$$

Current status of theory

- We are focusing on dilute situations.
- We have precisely evaluated collision integrals.
- The theoretical treatment for the temperature ratio seems to work for not-large size ratios, but has some troubles for large size ratios (V. Garzo).
- Flow curves are insensitive to the size dispersion.
- Perhaps, we will report the results in details in near future.

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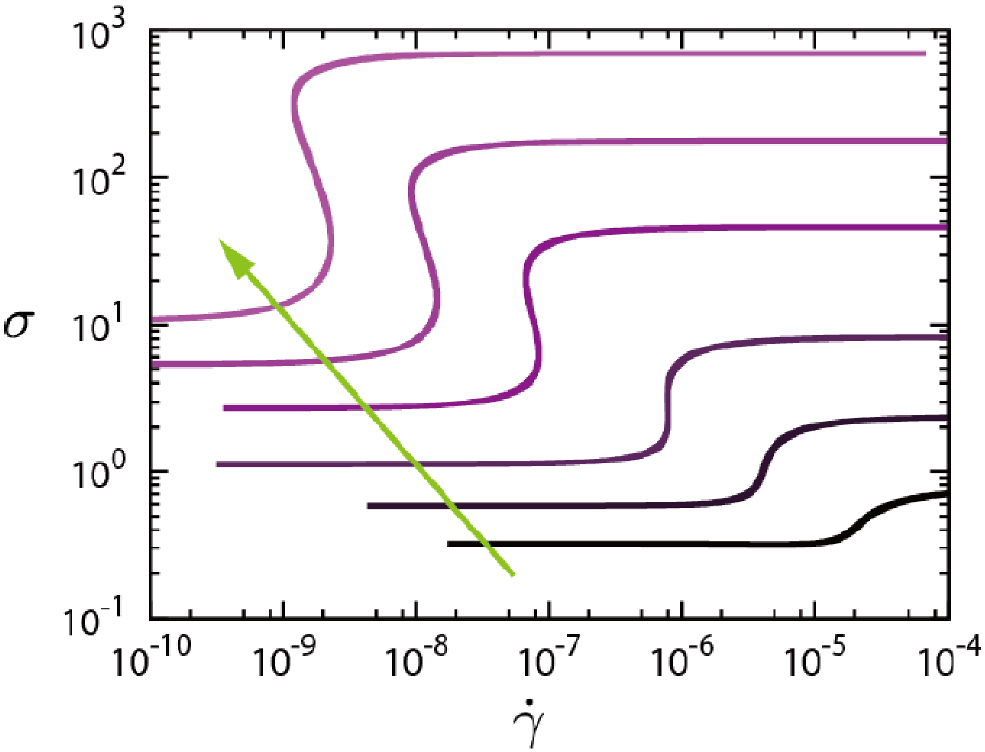
- From DST to continuous shear thickening (CST) at finite density
- Application to binary mixtures
- **Discussions**
- Conclusions

Effect of hydrodynamic interactions; shear thickening model

- The hydrodynamic interactions play crucial roles in moderately dense suspensions.
- It is difficult to analyze the serious model of hydrodynamically interacting suspensions.
- Nevertheless, it is easy to implement the hydrodynamic effect as a mean field by changing the drag coefficient.

Effect of mutual friction in dense systems

- The mutual friction plays an important role for dense systems.
- Kuniyasu Saitoh & HH are developing the kinetic theory of dense frictional dry granular systems.
- Listen to Kuni’s talk.



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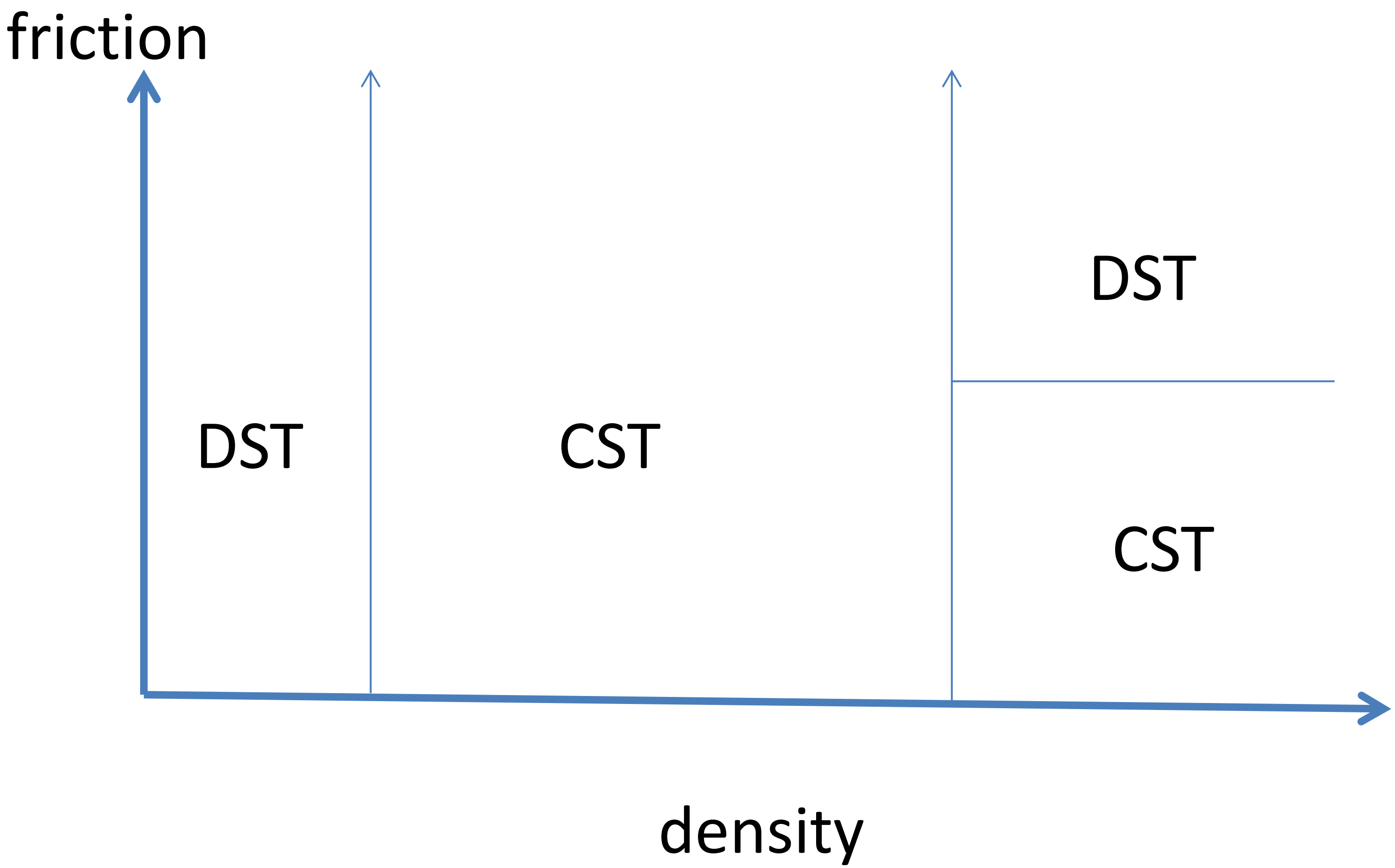
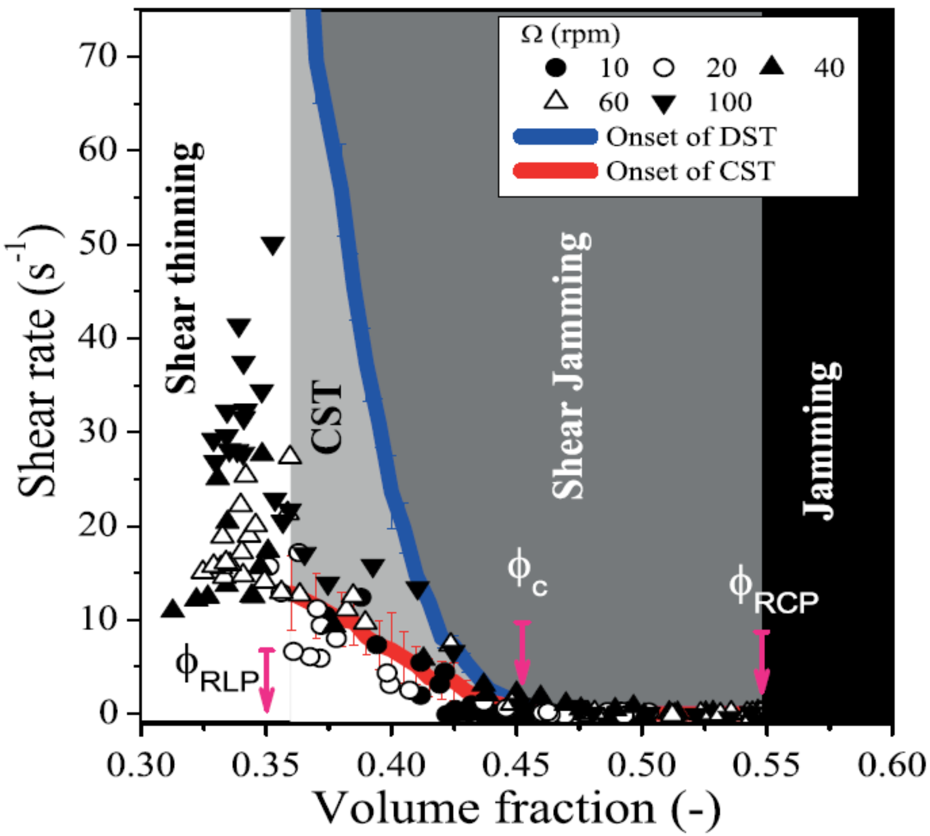
Conceptual phase diagram



Shear jammed state and DST

- DST for high density system is related to the shear jammed (SJ) state.
  - SJ may be a protocol dependent state for frictional grains.
- (Right) Bertland et al, PRL **114**, 098301 (2015) but it is under debate.
- This is a current hot subject in this field.



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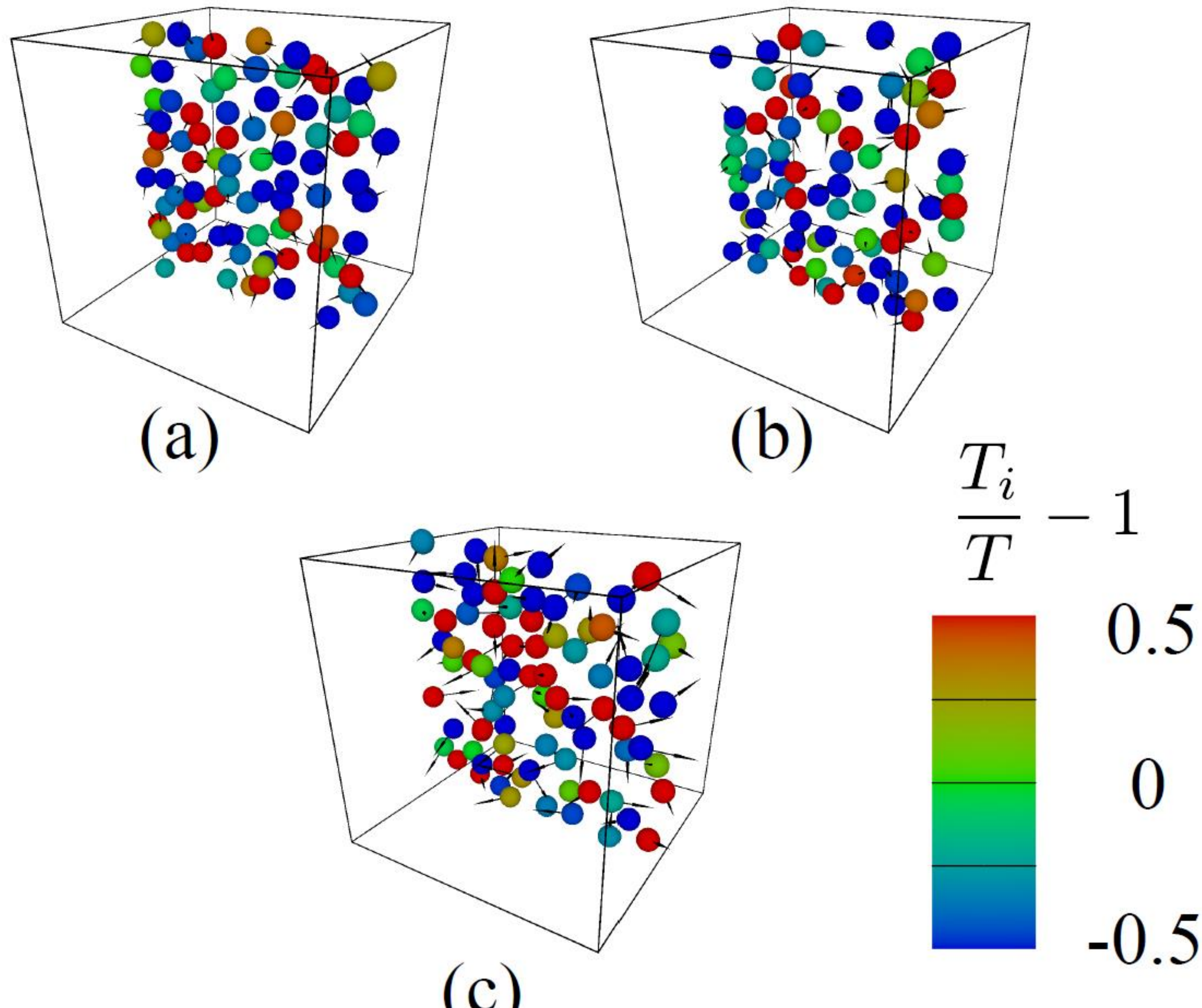
Conclusions for shear thickening

- We develop a simple kinetic theory for shear thickening.
- Discontinuous shear thickening (DST) can be reproduced for arbitrary T_{ex} and dilute situations.
- Normal stress difference is important.
- All of the theoretical results perfectly agree with simulation results for dilute cases.
- We also develop Enskog theory for moderately dense suspensions and find the existence a transition from DST to CST.
- See Hayakawa et al, PRE **96**, 042903(2017).

- Thank you for your attention.


(a)
(b)
(c)
$\frac{T_i}{T} - 1$
0.5
0
-0.5

Configurations