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Frontier research on glasses and related complex systems

Kinetic theory of inertial suspensions: Steady rheology and Mpemba effect

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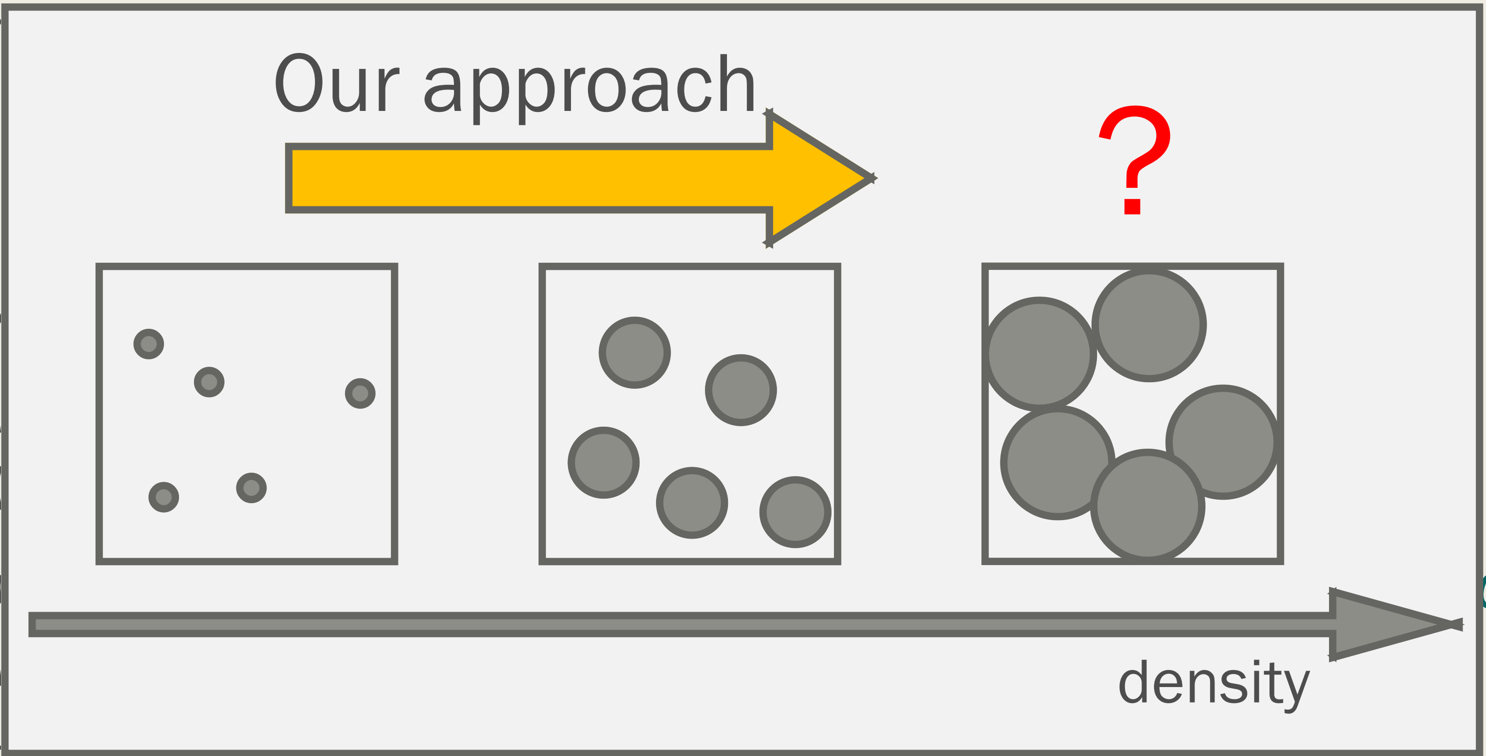
[3] Univ. Extremadura

☞ S. Takada, H. Hayakawa, A. Santos, and V. Garzó, Phys. Rev. E **102**, 022907 (2020)
S. Takada, H. Hayakawa, and A. Santos, Phys. Rev. E **103**, 032901 (2021).

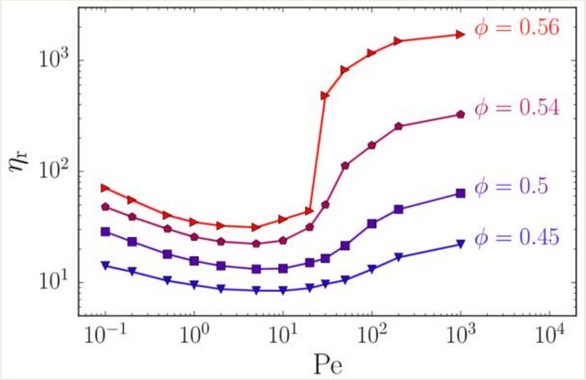
Why do we use Enskog theory?

- Enskog theory was derived almost 100 years ago.
- Enskog th
  for mode
- Applicabi
  - *Many* … *but* *NOT* *dense)*
  - *Rece*
    $\varphi \lesssim$ (
  - *Our o* … *d):*
    The t



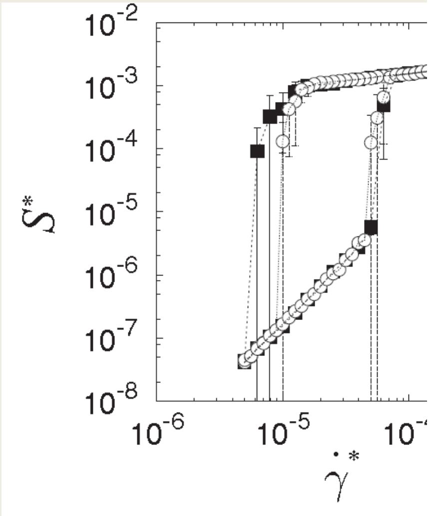
  - ➢ treat denser regime ($\varphi > 0.5$) near jamming density?
  - ➢ has several time scales. (can describe the relaxation?)
- We attempt to describe the rheology from a dilute side.

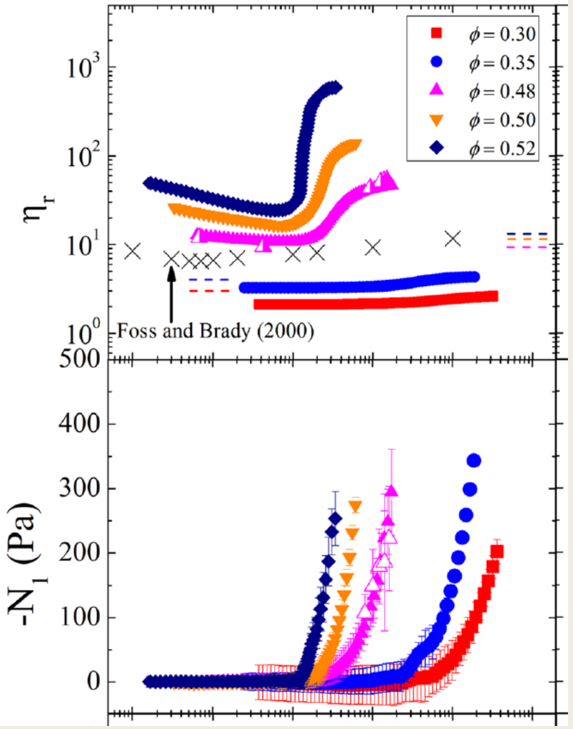
Shear thickening



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

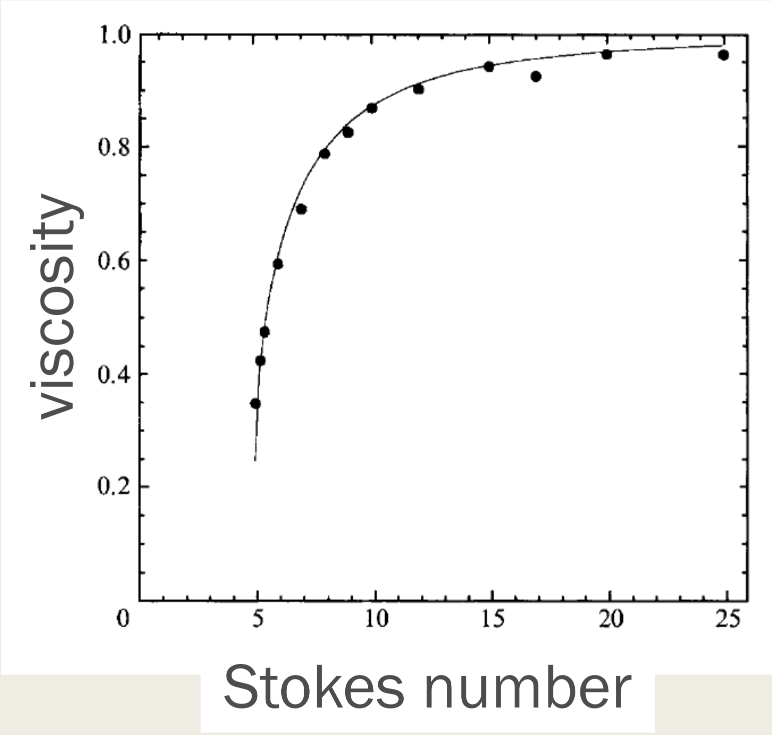
- Shear thickening:
  viscosity: $\eta_s(\varphi) = \sigma(\varphi)/\dot{\gamma} \nearrow$ against the shear rate $\dot{\gamma}$.
- Discontinuous shear thickening (DST):
  The viscosity discontinuously increases.
- DST is studied in many contexts and setups.
  - *DST for dense systems (simulations)*
    Mutual friction is important.
    M.Otsuki & H. Hayakawa, Phys. Rev. E ***83****, 051301 (2011)*
    R. Seto, et al., Phys. Rev. Lett. ***111****, 218301 (2013)*
  - *DST for colloidal systems (experiments)*
    Normal stress difference is also important.
    C. D. Cwalina & N.J. Wagner, J. Rheol. ***58****, 949 (2014)*
- Industrial applications: protective vest and traction control





Gas-solid suspensions

- Inertial suspensions (a model of aerosols)
- Homogeneity is kept.
- Relatively dilute system
  (theoretical treatment is available)



Previous (theoretical) study

☞ *Tsao and Koch, JFM* ***296****, 211 (1995)*

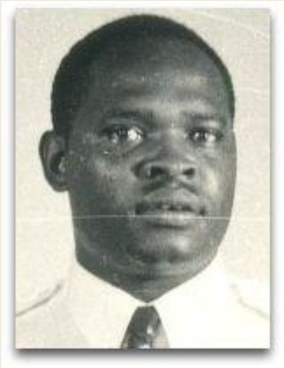
Kinetic theory of dilute gas-solid suspensions without thermal noise

⇒ Quenched-Ingnited transition

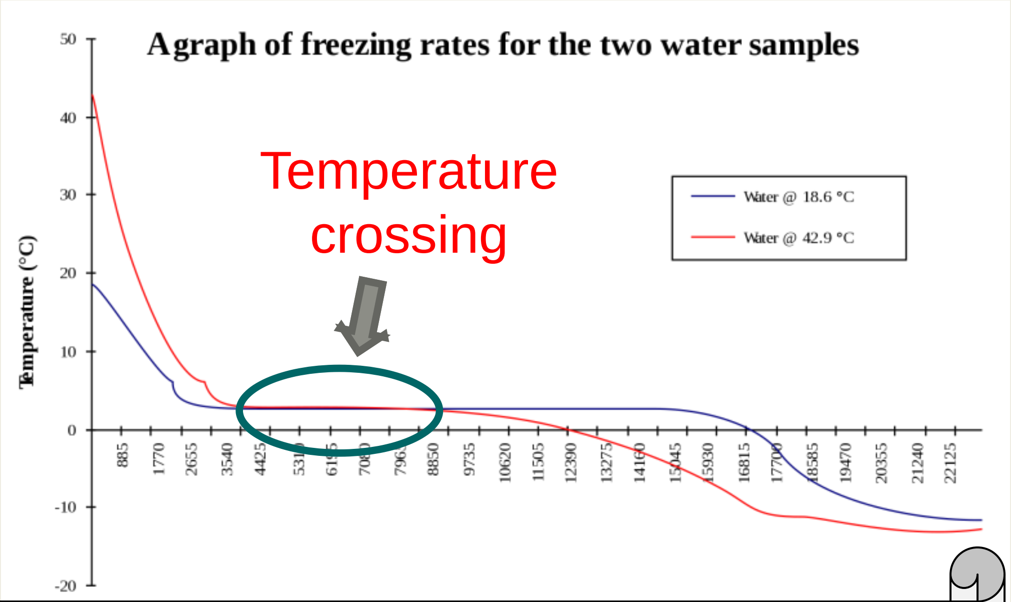
DST-like transition for **temperature**

but not for **viscosity**

Mpemba effect: Anomalous temperature relaxation



- E. B. Mpemba (1963) found that
“some hot water (ice cream mix; a typical suspension)
can freeze faster than cold water.”



Is it true?

Many debates to this phenomena

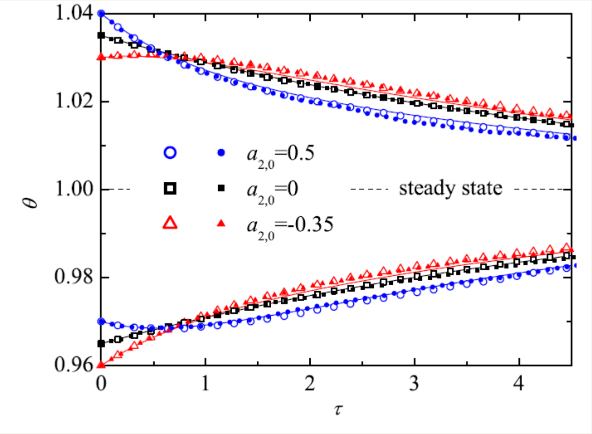
- Existence of many control parameters and setups.
- Poor reproducibility

Physics World

“Even if the Mpemba effect is real
— if hot water can sometimes freeze more quickly than cold —
it is not clear whether the explanation would be trivial or illuminating.”

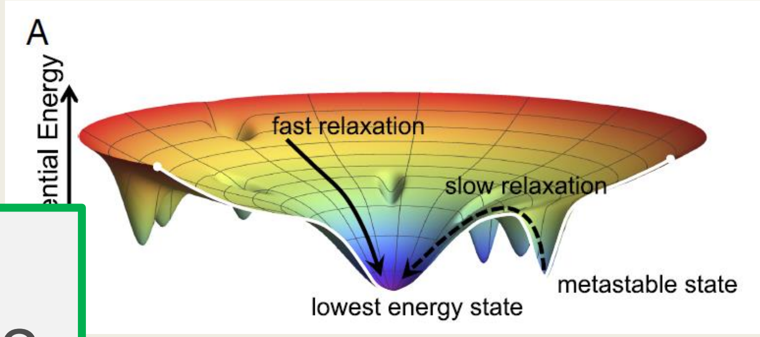
Modern perspective on Mpemba effect

- Freezing is complex… (supercooling, evaporation, convection…)
  ⇒ We focus on …
  "a hot fluid can have ***lower temperature*** *than a cold fluid"* as time goes on
- Inverse Mpemba effect in heating processes can exist.



Recent theoretical studies

- Granular gas (temperature)
  ☞ *Lasanta et al. PRL* ***119****, 148001 (2017)*
  Existence of both ME and inverse ME
  ⇒ origin: kurtosis of velocity distribution.
- Trapping process (dist. from equil.)
  ☞ *Lu & Raz, PNAS* ***114****, 5083 (2017)*
  slow relaxation by trapping at local minima.



Question:
But how can we control them?

Purpose of this talk

In this talk, we…

- construct the kinetic theory of the inertial suspensions.
- demonstrate that
  our theory gives a precise description of suspensions.
  - *DST-like behavior (ignited-quench transition) in dilute systems.*
  - *DST-like → CST-like as the density increases.*
  - *applicability to denser systems.*
- discuss anomalous relaxation processes.
  - *The normal Mpemba effect (NME) occurs quite naturally.*
  - *The anomalous ME (AME) also exists.*

1st part: General framework of Enskog theory

Langevin model for suspensions

Parameters
Packing fraction: φ
Restitution coeff.: e
Shear rate: $\dot{\gamma}$
Env. temp.: T_{env}

Suspended particles are described by

Langevin equation: $\dfrac{d\boldsymbol{p}_i}{dt} = \underbrace{-\zeta\boldsymbol{p}_i}_{①} + \underbrace{\boldsymbol{F}_i^{(\mathrm{imp})}}_{②} + \underbrace{m\boldsymbol{\xi}_i}_{③}$

$\boldsymbol{p}_i \equiv m(\boldsymbol{v}_i - \dot{\gamma} y_i \boldsymbol{e}_x) = m\boldsymbol{V}_i$: peculiar momentum

☞ *D. J. Evans & G. Morriss, "Statistical Mechanics of Nonequilibrium Liquids"*

①drag term

②impulsive force due to collisions

$$\boldsymbol{v}_1' = \boldsymbol{v}_1 - \frac{1+e}{2}(\boldsymbol{v}_{12}\cdot\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}, \qquad \boldsymbol{v}_2' = \boldsymbol{v}_2 + \frac{1+e}{2}(\boldsymbol{v}_{12}\cdot\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}$$

③thermal noise term satisfies

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

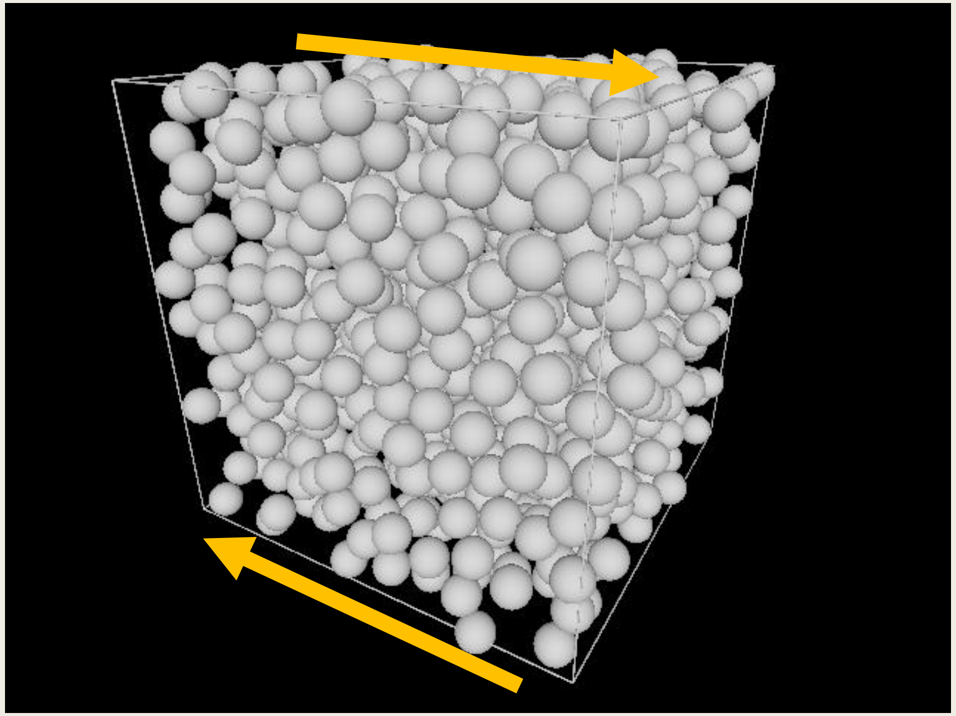
Langevin model for suspensions

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

Assumptions:

- drag ∝ solvent velocity (Stokesian)
- drag coefficient $\zeta = \mathrm{const.}$
- Existence of the noise term

  ⇒ The system can reach
  a thermal equilibrium state.



We also perform event-driven Langevin hard-core simulations.

☞ *A. Scala, Phys. Rev. E 86, 026709 (2012)*

Enskog kinetic equation for the inertial suspension

- Langevin model ⇔ kinetic (Enskog) equation

$$\left(\frac{\partial}{\partial t}-\boxed{\dot{\gamma}V_y\frac{\partial}{\partial V_x}}\right)f(\boldsymbol{V},t)=\boxed{\zeta\frac{\partial}{\partial \boldsymbol{V}}\cdot\left(\left[\boldsymbol{V}+\frac{T_{\rm env}}{m}\frac{\partial}{\partial \boldsymbol{V}}\right]f(\boldsymbol{V},t)\right)}+\boxed{J_{\rm E}\left(\boldsymbol{V}|f^{(2)}\right)}$$

shear — drag from the background — collision

- No inhomogeneity: $f(\boldsymbol{r},\boldsymbol{V},t)=f(\boldsymbol{V},t)$
- Collision integral:

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

- Decoupling: (two-body VDF)→(RDF)×(one-body VDF)×(one-body VDF)

$$f^{(2)}(\boldsymbol{v}_1,\boldsymbol{v}_2,t)=\underline{g_0(\varphi)}f(\boldsymbol{v}_1,t)f(\boldsymbol{v}_2,t)$$

radial distribution function (RDF)

Enskog kinetic equation for the inertial suspension

- Enskog equation

Evolution equation for the kinetic stress:

$$\frac{\partial}{\partial t}P^k_{\alpha\beta} + \dot{\gamma}\left(\delta_{\alpha x}P^k_{y\beta} + \delta_{\beta x}P^k_{y\alpha}\right) = -2\zeta\left(P^k_{\alpha\beta} - nT_{\rm env}\delta_{\alpha\beta}\right) - \Lambda_{\alpha\beta}$$

Kinetic stress: $P^k_{\alpha\beta} = m\int d\boldsymbol{V} V_\alpha V_\beta f(\boldsymbol{V},t)$

Moment of the collision integral: $\Lambda_{\alpha\beta} = -m\int d\boldsymbol{V} V_\alpha V_\beta J_{\rm E}(V|f,f)$

Closure: Grad's moment method

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

$\Pi_{\alpha\beta} \equiv \frac{P^k_{\alpha\beta}}{nT} - \delta_{\alpha\beta}$: dimensionless stress

$$f_{\rm M}(\boldsymbol{V}) = n\left(\frac{m}{2\pi T}\right)^{\frac{3}{2}}\exp\left(-\frac{mV^2}{2T}\right)$$

In principle, we can explicitly evaluate $\Lambda_{\alpha\beta}$.

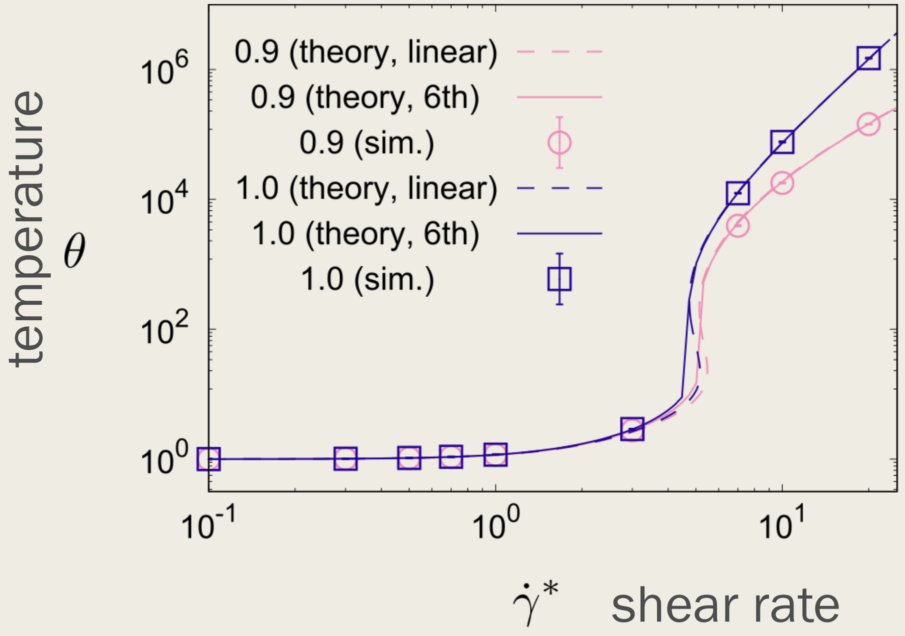
First, we consider the dilute limit, $P_{\alpha\beta} \simeq P^k_{\alpha\beta}$.

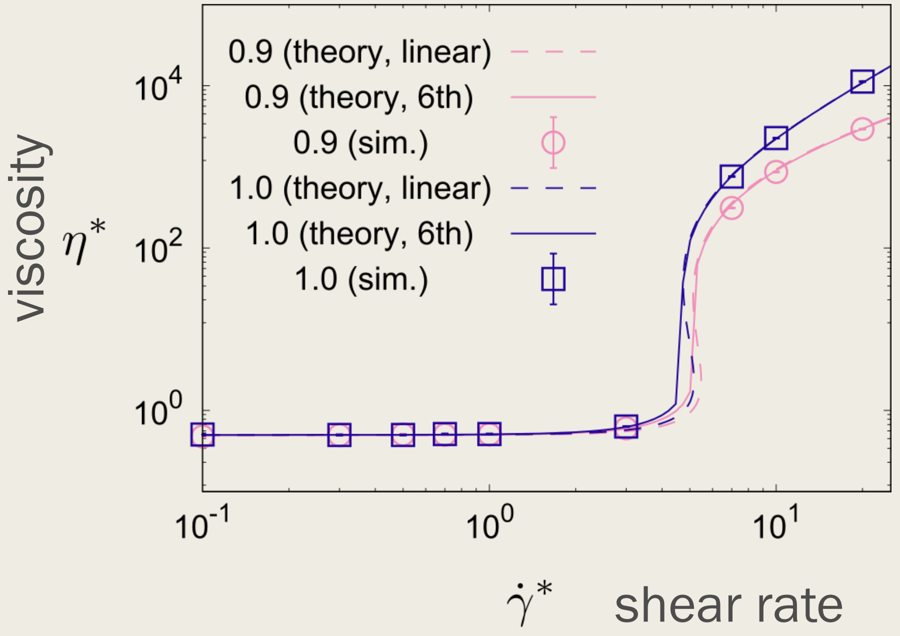
Results: DST in dilute suspensions

Flow curves for various restitution coefficient e

⇒ perfect agreement between theory and simulation

$\varphi = 0.01$





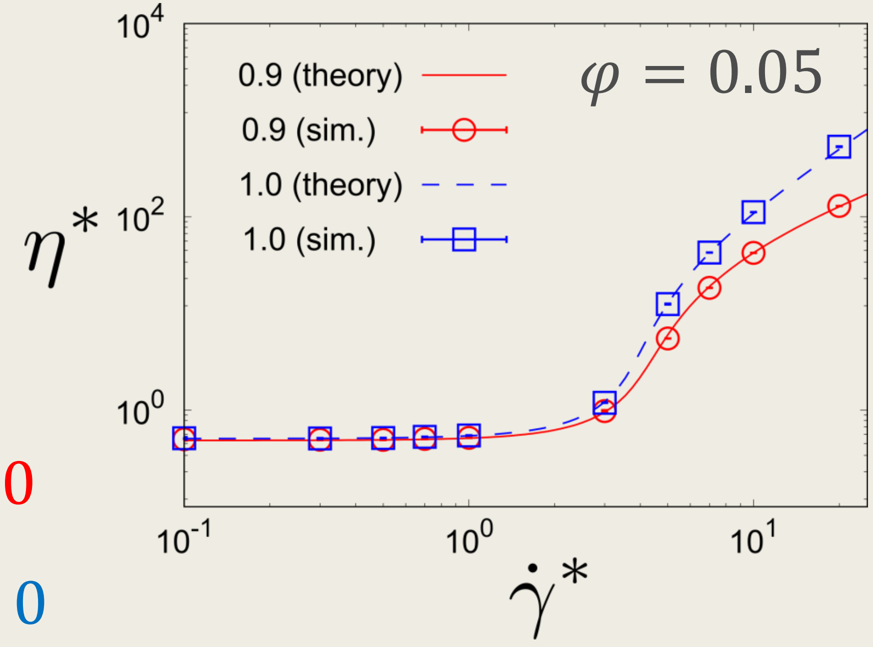
$\theta = T/T_{\mathrm{env}}$: dimensionless temperature
$\eta^* = \zeta\eta/(nT_{\mathrm{env}})$: dimensionless shear viscosity
$\dot{\gamma}^* = \dot{\gamma}/\zeta$: dimensionless shear rate

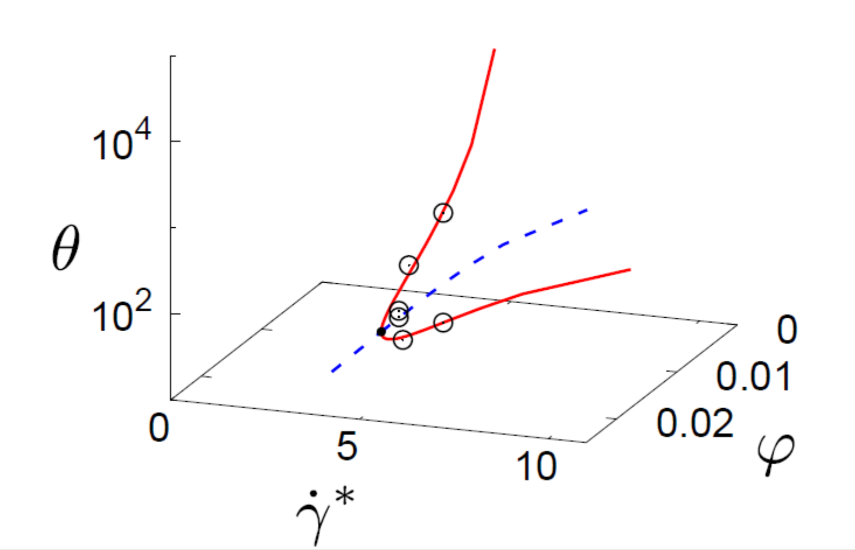
From "DST-like" to "CST-like" transitions

- Collisional stress $P^c_{\alpha\beta}$ plays an important role in dense cases.

$$P^c_{\alpha\beta} = \frac{1+e}{4} m\sigma^3 g_0 \int d\hat{\boldsymbol{\sigma}} \hat{\sigma}_\alpha \hat{\sigma}_\beta I^{(2)}(\hat{\boldsymbol{\sigma}})$$

- DST-like trans. becomes CST-like trans. as the density increases. ($\varphi_c \approx 0.0176$)





Red lines: $\frac{\partial \dot{\gamma}}{\partial \theta} = 0$

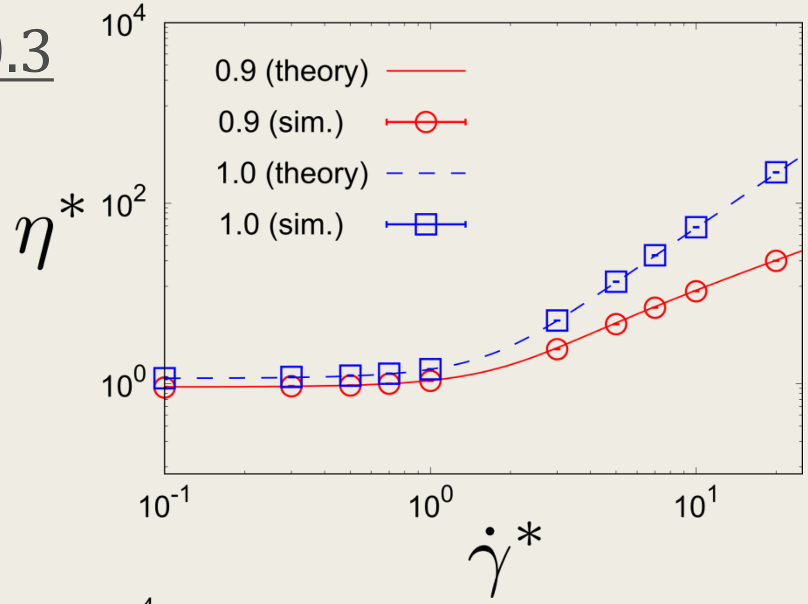
Blue line: $\frac{\partial^2 \dot{\gamma}}{\partial \theta^2} = 0$

- This is analogous to the first order transition.
  ☞ van der Waals fluid

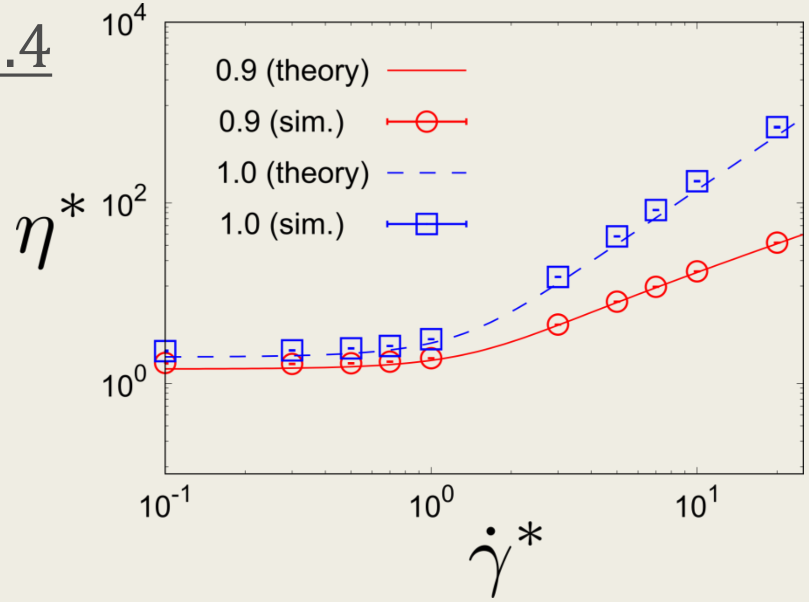
To what extent does the theory work?

Shear viscosity at finite densities

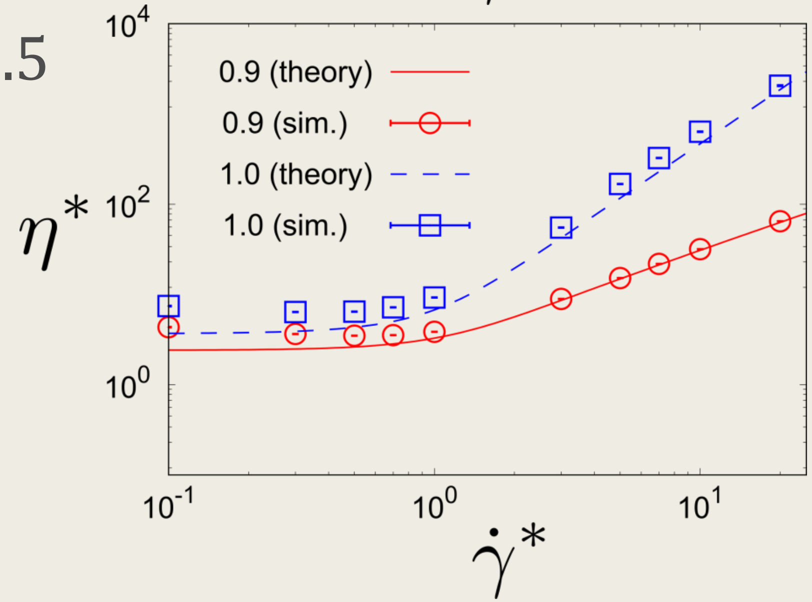
$\varphi = 0.3$



$\varphi = 0.4$



$\varphi = 0.5$



Our theory works well
without any fitting parameter
for $\varphi \lesssim 0.5$!
(slightly above the Alder trans. point)

Denser systems

- $\varphi \simeq 0.50$ is insufficient (or, rather dilute) for glass and jamming communities.

Question:
Is our theory applicable to denser situations?

- Monodisperse system is inappropriate for $\varphi \gtrsim 0.49$.
  $\Rightarrow$ Binary systems can avoid crystallization.
- We are now constructing the theory of binary mixtures (not yet completed).
- The theory can describe the long-time correlation?

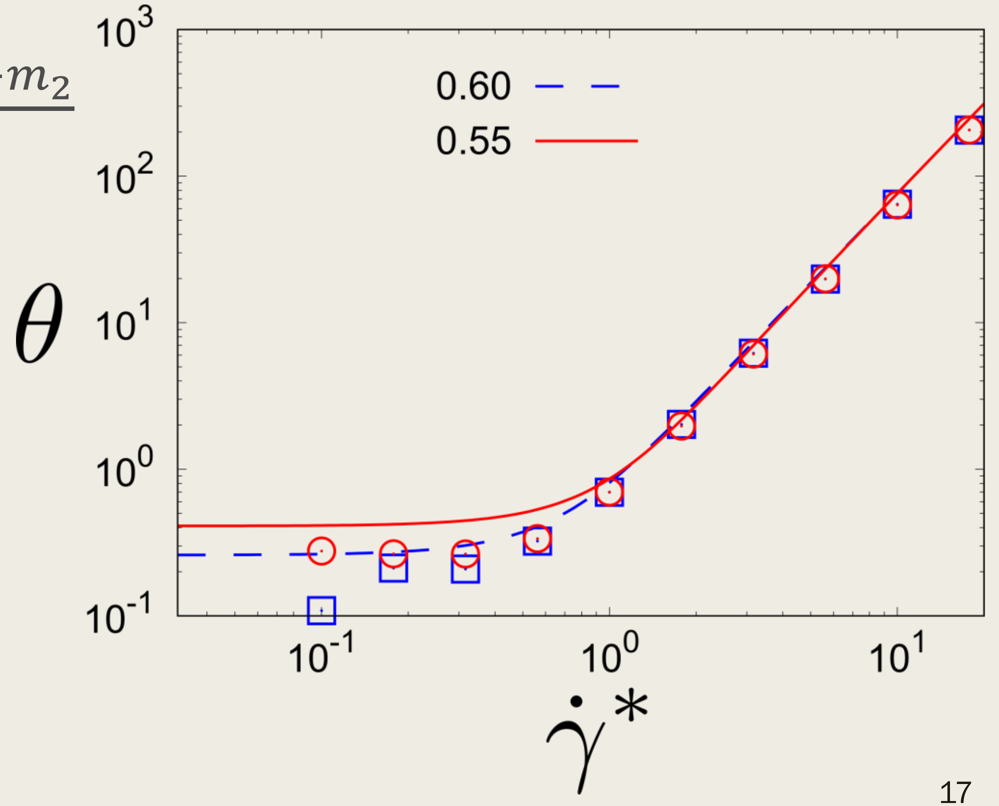
Flow curves for denser binary systems

- Trial to compare the simulation results with the theory
- Theory = monodisperse theory

  with RDF at contact $g_0(\varphi) = \frac{1-\frac{\varphi_f}{2}}{(1-\varphi_f)^3} \frac{\varphi_J-\varphi_f}{\varphi-\varphi_f}$ ☞ *S. Torquato, Phys. Rev. E* ***51****, 3170 (1995).*

- Simulation = bidisperse (size ratio 1:1.4).
  regard as monodisperse $\sigma = \frac{\sigma_1+\sigma_2}{2}, m = \frac{m_1+m_2}{2}$

- The theory qualitatively captures
  the behaviors in the high-shear regime.



Description of DST for dense suspensions

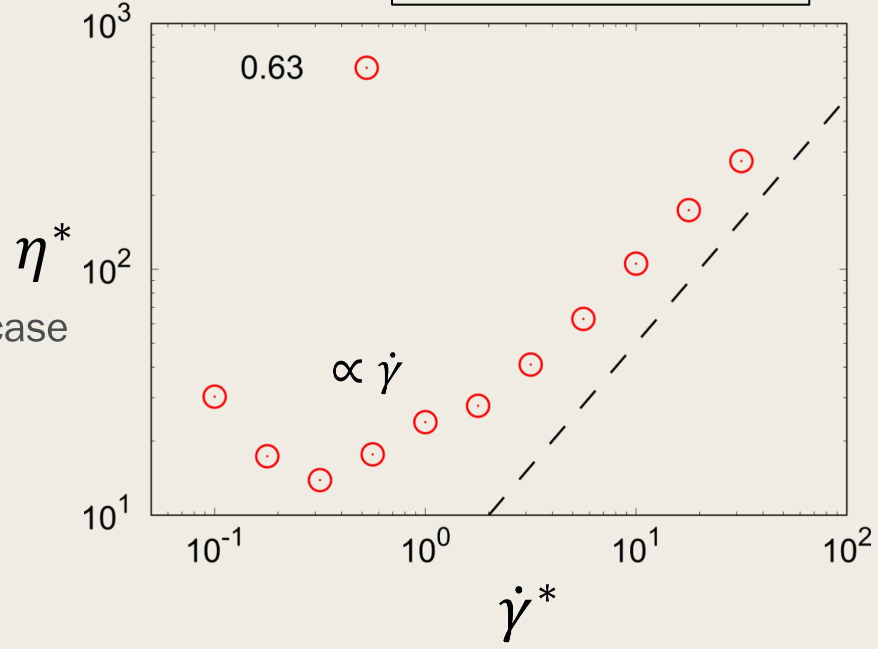
Question:
Can we describe DST for dense frictional suspensions by the kinetic theory?

Parameters:
$\varphi = 0.63$
$e_n = 0.9, e_t = 0.9$
$T^*_{\rm env} = 1$

Simulation for frictional hard-core models.
The answer is NO! ⇒ Why?

- Stable finite duration of contact must be important for DST.
- This stable contact can be described by the soft-core models.

☞ *S. Sugimoto & S. Takada, JPSJ* ***89****, 084803 (2020)* for dilute case



Low shear rate: crystallization effect
High shear rate: Bagnodlian

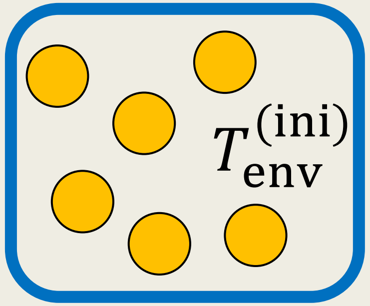
2nd part: Mpemba effect

Mpemba is NOT anomalous in inertial suspensions!

- Mpemba effect occurs quite naturally.
- For simplicity, we consider the elastic case ($e = 1$).
  Then, the equation of temperature becomes

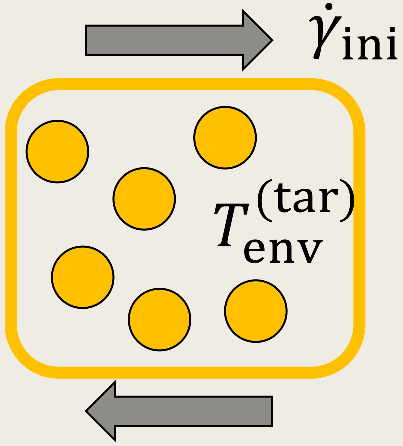
Eq. system must have faster cooling than noneq. system.
$\Rightarrow$ Initial overshoot is the origin of the Mpemba effect.

(Quasi-)Equilibrium system (T_{QE})



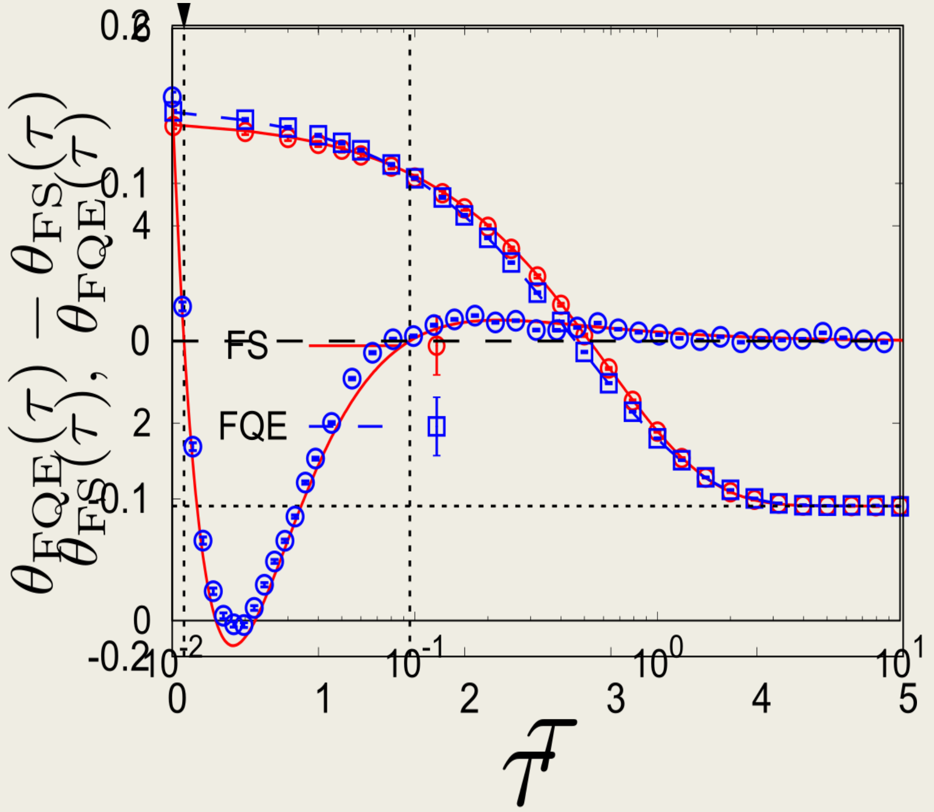
Viscous heating $= 0$ ($\because P_{xy}(0) = 0$)

Nonequilibrium system ($T_{\mathrm{F}} < T_{\mathrm{QE}}$)



Viscous heating > 0 ($\because P_{xy}(0) < 0$)

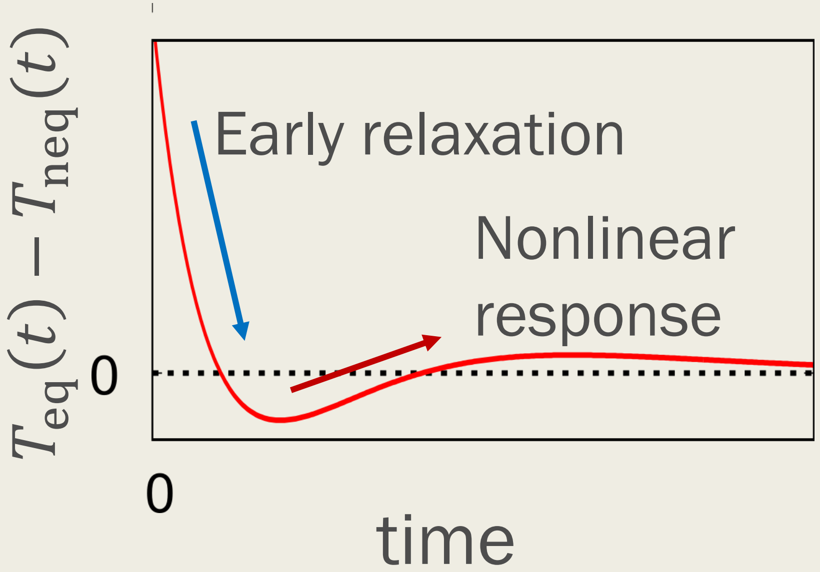
Typical time evolutions



- We call this as “NME+AME.”
- Good agreement without any fitting parameters. (Simulation: 100 samples)

Existence of
- normal Mpemba effect (NME) and
- anomalous Mpemba effect (AME)

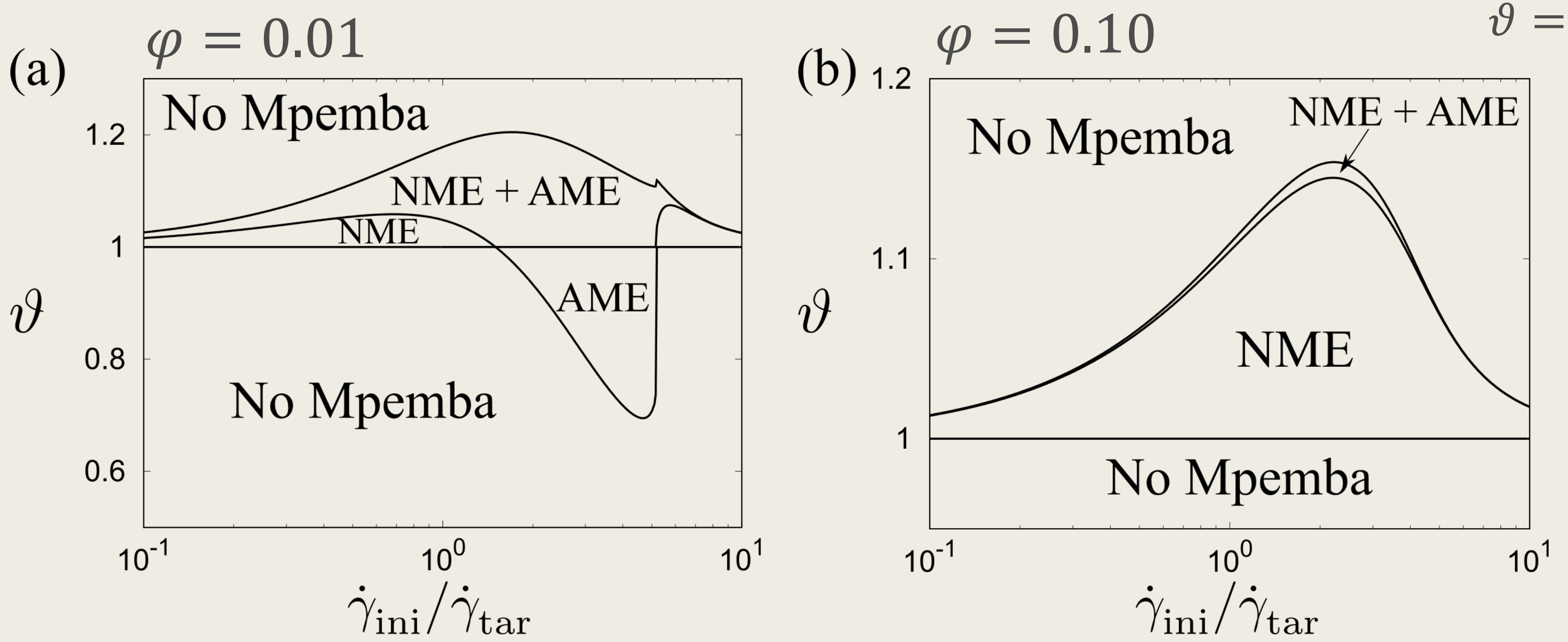
AME: nontrivial
= nonlinear consequence after the early relaxation.
≒ damped vibration after the overshoot



Phase diagram

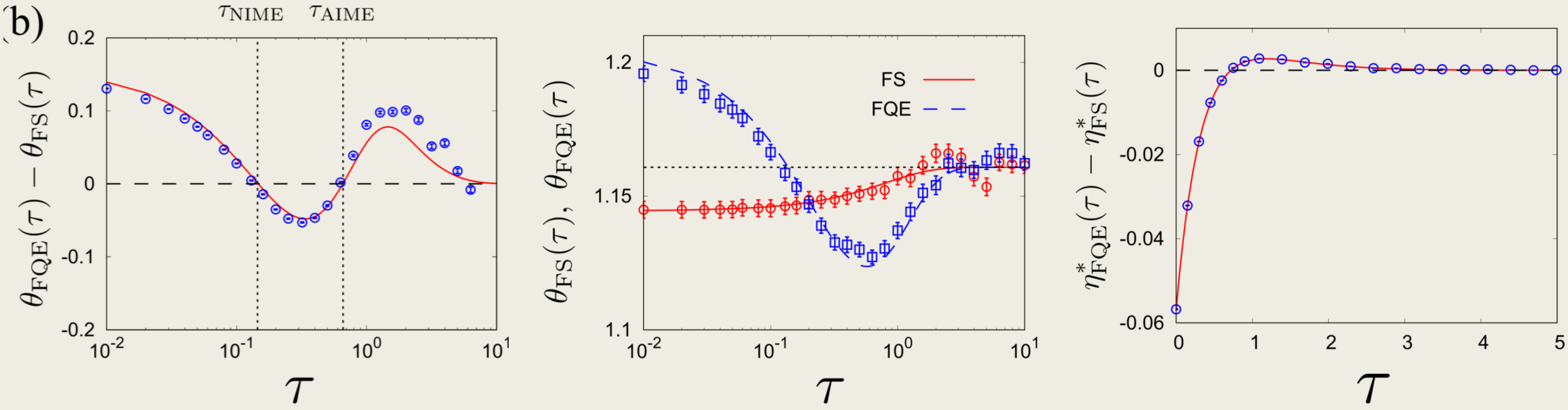
- The phase diamgram includes
  "No Mpemba," "NME," "AME," and "NME+AME."
- "AME" disappears at around at $\varphi = 0.04$.
- "NME+AME" tends to disappear at around $\varphi = 0.10$.

$$\vartheta = \frac{\theta_{\mathrm{FQE}}(0)}{\theta_{\mathrm{FS}}(0)}$$



Inverse, mixed, & viscosity Mpemba effects

- We also find the existence of
  - *inverse Mpemba effect (in heating process) and*
  - *mixed Mpemba effect (one in heating and another cooling processes).*



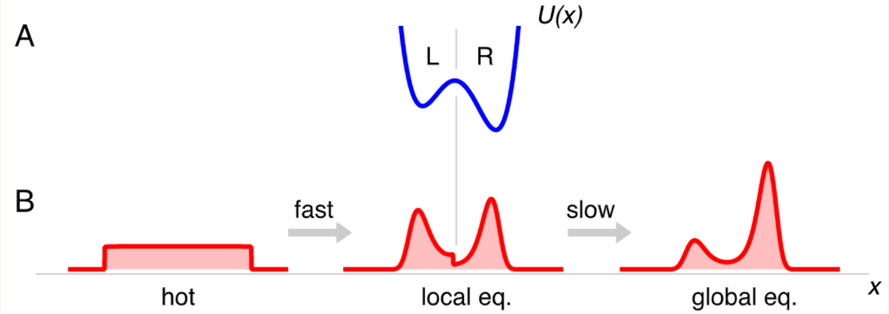
  - ***Mpemba effect for viscosity***

    ME is also observed for the viscosity. But, at most only once

Discussion:

- **Hydrodynamic interaction**
  Our current model is an oversimplified model.
  ⇒ For denser systems,
  the drag becomes the resistance matrix
  (instead of the constant drag force ζ).
  ☞ *Kim & Karrila, "Microhydrodynamics" (1991)*
  ⇒ The resistance depends on the configurations of particles.

- **Local potential trapping**
  Recent experiments
  Single colloidal particle is trapped
  in a potential by optical tweezers.
  ⇒ Mpemba effect = hopping process
  from one local minimum to another.



A. Kumar and J. Bechhoefer, Nature 584, 64 (2020).

Conclusion of the talk

- We have constructed the kinetic theory to describe the rheology of the inertial suspensions
- We have demonstrated that
  our theory gives a precise description of suspensions.
  - *DST-like behavior (ignited-quench transition) in dilute systems.*
  - *DST-like → CST-like as the density increases.*
  - *applicable to denser regime (not yet completed)*
- We have examined anomalous relaxation processes observed in the inertial suspension.
  - *Normal and anomalous Mpemba effects (NME and AME) when we control the parameters.*