Frictional Flow of Dense Granular Materials

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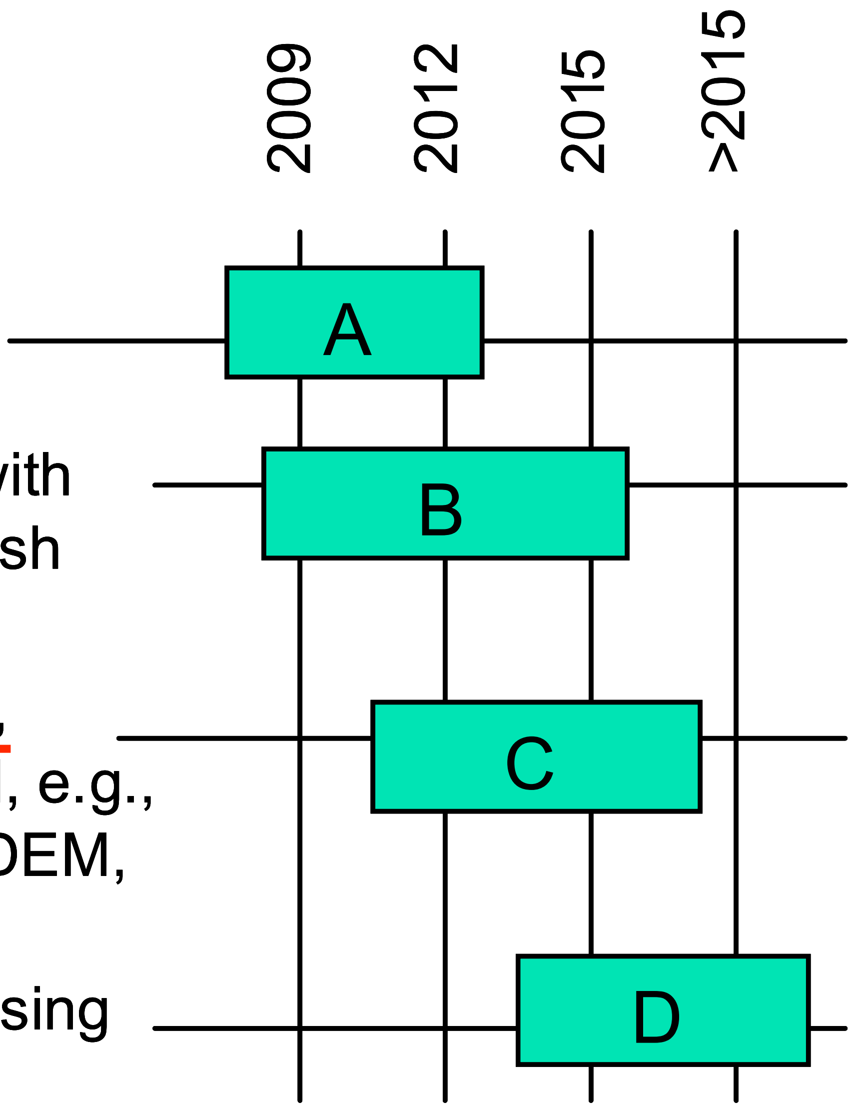
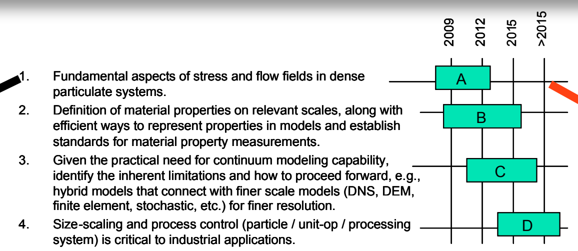
Roadmap for dense granular flow

1. Fundamental aspects of stress and flow fields in dense particulate systems.
2. Definition of material properties on relevant scales, along with efficient ways to represent properties in models and establish standards for material property measurements.
3. Given the practical need for continuum modeling capability, identify the inherent limitations and how to proceed forward, e.g., hybrid models that connect with finer scale models (DNS, DEM, finite element, stochastic, etc.) for finer resolution.
4. Size-scaling and process control (particle / unit-op / processing system) is critical to industrial applications.



Connection to roadmap

Key questions addressed:



Action taken in our project:

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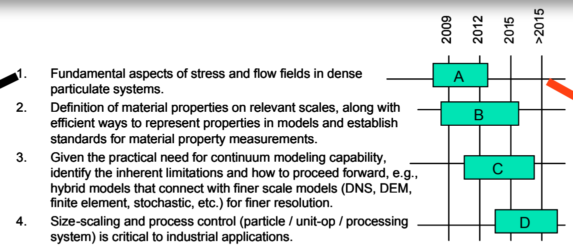

Action taken in our project:

- What defines the stress in quasi-static regime?

- Identified internal variables defining stress states.

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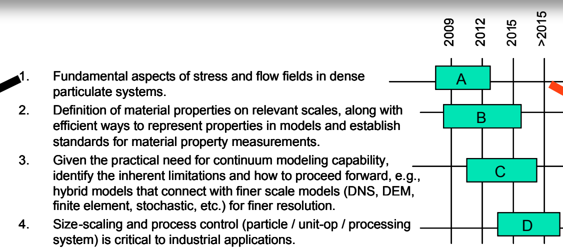

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- What defines the stress in quasi-static regime?
- What parameters control the transitions between granular states?

- Identified internal variables defining stress states.
- Demonstrated the connection between quasi-static transition with the jamming point.

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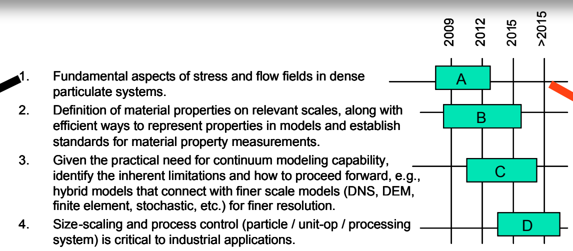

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- Continuum rheological models from quasi-static to rapid flow regimes?(Goal II in our project)

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- Developed a plasticity model for the quasi-static regime and linked to particle scale properties.

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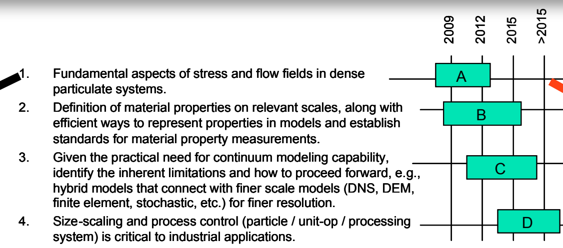

Key questions addressed:

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- How is stress transmitted?

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- Probed stress inhomogeneity and transmission in Jenike shear cell.

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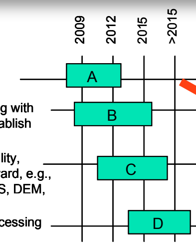

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Outline

- The continuum model development
- Its predictive capabilities demonstrated by applications to unsteady shear flows
- Future work

Dissipative plasticity model*

$$\sigma_{ij} = p\delta_{ij} - p\eta \frac{S_{ij}}{\sqrt{D : D}}$$

* D.G. Schaeffer. J. Differ. Equ. 66, 19, 1987 ; J.D. Goddard. JFM 568, 1, 2006

Dissipative plasticity model*

$$\sigma_{ij} = p\delta_{ij} - p\eta \frac{S_{ij}}{\sqrt{D:D}}$$

Deviatoric strain rate

Strain rate

- Stress is related to plastic deformation with rate independence

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Dissipative plasticity model*

$$\sigma_{ij} = p\delta_{ij} - p\eta \frac{S_{ij}}{\sqrt{D:D}}$$

Stress ratio

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Dissipative plasticity model*

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- Stress is related to plastic deformation with rate independence
- Pressure and stress ratio are modeled as functions of microstructural variables: coordination number and fabric tensor.

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- Stress is related to plastic deformation with rate independence
- Pressure and stress ratio are modeled as functions of microstructural variables: coordination number and fabric tensor.
- Stress is evolved through microstructural evolution.

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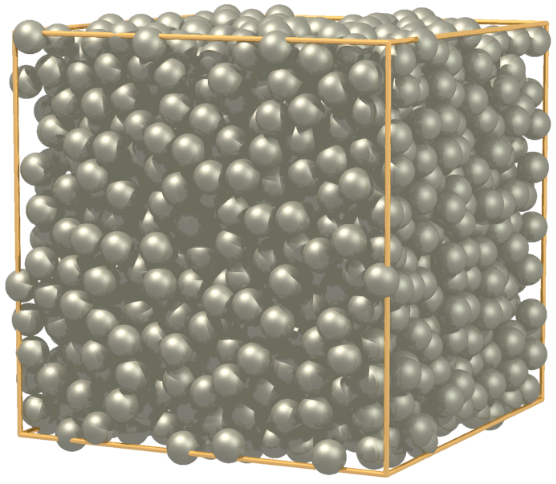
Model construction

- Simulate particle dynamics of homogeneous assemblies under isotropic compression or simple shear using discrete element method (DEM)
- Extract stress and structural information by averaging; seek constitutive relations.

Computational system

- 3D periodic domain without gravity
- 2000 mono-dispersed spherical particles
- Restitution coefficient: 0.7
- Inter-particle friction coefficient: *0.1-1*
- Simulate using the LAMMPS code*



Stress $$\sigma = \frac{1}{V}\sum_{i}^{N}\left[m_i\mathbf{C}_i\mathbf{C}_i + \sum_{j,j\neq i}\frac{1}{2}\mathbf{r}_{ij}\mathbf{F}_{ij}\right]$$

S. J. Plimpton. J Comp Phys, 117, 1-19 (1995) http://lammps.sandia.gov

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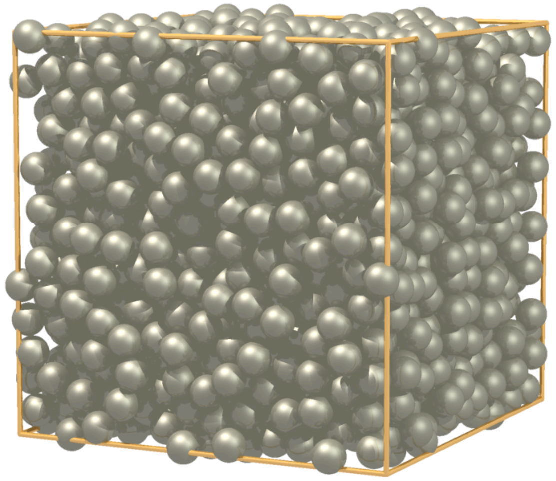

Small

Stress $$\sigma = \frac{1}{V}\sum_{i}^{N}\left[\cancel{m_i \mathbf{C}_i \mathbf{C}_i} + \sum_{j,j\neq i}\frac{1}{2}\mathbf{r}_{ij}\mathbf{F}_{ij}\right]$$

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Characterize microstructure

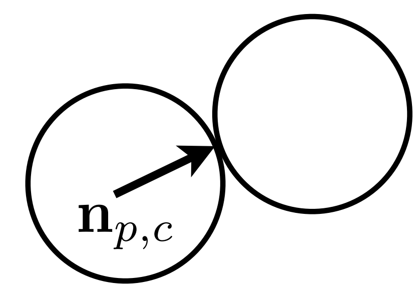
- Coordination number: average number of contacting neighbors

$$Z_2 = \frac{\sum_{p=1}^{N} \sum_{c=1}^{c_p \geq 2} 1}{N_2}$$

Exclude particles with zero or one contact

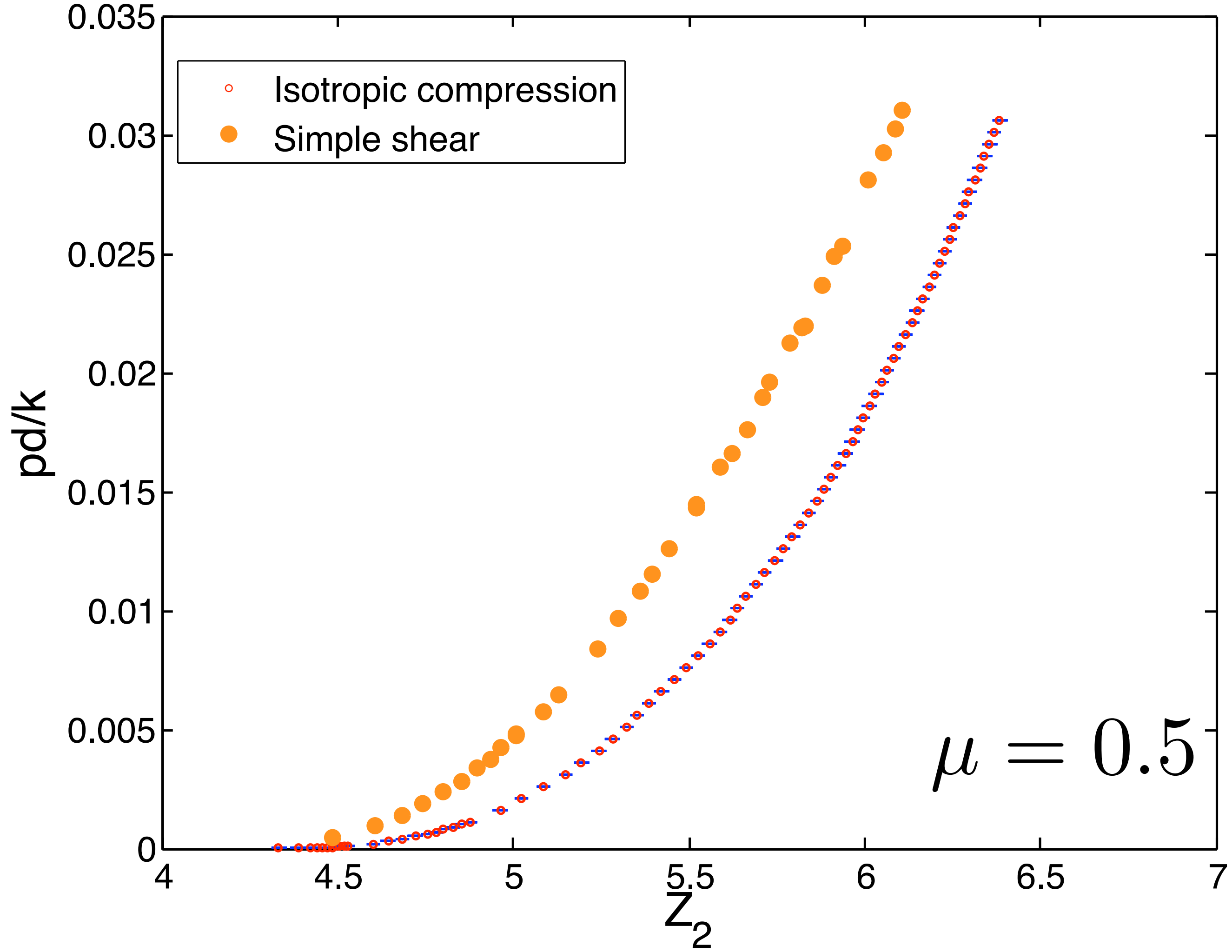
- Fabric tensor: average of tensor product of unit contact normals

$$\mathsf{A} = \frac{1}{N_{c2}} \sum_{n=1}^{N} \sum_{c=1}^{c_p \geq 2} \mathbf{n}_{\mathbf{p},\mathbf{c}} \mathbf{n}_{\mathbf{p},\mathbf{c}} - \frac{\mathbf{1}}{\mathbf{3}} \mathsf{I}$$



- A_{xz} magnitude indicates the microstructure anisotropy strength; sign indicates the anisotropy direction

Pressure equation



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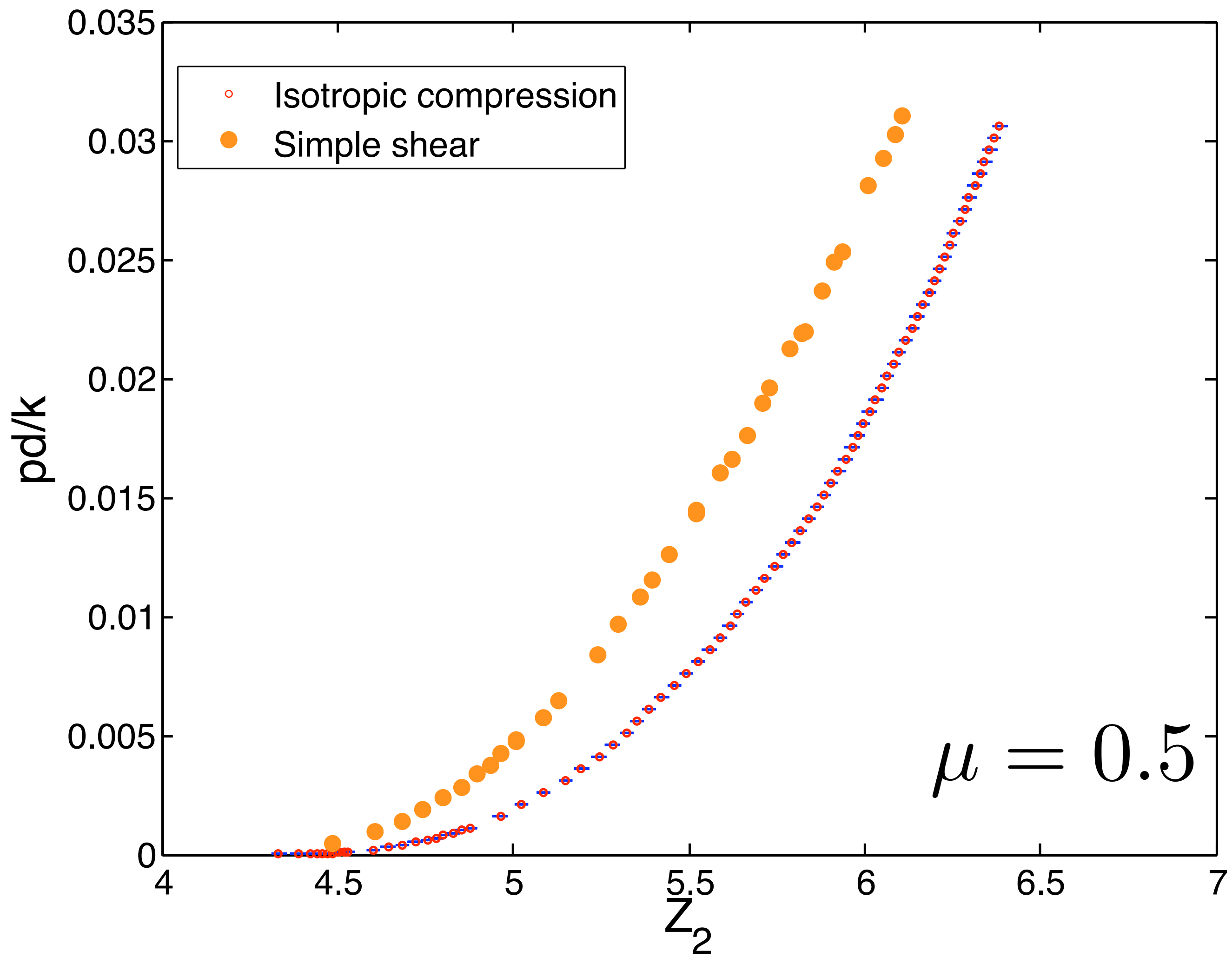
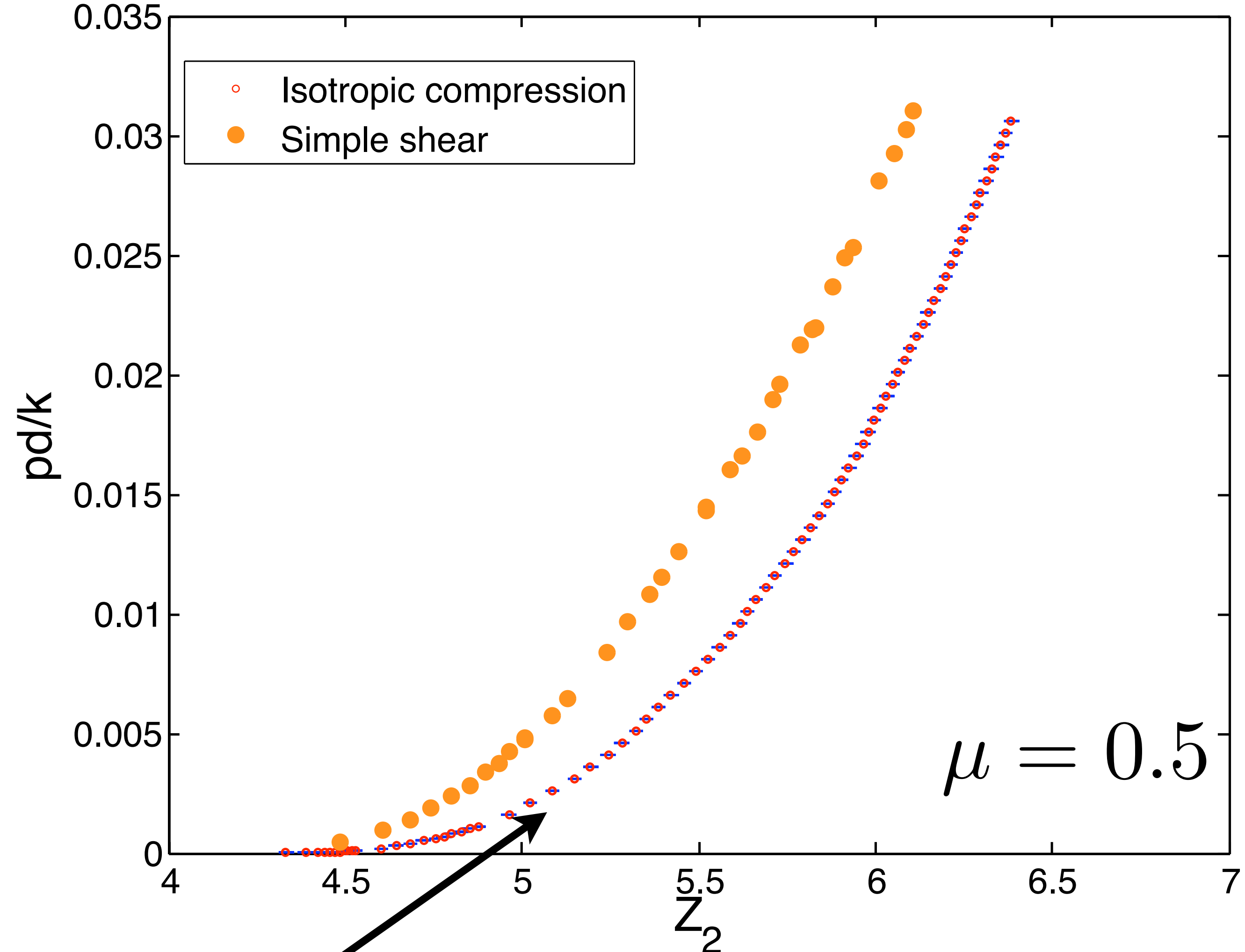


$$p = a(Z - Z_c)^b + \alpha_5(\mathsf{A} : \mathsf{A})(Z - Z_c)^{\alpha_6}$$

Pressure equation



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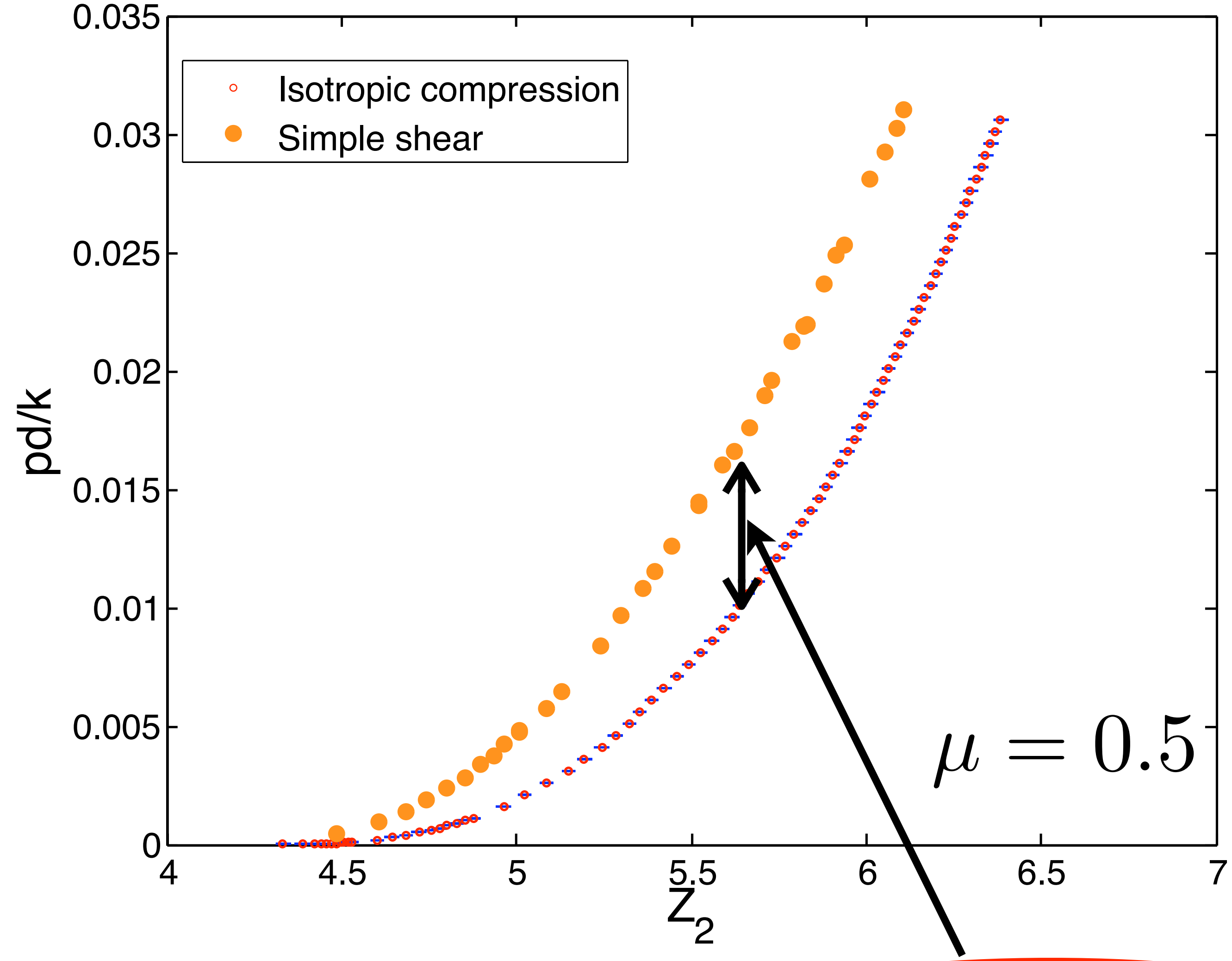
Isotropic pressure

$a = 0.0052, \;\; b = 2.48$

Pressure equation

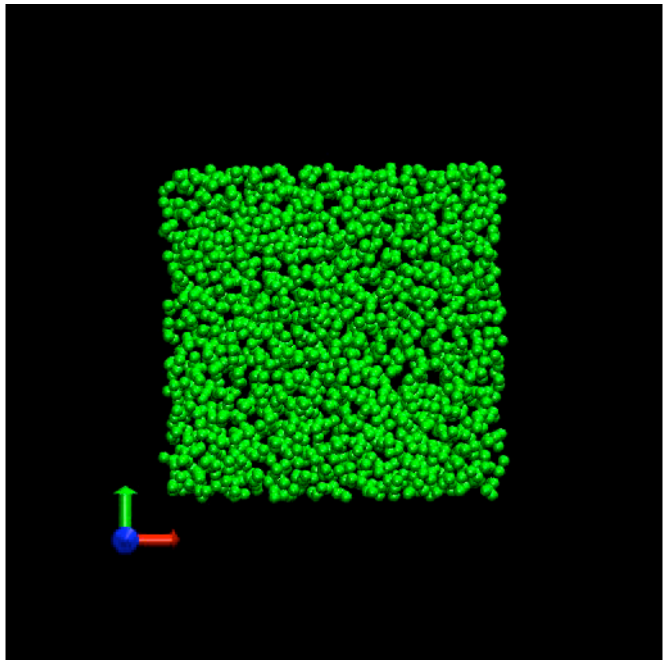


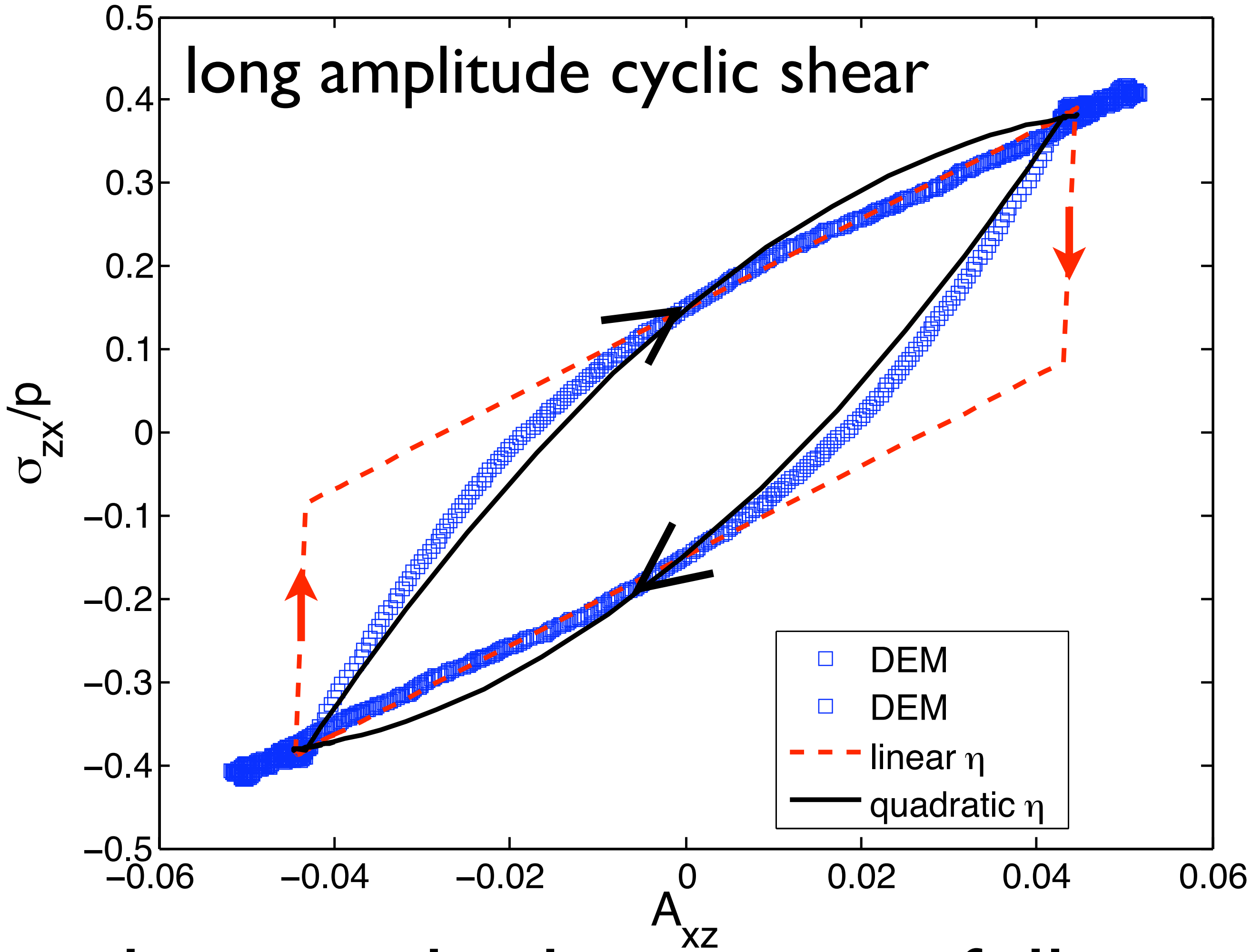
$$p = a(Z - Z_c)^b + \alpha_5(\mathsf{A} : \mathsf{A})(Z - Z_c)^{\alpha_6}$$

Excess pressure caused by structural anisotropy

$$\alpha_5 = 1.1,\ \alpha_6 = 1.2$$

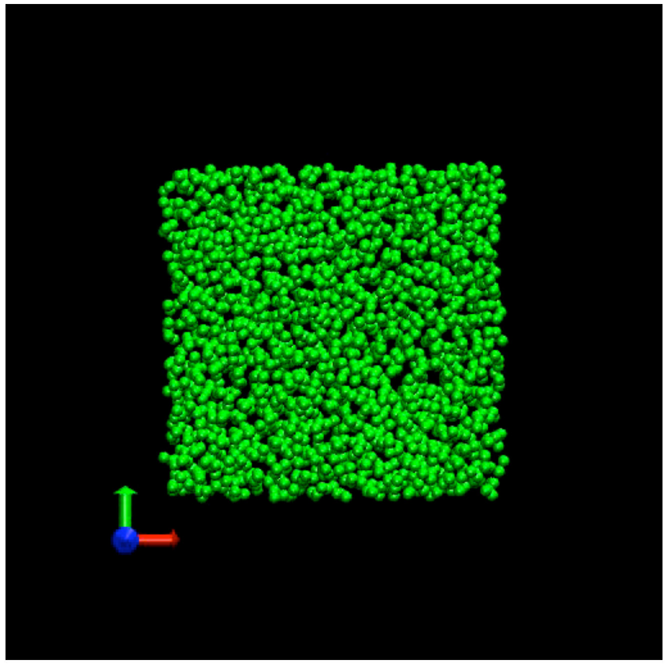
Shear stress ratio

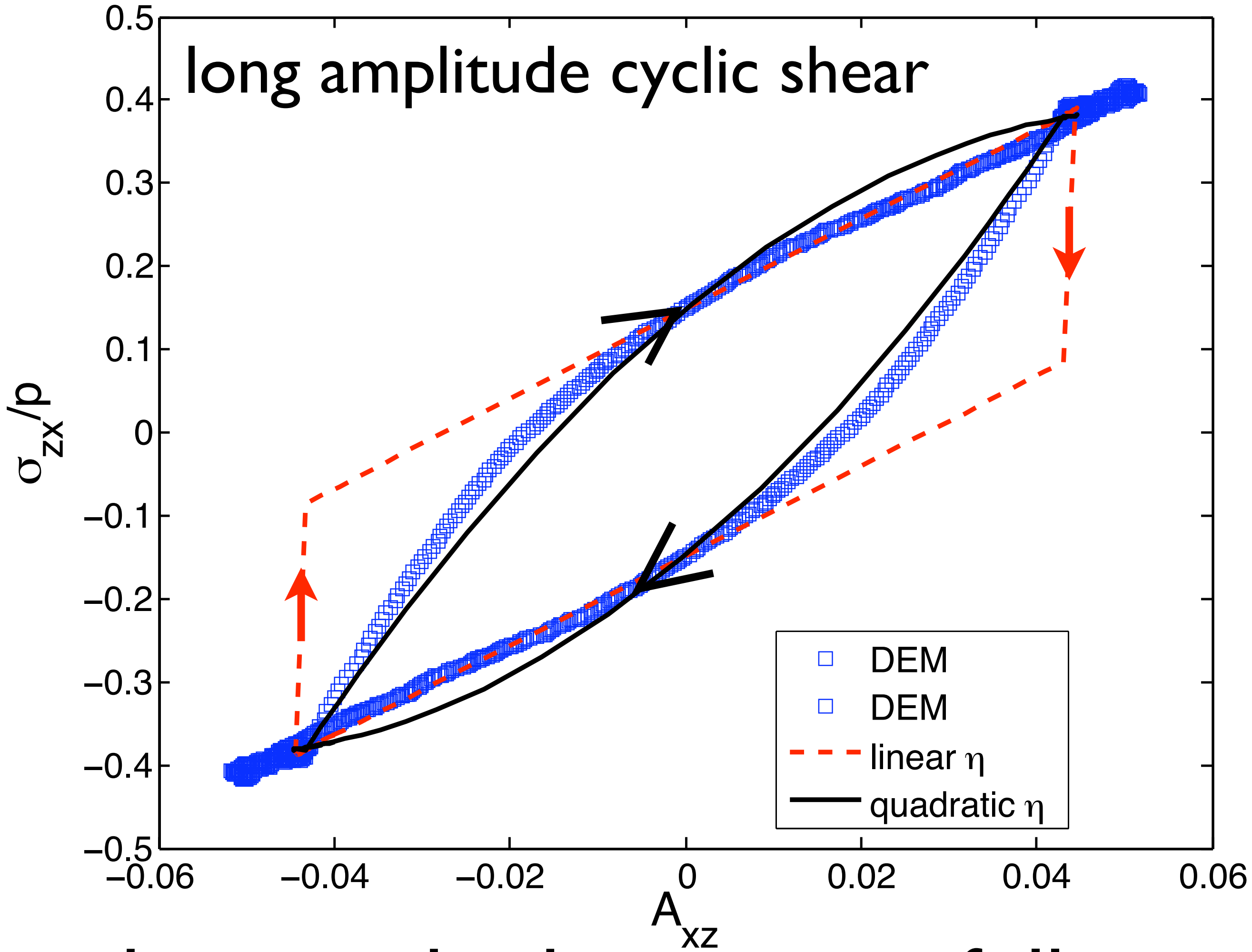




- Both steady and unsteady shear ratios following similar variation against anisotropy
- Modeled as function of fabric tensor

Shear stress ratio





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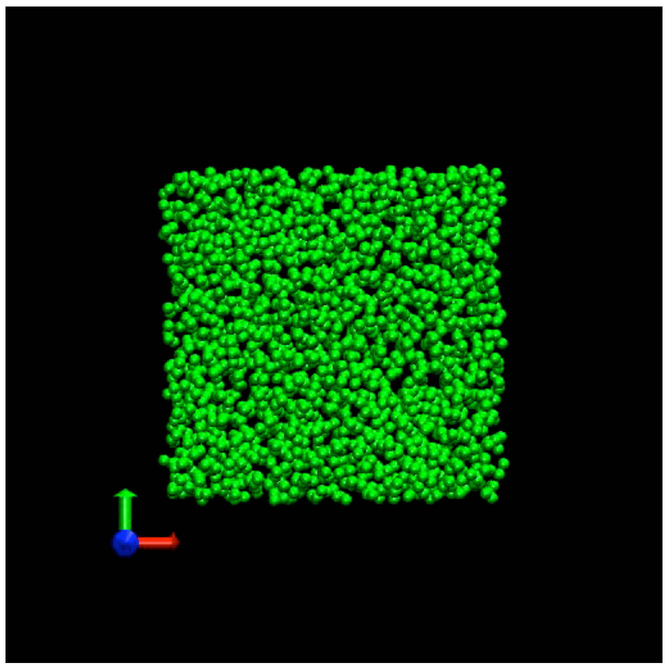
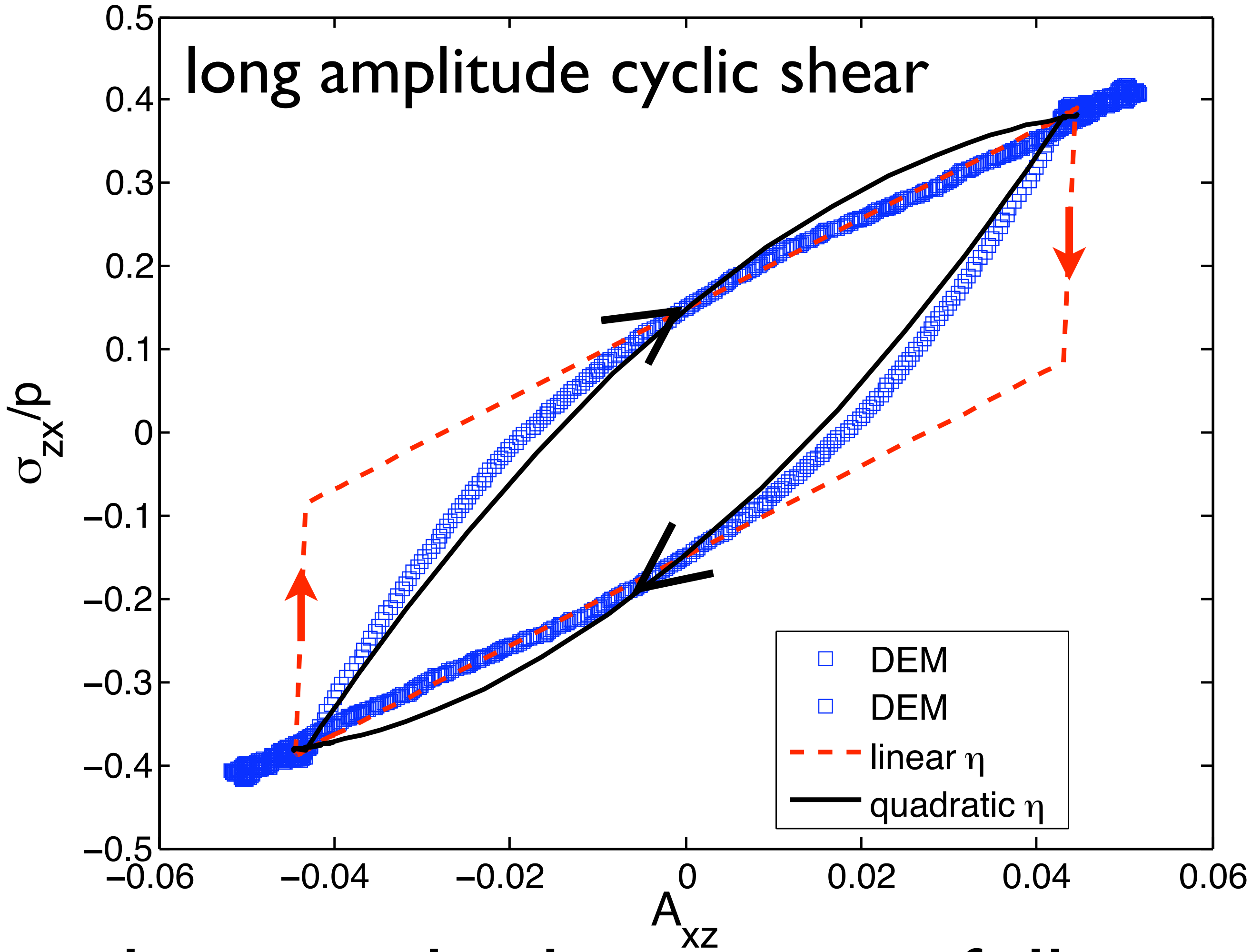
$$\eta = \beta_1 + \beta_2 \frac{\mathrm{A} : \mathrm{D}}{\sqrt{\mathrm{D} : \mathrm{D}}}$$

Shear stress ratio





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$$\eta = \beta_1 + \beta_2 \frac{\mathsf{A} : \mathsf{D}}{\sqrt{\mathsf{D} : \mathsf{D}}} + \beta_3 \frac{(\mathsf{A} : \mathsf{D})^2}{\mathsf{D} : \mathsf{D}}$$

Evolution equations

Coordination number

$$\dot{Z} = \alpha_1 \mathsf{A} : \mathsf{D} + \alpha_2 \sqrt{\mathsf{D} : \mathsf{D}} + \alpha_3 \sqrt{\mathsf{D} : \mathsf{D}} Z + \alpha_4 \mathrm{tr}(D) \quad \dot{Z} = \frac{dZ}{dt}$$

Fabric tensor

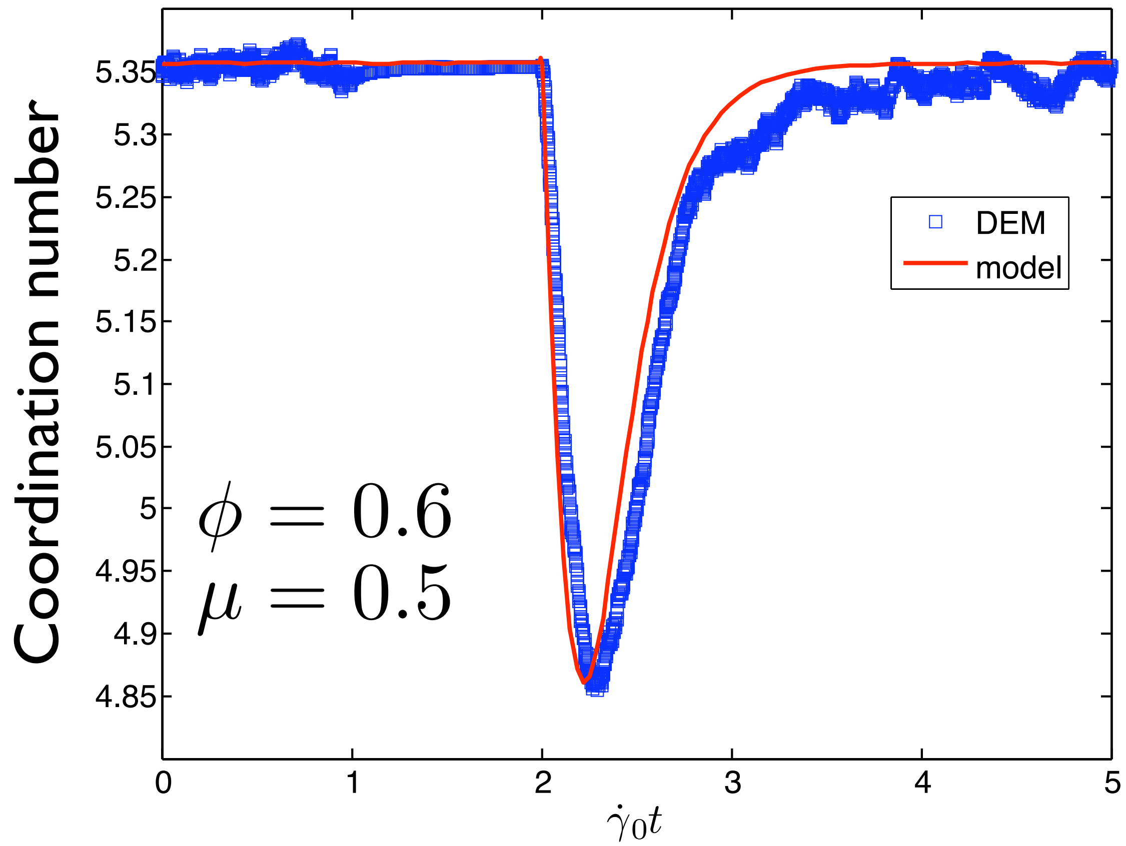
$$\mathring{\mathsf{A}} = c_1 \mathsf{S} + c_2 (\sqrt{\mathsf{D} : \mathsf{D}}) \mathsf{A} + c_3 (\mathsf{A} : \mathsf{D}) \mathsf{A}$$

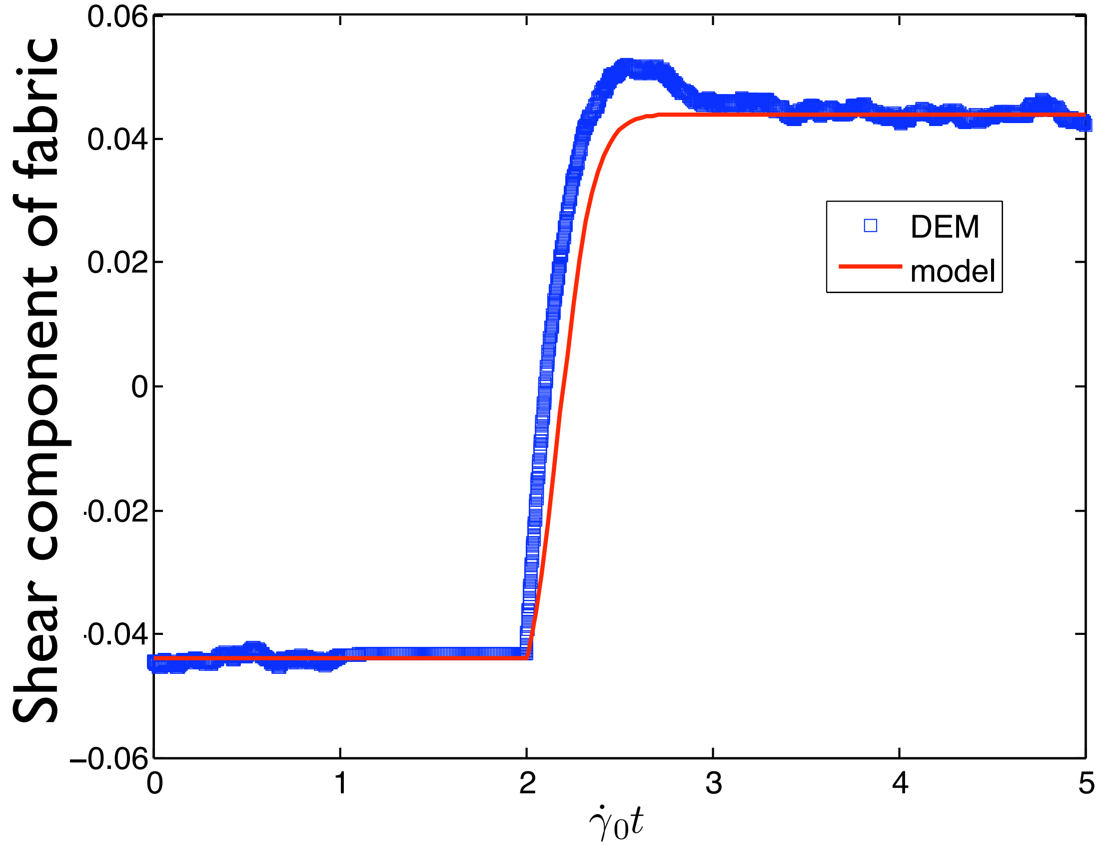
Jaumann derivative $\mathring{\mathsf{A}} = \frac{d\mathsf{A}}{dt} + \mathsf{A} \cdot \mathsf{W} - \mathsf{W} \cdot \mathsf{A}$

- Functions of A and D; satisfying frame indifference.
- Satisfy stability requirement.
- material constants, c and α, can be calibrated using DEM data.

Stickel, J. et al. A constitutive model for microstructure and total stress in particulate suspensions. Journal of Rheology, 50(4):379–413, 2006.

Constant volume shear reversal





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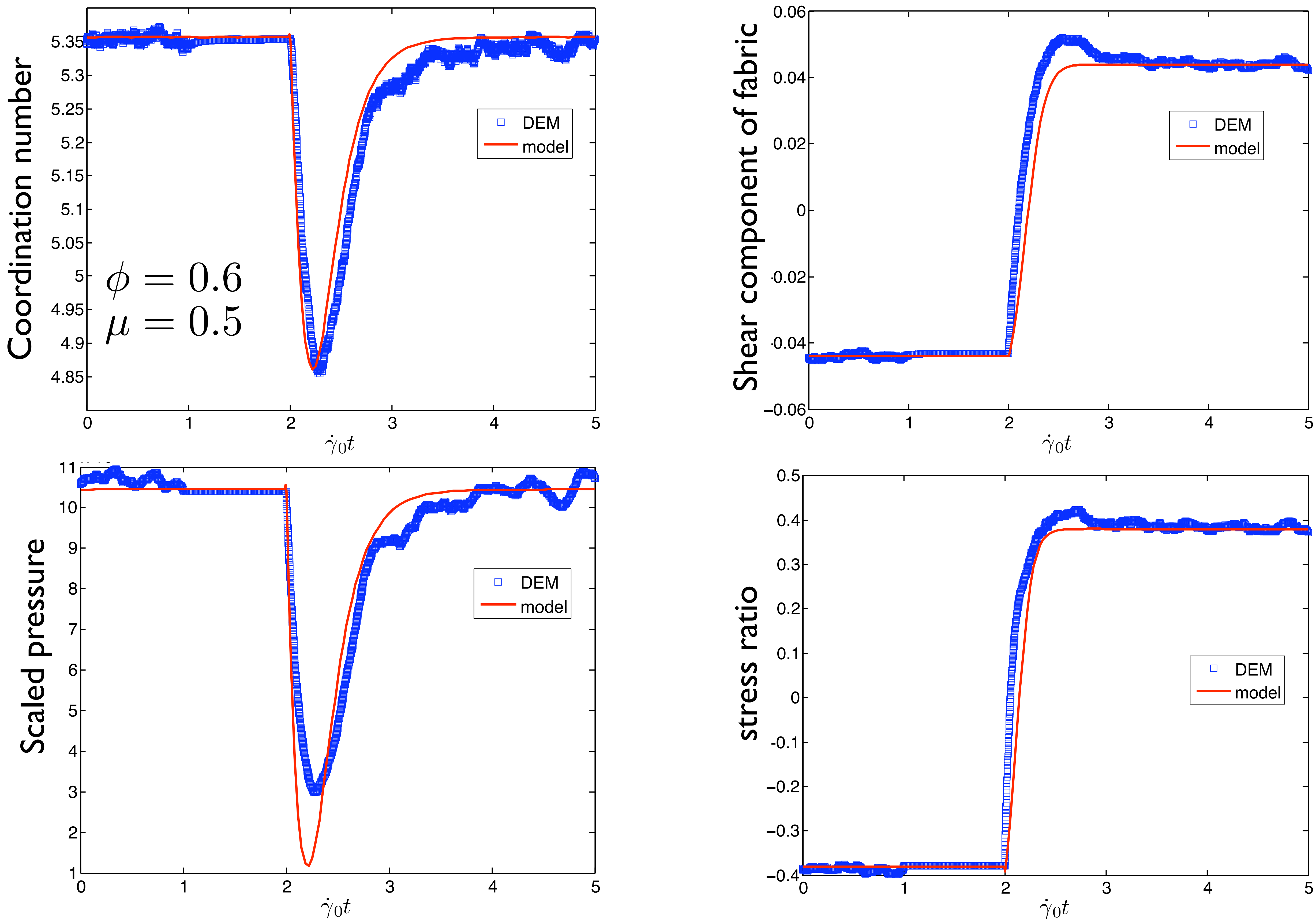
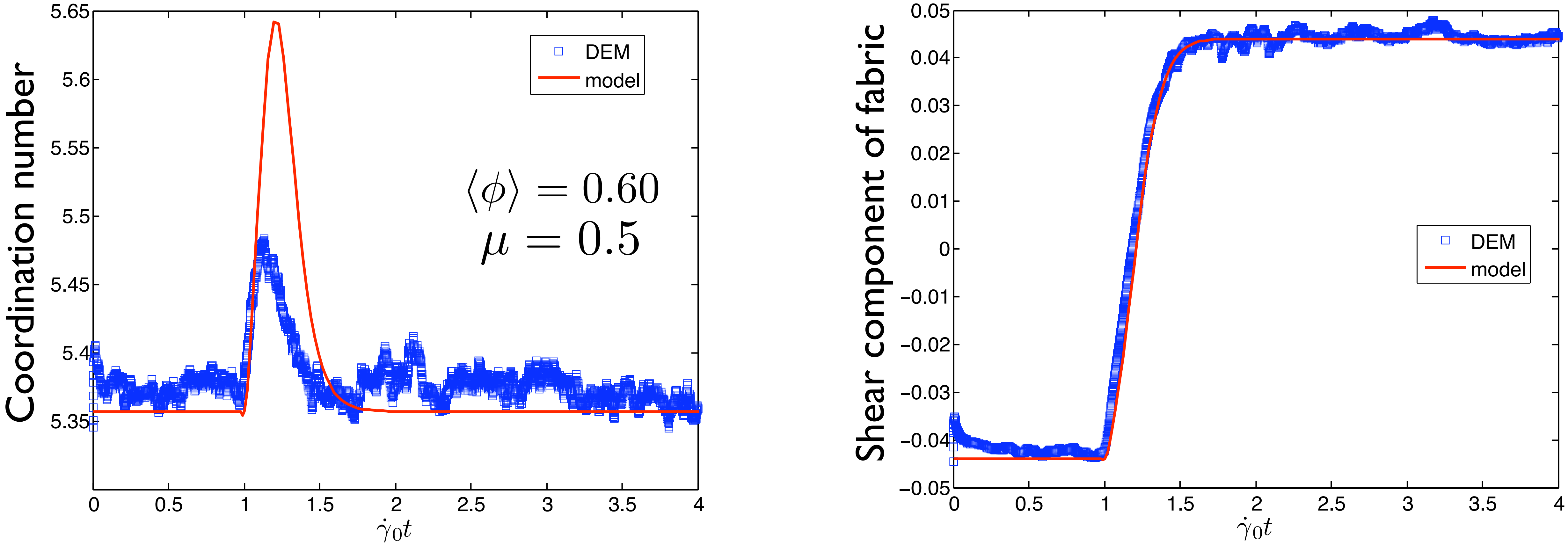


Constant pressure shear reversal



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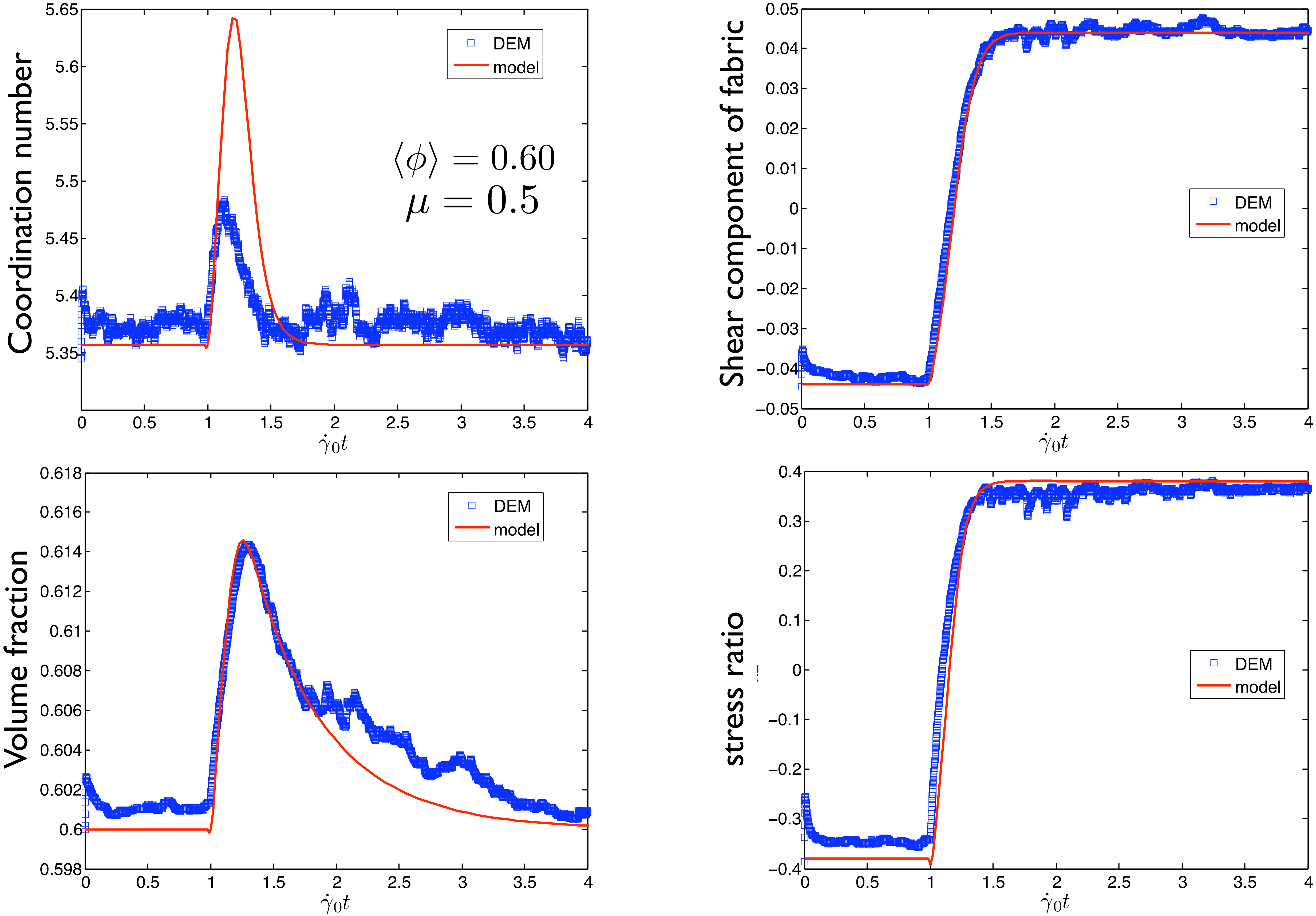
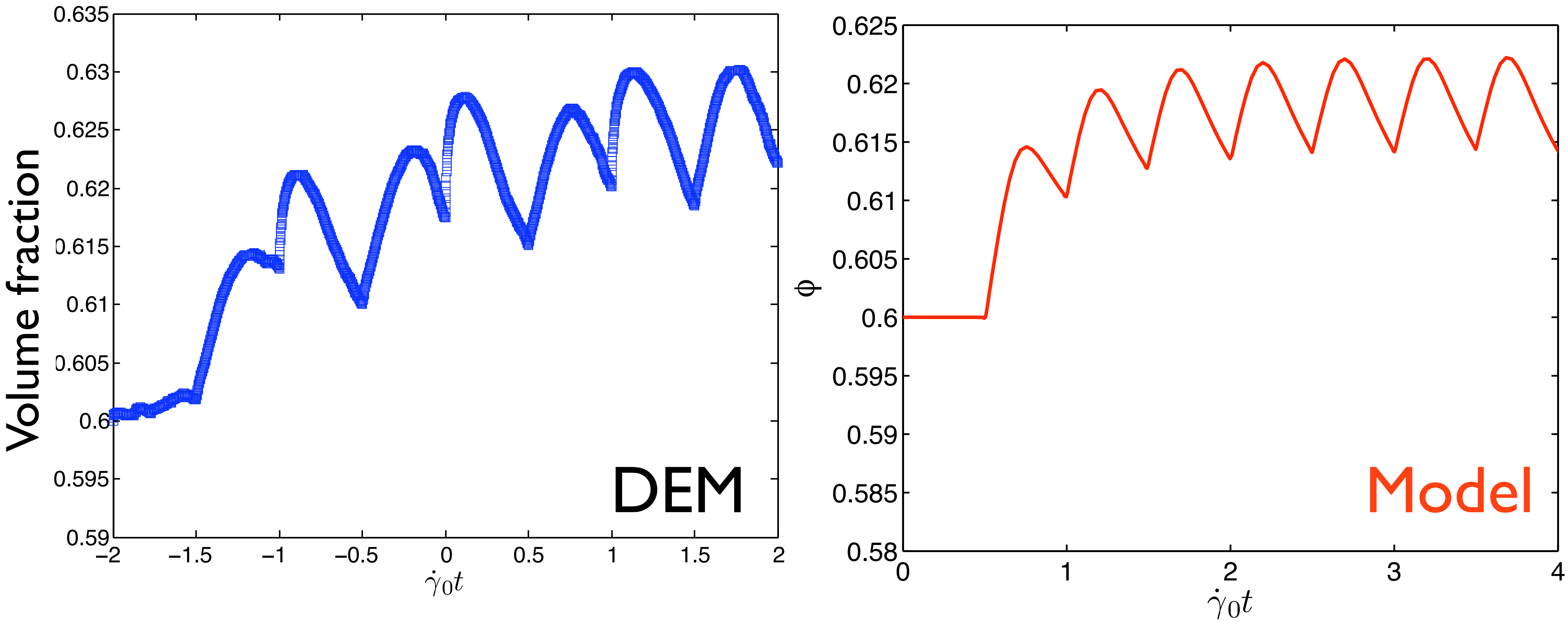


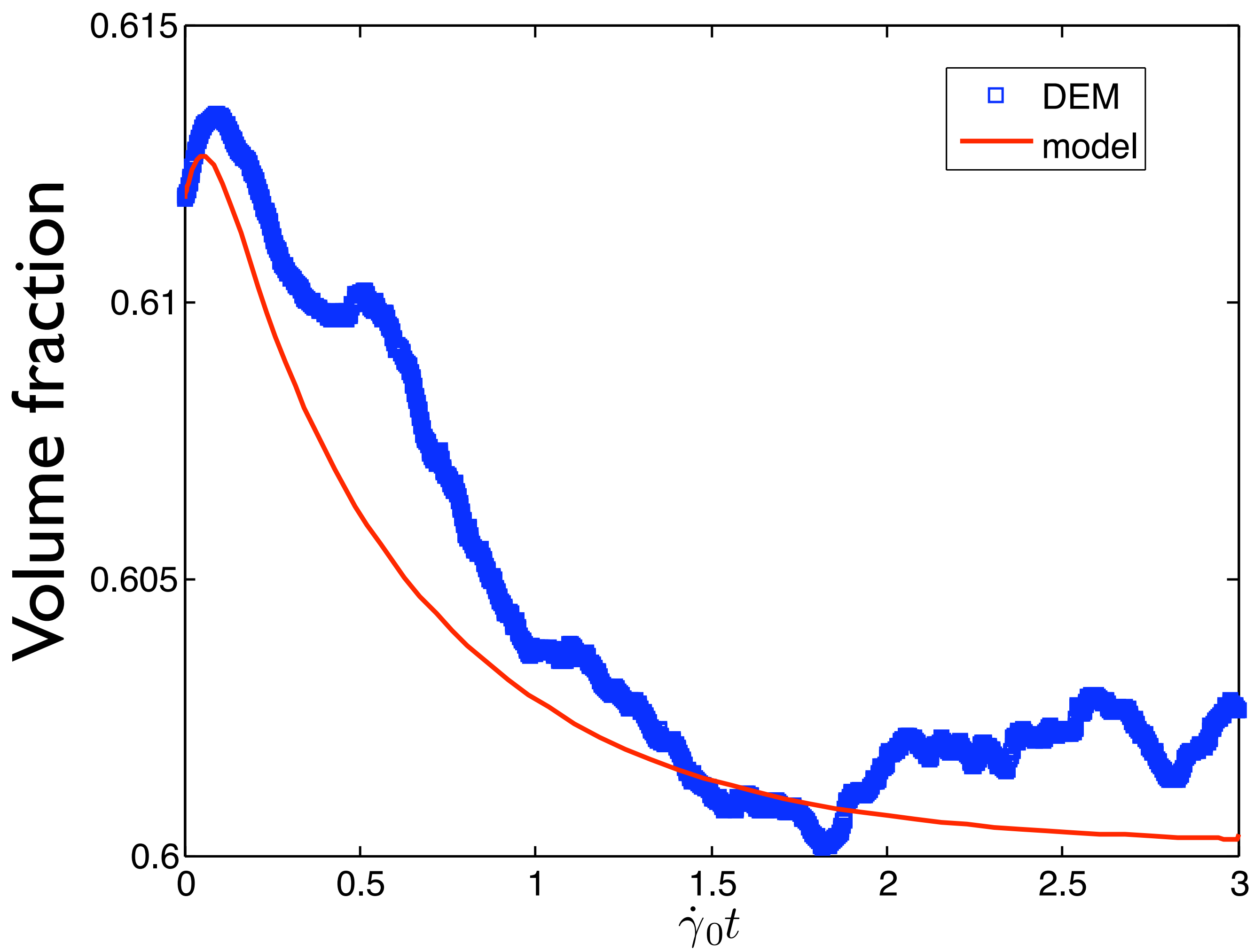
Constant pressure cyclic shear

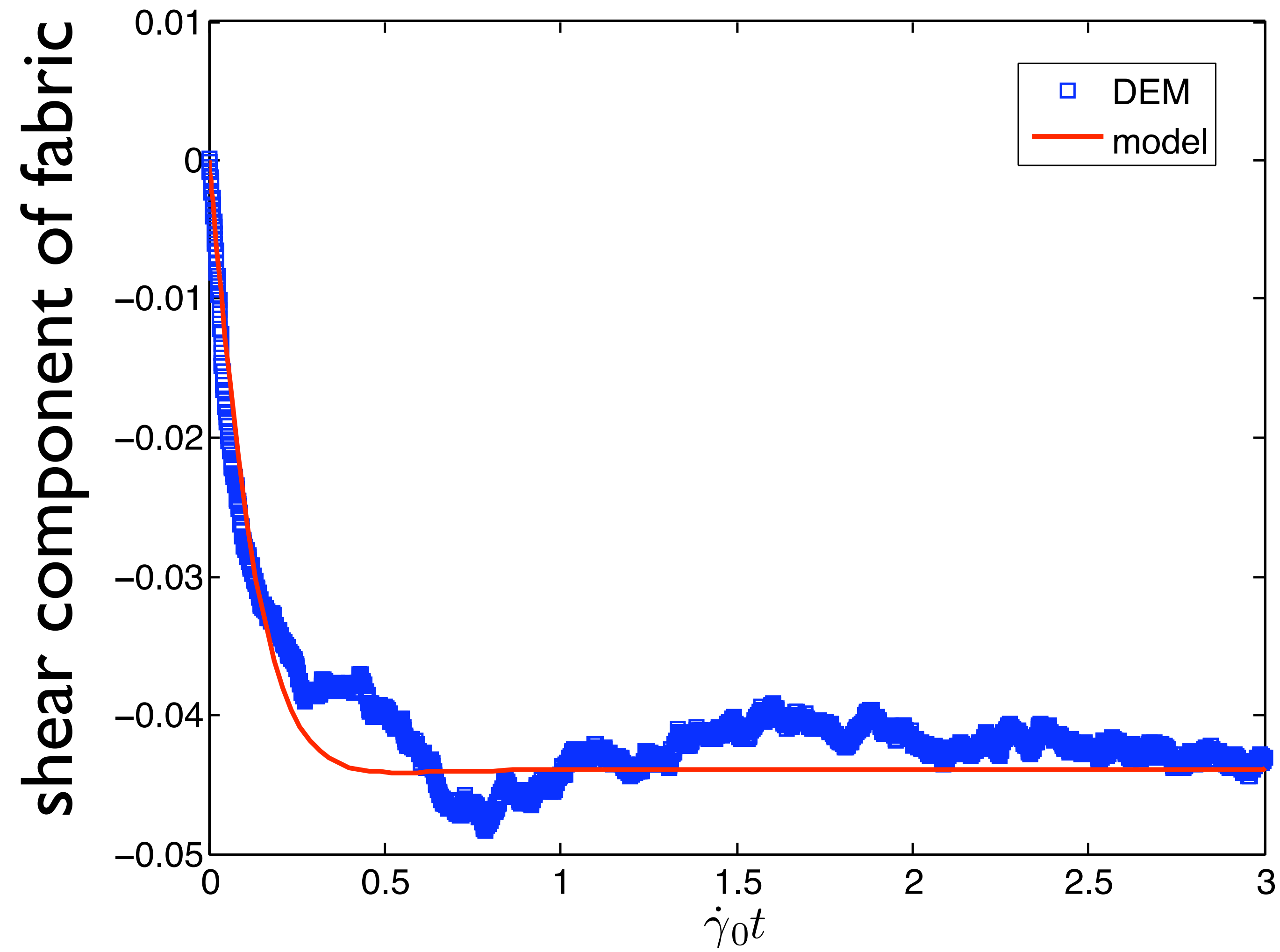


- Small strain amplitude ($\gamma_A = 0.5$) cyclic shear under constant pressure condition $\langle\phi\rangle = 0.60$ $\mu = 0.5$
- Lead to compaction as observed in experiments, e.g., Okada, 1992

Okada, N., Energy dissipation in inelastic flow of cohesionless granular media. PhD thesis, University of California, San Diego

Reynolds' dilatancy

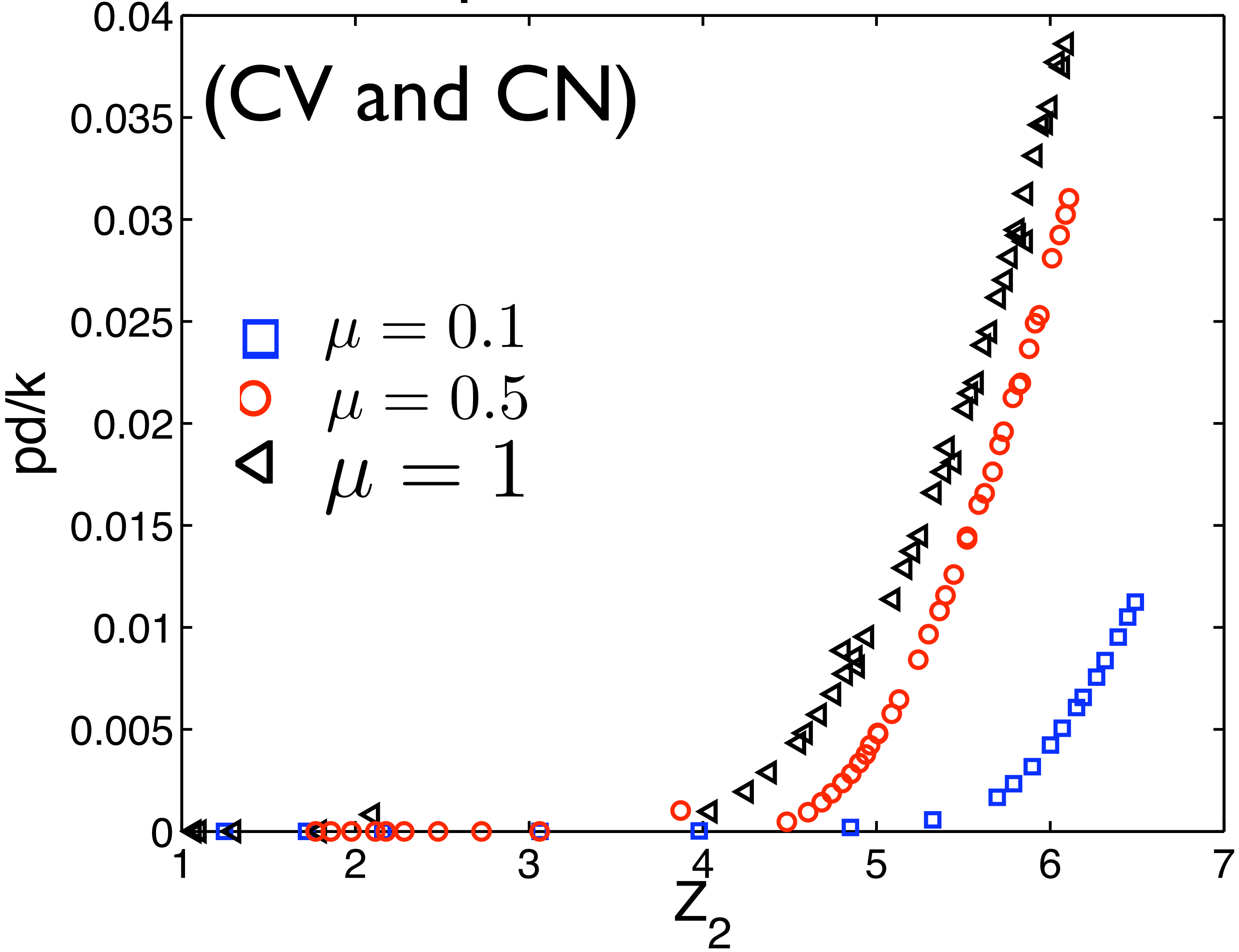




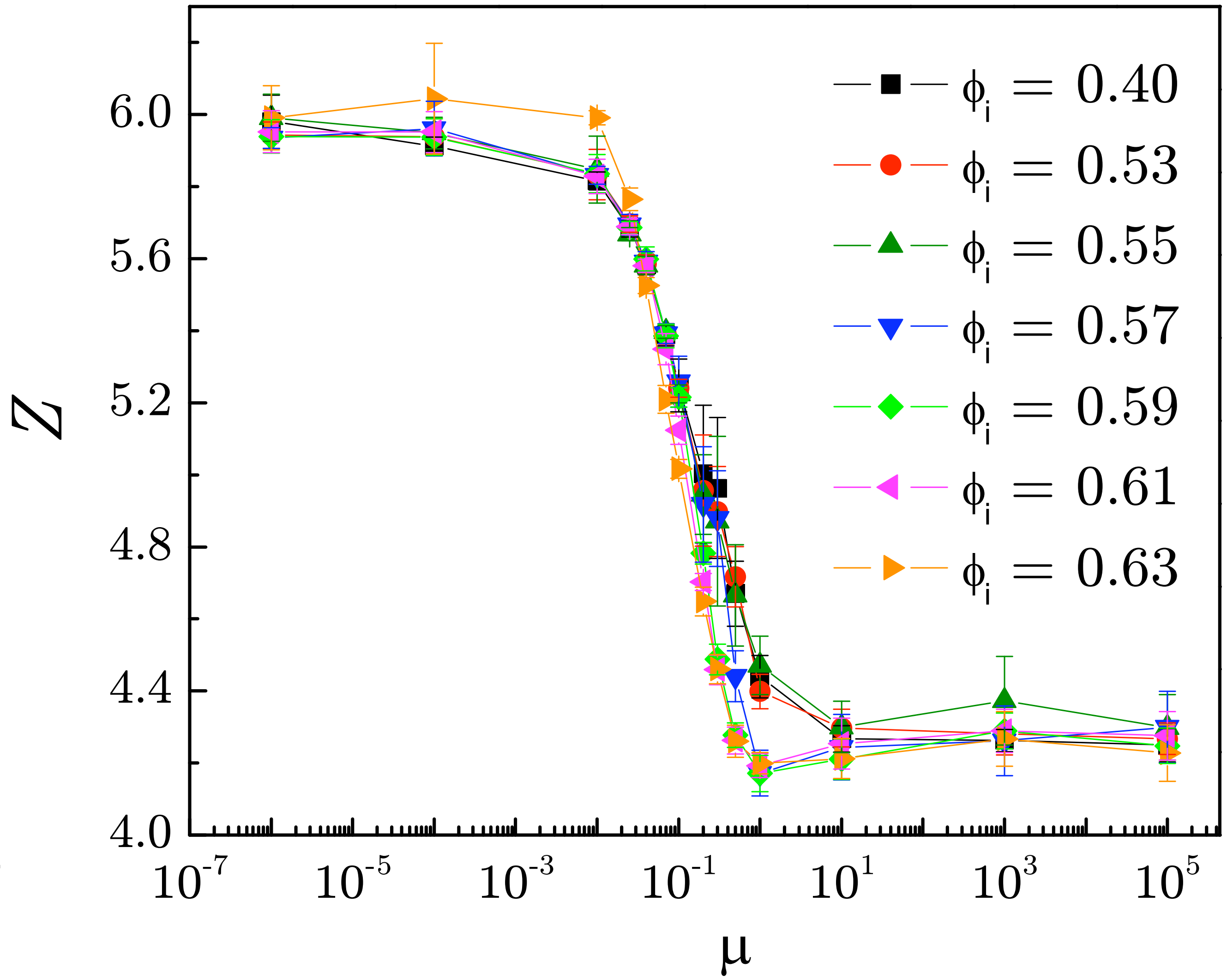
- Shear an initially isotropic assembly under constant pressure
- Model predicts correct dilation dynamics and steady state without fitting the dynamic data.

Friction dependence: pressure

Our simple shear data



Song et al. Jamming transition



- Pressure depends on friction.
- Transition point to quasi-static regime, Z_c, is related to jamming transition.

C. Song, P. Wang, and H. A. Makse. A phase diagram for jammed matter. *Nature*, 453(7195):629–632, 2008.

Friction dependence: pressure

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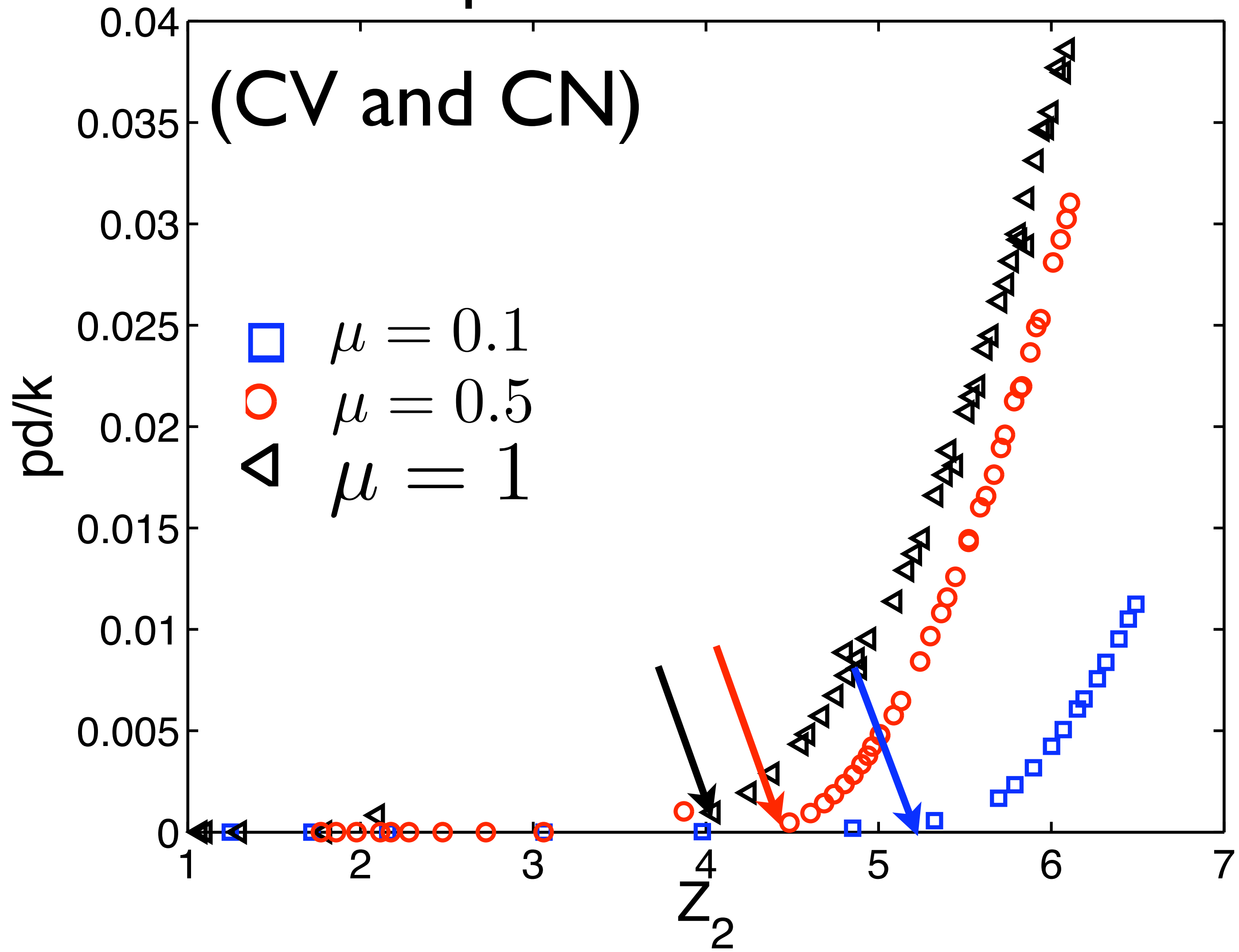

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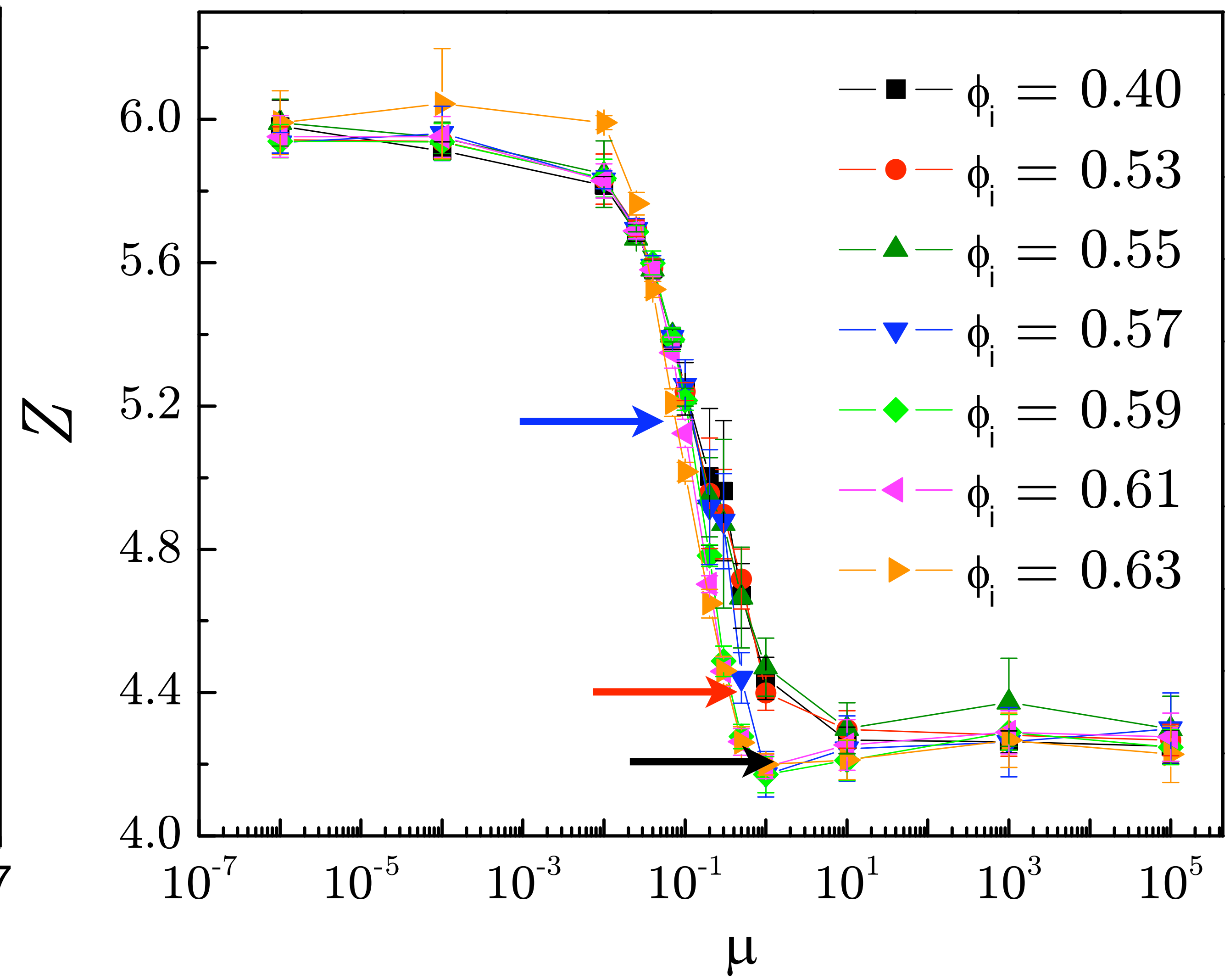

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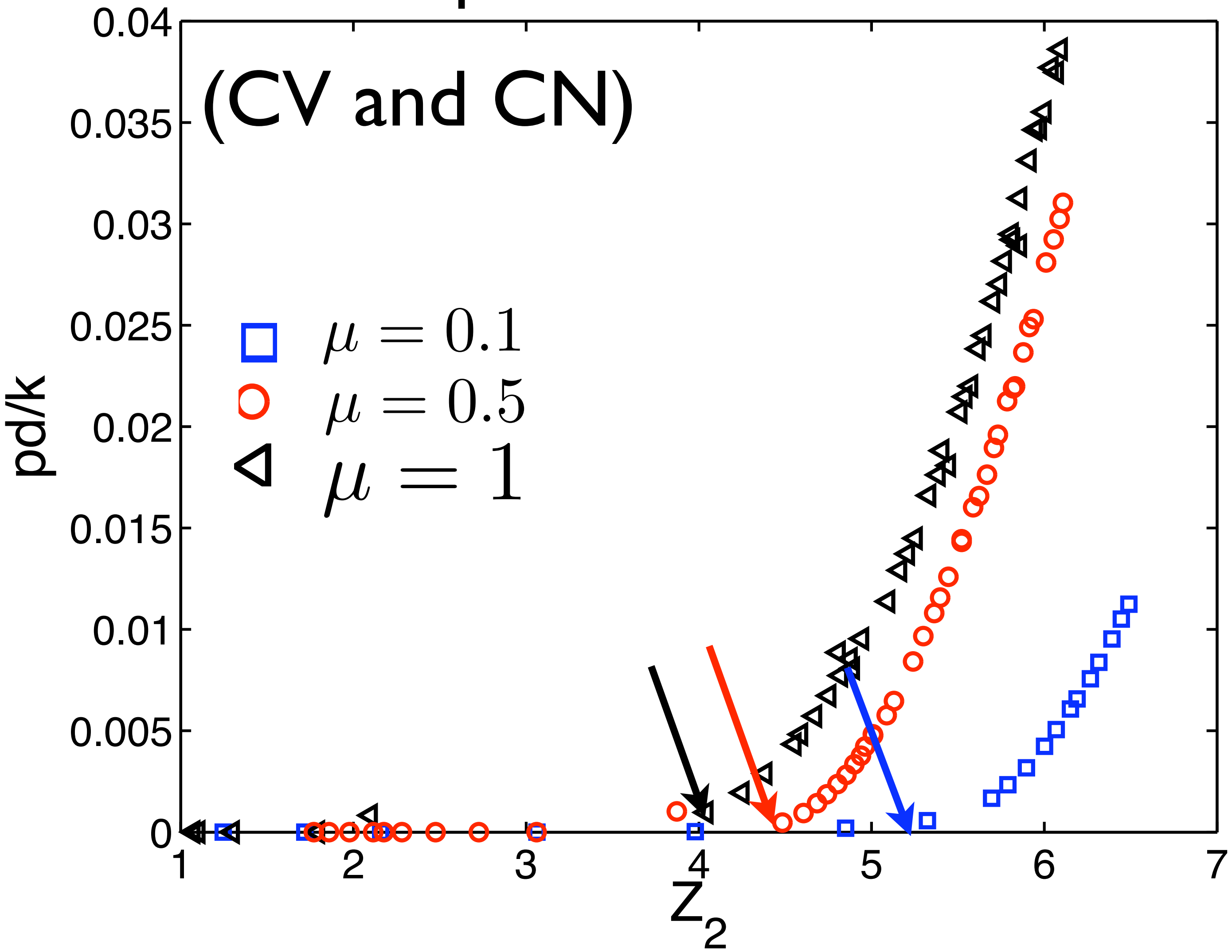

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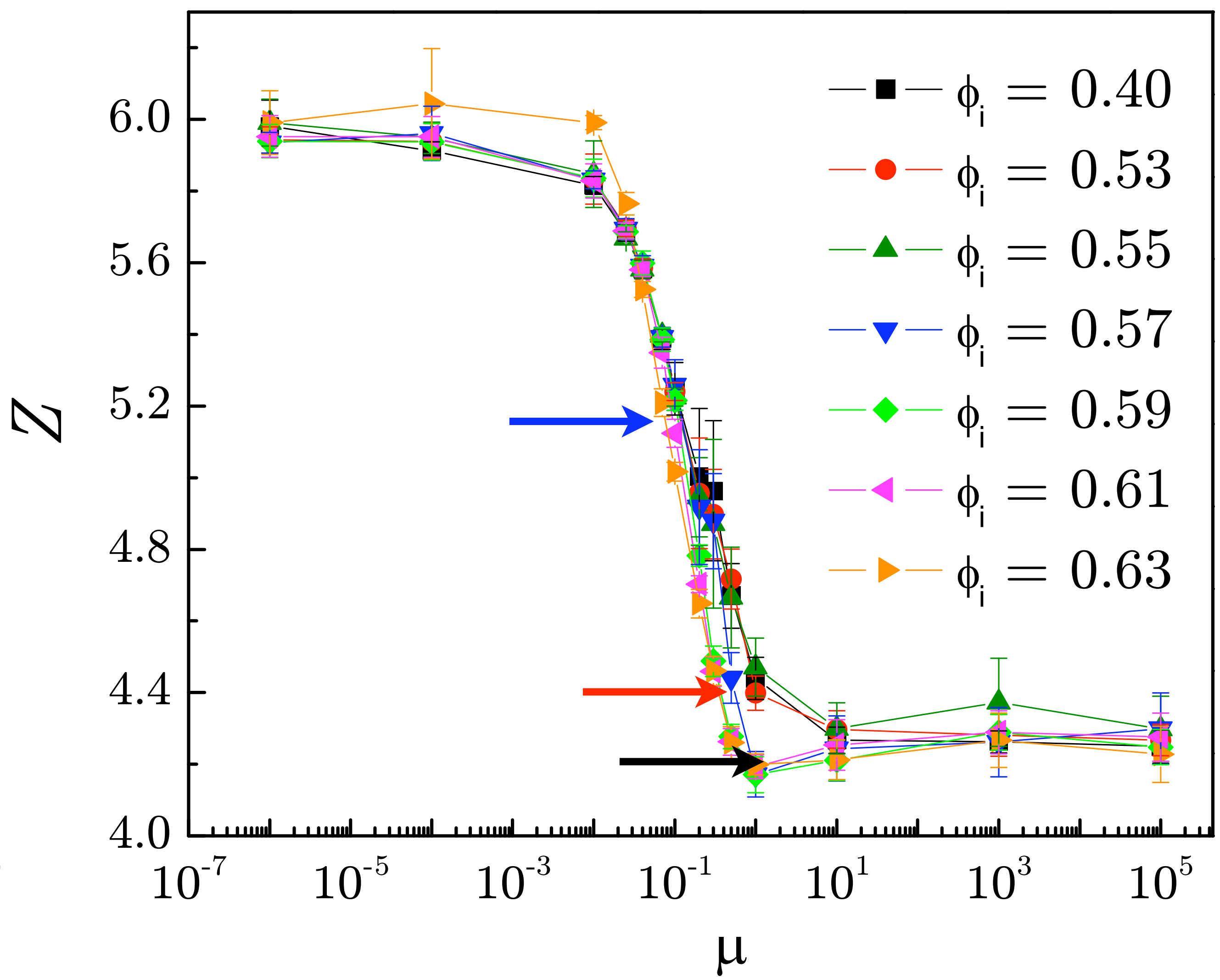

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$$p = a(Z - Z_c)^b + \alpha_5(\mathrm{A} : \mathrm{A})(Z - Z_c)^{\alpha_6}$$

$a, \ b, \ \alpha_5, \alpha_6$ depend on friction

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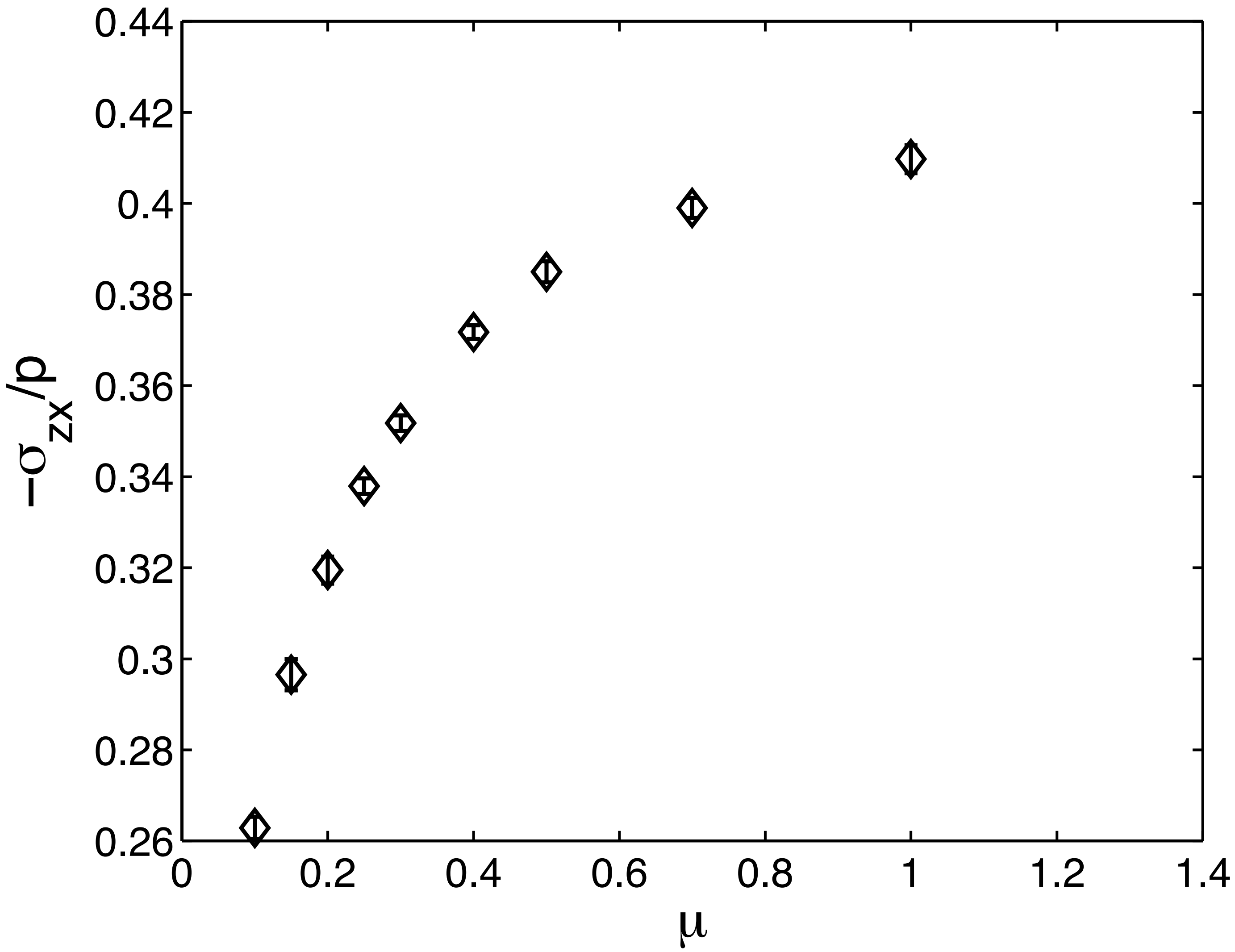
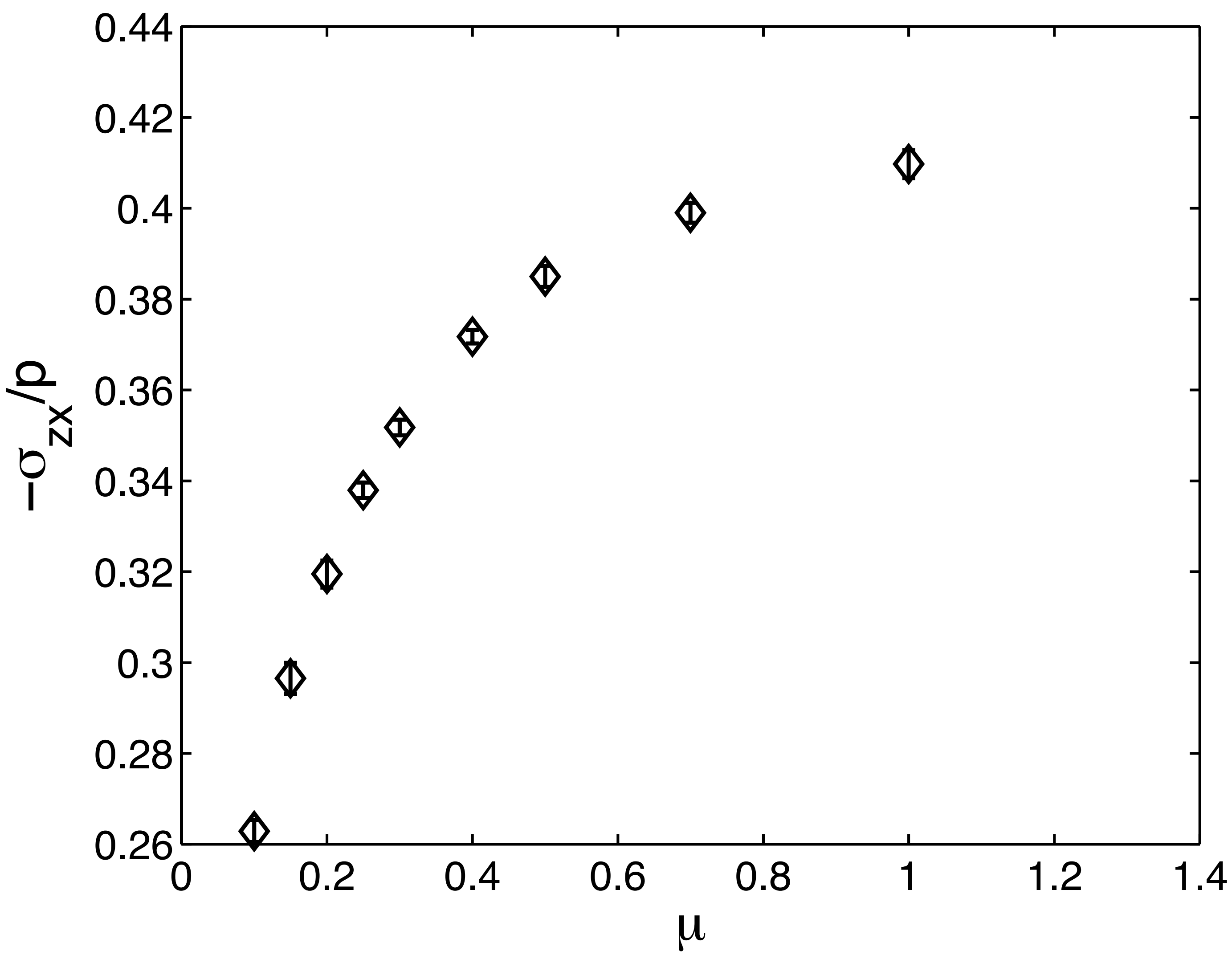
Friction dependence: stress ratio



- Simple shear data averaged over volume fractions
- Shear stress ratios increase magnitude as particle friction increases.

Friction dependence: stress ratio



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$\beta_1,\ \beta_2,\ \beta_3$ depend on friction

Summary: model recapitulation

$$\sigma_{ij} = p\delta_{ij} - p\eta\frac{S_{ij}}{\sqrt{D:D}}$$

Stress constitutive equation

Summary: model recapitulation

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- Closure relations linked to microstructure.
- Material constants depend on particle friction and elasticity.

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$$\boxed{\begin{aligned} \mathring{\mathsf{A}} &= c_1\mathsf{S} + c_2(\sqrt{\mathsf{D}:\mathsf{D}})\mathsf{A} + c_3(\mathsf{A}:\mathsf{D})\mathsf{A} \\ \dot{Z} &= \alpha_1\mathsf{A}:\mathsf{D} + \alpha_2\sqrt{\mathsf{D}:\mathsf{D}} + \alpha_3\sqrt{\mathsf{D}:\mathsf{D}}Z + \alpha_4\mathrm{tr}(D) \end{aligned}}$$

- Microstructure evolution equations.
- Material constants depend on volume fraction and friction.

Work in progress

- Simulate quasistatic triaxial compression/extension; Further test the continuum model against these DEM data.
- Study incipient yield behaviors and incorporate to the model.
- Extend the model to include strain rate-dependence.

Acknowledgment

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