Implementation and Refinement of a Comprehensive Model for Dense Granular Flows

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Monday, May 19, 2014

This work is supported by DOE-UCR grant DE-FE0006932.
Granular rheological behavior
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Ubiquitous in nature and widely encountered in industrial processes,
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Complex behavior: multiple regimes of rheology, jamming
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Shear flow of frictional particles in a periodic box
Granular rheological behavior

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- Complex behavior: multiple regimes of rheology, jamming

Shear flow of frictional particles in a periodic box

Shear flow of frictional particles with bounding walls
Computational methodology

- Simulate particle dynamics of homogeneous assemblies under simple shear using discrete element method (DEM).
  - Linear spring-dashpot with frictional slider.
  - 3D periodic domain without gravity
  - Lees-Edwards boundary conditions
- Extract stress and structural information by averaging.

Dense phase rheology: Questions asked
Flow regime map: What regimes of flow are observed in shear flow of soft, frictional, non-cohesive particles?
Dense phase rheology: Questions asked

- **Flow regime map**: What regimes of flow are observed in shear flow of soft, frictional, non-cohesive particles?

- **Effect of cohesion**: How does the addition of modest level of cohesion, such as in Geldart Group A particles change the flow regime map?
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Rheological models (non-cohesive particles)

  Steady state models that bridge various regimes
Flow regime map: What regimes of flow are observed in shear flow of soft, frictional, non-cohesive particles?

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- Modified kinetic theory
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- **Wall Boundary conditions**
Flow map

Previous studies
- Computational
- Experimental
Flow map

Quasi-static

\[ \hat{\gamma} \equiv \gamma d / \sqrt{k / (\rho_s d)} \]

\[ \hat{\rho} \equiv \rho d / k \]

\[ \mu = 0.5 \]

\[ \phi_c = 0.587 \]

Previous studies

- Computational

- Experimental
Flow map

Previous studies

- Computational

- Experimental
Flow map

Critical volume fraction $\phi_c$ and its flow curve $\hat{p} = \alpha \hat{\gamma}^m$ distinguish the three flow regimes.

Previous studies

- Computational

- Experimental
Flow map

\[
\hat{\gamma} \equiv \dot{\gamma} d / \sqrt{k / (\rho_s d)}
\]

\[
\hat{p} \equiv p d / k
\]

\[
\phi = 0.5 \quad + \phi = 0.52 \quad \bullet \phi = 0.54 \quad \diamond \phi = 0.55 \quad \star \phi = 0.56 \quad \times \phi = 0.57 \quad \triangle \phi = 0.578 \quad \blacklozenge \phi = 0.584 \quad \phi = 0.588 \quad \bigstar \phi = 0.594 \quad \times \phi = 0.6 \quad \star \phi = 0.61 \quad \bigstar \phi = 0.618 \quad \diamond \phi = 0.62 \quad \bullet \phi = 0.628 \quad \star \phi = 0.634 \quad \bigstar \phi = 0.638 \quad \times \phi = 0.64 \quad \diamond \phi = 0.648 \quad \bullet \phi = 0.65 \quad \bigstar \phi = 0.658 \quad \times \phi = 0.66 \quad \diamond \phi = 0.668 \quad \bullet \phi = 0.67 \quad \bigstar \phi = 0.678 \quad \times \phi = 0.68 \quad \diamond \phi = 0.688 \quad \bullet \phi = 0.69 \quad \bigstar \phi = 0.698 \quad \times \phi = 0.7 \quad \diamond \phi = 0.708 \quad \bullet \phi = 0.71 \quad \bigstar \phi = 0.718 \quad \times \phi = 0.72 \quad \diamond \phi = 0.728 \quad \bullet \phi = 0.73 \quad \bigstar \phi = 0.738 \quad \times \phi = 0.74 \quad \diamond \phi = 0.748 \quad \bullet \phi = 0.75 \quad \bigstar \phi = 0.758 \quad \times \phi = 0.76 \quad \diamond \phi = 0.768 \quad \bullet \phi = 0.77 \quad \bigstar \phi = 0.778 \quad \times \phi = 0.78 \quad \diamond \phi = 0.788 \quad \bullet \phi = 0.79 \quad \bigstar \phi = 0.798 \quad \times \phi = 0.8 \quad \diamond \phi = 0.808 \quad \bullet \phi = 0.81 \quad \bigstar \phi = 0.818 \quad \times \phi = 0.82 \quad \diamond \phi = 0.828 \quad \bullet \phi = 0.83 \quad \bigstar \phi = 0.838 \quad \times \phi = 0.84 \quad \diamond \phi = 0.848 \quad \bullet \phi = 0.85 \quad \bigstar \phi = 0.858 \quad \times \phi = 0.86 \quad \diamond \phi = 0.868 \quad \bullet \phi = 0.87 \quad \bigstar \phi = 0.878 \quad \times \phi = 0.88 \quad \diamond \phi = 0.888 \quad \bullet \phi = 0.89 \quad \bigstar \phi = 0.898 \quad \times \phi = 0.9 \quad \diamond \phi = 0.908 \quad \bullet \phi = 0.91 \quad \bigstar \phi = 0.918 \quad \times \phi = 0.92 \quad \diamond \phi = 0.928 \quad \bullet \phi = 0.93 \quad \bigstar \phi = 0.938 \quad \times \phi = 0.94 \quad \diamond \phi = 0.948 \quad \bullet \phi = 0.95 \quad \bigstar \phi = 0.958 \quad \times \phi = 0.96 \quad \diamond \phi = 0.968 \quad \bullet \phi = 0.97 \quad \bigstar \phi = 0.978 \quad \times \phi = 0.98 \quad \diamond \phi = 0.988 \quad \bullet \phi = 0.99 \quad \bigstar \phi = 0.998
\]

\[\phi_c = 0.587\]

- Critical volume fraction \(\phi_c\) and its flow curve \(\hat{p} = \alpha \hat{\gamma}^m\) distinguish the three flow regimes.

- Role of particle softness:
  - Large \(k\) \(\Rightarrow\) quasi-static or inertial regime
  - Small \(k\) \(\Rightarrow\) intermediate regime

Previous studies

- Computational

- Experimental
Pressure scalings for frictional particles

Scaled pressure and shear rate:\n\[
p^* = \frac{\hat{p}}{|\phi - \phi_c|^a}
\]
\[
\dot{\gamma}^* = \frac{\hat{\gamma}}{|\phi - \phi_c|^b}
\]

Choose exponents:\n\[
a = \frac{2}{3}
b = \frac{4}{3}
\]
Independent of \( \mu \)
Pressure scalings for frictional particles

Scaled pressure and shear rate:
\[
p^* = \hat{p}/|\phi - \phi_c|^a
\]
\[
\dot{\gamma}^* = \hat{\dot{\gamma}}/|\phi - \phi_c|^b
\]

Choose exponents:
\[
\begin{align*}
a &= 2/3 \\
b &= 4/3
\end{align*}
\]
Independent of \( \mu \)

Three pressure asymptotes:
\[
\frac{p_i}{|\phi - \phi_c|^{2/3}} = \alpha_i \left[ \frac{\dot{\gamma}}{|\phi - \phi_c|^{4/3}} \right]^{m_i}
\]
Pressure scalings for frictional particles

Scaled pressure and shear rate†:
\[ p^* = \hat{p} \left( \left| \phi - \phi_c \right| \right)^a \]
\[ \dot{\gamma}^* = \hat{\gamma} \left( \left| \phi - \phi_c \right| \right)^b \]

Choose exponents:
\( a = \frac{2}{3} \)
\( b = \frac{4}{3} \)

\( \mu=0.5 \)

• Three pressure asymptotes:

\[ \frac{p_i}{\left| \phi - \phi_c \right|^{2/3}} = \alpha_i \left[ \frac{\dot{\gamma}}{\left| \phi - \phi_c \right|^{4/3}} \right]^{m_i} \]

• Transitions between regimes blended smoothly
Pressure scalings for frictional particles

Scaled pressure and shear rate†:
\[ p^* = \hat{p} / |\phi - \phi_c|^a \]
\[ \dot{\gamma}^* = \hat{\gamma} / |\phi - \phi_c|^b \]

Choose exponents:
\[ a = 2/3 \]
\[ b = 4/3 \]

\[ \frac{p_i}{|\phi - \phi_c|^{2/3}} = \alpha_i \left[ \frac{\dot{\gamma}}{|\phi - \phi_c|^{4/3}} \right]^{m_i} \]

• Three pressure asymptotes:

• Transitions between regimes blended smoothly

S. Chialvo et al., PRE 85, 021305 (2012).
Dense phase rheology: Summary

- **Flow regime map**: What regimes of flow are observed in shear flow of soft, frictional, non-cohesive particles? (completed)

- **Effect of cohesion**: How does the addition of modest level of cohesion, such as in Geldart Group A particles change the flow regime map?

- **Rheological models (non-cohesive particles)**
  - Steady state models that bridge various regimes (completed)
    - S. Chialvo et al. PRE 85, 021305 (2012).
  - Modified kinetic theory

- **Wall Boundary conditions**
Kinetic-theory models

- Traditionally use kinetic-theory (KT) models for modeling inertial regime
- Most KT models designed for dilute flows of frictionless particles
Kinetic-theory models

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- Most KT models designed for dilute flows of frictionless particles.
- Can KT model be modified to capture dense-regime scalings?
Kinetic-theory models

- Traditionally use kinetic-theory (KT) models for modeling inertial regime
- Most KT models designed for dilute flows of frictionless particles
- Can KT model be modified to capture dense-regime scalings?
- Seek modifications to KT model of Garzó-Dufty (1999)†

Kinetic theory equations

Garzó-Dufty kinetic theory for simple shear flow

Pressure

\[ p = \rho_s H(\phi, g_0(\phi)) T \]

Energy dissipation rate

\[ \Gamma = \rho_s d \dot{\gamma} J(\phi) T^{3/2} \]

Shear stress

\[ \tau = \rho_s d \dot{\gamma} J(\phi) \sqrt{T} \]

Steady-state energy balance

\[ \Gamma - \tau \dot{\gamma} = 0 \]
Kinetic theory equations

Garzó-Dufty kinetic theory for simple shear flow

Pressure

\[ p = \rho_s H(\phi, g_0(\phi))T \]

Energy dissipation rate

\[ \Gamma = \frac{\rho_s}{d} K(\phi, e)T^{3/2} \]

Shear stress

\[ \tau = \rho_s d\gamma J(\phi)\sqrt{T} \]

Steady-state energy balance

\[ \Gamma - \tau\dot{\gamma} = 0 \]

Important quantities:

- Radial distribution function at contact \( g_0 = g_0(\phi) \)
  - Measure of packing
  - Diverges at random close packing
- Restitution coefficient \( e \)
  - Measure of dissipation
  - Has strong effect on temperature
Kinetic theory equations

Garzó-Dufty kinetic theory for simple shear flow

Pressure

\[ p = \rho_s H(\phi, g_0(\phi))T \]

Energy dissipation rate

\[ \Gamma = \frac{\rho_s}{d} K(\phi, e)T^{3/2} \]

Shear stress

\[ \tau = \rho_s d\dot{\gamma} J(\phi)\sqrt{T} \]

Steady-state energy balance

\[ \Gamma - \tau \dot{\gamma} = 0 \]

Modifications (in red)

Pressure

\[ p = \rho_s H(\phi, g_0(\phi, \phi_c(\mu)))T \]

Energy dissipation rate

\[ \Gamma = \frac{\rho_s}{d} K(\phi, e_{\text{eff}}(e, \mu))T^{3/2} \delta_{\Gamma} \]

Shear stress

\[ \tau = \tau_s + \rho_s d\dot{\gamma} J(\phi)\sqrt{T} \delta_{\tau} \]

Steady-state energy balance

\[ \Gamma - (\tau - \tau_s) \dot{\gamma} = 0 \]
Dense phase rheology: Summary

Flow regime map: What regimes of flow are observed in shear flow of soft, frictional, non-cohesive particles? (completed)

Effect of cohesion: How does the addition of modest level of cohesion, such as in Geldart Group A particles change the flow regime map?

Rheological models (non-cohesive particles)

- Steady state models that bridge various regimes (completed)
  S. Chialvo et al. PRE 85, 021305 (2012).
- Modified kinetic theory (completed)

Wall Boundary conditions
Cohesive particles

\[ p d / k \]

\[ \hat{\gamma} \equiv \dot{\gamma} d / \sqrt{k / \rho_s d} \]

\[ \text{Bo}^* = 0 \]

- \( \phi = 0.51 \)
- \( \phi = 0.53 \)
- \( \phi = 0.55 \)
- \( \phi = 0.57 \)
- \( \phi = 0.59 \)
- \( \phi = 0.6 \)
- \( \phi = 0.61 \)
- \( \phi = 0.62 \)
- \( \phi = 0.63 \)
Cohesive particles

\[ \hat{\gamma} \equiv \dot{\gamma}d/\sqrt{k/(\rho_s d)} \]

for \( Bo^* = 0 \)

and

\[ \hat{\gamma} \equiv \dot{\gamma}d/\sqrt{k/(\rho_s d)} \]

for \( Bo^* = 5.0E-06 \)

with symbols indicating different values of \( \phi \):
- \( \phi = 0.51 \)
- \( \phi = 0.53 \)
- \( \phi = 0.55 \)
- \( \phi = 0.57 \)
- \( \phi = 0.59 \)
- \( \phi = 0.6 \)
- \( \phi = 0.61 \)
- \( \phi = 0.62 \)
- \( \phi = 0.63 \)
Cohesive particles

\[
\hat{\gamma} \equiv \frac{\dot{\gamma} d}{\sqrt{k/(\rho_s d)}}
\]

\[
Bo^* \equiv F_{vdW}^{max} / kd \approx A / 24k_s^2_{\min}
\]
Cohesive particles

Bo* ≡ \( F_{vdW}^{\text{max}} / kd \approx A / 24ks_{\text{min}}^2 \)

\[ \hat{\gamma} \equiv \dot{\gamma}d / \sqrt{k/(\rho_s d)} \]
Cohesive particles

Quasi-static, inertial and intermediate regimes persist. A new cohesive regime emerges below the jamming conditions for equivalent non-cohesive particles.

$$Bo^* = \frac{F_{vdW}^{\text{max}}}{kd} \approx \frac{A}{24k\gamma_s^2}$$
Cohesive particles: Stress ratio

\[ \sigma = pl - p\eta \hat{S} \]

cohesion increases effective stress ratio
Dense phase rheology: Summary

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Effect of cohesion: How does the addition of modest level of cohesion, such as in Geldart Group A particles change the flow regime map? (work nearly complete, manuscript under revision)

Rheological models (non-cohesive particles)

Steady state models that bridge various regimes (completed)
S. Chialvo et al. PRE 85, 021305 (2012).

Modified kinetic theory (completed)

Wall Boundary conditions
Boundary vs. core regions

Core region
• comprises the bulk of the flow
• exhibits uniform flow properties
• obeys local, inertial-number rheological models*†

Boundary layer
• lies within ~10d of each wall
• exhibits large variations in field variables
• due to nonlocal conduction of pseudothermal energy

Boundary vs. core regions

**Core region**
- comprises the bulk of the flow
- exhibits uniform flow properties
- obeys local, inertial-number rheological models

**Boundary layer**
- lies within ~10d of each wall
- exhibits large variations in field variables
- due to nonlocal conduction of pseudothermal energy

**Questions:**
- How to define the slip velocity to get simple scaling to work?
- What if we want to avoid the need to resolve the small boundary layer?

Core rheology

Core region
- comprises the bulk of the flow
- exhibits uniform flow properties
- obeys local, inertial-number rheological models*†
  - interparticle friction coefficient $\mu$ affects yield stress ratio $\eta_s$
  - wall friction coefficient $\mu_w$ has no effect on rheological model

Inertial number:
$$I_{\text{core}} \equiv \frac{\dot{\gamma}_{\text{core}} d}{\sqrt{p_{\text{core}}/\rho_s}}$$
$$I_{\text{core}} \approx f(\phi) \text{ for } \phi < \phi_c(\mu)$$

Shear stress ratio:
$$\eta_{\text{core}} \equiv \frac{\tau_{\text{core}}}{p_{\text{core}}}$$
$$\eta_{\text{core}} = \eta_s(\mu) + \alpha I_{\text{core}}$$
Definitions of slip velocity

• Slip velocity: \( v_{\text{slip}} = v(\cdot) - v_w \)

• Options for velocity \( v(\cdot) \):
  
  a) ‘Standard’ slip velocity: based on translational velocity of particles at wall
  \( v_{\text{slip}}^{\text{tr}} = v^{\text{tr}} - v_w \)

  b) ‘Apparent’ slip velocity: based on extrapolated velocity from core region to wall
  \( v_{\text{slip}}^{\text{app}} = v^{\text{app}} - v_w \)

\( v^{\text{app}} \equiv \dot{\gamma}_{\text{core}} H/2 = v^{\text{tr}} - v' \)
Definitions of slip velocity

- **Slip velocity:**
  \[ v_{\text{slip}}^{(\cdot)} = v^{(\cdot)} - v_w \]

- **Options for velocity** \( v^{(\cdot)} \):
  
  c) ‘Surface’ slip velocity:
  based on relative velocity of particle surface at wall
  
  \[ v_{\text{surf}} = v_{\text{surf}} - v_w \]

  \[ v_{\text{surf}} = v^{\text{tr}} \pm \omega d/2 \]
Definitions of slip velocity

• Slip velocity: 
\[ v_{\text{slip}}^{(\cdot)} = v^{(\cdot)} - v_{w} \]

• Options for velocity \( v^{(\cdot)} \):
  c) ‘Surface’ slip velocity: based on relative velocity of particle surface at wall 
  \[ v_{\text{surf}}^{\text{slip}} = v_{\text{surf}} - v_{w} \]

\[ v_{\text{surf}} = v^{\text{tr}} \pm \omega d/2 \]

Question:
• Is one (or more) of these slip velocities amenable to a scaling collapse?
Velocity scales

- **Dimensionless slip velocity:**
  \[ I_{\text{slip}}^{(\cdot)} = \frac{v_{\text{slip}}^{(\cdot)}}{v_{\text{char}}} \]
  - Some slip velocity
  - Some characteristic velocity in the core

- **Options for \( v_{\text{char}} \):**
  a) **shear-rate-based\(^{\dagger}\):**
  \[ v_{\text{char}} = \dot{\gamma}d \]
  b) **stress-based\(^{*}\):**
  \[ v_{\text{char}} = \sqrt{p/\rho_s} \text{ or } \sqrt{\tau/\rho_s} \]
  c) **viscosity-based:**
  \[ v_{\text{char}} = \nu/\rho_s d = \tau/\rho_s \dot{\gamma}d \]

\(^{\dagger}\)Artoni et al. PRL 108, 238002 (2012).  
\(^{*}\)Artoni et al. PRE 79, 031304 (2009).
DEM results: dimensionless slip velocity

- Full collapse achieved by scaling of $\eta_{\text{core}} - \eta_s$:
  - $\eta_{\text{wall}} = \mu_w + \mu_w^*$
  - Critical wall friction coefficient $\mu_w^* \approx 0.33$ separates partial- and full-slip regimes

- Possible model form:
  $$ y = \frac{1.5 x^{2/3}}{(1 - x)^5} $$

- This form still requires solving for rotational velocity and boundary layer

$$ \begin{align*}
  v_{\text{slip}} &= v_{\text{surf}} - v_w \\
  v_{\text{surf}} &= v_{\text{tr}} \pm \omega d/2
\end{align*} $$

†Z. Shojaaee et al. PRE 86, 011302 (2012).
DEM results: dimensionless slip velocity

- Extend \( v_{\text{surf}} \) model to coarsely-resolved, translation-only problems

\[
I_{\text{slip}}^{\text{app}} = I_{\text{surf}}^{\text{slip}} + I_{\text{rot}} + I'
\]

from last slide
fit below

\[
I_{\text{rot}} = \frac{mI'}{(\eta_s - \eta_{s0})^2}
\]

(see figure)

\[
I' = \alpha(\eta - \eta_s)^\beta
\]

\[
\eta_{s0} = \eta_s(\mu = 0) = 0.105
\]

- Model can be coupled with simple rheological models (e.g. inertial-number models)
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- **Effect of cohesion:** How does the addition of modest level of cohesion, such as in Geldart Group A particles change the flow regime map? *(work nearly complete, manuscript under revision)*

- **Rheological models (non-cohesive particles)**
  - **Steady state models that bridge various regimes** *(completed)*
    S. Chialvo et al. PRE 85, 021305 (2012).
  - **Modified kinetic theory** *(completed)*

- **Wall Boundary conditions** *(work nearly complete, manuscript under preparation)*
Research questions: Looking ahead

- Complete wall boundary condition manuscript (Sebastian Chialvo)

- Implementation of the modified kinetic theory and the wall BCs in a CFD code (such as MFIIX) and testing. Will be collaborating with NETL researchers

- Implementation of the steady-shear rheology model in MFIIX and testing - already completed
Summary and future work

• Developed rheological model spanning three regimes of dense granular flow
• Proposed modified kinetic theory to capture rheological behavior for dense and dilute systems
• Developed boundary-condition model for dense flows
• Will soon implement MKT and wall BCs into MFIX continuum solver and test