CONSTITUTIVE MODEL DEVELOPMENT FOR FLOWS
OF GRANULAR MATERIALS

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Abstract

Granular flows are ubiquitous in both natural and industrial processes. When composed of dry, noncohesive particles, they manifest three different flow regimes — commonly referred to as the quasistatic, inertial, and intermediate regimes — each of which exhibits its own dependences on solids volume fraction, shear rate, and particle-level properties. The differences in these regimes can be attributed to microscale phenomena, with quasistatic flows being dominated by enduring, frictional contacts between grains, inertial flows by grain collisions, and intermediate flows by a combination of the two. Existing constitutive models for the solids-phase stress tend to focus on one or two regimes at a time, with a limited degree of success; the same is true of models for wall-boundary conditions for granular flows. Moreover, these models tend not to be based on detailed particle-level flow data, either from experiment or simulation. Clearly, a comprehensive modeling framework is lacking. The work in this thesis aims to address these issues by proposing continuum models constructed on the basis of discrete element method (DEM) simulations of granular shear flows. Specifically, we propose (a) a constitutive stress model that bridges the three dense flow regimes, (b) an modified kinetic-theory model that covers both the dense and dilute ends of the inertial regime, and (c) a boundary-condition model for dense, wall-bounded flows. These models facilitate the modeling of a wide range of flow systems of practical interest and provide ideas for further model development and refinement.
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Chapter 1

Introduction

Granular materials are a common class of matter composed of discrete, unbound, macroscopic particles that can act as a collective medium. Examples include natural materials such as sand, gravel, mineral powders, and cereals as well as manmade materials such as pills and catalyst pellets. It is clear from everyday experience that granular materials can exhibit both solidlike and fluidlike behavior depending on the forces they experience. For example, overturning a bucket of sand causes the contents to spill out and spread on the ground as would water or any other liquid; however, unlike a liquid, the material then comes to rest as a angled pile that is mechanically stable to small disturbances. This duality of behavior has been a cause for much of the scientific interest in granular matter.

Additionally, the variety of possible states of a granular material makes prediction of its behavior a complex engineering challenge with consequences for a wide array of industrial processes. Fluid catalytic cracking (FCC) units, used in petroleum refineries to crack crude oil into lighter, more valuable products, are an instructive example. In the riser section of the FCC unit, where the cracking reactions take place, the gaseous feedstock fluidizes catalyst powder to produce a dilute particulate phase whose flow behavior is dominated by gas-solid drag and inertial effects [1]. In contrast, the regenerator and standpipe, where catalyst particles are cleaned of their coke buildup and reintroduced into the riser, respectively,
exhibit denser flows where particle-phase stresses are more significant [2]. Development of models to capture flow behavior in these two distinct scenarios is an ongoing effort.

The most common approach for modeling granular and gas-solid flows on industrial scales is computational fluid dynamics (CFD). In particular, the finite volume method (FVM) is used to discretize and solve momentum- and mass-balance equations for each phase on a computational grid [3]; this method is combined with the two-fluid model (TFM), in which the fluid and solid phases are treated as interpenetrating continua [1, 4], to describe the behavior of each phase at every grid cell in the system. These balance equations are presented in Table 1.1. The continuity equations for the solids phase (Eq. 1.1) and gas phase (Eq. 1.2) are straightforward and relate the solids fraction $\phi$ to the solids velocity field $v$ and fluid velocity field $u$; in each, an accumulation ($\partial/\partial t$) term simply balances with a corresponding convective transport term. The momentum balance equations for the solids (Eq. 1.3) and fluid phases (Eq. 1.4), however, are more complex. Though they contain similar accumulation and convective terms (collectively known as the inertial terms) on the left-hand side of the equations, the right-hand side contains many additional contributions representing forces acting on each phase per unit volume of the mixture. These terms include (as read from left to right in Eq. 1.3) a stress divergence term for stress tensor $\sigma$, a generalized buoyancy term, an interphase interaction term $f$ (the most significant part of which is the drag force in gas-particle flows), and a gravitational body force term proportional to material density $\rho$. Here, $(\cdot)$ denotes the relevant phase — solids or gas. Of these quantities, three require additional closures to make solution of the system of equations possible: the gas-phase stress $\sigma_g$, the solids-phase stress $\sigma_s$, and the drag force $f$. The first of these quantities is, for most gas-solids flow problems, appropriately constituted simply with a Newtonian rheological model, but the latter two are less trivial to close. Indeed, much effort has been devoted to the development of models for the solids-phase stress (e.g. [5–8]) and interphase drag [9–12]. Since the work in this dissertation is concerned primarily with purely granular flows — that is, flows for which the solids are nearly unaffected by the flow of the gas, rendering $f \approx 0$ —
Table 1.1: Balance equations used in the two-fluid model (TFM) [1, 4].

Continuity Equations

\[
\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \mathbf{v}) = 0 \quad (1.1)
\]
\[
\frac{\partial (1-\phi)}{\partial t} + \nabla \cdot [(1-\phi) \mathbf{u}] = 0 \quad (1.2)
\]

Momentum Balance Equations

\[
\frac{\partial (\rho_s \phi \mathbf{v})}{\partial t} + \nabla \cdot (\rho_s \phi \mathbf{v} \mathbf{v}) = -\nabla \cdot \mathbf{\sigma}_s - \phi \nabla \cdot \mathbf{\sigma}_g + \mathbf{f} + \rho_s \phi \mathbf{g} \quad (1.3)
\]
\[
\frac{\partial [\rho_g (1-\phi) \mathbf{u}]}{\partial t} + \nabla \cdot [\rho_g (1-\phi) \mathbf{u} \mathbf{u}] = -(1-\phi) \nabla \cdot \mathbf{\sigma}_g - \mathbf{f} + \rho_g (1-\phi) \mathbf{g} \quad (1.4)
\]

the current focus hence turns to modeling the solids stress.

In the early modeling works, granular flow is presented as existing in either of two regimes. These regimes are readily observed in simple shear cell experiments [13–17] by varying the shear rate and allowing the bed to dilate or compact; a qualitative picture of this regime map is shown in Fig. 1.1. For low shear rates, the bed remains compact and stresses are observed to be independent of the shear rate \(\dot{\gamma}\); this regime is known as the quasistatic regime, and stresses here arise from enduring, multibody, frictional contacts between the grains. As shear rate is increased, the bed dilates and arrives at a regime in which stresses scale as the square of the shear rate; this regime is known as the inertial regime, and stresses here arise from nearly instantaneous, binary collisions between grains. However, it is noticed that there is a domain of shear rates in between the quasi-static and inertial regimes for which the stress scaling transitions smoothly from \(\dot{\gamma}^0\) to \(\dot{\gamma}^2\). This transitional or intermediate region is considered, in early works, not to be a truly separate regime but rather a zone of overlap between quasistatic and inertial behaviors. With this perspective, early models are aimed at capturing the transition by treating the intermediate regime as a superposition of
Figure 1.1: Qualitative regime map from early works on granular flows. The quasistatic regime, in which stresses are independent of shear rate $\dot{\gamma}$, occurs at low shear rates. High shear rates, on the other hand, give rise to the inertial regime, where stresses scale as the square of shear rate. The ‘intermediate’ region between these two regimes is not considered a separate regime so much as a transition between them. This regime map differs from those in Figure 1.2.

Quasistatic and inertial models, and thus stress models are decomposed into a rate-dependent part (exhibiting $\dot{\gamma}^2$-dependence) and a rate-independent part [7, 18]. However, it is never particularly clear when and to what extent each of these terms should contribute.

In his work from the late 1990s and early 2000s, Tardos presents the results of Couette cell experiments aimed at elucidating the reasons for this intermediate behavior [13, 14]. The experiments involve rotating an inner rough cylinder to shear an annulus filled with grains, with sensors inserted into the flow to measure stresses. The amount of dilation is controlled to some extent by overburdening the system with a static pile on top of the sheared section. Tardos observes that this inhibition to dilation is important for accessing the intermediate regime, suggesting that the solid volume fraction (and not just the shear rate) plays an
important role in the regime map. After compiling some of his data with those of some previous works [15–17], he notes that the intermediate regime is more prevalent for densely packed systems, underscoring the role of volume fraction in the location of the regimes.

Around the same time, Campbell presents results from a vast campaign of DEM simulations of shear flows near the regime boundaries. [19, 20]. For sheared soft-particle systems, Campbell identifies the dimensionless group

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

(1.5)

to be important to the rheology of the granular material. Here, \(d\) is the particle diameter, \(k\) is the (Hookean) particle stiffness, and \(\rho_s\) is the solid material density. Noting the dependence of pressure on shear rate in \(\phi-\hat{\gamma}\) space, he indeed observes three distinct regimes. However, their locations are somewhat different from the traditional view, as seen in Figure 1.2a (adapted from Ref. [19]). At low shear rates, the densest systems exist in the quasistatic regime, while less dense systems lie in the inertial regime. That is, the inertial regime is accessed by decreasing volume fraction, not by increasing shear rate as previously thought. Rather, increasing shear rate brings the system into the intermediate regime, or the elastic-inertial regime as Campbell calls it. This name comes from the role of particle softness or elasticity in this regime. As the particles are sheared more quickly, the extent of overlap during a collision increases, rendering the binary collision time of the particles an important timescale in the dynamics. In fact, the dimensionless shear rate \(\hat{\gamma}\) is simply the ratio of the binary collision time to the macroscopic deformation time.

Lois and Carlson [21] refine this regime map in their theoretical model based on length scales in grain networks. Figure 1.2b, adapted from their work, shows the regimes on a plot of volume fraction versus scaled shear rate. They argued that a critical volume fraction \(\phi_c\) separates the quasi-static and inertial regimes in the static limit, with this volume fraction corresponding to the jamming point of the assembly. The intermediate regime then emerges
Figure 1.2: Regime maps as presented by (a) Campbell [19] and (b) Lois and Carlson [21]. Both maps present a boundary at low \( \dot{\gamma} \) between quasistatic and inertial regimes that lies at a critical value of the volume fraction \( \phi \). As \( \dot{\gamma} \) increases, the intermediate regime emerges from this critical volume fraction to encompass a larger window of \( \phi \) values. This regime map suggests that the inertial regime is not accessed from the quasistatic regime simply by an increase in shear rate, in direct contrast to the map in Figure 1.1.
from this point to encompass an ever-growing window of volume fractions as the shear rate increases. This work is among the first of numerous attempts to quantify the rheology of soft spheres about a jamming transition.

Shortly thereafter, several works appear in the literature that identify convenient stress scalings based on simulations similar to Campbell’s but for frictionless spheres [22, 23] and disks [24, 25]. In particular, they find that the stress and shear rate can be scaled by powers of the distance \( \phi_c - \phi \) to the jamming point to collapse the data onto two branches, one above \( \phi_c \) and one below. The exact values of these exponents have been the subject of much debate, as has the shear-rate dependence of the intermediate-regime stresses, though most findings place the latter between 1/2 and 1. The form of these scalings is not simply the artifact of the numerical methods from which they are derived, however. Similar scaling exponents are found in rheometer experiments, for example, by Nordstrom et al. [26] for colloidal gel particles in water and by Seth et al. [27] for oil emulsions in water and water-glycerol solution. While Seth et al. do not explicitly present a scaling with respect to the distance to the jamming point, they do collapse their stress data by scaling it with respect to experimentally-measured yield stresses, which according to Nordstrom et al. scale as \((\phi_c - \phi)^2\). Clearly, these scalings are physically meaningful for frictionless systems, though 2D simulations suggest that they also hold for frictional systems, despite the fact that the jamming point \( \phi_c \) varies with the interparticle friction coefficient [28, 29]. The universality of these scalings requires that they be taken into account in future development of rheological models for granular materials.

Throughout the aforementioned works, various dimensionless shear rates have been presented, each one representing the competition of the macroscopic deformation time with some other time scale. Tardos [13, 14] finds the gravitational timescale to be convenient for his experiments, as it influences the dilation of the granular bed. Campbell, on the other hand, finds the particle stiffness to provide an important timescale that governs the entrance into the intermediate regime [19]. Separately, GDR MiDi [30] and others [8, 31] have proposed
using the inertial number, in which the particle-phase pressure provides the second time scale, interpreted as the characteristic time for microscopic particle rearrangement. This inertial number, defined as

\[ I \equiv \frac{\dot{\gamma} d}{\sqrt{p/p_s}} \]  (1.6)

has been shown to dictate the rheology of hard particles \( i.e. \) for which \( k \to \infty \). The plurality of possible scalings raises some important questions, including how these groups can be used to construct models that bridge the regimes observed in soft-particle and hard-particle flows.

All of the studies discussed above have involved flows only of dry, repulsive particles. If, however, we consider systems with cohesive van der Waals forces between the particles, we find yet another dimensionless group that comes into play — namely, a modified Bond number [32] defined as

\[ Bo^* \equiv \frac{F_{\text{max}}^{\text{vdw}}}{kd} \]  (1.7)

This quantity represents the ratio of the maximum attractive force \( F_{\text{max}}^{\text{vdw}}(A) \), which is a function of the Hamaker constant \( A \), to a characteristic repulsive force \( kd \) between two particles. Aarons and Sundaresan [32] have performed DEM simulations similar to those of Campbell [19] but with an added van der Waals force and are able to collapse data for different Bond numbers and shear rates. They also observe two prominent trends in the regime map. Firstly, the quasistatic regime widens to encompass a larger volume fraction domain, which is expected since the introduction of cohesion results in the formation of agglomerates that are more difficult to shear; it is hence also thought that cohesion decreases the critical volume fraction \( \phi_c \) separating the cohesive and inertial regimes. Secondly, the intermediate regime is observed to grow, an effect that has two micro-/mesoscopic causes: (1) the relevant length scale in cohesive flows is larger than in noncohesive flows because of the shearing of agglomerates rather than particles, so the ‘effective’ particle diameter increases;
and (2) because agglomerates can rearrange under compression, they are effectively softer than their constituent particles, so the ‘effective’ particle stiffness decreases. Inclusion of a larger $d$ and smaller $k$ in Eq. 1.5 yields a larger value of $\dot{\gamma}$ and therefore a larger intermediate regime that is easier to access. Clearly, understanding of the intermediate regime is critical to the understanding of dense flows of both cohesive and noncohesive granular material.

Finally, though significant advancement has been made in the development of rheological models for dense granular flows, there remains a lack of similarly developed models for boundary conditions (BCs) in wall-bounded flow systems. The vast majority of existing BC models are based on ad-hoc frictional-kinetic approaches [7], which fail to reproduce important $\dot{\gamma}$- and $\phi$-scalings of the stresses as aforementioned, or kinetic-theory (KT) approaches, which tend to involve simplifying assumptions about the nature of particle collisions that limit their range of applicability, typically, to dilute flows of frictionless [33] or slightly frictional [34, 35] particles. Recently, Artoni et al. [36] have performed particle simulations of dense flow down an inclined plane, the data from which they use to propose a simple, empirical model. While the small scope of their study leaves questions about the range of particle and flow properties for which the proposed model form and fitting constants are appropriate, the strategy used to develop this model is a new and productive step forward.

Indeed, the use of particle simulations to generate flow data for empirical model development is appealing for several reasons. For one, it generally involves fewer assumptions to be made about the velocity and spatial distributions of interacting particles that are necessary in kinetic-theory derivations; rather, the simulations solves for these distributions. Additionally, because of the rapid increases in computing power in recent years, large numbers of simulations can be performed to cover a wide range of particle and flow properties with no increase in complexity of the underlying methods. Finally, though the translation of simulation data into a coherent model is inherently empirical, the simulation allows access to micro- and mesoscopic information that is difficult to measure or even entirely inaccessible by experiment — for example, data related to the microstructure of particle contacts or the
gradients of solids fraction. For these reasons, we judge particle-based simulation approaches
to offer the most promising path forward for constitutive model development for granular
flows.

The overarching goal of the work presented in this dissertation is to elucidate the nature
of regime transitions in granular flows and develop continuum models that describe these
transitions. In addition, it is preferred that these models (1) be based on scaling laws eluci-
dated by particle simulations and consistent with dimensional analysis; (2) be applicable to
a wide range of flow types and particle properties; and (3) be ready for immediate implement-
tation and use in existing continuum-model solvers to simulate practical-scale flows. To meet
these goals, it is necessary to address a number of critical questions. For example, given that
ad-hoc approaches are generally used for regime bridging, what do particle simulations sug-
gest as appropriate functional forms for a comprehensive stress model? Additionally, in the
context of existing simulation studies that tend to be limited to small parameter spaces, do
changes to particle properties have a significant influence on each of the regime transitions?
How is the transition from dense to dilute regimes connected to micro- and mesostructural
variables, and is the dense-to-dilute transition microstructurally similar to the transitions
among dense regimes? To what extent are the assumptions made in the derivations of tra-
ditional kinetic-theory models valid for dilute and dense flows? And can local rheological
models be extended to include wall effects without a substantial increase in complexity?
These questions and others will be addressed presently.

To this end, the studies performed in this work use the discrete element method (DEM) [37]
to simulate simple shear flows of granular materials, from which field data are extracted and
used to develop continuum models. In Chapter 2, dense shear flows in periodic systems
are performed and used to develop a rheological model for flows in the three dense flow
regimes (of noncohesive particles): quasistatic, inertial, and intermediate. In Chapter 3, the
campaign of periodic shear simulations is expanded to include dilute systems; the data from
these simulations is used to construct modifications to an existing kinetic-theory rheological
model [38], including a bridging between dense- and dilute-regime closures. In Chapter 4, wall-bounded shear simulations are performed and used to construct BC models for several different definitions of slip velocity. Finally, Chapter 5 discusses the conclusions drawn from these efforts as well as potential directions for future investigation.
Chapter 2

Bridging granular rheology across three dense regimes

This chapter contains work that is published as “Bridging the rheology of granular ows in three regimes” by Chialvo, Sun, and Sundaresan in Physical Review E 85, 021305 (2012), which corresponds to Ref. [39]. Some changes and additions have also been included and are indicated with footnotes.
Overview of the Chapter

We investigate the rheology of granular materials via molecular dynamics simulations of homogeneous, simple shear flows of soft, frictional, noncohesive spheres. In agreement with previous results for frictionless particles, we observe three flow regimes existing in different domains of particle volume fraction and shear rate, with all stress data collapsing upon scaling by powers of the distance to the jamming point. Though this jamming point is a function of the interparticle friction coefficient, the relation between pressure and strain rate at this point is found to be independent of friction. We also propose a rheological model that blends the asymptotic relations in each regime to obtain a general description for these flows. Finally, we show that departure from inertial number scalings is a direct result of particle softness, with a dimensionless shear rate characterizing the transition.

2.1 Introduction

Flows of granular matter occur in numerous geophysical and industrial processes and, as such, have garnered the attention of researchers for many years. Early efforts to describe these flows focused on either dilute flows (where kinetic theories [5, 7, 38, 40] apply and which belong to the inertial regime) or very dense, slow flows (or quasistatic flows, for which plasticity models [6, 41] can be used). However, attention has turned recently to the interface between these two regimes in the context of a jamming transition, proposed to occur in granular and other soft matter [42]. Of particular interest are several works that find a critical rheology around this transition in flows of frictionless, soft spheres [22, 23, 26, 43] and disks [24, 25]. Furthermore, they find scalings for the mean normal and shear stresses with respect to volume fraction that apply over a wide range of volume fractions and shear rates. Granular materials, though, are typically considered stiff, frictional materials, and to date there has been little work on identifying a critical rheology [19, 28] for such matter despite significant progress in understanding their static jamming behavior [44–47]. In this
paper, we investigate the rheology of frictional granular matter about the jamming transition and discuss the construction of a rheological model for flows in the quasistatic, inertial, and intermediate (i.e. critical) regimes.

2.2 Simulation Methods

We perform computer simulations using a package of the discrete element method (DEM) [37] implemented in the molecular dynamics package LAMMPS [48]. In DEM, particles interact only via repulsive, finite-range contact forces. We employ a spring-dashpot model, for which the normal and tangential forces on a spherical particle $i$ resulting from the contact of two identical spheres $i$ and $j$ are†

$$
F^n_{ij} = f(\delta d) \left[ k_n \delta_{ij} n_{ij} - \gamma_n m_{\text{eff}} v^n_{ij} \right], \\
F^t_{ij} = f(\delta d) \left[ -k_t u^t_{ij} - \gamma_t m_{\text{eff}} v^t_{ij} \right],
$$

for overlap distance $\delta_{ij}$, particle diameter $d$, spring stiffness constants $k_n$ and $k_t$, viscous damping constants $\gamma_n$ and $\gamma_t$, effective mass $m_{\text{eff}} = m_i m_j / (m_i + m_j)$ for particle masses $m_i$ and $m_j$, relative particle velocity components $v^n_{ij}$ and $v^t_{ij}$, and elastic shear displacement $u^t_{ij}$.

A linear spring-dashpot (LSD) model is chosen by setting the function $f(x) = 1$, while a Hertzian model is set by $f(x) = \sqrt{x}/4$; note that the units of $k_n$ and $k_t$ are different for the two contact models in order to maintain consistent units of force. The LSD model will be used throughout this paper except where noted explicitly. By Newton’s Third Law, particle $j$ experiences the force $F_{ji} = -F_{ij}$. Particle sliding occurs when the Coulomb criterion $|F^t_{ij}| < \mu |F^n_{ij}|$ is not satisfied for particle friction coefficient $\mu$. Additionally, after setting $k_t/k_n = 2/7$ and $\gamma_t = 0$, we set $\gamma_n$ such that the restitution coefficient $e = \exp \left( -\gamma_n \pi / \sqrt{4k_n/m_{\text{eff}} - \gamma_n^2} \right) = 0.7$ in the LSD case.

Using the above contact model, assemblies of about 2000 particles in a periodic box

---

†Eqs. 2.1-2.2 contained a typographical error in the original publication in *Phys. Rev. E* [39].
are subjected to homogeneous steady simple shear at a shear rate $\dot{\gamma}$ via the Lees-Edwards boundary condition [49]. The box size, and hence the solids volume fraction $\phi$, are kept constant for each simulation. The macroscopic stress tensor is calculated as

$$\sigma = \frac{1}{V} \sum_i \left[ \sum_{j \neq i} \frac{1}{2} r_{ij} F_{ij} + m_i (v'_i)(v'_i) \right], \quad (2.3)$$

where $V$ is the box volume, $r_{ij}$ is the center-to-center contact vector from particle $j$ to particle $i$, and $v'_i$ is the particle velocity relative to its mean streaming velocity; from this result, an ensemble-averaged pressure $p = (\sigma_{xx} + \sigma_{yy} + \sigma_{zz})/3$ and shear stress $\tau = \sigma_{xz}$ can be extracted. All macroscopic quantities will be presented in dimensionless form, scaled by some combination of the particle diameter $d$, stiffness $k = k_n$, and solid density $\rho_s$. Since particles are assumed to overlap without deformation, we ensure that the average overlap is small (i.e. $\delta/d \approx pd/k \lesssim 0.07$).

### 2.3 Flow regimes

We performed a series of simple shear simulations over a range of shear rates and volume fractions reaching into all three flow regimes and for several particle friction coefficients between 0 and 1. Figure 2.1 shows the scaled pressure $pd/k$ versus the scaled shear rate $\dot{\gamma} = \dot{\gamma}d/\sqrt{k/(\rho_s d)}$ at various volume fractions for (a) $\mu = 0.5$ and (b) $\mu = 0.1$. At low shear rates, there is an observed separatrix occurring at a critical volume fraction $\phi_c$, which we identify as the jamming point; stresses scale quadratically with shear rate below $\phi_c$ but show no rate dependence above it. These two bands correspond to the inertial and quasistatic regimes, respectively. As shear rate increases, the quasistatic and inertial isochores approach a shared asymptote characteristic of the critical point in which dependence on the volume fraction vanishes; this region corresponds to the intermediate regime. Interestingly, the intermediate asymptote appears to be independent of the friction coefficient, in contrast to results at lower shear rates and despite the fact that $\phi_c = \phi_c(\mu)$. Values of $\phi_c$ for different
Table 2.1: Estimates of the critical volume fraction $\phi_c$ for different cases of the interparticle friction coefficient. The value of $\phi_c$ for the frictionless case agrees with the experimentally determined result of Nordstrom [26].

<table>
<thead>
<tr>
<th>$\mu$</th>
<th>0.0</th>
<th>0.1</th>
<th>0.3</th>
<th>0.5</th>
<th>1.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi_c$</td>
<td>0.636</td>
<td>0.613</td>
<td>0.596</td>
<td>0.587</td>
<td>0.581</td>
</tr>
</tbody>
</table>

cases of $\mu$ are presented in Table 2.1. It should be noted that these critical values inferred from dynamical behavior of sheared systems are unique for each case of $\mu$ and hence may differ from the jamming points of static packings, which are not unique and depend on the compactivity [45].

A better understanding of the regime transitions can be gained by constructing a regime map, or “phase diagram,” from the slopes of the curves in Figure 2.1. Such a map is shown in Figure 2.2. The intermediate regime is observed to lie in a window centered around $\phi = \phi_c$, and the width of this window is dependent on the value of the dimensionless shear rate. This feature has important implications for the modeling of dense granular flows. The large stiffness of granular materials such as sand or glass beads has been used to justify the modeling of granular particles as (infinitely) hard spheres. For such particles, dimensional analysis requires the traditional Bagnold scaling of the stresses (i.e. $p, \tau \sim \dot{\gamma}^2$), thereby rendering the intermediate and quasistatic regimes impossible. This picture is consistent with the vanishing of the intermediate regime observed in Figure 2.2 as $k \rightarrow \infty$. However, real granular materials do nevertheless have a finite stiffness. Therefore, in the context of building a general rheological model for granular flows, it is preferable to choose a framework that include all three regimes.

Another important observation from Figure 2.2 is the smoothness of the transitions between the regimes. This feature suggests that purely quasistatic, inertial, or intermediate flow is achieved only in certain limits. As $\dot{\gamma} \rightarrow 0$, we see quasistatic flow for $\phi > \phi_c$, inertial flow for $\phi < \phi_c$, and intermediate flow at $\phi = \phi_c$. We also see intermediate flow as $\dot{\gamma} \rightarrow \infty$ for all volume fractions over the wide range examined in this study. The smooth transitions
Figure 2.1: Dimensionless pressure vs. dimensionless shear rate for various volume fractions with (a) $\mu = 0.5$ and (b) $\mu = 0.1$. In both cases, three flow regimes are observed, each with the scalings $p \sim \dot{\gamma}^m$: a quasistatic regime with $m = 0$, an inertial regime with $m = 2$, and an intermediate regime with $m \approx 1/2$. At low $\dot{\gamma}$, a critical volume fraction $\phi_c$ separates the quasistatic and inertial regimes; values of $\phi_c(\mu)$ are given in Table 2.1.
Figure 2.2: Regime map for $\mu = 0.5$, with volume fraction vs. dimensionless shear rate. The intermediate regime occurs only at $\phi_c$ in the limit $\hat{\dot{\gamma}} \rightarrow 0$ but emerges from this point to encompass all volume fractions as $\hat{\dot{\gamma}} \rightarrow \infty$.

also suggest that the rheology at a particular $(\hat{\dot{\gamma}}, \phi)$ is a composite of contributions from low-$\hat{\dot{\gamma}}$ and high-$\hat{\dot{\gamma}}$ behaviors, and this notion will play a large role in our construction of a rheological model.

2.4 Critical volume fraction $\phi_c$

Because $\phi_c$ plays such an important role in governing the rheology in each of the three flow regimes, accurate estimation of its value for each case of $\mu$ is required for the construction of a valid rheological model. However, this task is made difficult by fluctuations of our measurements in time $t$. We observe a propensity for assemblies near $\phi_c$ to form and break force chains intermittently during the shearing process, resulting in stress fluctuations of several orders of magnitude as seen in Figure 2.3a. Though fluctuations occur at all volume fractions, their size relative to the mean is markedly large near the critical point. In Figure 2.3b the standard deviation $\sigma_p \equiv \sqrt{\langle p^2(t) \rangle - \langle p(t) \rangle^2}$ of the pressure, when scaled by the time-averaged pressure $p$, exhibits a spike centered slightly under $\phi_c$. This phenomenon increases
the potential error in the time-averaged stress values near the critical point, thereby limiting the precision of our \( \phi_c \) estimates to within about \( \pm 0.001 \).

Additionally, though \( \phi_c \) is certainly an important quantity, it is not necessarily the only or even the most influential parameter describing the jamming transition. The fact that stress can vary significantly at a constant volume fraction indicates that, while \( \phi \) is a useful predictor of time-averaged stresses, other state variables may be more suitable for predicting instantaneous stresses. This quality has been observed previously with the coordination number \( Z(t) \), for example, which was shown to exhibit a one-to-one correspondence with \( p(t) \) in the quasistatic regime \[29\]. Indeed, we observe that \( p(t) \) and \( Z(t) \) exhibit the same qualitative evolution in time (Figure 2.3c) and a similar \( \phi \)-dependence in their fluctuations (Figure 2.3d). Here we define \( Z(t) \equiv 2N_c(t)/N \) for \( N_c \) contacts occurring in the \( N \)-particle assembly. The \( p(t)-Z(t) \) relationship suggests that the critical point is better defined by some critical coordination number \( Z_c \). However, because our goal is the construction of a steady-state rheological model, it is convenient to ignore all dynamics and assume that \( Z_c \) and \( \phi_c \) correspond to the same conditions. We therefore proceed with \( \phi_c \) as the definition of the critical point for our model.

In addition to being a function of \( \mu \), the critical point has also been proposed to change with the restitution coefficient \( e \) \[50\], and such a \( \phi_c(e) \) has been used in a kinetic theory for frictional particles \[51\]. However, our DEM results do not support this conclusion, especially for frictional particles. As seen in Figure 2.4a-b for \( \mu = 0.5 \) and \( \mu = 0.1 \), the spike in the pressure fluctuations occurs at the same volume fraction for a given \( \mu \) regardless of the value of \( e \), suggesting that \( \phi_c = \phi_c(\mu) \) only. Even for the frictionless case (Figure 2.4c), where fluctuations tend occur over a wider range of volume fractions, there is no clear trend in the peak towards lower \( \phi \). One possible reason for the discrepancy is the methods used for determining \( \phi_c \). Because hard-sphere codes, used in Ref. \[50\], prohibit particle overlaps, they are unable to simulate sheared particle systems near or above \( \phi_c \) \[52\]. This shortcoming limits the performable simulations to one side of \( \phi_c \), thus requiring the critical point to be
Figure 2.3: Characteristics of the critical point for $\mu = 0.5$ and $\dot{\gamma} = 3.2 \times 10^{-5}$. (a) Pressure fluctuations in time are observed to become larger near the critical point. (b) The standard deviation of pressure, scaled by the mean pressure, exhibits a spike at $\phi_c$. (c-d) The coordination number fluctuations are similar to those of the pressure in terms of both dynamics and $\phi$-dependence.
Figure 2.4: Effect of changing the restitution coefficient on the pressure fluctuations for $\dot{\gamma} = 3.2 \times 10^{-5}$. Dotted lines demarcate the critical point $\phi_c$. For (a) $\mu = 0.5$ and (b) $\mu = 0.1$, the location of the spike in pressure fluctuations is independent of $\epsilon$. (c) Even for the frictionless case, there is little evidence to suggest $\phi_c = \phi_c(\epsilon)$.

estimated via extrapolation. Furthermore, while hard-sphere methods treat collisions as binary interactions, entrance into the quasistatic regime coincides with the development of multi-body interactions that persist even in the hard-sphere limit [53]. This conflict may render even-driven algorithms less accurate at resolving collisions upon approaching $\phi_c$ and perhaps result in an erroneous estimation of the value of $\phi_c$. Soft-sphere DEM, on the other hand, enables us to resolve multi-body contacts and simulate shear flows at any volume fraction on either side of $\phi_c$, thereby allowing us to interpolate the value of $\phi_c$. For these reasons, we expect the latter approach to provide more accurate $\phi_c$ estimates.
2.5 Pressure scalings and regime blending

It has been demonstrated in experimental [26] and computational [22–24] studies of frictionless particles that stress data will collapse onto two curves (one above $\phi_c$ and one below) upon scaling the stresses and shear rate by powers of $|\phi - \phi_c|$, the distance to jamming. This idea is consistent with several models of the radial distribution function, used in kinetic theories for the inertial regime, that diverge at close packing [54–56]. Such a collapse can be achieved for frictional particles as well, as shown in Figure 2.5, with

$$p^* = p / |\phi - \phi_c|^a \quad \dot{\gamma}^* = \dot{\gamma} / |\phi - \phi_c|^b$$

and constitutive exponents $a$ and $b$. This result for frictional disks was also found independently in Ref. [28]. From the collapse it is clear that an asymptotic power-law relationship between stress and shear rate exists for each flow regime $j$, and we can write the form of each asymptote as

$$p_j / |\phi - \phi_c|^a \sim \left( |\phi - \phi_c|^b \right)^{m_j}$$

where $m_{QS} = 0$, $m_{\text{Inert}} = 2$, and $m_{\text{Int}} = m^*$. The exponents $a$ and $b$ can be fitted from the DEM data, but the values are sensitive to the choice of $\phi_c$ used [23] and hence should be chosen with care. Our inertial regime data suggest that $p_{\text{Inert}} \sim |\phi - \phi_c|^{-2}$, which is consistent with previous results [8]; quasistatic regime data reveal that $p_{QS} \sim |\phi - \phi_c|^{2/3}$; and, as noted earlier, $p_{\text{Int}} \sim |\phi - \phi_c|^{0}$. These trends lead us to set $a = 2/3$, $b = 4/3$, and $m^* = 1/2$. The $m^*$ value is consistent with our fits of the intermediate asymptote (Table 2.1) and with experimental results [26, 43], and it is similar to other values proposed for frictionless particles using the linear spring-dashpot model [22, 23]. The value of $a$ used in Ref. [29] ($a = 1$), though different, still yields a decent collapse. However, in that work, $\phi_c$ is determined by extrapolation from the quasistatic regime, while here we interpolate it
from quasistatic and inertial regime data and furthermore verify it with stress fluctuation data, as described in Section 2.4; hence we believe our current $\phi_c$ values and the resulting $a$ value to be more accurate. We also point out that the above scaling exponents depend on the contact model used [22, 57]. Based on a small set of simple shear simulations with a Hertzian contact model, we observe the values of $a \approx 1$ and $m^* \approx 3/4$ to be larger than in the LSD case by a factor of $3/2$, which is consistent with previous results for static, jammed systems [44]. The value of $b$, however, remains the same for both contact models; note that in both cases $a = bm^*$ in order to satisfy the functional forms implied by the collapse. The resulting collapse for the Hertzian particles is shown in Figure 2.6.

Though the individual regime limits can be described using Eq. 2.5, the transitions between them have yet to be modeled. To this end, we employ a blending function $B$ of the form

$$B(y_1, y_2) = (y_1^w + y_2^w)^{1/w}$$

with $w > 0$ yielding an additive blend for the quasistatic-to-intermediate transition and $w < 0$ providing a harmonic blend for the inertial-to-intermediate transition. Figure 2.5 demonstrates the use of Eq. 2.6 with the asymptotic forms of Eq. 2.5 and $w = \pm 1$. The blended model is able to capture the pressure behavior continuously in shear rate for all three regime limits as well as the transitions; moreover, it does so without defining the stresses in piecewise fashion over arbitrary shear rate domains. Notably, it also predicts the narrowing intermediate window around $\phi = \phi_c$ in the limit of zero shear rate, as the quasistatic and inertial contributions to the stress become small near the jamming point. The general form of the pressure model based on the Hookean-case results can hence be written as

$$p = \begin{cases} p_{QS} + p_{Int} & \text{for } \phi \geq \phi_c \\ (p_{\text{Inert}}^{-1} + p_{\text{Int}}^{-1})^{-1} & \text{for } \phi < \phi_c \end{cases}$$

(2.7)
Figure 2.5: Collapse of pressure vs. shear rate curves from Figure 2.1 for (a) $\mu = 0.5$ and (b) $\mu = 0.1$. In both cases, the pressure is scaled as $p^* = p/|\phi - \phi_c|^{2/3}$ and the shear rate as $\dot{\gamma}^* = \dot{\gamma}/|\phi - \phi_c|^{4/3}$. A simple blending function (solid lines) captures regime asymptotes and transitions.
Figure 2.6: Collapse of pressure vs. shear rate curves for Hertzian particles with $\mu = 0.5$. The volume fractions (and legend) are the same as from Figure 2.1(a). Here, $p^* = p/|\phi - \phi_c|$, $\dot{\gamma}^* = \dot{\gamma}/|\phi - \phi_c|^{4/3}$, and $m^* \approx 3/4$. Regime asymptotes and transitions are captured by the same blending function (solid lines) as in the Hookean case.

with the individual regime contributions defined as

\[ p_{QS}d/k = \alpha_{QS}|\phi - \phi_c|^{2/3} \]  \hspace{1cm} (2.8)
\[ p_{\text{Int}}d/k = \alpha_{\text{Int}}\dot{\gamma}^{1/2} \]  \hspace{1cm} (2.9)
\[ p_{\text{Inert}}d/k = \alpha_{\text{Inert}}\dot{\gamma}^2 \]  \hspace{1cm} (2.10)

The pressure at $\phi = \phi_c$ can be calculated using either blend, since Eqs. 2.8 and 2.10 yield $p_{QS}(\phi = \phi_c) = 0$ and $p_{\text{Inert}}(\phi = \phi_c) = \infty$, which both yield $p = p_{\text{Int}}$ upon substitution into Eq. 2.7; this case is included with the quasistatic blending solely for the sake of simplicity. The constitutive parameter $\alpha_{QS}$ is a function of $\mu$, while $\alpha_{\text{Inert}}$ and $\alpha_{\text{Int}}$ are fairly $\mu$-independent. These and other model constants are given in Table 2.2.

There are a few features of Eqs. 2.7-2.10 that are worth noting. Firstly, for systems above the critical volume fraction, the blending function yields a model of Herschel-Bulkley form, which has been shown previously to capture the shear stress of soft-sphere systems [26, 43].
Table 2.2: Values of model constants

<table>
<thead>
<tr>
<th>( \mu )-dependent parameters</th>
<th>0.0</th>
<th>0.1</th>
<th>0.3</th>
<th>0.5</th>
<th>1.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \eta_s )</td>
<td>0.105</td>
<td>0.268</td>
<td>0.357</td>
<td>0.382</td>
<td>0.405</td>
</tr>
<tr>
<td>( \alpha_{QS} )</td>
<td>0.095</td>
<td>0.083</td>
<td>0.14</td>
<td>0.20</td>
<td>0.25</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( \mu )-independent parameters</th>
<th>( \alpha_{\text{Inert}} )</th>
<th>( \alpha_{\text{Int}} )</th>
<th>( I_0 )</th>
<th>( \alpha_1 )</th>
<th>( \beta_1 )</th>
<th>( \hat{\gamma}_0 )</th>
<th>( \alpha_2 )</th>
<th>( \beta_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.021</td>
<td>0.099</td>
<td>0.32</td>
<td>0.37</td>
<td>1.5</td>
<td>0.1</td>
<td>0.2</td>
<td>1.0</td>
<td></td>
</tr>
</tbody>
</table>

Additionally, the individual regime contributions are consistent with some known scalings. For example, the quasistatic pressure is proportional to the particle stiffness [29], while
\[ p_{\text{Inert}} = \alpha_{\text{Inert}} \rho_s (\dot{\gamma}_d)^2 / (\phi - \phi_c)^2 \]
rightly exhibits no dependence on \( k \) [5, 7, 38, 40]. Finally, the viability of the \( \phi \)-scaling in Eq. 2.10 for all \( \mu \) values suggests that the \( \phi_c = \phi_c(\mu) \) formulation could be a simple but effective step in improving current kinetic theory models.

2.6 Dimensionless groups and stress ratio model

It is possible to construct an analogous model for the shear stress as for the pressure, as previous works have shown \( \tau \) to exhibit similar scalings with respect to the distance to jamming [22, 23, 25]. However, because \( \tau \) and \( p \) both vary over several orders of magnitude, fitting them directly can result in poor predictions of their ratio, i.e. the shear stress ratio
\[ \eta \equiv \tau / p, \]
which varies over a much narrower range. For this reason, we choose to construct a model for \( \eta \) and then express the shear stress as \( \tau = \eta p \).

Some recent, successful rheological models for dense granular flows employ a dimensionless parameter called the inertial number as the basis for achieving stress collapses over a range of volume fractions and shear rates [8, 30, 31]. This inertial number
\[ I \equiv \dot{\gamma}_d / \sqrt{p / \rho_s} \]
is a ratio of the timescales of shear deformation and particle rearrangement, and the physics of granular flows of hard particles is said to be determined by the competition of these two mechanisms. When the particles have a finite stiffness, however, the binary collision time is nonzero and therefore presents yet another important timescale. With this point in mind,
we note that the dimensionless shear rate $\dot{\gamma}$ identified earlier is in fact the ratio of the binary collision time to the macroscopic deformation time [19], and we show here that it can be used along with the inertial number to characterize soft particle rheology.

In Figure 2.7 we plot the stress ratio versus the inertial number for $\mu = 0.5$. For the densest systems, i.e. for low $I$, $\eta$ exhibits a constant-value asymptote that we identify as the yield stress ratio $\eta_s = \eta_s(\mu)$; values of $\eta_s$ for different cases of $\mu$ are presented in Table 2.2. As $I$ increases, $\eta$ then also increases. These same observations were made in previous studies of particles in the infinitely-hard limit [8, 30, 31]. However, unlike in these works, we also observe significant scatter as $I$ becomes larger, which we will now show to be a consequence of the particle softness.

Because the inertial number models are designed for hard particles, we first limit our analysis to cases in which particle softness has little effect, i.e. for small $\dot{\gamma}$. Indeed, quasistatic and inertial regime data of $\eta$ versus $I$ from our DEM simulations collapse onto a single curve, with the quasistatic regime occurring for $I \lesssim 10^{-2}$ and inertial regimes occurring for $I \gtrsim 10^{-2}$. This collapse is seen in the inset of Figure 2.7a for $\mu = 0.5$. We model this curve as

$$
\eta_{\text{hard}}(I) = \eta_s(\mu) + \frac{\alpha_1}{(I_0/I)^{\beta_1} + 1}, \quad (2.11)
$$

where $I_0$, $\alpha_1$, and $\beta_1$ are parameters dictating the transition from quasistatic to inertial flow. This form is similar to that of Jop et al. [31]. Interestingly, the increase of $\eta$ from $\eta_s$ is nearly identical for all cases of $\mu \geq 0.1$ (Fig. 2.7b). Since the interparticle friction coefficient for most real granular materials falls in this range, we conveniently take one set of constitutive parameter values as suitable averages for our model; these values are presented in Table 2.2.

The form of $\eta_{\text{hard}}$ presented in Eq. 2.11 is not the only viable option. Another possibility is a simple power law, which can be written as $\eta_{\text{hard}}(I) = \eta_s + \alpha'_1 I^{\beta'_1}$. This form has been used previously by da Cruz and coworkers [8] with $\beta'_1 = 1$. A comparison between this form,
with $\beta'_1 = 1$ and $\alpha'_1 = 0.6$, and the one in Eq. 2.11 are shown in Figure 2.7b. The two models agree closely for all values of $I \lesssim 0.3$, with a departure occurring for larger $I$. However, with the inertial number models, we need to be concerned only with volume fractions greater than the freezing transition $\phi_f = 0.49$ [54], where traditional kinetic theories fail [51, 58]. At $\phi_f$, the kinetic theory of Garzó and Dufty [38] predicts $I = 0.83$, which is consistent with our DEM results and beyond which we can ignore disparities in the $\eta_{\text{hard}}$ predictions between the two models. Hence, though we continue with Eq. 2.11, we view both forms as being acceptable.

Though Eq. 2.11 captures low-$\hat{\gamma}$ behavior well, inclusion of higher-$\hat{\gamma}$ cases reveals a noticeable departure from the $\eta_{\text{hard}}(I)$ curve, as seen in Figure 2.7. Specifically, for a given value of $I$, the value of $\eta$ from an intermediate-regime flow is consistently lower than that given by the Eq. 2.11. This deviation is a consequence of particle softness and, in the context of our regime blending, grows in magnitude with the intermediate-regime contribution to the pressure. Figure 2.8a shows the connection between the magnitude of this departure $\eta_{\text{soft}} \equiv \eta_{\text{hard}} - \eta$ and $\hat{\gamma}$. This softness effect, similarly to $\eta_{\text{hard}}$, can be modeled as

$$\eta_{\text{soft}}(\hat{\gamma}) = \frac{\alpha_2}{(\hat{\gamma}_0/\hat{\gamma})^{\beta_2} + 1}, \quad (2.12)$$

where $\hat{\gamma}_0 = 0.1$, $\alpha_2 = 0.2$, and $\beta_2 = 1$ are constants describing the transition to intermediate flow. Finally, we can write

$$\eta(I, \hat{\gamma}) = \eta_{\text{hard}}(I) - \eta_{\text{soft}}(\hat{\gamma}), \quad (2.13)$$

and, by plotting $\eta^* \equiv \eta - \eta_s + \eta_{\text{soft}}$ vs. $I$ as in Figure 2.8b, we arrive at a collapse of the stress ratio data from all three regimes.
Figure 2.7: Behavior of the shear stress ratio with respect to inertial number. (a) Significant scatter is observed when data from all three regimes are included. Data are shown for $\mu = 0.5$ (see legend in Figure 2.1a). Inset: A good collapse is achieved, however, for cases in which $\dot{\gamma} \leq 3.2 \times 10^{-5}$. These cases correspond essentially to the quasistatic ($I \lesssim 10^{-2}$) and inertial regimes ($I \gtrsim 10^{-2}$) and are also indicated with a best-fit line (Eq. 2.11) in the main figure. Intermediate regime data lie below this line. (b) The increase in the stress ratio from the yield stress ratio for these small-$\dot{\gamma}$ cases collapses for $\mu \geq 0.1$. Eq. 2.11 captures these data well (solid line), as does the model of da Cruz et al. [8] for $I \lesssim 0.3$ (dashed line).
Figure 2.8: Shear stress ratio contribution from $\hat{\gamma}$ for all values of $\hat{\gamma}$ and $\mu \geq 0.1$. (a) The softness-induced departure $\eta_{\text{soft}}$ of the stress ratio from its hard-particle limit is essentially a function of only $\hat{\gamma}$. (b) The correction for particle softness yields a collapse of the data in all three regimes.
2.7 Generalized continuum model

Our rheological model therefore consists of Eqs. 2.7 - 2.10 for the pressure and Eqs. 2.11 - 2.13 for the shear stress ratio. Though the collapses can generally be improved by allowing the fitting parameters to be functions of $\mu$ rather than constants, the fits are nevertheless fairly good and hence justify the use of simpler forms.

While this model was developed for simple shear flows, it can be recast to handle general deformation types as done in Ref. [29]. First, we note that the strain rate tensor for simple shear flows is $D = \frac{1}{2} \dot{\gamma}(e_x e_z + e_z e_x)$ where $e_i$ are the unit vectors in the $i$ direction. This expression can be rearranged to yield

$$\dot{\gamma} = 2|D|, \quad (2.14)$$

where $|D| = \sqrt{\frac{1}{2} D^T : D}$ is the modulus of $D$, and $D$ is taken to correspond to general deformation types. Finally, we write the stress tensor as

$$\sigma = p(I - \eta \hat{S}) \quad (2.15)$$

where $p$ and $\eta$ are given by our model, $I$ is the identity tensor, and $\hat{S} = S/|D|$ with $S = D - \frac{1}{3} \text{tr}(D)$. Eqs. 2.14 and 2.15 allow our rheological model to handle flows in more complex geometries as are commonly found in real flow scenarios.

2.8 Normal stress differences†

The rheological model presented above describes the mean normal stress $p$ but does not address the issue of normal stress differences (NSDs), which have been observed in granular flows [59–62] and which are suspected to have important rheological consequences for these flows as they do for non-Newtonian liquids [63]. In the simulations we have performed,

†This section was not included in the original publication in Phys. Rev. E [39].
all three normal stress components have been measured, and hence we can make similar attempts to constitute the NSDs across the different flow regimes.

In Figure 2.9, the individual normal stresses $\sigma_{xx}$, $\sigma_{yy}$, and $\sigma_{zz}$ are scaled by the pressure

$$p = \frac{1}{3}(\sigma_{xx} + \sigma_{yy} + \sigma_{zz}),$$ (2.16)

and are plotted against stiffness-scaled shear rate $\dot{\gamma}$ for several volume fractions $\phi$ and an interparticle friction coefficient $\mu = 0.5$. These stress ratios correspond to the velocity, vorticity, and gradient directions, respectively. At low-to-medium shear rates, which correspond to the quasistatic regime for $\phi > \phi_c$ and to the inertial regime for $\phi < \phi_c$, the normal stress ratios exhibit little discernible dependence on the shear rate. That is, the individual normal stress components themselves display the same shear-rate scalings as the mean normal stress in both of these regimes. Their volume-fraction dependence, on the other hand, is substantial in the inertial regime and mostly disappears in the quasistatic regime. As shear rate increases, the curves for all volume fractions tend to converge to an intermediate asymptote exhibiting little $\phi$-dependence. Unfortunately, we are limited in our ability to analyze this asymptote, as we cannot perform simulations at very high shear rates due to unrealistically large particle overlaps. Furthermore, $\sigma_{ii}$ changes by at most about $0.05p$ as shear rate is varied over several decades, with most of the change occurring for shear rates much larger than those likely to be seen in flow scenarios of practical interest. For these reasons, we choose to neglect the rate-dependent behavior of the normal stress ratios and instead approximate them and the differences between them on the basis of their behavior at low shear rates. DEM data at high shear rates are presented nonetheless for reference.

Figure 2.10 presents the normal stress differences

$$N_1 = \sigma_{xx} - \sigma_{zz}$$ (2.17)
Figure 2.9: Normal stress components in the (a) flow, (b) vorticity, and (c) gradient directions for $\mu = 0.5$. 
Table 2.3: Critical volume fraction estimates for different cases of the interparticle friction coefficient $\mu$.

<table>
<thead>
<tr>
<th>$\mu$</th>
<th>$\phi_c$</th>
<th>$\phi^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.613</td>
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</tr>
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</tr>
</tbody>
</table>

and

$$N_2 = \sigma_{zz} - \sigma_{yy},$$

(2.18)

scaled by pressure, versus the scaled shear rate for $\mu = 0.5$, and from these data two qualitative trends emerge. Firstly, $N_1/p$ is positive at low volume fractions and negative at high volume fractions; and secondly, $N_2/p$ is a decreasing function of $\phi$ for low $\phi$ but an increasing one at high $\phi$. To look at these transitions more closely, we next plot the two scaled normal stress differences versus volume fraction for shear rates in the rate-independent regime, as seen in Figure 2.11. From Figure 2.11(a), it becomes clear that the sign change in $N_1/p$ occurs at volume fraction $\phi^*$ that is distinctly lower than the known jamming point $\phi_c$. This phenomenon has been observed in prior studies of both smooth hard disks [59] and frictional soft spheres [60]. It has been shown furthermore that $\phi^*$ varies with the particle coefficients of friction [60] and restitution [59, 60]. We too find a dependence of $\phi^*$ on $\mu$, though simulations for more volume fractions below $\phi^*$ are needed to pinpoint the transition precisely. Estimated values of $\phi^*$ and the corresponding values of $\phi_c$ for different $\mu$ are presented in Table 2.3. For $N_2/p$, we observe that the minimum occurs at about $\phi_c$ and varies linearly with $\phi$ on each side of the transition, though with a slightly different slope.

On the basis of the above results, we propose to constitute the normal stress differences as

$$N_1/p = \alpha_1(\phi - \phi^*)$$

(2.19)
Figure 2.10: (a) First and (b) second normal stress differences, scaled by pressure, versus scaled shear rate for $\mu = 0.5$. 

\begin{align*} 
\dot{\gamma} d / \sqrt{k / (\rho_s d)} & \quad \text{versus} \quad \frac{N_1}{p} \\
\dot{\gamma} d / \sqrt{k / (\rho_s d)} & \quad \text{versus} \quad \frac{N_2}{p} 
\end{align*}
and

\[ N_2/p = \begin{cases} 
\alpha_2(\phi - \phi_c) + \beta & \text{for } \phi \geq \phi_c \\
\alpha_3(\phi - \phi_c) + \beta & \text{for } \phi < \phi_c
\end{cases} \]  

(2.20)

where \( \alpha_i \) and \( \beta \) are in general a function of \( \mu \); for \( \mu = 0.5 \) we set \( \alpha_1 = -1.5, \alpha_2 = 0.67, \alpha_3 = -1.28, \) and \( \beta = 0.14. \) Individual stress components can then be calculated from the pressure and normal stress differences as

\[ \sigma_{xx} = p + \frac{2}{3}N_1 + \frac{1}{3}N_2 \]  

(2.21)

\[ \sigma_{yy} = p - \frac{1}{3}N_1 - \frac{2}{3}N_2 \]  

(2.22)

\[ \sigma_{zz} = p - \frac{1}{3}N_1 + \frac{1}{3}N_2. \]  

(2.23)

2.9 Implementation and testing of the rheological model in a continuum-model solver†

Lastly, we implement the proposed rheological model (neglecting NSDs) into the continuum-

†This section was not included in the original publication in *Phys. Rev. E* [39].
Table 2.4: Parameter values used in the hourglass test problem.

<table>
<thead>
<tr>
<th>Vessel height</th>
<th>Vessel width</th>
<th>Mouth width</th>
<th>Mesh size</th>
</tr>
</thead>
<tbody>
<tr>
<td>40 cm</td>
<td>20 cm</td>
<td>5 cm</td>
<td>0.5 cm</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Gas viscosity</th>
<th>Gas density</th>
<th>Particle density</th>
<th>Particle diameter</th>
<th>Particle stiffness</th>
<th>Friction coefficient</th>
<th>Restitution coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>18 $\mu$Pa·s</td>
<td>1.2 kg/m$^3$</td>
<td>2450 kg/m$^3$</td>
<td>0.53 mm</td>
<td>$10^6$ N/m</td>
<td>0.5</td>
<td>0.7</td>
</tr>
</tbody>
</table>

model solver MFIX and test its performance on the two-dimensional problem of flow in an hourglass, a common type of hopper. For this continuum-model simulation, the equations in Table 1.1 are discretized and solved on a 0.5-cm square mesh; the hourglass dimensions and physical properties are summarized in Table 2.4. The gas phase is considered, and the resulting drag force is described by the expression of Syamlal and O’Brien [10]. In addition, no-slip boundary conditions are used for both gas and solids. Finally, we also compare the predictions of the proposed model with those of MFIX’s default model, a frictional-kinetic model (as discussed in Chapter 1) that additively blends the plasticity model of Schaeffer [6] with the kinetic-theory model of Lun et al. [5]. This model solves a balance equation for granular fluctuation energy and as such offers the added benefits of including nonlocal effects, a feature missing from the proposed model formulation; however, it also does not conform to the regime map presented in Figure 1.2 and hence may be expected to predict poorly some qualitative behaviors of dense flows. The extent to which each of these features is important for this flow problem will be seen presently.

Beginning from an initial plug state (Fig. 2.12a) with solids volume fraction $\phi = 0.586$ (just below the critical volume fraction $\phi_c = 0.587$ for $\mu = 0.5$), the flow is observed to evolve differently using the two models. Notably, the new rheological model predicts ratholing (i.e. persistent core flow) in the upper chamber of the hourglass as well as the formation of a sandpile on the hourglass floor, both of which are consistent with experimental observations [64]. These flow predictions are a direct result of the model’s treatment of the regime
interfaces via the scalings of the stresses with respect to shear rate and volume fraction —
specifically, the rapid rise of the stresses in the limits of close packing and of zero shear rate. On the other hand, the kinetic-theory model predicts an unusual bubble formation above the orifice that one would not expect for such a dense flow and also fails to predict pile formation. While the coarseness of the mesh may reduce the quantitative accuracy of the predictions as a result of failure to predict cluster formation adequately [1], it would be insufficient to produce such qualitatively different behavior. Hence, the observed differences in the predictions can reliably be attributed to the differences in the model formulations. Furthermore, recent work by Schneiderbauer and coworkers [65] has shown that the proposed model, when combined with a kinetic-theory model for the dilute regime, predicts hopper discharge rates consistent with the Beverloo correlation [66], in contrast to the predictions of another frictional-kinetic model [67]. These results demonstrate the ability of the proposed rheological model to improve flow predictions in practical applications of dense granular flows.

2.10 Summary

We have investigated shear flows of dense frictional granular materials in all three flow regimes in order to gain a better understanding of the scalings within each regime and the transitions between them. We find scaling relations for the pressure with respect to both shear rate and the distance to the jamming point and, for the intermediate regime, observe identical power-law behavior for particles with different friction coefficients. Furthermore, we propose a simple blending function for patching each regime’s asymptotic form in order to predict pressure in between regimes. Finally, we decompose the shear stress ratio into contributions from two dimensionless shear rates, enabling us to quantify the effect of particle softness. These findings establish a framework for a global model for steady-state simple shear flows of dense granular matter.
Figure 2.12: Snapshots of solids fraction from gas-solid flow in an hourglass. Beginning from an initial state (a), a comparison is made between the predictions of the proposed rheological model (b-c) and MFIX’s default frictional-kinetic model [5, 6] (d-e). The new model predicts ratholing (core flow) in the upper chamber and pile formation on the hourglass floor, both in agreement with experimental observation [64]. The default model produces anomalous bubbles above the orifice and an even layer on the floor.
Chapter 3

Modified kinetic theory for dense and dilute granular flows

This chapter contains work that is published as “A modified kinetic theory for frictional granular ows in dense and dilute regimes” by Chialvo and Sundaresan in Physics of Fluids 25, 070603 (2013), which corresponds to Ref. [68].
Overview of the Chapter

Continuum modeling of granular and gas-solid flows generally involves the use of a kinetic-theory (KT) model for the particulate phase, and the most widely used KT models have been derived for dilute flows of smooth, frictionless spheres. In reality, however, granular particles are frictional and can achieve dense packing, and these features must be taken into account to improve rheological predictions in these flow scenarios. Existing approaches in the literature for producing closed-form KT-based models employ empirical modifications to adapt the original models for use in dense and frictional systems. In this article, we investigate the capacity for such modifications to improve the rheological predictions of the Garzó-Dufty (GD) KT model [V. Garzo and J. W. Dufty, “Dense fluid transport for inelastic hard spheres,” Phys. Rev. E 59, 5895-5911 (1999)]. On the basis of molecular dynamics simulations of homogeneous, simple shear flows of soft, frictional spheres, we propose a new expression for the radial distribution function at contact as well as modifications to the GD expressions for shear stress and energy dissipation rate. These changes account for dense-regime scalings observed in inertial-number models as well as the effects of interparticle friction while preserving the dynamic nature of the KT model.

3.1 Introduction

Granular rheology has been a commonly studied topic for many years owing in part to the diversity of behavior that granular flows exhibit. Depending on the local solids volume fraction $\phi$ and shear rate $\dot{\gamma}$, one can observe any of three distinct flow regimes [19, 21, 39]: 1) a quasi-static regime for $\phi$ exceeding the critical volume fraction $\phi_c$ in which pressure $p$ and shear stress $\tau$ are independent of shear rate; 2) an inertial regime below $\phi_c$ in which $p,\tau \sim \dot{\gamma}^2$; and 3) an intermediate regime occurring in a narrow window of volume fractions about $\phi_c$ in which $p,\tau \sim \dot{\gamma}^n$ with $0.5 \lesssim n \lesssim 1$. As particle stiffness $k \to \infty$, only the inertial regime can be observed, and, because granular particles are generally extremely hard, a large
subset of granular flows belong to the inertial regime.

Stresses in the inertial regime are typically modeled using the kinetic theory (KT) of granular gases, [5, 38, 40, 69] a class of dynamic models capable of predicting a variety of clustering behaviors. [1, 70] Development of these models involves following what we call the KT approach or KT analysis, which is the general process of evaluating the transport coefficients by moment analysis of the Boltzmann equation while making simplifying assumptions regarding the collision integral. These assumptions, which include the two-particle interaction model and the nature of the velocity distributions, will affect not only the regimes of validity for any resulting relations but also their attainability in closed form, as oftentimes the collision integral can only be evaluated numerically. The earliest and most widely used KT models have been derived for dilute flows of inelastic, smooth, frictionless spheres, [5, 38, 40, 69] though there also exist more sophisticated models that account for particle roughness by including tangential restitution and rotational degrees of freedom. [71, 72] We refer collectively to these two types of models, which consist of closed-form constitutive expressions, as traditional KT models.

Though all flows in the inertial regime are amenable to KT analysis, this regime in itself contains two ranges of volume fractions exhibiting somewhat different behavior. The first is the dilute inertial regime and encompasses volume fractions between zero and $\phi_f \approx 0.49$. In this range, traditional KT models exhibit generally good agreement with discrete particle simulations. On the other hand, for volume fractions between $\phi_f$ and $\phi_c$, which constitute the dense inertial regime, KT models are less successful, with discrepancies resulting from a few assumptions made in their derivation. For example, one typically assumes ‘molecular chaos,’ i.e. that the collisions of a particle with its neighbors are uncorrelated, allowing one to express the two-particle velocity distribution function as the product of the single-particle distribution functions (which are Gaussian). In dense flows, though, a particle will interact many times with the same neighbors [73, 74] as steric effects become predominant, thereby resulting in a non-Gaussian distribution of normal relative velocities. [75] Additionally, these
models assumes a small Péclet number $Pe \equiv \dot{\gamma}d/\sqrt{T}$, which represents the extent of departure from the equilibrium, isotropic state of an assembly of particles of diameter $d$ and with a granular temperature $T$. If $Pe << 1$, thermal forces predominate and preserve a nearly isotropic structure within the assembly. However, shear flows are distinctly nonequilibrium, as demonstrated by the emergence of prominent structural features including force chains [76] and anisotropy of the fabric of contacts, [29, 77, 78] which would not survive in a thermal system. This phenomenon arises in part because collisions between granular particles are dissipative, characterized by a restitution coefficient $e$ often not near unity that serves to increase $Pe$ by decreasing $T$. It is hence understandable that traditional KT models are unable to predict some features of the dense inertial regime, including the increase in $T$ near the critical volume fraction [79] and the saturation of the shear stress ratio $\eta \equiv \tau/p$ to its correct close-packing limit [30] $\eta_s$. Recent inertial-number models do predict the yield stress [8, 31, 39] but do not apply to dilute flows; they also do not account for important nonlocal effects [80] that KT can capture via conduction of pseudothermal energy. There is a need, therefore, for a rheological model that bridges the dense and dilute behaviors within the KT framework.

In addition to their dense-regime limitations, traditional KT models are derived assuming collisions of frictionless particles only and hence are unequipped to handle any dependence on the interparticle friction coefficient $\mu$. In reality, however, granular materials are frictional, and the value of $\mu$ has been shown to have a significant effect on stresses at least in the quasistatic regime, [29] where increasing $\mu$ generally increases the stress because of larger tangential interparticle forces arising from enduring contacts. Attempts to quantify the friction effect in the inertial regime, though, have been somewhat more limited. Many KT works have considered tangential restitution, [50, 71, 72, 75, 81] which similarly describes roughness but is nevertheless microscopically different from friction. A KT model that explicitly and accurately accounts for dependence on $\mu$ is currently lacking.

One important quantity in which friction, shearing, and large packing density all play an
important role is the radial distribution function at contact $g_0(\phi)$. Most expressions for $g_0$, in agreement with $g_0$ data extrapolated directly from equilibrium hard-sphere simulations, [54] predict its divergence at close packing, [54–56] i.e. $g_0 \sim (\phi_c - \phi)^m$ for some constant $m < 0$. However, shear simulations of discrete-particle assemblies suggest that these expressions significantly underpredict $g_0$ for systems far from equilibrium and featuring strong contact anisotropy. [79, 82] Additionally, these expressions tend to neglect the dependence of the critical volume fraction on the friction coefficient, which has been observed both in static systems [45] and sheared systems. [39] Since $\phi_c(\mu)$ determines the point at which the pressure diverges, any extension of KT to the dense regime must take this dependence into account.

Given the need for a KT model that spans dense and dilute regimes while accounting for anisotropy and interparticle friction, it is natural to attempt to revisit the KT approach without making the aforementioned inappropriate assumptions. Doing so would, in theory, yield a model applicable to a wide array of flows and particle types without the need for empirical fitting of rheological data. However, two major problems arise in this endeavor. Firstly, at the present time it does not appear possible to deduce closed-form expressions for the transport coefficients in the dense regime when employing the non-Gaussian relative velocity distribution function. [75] Because the rheological behavior of the material would need to be evaluated numerically for every given set of particle parameters, it is impractical to implement such a model into a continuum-model solver for application to large-scale flow problems. Secondly, this approach still does not avoid the need for empiricism, as the dense-regime relative velocity distribution function [75] and the radial distribution function at contact cannot yet be predicted a priori. Hence, it appears that the most promising path toward a comprehensive rheological model in the near term lies in empirical modification of existing closed-form KT models.

Indeed, such KT modifications have been proposed numerous times in the recent literature. [51, 83–85] Of particular interest are the changes proposed by Jenkins and coworkers for extending the commonly used theory of Garzó and Dufty [38] (GD), which is originally
derived for flows of frictionless, moderately dissipative spheres in the dilute regime. The first modification calls for introduction of a length scale $L$, which the authors call a ‘chain length,’ into the expression for the energy dissipation rate. [51] This length scale is said to represent the typical length of force chains that form in dense granular flows and that grow large upon approaching $\phi_c$. While the existence of a large or diverging length scale in such flows is a topic of debate, [21, 50, 86, 87] the use of such a functional form is nevertheless successful in qualitatively describing the dense-regime increase in temperature and decrease in shear stress ratio. The second modification is the replacement of the normal restitution coefficient with an “effective” restitution coefficient $e_{\text{eff}}(\mu, e) < e$ that accounts for the increased dissipation resulting from interparticle friction. [84] This substitution has been shown to improve stress predictions for dilute flows of slightly frictional particles. Modifications such as these are not only successful in improving the predictions of traditional KT models but moreover are convenient to constitute based on stress and temperature data from granular flow experiments and simulations.

In the present work, we assess the capacity for these two modifications to yield accurate model expressions by comparing their steady-state predictions for pressure, shear stress, and temperature with data obtained from discrete element method [37] (DEM) simulations of sheared particle assemblies; and, when these approaches prove insufficient, we propose additional corrections to bring the GD model predictions into closer agreement with those of the DEM simulations.

In the following sections, we present the original (GD) KT model, an explanation of our simulation methodology, and a validation of our simulations for the case of frictionless particles below $\phi_f$. We then demonstrate the stark disagreement between the GD model predictions and our DEM results above $\phi_f$ and for frictional particles at all volume fractions. Finally, we outline the steps taken to constitute various model quantities used in our modified KT expressions based on our DEM results.
3.2 Garzó–Dufty (GD) KT model

As aforementioned, the kinetic theory of choice for the modifications will be that of Garzó and Dufty, [38] which is designed for smooth, frictionless, moderately inelastic particles in the dilute regime. According to this model, for simple shear flows one can write the pressure \( p \) as

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

the shear stress \( \tau \) as

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

and the energy dissipation rate \( \Gamma \) as

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

Here, \( \rho_s \) is the solid material density, and the definitions of the dimensionless expressions \( H, J, \) and \( K \) and their components are

\[
H(\phi, e) = \phi[1 + 2(1 + e)\phi g_0],
\]

\[
J(\phi, e) = \frac{5\sqrt{\pi}}{96} \eta^*,
\]

\[
K(\phi, e) = \frac{12}{\sqrt{\pi}} \phi^2 g_0(1 - e^2),
\]

\[
\eta^* = \eta^*_k + \eta^*_c + \eta^*_b,
\]

\[
\eta^*_k = \frac{1 - \frac{2}{5}(1 + e)(1 - 3e)\phi g_0}{[1 - \frac{1}{4}(1 - e)^2 - \frac{5}{24}(1 - e^2)]g_0},
\]

\[
\eta^*_c = \frac{4}{5}(1 + e)\phi g_0 \eta^*_k,
\]

\[
\eta^*_b = \eta^*_k + \eta^*_c + \eta^*_b.
\]
and

\[ \eta^*_b = \frac{384}{25\pi}(1 + e)\phi^2 g_0. \]  

(3.10)

The quantities \( \eta^*_k \), \( \eta^*_c \), and \( \eta^*_b \) are the scaled kinetic, collisional, and bulk viscosity contributions, respectively. As per Jenkins and Berzi, [51] we have neglected here the very small contribution of all terms proportional to a quantity that Garzó and Dufty denote as \( c^*(e) \).

The radial distribution function at contact \( g_0(\phi) \) has been modeled in numerous ways, [54–56, 83, 88] but two formulations in particular have been validated by simulation data of frictionless hard spheres at equilibrium. The first of these is the Carnahan-Starling expression, [88]

\[ g_{0CS}^0 = \frac{1 - \phi/2}{(1 - \phi)^3}, \]

(3.11)

which is valid for systems below \( \phi_f \). The second is a modification to \( g_{0CS}^0 \) proposed by Torquato [54] for denser systems. Written as

\[ g_{0Torquato}^0 = \begin{cases} 
  g_{0CS}(\phi) & \text{for } \phi \leq \phi_f \\
  g_{0CS}(\phi_f)\frac{\phi_c - \phi_f}{\phi_c - \phi} & \text{for } \phi > \phi_f 
\end{cases}, \]

(3.12)

it differs from the Carnahan–Starling result only above \( \phi_f \), specifically by diverging at \( \phi_c \).

Because of its agreement with simulation data and its use in a recent KT work, [51] we will initially use Torquato’s \( g_0 \) formulation in the following section together with the GD equations for comparison with DEM results.

For steady-state simple shear flows we can write the granular energy balance as

\[ \Gamma - J_{vis} = 0 \]

(3.13)
where

\[ J_{vis} = \dot{\gamma} \tau \]  

(3.14)

is the viscous energy production rate. With this condition and Eqs. 3.2-3.3 we can solve for the GD steady-state temperature expression

\[ T_{GD}^{SS} = \left( \frac{J}{K} \right) (\dot{\gamma}d)^2. \]  

(3.15)

This result then allows us to obtain the steady-state GD pressure

\[ p_{GD}^{SS} = \left( \frac{JH}{K} \right) \rho_s (\dot{\gamma}d)^2 \]  

(3.16)

and shear stress

\[ \tau_{SS}^{GD} = \sqrt{\frac{J^3}{K}} \rho_s (\dot{\gamma}d)^2. \]  

(3.17)

Finally, the shear stress ratio \( \eta \) is found from Eqs. 3.1-3.2 to be

\[ \eta_{SS}^{GD} = \sqrt{\frac{JK}{H}}. \]  

(3.18)

We emphasize that these four expressions are valid only for simple shear flows that have reached steady state.

### 3.3 Simulation Methods

We use a package of the discrete element method [37] found in the molecular dynamics package LAMMPS [48] in order to simulate simple shear flows of discrete, uniform, spherical particles. These particles interact via a linear spring-dashpot (LSD) model, which gives the
normal and tangential forces on a particle $i$ caused by contact with a particle $j$ as

\[ F^n_{ij} = k_n \delta_{ij} n_{ij} - \gamma_n m_{eff} v^n_{ij} \]
\[ F^t_{ij} = -k_t u^t_{ij} - \gamma_t m_{eff} v^t_{ij} \]  

for overlap distance $\delta_{ij}$, particle diameter $d$, spring stiffness constants $k_n$ and $k_t$, viscous damping constants $\gamma_n$ and $\gamma_t$, effective mass $m_{eff} = m_i m_j / (m_i + m_j)$ for particle masses $m_i$ and $m_j$, relative particle velocity components $v^n_{ij}$ and $v^t_{ij}$, and elastic shear displacement $u^t_{ij}$. We choose to set $k_t / k_n = 2/7$ and $\gamma_t = 0$ as done in some previous works [39, 89] and by doing so can set $\gamma_n$ in order to produce the desired restitution coefficient according to the expression $e = \exp \left( -\gamma_n \pi / \sqrt{4 k_n / m_{eff} - \gamma_n^2} \right)$. While experiments have revealed a dependence of the restitution coefficient on the particle impact velocity, [90] a behavior captured by some nonlinear spring-dashpot models, [91] kinetic theory models assume a constant $e$ as produced by the LSD model. Hence, for ease of comparison we neglect more complex, nonlinear behavior.

Samples are prepared by placing 2000 particles on a simple cubic lattice in a periodic box, assigning random, normally distributed initial velocities to the particles, and allowing the assembly to evolve in order to lose any memory of the initial configuration. The assembly then undergoes a simple shear deformation with shear rate $\dot{\gamma}$ imposed via the Lees-Edwards boundary condition, [49] which allows for the system to remain homogeneous during the shearing process. The shearing motion proceeds until the system reaches a steady state and remains there for sufficient time to collect proper statistics as determined by the saturation of the time-averaged stresses. From the particle interaction forces and the constant box volume $V$, we can calculate the macroscopic stress tensor as

\[ \sigma = \frac{1}{V} \sum_i \left[ \frac{1}{2} \mathbf{r}_{ij} \mathbf{F}_{ij} + m_i (v^t_i)(v^t_i) \right] \],  

where $\mathbf{r}_{ij}$ is the contact vector from the center of particle $j$ to the center of particle $i$, and $v^t_i$
is the particle fluctuating velocity (i.e. its velocity relative to its mean streaming velocity). From this tensor we can calculate the ensemble-averaged pressure \( p = (\sigma_{xx} + \sigma_{yy} + \sigma_{zz})/3 \) and shear stress \( \tau = \sigma_{xz} \). Because we limit the focus of our study to inertial regime flows, i.e. flows with \( \phi < \phi_c \) and \( \dot{\gamma} \equiv \dot{\gamma} d/\sqrt{k/\rho_s d} \lesssim 10^{-3} \) [Ref. [39]], it is appropriate to scale our stress data by the quantity \( \rho_s (\dot{\gamma} d)^2 \), where \( \rho_s \) is the solid material density and \( d \) is the particle diameter; similarly we scale the temperature data by \( (\dot{\gamma} d)^2 \). We also have confirmed this Bagnold scaling by running a small set of simulations with varying values of \( k \) and observing no substantial changes in the predicted temperature or stresses.

### 3.4 Results

#### 3.4.1 Comparison of KT with DEM of frictionless particles

If the kinetic theory is to be extended to frictional and dense flows based on DEM data, we must demonstrate first that the continuum and discrete models make similar stress and temperature predictions for frictionless particle flows at low-to-moderate volume fractions. Such a comparison is shown in Fig. 3.1, with scaled pressure, shear stress ratio, and scaled temperature plotted versus volume fraction.

Indeed, as expected, the predictions of the two models display good agreement up to \( \phi \approx \phi_f \). For higher volume fractions, however, there appear three salient discrepancies: 1) the scaling of \( p \) with respect to \( \phi \), 2) the close-packed limit of the shear stress ratio, and 3) the scaling of \( T \) with respect to \( \phi \). Of course, the original kinetic theory cannot be expected, as explained earlier, to capture dense flow behavior. However, the good agreement at the low volume fractions for which the original GD model was designed validates our use of DEM for model construction.
Figure 3.1: Results from DEM simulations of steady state simple shear flows of frictionless particles. (a) Scaled pressure, (b) shear stress ratio, and (c) scaled temperature are plotted versus volume fraction for various cases of the restitution coefficient $e$. The predictions of GD kinetic theory with Torquato’s radial distribution function [54] and $\phi_c = 0.636$ are shown with solid lines. GD and DEM are in good agreement for volume fractions of $\phi \lesssim \phi_f = 0.49$ but depart above this point.
3.4.2 Comparison of KT with DEM of frictional particles

When the particles are made frictional, on the other hand, the DEM data departs markedly from the GD predictions, as seen in Fig. 3.2 for $\mu = 0.5$. In addition to its aforementioned dense-regime shortcomings, the GD model now substantially overpredicts the pressure and temperature for $\phi \lesssim \phi_f$ while also underpredicting the shear stress ratio. This behavior is unsurprising, as the GD model is not designed for such systems, and is explained by the additional source of dissipation of pseudothermal energy provided by interparticle friction during collisions between particles. [84] Additionally, the assumption that the critical volume fraction $\phi_c$ is independent of $\mu$ leads the model to predict incorrectly the location of the dense-limit pressure divergence. As expected based on its derivation, the GD model is unequipped to handle either friction or dense packing, and adaptations must be made to extend its applicability to these conditions.

Based on the discrepancies observed between the GD and DEM predictions and on previous approaches to constitutive model refinement, our strategy for modifying the kinetic theory equations will be as follows:

1. The energy dissipation $\Gamma$ (Eq. 3.3) will be modified to include 1) an effective restitution coefficient [84] $e_{\text{eff}} = e_{\text{eff}}(e, \mu)$ in the $K$ term to capture $\mu$-functionality and 2) a multiplicative correction factor $\delta_\Gamma$ related to the chain length [51] to capture dense-regime trends with respect to $\phi$.

2. A new expression will be proposed for the radial distribution function at contact $g_0$ that will diverge at close packing in a manner concordant with our DEM data and that is specifically for use in nonequilibrium systems.

3. The shear stress $\tau$ will be decomposed into a yield stress and an inertial stress, the latter of which will be similar to Eq. 3.2 except augmented with a multiplicative correction factor $\delta_\tau$ (analogous to the adjustable parameter that appears in the $\tau$ expression of some previous kinetic theories [1, 7, 69]). This factor will transition from a dilute-
Figure 3.2: Results from DEM simulations of steady state simple shear flows of frictional particles with $\mu = 0.5$. (a) Scaled pressure, (b) shear stress ratio, and (c) scaled temperature are plotted versus volume fraction for various cases of the restitution coefficient $e$. The predictions of GD kinetic theory with Torquato’s radial distribution function [54] and $\phi_c = 0.636$ are shown with solid lines. GD and DEM are in very poor agreement, even for the dilute regime.
regime limit of $\delta^\text{dil}$ that accounts for $\mu$-functionality at low $\phi$ to a dense-regime limit $\delta^\text{dense}$ that will force $\eta$ to obey an inertial-number model [8, 30, 31, 39] for $\phi \gtrsim \phi_f$.

The correction factors will be applied to the dynamic GD equations and, as a result, will change the steady-shear GD predictions produced by imposing Eq. 3.13. The expressions chosen for these corrections, therefore, will be motivated by the steady-state values of the temperature, pressure, and shear stress calculated from our simple shear simulations.

### 3.4.3 Constituting the DEM results

**DEM temperature**

We will focus first on corrections to capture the DEM temperature. Because the behavior of the temperature is qualitatively different in the dense and dilute regimes, we will analyze each case separately. In the dilute regime, temperature is observed to drop upon increasing the friction coefficient from zero, and following the approach of Jenkins and Zhang [84] we seek to define an *effective* restitution coefficient that describes the total energy loss due to inelasticity and friction during an interparticle collision. To do so, we rewrite Eq. 3.15 by replacing $e$ in the $K$ term of the denominator with $e_{\text{eff}} = e_{\text{eff}}(e, \mu)$. The value of the effective restitution coefficient is then chosen to reproduce the temperature found in dilute-regime DEM simulations. Based on the DEM data, we find the expression

$$e_{\text{eff}} = e - f(\mu)$$

(3.22)

with

$$f(\mu) = \frac{3}{2} \mu \exp(-3\mu)$$

(3.23)

to provide a good fit. A comparison is made in Fig. 3.3 between this form and that derived by Jenkins and Zhang [84] for small values of $\mu$. (We note that their expression for $f$ has
Figure 3.3: The dependence of the frictional part $f(\mu)$ (Eq. 3.23) of the effective restitution coefficient $e_{\text{eff}}$ on the interparticle friction coefficient $\mu$. Our expression agrees with that of Jenkins and Zhang [84] for small values of $\mu$.

a very small dependence on $e$, which we have neglected.) For $\mu \lesssim 0.2$ the two expressions show good agreement but begin to depart thereafter. In particular, following our data, our expression for $f(\mu)$ decreases for larger values of the friction coefficient, seeming to predict lower dissipation for more frictional particles. This nonmonotonic dependence is consistent with the previous finding that the translational temperature reaches the same steady-state values for the zero- and infinite-friction cases. [85] We thus can write

$$T_{\text{DEM}}^{\text{dil}} = \left(\frac{J}{K'}\right) (\gamma d)^2$$

with

$$K'(\phi, e, \mu) = \frac{12}{\sqrt{\pi}} \phi^2 g_0 (1 - e_{\text{eff}}^2)$$

$$= K(\phi, e) \left(\frac{1 - e_{\text{eff}}^2}{1 - e^2}\right).$$
For volume fractions above $\phi \approx \phi_f$, an additional correction is needed to capture the increase in temperature with $\phi$ [Ref. [79]], as the original GD model predicts a monotonically decreasing temperature. Plotting the dimensionless temperature versus the distance to the critical volume fraction $\phi_c - \phi$, as in Fig. 3.4, we observe that

$$T_{\text{DE}M}^{\text{dense}} = \frac{\alpha_1 (\dot{\gamma} d)^2}{(\phi_c - \phi)^{1/2}}, \quad (3.27)$$

a power law that is robust to changes in $e$ and $\mu$. The transition in temperature between the dilute and dense regimes can be captured conveniently by

$$T_{\text{DE}M} = \max(T_{\text{DE}M}^{\text{dil}}, T_{\text{DE}M}^{\text{dense}}) \quad (3.28)$$

or equivalently

$$T_{\text{DE}M} = M(\phi, e, \mu)(\dot{\gamma} d)^2 \quad (3.29)$$

with

$$M(\phi, e, \mu) = \max \left( \frac{J}{K^2}, \frac{\alpha_1}{[\phi_c - \phi]^{1/2}} \right). \quad (3.30)$$

This form succeeds in capturing the sharp transition between the two behaviors as well as the loss of $e$-dependence observed in the close-packing limit, as seen in the comparison of Eq. 3.29 with the DEM temperature in Fig. 3.5. Moreover, it succeeds in reproducing the $e$-dependence of the volume fraction at which the dilute-to-dense crossover occurs without needing to specify this point explicitly. There is some minor quantitative disagreement in very dilute cases ($\phi \lessapprox 0.2$), but we will neglect them here and reserve this topic for the Discussion (Section 3.5).
Figure 3.4: Dense-regime temperature from DEM simulations. Symbols are the same as in Figs. 3.1-3.2. Scaled temperature versus volume fraction is shown for $\mu = 0.5$. A power law of slope $-1/2$ is observed (solid line) close to $\phi_c$, and the transition from dilute to dense behavior occurs for lower $\phi$ as $\epsilon$ decreases. The power-law fit is reasonably good for all cases of $\mu$. 
Figure 3.5: Comparison of the new steady-state temperature model with DEM results. Scaled temperature versus volume fraction is shown for (a) $\mu = 0.1$ and (b) $\mu = 0.5$. The agreement observed here between the KT and DEM predictions is substantially better than in Fig 3.2. Symbols are the same as in Figs. 3.1-3.2.
DEM pressure

With the temperature now described accurately, we turn our attention to the pressure, which depends primarily on $T$ and the contact value $g_0(\phi)$ of the radial distribution function. As demonstrated in Fig. 3.2a, the scaling of the pressure with respect to volume fraction in the dense regime observed using DEM is in disagreement with the GD model when Torquato’s $g_0$ expression [54] for frictionless spheres at equilibrium is used. Moreover, substitution of the temperature given by Eq. 3.29 into Eq. 3.1 is insufficient to resolve the disparity. In fact, based on literature results [8, 39] showing that $p \sim (\phi_c - \phi)^{-2}$ and our finding here that $T \sim (\phi_c - \phi)^{-1/2}$ in the dense regime, we would expect to see $g_0 \sim (\phi_c - \phi)^{-3/2}$. By plotting DEM results for $p/\rho_s \phi T$, which goes as $g_0$ in the dense regime, versus $\phi_c - \phi$ as in Fig. 3.6a, we indeed observe this power law quite clearly. The -3/2 power also lies in the range of exponent values measured for the collision frequency (which is proportional to $g_0$) in sheared hard-sphere systems. [50] Hence, we propose to represent $g_0$ as

$$g_0 = g_0^{CS} + \frac{\alpha_2 \phi^2}{(\phi_c(\mu) - \phi)^{3/2}}$$

with $\alpha_2 = 0.58$ for all $e$ and $\mu$. Note that we allow $\phi_c$ to vary with $\mu$ as per Chialvo et al. [39] A comparison of this form with those of Torquato and Carnahan–Starling is given in Fig. 3.7. The larger exponent in our proposed model for sheared systems (-3/2) compared with that of Torquato’s model for equilibrium systems (-1) results in a stronger divergence at close packing. This phenomenon can be explained physically by recalling that sheared systems exhibit strong orientational anisotropy of collisions. In a sheared assembly, a reference particle will experience collisions concentrated preferentially along the compression axis of shear, while in isotropic systems these collisions are distributed uniformly in all directions. This crowding of collisions into a smaller spatial window in the sheared case results in a higher effective contact value of the radial distribution function for a given packing fraction.
Using the proposed $g_0$ model along with our DEM temperature in the GD pressure equation, we are able to improve the kinetic-theory predictions of the pressure for the entire range of $\phi$ and for all $e$ and $\mu$ investigated (Fig. 3.8). As mentioned above for the temperature, there is some disagreement for $\phi \lesssim 0.2$, though the $\mu$-independence of $p/\rho_s \phi T$ indicates that improved prediction of $T$ in this range would mitigate or eliminate this error.

Because the collisional contribution to the pressure contains a factor of $(1 + e)$, one could ask whether the effective restitution coefficient should appear here as well. To address this question, we examine the behavior of $p/\rho_s \phi T$ from dilute-regime DEM simulations as the friction coefficient is varied. According to the GD model $p/\rho_s \phi T = 1 + 2(1 + e) \phi g_0$, so replacement of $e$ here with $e_{\text{eff}}$ is justified only if a $\mu$-dependence is observed. As seen in Fig. 3.6b, no such dependence is observed in the simulations, and hence we maintain the original form.

**DEM shear stress ratio**

Finally, we must attempt to capture the DEM shear stress, which, since we have now described the pressure, can be achieved by simply modeling the shear stress ratio $\eta$. Before investigating any further corrections, however, we first test whether the modifications done so far are sufficient to capture the DEM trends. In Fig. 3.9, we compare the DEM $\eta$ values with the predictions of the original GD model (Eqs. 3.1-3.2) augmented only with $e_{\text{eff}}$ from Eq. 4.27, a chain length correction that reproduces the temperature as per Eq. 3.30, and the new $g_0$ expression from Eq. 3.31. This set of corrections would involve setting $\delta_c = 1$ and is analogous to the model of Jenkins and Berzi. [51] As seen in the figure, there is somewhat of an improvement in that this modified GD model now predicts an increased in $\eta$ due to friction in the dilute regime and a decrease in $\eta$ as $\phi$ approaches $\phi_c$. However, this model continues to underpredict the effects of friction and still fails to produce a yield stress ratio at close packing. Hence, a further shear stress correction is necessary to reproduce the DEM $\eta$ results quantitatively.
Figure 3.6: Behavior of the quantity \( p/\rho_s \varphi T \) from DEM simulations in (a) the dense regime with \( \mu = 0.5 \) and (b) the dilute regime with \( e = 0.9 \). (a) The clear power-law dependence with slope \(-3/2\) (solid line) suggests that \( g_0 \sim (\phi_c - \phi)^{-3/2} \) in the dense regime, in disagreement with Torquato’s equilibrium results. [54] (b) Varying the friction coefficient \( \mu \) has no effect on this quantity in the dilute regime, indicating that \( e \) need not be replaced with \( e_{\text{eff}} \) in the pressure equation (Eq. 3.1). Similar results are obtained for other cases of \( \mu \) and \( e \).
Figure 3.7: Comparison of the $g_0$ expression proposed in Eq. 3.31 with those of Torquato [54] (Eq. 3.12) and Carnahan–Starling [88] (Eq. 3.11). The proposed and Torquato expressions are plotted for both $\mu = 0.0$ and $\mu = 0.5$, with $\phi_c$ depending on $\mu$. Both of these models approach the Carnahan–Starling model in the dilute regime, while their dense-regime behaviors differ in their scaling with respect to $(\phi_c - \phi)$.
Figure 3.8: Comparison of the new steady-state pressure model with DEM results. Scaled pressure versus volume fraction is shown for (a) $\mu = 0.1$ and (b) $\mu = 0.5$. The agreement observed here between the KT and DEM predictions is substantially better than in Fig 3.2. Symbols are the same as in Figs. 3.1-3.2.
Figure 3.9: Comparison of the DEM shear stress ratio values with the GD model modified to include only $e_{\text{eff}}$ and the new $g_0$ expression (i.e. $\delta_\tau = 1$ as per Jenkins and Berzi [51]). The agreement observed here between the modified GD and DEM predictions is somewhat better than in Fig 3.2, though the effect of friction is underestimated and a finite yield stress ratio is still not predicted. Results are shown for $\mu = 0.5$, though these trends are observed for all $\mu$. Symbols are the same as in Figs. 3.1-3.2.
The proposed $\eta$ model must not only predict the dilute- and dense-regime behaviors in the respective limits of $\phi \to 0$ and $\phi \to \phi_c$ but must also capture the transition between the two. In the case of pressure and temperature, the dilute-to-dense transitions involve changes of orders of magnitude, facilitating the bridging effort by allowing simple additive or switch models. However, the shear stress ratio varies over a much smaller range – always within the same order of magnitude – and the subtler transition will require a different bridging form.

In the dilute regime, we define $\psi(\mu, e, \phi) \equiv \eta(\mu, e, \phi) / \eta(\mu = 0, e, \phi)$ in order to quantify the departure of the shear stress ratio from the frictionless case. We then estimate a $\phi$-averaged value of $\psi$ for each case of $\mu$ and $e$, with weighting given more heavily to volume fractions between approximately between 0.2 and 0.4. The expression

$$\psi(\mu, e) = 1 + \frac{3}{10}(1 - e^2)^{-2/3}[1 - \exp(-8\mu)]$$

(3.32)

is found to provide a reasonably good fit while also satisfying some physical criteria, including the diminished influence of friction for more inelastic particles and the requirement that $\psi \to 1$ as $\mu \to 0$. The exponential $\mu$-dependence here is similar in form to that proposed for constitutive coefficients in a recent quasi-static model [29]; it also agrees with our observations that the effect of $\mu$ on $\eta$ is monotonic, unlike for $T$, and saturates quickly as $\mu$ exceeds about 0.3. The dilute shear stress ratio is then written as

$$\eta_{DEM}^{dilute} = \eta_{SS}^{GD} \psi.$$ (3.33)

In the dense regime, existing models for the shear stress ratio tend to take the form $\eta = \eta(I)$, where

$$I \equiv \frac{\dot{\gamma}d}{\sqrt{p/\rho_s}}$$

(3.34)

is the inertial number and can be interpreted as a ratio of the timescales of macroscopic shear
deformation to microscopic particle rearrangement. Though this quantity has been shown
to dictate granular rheology in the dense regime, [8, 30, 31, 39] it is not particularly useful in
colorizing dilute-regime behavior, in part because $I$ is not monotonic in $\phi$ over the entire
range of volume fractions. [58] Specifically, when evaluated using the steady-shear pressure,
$I$ approaches zero in both the dense and dilute limits, achieving a maximum around $\phi \approx 0.2$.
For this reason, we modify slightly the definition of the inertial number to

$$I' \equiv \frac{\dot{\gamma} d}{\phi \sqrt{p/\rho_s}} = I/\phi$$

(3.35)

in order to provide a monotonic $I'(\phi) \) dependence. With $I' \to 0$ representing the dense limit
and $I' \to \infty$ representing the dilute limit, we now can model the transition from dense to
dilute behavior using a function of $I'$.

Conveniently, the original GD expression for the shear stress ratio can be expressed in
terms of this inertial number. By combining Eqs. 3.1-3.2, we obtain

$$\eta_{GD} = \beta_{GD}(\phi) I'$$

(3.36)

with $\beta_{GD}(\phi) \equiv \phi J/\sqrt{H}$. Similarly, our DEM $\eta$ from Eq. 3.33 along with the DEM temper-
ature from Eq. 3.29 yields

$$\eta_{DEM}^{\text{dilute}} = \beta(\phi) I'$$

(3.37)

with

$$\beta(\phi) \equiv \phi \psi J \sqrt{K/K' H}.$$  

(3.38)

These expressions look similar in form to the dense-regime inertial-number model proposed
except that the latter contains a constant yield stress ratio $\eta_s$ added to the linear term. To obtain a comprehensive expression for $\eta$, we therefore can proceed with a linear dependence on the inertial number and simply allow its prefactor to transition between dense and dilute expressions. We propose to achieve this transition using a blending function

$$B(\alpha, \beta) = \alpha + (\beta - \alpha) \chi(I')$$  \hspace{1cm} (3.40)

defined in terms of a quantity $\chi(I')$ that transitions from zero to unity according to

$$\chi(I') = \frac{1}{(I_0/I')^{1.5} + 1}.$$  \hspace{1cm} (3.41)

The forms of $B$ and $\chi$ are motivated by the $\eta(I)$ models of Jop et al. [31] and Chialvo et al., [39] though the 1.5-power from the latter is chosen because a power greater than unity is needed to achieve a complete $\alpha$-to-$\beta$ transition. We then propose to write the shear stress ratio as

$$\eta_{DEM} = \eta_s(\mu) \chi_s + B(\alpha, \beta) I',$$  \hspace{1cm} (3.42)

with

$$\chi_s = 1 - \chi.$$  \hspace{1cm} (3.43)

so that, as volume fraction decreases, the contributions of $\eta_s$ and $\alpha$ disappear commensurately. A comparison between this steady-state $\eta$ model and the DEM results is shown in Fig. 3.10. As with the temperature and pressure, the fit for $\eta$ is best for $\phi \gtrsim 0.2$. Addi-
tionally, though we find a small dependence of $\alpha$ on $\mu$ near $\mu = 0$, $\alpha$ is nearly constant with respect to $\mu$ for $\mu \gtrsim 0.1$; since most practical systems feature particles with friction coefficients in this range, we hence will assume $\alpha$ to be constant as in Ref. [39].

### 3.4.4 Modified dynamic equations

Having now captured the steady-shear DEM results of $T$, $p$, and $\eta$, we can now use these updated expressions to define correction factors to the dynamic GD equations. First, the pressure equation remains unchanged from Eq. 3.1 except that $g_0$ is given by Eq. 3.31. Next we write the new shear stress expression as the sum of a yield stress and an inertial stress, i.e.

$$\tau = \tau_s + \tau_{\text{inertial}}$$  \hspace{1cm} (3.44)

with

$$\tau_s = \eta_s \chi_s p$$  \hspace{1cm} (3.45)

and

$$\tau_{\text{inertial}} = B(\alpha, \beta) I' p.$$  \hspace{1cm} (3.46)

We also stipulate that only the inertial part $\tau_{\text{inertial}}$ will contribute to the viscous energy production rate – that is,

$$J_{\text{vis}} = \tau_{\text{inertial}} \dot{\gamma}.$$  \hspace{1cm} (3.47)

This decomposition, though not necessary to predict a minimum flow angle in KT-type models, [81] is advantageous because it reproduces the observed dense-regime $\eta$ behavior while
Figure 3.10: Comparison of the new steady-state shear stress ratio model with DEM results. Shear stress ratio versus volume fraction is shown for (a) $\mu = 0.1$ and (b) $\mu = 0.5$. The agreement observed here between the KT and DEM predictions is substantially better than in Fig 3.2. Symbols are the same as in Figs. 3.1-3.2.
also leaving open the possibility for $\eta_s$ to be a function of microstructural variables (e.g. coordination number and fabric tensor [29]) that become rheologically important in close-packed systems and that could evolve independently of the KT equations; it also maintains the linear term in $I'$ that naturally arises from the original GD model. As aforementioned, we can write $\tau_{\text{inertial}}$ alternatively as the GD expression for $\tau$ modified with a correction factor, i.e.

$$\tau_{\text{inertial}} = \tau_{\text{GD}} \delta_\tau$$

with $\tau_{\text{GD}}$ given by Eq. 3.2 and

$$\delta_\tau = \frac{\alpha}{\beta} + \left[ 1 - \frac{\alpha}{\beta} \right] \chi.$$  

Finally, the new energy dissipation rate expression is written as

$$\Gamma = \frac{\rho_s}{d} K'(\phi, e, \mu) T^{3/2} \delta_\Gamma.$$  

By solving the steady-state condition in Eq. 3.13 and requiring $T = T_{\text{DEM}}$ from Eq. 3.29 and $\tau/p = \eta_{\text{DEM}}$ from Eq. 3.42, we can easily define the correction factor

$$\delta_\Gamma = \left( \frac{\beta \sqrt{H}}{K'M} \right) \delta_\tau.$$  

We note that for frictionless particles in the dilute regime the original GD expressions are recovered. Additionally, the correction factor $\delta_\Gamma$ is related to the chain length $L$ of Jenkins and Berzi, [51] with $L/d = \delta_\Gamma^{-1}$. This chain length is equal to the particle diameter in the dilute limit and grows rapidly as $\phi \to \phi_c$. It also produces $T \sim g_0^{1/3}$ under steady shear, a result similar to Jenkins and Berzi’s prediction that $T \sim g_0^{2/3}$.

It is important to mention that we have not addressed the need for corrections to the
Table 3.1: Summary of model equations.

<table>
<thead>
<tr>
<th>Primary Equations</th>
<th>Secondary Equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure: ( p = \rho_s HT )</td>
<td>( g_0^{CS} = \frac{1 - \phi/2}{(1 - \phi)^3} )</td>
</tr>
<tr>
<td>Shear stress: ( \tau = \tau_s + \tau_{\text{inertial}} )</td>
<td>( g_0 = g_0^{CS} + \frac{\alpha_2 \phi^2}{[\phi_c(\mu) - \phi]^{3/2}} )</td>
</tr>
<tr>
<td>( \tau_s = \eta_s \chi p )</td>
<td>( e_{\text{eff}} = e - f(\mu) )</td>
</tr>
<tr>
<td>( \tau_{\text{inertial}} = \beta I' \delta_{\tau} )</td>
<td>( f(\mu) = \frac{3}{2} \mu \exp(-3\mu) )</td>
</tr>
<tr>
<td>( \Gamma = \frac{\rho_s}{d} K'T^{3/2} \delta_{\Gamma} )</td>
<td>( \psi = 1 + \frac{3}{10} (1 - e^2)^{-2/3} [1 - \exp(-8\mu)] )</td>
</tr>
<tr>
<td>( J_{\text{vis}} = \tau_{\text{inertial}} \dot{\gamma} )</td>
<td>( I' = \frac{\dot{\gamma} d}{\phi \sqrt{p/\rho_s}} )</td>
</tr>
<tr>
<td>( \delta_{\tau} = \frac{\alpha}{\beta} + \left[ 1 - \frac{\alpha}{\beta} \right] \chi )</td>
<td>( \chi = \frac{1}{(I_0/I')^{1.5} + 1} )</td>
</tr>
<tr>
<td>( \delta_{\Gamma} = \left( \frac{\beta \sqrt{H}}{K'M} \right) \delta_{\tau} )</td>
<td>( \chi_s = 1 - \chi )</td>
</tr>
<tr>
<td>( \beta = \phi \psi J \sqrt{\frac{K}{K'M}} )</td>
<td>( K'(\phi, e, \mu) = K(\phi, e) \left( \frac{1 - e_{\text{eff}}^2}{1 - e^2} \right) )</td>
</tr>
<tr>
<td>( H(\phi, e) = \phi [1 + 2(1 + e)\phi g_0] )</td>
<td>( M(\phi, e, \mu) = \max \left( \frac{J}{K'^{\mu}} \left( \frac{\alpha_1}{[\phi_c - \phi]^{1/2}} \right) \right) )</td>
</tr>
<tr>
<td>( J(\phi, e) = \frac{5 \sqrt{\pi}}{96} \eta^* )</td>
<td></td>
</tr>
<tr>
<td>( K(\phi, e) = \frac{12}{\sqrt{\pi}} \phi^2 g_0 (1 - e^2) )</td>
<td></td>
</tr>
<tr>
<td>( \eta^* = \eta_k^* + \eta_c^* + \eta_b^* )</td>
<td></td>
</tr>
<tr>
<td>( \eta_k^* = \frac{1 - \frac{2}{5}(1 + e)(1 - 3e)\phi g_0}{[1 - \frac{1}{4}(1 - e)^2 - \frac{5}{24}(1 - e^2)]g_0} )</td>
<td></td>
</tr>
<tr>
<td>( \eta_c^* = \frac{4}{5} (1 + e) \phi g_0 \eta_k^* )</td>
<td></td>
</tr>
<tr>
<td>( \eta_b^* = \frac{384}{25 \pi} (1 + e) \phi^2 g_0 )</td>
<td></td>
</tr>
</tbody>
</table>
Table 3.2: Values of model constants. Values of the critical volume fraction $\phi_c$ and the yield stress ratio $\eta_s$ are taken from Ref. [39].

<table>
<thead>
<tr>
<th>$\mu$-dependent parameters</th>
<th>0.0</th>
<th>0.1</th>
<th>0.3</th>
<th>0.5</th>
<th>1.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi_c$</td>
<td>0.636</td>
<td>0.613</td>
<td>0.596</td>
<td>0.587</td>
<td>0.581</td>
</tr>
<tr>
<td>$\eta_s$</td>
<td>0.105</td>
<td>0.268</td>
<td>0.357</td>
<td>0.382</td>
<td>0.405</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\mu$-independent parameters</th>
<th>$I_0$</th>
<th>$\alpha$</th>
<th>$\alpha_1$</th>
<th>$\alpha_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.2</td>
<td>0.36</td>
<td>0.06</td>
<td>0.58</td>
</tr>
</tbody>
</table>

Pseudothermal energy conductivity $\lambda$ to account for interparticle friction and dense packing. Because our simulation approach produces homogeneous shear with no temperature gradients, it cannot be used to measure conductivity. Hence, we are unable to assess the original model or recommend any new corrections. However, we briefly mention two simple options. First, Jenkins and Berzi [51] left the original GD expression for $\lambda$ unchanged, which is tantamount to setting $\lambda = \lambda_{GD}\delta\lambda$ with $\delta\lambda = 1$. The other option is to assume, based on the fact that the transport coefficients exhibit similar trends with respect to volume fraction, that $\delta\lambda = \delta_T$. Though we cannot address this issue in the present study, we offer these two options and reserve their assessment for future work.

The complete model consists of the equations listed in Table 3.1 along with the constant parameters in Table 3.2. As in the original GD model, all quantities are given as explicit functions of local system parameters (namely, volume fraction and shear rate) and particle-level properties (namely, material density, diameter, restitution coefficient, and friction coefficient).

### 3.5 Discussion

When applied to steady simple shear flows, the above dynamic model reproduces the temperature, pressure, and shear stress ratio results presented earlier in Figs. 3.5, 3.8, and 3.10.
that the original GD theory is unable to predict. Moreover, the basic forms of the corrections used to achieve the improved performance all have precedent in the literature, as previous authors have proposed effective restitution coefficients to capture the effects of friction, [51, 84] adjustable prefactors in the shear stress equation, [1, 7, 69] a characteristic chain length in the energy dissipation equation, [51] and expressions for the radial distribution function at contact that are based on simulation data. [54, 82] Our work here builds upon these approaches and provides closures for the corrections in terms of local flow variables and particle properties.

An important finding of the present work is that corrections to the energy dissipation rate expression, such as those proposed by Jenkins and coworkers, [51, 84] are insufficient on their own for extending traditional KT models to describe frictional and dense systems. Some aspects of the predictions are improved: the ‘chain length’ correction reproduces an increase in temperature and a decrease in the shear stress ratio in the dense regime, and the effective restitution coefficient captures a decrease in temperature and pressure in the dilute regime as interparticle friction is increased. However, even when one constitutes these corrections based on DEM data, disparities between KT and DEM temperature and stresses remain. Hence, we choose to supplement the ‘chain length’ and effective restitution coefficient with a modified radial distribution function at contact (to capture pressure), a correction factor to the shear stress, and decomposition of the shear stress into inertial and yield components. Though there are certainly other approaches one can take, they will necessarily involve modifications in the pressure and shear stress expressions. This point is consistent with the finding of Kumaran [50, 75] that dense packing and particle roughness result in changes in the collision frequency and velocity distribution functions of a granular medium; in the full KT approach, the model expressions for energy dissipation rate, pressure, and shear stress are all derived from collision integrals involving the velocity distribution functions, so any change in the latter will necessarily produce changes in all of the former, not just the dissipation rate.
The proposed model has some key advantages over existing rheological models for granular materials. The first is its handling of the effects of friction. By acknowledging the decrease in $\phi_c$ upon increasing friction, the new model correctly predicts a corresponding increase in pressure in the dense regime. Previous kinetic theories accounting for friction neglect this effect and hence predict a decrease in pressure at all volume fractions resulting from increased dissipation and decreased temperature. [51, 84] Secondly, while kinetic theory has long been used for modeling dilute flows, and while inertial-number models have proven successful for many dense flows, only very recently have the two been bridged to handle systems with wide variations in packing. [65] Although this model did not account for interparticle friction or for dense-regime $\epsilon$-dependence, the good agreement between its predictions and experimental results for a number of flow problems is quite promising and motivates the more general bridging performed here. Finally, the recasting of the inertial-number description into a kinetic theory framework 1) makes the model compatible with boundary conditions involving granular temperature that are more sophisticated than the simple no-slip condition and 2) enables the model to account for nonlocal effects via the conduction of pseudothermal energy. Inertial-number models are typically coupled with the no-slip wall conditions whose validity may be questionable depending on system and particle properties (an issue we aim to address in a later work), while KT models afford the option of wall slip conditions connected to fluctuating energy and the inelasticity of particle-wall collisions. [7, 34] This fluctuating energy, furthermore, can vary spatially and produce nonlocal rheological effects, which recent work has shown to be of substantial importance even in the dense systems for which inertial-number models were designed. [80] While the ‘fluidity’ approach in Ref. [80] (and also Ref. [[92]]) is currently limited to the dense regime, the extended KT scheme presented here offers a way to account for nonlocality over the full range of volume fractions below jamming.

On the other hand, the proposed model does exhibit several weaknesses resulting in part from the approach taken in its development. Among the most salient of these is the
overprediction of granular temperature in the very dilute regime \((\phi \lesssim 0.2)\). Had we allowed the effective restitution coefficient to vary with volume fraction, we would have been able to capture the temperature more closely in this region. However, because the \(\phi\)-dependence is neither simple nor consistent across all cases of \(e\) and \(\mu\), we choose to define \(e_{\text{eff}}(e, \mu)\) as a constant, with higher importance placed on capturing cases where \(\phi \gtrsim 0.2\). This definition is also more satisfying since \(e_{\text{eff}}\) is conceptually a particle property rather than an ensemble one. The disparity in very dilute cases, rather than arising from a poorly constituted \(e_{\text{eff}}\), is more likely the result of neglecting rotational degrees of freedom. The GD model is derived for smooth, frictionless particles and hence does not track rotational kinetic energy. In this context, conversion of translational energy to rotational energy is treated as an additional mode of translational energy dissipation, and so the parameter \(e_{\text{eff}}\) must encapsulate both real energy dissipation and loss to rotation. The extent of to which one mode predominates over the other may vary with volume fraction and therefore invalidate the assumption of a constant effective restitution coefficient. This problem is mitigated, though, by the fact that flow problems of practical interest manifesting such dilute regions tend to be heavily fluidized; hence, flow behavior in these regions is dictated primarily by the fluid-particle drag law, rendering any error in the solids-phase stress model rather inconsequential. Dense-phase predictions of the solids-phase stress, therefore, are most important to capture, and the corrections outlined in this work are weighted accordingly.

Another weakness of the present model is its reliance on empiricism, particularly in the corrections for the shear stress. Some of this need can likely be alleviated by considering rotational degrees of freedom, as the GD model and our modified version of it do not account for the dependence of the shear stress on the rotational temperature. It is possible, therefore, to start not with the GD model as the basis for modifications to account for friction and dense packing but rather with another existing KT model that considers particle rotation.\[71, 72\] The effects of friction can be included in such models by defining not only an effective normal restitution coefficient as done here but also an effective tangential restitution
coefficient, which has been employed previously with some success. [85] The inclusion of dense-regime effects can then be pursued as per the present work by defining a ‘chain length’ correction and a new $g_0$ expression. Even these tasks are encumbered by the empirical approach, as there is little agreement in the literature in regard to the precise dense-regime scalings for the stresses and temperature with respect to $\phi_c - \phi$ [Ref. [25]]. Our findings that $T \sim (\phi_c - \phi)^{-1/2}$, $g_0 \sim (\phi_c - \phi)^{-3/2}$, and $p \sim (\phi_c - \phi)^{-2}$ in the dense regime are simply our best estimates based on our DEM data, and more work needs to be done to determine the reason for the variety of exponents proposed in the literature. Finally, the determination of $\phi_c$ itself must be done empirically and as such has produced varying results. In particular, among recent works considering ‘rough’-particle shear flows, one finds that $\phi_c$ is independent of the normal restitution coefficient and is purely a function of $\mu$ [Ref. [39]] while others show $\phi_c$ to vary with both normal and tangential restitution coefficients. [50, 93] These works agree in their finding that roughness, whether measured by friction or tangential restitution, decrease $\phi_c$ from its value in the smooth, frictionless case ($\phi_c \approx 0.64$), but the contrary results regarding the influence of the normal restitution coefficient are hitherto unexplained and merit further study. The DEM data in the present work supports the idea that $\phi_c(\mu)$, and since this data forms the basis for our empirical modifications to the GD model we move forward with such a form.

Related to the jamming point $\phi_c$ is the rise of the particle stiffness $k$ as a rheologically important parameter. The KT approach assumes that particle collisions are instantaneous and hence that particles are infinitely hard (i.e. $k \to \infty$). For this reason, in the present work we have made certain to consider only cases in which Bagnold scaling holds and hence the finite stiffness plays no role — that is, cases in the inertial regime. A truly complete rheological model, however, would be capable of describing both infinitely and finitely stiff particles and hence would span the inertial, quasistatic, and intermediate regimes. Much work has been done recently to elucidate differences between hard- and soft-particle rheology [93, 94] and to quantify the rheology of soft particles in elastic and inertial regimes. [19, 21, 22, 24–
One recent work proposes a way to bridge the rheology of the inertial regime with the two elastic regimes by smoothly incorporating stiffness dependence to an extent governed by the dimensionless parameter $\dot{\gamma} \equiv \dot{\gamma}/\sqrt{k/\rho_d d}$. Such an approach can be applied regardless of the choice of inertial-regime model, including the one described here, and could conceivably be coupled with more complex plasticity or hypoplasticity models for quasistatic flows.

A final drawback of the current approach is that the modifications made to the GD model, while appealing to micro- or mesoscopic concepts, are all rheological (i.e. macroscopic) in nature. In deriving KT models, one generally begins by describing the details of a single collision and the velocity distribution of a pair of particles — that is, model construction begins at the microscale and builds upwards. The approach taken here, though, makes measurements at the macroscopic level and uses them to constitute parameters that have a physical interpretation at smaller scales. The chain length correction, for example, can be interpreted as a mesoscopic length of a typical granular chain [51] or microscopically as the result of dense-regime velocity correlations. [50] The effective restitution coefficient is a microscopic metric of dissipation during the collision of two particles. [84] The radial distribution function at contact $g_0$ is already microscopic in nature, and our modification to it accounts in a phenomenological way for anisotropy of particle collisions (which is also a microscale effect). The correction to the shear stress, on the other hand, is mostly rheological, though the inertial number that appears therein can be interpreted as a ratio of timescales of macroscopic shear and microscopic particle rearrangement. [8] In some regard, however, the connection between our proposed values for the micro-/mesoscale quantities and their physically measurable counterparts is one of analogy more so than equality.

An alternative approach to the present one is, of course, to perform a rigorous KT derivation that includes provisions for friction and dense packing. The problem with this approach, as discussed in the Introduction, is the difficulty in obtaining a closed-form model. A collision integral involving a tangential impulse proportional to the normal one (via $\mu$)
appears to require numerical solution, as does the integral for the non-Gaussian relative velocity distribution function that arises in dense flows [75] — and even this distribution function is determined empirically. For the time being, the most promising approach toward developing a comprehensive rheological model appears to be modification of existing KT models for dilute flows of frictionless particles.

3.6 Summary

We investigate the influence of dense packing and interparticle friction on granular rheology in the inertial regime. From DEM simulations of homogeneous simple shear flows we observe good agreement with the kinetic theory (KT) of Garzó & Dufty [38] (GD) in regard to predictions of pressure, shear stress ratio, and temperature in the case of frictionless particles below $\phi_f \approx 0.49$; however, for denser systems or for frictional particles, there is a substantial discrepancy between the simulation and GD results. Based on previous strategies in the literature for modifying the kinetic theory, we propose simple corrections to the GD model to bring its predictions closer to those of our DEM simulations. These corrections include an effective restitution coefficient to capture the increased dissipation resulting from friction, [84] a chain length correction to the energy dissipation rate, [51] a new expression for the radial distribution function at contact, and a correction factor to the shear stress equation to reflect the influence of friction in the dilute regime as well as to reproduce inertial-number scalings in the dense regime. [8, 30, 31, 39] These new terms are then constituted in terms of particle-level properties and system parameters from our DEM simulations to produce a more complete rheological model. This model may then be implemented in continuum-model simulations to investigate large-scale flows of frictional particles over a wide range of volume fractions such as those found in numerous important flow problems including chutes, hoppers, and fluidized beds.
Chapter 4

Boundary conditions for dense granular flows
Overview of the Chapter

Continuum modeling of granular materials in most practical applications requires specification of boundary conditions at the walls of the system geometry. Unlike with molecular fluids, which under most circumstances obey no-slip behavior, granular materials exhibit complex and varied slip behavior depending on flow-field conditions and particle-particle and particle-wall interaction properties. The nature of these dependencies becomes more challenging to investigate from a theoretical perspective in dense flows, which are less amenable to the traditional kinetic-theory approach and therefore require more empirical modeling strategies. Additionally, practical continuum modeling applications tend not to consider particle rotation or resolve near-wall boundary layer formation of the particulate phase, tasks which can add undesired model complexity and computational expense to the problem. In this work, we expand upon previous simulation studies of wall-bounded granular flows by investigating slip behavior in simple-shear simulations of soft, frictional spheres over a range of volume fractions and friction coefficients. We introduce a novel scaling based on granular viscosity and use it to collapse data of the ‘surface’ slip velocity, which includes rotational and boundary-layer velocity contributions, and propose an empirical model for use in finely-resolved flow problems considering both translational and angular velocity fields. We then separately constitute the rotational contribution to produce a slip velocity model for use in finely-resolved, translation-only flow problems. Finally, we coarse-grain the model by subsuming the boundary-layer contribution into the boundary condition, in analogy to the wall functions used in turbulence modeling, to produce a constitutive expression for use in coarsely-resolved flows considering only translational motion — *i.e.* the vast majority of applications.
4.1 Introduction

Flows of granular material are found in many industrial and natural processes, and attempts to model these flows often rely on continuum approaches. The development of rheological models for granular materials has progressed substantially over the past three decades. For dilute flows, numerous kinetic-theory models have been developed [5, 38, 40, 69, 71, 72]; for dense flows, inertial-number models have proven successful [8, 31, 39]; and recently methods to bridge dense and dilute behavior have been proposed [65, 68]. However, application of these rheological models to practical flow problems requires the specification of boundary conditions (BCs) at the system walls, and similarly advanced development of robust BC models to predict wall slip behavior remains an open challenge.

Most of the development of wall BCs for granular flows has been limited to dilute flows. Models for this regime generally track the granular fluctuation energy in addition to velocity and volume fraction and hence require two BC equations: one for the shear stress and one for the flux of fluctuation energy [7, 33]. Both equations contain explicit dependences on the slip velocity as well as particle/wall properties such as the normal [7, 33–35, 96, 97] and tangential [34, 35, 96, 97] restitution coefficients, the particle-wall friction coefficient [34, 35, 96], and the (phenomenological) specularity coefficient [7]. These BC models are coupled with kinetic-theory rheological models that relate stresses to fluctuation energy, which itself evolves dynamically according to a balance equation containing a (nonlocal) flux term. In the dense regime, however, traditional kinetic-theory rheological models are less successful because different physics predominate under dense and dilute conditions, with dilute flows characterized by uncorrelated binary collisions (often termed ‘molecular chaos’) while dense flows exhibit correlations in relative velocity distributions [75]. Inertial-number models [8, 31, 39], in which the stresses (and/or the shear stress ratio) are simple algebraic functions of particle concentration and shear rate, have been shown to yield reasonably good predictions of velocity profiles in dense flow systems [31, 65]. It is natural to expect, therefore, that dilute-regime BC models likewise would underperform when applied to dense flow problems.
and would necessitate the development of new BC formulations specifically for dense flows.

Indeed, recent work by Artoni and coworkers [36, 98] has revealed details about slip behavior in dense granular flows, on the basis of which the authors propose new BC expressions. However, their investigations were limited to two-dimensional systems of polygonal particles with a limited range of particle concentrations, wall friction coefficients, and particle properties. Shojaaee et al. build upon this work by expanding the range of particle and wall friction coefficients investigated but do not provide a constitutive model for the slip velocity [99, 100]. These efforts thus motivate the first aim of the current chapter, which is the development of a wall BC model applicable to flows with a wide array of particle/wall friction coefficients and solids concentrations within the dense regime.

Whether modeling dense or dilute flows, there remains another problem with specifying wall BCs for continuum modeling of practical flow systems: resolution of the boundary layer near the wall. Existing BC models relate the slip velocity to field variables evaluated at the wall; these field variables can vary substantially over the thickness of the boundary layer, which is generally $\sim 10d$ in thickness [30]. Hence, meaningful application of the BC requires adequately resolving the flow in the boundary layer. The computational costs of this task, though, are prohibitively high for most systems of practical interest (such as fluidized beds, risers, and hoppers), whose length scale of $O(1 \text{ m})$ is much larger than the particle diameter of $O(100 \mu\text{m})$. Eliminating the need to resolve the near-wall region would result in substantial savings in computational time. Additionally, in continuum simulations a boundary layer is predicted only if nonlocal conduction terms are included in the rheological model. These nonlocal terms can appear, for example, as a conduction term in the balance equation for granular energy (e.g. [5, 7, 38]) or in equations for other attributes such as ‘fluidity’ [80] or an order parameter related to the fraction of ‘fluidlike’ interparticle contacts [101, 102]. However, such equations, by virtue of being partial differential equations, add substantial complexity to the model that further increases computational time with respect to that required by a simple, algebraic rheological model. The reason is that numerical solution
of the additional scalar field requires another iteration procedure to account for the field’s spatial gradients. This burden does not exist with an algebraic formulation, a benefit that, in the case of kinetic-theory modeling of granular flows, has motivated the use of local, algebraic versions of the granular energy equation that remove gradient terms and simply equate production and dissipation terms [103, 104]. Therefore, the development of a BC model that subsumes the boundary layer and can be paired with a local rheological model is of practical interest, and such is the second aim of the current chapter.

4.2 Simulation Methods

We perform computer simulations using a package of the discrete element method (DEM) [37] implemented in the molecular dynamics package LAMMPS [48]. Particles interact only via repulsive, finite-range contact forces. We employ a linear spring-dashpot (LSD) model, for which the normal and tangential forces on a spherical particle $i$ resulting from the contact of two identical spheres $i$ and $j$ are

$$F^n_{ij} = k_n \delta_{ij} n_{ij} - \gamma_n m_{\text{eff}} v^n_{ij}$$

$$F^t_{ij} = -k_t u^t_{ij} n_{ij} - \gamma_t m_{\text{eff}} v^t_{ij},$$

for overlap distance $\delta_{ij}$, particle diameter $d$, spring stiffness constants $k_n$ and $k_t$, viscous damping constants $\gamma_n$ and $\gamma_t$, effective mass $m_{\text{eff}} = m_i m_j / (m_i + m_j)$ for particle masses $m_i$ and $m_j$, relative particle velocity components $v^n_{ij}$ and $v^t_{ij}$, and elastic shear displacement $u^t_{ij}$. By Newton’s Third Law, particle $j$ experiences the force $F_{ji} = -F_{ij}$. Particle sliding occurs when the Coulomb criterion $|F^t_{ij}| < \mu |F^n_{ij}|$ is not satisfied for particle friction coefficient $\mu$. Additionally, after setting $k_t/k_n = 2/7$ and $\gamma_t = 0$, we set $\gamma_n$ such that the restitution coefficient $e = \exp\left( -\gamma_n \pi / \sqrt{4k_n m_{\text{eff}} - \gamma_n^2} \right) = 0.7$. We likewise set a wall-particle friction coefficient $\mu_w$, wall stiffness $k_w = k$, and wall restitution coefficient $e_w = e$. Finally, the
Macroscopic stress tensor is calculated as

\[
\sigma = \frac{1}{V} \sum_i \left[ \sum_{j \neq i} \frac{1}{2} r_{ij} F_{ij} + m_i (v'_i)(v'_i) \right],
\]

where \( V \) is the box volume, \( r_{ij} \) is the center-to-center contact vector from particle \( j \) to particle \( i \), and \( v'_i \equiv v_i - \langle v \rangle (x) \) is the particle fluctuation velocity, i.e. the difference between its instantaneous velocity \( v_i \) and the time-averaged streaming velocity \( \langle v \rangle \) at position \( x \). The mean streaming velocity is zero in the \( y \)- and \( z \)-directions but is not known in the \( x \)-direction at runtime; it must be calculated in post-processing.

Two wall boundaries are placed at \( y = \pm H/2 \), and the gap of height \( H \) between them is filled with particles to achieve the desired ensemble-average volume fraction \( \bar{\phi} \). Shear is then induced by moving the top wall at a velocity \( +U_{\text{wall}} \) and the bottom wall at a velocity \( -U_{\text{wall}} \) in the \( x \)-direction. Shearing proceeds for a dimensionless time of \( \dot{\gamma}_{\text{wall}} t = 1000 \) to ensure that steady state has been reached; here, \( \dot{\gamma}_{\text{wall}} \equiv 2U_{\text{wall}}/H \) is the apparent shear rate, which will differ from the actual local shear rate \( \dot{\gamma} \) because of wall slip. During the simulation, 1000 snapshots of particle position, velocity, and stress are saved for post-processing. In post-processing, we perform a volume-weighted binning to calculate the field variables; that is, a particle whose volume crosses one or more bin boundaries will have its contribution to the volume fraction, velocity, etc. distributed across the bins in proportion to the fraction of its volume lying in each bin. Quantities reported as boundary values and denoted as \( \langle \cdot \rangle_w \) are, in fact, measured at a distance of \( d/2 \) away from the wall, as this is the closest point to the wall that a particle center can reach; the best location for wall measurements, however, is a small but still open question [105]. After performing the binning procedure on each snapshot, the snapshots are then averaged together to yield time-averaged quantities. From the stress data, we calculate a shear stress \( \tau \equiv \frac{1}{2}(\sigma_{xy} + \sigma_{yx}) \) and an approximate pressure \( p \equiv \frac{1}{2}(\sigma_{yy} + \sigma_{zz}) \). This pressure is approximate since it excludes the normal stress in the flow direction, the data for which are unreliable because the (nonzero) true streaming velocity at a given position...
will deviate from the mean value calculated for the bin containing this position. However, since normal stress differences are typically of the order of 10% of the mean normal stress for shear flows [29], we consider this approximation acceptable. We can then define the shear stress ratio, also commonly called the bulk friction coefficient, as $\eta \equiv \tau/p$ and the granular viscosity as $\nu \equiv \tau/\dot{\gamma}$. All macroscopic quantities will be presented in dimensionless form, scaled by some combination of the particle diameter $d$, stiffness $k = k_n$, and solid material density $\rho_s$.

### 4.3 Results

#### 4.3.1 Core and boundary regions

As described in previous works [99, 106], wall-bounded shear flows exhibit two regions of flow: 1) a central or core region characterized by spatially-invariant, local rheology and 2) a boundary region within about $10d$ of each wall featuring strong gradients in shear rate $\dot{\gamma}$ and volume fraction $\phi$ due to non-local conduction of granular energy. Indeed we observe these regions in our simulations, as demonstrated in Figure 4.1, where exponential tails towards the walls are clearly visible for the shear rate, volume fraction, and granular temperature. The measured pressure $p$ and shear stress ratio $\eta$ are found to obey local, inertial-number rheological behavior [8, 39] in the core region, as shown in Figure 4.2. This local behavior in the core supports the notion that a BC model that absorbs the near-wall behavior can be successfully coupled with a simple, local rheological model without the need for inclusion of further complexity to the rheology.

For some combinations of parameters, we observe that the friction of the walls is insufficient to generate sustained shear in the particle assembly, a phenomenon that has also been observed in a previous work using the contact dynamics method [100]. In an effort to determine whether this non-shearing state is dependent on initial configuration, we perform low-$\mu_w$ simulations starting with a pre-sheared initial condition, i.e. one generated from
Figure 4.1: Profiles of (a) velocity, (b) shear rate, (c) volume fraction, and (d) granular temperature vs. position between wall boundaries for $\mu = \mu_w = 0.5$ and $\tilde{\phi} = 0.55$. Quantities are scaled by wall velocity $U_{\text{wall}}$ and gap width $H$. A core region with spatially invariant rheological properties is observed to lie between boundary layers of thickness $\sim 10d$ at each wall. Exponential tails are observed in the boundary layers.
Figure 4.2: Comparison of core data for (a) scaled pressure and (b) shear stress ratio with predictions of the local rheological model of Chialvo et al. [39]. Reasonably good agreement between the two confirms the locality of the rheological behavior in the core.
shearing with a sufficiently frictional wall. As seen in Figure 4.3a, such a simulation begins with a volume fraction profile qualitatively similar to that in Figure 4.1c; however, as shearing progresses under the new, low-\(\mu_w\) conditions, the particle layers closest to the wall lose pseudothermal energy and begin to accumulate near the wall. This movement of particles towards the wall results in a depletion of particles in the core, producing a profile that is inverted with respect to the core-concentrated, fully sheared case. Additionally, the cooling process is accompanied by ordering of the particles near the wall (Figure 4.1a) and by a slow decrease in the observed shear rate over time (Figure 4.1b). Because our aim in this study is to develop a BC model for amorphous granular media, we deem it more valuable at present to focus our attention on the range of \(\mu_w\) values that produces sustained shear.

Previous two-dimensional shear simulations suggest that the lower bound for this range is \(\mu_w^* \approx 0.25\) [100]; our simulations in three dimensions suggest a different value of \(\mu_w^* \approx 0.33\). While it is possible that this critical value of the particle-wall friction coefficient should vary with particle and flow parameters, more cases of \(\mu_w\) near \(\mu_w^*\) need to be simulated in order to elucidate the dependences on these parameters. This task is outside the scope of the present work and is reserved for follow-up studies.

### 4.3.2 Dimensionless slip velocities and BC model

In seeking a BC model, there are several different definitions of slip velocity that one can consider. Specifically, these definitions differ in how the velocity of the granular medium is described. The options described below are summarized in Table 4.2. We note that, for the sake of simplicity, all the velocities presented in this section are scalars and correspond to the \(x\)-component of the velocity profile, \(v_x(y)\), generated by the simple-shear geometry described above; more specifically, the velocities are measured adjacent to the wall located at \(y = +H/2\) and are therefore positive. A generalization of our models to arbitrary flows and geometries is provided in Subsection 4.3.4.

For a wall-shear flow the simplest definition of the slip velocity is the difference between
Figure 4.3: Example case of shear localization when starting from a pre-sheared state with $\mu = 0.5$, $\mu_w = 0.3$, and $\bar{\phi} = 0.55$. (a) A plot of volume fraction versus position reveals migration over time of particles away from the core and towards the walls, where they begin to show signs of ordering. (b) Velocity profiles at different shear times indicate progressive cooling of the assembly towards an isotropic state, with unsheared plugs growing over time at each wall.
the velocity $U_{\text{wall}}$ of the wall itself and the translational velocity $v_w$ of the particle layer immediately adjacent to the wall – that is,

$$v_{\text{slip}} \equiv U_{\text{wall}} - v_w,$$  \hfill (4.4)

This translational slip velocity has been commonly used in previous works, most notably in the model of Johnson and Jackson [7] that is frequently used in gas-solid two-fluid model simulations [107]. While this definition is straight-forward to use since all continuum models track the translational velocity of the solids, it does not include any rotational motion of the particles at the wall. This exclusion is certainly significant, as a particle that rolls along a wall without slipping will nevertheless have a nonzero translational slip velocity. In fact, the best measure of true slip utilizes the velocity of the particles’ surface that is in contact with the wall rather than the translational velocity of its center of mass. We define this surface slip velocity as

$$v_{\text{surf}}_{\text{slip}} \equiv U_{\text{wall}} - v_{w, \text{surf}},$$  \hfill (4.5)

where the rotational velocity of the particles at the wall

$$v_{w, \text{rot}} \equiv \omega_w d/2$$  \hfill (4.6)

is added to the particles’ translational velocity to yield the velocity of the particles’ surface

$$v_{w, \text{surf}} \equiv v_w + v_{w, \text{rot}}.$$  \hfill (4.7)

Here, $\omega_w$ is the angular velocity of the particles at the wall; for this flow geometry, only the $z$-component has a nonzero time-averaged value, which is positive at both walls. This surface slip velocity has been used recently in the works of Artoni et al. [36, 98] to describe
slip behavior. While this definition is a better descriptor of slip behavior, its use in continuum modeling requires the tracking of the rotational motion of the solids phase, a level of complexity that is computationally more expensive and not commonly used. In both of the above definitions, though, the major computational cost comes from the need to resolve the boundary layer since both the translational and rotational velocities exhibit significant gradients within $\sim 10d$ of the wall – see Figure 4.1a. Hence, while not microscopically descriptive, it would be convenient to constitute a model for an ‘effective’ slip velocity based on a particle velocity extrapolated from the linear core profile to the wall. This \textit{apparent solids velocity} $v_{\text{app}}$ can be defined as

$$v_{\text{slip}} = U_{\text{wall}} - v_{\text{app}}$$

(4.8)

where the apparent solids velocity is

$$v_{\text{app}} = \dot{\gamma}_{\text{core}} H/2,$$

(4.9)

and the difference between the apparent and translational velocities – which we term the \textit{boundary-layer velocity contribution} – is

$$v'_{\text{w}} = v_{\text{w}} - v_{\text{app}}.$$

(4.10)

These definitions are denoted on an example velocity profile in Figure 4.4. In this work, we aim to constitute models useable at all levels of resolution and complexity, and hence we investigate the amenability of all the slip velocities to scaling collapses.

Just as there are numerous slip velocities and velocity contributions, there are likewise several different options for scaling the velocities. We generally define the dimensionless slip
Table 4.1: Definitions of velocities and slip velocities, specified at the wall located at $y = H/2$.

<table>
<thead>
<tr>
<th>Velocity</th>
<th>Definition</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>$U_{\text{wall}}$</td>
<td>$v(y = H/2)$</td>
<td>Velocity of the wall</td>
</tr>
<tr>
<td>$v_w$</td>
<td>$\gamma_{\text{core}} H/2$</td>
<td>Translational velocity (of the solids) at the wall</td>
</tr>
<tr>
<td>$v_{\text{app}}$</td>
<td>$v_w - v_{\text{app}}$</td>
<td>Translational velocity extrapolated to the wall</td>
</tr>
<tr>
<td>$v'_w$</td>
<td>$\omega(y = H/2)d/2$</td>
<td>Boundary-layer velocity contribution at the wall</td>
</tr>
<tr>
<td>$v_{\text{tot}}$</td>
<td>$v_w + v_{\text{rot}}$</td>
<td>Rotational velocity at the wall (in the direction of $U_{\text{wall}}$)</td>
</tr>
<tr>
<td>$v_{\text{surf}}$</td>
<td>$v_{\text{app}}$</td>
<td>Velocity of the particle surfaces at the wall</td>
</tr>
</tbody>
</table>

$\gamma_{\text{core}}$ region

Figure 4.4: Example velocity profile with the apparent wall velocity denoted.
velocity as

\[ I_{slip}^{(i)} = \frac{v_{slip}}{v_{char}} \]  

for some velocity scale \( v_{char} \). Choices for \( v_{char} \), which in general can be measured at the wall or in the core, include:

1. \( U_{wall} \), simply the wall velocity;

2. \( \dot{\gamma}d \), a shear-rate-based scale proposed by Artoni [36];

3. \( \sqrt{p/\rho_s} \), a stress-based scale used by Artoni [98] and analogous to that in the inertial-number definition [8, 39]; and

4. \( \nu/\rho_s d \) (= \( \tau/\rho_s \dot{\gamma}d \)), a viscosity-based scale that seems not to have been considered in the prior literature.

The first of these options, \( U_{wall} \), is an awkward choice for general flow problems since a BC with slip velocity scaled in this manner cannot be applied to a system with a stationary wall. Nevertheless, it is a useful reference velocity in this bounded shear flow example, in part because it is independent of particle and wall properties and the state of the particle assembly. We hence employ this scaling in Figure 4.5 to show the effect of \( \mu \), \( \mu_w \), and \( \phi \) on surface slip velocity data. Here, an ordinate value of zero corresponds to a no-slip state while a value of unity corresponds to a full-slip state. Unsurprisingly, we observe that slip decreases as wall friction increases, with zero slip occurring as \( \mu_w \rightarrow \infty \). There are also less straightforward dependences on \( \mu \) and \( \phi \) (or, equivalently, the distance to the jamming point \( \phi_c - \phi \)) that become clearer with the use of the other velocity scaling options.

Next we assess the ability of the suggested scalings of Artoni et al. [36, 98] to collapse the surface slip velocity data for an array of values of \( \mu \), \( \mu_w \), and \( \phi \). In Figure 4.6a, the shear-rate-based scaling is used, and the resulting dimensionless slip velocity is plotted versus \( \eta/\mu_w \) — the quantity suggested in Refs. [36, 98] as the determinant of slip behavior. As seen in
Figure 4.5: Surface slip velocities, scaled by wall velocity, vs. $\phi_c - \phi$ for (a) $\mu = 0.5$ and (b) $\mu = 1.0$ for various $\mu_w$. Slip is observed to increase with decreasing $\mu_w$. 

\[
\mu_w = 1.0, 
\mu_w = 0.7, 
\mu_w = 0.5 
\]
the figure, however, there is significant scatter for low values of $\eta/\mu_w$, which correspond to volume fractions closest to $\phi_c$. Additionally, for any given combination of friction coefficients, one can observe nonmonotonic behavior of the scaled slip velocity, which is in contrast to the behavior of the model proposed in Ref. [36]. We do note that, for the purpose of this scaling, Artoni et al. measure the shear rate at the wall, a task that is simple in their gravity-driven chute-flow simulations because of the rather small spatial dependence of $\dot{\gamma}$; in our shear-flow simulations, however, the shear rate varies sharply near the wall, making extrapolation of $\dot{\gamma}_w$ difficult. By contrast, the shear rate is constant in the core region of the shear flow and thus is substantially easier to measure with confidence. We hence use $\dot{\gamma}_\text{core}$ as the basis for the scaling here while also noting that our use of estimated values of $\dot{\gamma}_w$ does not improve the ability of this scaling to collapse the data (results not shown).

With the limitations of the $\dot{\gamma}$-based scaling in mind, we then test the pressure-based scaling of Ref. [98] in Figure 4.6b and find that, while it resolves the issue of nonmonotonicity, it remains unable to collapse the various simulated cases in a satisfactory manner when paired with the same abscissa. If plotted against $\eta - \eta_s$ as in Figure 4.6c, however, the pressure scaling somewhat collapses the data for different cases of $\mu$ and $\phi$ onto separate curves for each case of $\mu_w$. There is also, though, a slight suggestion of a non-zero $y$-intercept in the data, which we find difficult and ultimately undesirable to constitute—no combination of $\eta$, $\eta_s$, $\mu_w$, $\mu$, $\phi$, or $\phi_c$ in the ordinate or abscissa is found to remove this feature. For this reason as well as some persisting scatter, it appears that there is room for improvement, which we aim to address by changing the velocity scale.

Indeed, when the surface slip velocity is scaled using the viscosity-based scaling, \textit{i.e.}

$$I_{\text{slip}} = \frac{v_{\text{slip}}}{\nu_{\text{core}}/\rho_s d},$$

(4.12)

the data similarly collapse to distinct curves for each case of $\mu_w$, as seen in Figure 4.6d; the $y$-intercept is also pushed towards zero. The additional step of collapsing these distinct
curves requires that the abscissa — chosen here as $\eta - \eta_s$ — be augmented with a dependence on the wall friction coefficient as is done in Figures 4.6a-b. With the abscissa written in the form $(\eta - \eta_s)/f(\mu_w)$, we find that the function

$$f(\mu_w) = \mu_w + \mu^* - \eta_s$$

(4.13)

produces the best collapse of the data, as demonstrated in Figure 4.7. The quantity $\mu^*_w = 0.33$, as aforementioned, represents the critical wall friction coefficient below which the moving walls are unable to overcome the internal friction of the granular layer and produce shear [100]. The robustness of this collapse is further tested for various cases of wall separation distance $H$ and wall velocity $U_{wall}$; these data, shown in Figure 4.8, reveal the insensitivity of the collapse to system parameters. Finally, we generate an approximate fit to the collapsed data of

$$I_{slip} = \frac{1.5x^{2/3}}{(1 - x)^5}$$

(4.14)

with

$$x \equiv \frac{\eta - \eta_s}{f(\mu_w)}$$

(4.15)

in order to produce a useable surface slip velocity model for finely-resolved simulations tracking rotational particle motion.

The BC model in Eq. 4.14 can be applied to continuum modeling of shear flow problems in which both translation and rotational velocity fields are solved with sufficient resolution to capture the boundary layer. In such an application, it is clear that the values of $v_w$ and $\omega_w$ should be measured at the wall. The location for measurement of $\nu_{core}$, though, is to some extent a choice of the modeler; the only requirement is that it be measured outside the boundary layer, i.e. at least $10d$ away from the wall. This question is discussed in more
Figure 4.6: Scaled surface slip velocity versus scaled shear stress ratio using velocity scales based on (a) core shear rate $\dot{\gamma}_{\text{core}}$, (b-c) pressure $p$, and (d) core viscosity $\nu_{\text{core}}$. In (a) and (b), the abscissa is that used in Refs. [36, 98], and the slip data appear not to collapse as reported in those works. In (c), a new abscissa is used that somewhat collapses the data for different cases of $\mu$ and $\phi$ onto separate curves for each case of $\mu_w$. However, there is a slight suggestion of a non-zero $y$-intercept in the data, which is undesirable to constitute. In (d), this new abscissa is paired with a new velocity scaling, which reduces the scatter of the previous scaling and pushes the $y$-intercept to zero. The further collapsing of $\mu_w$ cases is performed in Figure 4.7.
Figure 4.7: Viscosity-scaled surface slip velocity versus scaled shear stress ratio. The function $f(\mu_w)$ is defined in Eq. 4.13. The scalings produce a collapse of the data for different cases of $\mu_w$, $\mu$, and $\phi$.

detail in Section 4.3.4.

4.3.3 Extension of BC model to problems with coarse resolution and/or considering only translational motion

Though Eq. 4.14 can predict the surface slip velocity over a wide range of dense flow scenarios, it will lose accuracy in continuum simulations that are coarsely resolved or that do not track the angular velocity of the granular material – scenarios that constitute the vast majority of practical granular and multiphase simulation efforts. Hence, we turn our attention to extending the BC model for application to these cases.

The strategy employed here for this extension is to constitute the unknown quantities representing rotational velocity and boundary-layer velocity contribution in terms of known, core quantities. We begin by applying the same viscosity-based scaling used earlier to define

$$I_{\text{rot}} \equiv \frac{v_{\text{rot}}}{v_{\text{core}}/\rho_s d}$$

(4.16)
Figure 4.8: Viscosity-scaled surface slip velocity versus scaled shear stress ratio for various dimensionless values of (a) wall spacing and (b) wall velocity with $\mu = \mu_w = 0.5$. The scaled wall velocity is defined here as $U_{wall}^* \equiv U_{wall}/\sqrt{k/\rho_s d}$. The collapse afforded by the slip velocity scaling is robust to changes in these system parameters.
and

\[ I' \equiv \frac{v'_w}{\nu_{\text{core}}/\rho_d}. \] (4.17)

Next, we note that both \( v_{\text{rot}} \) and \( v' \) are essentially zero in the core but become significant in the near-wall region [106], as seen in Figure 4.4 and Figure 4.1a. Indeed, their similar near-wall gradients suggest the possibility of a simple relationship between the two, which is confirmed by the plotting \( I_{\text{rot}} \) versus \( I' \) in Figure 4.9a. Here, we observe an approximately linear relationship that is independent of the chosen velocity scaling and whose slope depends primarily on \( \mu \). This \( \mu \) dependence appears to be nearly exponential in a manner similar to the variation of \( \eta_s \) with \( \mu \). We are hence able to collapse the data from Figure 4.9a to a single curve, seen in Figure 4.9b, by scaling the abscissa by the quantity \( \eta_s(\mu) - \eta_{s0} \), where \( \eta_{s0} = \eta_s(\mu = 0) \); values of \( \eta_s \) can be obtained from simulation data [39] or calculated from the fitted function [29]

\[ \eta_s = \eta_{s0} + (\eta_{s\infty} - \eta_{s0})g(\mu), \] (4.18)

where \( \eta_{s0} = 0.105 \), \( \eta_{s\infty} = \eta_s(\mu = \infty) = 0.405 \), and \( g(\mu) \) is defined as

\[ g(\mu) = 1 - \exp(-6\mu). \] (4.19)

We can then relate the scaled velocities by

\[ I_{\text{rot}} = mI' \] (4.20)
with
\[ m = \frac{(\eta_{\infty} - \eta_0)^2}{\left(\eta_s(\mu) - \eta_0\right)^2} \]  
\[ = \frac{1}{g^2(\mu)}. \]  
(4.21)
(4.22)

Finally, we write the translational slip velocity in dimensionless form as
\[ I_{\text{slip}} = \frac{v_{\text{slip}}}{\nu_{\text{core}}/\rho_s d}, \]  
(4.23)

and constitute it as
\[ I_{\text{slip}} = I_{\text{surf}}^{\text{slip}} + I_{\text{rot}}, \]  
(4.24)

with \( I_{\text{surf}}^{\text{slip}} \) given by Eq. 4.14 and \( I_{\text{rot}} \) given by Eq. 4.20.

Functionally, Eq. 4.20 augments the \( I_{\text{surf}}^{\text{slip}} \) model in Eq. 4.14 to create a BC model applicable to continuum-modeling problems without explicit solution of the angular velocity field. For such cases, the near-wall angular velocity is algebraically related to the near-wall boundary-layer velocity contribution \( v' \), which can be extracted from the translational velocity field provided it is solved with sufficient resolution to capture the \( \sim 10d \)-thick boundary layer. Specifically, we apply Eqs. 4.9-4.10 to obtain
\[ v' = v_w - \gamma_{\text{core}} H/2, \]  
(4.25)

which is easily evaluated since the right-hand side contains known quantities. As aforementioned, for shear flows \( \gamma_{\text{core}} \) can be measured at any chosen location in the core.

In a similar fashion, we next attempt to constitute \( I' \) in order to eliminate the need for boundary layer resolution. The boundary contribution to the translational velocity is again observed to depend on the distance to the jamming point as well as particle and wall friction
coefficients; as with $I_{\text{slip}}^{\text{surf}}$, there is also a dependence on the restitution coefficient. These dependences are seen in Figure 4.10a. By approximating the relationship between $I'$ and $\eta - \eta_s$ as linear, we calculate a slope for each case and fit the slope data to the form of

$$m' = 23.4 \left( 1 - e_{\text{eff}}^2 \right) \arctan \left[ 6 \left( \frac{\mu_w}{\eta_s} - 1 \right) \right].$$

(4.26)

Here, $e_{\text{eff}}$ is the effective restitution coefficient [68], which empirically describes the collisional loss of translational velocity resulting from inelasticity and friction as

$$e_{\text{eff}} = e - \frac{3}{2} \mu \exp(-3\mu).$$

(4.27)

We then write

$$I' = m'(\eta - \eta_s)$$

(4.28)

and can calculate the apparent slip velocity, defined as

$$I_{\text{app}}^{\text{slip}} = \frac{v_{\text{slip}}^{\text{app}}}{\nu_{\text{core}}/\rho_s d}.$$  

(4.29)

from

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

(4.30)

$$= I_{\text{slip}} + I'.$$

(4.31)

### 4.3.4 Generalized BC model

Though the model expressions presented above are developed on the basis of simple-shear simulation results, they can be easily recast to handle general flow problems. To this end,
Figure 4.9: Scaled rotational velocity vs. scaled boundary-layer velocity contribution (a) without and (b) with the prefactor \( m \) on the abscissa; \( m \) is defined in Eq. 4.22. A linear relationship between the two exists for all cases considered, regardless of how the velocities are nondimensionalized.
Figure 4.10: Scaled boundary-layer velocity contribution vs. scaled shear stress ratio (a) without and (b) with the prefactor $m'$ on the abscissa. The prefactor is defined in Eq. 4.26.
we begin by rewriting all the aforementioned velocities in vectorial form. The surface slip velocity can thus be written as

\[ \mathbf{v}_{\text{surf}} \equiv \mathbf{U}_{\text{wall}} - \mathbf{v}_{\text{w}}^\text{surf}, \]  

(4.32)

with

\[ \mathbf{v}_{\text{w}}^\text{surf} \equiv \mathbf{v}_{\text{w}} + \mathbf{v}_{\text{rot}}^\text{w} \]  

(4.33)

and

\[ \mathbf{v}_{\text{rot}}^\text{w} \equiv \left( \frac{d}{2} \right) \omega_{\text{w}} \times \mathbf{n}. \]  

(4.34)

Here, \( \mathbf{n} \) is the unit normal vector from the particle center to the wall. We then note that, in the simple-shear example above, the scalar slip velocity is simply the magnitude of the slip velocity vector — that is,

\[ v_{\text{surf}} \equiv |\mathbf{v}_{\text{surf}}|. \]  

(4.35)

We can then continue to define \( I_{\text{slip}}^\text{surf} \) as in Eq. 4.12 and constitute it as in Eq. 4.14. In similar fashion, we can write

\[ \mathbf{v}_{\text{slip}} \equiv \mathbf{U}_{\text{wall}} - \mathbf{v}_{\text{w}}, \]  

(4.36)

and

\[ v_{\text{slip}} \equiv |\mathbf{v}_{\text{slip}}|. \]  

(4.37)
define $I_{\text{slip}}$ as in Eq. 4.25 and constitute it with Eqs. 4.24, 4.20, and 4.28. Finally, we write

$$v_{\text{slip}}^{\text{app}} \equiv U_{\text{wall}} - v_{w}^{\text{app}}$$  \hspace{1cm} (4.38)$$
and

$$v_{\text{slip}}^{\text{app}} \equiv |v_{\text{slip}}^{\text{app}}|, \quad (4.39)$$

with $I_{\text{slip}}^{\text{app}}$ defined in Eq. 4.29 and constituted in Eqs. 4.31, 4.20, and 4.28.

In addition to the velocities, we must also generalize the definition of the viscosity in the core. This definition is trivial in the case of a shear flow since the rough location of the core is known prior to solving for the flow fields and since the core features spatially-invariant rheological properties. These features ensure that the BC model will be unaffected by the choice of $\nu_{\text{core}}$ so long as it is measured at a location that is beyond $10d$ of the walls. However, the definition of a core viscosity becomes less clear in general flow scenarios, where the viscosity (and shear rate and volume fraction) may vary with position throughout the domain. One can reason, though, that the core viscosity succeeds in collapsing slip velocity data in our shear flow simulations because of the proximity of the core to the wall; that is, the core influences the wall behavior because the two regions are separated by only $10d$.

This observation motivates us to recommend measuring the core viscosity at a distance of $10d$ from the wall, \textit{i.e.}

$$\nu_{\text{core}} \equiv \nu(x = x_{\text{wall}} + (10d)n), \quad (4.40)$$

where $x_{\text{wall}}$ is the local position of the wall. If the computational mesh is sufficiently coarse, though, the first grid cell may lie further than $10d$ from the wall, so viscosity information would be unavailable at the desired distance from the wall. In such a scenario, the viscosity can instead be taken at the first interior grid cell. This position ensures measurement of
Table 4.2: Summary of model equations.

<table>
<thead>
<tr>
<th>Equation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I_{\text{surf}} = \frac{\eta - \eta_s}{\mu + \mu_s - \eta_s}$</td>
<td>Surface slip velocity</td>
</tr>
<tr>
<td>$I_{\text{slip}} = I_{\text{surf}} + I_{\text{rot}}$</td>
<td>Translational slip velocity</td>
</tr>
<tr>
<td>$I_{\text{app}} = I_{\text{slip}} + I'$</td>
<td>Apparent translational slip velocity</td>
</tr>
<tr>
<td>$I_{\text{rot}} = mI'$</td>
<td>Rotational velocity at the wall</td>
</tr>
<tr>
<td>$I' = m'(\eta - \eta_s)$</td>
<td>Boundary-layer velocity contribution at the wall</td>
</tr>
</tbody>
</table>

rheological information relevant to the slip behavior while still characterizing core (i.e. local) rheology.

4.4 Discussion

The constitutive equations presented in the previous section allow for the prediction of the slip velocity in finely- or coarsely-resolved solution of continuum models that either include or neglect the angular velocity field. The BC expressions contain explicit dependencies on numerous important particle and wall parameters, including (1) microscopic parameters such as the particle-particle friction coefficient $\mu$, particle-wall friction coefficient $\mu_w$, and the particle restitution coefficient $e$, as well as (2) continuum parameters that depend on the microscopic parameters such as the yield stress ratio $\eta_s$ and the effective restitution coefficient $e_{\text{eff}}$. These aspects — flexibility and range of application — are the primary strengths of the presented model.

Another notable feature of the model is the viscosity-based characteristic velocity $v_{\text{char}} = \nu_{\text{core}} / \rho_s d$ that is used to scale the slip velocities and velocity contributions. Previous BC models have cast the slip velocity as being proportional to a characteristic shear velocity $\dot{\gamma}d$ [36], a characteristic particle rearrangement velocity $\sqrt{p/\rho_s}$ [98], or a characteristic fluctuating velocity $\sqrt{\bar{T}}$ [7]. Each of these has its advantages and disadvantages. The quantity $\dot{\gamma}d$ is a valid velocity scale for all flow problems but does not contain any explicit dependences on volume fraction, which appear to be necessary to eliminate the nonmonotonicity of the scaled
slip velocity observed in Figure 4.6a; the $\phi$-dependence must therefore be constituted in the model prefactors — a task that is certainly possible but may be tedious for a large parameter space (i.e. $\phi$, $\mu$, $e$, etc.). The pressure-based scale introduces such a $\phi$-dependence, albeit in a way that is not conducive to a general collapse (as far as we could identify); this scale is also not a useful velocity scale in quasistatic flows [36], where pressure becomes independent of shear rate [39]. Finally, the temperature-based scaling, in a continuum-modeling context, not only requires the solution of a balance equation for the fluctuation energy but moreover requires that this energy balance model be representative of the physics of dense flows; most models for $T$ are based on kinetic theory and have been designed for flows in which $\phi \lesssim 0.5$ (with some exceptions [51, 68, 75]). The viscosity-based scaling, therefore, combines several of the benefits of the other scales but without their drawbacks.

On the other hand, the presented model has a number of weaknesses, perhaps the largest of which is the heavy reliance on empiricism. Indeed, not only the fitting constants but even the functional forms of some of the model equations may appear difficult to justify from a purely microscopic, physical basis. To some extent, this empiricism is a product of the large parameter space considered in this work; the range of $\phi$, $\mu$, $\mu_w$, and $e$ studied in our simulations requires substantial effort to find common functional dependences. The kinetic-theory framework has proven useful in past investigations of rheological [71, 72] and slip behavior [34, 35] of inelastic, frictional/rough particles, producing explicit dependences on these same parameters. However, the assumptions typically made when utilizing the kinetic-theory approach can limit the range of applicability of the derived constitutive equations. Most importantly, the assumption of molecular chaos limits the model validity to volume fractions less than about 0.5, outside the dense regime of interest here. The use of kinetic theory along with velocity distribution data from dense-regime simulations, an approach taken by Kumaran [75], could reduce the need for empiricism, though it is not clear that this approach would produce closed-form expressions for the stresses as needed for practical continuum-modeling work. Hence, the approach we propose here is an interim solution until
models firmly grounded on underlying physics are rigorously derived. Despite the empirical strategy, many of the model parameters, though fitted from simulation data, have direct or approximate physical meanings. For example, $\eta_s$ is the yield stress ratio for the particle assembly, while $\eta - \eta_s$ is the distance to the yield stress ratio. The effective restitution coefficient $e_{\text{eff}}$ appears in terms of $1 - e_{\text{eff}}^2$, which is an approximate measure of the collisional loss of kinetic energy due to the combined effects of inelasticity and friction [68]. The term $\mu_w*$ represents approximately the minimum required amount of wall friction to sustain shear, and its value of 0.33 is, perhaps not by pure coincidence, also the value of $\mu$ at which $e_{\text{eff}}$ is minimized, suggesting a possible microscopic reason for the failure to thermalize the particle assembly when $\mu_w = \mu_w*$. While a more sound theoretical basis for the BC model is certainly desirable, the model presented here provides usable expressions for the slip velocity while also providing clues as to the possible forms and scalings that a detailed theoretical treatment might produce.

Finally, the BC model does not adequately address cases of unsteady particle cooling. As mentioned in Section 4.3.1, in some simulated cases the dissipation of granular energy is too high at the walls to allow sustained shear to occur. While we do observe an approximate regime boundary between shearing and non-shearing cases at a critical value of $\mu_w$ as did Shojaee et al. [100], we do not conduct a thorough investigation of the nature of this transition. The reason for limiting our analysis to steady systems is the difficulty in obtaining meaningful measurements of continuum field variables that vary both in space and time while maintaining high spatial and temporal resolution. In the case of our steady simulations, high spatial resolution is facilitated by time-averaging over long simulation times; this approach is impeded if the dependence on time is also to be measured. Moreover, the resolution in time and space cannot be improved by increasing the system size, as the field variables of interest in the shear flow vary over distances of $\sim 10d$, a distance that is independent of the number of particles being considered. Overcoming these challenges to produce a dynamic BC model would represent a substantial, standalone effort and is therefore outside the scope
of the present study.

4.5 Summary

Solution of granular flow problems by continuum methods requires specification of wall boundary conditions, expressions for which have not been fully established for dense flow scenarios. Additionally, continuum methods are limited in the case of most practical flow problems by the need for (1) coarse resolution of the flow field and (2) simple flow models that consider only translational motion, as both of these choices reduce computational cost. On the basis of DEM simulations for a wide array of particle and wall properties, we propose a constitutive expression for the slip velocity for use in finely-resolved continuum simulations tracking particle rotation. We then constitute additional terms that, when added to this slip velocity model, extend its validity to coarsely-resolved, translation-only flow descriptions. The presented model hence offers flexibility to the modeler in regard to the level of resolved detail while reducing the loss of accuracy, thereby allowing for improved flow predictions across a wide range of practical flow problems.
Chapter 5

Summary and future work

5.1 Summary

The preceding chapters have presented work performed to address several important questions of both academic and industrial interest in the area of granular flow modeling. Their content is summarized below, with a brief discussion of ongoing and future work thereafter.

In Chapter 2, a rheological model has been proposed, on the basis of discrete element method (DEM) simulations of simple shear flows, for flows of dense granular material in three different flow regimes. The presented model has several key features not exhibited in prior models. For one, it includes explicit dependences on the interparticle friction coefficient — most notably in the critical (i.e. jamming) volume fraction, a dependence not previously appreciated in a continuum-modeling context. Additionally, the model is unique in its approach for bridging the stress behavior in the different regimes. For the pressure model, an expression for the low shear-rate limit is chosen based on whether the flow is above or below the jamming point, which correspond to the quasistatic and inertial regimes, respectively; on this same basis, the low shear-rate expression is then blending either additively or harmonically, respectively, with a common high shear-rate expression representing the intermediate regime. The use of such a blending form, though fairly simple, has not been
demonstrated or utilized to our knowledge in prior granular modeling work. Finally, the behavior of the shear stress ratio (\(i.e.\) the ratio of shear stress to pressure) is shown to be an additive combination of contributions from two dimensionless groups: the inertial number and the stiffness-scaled shear rate. These contributions are constituted to produce a model for the shear stress ratio, the first time a so-called inertial-number model has been extended to include particle softness effects.

In Chapter 3, the inertial-regime portion of the dense-phase rheological model is extended to cover dilute granular flows. We show that, though the kinetic-theory (KT) model of Garzó and Dufty [38] predicts stresses accurately for frictionless particles, interparticle friction decreases the prediction accuracy considerably, often by orders of magnitude in the case of the pressure model. This observation is significant because KT models, most of which are derived for frictionless particles, are nevertheless frequently used to attempt to model frictional-particle flows. Additionally, we propose corrections to the Garzó–Dufty model to bring it into agreement with DEM data. These corrections, though empirical, are guided by micro- and mesoscopic concepts, including (1) an effective restitution coefficient accounting for frictional dissipation in binary collisions, (2) a phenomenological expression for the radial distribution function at contact accounting for collisional anisotropy, and (3) a ‘chain length’ characterizing the development of a correlation length larger than the particle diameter. The resulting model is the first to capture particle simulation results in both dense and dilute regimes using closed-form expressions.

In Chapter 4, a boundary-condition (BC) model is presented for flow of dense granular material past a frictional wall. DEM simulations are performed for a wide parameter set far exceeding that of previous simulation-based BC studies; this parameter space includes different values of volume fraction, shear rate, interparticle friction coefficient, particle-wall friction coefficient, and system size. We then demonstrate that previously proposed scalings for the slip velocity do not adequately describe the data from this wider space of flow conditions and propose a new scaling based on the solids-phase viscosity that accomplishes this
task. Along with a constitutive expression for the slip velocity, we finally present expressions that, when added to the slip-velocity expression, constitute a coarse-grained ‘effective’ slip-velocity model applicable to coarsely-resolved continuum-model simulations. The viscosity-based scaling and the coarse-graining approach are novel contributions that provide both immediately useable models as well as lessons for future BC model development.

5.2 Future work

The regime map presented in Chapter 2 is valid for dense flows of noncohesive granular materials, but many granular flow problems involve at least some weak cohesion — e.g. clumping of powders induced by humidity. The macroscopic effects of the added attractive force are known, on the basis of everyday observation, to include the facilitated development of a yield stress, a characteristic associated with the quasistatic regime; it would seem, then, that cohesion either widens the quasistatic regime or produces a new regime with similar flow characteristics. Additional simulation work to address these questions is a straightforward task, and dimensional analysis would be expected to inspire similar regime-bridging methods as in the noncohesive model development.

Though the model in Chapter 2 is capable of describing flows across three flow regimes, it is only able to do so at steady state. Therefore, another interesting though presumably more complex issue is that of constructing a bridged microstructural evolution model capable of describing dynamic flow behaviors — for example, the increase in pressure during shear start-up from a static initial state, or gradual compaction of a particle bed when subjected to oscillatory shear. The primary challenge in this task lies in linking the microstructural variables that are relevant in the different regimes. In the dilute inertial regime, granular temperature is the only relevant microstructural variable, as collisions are binary and nearly isotropic; in the quasistatic regime, coordination number and the fabric anisotropy tensor of interparticle contacts are the two important; in the dense inertial and intermediate regimes,
it is possible that all three of these variables are important. Once a bridged evolution model has been constructed, connecting the microstructure to the stress state should be straightforward, following the expressions from previously developed models for the inertial and quasistatic regimes individually.

Finally, all of the simulation work here has been for simple-shear flows, and the models developed on the basis of these simulations have presumed a particular way to generalize the results to other deformation types. However, previous experimental work on soils [108] and simulation work on frictionless particles [109] reveal that different stress states can develop from triaxial and biaxial compression tests, and the source of the discrepancy likely lies in the microstructure that develops during the shearing process. Extension of the aforementioned microstructural evolution models to include a dependence on the full deformation rate tensor rather than simply its magnitude would therefore be of value.
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