EFFECT OF PARTICLE SURFACE FRICTION ON CONSTITUTIVE RELATION FOR STEADY GRANULAR FLOW

KEN KAMRIN† AND GEORG KOVAL*

†Department of Mechanical Engineering
Massachusetts Institute of Technology (MIT)
Cambridge, MA 02139, USA
e-mail: kkamrin@mit.edu, web page: http://web.mit.edu/kkamrin/www/

*ICube Laboratory
National Institute of Applied Sciences of Strasbourg (INSA)
24 Bd de la Victoire, 67084 Strasbourg, France
e-mail: georg.koval@insa-strasbourg.fr, web page:

Key words: Granular behavior, Nonlocal rheology, Discrete element simulations.

Abstract. Nonlocal behavior based on the concept of nonlocal granular fluidity has demonstrated predictive capabilities in multiple geometries for (inertial and quasi-static) granular flow [1]. We investigate the effect of the surface friction of the grains on the continuum parameters, with a focus on the nonlocal amplitude, the model’s one new parameter. In our study, two-dimensional discrete element simulations of flowing disks are compared to numerical solutions of the nonlocal model in planar shear and several annular shear geometries. We observe an increase of the nonlocal amplitude as the surface friction decreases. This effect becomes especially stronger for very low values of coefficient of friction.

1 INTRODUCTION

Dry granular materials are ubiquitous in day-to-day life (geotechnical matter, raw materials, food grains, pharmaceuticals) and are the world’s second-most handled industrial material, second to water. While modeling efforts for these materials go back over two centuries, originating with Coulomb’s pioneering work, a precise continuum description for granular deformation has remained an elusive goal. In recent years, however, notable progress has been made on the specific question of how to predict well-developed flows of dense, dry granular media. A major development was the advent of the “inertial rheology”, a local constitutive description of flowing grains, ascribing a direct relationship
between the local stress state and the strain-rate [2, 3]. The particular relationship that emerges can be understood through dimensional analysis of planar simple shearing of a material composed of stiff, round grains with frictional viscoelastic contacts, and takes the form of a dimensionless relationship

\[ \mu = \mu_{\text{loc}}(I), \quad I = \dot{\gamma} \sqrt{m/P}, \quad \mu = \tau/P, \]  

(1)

where \( \mu \) is the ratio of shear stress \( \tau \) and normal pressure \( P \), and \( I \) is the inertial number, where \( \dot{\gamma} \) is the shear rate and \( m \) is the mean mass of a grain. This relation agrees with earlier scaling relations stemming back to Bagnold [4]. The inertial number can be understood as a ratio of the macroscopic time-scale of applied shearing, to the microscopic or inertial time. The precise function for \( \mu_{\text{loc}}(I) \) is empirically fit from planar simple shearing data and is characterized by a yield condition \( \mu_s \) such that \( \mu_{\text{loc}}(I \to 0) = \mu_s \), rendering the relation akin to that of a pressure-dependent yield stress fluid. This rheology has also been coupled to a granular elasticity relation [5], thereby closing the system mathematically to compute stress and velocity in flowing or static grains, producing a general mechanical law.

The inertial rheology works well in describing uniform flows (e.g. planar shearing) over a wide range of flow rates [2]. It can also be isotropically extended to a fully 3D rheology and is able to represent nonuniform flows at rapid rates [3]. However, in slower, quasi-static zones of flow (i.e \( I \lesssim 10^{-3} \)) in nonuniform flow geometries, the one-to-one inertial relation between \( \mu \) and \( I \) is violated [6], and inertial rheology flow predictions are incorrect. The behavior displayed in these zones is unexplainable through any local relation because the bulk stress/strain-rate behavior appears to vary with the macroscopic geometry, even when the local kinematics are identical. This has motivated the search for an appropriate nonlocal model, able to account for such geometric effects, by inclusion of an explicit length-scale based on the mean grain diameter, \( d \).

A nonlocal rheology that has recently emerged, the “nonlocal granular fluidity” (NGF) model, appears to have addressed this issue, and demonstrates the ability to quantitatively predict granular flows in many disparate geometries, in both rapid and quasi-static regimes [1, 7]. Specifically, NGF (in its reduced scalar form) is composed of the system

\[ g \equiv \frac{\dot{\gamma}}{\mu}, \quad g_{\text{loc}}(\mu, P) = \frac{\dot{\gamma}_{\text{loc}}(\mu, P)}{\mu} = \mu_{\text{loc}}^{-1}(\mu) \sqrt{P/m}, \quad g = g_{\text{loc}} + \xi^2 \nabla^2 g. \]  

(2)

The field \( g \) is the granular fluidity, and \( \xi \) is the plastic cooperativity length, which is proportional to \( d \). Note that in planar shear, flow gradients vanish and the above reduces appropriately to the local rheology; but in the presence of gradients, the Laplacian term “spreads” fluidity based on \( \xi \). As verified in multiple ways in [1, 7], \( \xi \) is in fact not a constant length; as in [7] we use a form inspired by [8]

\[ \xi = \frac{A}{\sqrt{|\mu - \mu_s|} d}, \]  

(3)
a form consistent with past work on jamming in amorphous media [9, 10] in that it diverges approaching a yield, or jamming point. The parameter $A$, the dimensionless nonlocal amplitude, is the only new parameter in the model, which quantifies the spatial extent of cooperativity in the flow.

With the successes of NGF, a key question to ask is: What is the connection between properties of the grains themselves and the continuum parameters/functions of the model, most importantly the new parameter $A$? To be able to answer this question is potentially of great value, as it would provide more complete upscaling between the micro and macroscales, and move toward the ability to predict a granular flow with NGF upon mere examination of the individual grains. There are limitless grain properties to consider; we are aware of past studies that have looked at connections to the grain shape [11], polydispersity [12], and surface roughness [13], but all have focused on the local response only. In this paper, we seek to provide a first step to the broader, nonlocal, scenario by investigating how the NGF model parameters depend on a single pertinent grain parameter while controlling all others. The property we will vary is the surface friction coefficient, $\mu_{\text{surf}}$, which is a property expected to have a nontrivial effect down into the quasi-static regime for which the effect of nonlocality is the most obvious.

Our general strategy is to simulate flows in planar shear to measure the local response function $\mu_{\text{loc}}(I)$, and then to fit $A$ by simulating the same material in a family of annular shear geometries, which brings out the nonlocal phenomena clearly. To fit $A$ we must calculate NGF solutions for comparison against the DEM, which we do numerically using Mathematica 10. Due to the symmetry of the annular cell geometry, the fluidity partial differential equation reduces to an ordinary differential equation, greatly simplifying the numerical solution process.

Details of the discrete-particle simulations are described next, followed by details of the parameter extraction and results.

2 DISCRETE ELEMENT SIMULATIONS

2.1 Studied geometries

The model is compared to two-dimensional annular and planar systems (see Figure 1). The annular geometry is defined by its inner radius $R$ and outer radius $R_o$. The gap between the walls is equal to $50d$ on the planar geometry and equal to $2R$ on the annular geometry ($R_o = 3R$), which avoids any disturbing effect of the walls on the material behavior. The granular material is composed by dissipative disks of average diameter $d$ (a polydispersity of 20% prevents crystallization) and average mass $m$. The shear stress is fully mobilized by the relative motion of two rough walls made of contiguous glued grains of a diameter equal to $2d$. We prescribe the tangential inner wall velocity $V_w$ and the normal stress $P_w$. We define the (measured) shear stress at the inner wall $S$.

We take advantage of the symmetry of the simulated systems introducing periodic boundary conditions along the tangential direction. The annular cell is represented by
an angular sector $\Theta$, while the plane shear cell presents a width equal to $50d$ (see [6] for more details). Table 1 describes the dimensions of the annular shear cells.

<table>
<thead>
<tr>
<th>$R/d$</th>
<th>$\Theta/(2\pi)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_{25}$</td>
<td>25</td>
</tr>
<tr>
<td>$R_{50}$</td>
<td>50</td>
</tr>
<tr>
<td>$R_{100}$</td>
<td>100</td>
</tr>
</tbody>
</table>

Table 1: Dimensions of the annular shear cells.

2.2 System parameters

The contacts are described by a standard spring-dashpot law defined by a damping coefficient, the coefficient of friction $\mu_{surf}$, and the elastic stiffness parameters $k_n$ and $k_t$. Physically we can relate the damping coefficient to the coefficient of restitution $e$ which describes the dissipation of energy during a chock. We perform simulations with standard molecular dynamics method as in Refs. [1, 2, 6].

Dimensional analysis allows us to reduce the number of parameters to few dimensionless quantities. We adopted the relation $k_t/k_n = 0.5$ and $e = 0.1$, two parameters with nearly no influence in dense granular flows [2]. We set the relation between the normal stiffness and the confining pressure $k_n/P_w = 10^4$ in order to simulate quasi-rigid grains.

Similar to the inertial number $I$, we can define the dimensionless wall velocity $V$:

$$V = \frac{V_w}{d} \sqrt{\frac{m}{P_w}},$$

which describes the shear state in the scale of the system.
The local behavior of each granular material \( \mu_{\text{loc}}(I) \) is obtained by plane shear simulations at different values of \( V \) (0.005, 0.025, 0.05, 0.25, 0.5, 2.5, 5.0 and 7.5). The non-local behavior is obtained in the annular cells with \( V = 2.5 \), where a transition between inertial to quasi-static regime is observed from the inner to the outer wall.

We analyze the effect of different materials with a wide range of coefficients of friction \( \mu_{\text{surf}} \) (0, 0.025, 0.05, 0.1, 0.2, 0.4 and 0.8) in all shear cells.

### 2.3 Steady shear states

Initially, the particles are randomly disposed inside the cells, producing very loose samples. As observed by [6], the system reaches a steady state, characterized by constant time averaged profiles of velocity and stress, after a short transient inferior to the shear length \( V \Delta t \approx 50 \) (where \( \Delta t \) is the simulation time). In practice, we adopt the conservative steady state condition \( V \Delta t = 100 \). All quantities results of a time average of 400 steps distributed over the distance \( V \Delta t \approx 200 \). The material bulk behavior is obtained from space averages of the whole sample (excepting the very first layers near the walls) in plane shear. Annular results are analyzed by radial profiles smoothed through central moving averages of \( d \) length.

### 3 CONTINUUM PARAMETER EXTRACTION

Because the nonlocal effect is characterized by its ability to remove uniqueness of the local rheological connection between \( \mu \) and \( I \) apparent in gradient-free flow geometries, it is sensible to calibrate \( A \) based on how the \( \mu \) and \( I \) fields in the annular cell differ from the \( \mu_{\text{loc}} \) relation in planar shear. Our calibration strategy takes a few steps. For each value of \( \mu_{\text{surf}} \):

1) The inertial rheology, given by the function \( \mu_{\text{loc}} \), is fit by conducting a sequence of planar shear DEM simulations of different prescribed \( I \), measuring \( \mu \). The result is then fit to a general mathematical form; we have found the following form appropriate,

\[
\mu = \mu_{\text{loc}}(I) = \mu_0 + bI + (\mu_s - \mu_0) \exp(-I/C),
\]

see Figure 2 for example. A simple linear relation between \( \mu \) and \( I \) is often assumed, but the above nonlinear form permits us to better fit data for low \( \mu_{\text{surf}} \) grains for which past studies have revealed a non-negligible curvature of the \( \mu_{\text{loc}} \) function at low \( I \) [2].

2) Three separate annular shear flow DEM simulations are conducted, for \( R = 25, 50 \) and 100\( d \). Coarse-grained data is recorded when steady state is reached. The stress distributions obtained, for each \( R \), are fit to the mechanically justified relations

\[
\mu(r) = \frac{S_w R^2}{r^2 P(r)}, \quad P(r) \cong P_w.
\]
K. Kamrin and G. Koval

Figure 2: Relationship between local parameters and the fit-form for the inertial rheology.

The former relation is implied from torque balance, and always well-fit to DEM data, and the latter is valid based on our own data as well as others' in this particular geometry [1, 6]. Here, $S_w$ is the shear stress acting on the inner wall.

3) Numerical simulation of NGF is begun by inputting the above fit for $\mu(r)$, the local flow-rate $\dot{\gamma}_{loc}(r)$ as obtained applying the inertial rheology, and a guess for $A$. The fluidity system, Equations 2, is then solved for $g(r)$, in the three annular shear geometries, assuming $g = g_{loc}$ on the boundaries. We have used this boundary condition in past annular shear flow solutions with success [1], however, the question of the precise form of the fluidity boundary condition is still open. Once $g(r)$ is computed, $I(r)$ is obtained trivially from its definition in Equation 1.

4) Plots of $\mu$ vs $I$ are made for all three annular shear NGF solutions, and compared directly against scatter-plots of those of the DEM. $A$ is varied under a simple bisection calibration approach until the NGF solutions best match those of the DEM. We judge the match over two decades of $I$, from 0.0005 to 0.05, which is low enough to cover a broad range of behavior dominated by the nonlocal effect but still large enough to capture the transition zone where the local influence diminishes.

4 RESULTS

Seven different surface roughness values: $\mu_{surf} = 0, 0.025, 0.05, 0.1, 0.2, 0.4, 0.8$ are covered by our tests. Figure 3 shows the results of our fitting of the inertial rheology to the planar shear DEM data for each $\mu_{surf}$. The parameters corresponding to each fit can be viewed in Table 2 (Local). Overall, the local fitting form appears sufficient. Figure 5 indicates the clear trend of the bulk static friction coefficient $\mu_s$, monotonically decreasing albeit nonlinearly with $\mu_{surf}$, in good agreement with past work on roughness effects in the inertial rheology [13]. The decreasing amount of curvature in the plots for larger $\mu_{surf}$ is captured by the decreasing separation between $\mu_s$ and $\mu_0$ as $\mu_{surf}$ increases.

The calibrated values of the nonlocal amplitude, $A$, are also presented in Table 2 along
Figure 3: Planar shear flows: DEM data (squares) and selected fit functions per Equation 5 (dashed lines) corresponding to all seven particle surface frictions, displayed simultaneously in (a) linear and (b) semilog.

<table>
<thead>
<tr>
<th>Continuum parameters</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Nonlocal</td>
<td>Local</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\mu_{\text{surf}}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.8</td>
<td>0.84</td>
<td>0.290</td>
<td>0.300</td>
<td>1.50</td>
<td>0.014</td>
</tr>
<tr>
<td>0.4</td>
<td>0.80</td>
<td>0.265</td>
<td>0.270</td>
<td>1.45</td>
<td>0.025</td>
</tr>
<tr>
<td>0.2</td>
<td>0.85</td>
<td>0.245</td>
<td>0.250</td>
<td>1.35</td>
<td>0.020</td>
</tr>
<tr>
<td>0.1</td>
<td>0.83</td>
<td>0.205</td>
<td>0.215</td>
<td>1.35</td>
<td>0.033</td>
</tr>
<tr>
<td>0.05</td>
<td>0.97</td>
<td>0.170</td>
<td>0.200</td>
<td>1.20</td>
<td>0.025</td>
</tr>
<tr>
<td>0.025</td>
<td>1.03</td>
<td>0.145</td>
<td>0.185</td>
<td>1.20</td>
<td>0.022</td>
</tr>
<tr>
<td>0</td>
<td>1.05</td>
<td>0.106</td>
<td>0.160</td>
<td>1.25</td>
<td>0.011</td>
</tr>
</tbody>
</table>

Table 2: Calibrated model parameters for all different grain frictions.

with the corroborating plots in Figure 4, where NGF outcomes for $\mu$ vs $I$ in the four different geometries are compared directly to those of the DEM, for each $\mu_{\text{surf}}$. The degree of agreement between DEM data and the NGF model, for each $\mu_{\text{surf}}$, as seen in the figure, lends confidence to the fits for $A$ and the effectiveness of the NGF model. However, there is some bumpiness evident in the extracted $A$ vs $\mu_{\text{surf}}$ relation (Figure 5), which could arise from sampling uncertainties in the DEM combined with the sensitive four-step calibration process used to obtain $A$. The latter point reflects the nature of $A$ within the system as that of a coefficient of a high-order derivative of an implicitly solved variable $g$, which precludes a straightforward measurement scheme for $A$ from DEM data.

In Figure 4, it is interesting to note that the degree of deviation from the local (i.e. planar shear) data appears to decrease as $\mu_{\text{surf}}$ decreases, yet $A$ is actually increasing with decreasing $\mu_{\text{surf}}$ (see Figure 5). This may seem counterintuitive, but it can be explained. Indeed, if all all other model parameters are held fixed, the extent of deviation from...
Figure 4: Calibrated NGF model [c.f. Table 2] (lines), vs DEM data (symbols) for planar shear (●) and annular shear geometries with $R = 25d$ (●), 50d (■), 100d (▲).
locality always grows with $A$ and vanishes as $A$ vanishes, in a given geometry. However, as $\mu_{\text{surf}}$ varies, the other NGF model parameters are not staying fixed. In other words, if deviation from locality were assigned a measure, one might say $A$ acts as an amplifier of deviation, but the term it amplifies depends on the other model parameters.

Our results suggest three conclusions about $A$. The first is that, unless the surface friction is very small ($\leq 0.1$), the nonlocal amplitude does not appear to vary to a significant extent with $\mu_{\text{surf}}$ (neither does $\mu_s$). Secondly, in the case of small $\mu_{\text{surf}}$, $A$ actually displays an increasing behavior as $\mu_{\text{surf}}$ decreases, as previously noted. The third is that the overall size of $A$ remains order-one over the range of $\mu_{\text{surf}}$ considered — even as the increasing behavior of $A$ with decreasing $\mu_{\text{surf}}$ becomes evident, this increase is much less than an order of magnitude. The order-one nature of $A$ agrees with past NGF work [1, 7].

5 CONCLUSIONS

We have performed the first upscaling study to link the recent Nonlocal Granular Fluidity model for granular flow directly to particle properties. Our parameter study has focused on the effect of particle roughness, corroborating past work on local rheology dependences and revealing a number of conclusions about its effect on the nonlocal amplitude. Perhaps the over-riding point is that $A$ is influenced by $\mu_{\text{surf}}$ but not tremendously. Viewing $A$ as an indicator of the amount by which flow at one place disturs material at another, this result would support the idea that $A$ is mostly a reflection of the geometric constraints involved in particles moving past other particles in a dense packing, and not so much a product of the contact interaction details. It remains future work to continue such a study to analyze the effects of varying other particle properties individually (like shape and polydispersity), or combinations of properties. From a physical standpoint, it also remains to attempt a theoretical understanding for these results. This is a non-
trivial task, but might be achievable by revisiting of the existing theoretical derivation for nonlocal fluidity.

REFERENCES


