A Lattice-Based Cellular Automata Modeling Approach for Granular Flow Lubrication

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Liquid lubricants break down at extreme temperatures and promote stiction in micro-/nanoscale environments. Consequently, using flows of solid granular particles as a "dry" lubrication mechanism in sliding contacts was proposed because of their ability to carry loads and accommodate surface velocities. Granular flows are highly complex flows that in many ways act similar to fluids, yet are difficult to predict because they are not well understood. Granular flows are composed of discrete particles that display liquid and solid lubricant behavior with time. This work describes the usefulness of employing lattice-based cellular automata (CA), a deterministic rule-based mathematics approach, as a tool for modeling granular flows in tribological contacts. In the past work, granular flows have been modeled using the granular kinetic lubrication (GKL) continuum modeling approach. While the CA modeling approach is constructed entirely from rules, results are in good agreement with results from the GKL model benchmark results. Velocity results of the CA model capture the well-known slip behavior of granular flows near boundaries. Solid fraction results capture the well-known granular flow characteristic of a highly concentrated center region. CA results for slip versus roughness also agree with GKL theory. [DOI: 10.1115/1.2164466]

Introduction

The increased capacity of turbine engines at higher thermodynamic efficiencies in the future can result in high temperatures on the order of 800°C. At temperatures greater than 500°C, however, conventional liquid lubricants fail. Additionally, liquid lubricants promote stiction that is detrimental to the successful operation of micro-/nanoscale systems, such as MEMs devices. Consequently, researchers have proposed innovative forms of particulate lubrication that can lower friction and prevent wear in sliding contact interfaces [1–4]. One type of particulate lubricant is known as a granular flow [2,5–7]. In a sliding contact, granular flows have demonstrated the ability to act as a hydrodynamic fluid by exhibiting the ability to carry loads and accommodate surface velocity differences.

Since granular flows behave like fluids, modified Navier–Stokes equations have been used to model them as a continuum, where the discrete granules are analogous to dense fluid molecules [2,8–10]. Navier–Stokes equations themselves can only be solved for the simplest cases, and when they are modified for use with granular flows, they become increasingly more complex. For example, a simple one-dimensional granular flow problem becomes nonlinear when coupled with equations for the granular flow velocity and solid fraction (i.e., granular density). Particle dynamic simulations—the granular flow analog to molecular dynamic (MD) simulations—have also been employed to model granular flows acting as lubricants [6,11–14]. However, they are usually computationally expensive for vast numbers of particles, which can be problematic as the film height to particle diameter ratio increases. Lattice-based cellular automata (CA) present a simple, flexible, and computationally inexpensive approach for this problem. CA employs rule-based mathematics to describe physical processes that are subsequently converted into computer simulations that display emergent system behavior. While granular flows exhibit continuum behavior, this behavior is the result of discrete granules being energized by surface and neighboring particle collisions. Since the localized granular interactions form the basis of the global granular flow behavior, the CA modeling approach that is based on local rules is an attractive approach. The current work employs a lattice-based CA modeling approach to the problem of granular flows in a Couette interface. Continuum modeling results that have predicted granular behavior in Couette flow environments are used as a benchmark for determining the effectiveness of CA in modeling granular flows.

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Background

Granular Flow Experiments. In past shear cell experiments, dry metal granular beads with varying diameters between 0.61 and 0.71 mm were placed in an annular shear cell [15]. From these experiments, efforts were made to formulate a continuum lubrication equation for granular flows. Two modes of lubrication effects were observed in the shear cell, as described [5]. At lower speeds, there are strong and long-lasting contact forces between the highly compacted beads and the surfaces. This mode is called granular *contact* lubrication. Load grinding noises occur, with jerky motion, and the friction coefficient was near unity. At some increased critical speed the particles become separated due to increased agitation; the motion smoothens out, and friction falls suddenly. They called this mode a transition to granular kinetic lubrication. As the speed increases, granular *kinetic* lubrication (GKL) becomes the mode of operation. GKL is characterized by a load carrying capacity due to the shear and normal forces created by the colliding particles against the upper surface. Both the continuum and lattice-based cellular automata models developed and represented in this work model the GKL regime.

Continuum Modeling Simulations. Kinetic theory uses molecular models and the methods of statistical mechanics to relate the behavior of the individual particles to that of the bulk flow. For dense gases, the kinetic theory was originally used to characterize the stress on the surface resulting from the transport of momentum from the colliding gaseous molecules [16]. Haff used the kinetic theory approach to model granular flows noting that the individual granules are treated as "molecules of granular fluid" [8]. A key difference between real molecules and granular par-

ticles is that colliding molecules undergo perfectly elastic collisions, which means that kinetic energy is conserved. The colliding granular particles however, inelastically collide, causing loss of kinetic energy.

Lun et al. [7] analyzed the interaction of granules in a flow using a statistical approach. They describe the movement of inelastic particles in Couette flows with variable coefficients of restitution. The conservation equations of mass continuity, momentum, and energy have terms that must be quantified by constitutive relations for granular flows. Lun uses an approach that considers the collisional contributions to the constitutive equations as well as the kinetic contribution to the constitutive equations.

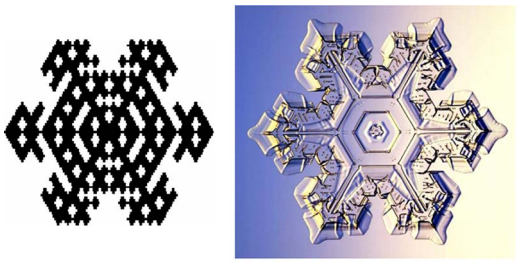
Zhou and Khonsari [17] utilized Lun's constitutive relationships for the flow field, a modified version of the Hui et al. [9] boundary conditions for momentum, and the Jenkins and Richman [18] boundary conditions for energy, to predict the behavior of the granular flow being sheared between parallel plates. Sawyer and Tichy used a particle dynamics approach alongside a similar continuum approach and interpreted their results in light of the shear cell experiments [10]. Higgs and Tichy employed a robust continuum modeling approach that applied the rigorous Jenkins-Richman boundary conditions to the modified granular forms of Navier–Stokes equations [2]. The resulting granular velocity and solid fraction from their effort will serve as a benchmark for validating the capabilities of the lattice-based cellular automata modeling approach introduced in this work.

Cellular Automata Simulations. Lattice-based CA are discrete dynamical systems whose behavior is specified in terms of local relationships. Space is represented by a uniform grid made up of many discrete cells, each of which should be in one of a finite number of defined states. Cells may change states only at fixed, regular intervals of time. States are updated in accordance with fixed rules that depend on cell value and the values of neighboring cells.

Cellular automata (CA) are commonly misinterpreted as "computational methods," but actually they are "computational models" [19]. "Computational methods" are used for obtaining numerical solutions to existing theoretical models usually in the form of partial differential equations. Some common computational methods are finite differencing, finite volume, and finite elements methods. "Computational models" are an alternative to theoretical models. Computational models are developed by understanding the underlying processes of the interested phenomena and translating this understanding into rules. Algorithms are developed from the rules that simulate the phenomena. CA computational models can be easily implemented as algorithms directly on computers. Conversely, theoretical models describe the physical system as mathematical equations and then use computational methods to solve them.

One important detail to note about CA models is that they can be developed based on rules constructed from simple observations and experiments. The fact that CA models can be independent of theoretical models is of great relevance at this time. It bridges the gap between cutting edge experimental work and rapidly growing computational capabilities by bypassing the bottle neck of theory and higher-order mathematical development. In many fields that feature complex phenomena, sophisticated experimental studies are established but theory is far lagging behind as is the case in granular flows. CA gives an alternative framework to model these experiments in terms of algorithms to take advantage of current computational capabilities. Similar to other models, the validity of the CA model is established by first comparing the results to actual experiments. Upon attaining satisfactory agreement, the CA model can subsequently be modified to study further cases. CA is potentially useful for studying a variety of physical systems.

Lattice-Based Cellular Automata in Physical Systems. Cellular automata were introduced by Von Neumann as a part of his research on evolutionary biological systems [20]. Later, many applications in nonbiological fields were found for CA, since it is a flexible abstract formalism that can be adapted to a desired application. Among these, the modeling of physical systems has emerged as one of the primary areas of application. Many independent investigations have confirmed the feasibility of such an application [21–23]. Some of the fields in which CA are actively used are fluid dynamics [24–26], diffusion reactions [27–29], crystal growth [30,31], galaxy formation, [32,33] and the formation of biological systems [34–36]. One well-known CA simulation is crystal growth in snowflake formation. Simple rules describing the thermodynamic evolution of the snowflake yielded the simulation of the evolving snowflake. Figure 1 shows both an image from the simulation based on the rules from Wolfram [21] and a photo of an actual mature snowflake. The relevance of CA as an alternative to conventional calculus-based approaches for modeling physical systems is evident from the myriad of successful applications.



(*a*) (*b*)

Fig. 1 Crystal growth of the snowflake simulation. (*a*) Image from the cellular automata simulation. (*b*) Photograph of a mature snowflake [59]

Lattice-Based Approaches in Discrete Particulate-Type Flows. First-principle continuum-based physics models are continuing to advance. However, they oftentimes fail at producing accurate models when predicting very complex physical phenomena such as turbulence or multicomponent flows. They also are becoming inapplicable, as processes are increasingly pertaining to smaller length scales. The lattice Boltzmann method (LBM) is a lattice-based modeling approach that has been applied to molecular lubrication of data storage devices [37]. In some ways, granular lubrication flows mimic molecular lubricants since both of their global behaviors are defined by the local and discrete interactions, such as their respective particle–particle and particle–boundary collisions. Additionally, nanomanufacturing processes such as chemical mechanical polishing (CMP) [38–41] feature slurries used for polishing and planarizing semiconductor wafer surfaces. Slurries are multicomponent particulate flows that have also been modeled using lattice-based approaches [42,43].

Lattice-Based CA Approaches in Granular Flows. Granular flows exhibit many peculiar and unusual characteristics. Theoretical models capturing these characteristics are very complicated and difficult to solve. They are hindered by the complexity of higher-order nonlinear differential equations. For this reason many alternate approaches have been attempted like Molecular dynamics [6,11–14], lattice–Boltzmann [44], Monte Carlo [45,46], and others. CA modeling was one such attempt. Most of the CA models, however, concentrate on modeling one of the specific aspects of granular flows like size segregation [47–49], heap formation [50–52], complex flow patterns in pipes [53,54], peculiar flow down hoppers and silos [48,55,56], and others. Some of them tried to develop one generalized CA framework to model all the characteristics inherent in granular flow [57,58]. But to best of our knowledge, no CA model has been applied to granular flow from a tribological perspective.

Theory

The models discussed in this work predict the behavior of the annular shearing flow of identically sized glass spheres. The simulation mimics a small polar-rectangular region of an actual experimental annular shear cell [5], which is approximated as being a parallel Couette shear cell with only one surface moving. This is how it would appear if a segment of the annular shear cell were unwrapped and the bottom surface moved relative to the fixed top surface.

Continuum Simulation of Shear Cell. The top wall is stationary, while the bottom wall moves with a velocity $u=U$ in the positive x direction. The flow is a steady ($\partial/\partial t=0$), fully developed ($\partial/\partial x=0$), and the normal velocity is zero. The flow only varies across the film, i.e., the dependent variables are only functions of the cross-film coordinate y. The infinitely wide bearing assumption ($\partial/\partial z=0$) was used.

The Governing Equation for Velocity and Solid Fraction. The constitutive relationships developed by Lun [7] were substituted in the governing equations and applied to this problem. The governing ordinary differential equation, Eq. (1), for the mixture velocity $u(y)$ can be determined by simplifying the x component of the momentum equation. Similarly, the governing differential equation, Eq. (2), for the solid fraction $\nu(y)$ is deduced from the granular form of the energy equation

$$\left(\frac{d^2u}{dy^2}\right)+B_1[\nu(y)]\left(\frac{d\nu}{dy}\right)\left(\frac{du}{dy}\right)=0 \tag{1}$$

$$\frac{d\nu^2(y)}{dy^2}+\left[B_2[\nu(y)]\left(\frac{d\nu(y)}{dy}\right)^2\right]+B_3[\nu(y)]+B_4\left(\frac{du(y)}{dy}\right)^2=0 \tag{2}$$

The details of the B coefficients and Eqs. (1) and (2) can be found in Higgs and Tichy [2].

Boundary Conditions. The boundary conditions for the velocity u and the solid fraction ν are obtained from Jenkins and Richman [18] and are shown below in Eqs. (3) and (4), respectively.

$$\left[\frac{du(y)}{dy}-RB_5[\nu(y)]u_s\right]_{y=0,H}=0 \tag{3}$$

$$\left[\pm\frac{d\nu(y)}{dy}+RB_6[\nu(y)] \quad \nu+RB_7[\nu(y)] \quad u_s^2\pm RB_8[\nu(y)] \quad u_s\frac{du(y)}{dy}\right]_{y=0,H}=0 \tag{4}$$

where R is a roughness factor and u_s is the slip velocity. The slip velocities at the lower and upper walls are

$$\text{(a)} \quad Y=0: \quad u_s=U-u(0)$$

$$\text{(b)} \quad y=H: \quad u_s=-u(H) \tag{5}$$

The roughness factor R varies as $0\leqslant R\leqslant 1$, where $R=0$ corresponds to a smooth surface, and $R=1$ to a very rough surface, where slip is minimum. While the literature has interpreted the roughness factor R in several ways, the authors employ the definition of R as the fraction of granule that fits in the gap between the wall disk "asperities" [18]. This definition is straightforward to implement in experiments, as shown in Fig. 2.

Cellular Automata Simulation of Shear Cell. To employ CA for this problem, the first step is to discretize a region of the shear cell. A two-dimensional rectangular grid, with unit length equal to the diameter of the granule is created. The length and height of the grid correspond to the length and thickness of granular film. Two types of particles constitute the grid; boundary particles and object particles (see Fig. 3). Boundary particles are special particles that collectively define the upper and the lower wall. Object particles, which represent the granules, can move with discrete steps on the grid space. Unless otherwise mentioned, "particles" refer to object particles (i.e., granules). Since periodic boundary conditions were implemented, particles going out of the grid on the left side will come back on the right side, and *vice versa*. Each grid location can be either empty or filled with one particle only. This captures the volume solid fraction property of the granular flow. Along with film parameters, other material properties of the boundary and granules have to be input into the simulation. For example, the coefficient of restitution and roughness factor are assigned to the walls and particles.

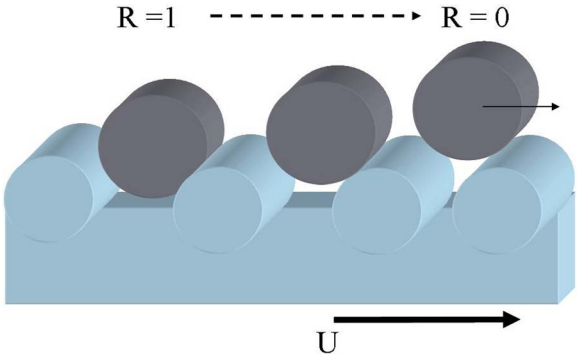


Fig. 2 Schematic of roughness factors

The simulation should also be capable of mimicking the dynamic granular behavior. The movement of the particle is obtained by updating its coordinates at each time step, and the movement must have a direction and speed. Being a rectangular grid, the particle can have one of eight discrete directions (see Fig. 4). The speed of the particle is defined by "time factors," which represents the number of steps before the particle can advance one grid step. The fastest speed that can be implemented is one grid step in one time step (i.e., time factor=1). The current grid location, direction, and speed can completely define the movement of the particle. The lower wall is moving and energizing the system, so we assign the maximum speed in the 1-direction to all the boundary particles that define the lower wall.

Next, the rules of evolution for the simulation are developed. In this case the evolution is the movement of the granules and granular collisions. Granular collisions can be particle–particle or particle–wall collisions. Rules for movement require updated coordinates; the direction and the speed remain the same. In a collision, the position remains the same, but direction and speed change. For simplicity, the rules for updating direction and speed are implemented separately, and there will be a separate set of rules for boundary interactions and particle–particle interactions. Figure 5 graphically summarizes all the rules for updating the direction for boundary interactions. All these rules are intuitive and can be determined experimentally by observing balls collide in a billiard-type apparatus. Figure 6 summarizes the rules for

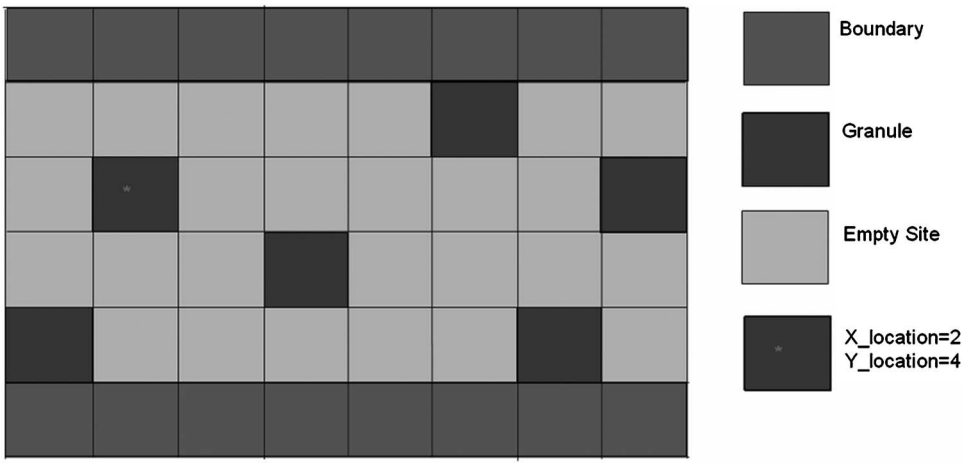


Fig. 3 Schematic of the Cellular Automata model

updating the directions for particle–particle collisions. An important assumption here is that all of the other particles except the one being updated are fixed. In cases where there are two possible resulting directions, one of the resulting directions is chosen randomly. An important detail to note is that while collisions can result in numerous post-collision directions, the simulation discretizes them into only eight directions.

When the particle collides with the boundary, its change in velocity depends on the coefficient of restitution (e_w) and the roughness (R) of the wall. The speed of the particle is updated using

$$u_{p,f} = u_{p,i} + R(U - u_{p,i}) \tag{6}$$

$$u_{p,f} = U - e_w(U - u_{p,i}) \tag{7}$$

Similarly when there is a particle–particle collision, the speed of both the particles is updated according to Eqs. (8) and (9), which depend on the coefficient of restitution (e_p) of the particles. While Eqs. (8) and (9) are standard in theory, they are empirical relations derived from experiments. Thus, we are not violating the property of CA that it can be built independent of any presupposed mathematical physics-based theory, namely first-principal differential equations

$$u_{p1,f} = ((1 - e_p)u_{p1,i} + (1 + e_p)u_{p2,i})/2 \tag{8}$$

Fig. 4 Eight possible directions of motion

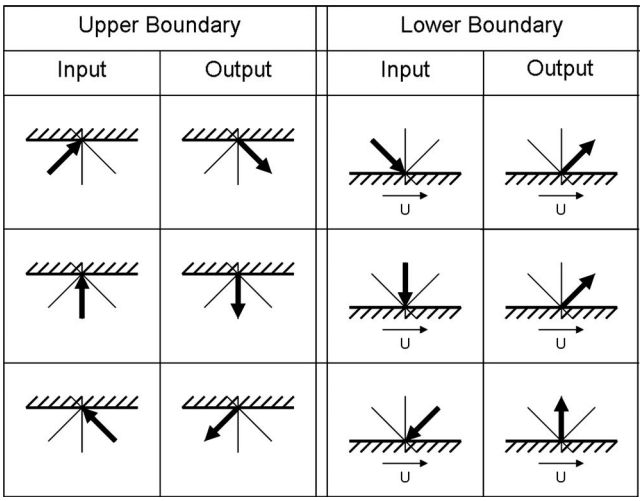


Fig. 5 Rule for boundary interaction

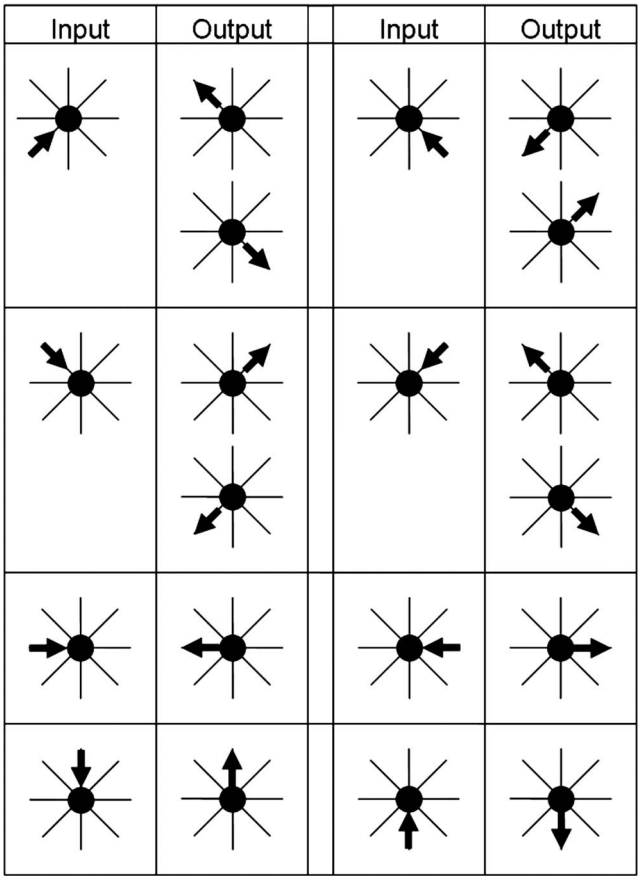


Fig. 6 Rule for interparticle interaction

$$u_{p2,f} = ((1 - e_p)u_{p2,i} + (1 + e_p)u_{p1,i})/2 \quad (9)$$

The simulation takes the dimensions of the shear cell and solid fraction as inputs. Based on this information it calculates the number of granules in the shear cell, which remains constant through out the simulation. Before starting the simulation, the granules are given initial conditions, such as a random and a unique grid location. This makes the initial distribution of particles random. Additionally, granules are assigned random directions and given an initial velocity. This is necessary to start the processes of granular collisions. However, this initial velocity is much smaller compared to the velocity of the lower wall.

The system evolves in discrete time steps, where the location, direction, and speed of the particles are updated each step. Particles are consecutively updated in each time step and when one particle is being updated the others are assumed to be at rest. The order of the particles is shuffled in each time step to avoid any bias. This makes the current work fall under the category of asynchronous CA, which results in a loss of the parallel processing capability that the more robust CA models possess. However, the simplicity of the algorithm more than compensated for the loss of this feature. Whenever each particle was updated, its current location is retrieved and its neighboring locations in all eight directions are determined using periodic boundary conditions. Depending on the direction, the corresponding neighboring site is checked to see if it is occupied or not. If the neighboring site is empty, the coordinates of the particle are updated. If the neighboring site is occupied, it is checked to see if it is filled by a boundary particle or a granule. The appropriate rule is then applied from the table to determine the new velocity and the direction. Subsequently, it attempts to move again in the new resulting direction. This is repeated until an empty neighboring site is found or all the possible directions are exhausted. Collisions are assumed to be instantaneous, so each particle can have multiple collisions in one time step. Once the position, direction, and the velocity of the particle are updated according to the rules, this particle is fixed and the next particle is updated.

The simulation has to run until it reaches a steady state. The way to determine the number of steps required to reach the steady state is to keep running the simulation for increasing number of time steps. Whenever consecutive readings match, it implies that steady state is reached. Once the simulation is complete, the position, velocity, and direction data at steady state are tabulated. The algorithm outlined above was implemented in " MATHEMATICA® 5" on a 3.2 GHz processor with 2 GB ram. Simulations handling 850 particles for 10,000 time steps were processed in 1.92 h.

Results

Continuum Modeling Simulation. The parameter values used are those approximating the experiments of Yu et al. [1]: $U=2$ m/s, $e_p=0.85$, $e_w=0.65$; $\rho_p=2550$ kg/m^3; $d=0.787$ mm; $H=4$ mm; $R=0.65$. (The last parameter is simply an assumption) The solid fraction, $\nu_{\max}=0.65$ refers to the theoretically maximum possible solid fraction while filling up rectangular space with spherical particles. The length of the cell is not relevant since the flow is fully developed and the granular properties do not vary with length.

CA "Modeling" Simulation. The input conditions of the simulation are correlated to the theoretical model as best as possible. The coefficient of restitutions and roughness factor has a direct correspondence in both the models. So we set $e_p=0.85$, $e_w=0.65$, and $R=0.65$. The height of the film and the length of the film are input in terms of the diameter of the particle. $H=10d$ and $L=100d$, where d is the diameter of the particle. In the initial solid fraction $\nu=0.85$ it is important to note that since the CA simulation has rectangular particles, it can have a maximum solid fraction of one. The bottom wall that is energizing the granules is assigned the maximum velocity in the model. The height and velocity are made dimensionless to compare the plots of both the models. Hence the actual value of the film height and the wall velocity are not required.

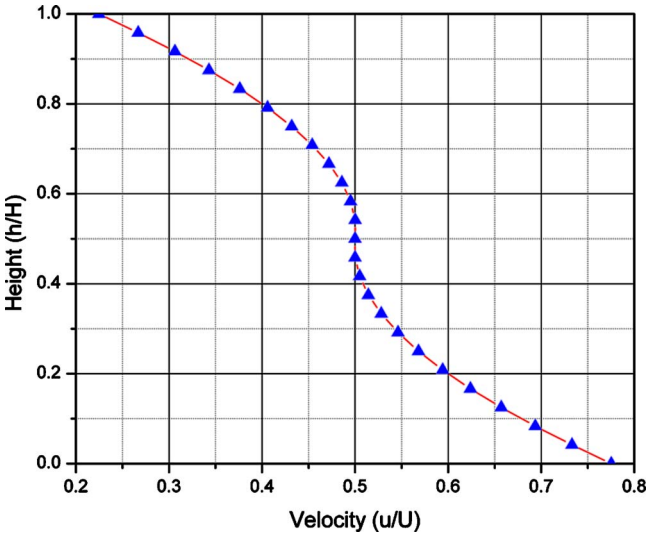


Fig. 7 Velocity versus height from theoretical model

Model Comparisons. Figure 7 shows the granular velocity for the GKL continuum model across the film. There is slip at the upper and lower boundaries, as is evident by the deviations from the wall velocities. For example, the lower wall moves with a velocity of $u=U$, and the top wall is stationary ($u=0$). The no-slip boundary condition is not in effect, as the flow velocity at the lower and upper walls are not $u=U$ and $u=0$, respectively. The CA simulation also captures the slip behavior of the granular flow, as seen in Fig. 8. However, the linearly decreasing trend of the curve looks more like that of a Newtonian Couette flow. It did not capture the nonshearing vertical region in the center. Figure 9 shows the solid fraction across the channel for the GKL model. The flow is dilute at the lower and upper walls because these walls are the major energy source and sink to the flowing granules. Consequently, the region farthest from the walls—the center region—is the most dense. This is also a common characteristic of granular flows in Couette cells. The solid fraction results of the

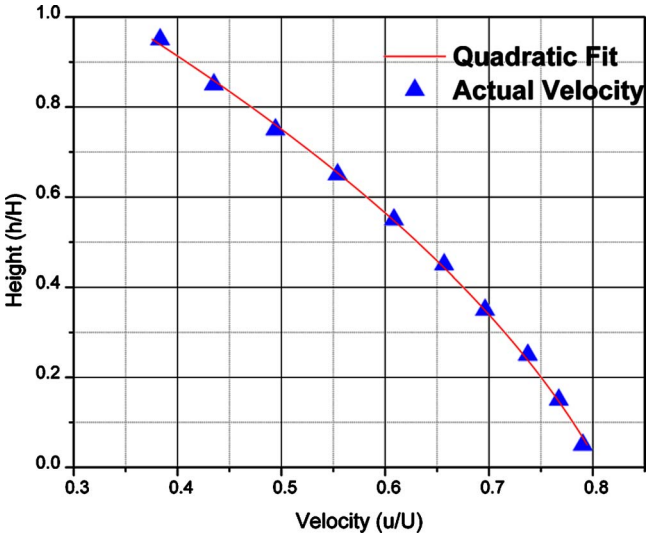


Fig. 8 Velocity versus height from CA model

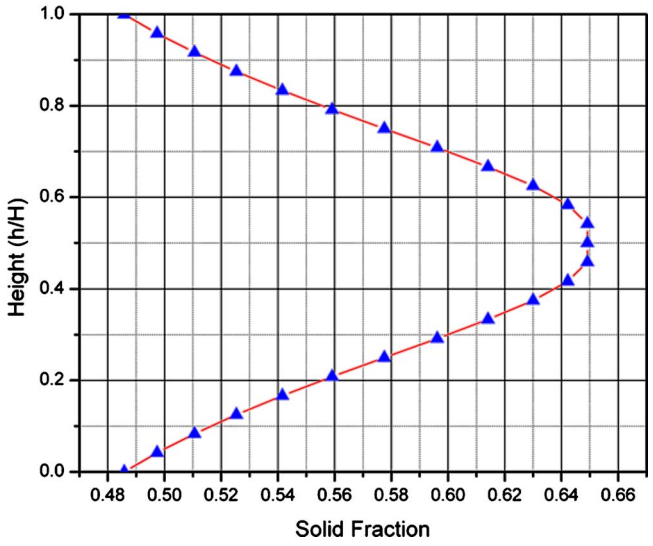


Fig. 9 Solid fraction versus height from theoretical model

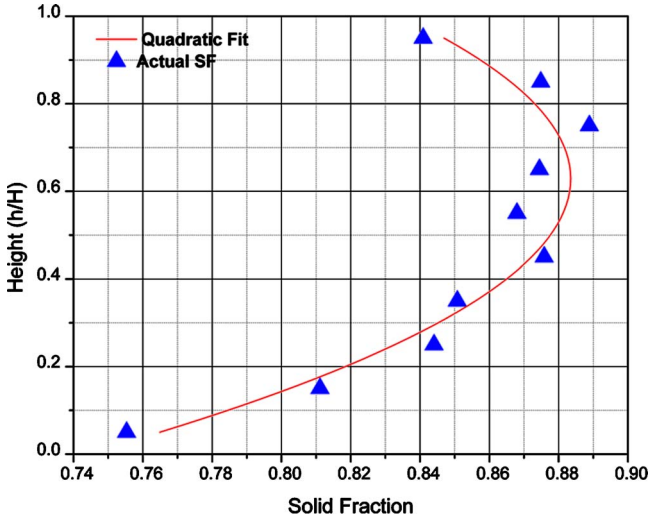


Fig. 10 Solid fraction versus height from CA model

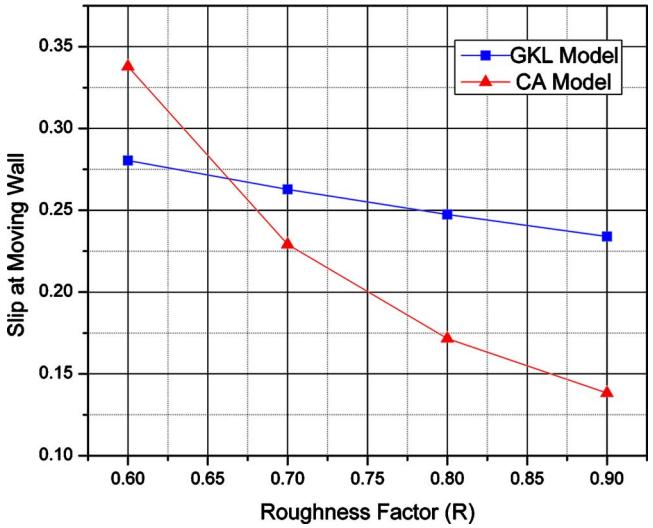


Fig. 11 Roughness factor versus slip from GKL model and CA model

CA simulation in Fig. 10 also capture the maximum solid fraction region. However, the profile is asymmetrical. The actual range is different for both the profiles, because CA simulation has rectangular particles. However they show that solid fractions are close to their maximum possible values at the center region. Figure 11 shows the variation of slip at the lower wall that is moving as the roughness factor R varies. Both the models show that the slip decreases with increased roughness, which is expected. The deviations in the results from the CA model are attributed to the fact that the simulation is discrete in nature and that the rules employed were based on the simplest understanding of colliding spheres. Thus, certain disagreements between the continuum and lattice-based CA results do not indicate that either model is flawed.

Conclusion

Granular flows are believed to macroscopically display continuum behavior over time, but this behavior is composed of interactions of discrete particles. In this work we describe the usefulness of employing CA, which is a discrete particle simulation technique, as a tool for modeling granular flows in lubrication-type systems. In the past, granular flows were modeled using continuum and molecular dynamics modeling approaches. The continuum modeling approach known as the granular kinetic lubrication (GKL) model has been successful at predicting trends gleaned from experiments conducted with granules in a Couette shear cell. The average velocity and solid fraction from CA simulations of granules in a Couette cell were compared to results from the GKL model. The trends have satisfactory agreement considering the following:

- the computational cost of employing CA to the granular flow problem is much more inexpensive than the continuum modeling approach;
- the simplicity of the rules describing local granular collisions yielding the correct global behavior;
- CA results for velocity capture the well-known slip behavior of granular flows near boundaries;
- CA results for solid fraction capture the well-known characteristic of the high concentration of granules in the center region, and a lower concentration of granules at the boundaries;
- CA results for slip versus roughness agrees with the GKL model;
- CA provides an alternative rule-based mathematics approach to elaborate first-principle physics-based differential equations.

Lattice-based cellular automata simulations have the potential for modeling complex systems where theoretical physics-based mathematical models prove computationally expensive or unsolvable. Using lattice-based cellular automata for modeling complex tribological systems, such as lubricating granular flows, could prove useful in providing answers where traditional tribology and physics-based models cannot.

Acknowledgment

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Nomenclature

d = diameter of the granules
H = height of the film
L = length of the film
U = velocity of the bottom wall
e_w = coefficient of restitution between the wall and the granules

e_p = coefficient of restitution between the granules
R = roughness factor of the wall
ν = solid fraction
u = mixture velocity of granules
u_p = velocity of discrete granular particle
u_s = slip velocity
B = coefficients from [2]

Subscripts

i = before the collision
f = after the collision
1 = first particle
2 = second particle

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