**Units/Parameters:**

In our simulations, we chose to express quantities in terms of three fundamental values: $m$ (particle mass), $d$ (particle diameter), and $\tau$ (timestep, which is equivalent to $(g/d)^{0.5}$, where $g$ is the acceleration due to gravity). Typical values of $d$ are $\sim1$ mm, which is the baseline value we used in testing. Particle masses are expected to be on the order of magnitude of $10^{-7}$ kg, based on this particle size. For a diameter $d$ of 1 mm, the simulation timestep $\tau$ is approximately 0.01 s. We also specify both normal and tangential components of an elastic constant $k$ and viscoelastic damping constant $\gamma$. In our model, the tangential component $k_t$ is $2/7 k_n$, and $\gamma_t = 1/2 \gamma_n$.

Although in our initial tests we have chosen somewhat general values, we will eventually consider materials feasible for manufacturing with specific $m$ and $k$. The materials we will consider are zirconia, acrylic, and melamine. These materials span a wide range of Young’s modulus values, and should yield varying results. Currently, we are using a normal elastic constant of 200,000 $mg/d$ for initial testing, as this value was appropriate for previous studies involving simulation of hopper flow of granular materials. Testing will determine whether or not this value is appropriate, and whether or not it can be reduced further without affecting the particle dynamics.

Based on the following calculations, our estimated $k$ values for the materials we are interested in could vary from $10^{10}$ to $10^{11} m/d\tau^2$. These are calculated from using the Young’s modulus, Poisson ratio $\nu$, and mass of each particle $m$. The normal and tangential elastic constants in the Hertzian model are calculated by $k_n = 4G/(3(1-\nu))$, where the shear modulus, $G = E/(2(1+\nu))$, and $k_t = 4G/(2-\nu)$. Tests will have to be done to determine if the particle dynamics are significantly affected by reducing $k$ for the simulations.

**Shear cell/Pouring routine:**

The shear cell is a well-established experimental geometry with which our simulation results can be compared. Our shear cell geometry is constructed in LAMMPS as a cylindrical region of granular particles of radius $36d$ and height $10d$, where $d$ is the diameter of the granular particles under consideration. The cylinder is centered around the $z$-axis with the base at $z = 0$. The top and bottom plates of the shear cell are modeled in LAMMPS with two extra cylindrical layers of particles of diameter $36d$ and height $2d$. By doing this, the top and bottom plates, which are subject to a prescribed displacement or force, have rough surfaces that make good contact with the particles in the cell. This apparatus is constructed by first pouring the particles into the shear cell from a height approximately two times the height of the shear cell. For the cell of height $14d$, the insertion region from which the particles fall (under the influence of gravity), is a cylindrical region from $z = 27$ to $z = 30$ of diameter $35.5d$ (to keep $d$ diameter particles from hitting the walls of the cell). Particles fill this region with a specified volume fraction (0.1) until the desired
number of particles have been inserted. The volume fraction can be increased to simulate a faster pouring rate, which is expected to reduce the packing fraction of the particles. The number of particles inserted is chosen based on the number of particles which is expected to fill the desired volume based on the random close pack arrangement for spheres (64%). For our default geometry, this is about 65,000 particles, a number which may vary depending on other considerations (see later sections). The particles interact with each other via a Hookean contact model for granular materials built into LAMMPS, and are assumed to interact with the walls of the shear cell by the same frictional interaction.

Cylindrical shear cell of radius $36d$ and height $14d$. The bottom plate remains fixed and the top plate undergoes a shearing motion.

Particles being poured into the shear cell.
Shearing motion:

After the particles are poured into the shear cell, the particles are separated into three categories: top plate, bottom plate, and free particles, as discussed above. The particles in the bottom plate remain fixed, while the particles in the top plate are subject to a constant external force acting downward on the plate. This force is the equivalent of a pressure of $3 \times 10^4$ Pa, and is an approximation of the vacuum pressure the particles will experience when the granular membrane cavity is evacuated. If we assume a particle density of 1000 kg/m$^3$, for the full-scale shear cell geometry, this is a downward force of $2.3328 \times 10^7 \frac{md}{\tau^2}$. With each timestep, the force from the particles on the plate is calculated, and the plate’s position is updated with a first-order integration scheme, which should be sufficient considering the relatively slow movement of the particles. The plate is assumed to be rigid, so all particles within the plate are subject to the same acceleration at each timestep. The plate is also twisted as specified by a period of oscillation $T$. The plate can move in two ways: continuous rotation or oscillation over a smaller angular range. The period specified either corresponds to the time for one continuous rotation, or one sinusoidal oscillation. The current baseline test runs with a timestep of $10^{-4} \tau$ for $2.5 \times 10^6$ timesteps, or 2.5 seconds, which rotates the plate through 180 degrees ($T = 500 \tau = 5$ s). The current oscillations have $T = 50 \tau$, which twists the plate at roughly the same angular velocity as the continuous rotation. During this shearing motion, the gravitational force applied in the pouring step is turned off, as we are primarily interested in a microgravity environment.

Preliminary Results:

So far, the simulations run have been somewhat of an exploratory exercise. Basically, our goal was to identify types of materials that exhibit different responses in the shear cell environment. We also wanted to identify what kinds of simplifications could be made to make our simulations more computationally tractable. In these initial tests, we considered a range of elastic constants, three different size geometries for the shear cell, gravity vs. no gravity, bidisperse vs. monodisperse compositions, different pouring rates, and continuous and oscillatory plate movement. Results are written to an output file every 100 timesteps, measuring the force and torque on the plate, as well as its position over time. We present some of the more interesting results from our initial analysis, which motivate further testing. We are primarily interested in the torque applied to the top plate in the z-direction, as this best characterizes the response of the granular material to the shearing force.
Geometric scaling:

Continuous rotation:
These simulations are run for a continuous half rotation for three different geometries: the full scale geometry specified previously, a half-radius version, and a half-scale version. The latter two have a modified external force \((5.832 \times 10^6 \text{ md/}t^2)\) that is scaled by the plate’s area to maintain equivalent pressure. These simulations used an elastic constant \(k = 200,000\).

For this first set of results, I will present all of the output data to illustrate a few ideas, but have truncated the subsequent results to highlight more interesting phenomena.

Force on plate vs. time (continuous rotation):

The above plots show the force acting on the top plate of the shear cell by the granular material. The three geometries are displayed in different colors as indicated by the legend. Note that the magnitude of the forces in the x and y-directions is two orders of magnitude smaller than the magnitude of the force in the z-direction. As discussed above, the reaction force of the granular material on the plate is smaller by a factor of four for the half-radius and half-scale configurations due to the external force being scaled by the area of the plate. While the forces in the z-direction reach an equilibrium value quickly, the forces in the x and y-directions are much more noisy due to the constant rotation of the plate. The initial damped oscillations in the force in the z-direction occur until the applied external force and the reaction force from the particles equilibrate. This effect is more pronounced for less stiff materials (lower elastic constant).
The above plots show the torques acting on the top plate by the granular material in the x, y, and z-directions. Again, the magnitude of the torque in the z-direction is much larger (one order of magnitude) than the torques in the z and y-directions. The main quantity of interest in our simulations is the torque in the z-direction, as it tells us how resilient the granular material is to our rotational shearing motion. We can see that initially, there is some transient effect, likely to do with initial rearrangement of the grains, that creates a greater torque response on the plate in the z-direction. The half-scale and half-radius geometries create a torque response in the z-direction that is one-eighth the response compared to the full-scale configuration. Dimensional analysis shows us that this is an expected result. Given that we are keeping the pressure constant, the force applied by the plate is a factor of four larger for the full-scale configuration. Additionally, another $r$ (radius) term contributes from the cross product of the radius with the force in the torque calculation. Thus, it is expected that the torque would scale as $r^3$. 
Displacement vs. time (continuous rotation):

The plots above show the position, velocity, and acceleration of the top plate in the z-direction. As in the plots before, we can see the transient damped oscillations in all three plots before equilibrium values are reached. The differences in the equilibrium z-position reached in the top graph could have to do with either the depth or width of the shear cell.

**Oscillatory motion**

For these simulations, we oscillated the top plate with a frequency of 50 $\tau$ for the three different configurations, as specified above. These simulations used $k = 2,000,000$ because upon running simulations for lower elastic constants, the particles were found to leave the system due to the extreme forces imposed on them.

**Torque (z-direction) vs. time (oscillatory motion):**
The plot above shows the torque response from three different scale configurations for oscillatory motion of the top plate. The torque changes direction along with the oscillation of the top plate. Interestingly, as with the continuous rotation, the torque for the half-scale and half-radius configurations appear to be the same. Previous studies have shown that the structure of packings, and thus the torque response, can change drastically over a very long period of shearing (for both oscillatory motion and continuous rotation). Seeing similar behaviors in all three geometries is useful, as our scaled down geometry could run for longer time periods much quicker.

Shown above are the three geometrical configurations of the cylindrical shear cell.
Different elastic constants:

Continuous rotation:
The following simulations are for continuous rotation with elastic constants of 40,000 (low $k$), 200,000 (medium $k$), and 2,000,000 (high $k$). While less accurate, the purpose of lowering the elastic constant from its true value is that it allows us to increase the timestep, speeding up the simulation. The timestep scales as $k^{1/2}$, so appropriate timesteps for the three simulations are 0.0002 \( \tau \), 0.0001 \( \tau \), and 0.000025 \( \tau \), respectively. The number of timesteps was altered accordingly to ensure the same simulation time for each.

Torque (z-direction) vs. time (continuous rotation):

Displacement (z-direction) vs. time (continuous rotation):

The two plots above illustrate some problems with using a smaller (less stiff) elastic constant. The elastic constants of 2,000,000; 200,000; and 40,000 are plotted in red, blue, and green, respectively. As the elastic constants are increased, there seems to be some convergence towards a torque value. Ideally, the elastic constant that we choose would not alter the torque response too much from the true value. An effect that is better seen in our simulation movies is that lower elastic constants make the material less stiff. In the second plot, this is seen in the larger and longer lasting damped oscillations of the plate displacement in the z-direction at the beginning of the simulation. Additionally, the displacement towards which the plate equilibrates is much different due to the amount the material ‘gives’ under pressure. This will significantly affect another value that we are interested observing over time, the packing fraction.
The previous two pictures illustrate some of the complications when dealing with lower elastic constants. I first tried to use a constant an order of magnitude lower than the medium $k$ value (20,000), but ran into problems with particles leaving the system. I eventually settled on using a slightly higher elastic constant, $k = 40,000$. Still, the less stiff elastic constants created large forces on certain particles, which would force them out of the system. I first tried to increase the thickness of the top plate to prevent particles from leaving the cell at the top, but the particles still escaped through the top and sides. I attempted to see if lowering the timestep would help remedy the problem, but this is wrongheaded, as the entire point of low $k$ values was to increase the timestep. The first picture shows a particle forced out on the right side of the system (this is much more easily observed in simulation videos). The second image illustrates another issue which happens for low $k$ values, the top plate bursting. Intuitively, the clean break lines seem to hint at some error related to the way MPI distributes the particles across processes. I have been able to resolve similar problems by simply running the simulation on a single process, however the nature of this problem may point to some other issue, or simply indicate the $k$ is too low in this case. It is possible that the low $k$ values create very large forces, leading to a buffer overflow or some other memory issue. This problem is not especially worrisome since it only occurs for physically unrealistic systems.
As a note, initially using $k = 20,000$ would cause the simulation to blow up immediately, which I was able to resolve by applying a gradual, linearly increasing applied force to the top plate over the first 10,000 timestep. This is just an extreme case of the damped oscillations seen at the start of many of the simulations.

**Bidisperse composition:**

A bidisperse simulation with 50-50 composition of particles with $d = 1.2$ mm and $d = 0.8$ mm is compared with a monodisperse continuous rotation. These simulations used $k = 200,000$.

**Torque (z-direction) vs. time (continuous rotation)**

The plot above is the torque in the z-direction measured for a monodisperse vs. a bidisperse packing. Although the composition in the bidisperse was chosen without much consideration, we immediately see a noticeable difference in the torque. All other measured values were virtually identical. This is an area that is ripe for further exploration, as we can explore many different packing configurations with different particle diameters and percent compositions. For our partners at Bethcare, it is a clear demonstration for their investors relatively simple changes to the granular material can change its properties.

The image above shows a poured bidisperse composition of $d = 0.8$ mm and $d = 1.2$ mm.
Faster pouring/Lower packing fraction:

These simulations compare two compositions with different packing fractions. The cell that was created with a faster pouring rate (inserted into the cell with a higher volume fraction or density), which leads to a lower packing fraction. These simulations used $k = 200,000$.

Displacement (z-direction) vs. time (continuous rotation):

The above plot shows the displacement in the z-direction of the top plate during shearing after a normal pour and a faster pour. The faster pouring rate uses an volume fraction of 0.2 for particle insertion compared to 0.1 for the normal pouring rate. Although there was no discernible difference in the torque response of the plate, the plot above does show that a different pouring rate leads to a different plate displacement, which could be a result of a change in the packing fraction. However, given that the plate particles are frozen into place after the pouring step according to their position ($z > 12$ and $z < 2$), we would be comparing two compositions with different packing fractions but also different numbers of particles. Also, the surface profile of the plates (mainly to top plate) would be significantly different. If we wanted a better comparison of the role of the packing fraction alone, we would have to modify the method of initialization of our simulation.

The above two pictures show the cell after regular and faster pours, respectively. It is hard to notice a difference, but the second cell should have a lower packing fraction.
Gravity:

These simulations show a continuous rotation with $k = 200,000$ with gravity compared to the microgravity environment (no gravity) used for all other simulations.

Torque (z-direction) vs. time (continuous rotation):

The plot above shows that there is no significant difference in the torque response in the z-direction of our shear cell with gravity compared with no gravity. This is likely due to the fact that the force applied to the top plate is much greater than the force of gravity on the particles, so there is not much difference in the way the particles behave. If we were to reduce the force applied to the top plate, we would likely see a difference in the torque response.

Future plans:

From our preliminary results, we have identified a few key areas that warrant further exploration. After meeting with our collaborators at Bethcare, we have decided to further explore the torque response of a shear cell consisting of a wide variety of bidisperse particle configurations, such as different size particles and different percent compositions. This should yield some interesting scientific results, as well as provide useful insight for potential prosthetic membrane materials. We are also interested in how the long-term structure of the packing evolves using longer simulations (currently our simulations only run for several seconds). In order to do this, we will need more computing power, so I am looking to get our simulations running on Harvard’s research computing clusters. To analyze the structure of the packing, we will use a Voronoi tessellation package for post-processing.

If there is time, some other things that could be considered are the effects of gravity under a lower force applied to the top plate, the effect of the number of particle layers in the shear cell, particle-level wear, and more realistically modeling bottom layer of the plate (it is currently a very uniform, non-random packing because it is formed from the first particles poured into the cell).