

PEBBLES Operation and Theory Manual

Joshua Cogliati
Abderrafi Ougouag

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INL/EXT-10-19305: PEBBLES Operation and Theory Manual

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Chapter 1

Overview of PEBBLES

The PEBBLES code is a computer program designed to simulation the motion, packing and vibration of spheres that undergo various mechanical forces including gravitation, Hooke's law force and various friction forces. The frictional forces include true static friction that allows non-zero angles of repose. Each pebble is individually simulated using the distinct element method.

Chapter 2

Overview of Running PEBBLES

Running PEBBLES generally requires three things. First is the geometry specification that describes the arrangement of the container for the vessel. Next is any type of motion inducing parameters such as an earthquake simulation or recirculation of the pebbles. Last are the tallies of variables that are desired. Sometimes multiple simulations are chained together manually, for example a recirculation that outputs the save data followed by a second run of PEBBLES that loads the data and simulates an earthquake.

Several simulation types that are supported by PEBBLES. The first is simulations to determine the effects and parameters of the recirculation. The second is to investigate packing arrangements of the pebbles. The third is to simulate the effects of vibration motion on the vessel. For all of these, a variety of tally types are provided including dust production estimation, force tallying, velocity tallying and also the raw position data is available.

Chapter 3

Theory

3.1 Overview of History of granular and Pebble simulation

A variety of simulations of the motion of discrete elements have been created for different purposes. Lu, Abdou and Ying applied a discrete element method (DEM) to determine the characteristics of packed beds used as fusion reactor blankets[13]. Jullien, Pavlovitch and Meakin used a DEM to determine packing fractions for spheres using different non-motion methods[14]. Soppe used a rain method (lower spheres down until they reach other ones) to determine pore structures in different sized spheres[15]. Freund et al. used a rain method for fluid flow for chemical processing[16].

Kohring created a 3-D discrete element method simulation to study diffusional mixing and provided the time derivatives for the simulation, but not the details of the calculation of static friction[17]. Haile discusses both how to simulate hard spheres (which is impractical for many PEBBLES simulations due to the frequent and continuous contact between spheres) and soft spheres using just the potential energy which is insufficient for modeling the motion[18]. The dissertation by Ristow described multiple methods for simulation of granular materials. On Ristow's list was a model similar to that used in the preliminary work supporting this proposal. Ristow's dissertation provided an overview of simulating static friction[19]. Vu-Quoc and Zhang created a model for particle flow simulations which was used for simulation of particle flow in chutes[20]. Their model included a detailed description of static friction calculation that was computationally tractable yet still based on the complete and complicated friction model of Mindlin and Deresiewicz[5]. To determine particle flows, Wait developed a discrete element method which included dynamic friction, but the model did not include static friction[21]. Multiple other discrete element codes have been created, and PEBBLES is similar to several of the full motion models.

3.2 Methods of simulation of dynamic effects

The PEBBLES simulation tracks each individual pebble's velocity, position, angular velocity and static friction loadings. The following classical mechanics differential equations are used for calculating the time derivatives of those variables:

$$\frac{d\mathbf{v}_i}{dt} = \frac{m_i \mathbf{g} + \sum_{i \neq j} \mathbf{F}_{ij} + \mathbf{F}_{ci}}{m_i} \quad (3.1)$$

$$\frac{d\mathbf{p}_i}{dt} = \mathbf{v}_i \quad (3.2)$$

$$\frac{d\omega_i}{dt} = \frac{\sum_{i \neq j} \mathbf{F}_{\parallel ij} \times r_i \hat{\mathbf{n}}_{ij} + \mathbf{F}_{\parallel ci} \times r_i \hat{\mathbf{n}}_{ci}}{I_i} \quad (3.3)$$

$$\frac{ds_{ij}}{dt} = \mathbf{S}(\mathbf{F}_{\perp ij}, \mathbf{v}_i, \mathbf{v}_j, \mathbf{p}_i, \mathbf{p}_j, \mathbf{s}_{ij}) \quad (3.4)$$

where \mathbf{F}_{ij} is the force from pebble j on pebble i , \mathbf{F}_{ci} is the force of the container on pebble i , \mathbf{g} is the gravitational acceleration constant, m_i is the mass of pebble i , \mathbf{v}_i is the velocity of pebble i , \mathbf{p}_i is the position vector for pebble i , ω_i is the angular velocity of pebble i , $\mathbf{F}_{\parallel ij}$ is the tangential force between pebbles i and j , $\mathbf{F}_{\perp ij}$ is the perpendicular force between pebbles i and j , r_i is the radius of pebble i , I_i is the moment of inertia for pebble i , $\mathbf{F}_{\parallel ci}$ is the tangential force of the container on pebble i , $\hat{\mathbf{n}}_{ci}$ is the unit vector normal to the container wall on pebble i , $\hat{\mathbf{n}}_{ij}$ is the unit vector pointing from the position of pebble i to that of pebble j , \mathbf{s}_{ij} is the current static friction loading between pebbles i and j , and \mathbf{S} is the function to compute the change in the static friction loading. The static friction model contributes to the $\mathbf{F}_{\parallel ij}$ term which is also part of the \mathbf{F}_{ij} term. Figure 3.1 illustrates the principal vectors with pebble i going in the \mathbf{v}_i direction and rotating around the ω_i axis, and pebble j going in the \mathbf{v}_j direction and rotating around the ω_j axis.

The mass and moment of inertia are calculated assuming spherical symmetry and allowing for the spheres to have a different density in an inner spherical core. With this assumption the following equations hold:

$$m = \frac{4}{3}\pi [\rho_c r_c^3 + \rho_o (r_o^3 - r_c^3)] \quad (3.5)$$

$$I = \frac{8}{15}\pi [\rho_c r_c^5 + \rho_o (r_o^5 - r_c^5)] \quad (3.6)$$

where r_c is the radius of inner zone of the pebble, r_o is the radius of whole pebble, ρ_c is the average density of center region and ρ_o is the average density of outer region. For example, a tennis ball would have an effectively zero density center region since they are hollow.

The dynamic (or kinetic) friction model is based on the model described by Wait[12]. Wait's and PEBBLES model calculates the dynamic friction using

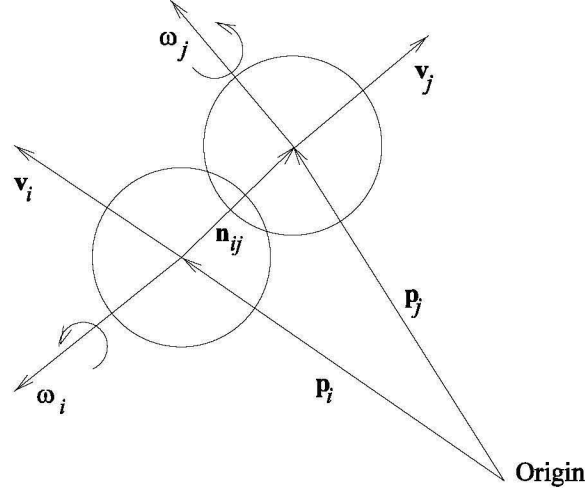


Figure 3.1: Principle Vectors in the Interaction of Two Pebbles

a combination of the relative velocities and pressure between the pebbles, as shown in Equations (3.7) and (3.8):

$$\mathbf{F}_{\perp ij} = h l_{ij} \hat{\mathbf{n}}_{ij} - C_{\perp} \mathbf{v}_{\perp ij}, l_{ij} > 0 \quad (3.7)$$

$$\mathbf{F}_{d\parallel ij} = -\min(\mu |\mathbf{F}_{\perp ij}|, C_{\parallel} |\mathbf{v}_{\parallel ij}|) \hat{\mathbf{v}}_{\parallel ij}, l_{ij} > 0 \quad (3.8)$$

where C_{\parallel} is the tangential dashpot constant, C_{\perp} is the normal dashpot constant, $\mathbf{F}_{\perp ij}$ is the normal force between pebbles i and j , $\mathbf{F}_{d\parallel ij}$ is the tangential dynamic friction force between pebbles i and j , h is the normal Hooke's law constant, l_{ij} is the overlap between pebbles i and j , $\mathbf{v}_{\parallel ij}$ is the component of the velocity between two pebbles perpendicular to the line joining their centers, $\mathbf{v}_{\perp ij}$ is the component of the velocity between two pebbles parallel to the line joining their centers, \mathbf{v}_{ij} is the relative velocity between pebbles i and j and μ is the kinetic friction coefficient. Equations (3.9-3.12) relate supplemental variables to the primary variables:

$$\mathbf{F}_{ij} = \mathbf{F}_{\perp ij} + \mathbf{F}_{\parallel ij} \quad (3.9)$$

$$\mathbf{v}_{\perp ij} = (\mathbf{v}_{ij} \cdot \hat{\mathbf{n}}_{ij}) \hat{\mathbf{n}}_{ij} \quad (3.10)$$

$$\mathbf{v}_{\parallel ij} = \mathbf{v}_{ij} - \mathbf{v}_{\perp ij} \quad (3.11)$$

$$\mathbf{v}_{ij} = (\mathbf{v}_i + \omega_i \times \mathbf{r}_i \hat{\mathbf{n}}_{ij}) - (\mathbf{v}_j + \omega_j \times \mathbf{r}_j \hat{\mathbf{n}}_{ji}) \quad (3.12)$$

The friction force is then bounded by the friction coefficient and the normal force, to prevent it from being too great:

$$\mathbf{F}_{f\parallel ij} = \mathbf{F}_{s\parallel ij} + \mathbf{F}_{d\parallel ij} \quad (3.13)$$

$$\mathbf{F}_{\parallel ij} = \min(\mu|\mathbf{F}_{\perp ij}|, |\mathbf{F}_{f\parallel ij}|)\hat{\mathbf{F}}_{f\parallel ij} \quad (3.14)$$

where $\mathbf{F}_{s\parallel ij}$ is the static friction force between pebbles i and j , $\mathbf{F}_{d\parallel ij}$ is the kinetic friction force between pebbles i and j , h_s is the coefficient for force from slip, s_{ij} is the slip distance perpendicular to the normal force between pebbles i and j , v_{\max} is the maximum velocity under which static friction is allowed to operate, and μ is the static friction coefficient when the velocity is less than v_{\max} and the kinetic friction coefficient when the velocity is greater. These equations fully enforces the first requirement of a static friction method, $|\mathbf{F}_s| \leq \mu|\mathbf{F}_{\perp}|$.

3.3 Integration

When all the position, linear velocity, angular velocity and slips are combined into a vector \mathbf{y} , the whole computation can be written as a differential formulation in the form:

$$\mathbf{y}' = \mathbf{f}(t, \mathbf{y}) \quad (3.15)$$

$$\mathbf{y}(t_0) = \mathbf{y}_0 \quad (3.16)$$

This can be solved by a variety of methods with the simplest being Euler's method:

$$\mathbf{y}_1 = \mathbf{y}_0 + \Delta t \mathbf{f}(t, \mathbf{y}_0) \quad (3.17)$$

In addition, both the Runge-Kutta method and the Adams-Moulton method can be used for solving this equation. These methods improve the accuracy of the simulation. However, they do not improve the wall-clock time at the lowest stable simulation, since the additional time required for computation negates the advantage of being able to use somewhat longer time-steps. In addition, when running on a cluster, more data needs to be transferred since the methods allow non-contacting pebbles to affect each other in a single 'time-step calculation'.

3.4 Geometry equations

For any geometry interaction, two things need to be calculated, the overlap distance l (or, technically, the mutual approach of distant points) and the normal to the surface \hat{n} . The input is the radius of the pebble r and the position of the pebble, \mathbf{p} with components \mathbf{p}_x , \mathbf{p}_y , and \mathbf{p}_z

For the floor contact this is:

$$l = (\mathbf{p}_z - r) - \text{floor_location} \quad (3.18)$$

$$\hat{n} = \hat{z} \quad (3.19)$$

For cylinder contact on the inside of a cylinder this is:

$$pr = \sqrt{\mathbf{p}_x^2 + \mathbf{p}_y^2} \quad (3.20)$$

$$l = (pr + r) - \text{cylinder_radius} \quad (3.21)$$

$$\hat{n} = \frac{-\mathbf{p}_x}{pr} \hat{x} + \frac{-\mathbf{p}_y}{pr} \hat{y} \quad (3.22)$$

For cylinder contact on the outside of a cylinder this is:

$$pr = \sqrt{\mathbf{p}_x^2 + \mathbf{p}_y^2} \quad (3.23)$$

$$l = \text{cylinder_radius} + r - pr \quad (3.24)$$

$$\hat{n} = \frac{\mathbf{p}_x}{pr} \hat{x} + \frac{\mathbf{p}_y}{pr} \hat{y} \quad (3.25)$$

For contact on the inside of a cone defined by the $\text{radius} = mz + b$:

$$pr = \sqrt{\mathbf{p}_x^2 + \mathbf{p}_y^2} \quad (3.26)$$

$$z_c = \frac{m(pr - b) + z}{m^2 + 1} \quad (3.27)$$

$$r_c = mz_c + b \quad (3.28)$$

$$x_c = (r_c/pr) \mathbf{p}_y \quad (3.29)$$

$$y_c = (r_c/pr) \mathbf{p}_x \quad (3.30)$$

$$\mathbf{c} = x_c \hat{x} + y_c \hat{y} + z_c \hat{z} \quad (3.31)$$

$$d = \mathbf{p} - \mathbf{c} \quad (3.32)$$

$$l = |d| + r, r_c < pr \quad (3.33)$$

$$\hat{n} = -\hat{d}, r_c < pr \quad (3.34)$$

$$l = r - |d|, r_c \geq pr \quad (3.35)$$

$$\hat{n} = \hat{d}, r_c \geq pr \quad (3.36)$$

These equations are derived from minimizing the distance between the contact point \mathbf{c} and the pebble position \mathbf{p} .

For contact on a plane defined by $ax + by + cz + d = 0$ where the equation has been normalized so that $a^2 + b^2 + c^2 = 1$, the following is used:

$$dp = a\mathbf{p}_x + b\mathbf{p}_y + c\mathbf{p}_z + d \quad (3.37)$$

$$l = r - dp \quad (3.38)$$

$$\hat{n} = a\hat{x} + b\hat{y} + c\hat{z} \quad (3.39)$$

3.5 Simulation of Static Friction

The static friction model has two key tasks: the force from stuck slip must be updated based on relative motion of the pebbles, and the current direction of the force must be calculated, since the pebbles can rotate in space.

3.5.1 Use of Parallel Velocity for Slip Updating

The true method for updating the stuck slip force of elastic spheres is to use the R. D. Mindlin and H. Deresiewicz method[5], which requires computationally and memory intensive calculations to track the forces. However, a simpler method described by Cundall and Strack[6], uses the integration of the parallel relative velocity as the displacement, is used to approximate the force. The essential idea is that the farther the pebbles have stuck slipped at the contact point, the greater the counteracting static friction force needs to be. This is what happens under more accurate models such as Mindlin and Deresiewicz. This assumption imposes two approximations: (1) the amount that the force changes is independent of the normal force, (2) the true hysteretic effects, which depend on loading history details, are ignored. For simulations where the exact dynamics of static friction are important, these could potentially be serious errors. However, since static friction only occurs when the relative speed is low, the dynamics of the simulation are usually unimportant. Thus, for most circumstances, the approximation that can be used to describe the rate of change of the magnitude and non-rotational change of the stuck slip is

$$\frac{ds_{ij}}{dt} = \mathbf{v}_{\parallel ij}. \quad (3.40)$$

Vu-Quoc, Zhang, and Walton developed a 3-D discrete-element method for granular flows[7]. They used a simplification of the Mindlin and Deresiewicz model for calculating the stuck slip magnitude, and projected the stuck slip onto the tangent plane for each time step to rotate the stuck slip force direction. This correctly rotates the stuck slip, but requires that the rotation of the stuck slip be done as a separate step since this is not written in a differential form.

Silbert et al. describe a 3-D differential version of the Cundall and Strack method[8, 9]. The literature states that particle wall interactions are done identically to the particle-to-particle interactions (with no derivation or justification provided). The amount of computation of the model is less than the Vu-Quoc, Zhang, and Walton model. This model was used to model pebble bed flow[10, 11].

3.5.2 Rotation of Stuck Slip

The static friction force must also be rotated so that it is in the plane of contact between the two pebbles. When there is a difference between the pebbles' center velocities, which changes in the relative pebble center location, change in the direction in the stuck-slip occurs. That is:

$$\mathbf{p}_{in+1} - \mathbf{p}_{jn+1} \approx \mathbf{p}_{in} - \mathbf{p}_{jn} + (\mathbf{v}_{in} - \mathbf{v}_{jn})\Delta t \quad (3.41)$$

First, let $\mathbf{n}_{ijn} = \mathbf{p}_i - \mathbf{p}_j$ and $d\mathbf{n}_{ijn} = \mathbf{v}_i - \mathbf{v}_j$. The cross product $-d\mathbf{n}_{ijn} \times \mathbf{n}_{ijn}$ is perpendicular to both \mathbf{n} and $d\mathbf{n}$ and signed to create the axis around which \mathbf{s} is rotated in a right-handed direction. Then, using the cross product of the axis and \mathbf{s} , $-(d\mathbf{n}_{ijn} \times \mathbf{n}_{ijn}) \times \mathbf{s}_{ijn}$ gives the correct direction that \mathbf{s} should be increased.

Next, determine the factors required to make the differential the proper length. By cross product laws,

$$|-(d\mathbf{n}_{ijn} \times \mathbf{n}_{ijn}) \times \mathbf{s}_{ijn}| = |d\mathbf{n}_{ijn}| |\mathbf{n}_{ijn}| |\mathbf{s}_{ijn}| \sin \theta \sin \phi \quad (3.42)$$

where θ is the angle between \mathbf{n}_{ijn} and $d\mathbf{n}_{ijn}$, and ϕ is the angle between $d\mathbf{n}_{ijn} \times \mathbf{n}_{ijn}$ and \mathbf{s}_{ijn} . The relevant vectors are shown in Figure 3.2.

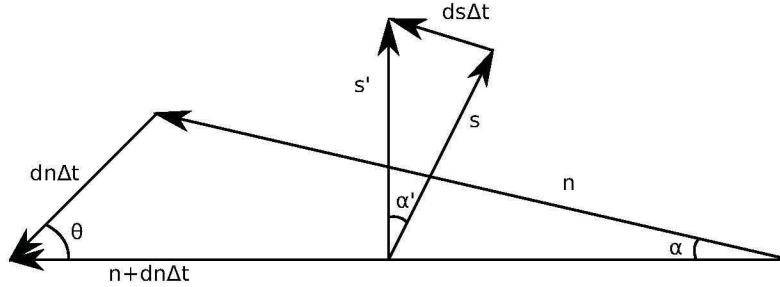


Figure 3.2: Static Friction Vectors

The goal is to rotate \mathbf{s} by angle α' , which is the 'projection' into the proper plane of angle α that \mathbf{n} rotates by. Since the direction has been determined, for simplicity the figure leaves the indexes off, and concentrates on determining the lengths. In Figure 3.2, \mathbf{s} is the old slip vector, \mathbf{s}' is the new slip vector, \mathbf{n} is the vector pointing from one pebble to another. The vector $d\mathbf{n}\Delta t$ is added to \mathbf{n} to get the new \mathbf{n}' , $\mathbf{n} + d\mathbf{n}\Delta t$. The initial condition is that \mathbf{s} and \mathbf{n} are perpendicular. The final conditions are that \mathbf{s}' and \mathbf{n}' are perpendicular, and that \mathbf{s} and \mathbf{s}' are the same length and that \mathbf{s}' is the closest vector to \mathbf{s} as it can be while satisfying the other conditions. There is no requirement that \mathbf{s} or \mathbf{s}' are coplanar with $d\mathbf{n}\Delta t$ (otherwise α' would be equal to α). From the law of sines we have:

$$\frac{|d\mathbf{n}\Delta t|}{\sin \alpha} = \frac{|\mathbf{n}|}{\sin \theta} \quad (3.43)$$

so

$$\sin \alpha = \frac{|d\mathbf{n}\Delta t| \sin \theta}{|\mathbf{n}|}, \quad (3.44)$$

The projection to the correct plane occurs in Figure 3.3. First, by using ϕ , the length of \mathbf{s} is projected to the plane. Note that ϕ is the angle both to \mathbf{s} and to \mathbf{s}' . So, the length of the line on the $d\mathbf{n} \times \mathbf{n}$ plane is $|\mathbf{s}| \sin \phi$, and the length of the straight line at the end of the triangle is $|\mathbf{s}| \sin \phi \sin \alpha$ (note that the chord length is $|\mathbf{s}|(\sin \phi)\alpha$, but as Δt approaches 0 the other can be used). From these calculations, the length of the $d\mathbf{s}\Delta t$ can be calculated with the following formula:

$$d\mathbf{s}\Delta t = \frac{|\mathbf{s}| \sin \phi |d\mathbf{n}\Delta t| \sin \theta}{|\mathbf{n}|}, \quad (3.45)$$

Since $|-(d\mathbf{n}_{ij} \times \mathbf{n}_{ijn}) \times \mathbf{s}_{ijn}| = |d\mathbf{n}_{ij}| |\mathbf{n}_{ijn}| |\mathbf{s}_{ijn}| \sin \theta \sin \phi$, the formula for the rotation is

$$\mathbf{s}_{ijn+1} = -\frac{(d\mathbf{n}_{ijn} \times \mathbf{n}_{ijn}) \times \mathbf{s}_{ijn}}{|\mathbf{n}|^2} \Delta t + \mathbf{s}_{ijn}. \quad (3.46)$$

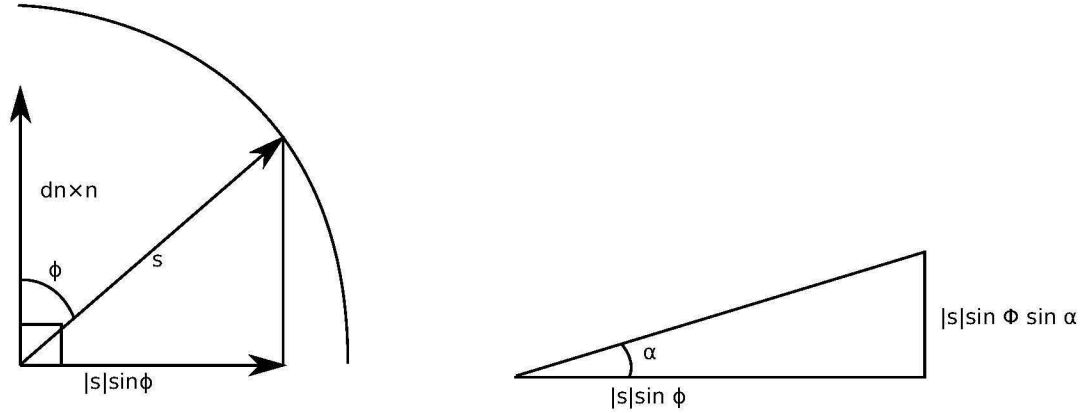


Figure 3.3: Projections to $d\mathbf{s}$

As a differential equation this is

$$\frac{d\mathbf{s}_{ij}}{dt} = -\frac{[(\mathbf{v}_i - \mathbf{v}_j) \times (\mathbf{p}_i - \mathbf{p}_j)] \times \mathbf{s}_{ij}}{|\mathbf{p}_i - \mathbf{p}_j|^2}. \quad (3.47)$$

By the vector property $a \times (b \times c) = b(a \cdot c) - c(a \cdot b)$ and, since $(\mathbf{p}_i - \mathbf{p}_j) \cdot \mathbf{s}_{ij} = 0$, this can be rewritten per the version in Silbert et al. as

$$\frac{d\mathbf{s}_{ij}}{dt} = -\frac{(\mathbf{p}_i - \mathbf{p}_j)(\mathbf{s}_{ij} \cdot (\mathbf{v}_i - \mathbf{v}_j))}{|\mathbf{p}_i - \mathbf{p}_j|^2}. \quad (3.48)$$

Differential Equation for Surface Slip Rotating

It might seem that the wall interaction could be modeled the same way as the pebble-to-pebble interaction. For sufficiently simple wall geometries this may be possible, but more complicated vessel geometries violate some of the assumptions that underpin the derivation. For a flat surface, there is no rotation, so the formula can be entirely dropped. For a spherical surface, it would be possible to measure the curvature at pebble to surface contact point in the direction of relative velocity to the surface. This curvature could then be used as an effective radius in the pebble-to-pebble formulas.

Vessel walls allowed in PEBBLES can have additional features that violate assumptions made for the derivation. For surfaces such as a cone, the curvature is not in general constant, because the path can follow elliptical curves. As well, the curvature has discontinuities where different parts of the vessel join together (for example, in a transition from the outlet cone to the outlet chute). At these transitions, the assumption that the slip stays parallel to the surface fails because the slip is parallel to the old surface, but the new surface has a different normal.

The PEBBLES code uses an approximation of the rotation delta to deal with complications with using the pebble-to-pebble interaction. This is similar to the Vu-Quoc et al[7]. method of adjusting the slip so that it is parallel to the surface each time. Every time the slip is used, a temporary version properly aligned to the surface is computed and used for the force. When the derivatives are calculated, a rotation to move the slip to be more parallel to the surface is computed as described in the next paragraph.

The rotation is computed as follows. Let the normal direction of the wall at the point of contact of the pebble be \mathbf{n} , and the old stuck-slip be \mathbf{s} . Let a be the angle between \mathbf{n} and \mathbf{s} . $\mathbf{n} \times \mathbf{s}$ is perpendicular to both \mathbf{n} and \mathbf{s} and so this cross product is the axis that needs to be rotated around. Then $(\mathbf{n} \times \mathbf{s}) \times \mathbf{s}$ is perpendicular to this vector, so it is either pointing directly towards \mathbf{n} if a is acute or directly away from \mathbf{n} if a is obtuse. To obtain the correct direction, this vector is multiplied by the scalar $\mathbf{s} \cdot \mathbf{n}$ which has the correct sign from $\cos a$. The magnitude of $(\mathbf{s} \cdot \mathbf{n})[(\mathbf{n} \times \mathbf{s}) \times \mathbf{s}]$ needs to be determined for reasonableness. We define the angle b , which is between $(\mathbf{n} \times \mathbf{s})$ and \mathbf{s} . By these definitions the magnitude is $(|\mathbf{s}||\mathbf{n}|\cos a)[(|\mathbf{n}||\mathbf{s}|\sin a)|\mathbf{s}|\sin b]$. b is a right angle since $\mathbf{n} \times \mathbf{s}$ is perpendicular to \mathbf{s} , so $\sin b = 1$. Collecting terms gives the magnitude as $|\mathbf{s}|^3|\mathbf{n}|^2\cos a\sin a$ which is divided by $|\mathbf{n} \times \mathbf{s}||\mathbf{n}||\mathbf{s}|$ to give the full term the magnitude $|\mathbf{s}|\cos a$. This is the length of the vector that goes from \mathbf{s} to the plane perpendicular to \mathbf{n} . This produces Equation 3.49, which can be used to ensure that the wall stuck-slip vector rotates towards the correct direction.

$$\frac{d\mathbf{s}}{dt} = (\mathbf{s} \cdot \mathbf{n}) \frac{[(\mathbf{n} \times \mathbf{s}) \times \mathbf{s}]}{|\mathbf{n} \times \mathbf{s}||\mathbf{n}||\mathbf{s}|} \quad (3.49)$$

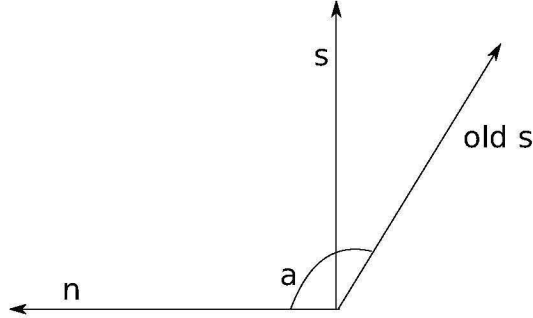


Figure 3.4: Static friction vectors for wall

3.5.3 Use of Slip

The value of the slip is used to calculate the force of static friction as in

$$\mathbf{F}_{s\parallel ij} = -h_s \mathbf{s}_{ij}, |\mathbf{v}_{v\parallel ij}| < v_{max}. \quad (3.50)$$

The friction force is then bounded by the friction coefficient and the normal force, to prevent it from being too great as

$$\mathbf{F}_{f\parallel ij} = \mathbf{F}_{s\parallel ij} + \mathbf{F}_{d\parallel ij} \quad (3.51)$$

and

$$\mathbf{F}_{\parallel ij} = \min(\mu |\mathbf{F}_{\perp ij}|, |\mathbf{F}_{f\parallel ij}|) \hat{\mathbf{F}}_{f\parallel ij} \quad (3.52)$$

where $\mathbf{F}_{s\parallel ij}$ is the static friction force between pebbles i and j , $\mathbf{F}_{d\parallel ij}$ is the kinetic friction force between pebbles i and j , h_s is the coefficient for force from slip, \mathbf{s}_{ij} is the slip distance perpendicular to the normal force between pebbles i and j , v_{max} is the maximum velocity under which static friction is allowed to operate, and μ is the static friction coefficient when the velocity is less than v_{max} and the kinetic friction coefficient when the velocity is greater. These equations fully enforces the first requirement of a static friction method, $|\mathbf{F}_{\parallel}| \leq \mu |\mathbf{F}_{\perp}|$.

Chapter 4

Input Description

4.1 Introduction

directive *var1 var2*

Default: **directive** *num1 num2*

The variables are numbers input, and the default is what happens if no directive is given.

done

Terminates input and starts the program running. This is the only mandatory part of the input. Multiple done commands have no effect.

rem *stuff*

Remark. Allows comments in the input file. Allows commenting out lines. Ignored by pebbles.

4.2 Parameters

runs *number*

Default: **runs** *10000*

How many time-steps are run. This multiplied by alpha gives the total time that the simulation simulates.

number_of_pebbles *number*

Default: **number_of_pebbles** *1000*

The total number of pebbles in the simulation.

initial_time *time*

Default: **initial_time** *0.0*

The initial time used to start the simulation. This will allow the various times to be modified, such as the earthquake start times and such.

kinetic_friction *friction_coefficient*
Default: **kinetic_friction** 0.1

The kinetic friction coefficient.

static_friction_new *friction_coefficient static_friction_hooke velocity_max_sqr*

The static friction coefficients. The *friction_coefficient* limits the amount of friction to *friction_coefficient*normal_force*. The *static_friction_hooke* is how much force there is related to the distance slipped. The *velocity_max_sqr* is the maximum velocity squared that static friction operates in.

static_friction_new2 *friction_coefficient static_friction_hooke surface_static_friction_hooke velocity_max_sqr*

The static friction coefficients. The *friction_coefficient* limits the amount of friction to *friction_coefficient*normal_force*. The *static_friction_hooke* is how much force there is related to the distance slipped between pebbles. The *surface_static_friction_hooke* is how much force there is related to the distance slipped between the pebble and the surface. The *velocity_max_sqr* is the maximum velocity squared that static friction operates in.

static_friction_new3 *pebble_pebble_friction_coefficient pebble_pebble_static_friction_hooke surface_friction_coefficient surface_static_friction_hooke velocity_max_sqr*

The static friction coefficients. The two *friction_coefficient* limit the amount of friction to *friction_coefficient*normal_force*. The *pebble_pebble* one is used between two pebbles, and the *surface* one is used between pebbles and the surface. The *static_friction_hooke* is how much force there is related to the distance slipped between pebbles. The *surface_static_friction_hooke* is how much force there is related to the distance slipped between the pebble and the surface. The *velocity_max_sqr* is the maximum velocity squared that static friction operates in. This version allows separate values for the pebble to pebble static friction coefficient and the pebble to surface coefficient.

alpha *time_step*
Default: **alpha** 0.0001

The time step between each iteration of the model. Each time-step takes this long in simulation time. The unit is seconds.

dash_pot *dash_pot_constant*
Default: **dash_pot** 2.0

The dashpot damping coefficient. Large values of this tend to make the model unstable (may need to decrease the timestep if this is increased).

dash_pot2 *normal_dash_pot_constant transverse_dash_pot_constant*
Default: **dash_pot2** 2.0 2.0

The separate dashpot damping coefficients. The normal is used for normal velocity, and the transverse is used for transverse velocities.

seed *random_seed*
Default: **seed** 256

The random number to seed the random number generator with. Put in different values to get different initial conditions. The random number generator is mostly used to find initial pebble locations.

pebble_pebble_hooke *constant*
Default: **pebble_pebble_hooke** 10000.0

The pebble_pebble hooke constant in $\text{kg}\cdot\text{m}/(\text{m}\cdot\text{s}^2)$

pebble_vessel_hooke *constant*
Default: **pebble_vessel_hooke** 10000.0

The pebble vessel hooke constant in $\text{kg}\cdot\text{m}/(\text{m}\cdot\text{s}^2)$

pebble_radius *center_radius outside_radius*
Default: **pebble_radius** 0.0 0.1

The center radius is the radius of the inner region. The outside radius is the radius of the pebble in meters. If the center_radius is 0.0 then the pebble has uniform density.

pebble_density *center_density outside_density*
Default: **pebble_density** 0.0 2.0

The density of the pebble in kg/m^3 . Used to calculate mass and moment of inertia. The first value is the density of the center region. The second value is the density of the region outside the outer region. For example, a tennis ball would have a center region density of 0.0 (or air) and an outside density that matched rubber.

recirculate *recirculation_height door_closed_time first_door_open_time hole_size hole_depth*

Creates a door at the bottom of the cone. The door will first open at first_door_open_time and then it will close for door_closed_time every time that a pebble falls through. The pebbles will be dropped from recirculation_height (make sure that is above all the pebbles). Makes the door pebble_radius *

hole_size The **hole_depth** is the distance below the end of the cone that the door is and is in meters. This allows a short cylinder to be placed below the cone to simulate the drainage tube. It is recommended that **recirculate_params** be used instead since it splits out the geometry changes from the recirculation parameters.

recirculate_params *recirculation_height door_closed_time first_door_open_time*

Causes the pebbles to be recirculated. The door will first open at **first_door_open_time** and then it will close for **door_closed_time** every time that a pebble falls through. The pebbles will be dropped from **recirculation_height** (make sure that is above all the pebbles). Make sure that a exit chute has been created.

ppf_filename *base_filename*

The filename must be of the format abcdefgh00 where there are eight letters followed by two digits that are ignored. The last two characters are replaced by the MPI processor rank, and debugging and timing information is put in the file. This directive is ignored for the single processor pebbles7 and pebbles9 program.

linear_static_friction_cutoff

If this is turned on, then the model will use a $1 - v_{\text{transverse}}/v_{\text{static_max}}$ for the static friction cutoff. Otherwise, 1 will be used.

sort_pebbles

If this is added, after the pebbles are initially loaded, it will sort them by height. In general, this should be included, since it speeds up the program by increasing memory locality which improves cache usage.

zero_long_slips_mult *mult*

Zeros slips that are longer than $\text{mult} * \text{normal_force} * \text{static_friction_coefficient}$

integration_method *method*

In pebbles9 this is used to determine the integration method used. Methods available are euler, runge_kutta, adams_bashforth and adams_moulton. In pebbles10 only euler and runge_kutta are available.

4.3 Tallies

dump_frequency *frequency*

Default: **dump_frequency** 100000

How often a dump of the overlaps between pebbles is done. This is always done at the end. Units of timesteps.

display_frequency *frequency*

Default: **display_frequency** 1000

How often the data for the pebbles is displayed. This includes the position, velocities and static friction loadings for all the pebbles. Units in terms of timesteps. Note that these can be loaded from with appropriate processing, and used as restart files.

position_display_frequency *frequency*

Default: **position_display_frequency** 100000000

How often just the positions of the pebbles are displayed. Units in terms of timesteps. This will dump less information to the output so disk space is not quite as much of an issue.

energy_display_frequency *frequency*

Default: **energy_display_frequency** 100

How often to display the total energies. Units in terms of timesteps.

velocity_tally *start_time frequency*

Starts tallying the velocity from start time every frequency. Frequency is number of time steps to wait to do each tally.

probability_table *start_time frequency delta_size*

Starts the probability tally at start_time every frequency. Frequency is the number of time steps to wait to do each tally. delta_size specifies the size of the grid that the probabilities are done on.

calculate_pebble_wear

If this is turned on, calculates the sum of the normal force $^{4/3}$ *distance for the pebble slips. This number is proportional to the volume of material produced by adhesive wear.

normal_force_wear_exponent *exponent*

Default: **exponent** 2.0/3.0

Allows a different exponent to be used for the pebble wear calculation.

wear_velocity_bins *number list of bins*

This allows wear values to be calculated for different velocity bins. For example, if this is wear_velocity_bins 2 1.0 2.0 then three bins of wear tallies will be calculated, wear up to 1.0 m/s, wear from between 1.0 and 2.0, and wear from above 2.0.

calculate_force_tally

If this is turned on, a sum of the force on pebbles at different points in the vessel is done.

4.4 Packing

initial_packing *value*

Default: **initial_packing** *0.10*

The initial density of the pebbles. Should not be greater than 0.15 or the model may get into infinite loops trying to get started (or at least appears to act that way). In general `random_packing_method` should be used instead.

random_packing_method *mult*

An alternative method of packing. This uses the PRIME method which generates a large number of pebble positions and finds the non-overlapping ones. This can produce higher packing fractions than the `initial_packing` method. The larger the `mult`, the higher the packing density, but the slower the method. Using 100000 results in a packing fraction above 0.5.

cone_packing *opening_size height*

Cone packing creates a cone above the vessel with an opening radius size that is `opening_size` in meters and the bottom is at `height` and has a 45 degree angle. Then, the pebbles are initially put above the cone and drop down through the hole into the vessel. This is more realistic than the other packing method, but slower.

cone_packing_chute *opening_size height chute_height*

Cone packing creates a cone above the vessel with an opening radius size that is `opening_size` in meters and the bottom is at `height` and has a 45 degree angle. Then, the pebbles are initially put above the cone and drop down through the hole into the vessel. This is more realistic than the other packing method, but slower. The `chute_height` is a cylinder starting at `height` and going down by `chute_height` meters and is to make the pebbles go straighter.

4.5 Loading and Saving

dump_positions *filename*

At the end of the run, dumps the positions of the pebbles to a file.

dump_positions_mult *filename mult*

Same as `dump_positions`, except that it multiplies the positions by the `mult` factor. Since the positions are in meters, if you say want them in cm, then the `mult` should be 100.0, and so forth.

load_positions *filename*

At the start of the run, loads the positions of the pebbles from a file. The positions should be in three floating point numbers separated by spaces. They are x,y,z in meters.

load_positions_divide *filename divide*

Same as load_positions, except that it divides the positions by the divide factor. Since the positions are in meters, if you say want to load them from say cm, then the divide should be 100.0, and so forth.

load_pebble_info *filename*

Loads all the info from the file. Same format as the dumps that occur to standard out. load_pebble_save is generally preferred unless there is no slip or surface slip data.

load_pebble_slips

Loads the slips from a file in addition to all the other data. Ignored if load_pebble_info does not also appear in the file.

load_pebble_surface_slips

Loads the surface slips from a file in addition to all the other data. Ignored in if load_pebble_info does not also appear in the file.

load_pebble_save *filename*

Loads all the pebble info from the file. Same format as the dumps that occur to standard out. Loads both the slips and the surface slips.

4.6 Earthquake

earthquake_enable *number_of_waves*

Default: **earthquake_enable** 0

Enables number_of_waves of earthquake waves. The number must at least be the number of earthquake waves that are later defined. Must appear before any definition of an earthquake wave.

earthquake_sine_wave *start_time end_time d_x d_y d_z period initial_cycle*

The wave runs between the start time and the end time (in terms of seconds). The d_x, d_y, and d_z are displacements that the earthquake does. So, d_x = d_y = 0 and d_z = 1.0 would be a earthquake that caused a 1.0 meter displacement in the upward direction, followed by a 1.0 displacement in the downward direction. The period is the time that the earthquake takes to cycle back to the beginning. The initial cycle is between 0 and 2*pi and determines where in the sine wave a cycle starts.

earthquake_sine_wave_offset *start_time end_time d_x d_y d_z period
initial_cycle offset*

The same as earthquake sine wave, except there is a default offset. If the offset is zero, then it is exactly as the earthquake_sine_wave. If it is 1 then the displacement runs from 2.0*displacement to 0.0*displacement, instead of 1.0*displacement to -1.0*displacement.

tabular_earthquake *earthquake_start table_data_delta table_length filename*

The earthquake_start is the time that the earthquake data starts. The table_data_delta is the time between each piece of data in the table. Note that table_data_deltas less than the alpha value are not well handled in the current code (It won't crash, but the frequency spectrum will be destroyed). The table_length is the number of sample values. The filename is the name of the file to load the data from. The data should be in lines of x,y,z displacement values. The velocity is calculated by subtracting successive values.

4.7 Geometry Section

There can be one geometry section. It start with a **start_geometry** line and ends with a **end_geometry** line. In between, it can have unions, which consist of multiple objects that are combined together to form one object. A union is started with a **start_union** line and ended with a **end_union** line. In a union there can be the following objects. The geometry section can also have inlets, which specify where the recirculating pebbles enter.

inlet *px py pz vx vy vz*

Specifies the initial position x,y, and z and the initial velocity x, y, and z when a pebble is removed from the bottom of the vessel.

4.7.1 Geometry Objects

block *xmin ymin zmin xmax ymax zmax*

Creates a rectangular parallelepiped box with corners at xmin, ymin, zmin and xmax, ymax, and zmax. The minimum values must be less than the maximum values for each dimension.

cylinder *radius xcenter ycenter zmin zmax*

Creates a vertical cylinder between zmin and zmax centered at xcenter and ycenter with the supplied radius.

plane *a b c d*

Creates a plane defined by the equation $ax + by + cz + d = 0$. The normal for this plane is a vector formed by normalizing $a\hat{x} + b\hat{y} + c\hat{z}$. For example, **plane** 0.0 0.0 1.0 -8.0 would form a floor at height 8.0, and **plane** 0.0 0.0 -1.0 8.0 would form a ceiling at height 8.0, and **plane** 0.0 0.0 -0.5 4.0 would also form a ceiling at height 8.0.

4.7.2 Indentations

Indentations are depressions in a wall. Right now, they are only supported on the main wall specified by the **vessel_radius** directive. A pattern is created by intersecting multiple planes. These patterns are then replicated between a minimum and a maximum height, at each row and at each angle specified for the row.

The indentations occur between the minimum and maximum height specified. Rows are specified by providing a minimum, and all the angles that indentations occur at in that row.

start_pattern

Starts a pattern block. Must be inside an indentation block. The only thing inside should be **plane** directives.

end_pattern

Ends a pattern block.

min_max *minimum maximum*

This must be inside an indentation block and before any rows. It specifies the minimum and the maximum heights that indentations are allowed.

start_row

This starts a row block. It must be inside an indentation block.

end_row

This ends a row block.

row_min *min*

This specifies the minimum location (and zero point) of a row. The row goes to either the next row's minimum location or the indentation's maximum location. This must be in a row block.

angle *angle*

This specifies an angle that an indention pattern is used. This must be in a row block, and multiple angles can be specified.

angles *angle_count angle1 angle2 ...*

This specifies multiple angles that an indentation pattern is used. This must be in a row block, and this can be repeated. The *angle_count* is the number of angles that follow in that line.

```
vessel_radius 0.0 0.15
start_geometry
start_indentation
start_pattern
plane -1.0 0.0 0.0 0.25
plane 1.0 0.0 0.0 0.25
plane 0.0 -1.0 0.0 0.05
plane 0.0 1.0 0.0 0.05
plane 0.0 0.0 -1.0 0.5
plane 0.0 0.0 1.0 0.0
end_pattern
min_max 0.4 2.0
start_row
row_min 0.4
angle 0.0
end_row
start_row
row_min 1.0
angle 90.0
angle -45.0
angle 180.0
end_row
end_indentation
end_geometry
```

4.8 Other Geometry

vessel_radius *inside_radius outside_radius*

Default: **vessel_radius** *0.0 1.0*

The size of the cylinder the vessel is in. Pebbles go between the inside radius and the outside radius. If the *inside_radius* is 0.0 then the container is a cylinder instead of an annulus.

rectangular_vat *x_wall y_wall*

Creates a rectangular vat instead of a cylindrical. Use with a cone chute underneath is untested. The *x_wall* parameter is the distance that *x_wall* is from the center in meters, so the vat's floor area is $4.0 * x_wall * y_wall$.

floor_location *height*

Default: **floor_location** 0.0

Sets the height of the floor. Below this value the pebbles are forced up by the hookes law force.

cone *location slope*

Creates a cone starting at location height and going down at slope slope. Slope 0.0 would be straight down, and 1.0 would be 45 degrees. Uses formula $\text{radius} = m * z + \text{constant}$

number_of_cones *number_of_cones*

Creates the specified number of cones located radially spaced around the vessel center.

offset_inlet_holes

Offsets the inlet holes and the cone packing cones from the holes that are in the base.

exit_chute *hole_size hole_depth*

Creates a door at the bottom of the cone. Makes the door $\text{pebble_radius} * \text{hole_size}$ The hole_depth is the distance below the end of the cone that the door is and is in meters. This allows a short cylinder to be placed below the cone to simulate the drainage tube. If you want recirculation, use the `recirculate_params` function. Note that these parameters are also set if `recirculate` is used instead of `recirculate_params`.

Chapter 5

Methods of Packing

The PEBBLES code has three different methods of packing, or creating an initial condition. One of these needs to be chosen when an existing save file is not used. The simplest is the drop and compact method. For this method, an initial very low density packing is created (typically 15% filled) and then gravity is used to compact the pebbles. This method has two issues. First, the simulation can use a fair amount of time simulating the falling of the pebbles until they reach their final position. Second, depending on the number of pebbles and the cross sectional area of the vat, the pebbles that are above can cause excess compression of the pebbles that are below, and static friction can lock in part of this compression. This results in non-physical configurations.

The second method is the PRIME method developed by Kloosterman and Ougouag [22]. In this method large numbers of random positions (on the order of 100,000 more than will fit) are generated. The random positions are sorted by height, and starting at the bottom, the ones that fit are kept. Figure 5.1 illustrates this process. This generates packing fractions of approximately 0.55. Then they are allowed to fall to compact. This compaction takes less time than starting with a 0.15 packing fraction.

The last method is to automatically generate virtual chutes above the vessel where the actual inlet chutes are, and then loads the pebbles into the chutes. Figure 5.2 shows this in progress. This allows locations that have piles where the inlet chutes are, but can be done quicker than a recirculation. The other two methods generate flat surfaces at the top, which is unrealistic, since the surface of a recirculated vessel will have cones under each inlet chute.

Each of these methods will result in somewhat different initial configurations. The packing fraction and the vertical packing fraction distribution will be different depending on the method chosen and the parameters given to the method.

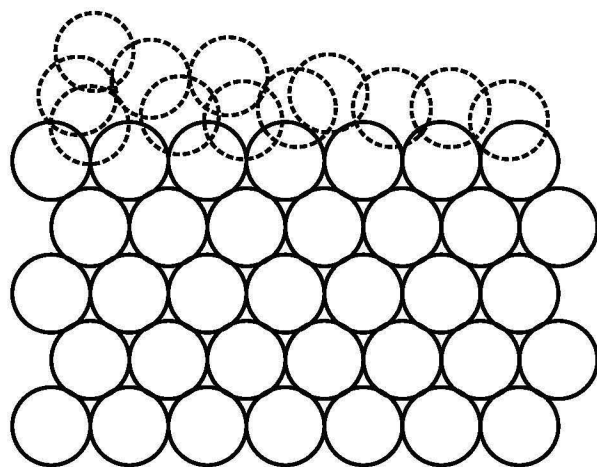


Figure 5.1: PRIME Method Illustration

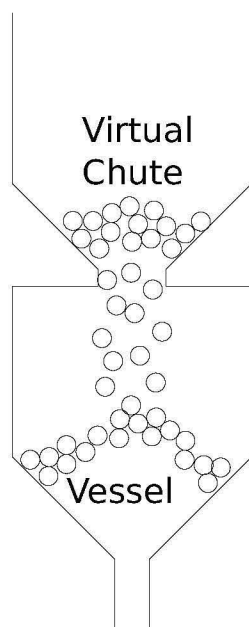


Figure 5.2: Virtual Chute Method

Chapter 6

Recirculation Simulation

The recirculation is simulated by moving a pebble from the bottom of one of the outlet chutes to an inlet location. Essentially, PEBBLES creates a flat door at the bottom of the outlet chutes. The lowest pebble is removed when the door is opened. If there are multiple outlet chutes, one pebble is removed from one of the chutes. The code cycles through all the outlet chutes, so that each time a different chute is used.

Pebbles are dropped in at the top. The location is selected by the input file. By default they are dropped in at the recirculation height directly above the center of the outlet chute with no initial velocity. They can also be dropped offset from the outlet chute. Alternatively the exact locations and the initial velocity of the pebbles can directly be specified in the geometry section.

Chapter 7

Earthquake Simulation

For each time, the simulation calculates both a displacement and a wall velocity.

For the sum of waves method, the displacement is calculated by:

$$\mathbf{d} = \sum_i \mathbf{D} \left[\sin \left((t - S) \frac{2.0\pi}{p} + c \right) + o \right] \quad (7.1)$$

where t is the current time, S is the time the wave starts, p is the period of the wave, c is the initial cycle of the wave, o is the offset, and \mathbf{D} is the maximum displacement.

The velocity is calculated by:

$$\mathbf{m} = \sum_i \frac{2\pi\mathbf{D}}{p} \cos \left((t - S) \frac{2\pi}{p} + c \right) \quad (7.2)$$

For the tabular data, the displacement and velocity are calculated by:

$$\mathbf{d} = (1 - o)T_k + oT_{k+1} \quad (7.3)$$

$$\mathbf{m} = \frac{1}{\delta}(T_{k+1} - T_k) \quad (7.4)$$

where T_i is the displacement at the i 'th timestep, o is a number between 0 and 1 that specifies where 0 is the start of the timestep and 1 is the end, and δ is the time in seconds between timesteps.

All the displacements are summed and the code then adjusts each pebble's velocity and position:

$$\mathbf{p} = \mathbf{p} + \mathbf{d} \quad (7.5)$$

$$\mathbf{v} = \mathbf{v} + \mathbf{m} \quad (7.6)$$

$$(7.7)$$

Chapter 8

Sample inputs

These are sample inputs that can be used to testing pebbles or as the basis for other inputs.

8.1 Sample Packing Input

```
rem Sample Packing input
vessel_radius 0.0 0.5
pebble_radius 0.01 0.02
runs 10000
kinetic_friction 0.4
static_friction_new3 0.6 1.0e6 0.6 1.0e6 0.01
alpha 0.0001
dash_pot2 200.0 200.0
pebble_pebble_hooke 1.0e6
pebble_vessel_hooke 1.0e6
pebble_density 2000.0 1000.0
random_packing_method 100000
use_simple_integrator
floor_location 0.0
no_linear_static_friction_cutoff
decrease_long_slips 1.1 1.0
sort_pebbles
done
```

8.2 Sample Extended Input

```
vessel_radius 0.0 1.0
number_of_pebbles 10000
rem 30 degrees from surface, or 60 degrees from wall
cone 0.0 1.73205
```

```

start_geometry
inlet 0.0 0.5 3.0 0.0 -0.1 0.0
inlet 0.0 -0.5 3.0 0.0 0.1 0.0
start_union
cylinder 0.2 0.5 0.0 -8.0 8.0
block 0.5 -0.2 -8.0 2.0 0.2 8.0
end_union
start_union
cylinder 0.2 -0.5 0.0 -8.0 8.0
block -2.0 -0.2 -8.0 -0.5 0.2 8.0
end_union
end_geometry
pebble_radius 0.01 0.02
runs 20000
kinetic_friction 0.4
static_friction_new3 0.6 1.0e6 0.6 1.0e6 0.01
alpha 0.0001
dash_pot2 200.0 200.0
pebble_pebble_hooke 1.0e6
pebble_vessel_hooke 1.0e6
pebble_density 2000.0 1000.0
random_packing_method 10000
dump_frequency 100000000
display_frequency 10000000
position_display_frequency 1000000
use_simple_integrator
floor_location -8.0
recirculate_params 3.0 0.25 1.0
exit_chute 8.0 2.0
seed 512
no_linear_static_friction_cutoff
decrease_long_slips 1.1 1.0
sort_pebbles
done

```

8.3 Sample Packing and Recirculation

```

rem flow test
vessel_radius 0.0 0.20
pebble_radius 0.01 0.02
rem 10% recirculation (500*0.1+1)/0.0001
runs 510000
number_of_pebbles 2000
kinetic_friction 0.4
static_friction_new3 0.6 1.0e6 0.6 1.0e6 0.01

```



```

alpha 0.0001
dash_pot2 200.0 200.0
pebble_pebble_hooke 1.0e6
pebble_vessel_hooke 1.0e6
pebble_density 2000.0 1000.0
use_simple_integrator
floor_location -8.0
cone 0.0 1.0
recirculate_params 1.6 0.25 1.0
exit_chute 5.5 0.0
no_linear_static_friction_cutoff
decrease_long_slips 1.1 1.0
sort_pebbles
seed 256
done

pebbles9 pack_and_recirc > pack_and_recirc.out
get_run pack_and_recirc.out 510000 | get_save_info > pack_and_recirc_save

```

8.4 Sample Earthquake input

The following loads from the packing and recirculation example, but could also be generated new by replacing the load_pebble_save with a random_packing_method directive.

```

rem earthquake sample input
vessel_radius 0.0 0.20
pebble_radius 0.01 0.02
runs 100000
number_of_pebbles 2000
kinetic_friction 0.4
static_friction_new3 0.6 1.0e6 0.6 1.0e6 0.01
alpha 0.0001
dash_pot2 200.0 200.0
pebble_pebble_hooke 1.0e6
pebble_vessel_hooke 1.0e6
pebble_density 2000.0 1000.0
use_simple_integrator
floor_location -8.0
cone 0.0 1.0
exit_chute 5.5 0.0
no_linear_static_friction_cutoff
decrease_long_slips 1.1 1.0
sort_pebbles
earthquake_enable 2
earthquake_sine_wave_offset 2.0 8.0 0.248 0.0 0.0 1.0 -1.5707963 1.0

```

```
load_pebble_save pack_and_recirc_save  
seed 256  
done
```

Chapter 9

Post processing tools

There are several tools that can be used for post processing the PEBBLES output. These include data splitters, data readers and packing fraction calculations.

get_run *time_step_number filename*

zget_run *time_step_number filename.gz*

The script **get_run** and the compressed file version **zget_run** get a specific time-step from the pebbles output. This is used by specifying the filename and the time-step number (like **get_run 1000 packing_output**).

get_save_info [*filename*]

This command takes either a filename or the standard input and outputs only the portions that are valid portions of a save file. This is usually used with the **get_run** command. Typical use would be **get_run pack_and_recirc.out 600000 | get_save_info > pack_and_recirc_save** which can then be used with **load_pebble_save** in a different input.

get_energy *filename*

zget_energy *filename.gz*

Extracts the energy displays from the program. This is a simple way to check the progress of an input since the time is included in the display. It also can be used to check if a packing run has sufficiently slowed down by looking at the linear and rotational energy. Geometry problems also show up if substantial amounts of energy are being injected into the system. However, earthquakes and recirculation also add energy to the system, and the compression energy is not tallied into the total.

split_data *filename directory_name [frequency [skips]]*

This command splits out the different time-steps of the file into the directory. This split up data can then be used by other programs such as plotters or the packing fraction calculation. The split can be done at different powers of 10 frequencies. Also, the only every skip can be calculated. For example, if the output was displayed every 100 times, and every thousandth output was desired, the command would be `split_data filename filename_dir 100 10`

bin_count *filename* [*cylinder_radius* [*cylinder_bottom* *cylinder_top* [*pebble_radius* [*center_radius*]]]]

This command calculates the packing fraction from a save file. This is calculated both vertically and radially. In order to do this, it needs to know the cylinder radius and the inner cylinder radius so that the area that is encompassed can be calculated. It also needs to know the pebble radius so that area and volume can be calculated, and for calculating the radial packing fraction, the cylinder bottom and top need to be specified so that area can be calculated correctly. Note that these should be included in the actual area that is filled with pebbles, so that the fraction calculation does not calculate over empty space.

For determining the volume of a sphere that is inside vertical slice the formula

$$a = \max(-r, bot - z) \quad (9.1)$$

$$b = \min(r, top - z) \quad (9.2)$$

$$v = \pi \left[r^2(b - a) + \frac{1}{3}(a^3 - b^3) \right] \quad (9.3)$$

where r is the pebble radius, bot is the bottom of the vertical slice, top is the top of the vertical slice and z is the vertical location of the pebble center.

To determine the area inside a vertical and radial slice, two auxiliary functions are defined, one which has the area inside a radial 2d slice, and another which has the area outside a radial 2d slice.

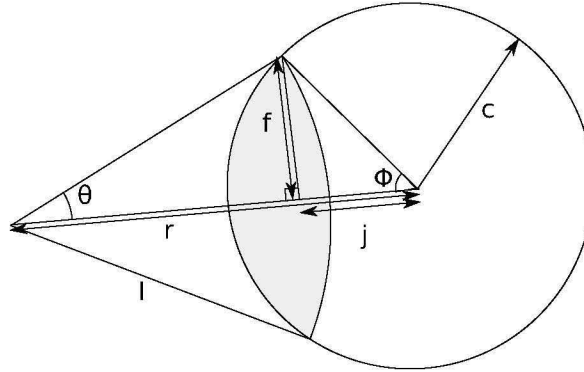


Figure 9.1: Area inside geometry

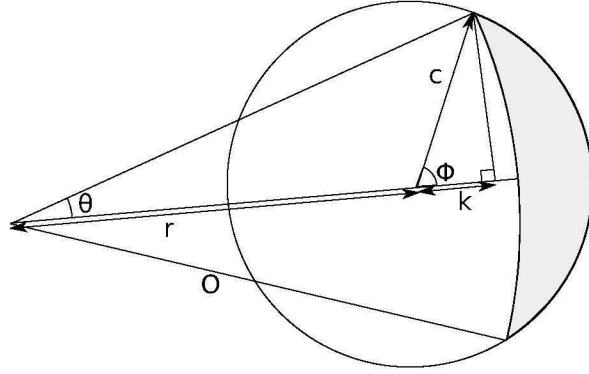


Figure 9.2: Area outside geometry

Figure 9.1 shows the area that is inside both a circle of radius c and a radial slice of I . The circle is r from the center of the radial circle. Auxiliary terms are defined, which include f , the distance from the intersection of the segment of the radial circle perpendicularly to the center line, j the distance to the intersection of f , θ the angle of segment, and ϕ the angle from the segment intersection on the circle side. The `area_inside` function has the following definition:

$$a_i = 0.0 \quad \text{if } I < r - c \quad (9.4)$$

$$a_i = \pi c^2 \quad \text{if } r + c < I \quad (9.5)$$

$$a_i = \pi I^2 \quad \text{if } I < r + c \text{ and } I < c - r \quad (9.6)$$

$$\text{otherwise} \quad (9.7)$$

$$j = \frac{r^2 + c^2 - I^2}{2r} \quad (9.8)$$

$$f = \sqrt{c^2 - j^2} \quad (9.9)$$

$$\theta = 2 \arccos \frac{I^2 + r^2 - c^2}{2Ir} \quad (9.10)$$

$$\phi = 2 \arccos \frac{r^2 + c^2 - I^2}{2rc} \quad (9.11)$$

$$a_i = \frac{1}{2} c^2 \phi + \frac{1}{2} I^2 \theta - fr \quad (9.12)$$

Figure 9.2 shows the area that is outside the radial slice, but inside the circle. The radial slice has a radius of O . The new auxiliary term k is the distance from the circle's center to the perpendicular intercept. The `area_outside` function has the following definition:

$$a_o = 0.0 \quad \text{if } O > c + r \quad (9.13)$$

$$a_o = \pi c^2 \quad \text{if } c - r > O \quad (9.14)$$

$$a_o = \pi c^2 - \pi O^2 \quad \text{if } O < r + c \text{ and } O < c - r \quad (9.15)$$

$$\text{otherwise} \quad (9.16)$$

$$k = \frac{O^2 - r^2 - c^2}{2r} \quad (9.17)$$

$$m = \sqrt{c^2 - k^2} \quad (9.18)$$

$$\theta = 2 \arccos \frac{k + r}{O} \quad (9.19)$$

$$\phi = 2 \arccos \frac{k}{c} \quad (9.20)$$

$$a_o = \left(\frac{1}{2}c^2\phi - mk\right) - \left(\frac{1}{2}O^2\theta - m(k + r)\right) \quad (9.21)$$

Then, the total volume in a radial slice can be determined from the computation:

$$a = \max(-r, \text{bot} - z) \quad (9.22)$$

$$b = \min(r, \text{top} - z) \quad (9.23)$$

$$v_t = \pi \left[R^2(b - a) + \frac{1}{3}(a^3 - b^3) \right] \quad (9.24)$$

$$v_i = \int_a^b \text{area_inside}(c = \sqrt{R^2 - z^2}) dz \quad (9.25)$$

$$v_o = \int_a^b \text{area_outside}(c = \sqrt{R^2 - z^2}) dz \quad (9.26)$$

$$v = v_t - v_i - v_o \quad (9.27)$$

Chapter 10

Approximations

The PEBBLES simulation uses soft spheres. Physically, there will be deflection of spheres under pressure (even the pressure of just one sphere on the floor), but the true compression is much smaller than what is actually modeled in typical inputs (such as the example inputs provided). In these inputs for PEBBLES, the forces are chosen to keep the compression distance at a millimeter or below. Another effect related to the physics simulation is that force is transmitted via contact. This means the force from one end of the vessel is transmitted at a speed related to the time-step used for the simulation, instead of the speed of sound.

The physics models do not take into account several physical phenomena. The physics do not handle pure spin effects, such as when two pebbles are contacting and are spinning with an axis around the contact point. This should result in forces on the pebbles, but the physics model does not handle this effect since the contact velocity is calculated as zero. In addition, when the pebble is rolling so that the contact velocity is zero because the pebble's turning axis is parallel to the surface and at the same rate as the pebble is moving along the surface, there should be rolling friction, but this effect is not modeled either. As well, the equations used assume that the pebbles are spherically symmetric.

The physics model does not match classical Hertzian or Mindlin and Deresiewicz elastic sphere behavior. The static friction model is a simplification and does not capture all the hysteretic effects of true static friction. Effectively, this means that h_s , the coefficient used to calculate the force from slip, is not a constant. In order to fully discuss this, some features of these models will be discussed in the following paragraphs.

Since closed-form expressions exist for elastic contact between spheres, they will be used, instead of a more general case which lacks closed-form expressions. Spheres are not a perfect representation of the effect of contact between shapes such as a cone and a sphere, but should give an approximation of the size of the effect of curvature.

The amount of contact area and displacement of distant points for two spheres or one sphere and one spherical hole (that is negative curvature) for

elastic spheres can be calculated via Hertzian theory[23]. For two spherical surfaces the following variables are defined:

$$\frac{1}{R} = \frac{1}{R_1} + \frac{1}{R_2} \quad (10.1)$$

and

$$\frac{1}{E^*} = \frac{1 - \nu_1^2}{E_1} + \frac{1 - \nu_2^2}{E_2} \quad (10.2)$$

with R_i the i th's sphere's radius, E_i the Young's modulus, ν_i the Poisson's ration of the material. For a concave sphere, the radius will be negative. Then, via Hertzian theory, the contact circle radius will be:

$$a = \left(\frac{3NR}{4E^*} \right)^{1/3} \quad (10.3)$$

where N is the normal force. The mutual approach of distant points is given by:

$$\delta = \frac{a^2}{R} = \left(\frac{9N^2}{16RE^{*2}} \right)^{1/3} \quad (10.4)$$

Notice that the above differs compared to the Hooke's Law formulation that PEBBLES uses. The maximum pressure will be:

$$p_0 = \frac{3N}{2\pi a^2} \quad (10.5)$$

So as a function of the radii R_1 and R_2 , the circle radius of the contact will be:

$$a = \left(\frac{3N}{4E^*} \left[\frac{1}{R_1} + \frac{1}{R_2} \right]^{-1} \right)^{1/3} \quad (10.6)$$

If m is used for the multiple of negative curvature sphere of the radius of the other, then the equation becomes:

$$a = \left(\frac{3N}{4E^*} \left[\frac{1}{R_1} - \frac{1}{mR_1} \right]^{-1} \right)^{1/3} \quad (10.7)$$

which can be rearranged to:

$$a = \left(\frac{3NR_1}{4E^*} \right)^{1/3} \left(1 - \frac{1}{m} \right)^{-1/3} \quad (10.8)$$

From this equation, as m increases, it has less effect on contact area, so if R_2 is much greater than R_1 , the contact area will tend to be dominated by R_1 rather than R_2 . For example, typical radii in PEBBLES might be 18 cm outlet

chute and a 3 cm pebble, which would put m at 6, so the effect on contact area radius would be about 33% difference compared to pebble to pebble contact area radius, or 6% compared to a flat surface.¹

To some extent, the actual contact area is irrelevant for calculating the maximum static friction force as long as some conditions are met. Both surfaces need to be of a uniform material. The basic macroscopic description $|F_S| \leq \mu|N|$ needs to hold, so changing the area changes the pressure $P = N/a$, but not the maximum static friction force. If the smaller area causes the pressure to increase enough to cause plastic rather than elastic contact, then through that mechanism, the contact area would cause actual differences in experimental values. PEBBLES also does not calculate plastic contact effects.

The contact area causes an effect through another mechanism. The tangential compliance in the case of constant normal and increasing tangential force, that is the slope of the curve relating displacement to tangential force, is given in Mindlin and Deresiewicz as:

$$\frac{2 - \nu}{8\mu a} \quad (10.9)$$

Since the contact area radius, a , is a function of curvature, the slope of the tangential compliance will be as well, which is another effect that PEBBLES' constant h_s does not capture.

In summary for the static friction using a constant coefficient for h_s yields two different approximations. First, using the same constants for wall contact when there is different curvatures is an approximation that will give somewhat inconsistent results. Since the equations for spherical contact are dominated by the smaller radius object, this effect is somewhat less but still exists. Second, using the same constant coefficient for different loading histories is a approximation. For a higher fidelity, these effects need to be taken into account.

¹ Sample values of $k = (1 - \frac{1}{m})^{-1/3}$: $m = -1, k = 1.26$ for sphere to sphere, $m = 6, k = 0.94$ sphere to outlet chute and $m = \infty, k = 1$ sphere to flat plane.

Chapter 11

Estimating Run-times

The code theoretically scales as a function of the number of time-steps times the number of pebbles. In practice, the time for running increases somewhat faster because there are less edge pebbles (which have fewer pebble to pebble contacts) and less fit in the cache.

Chapter 12

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