Macroscopic Mechanical Description of Granular Media Using Frictional Contact Mechanics

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1 Problem Setting

Loss of stress support caused by hydrate dissociation may result in a significant reduction of rock strength. The strength of a hydrate-bearing sedimentary formation is a function of the strengths of inter-granular bonds and the interactions between the rock grains and the hydrates in the pore space. Myriads of such bonds and interactions define the macroscopic rock strength parameters. We expect that the history or hydrate formation has a great impact on the character of hydrate distribution and, consequently, on the possible scenarios of failure of a hydrate-bearing rock.

Here we formulate a model of the macroscopic response of a deforming rock mass to the microscopic forces and displacements. Our model does not yet include the effects of hydrate dissociation, but the model's microscopic nature provides a robust framework to include these effects in the future.

Here we present the mechanical problem of deformation of granular media. We are interested in describing the macroscopic behavior of a rock mass, in response to, e.g., changes in applied stress or to imposed displacements. This description will be made based on the microscopic response of a pack of grains. We are not interested in a detailed description, such as the shapes of the deformed interfaces, but rather in a more general one, e.g., in the displacements of the centers of mass due to local deformations. This approach is consistent with the assumptions used to develop the contact theories which are based on linear elastic description of the bodies, where the effect of the contact is only felt in a region which is close to the contact surface, while the rest of the body experiences a rigid motion.

The approach we are using is discrete elements which are spheres of different radii and elastic properties. The solid spheres are considered to be elastic, and the deformations are small. The pack is contained within a semi-rigid box, made of planar surfaces which are stiffer than the spheres. Note that even when the Hertzian contact is employed (i.e. normal contact forces only), based on the assumptions of linear elastic bodies in contact, the problem immediately becomes non-linear due to the non-linear boundary conditions, since the contact area is a non-linear function of the displacements. In this work the tangential forces and torsion are also considered.

Equilibrium configuration (described by the location of the centers of mass of the spheres and their rotations) will be attained when the sums of forces and moments on each sphere are identically zero, and thus is such that it satisfies a system of equations of the size equal to the number of degrees of freedom. Assuming that the forces (and the moments produced by them) are potential, i.e., ignoring slip, the residual forces and moments are the gradient of the potential energy. Thus, seeking the solution to this problem can be viewed either as solving a system of algebraic equations or, formulated in a variational setting, as a minimization of the total potential energy of the pack. In other words, the displacements (linear and angular) that minimize the potential energy are the ones that correspond to zero residual forces and moments. Here we will consider two cases:

1. Start from an undeformed pack, where the contacts are formed by the additional loading (they are singular), and
2. Start from a prestressed configuration, where some stresses and deformations have already occurred, and the pack is in static equilibrium.

Both cases will be analyzed as static, with inertial effects neglected.

2 Contact Forces, Moments and Elastic Deformations

This section describes the forces, moments and potential energies that result from the relative deformations of grain bodies. These quantities can be calculated from the kinematics, i.e., from the geometry of the pack. This section contains explicit formulae for calculating the forces, moments and energies that will be used to obtain the equilibrium configuration.

A given 3D configuration includes knowing 6 degrees of freedom that describe the location and orientation of each sphere in space. From this knowledge, the displacement of each sphere with respect to its position in the undisturbed configuration can be obtained:

- $\boldsymbol{\delta r}_i = \boldsymbol{r}_i - \boldsymbol{r}_{0i}$ is the vector of linear displacements of the center with respect to a fixed coordinate system (mutual to all spheres), where $\boldsymbol{r}_i$ is the radius vector from a fixed origin of a cartesian coordinate system, see Figure 1, and subscript 0 denotes the initial unperturbed[1] configuration. The total relative displacement of sphere i w.r.t. j is $\boldsymbol{\delta r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_{0i} - (\boldsymbol{r}_j - \boldsymbol{r}_{0j})$.

[1] Either undeformed, or prestressed, i.e. before the application of an additional loading/deformation.

- $\boldsymbol{\Omega}_i$ is the rotation vector, i.e. rotation of each sphere around its center by a magnitude Ω_i and around an axis in the direction of $\boldsymbol{\Omega}_i$ (using the right-hand rule).

For a given configuration, from which the relative displacements of sphere i with respect to each of its neighbors is calculated, the task is to find the forces and moments that act on each sphere, which are transmitted through the contact regions, and the elastic potential energy associated with these deformations. Note that if the spheres are not in contact, no forces/moments are assumed to be acting between them, and since there is no deformation, no potential energy is associated with the relative displacements. Also note that the displacements are currently restricted to be small enough to comply with the linear elastic theory. Additional restrictions will enable linearizing the relations and obtaining a system of linear equations, to be discussed in Section 3.2.

2.1 Hertzian Normal Contact Forces

Hertzian contact theory (Hertz, 1882) assumes that each body can be approximated by an elastic half-space. This assumption is based on the fact that the contact area is much smaller than the size of the body and its radius of curvature, and that the deformations are sufficiently small so that linear small strain theory can be applied. It is observed that the contact stresses are highly concentrated close to the contact region, and they decrease rapidly in intensity with the distance from the contact area, so that the domain of influence lies close to the contact interface. With these assumptions, the following constitutive relation between the local deformations and the contact force was developed

$$\boldsymbol{P}_{ij} = \left[\frac{4}{3}E_{ij}^{*}\sqrt{R_{ij}}h_{ij}^{\frac{3}{2}}\right]\frac{\boldsymbol{r}_{ij}}{||\boldsymbol{r}_{ij}||} \tag{1}$$

where $h_{ij} = R_i + R_j - ||\boldsymbol{r}_i - \boldsymbol{r}_j||$ is the mutual approach, i.e. the decrease[2] of distance between the spheres from the state of initial contact (i.e. at a point). R_i, E_i and ν_i are the radius, the Young modulus, and the Poisson ratio of sphere i, respectively, and $\frac{1}{E_{ij}^{*}} = \frac{(1-\nu_i^2)}{E_i} + \frac{(1-\nu_j^2)}{E_j}$ and $\frac{1}{R_{ij}} = \frac{1}{R_i} + \frac{1}{R_j}$. $\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$ is a vector between the center of sphere i to j, which is the direction of compressive force on i due to the contact with j.

For the case of s grain in contact with a fixed planar boundary (see Figure 1), the force is

$$\boldsymbol{P}_{ij} = \left[\frac{4}{3}E_{ij}^{*}\sqrt{R_{ij}}h_{ij}^{\frac{3}{2}}\right]\boldsymbol{n}_j \tag{2}$$

$h_{ij} = R_i - (\boldsymbol{r}_i - \boldsymbol{x}_j)\cdot\boldsymbol{n}_j$, and $\boldsymbol{x}_j$ is the radius vector to an arbitrary point on the planar boundary j. Note that for a planar boundary, $R_j \to \infty$ so that $R_{ij} \to R_i$. Hertzian contact theory also provides the radius of the contact area as

$$a_{ij} = \left(\frac{3P_{ij}R_{ij}}{4E_{ij}^{*}}\right)^{\frac{1}{3}} = \sqrt{R_{ij}h_{ij}} \tag{3}$$

[2]Note that Eq. 1 is accounting for compressive force only, thus it is valid for $h_{ij} \geq 0$ only.

Since the normal contact forces are the gradient of the potential energy U^n_{ij} of each contact, $\boldsymbol{P}_{ij} = -\frac{\partial U_{ij}}{\partial \boldsymbol{\delta r}_{ij}}$, this energy can be derived by integration of the contact force along the relative displacement (see, e.g. Eq. 9.15 in Landau and Lifshitz, 1986)

$$U^n_{ij} = \int_{\boldsymbol{r}_{ij}}^{(\boldsymbol{r}_{ij}+\boldsymbol{\delta r}_{ij})} \boldsymbol{P}_{ij} \cdot d\boldsymbol{r}'_{ij} = \frac{8E^*_{ij}\sqrt{R_{ij}}}{15}(h_{ij})^{\frac{5}{2}} \tag{4}$$

2.2 Frictional Contact

Since surfaces are never perfectly smooth, friction will oppose tangential motion between bodies in contact. This friction will cause tangential stresses/twisting moments to develop between the bodies, which in turn will cause shear deformations/torsion. To remain within theory of elasticity we will restrict this discussion to elastic deformations only, i.e. neglecting slip[3] and considering static friction only. Slip will cause energy losses due to friction, and forces can no longer be considered as potential. The formulae below were originally derived by Mindlin, 1949.

Singularities of streses/displacements at the edge of the contact area suggest that there is always some slip occurring (which removes these singularities). Thus, the applicability of the following formulae will be limited to small increments of forces/displacements applied to the spheres, as it is seen that the compliance of a pair obtained with the no-slip assumption is identical with the initial compliance obtained from solutions which account for some slip (Deresiewicz, 1958). The influence of slip was thoroughly investigated by Mindlin and Deresiewicz, 1953.

The no-slip assumption means that the shear stresses should be everywhere smaller than the limiting friction, which could be determined by, e.g., Amonton's law of friction (Johnson, 1987). Due to symmetry, it is usually assumed (see, e.g. Mindlin, 1949, Mindlin and Deresiewicz, 1953 or Johnson, 1987) that the tangential forces do not have a major influence on the pressure distribution (and thus on the contact area), i.e., they could still be determined using Hertzian normal contact. Bodies will move relative to each other, where distant points (i.e. away from contact area) will have rigid displacements, and points on the contact surface will deform by elastic displacements. These rigid displacements are equivalent to the rigid normal displacement considered in developing the normal Hertzian contact theory.

Under the assumption that slip is negligible, and that the tangential stresses do not interfere with the contact area and pressure, the resulting tangential "rigid" displacements are independent of the position, and thus the sum of overall displacements of two points originally in contact is constant throughout the contact area. Furthermore, in the case of similar elastic coefficients, the tangential displacements of such points will be similar in magnitude and opposite in sign (i.e. relative displacement will split evenly between the two bodies).

[3] Slip is the relative motion of two points on the opposite sides of the contact interface that were originally touching each other.

2.2.1 Tangential Force Due to Relative Tangential Displacements

This section deals with symmetrically distributed tangential stresses that will not cause any twisting moments, but rather only moments around an axis parallel to the contact area. For the contact of spherical bodies, using analogy with the development of the normal stresses leading to a uniform normal displacement (i.e. a rigid punch), the tangential stress distribution that gives rise to uniform tangential displacement within the contact area is (Mindlin, 1949)

$$q_x(r) = q_0(1 - r^2/a^2)^{-1/2} \tag{5}$$

where the x-direction is chosen such that it is the direction of the tangential displacement (no stresses appear in the perpendicular tangential direction y), a is the radius of the contact area, and q_0 is the tangential stress at the original contact point. Since coupling between the normal and the tangential tractions and deformations is neglected, the contact area a is determined from the normal contact, as in Eq. 3. The corresponding displacement at the interface of sphere i is

$$u_{xi} = q_0 a \frac{\pi(2 - \nu_i)}{4G_i} \tag{6}$$

where G_i is the shear modulus of sphere i (also referred to as the "modulus of rigidity"). The total relative displacement of two spheres (i.e., the relative rigid displacement between 2 distant points) is $\delta_x = u_{x1} - u_{x2}$, and the resultant tangential force $Q_x = 2\pi a^2 q_0$ acting on the spheres (equal in magnitude, opposite in sign) can be related to this displacement as $\delta_x = \frac{Q_x}{8a}(\frac{2-\nu_1}{G_1} + \frac{2-\nu_2}{G_2})$. Denoting the relative tangential displacement vector (in the x direction) by $\boldsymbol{\delta}_{ij}^{t(Lin)}$ and the corresponding tangential force vector by $\boldsymbol{Q}_{ij}^{(Lin)}$, the above formula can be rewritten in vector form as

$$\boldsymbol{Q}_{ij}^{(Lin)} = -8a_{ij}\left(\frac{2-\nu_i}{G_i} + \frac{2-\nu_j}{G_j}\right)^{-1} \boldsymbol{\delta}_{ij}^{t(Lin)} \tag{7}$$

where the superscript (Lin) denotes the part which is due to the linear relative displacements. Another part will be added due to relative rotations. To obtain the relative (with respect to the contact surface) tangential displacement of sphere i with respect to j, $\boldsymbol{\delta}_{ij}^{t(Lin)}$, subtract the normal component[4] of relative displacement

$$\boldsymbol{\delta}_{ij}^{n} = \begin{cases} \left(\boldsymbol{\delta r}_{ij} \cdot \frac{\boldsymbol{r}_{0ij}}{||\boldsymbol{r}_{0ij}||}\right)\frac{\boldsymbol{r}_{0ij}}{||\boldsymbol{r}_{0ij}||} & \text{for sphere-sphere contact} \\ (\boldsymbol{\delta r}_i \cdot \boldsymbol{n}_j)\boldsymbol{n}_j & \text{for contact with boundary} \end{cases} \tag{8}$$

from the total relative displacement $\boldsymbol{\delta r}_{ij}$ to get the part which is due to linear displacements,

$$\boldsymbol{\delta}_{ij}^{t(Lin)} = \boldsymbol{\delta r}_{ij} - \boldsymbol{\delta}_{ij}^{n} \tag{9}$$

The minus sign in Eq. 7 is due to the fact that the tangential force that acts on sphere i, $\boldsymbol{Q}_{ij}^{(Lin)}$, is opposing the direction of the rigid tangential motion $\boldsymbol{\delta}_{ij}^{t(Lin)}$. The anti-symmetry

[4] The normal component of relative displacement between 2 spheres can be found by the projection along the original normal direction.

of i and j in Eq. 7 is expected, since the tangential force that acts on the 2 spheres (from 2 sides of the interface) should be equal in magnitude and opposite in sign. Eq. 7 shows a linear relation between the tangential displacement and the force. This is different than the normal loading case, where the nonlinearity is due to the change in contact area with the pressure. Note that the stress distribution in Eq. 5 leads to infinite tangential stresses at the edges of the contact area, thus partial slip at the edges is usually considered. This slip is not accounted for in the current formulation.

2.2.2 Tangential Force Due to Relative Rotation

Relative rotation around an axis which lies in the contact plane (for two spheres it is perpendicular to the line adjoining the centers in the undeformed configuration), will exert tangential forces on the contact area, which could be estimated by Eq. 7. Note that this is only an approximation, since the distribution of tractions will be different in the case of pure rotation around a horizontal axis and relative tangential displacement, even if the tangential force produced is the same. Moreover, rotation will affect the normal tractions, an effect which is usually neglected. In the following discussion we will use a relative tangential displacement which is due to the pure rotation to calculate the resulting tangential force. Note that the rotation vector is not limited to lie in the contact plane, i.e. torsion could develop at the interface. This torsion will be discussed in the next section.

Consider a pair of spheres compressed together with a normal force P, where each sphere is rotating around its center. This rotation is characterized by the rotation vectors $\boldsymbol{\Omega}_i$ and $\boldsymbol{\Omega}_j$, respectively. Note that for the case of contact with a fixed boundary, $\boldsymbol{\Omega}_j = \mathbf{0}$. This rotation is considered to be rigid everywhere, except for the neighborhood of the contact areas, where it is assumed that there is no slip (i.e. the tangential traction is everywhere smaller than the pressure times the limiting friction coefficient). The no-slip assumption implies that the spheres remain “stuck” together at the contact interface, with a constant contact area[5], so that the tangential displacements of both spheres are uniform and identical from both sides of the contact area . The relative (with respect to the original contact area) tangential component of the elastic displacement at the interface $\boldsymbol{\delta}_i^{t(Rot)}$ could be calculated from the rotation of sphere i, by the cross product

$$\boldsymbol{\delta}_i^{t(Rot)}\Big|_{j=fixed} = \boldsymbol{\Omega}_i \times \boldsymbol{R}_{ij} \tag{10}$$

where the superscript Rot denotes the fact that this tangential component is due to rotation, and $\boldsymbol{R}_{ij}$ is a vector of magnitude R_i (radius of sphere i) which is directed along the line from the unperturbed center of sphere i to the original contact point,

$$\boldsymbol{R}_{ij} = \begin{cases} (\boldsymbol{r}_{0j} - \boldsymbol{r}_{0i})\frac{R_i}{R_i+R_j} & \text{for sphere-sphere contact} \\ R_i \boldsymbol{n}_j & \text{for contact with boundary} \end{cases} \tag{11}$$

where $\boldsymbol{n}_j$ is a unit vector normal to the boundary j pointing towards sphere i, see Figure 1. The cross-product in Eq. 10 automatically excludes the component of rotation which will cause torsion (since it is aligned with $\boldsymbol{R}_{ij}$), and thus one does not need to decompose the rotation vector into the tangential and normal components with respect to the contact plane in order to calculate the resulting tangential displacement by Eq. 10. The effect of torsion

[5] It is further assumed that the contact area and the pressure are unaffected by the tangential stresses.

will be considered in the next section.

For the case of contact with a fixed boundary, $\boldsymbol{\delta}_i^{t(Rot)}$ is the relative rotation with respect to that body, denoted by $\boldsymbol{\delta}_{ij}^{t(Rot)}$. For the contact of two spheres, one needs to superimpose the effect of the rotations of the two to obtain the total effect[6]. Note that even though rotation vectors are not commutative (except for the case of infinitesimal rotations), it is possible to calculate the relative linear displacement (the consequence of the relative rigid rotation) of sphere i with respect to j as

$$\boldsymbol{\delta}_{ij}^{t(Rot)} = \boldsymbol{\Omega}_i \times \boldsymbol{R}_{ij} - \boldsymbol{\Omega}_j \times \boldsymbol{R}_{ji} \tag{12}$$

and obtain the tangential resultant force acting on each sphere using $\boldsymbol{\delta}_{ij}^{t(Rot)}$ as the tangential displacement in Eq. 7. To obtain the total tangential displacement $\boldsymbol{\delta}_{ij}^t$ (due to linear displacement and rotation), add the two corresponding tangential displacement vectors, $\boldsymbol{\delta}_{ij}^t = \boldsymbol{\delta}_{ij}^{t(Lin)} + \boldsymbol{\delta}_{ij}^{t(Rot)}$. In the case of two contacting spheres, this vector is

$$\boldsymbol{\delta}_{ij}^t = \boldsymbol{\delta r}_{ij} - \left(\boldsymbol{\delta r}_{ij} \cdot \frac{\boldsymbol{r}_{0ij}}{||\boldsymbol{r}_{0ij}||}\right)\frac{\boldsymbol{r}_{0ij}}{||\boldsymbol{r}_{0ij}||} - \frac{1}{R_i + R_j}\Big[(R_i\boldsymbol{\Omega}_i + R_j\boldsymbol{\Omega}_j) \times \boldsymbol{r}_{ij}\Big] \tag{13}$$

whereas for the case of contact with a fixed planar boundary, the total vector is

$$\boldsymbol{\delta}_{ij}^t = \boldsymbol{\delta r}_i - (\boldsymbol{\delta r}_i \cdot \boldsymbol{n}_j)\boldsymbol{n}_j + R_i\boldsymbol{\Omega}_i \times \boldsymbol{n}_j \tag{14}$$

Using the total tangential displacement in Eq. 7 provides the tangential force due to relative tangential displacements and rotations,

$$\boldsymbol{Q}_{ij}(\boldsymbol{\delta}_{ij}^t) = -8a_{ij}\left(\frac{2-\nu_i}{G_i} + \frac{2-\nu_j}{G_j}\right)^{-1}\boldsymbol{\delta}_{ij}^t \tag{15}$$

2.2.3 Elastic Potential Energy of Tangential Deformations

The elastic potential energy related to the deformations described above can be found by integrating the resultant force over the displacement in the direction of that force (dot product of the force vector and the displacement vector)[7], i.e. for a tangential force Q which causes a displacement of $\delta^{t(Rot)}$ the associated potential energy would be

$$U^{t(Lin)}(\delta^{t(Lin)}) = \int_0^{\delta^{t(Lin)}} Q^{t(Lin)}(\delta^{t(Lin)})d\delta^{t(Lin)} \tag{16}$$

The potential energy associated with the relative rotation Ω could be computed in a similar way[8], i.e., the tangential force as a function of rotation is integrated over the linear displacement which results from the rotation

[6] Summing the displacements and obtaining the force is identical to summing the two forces resulting from each rotation of a single sphere keeping the other fixed.

[7] In the one dimensional case, the energy is $U(x') = -\int_0^x F(x')dx'$. In Eq. 16 the minus sign is omitted since the force in the original expression is the force exerted by the elastic deformation, while the force in the above equation is the force required to cause that deformation.

[8] It is identical to integrating the moment along the rotation angle, as $M = QR$ and $\Omega = \delta^t/R$ where R is the sphere radius.

$$U^{t(Rot)}(\Omega) = \int_0^{\Omega} M(\Omega)d\Omega = \int_0^{\delta^{t(Rot)}(\Omega)} Q^{t(Rot)}(\delta^{t(Rot)}(\Omega))d\delta^{t(Rot)}(\Omega) \tag{17}$$

The potential energy associated with both deformations is thus

$$U_{ij}^t(\boldsymbol{r}_i, \boldsymbol{r}_j, \boldsymbol{\Omega}_i, \boldsymbol{\Omega}_j) = 4a_{ij}\left(\frac{2-\nu_i}{G_i} + \frac{2-\nu_j}{G_j}\right)^{-1}(\delta_{ij}^t)^2 \tag{18}$$

where δ_{ij}^t is the magnitude of the relative tangential displacement vector between the spheres, due to both linear and angular displacements, thus it is a function of $\boldsymbol{r}_i, \boldsymbol{r}_j, \boldsymbol{\Omega}_i, \boldsymbol{\Omega}_j$. Note that because of the presence of the contact area a, this energy is also an explicit function of the normal component, which in turn is a function of $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$. Note that Eq. 18 holds only in the case of contact between the spheres, since U_{ij}^t must vanish otherwise, even though $\delta_{(ij)}^t$ might be nonzero.

2.2.4 Torsional Elastic Deformations and Twisting Moments

Rotation around an axis along the line connecting the centers will cause a twisting moment, which will induce torsional deformation. Similarly to our handling of tangential stress, it is assumed that the bodies rotate rigidly everywhere except for the neighborhood of the contact areas, where elastic deformation is assumed. Since it is assumed that there is no slip, and that no normal traction component or distortion in the contact plane results from this rotation (Mindlin, 1949 and Deresiewicz, 1958), these moments will induce only torsional deformations.

Considering a pair of identical spheres with similar elastic properties, assuming no slip, the torsional compliance that relates the moment to the rotation angle in the case of twisting couple of magnitude M_{ij}^{tor} is (Mindlin, 1949)

$$M_{ij}^{tor} = \frac{8}{3}Ga_{ij}^3\Omega_{ij}^{tor} \tag{19}$$

where Ω_{ij}^{tor} is the relative rotation of the two bodies in a direction normal to the contact surface, denoted by superscript *tor*. The direction of the moment can be easily found from the requirement that the moment opposes the direction of rotation. To obtain the relative rotation, we will use the fact that we will eventually deal with the incremental formulation (restricted to small deformations). Considering infinitesimal rotation of the spheres around their centers, $\boldsymbol{\Omega}_i$, the component of rotation of each sphere around an axis which is perpendicular to the contact surface would be $\boldsymbol{\Omega}_i^{tor}\big|_{j=fixed} = (\boldsymbol{\Omega}_i \cdot \boldsymbol{R}_{ij})\boldsymbol{R}_{ij}$. For contact with another sphere, the rotation of that sphere around the same axis is $\boldsymbol{\Omega}_j^{tor}\big|_{i=fixed} = (\boldsymbol{\Omega}_j \cdot \boldsymbol{R}_{ij})\boldsymbol{R}_{ij}$. Since these rotations are around the same (parallel) axis, the relative rotation of i with respect to j is obtained by taking the difference, as

$$\boldsymbol{\Omega}_{ij}^{tor} = \boldsymbol{\Omega}_i^{tor} - \boldsymbol{\Omega}_j^{tor} = [(\boldsymbol{\Omega}_i - \boldsymbol{\Omega}_j) \cdot \boldsymbol{r}_{0ij})]\boldsymbol{r}_{0ij} \tag{20}$$

where for contact with a fixed plane, $\boldsymbol{\Omega}_{ij}^{tor} = \boldsymbol{\Omega}_i^{tor}\big|_{j=fixed}$. For the case of non-uniform elastic properties, the relation in Eq. 19 will transform into (Johnson, 1987)

$$\boldsymbol{M}_{ij}^{tor} = -\frac{16}{3} a_{ij}^3 \left(\frac{1}{G_i} + \frac{1}{G_j} \right)^{-1} \boldsymbol{\Omega}_{ij}^{tor} \tag{21}$$

where $\boldsymbol{M}_{ij}^{tor}$ is the moment applied on sphere i by sphere j due to a relative rotation of $\boldsymbol{\Omega}_{ij}^{tor}$. The energy associated with the torsion, calculated as the integral of the moment along the rotation angle, is

$$U_{ij}^{tor} = \frac{8}{3} a_{ij}^3 \left(\frac{1}{G_i} + \frac{1}{G_j} \right)^{-1} (\Omega_{ij}^{tor})^2 \tag{22}$$

where Ω_{ij}^{tor} is the magnitude of the relative tangential displacement between the spheres.

As in the case of tangential displacements, singularities at the edge of the contact area suggest that some slip in a circumferential direction takes place over an annular area. This limits the use of Eq. 21 and Eq. 22 to cases of large limiting friction relative to the actual stresses developed in the contact area. Intuitively, the stresses produced by this motion would be smaller compared with those created by tangential displacements and rotation around horizontal axis; however, twisting has a very important role in determining the strength of contact (Hills, 1986), and should be considered carefully when failure is involved.

2.2.5 Moments

While the normal resultant force induced at the contacts acts along the line connecting the centers, and thus does not apply a moment[9], the tangential forces (Eq. 15) will. Since the deformations are considered to be small, the tangential forces at the contacts could be considered as acting on the original contact point (before perturbation applied). Thus the arm from sphere i center to the contact is described by $\boldsymbol{R}_{ij}$. The moments are calculated by the cross product of the arm and the force, so that the moment acting on sphere i is produced by the tangential force $\boldsymbol{Q}_{ij}$ is[10]

$$\boldsymbol{M}_{ij}^{t} = \boldsymbol{R}_{ij} \times \boldsymbol{Q}_{ij} \tag{23}$$

Note that this moment is a function of both linear tangential displacements and rotations around an axis parallel to the contact plane. Upon inserting the explicit expression for $\boldsymbol{R}_{ij}$, and for $\boldsymbol{Q}_{ij}$ as a function of $\boldsymbol{\delta}_{ij}^{t}$, using the vector triple product $\boldsymbol{A} \times (\boldsymbol{B} \times \boldsymbol{C}) = \boldsymbol{B}(\boldsymbol{A} \cdot \boldsymbol{C}) - \boldsymbol{C}(\boldsymbol{A} \cdot \boldsymbol{B})$, and the fact that cross products of parallel vectors will vanish, the resulting equation could be simplified to,

$$\begin{aligned} \boldsymbol{M}_{ij}^{t} = -8 a_{ij} \left(\frac{2-\nu_i}{G_i} + \frac{2-\nu_j}{G_j} \right)^{-1} \frac{R_i}{R_i + R_j} \Bigg\{ & - \boldsymbol{r}_{0ij} \times \boldsymbol{\delta r_{ij}} \\ & + \frac{1}{R_i + R_j} \Big(||\boldsymbol{r}_{0ij}||^2 (R_i \boldsymbol{\Omega}_i + R_j \boldsymbol{\Omega}_j) - (\boldsymbol{r}_{0ij}) \big[\boldsymbol{r}_{0ij} \cdot (R_i \boldsymbol{\Omega}_i + R_j \boldsymbol{\Omega}_j) \big] \Big) \Bigg\} \end{aligned} \tag{24}$$

[9] Assuming small deformations so that bodies remain spherical, the center of mass remains at the sphere center.

[10] Note that the force is perpendicular to the arm, so that the magnitude of the moment is simply $R_i ||\boldsymbol{Q}_{ij}||$. The vectorial notation is needed though for determining the direction of the moment.

for the case of sphere-sphere contact, and to

$$\boldsymbol{M}_{ij}^t = -8a_{ij}\left(\frac{2-\nu_i}{G_i}+\frac{2-\nu_j}{G_j}\right)^{-1} R_i\Big[\boldsymbol{n}_j \times \boldsymbol{\delta r}_i + R_i\boldsymbol{\Omega}_i - \boldsymbol{n}_j\big(\boldsymbol{n}_j \cdot R_i\boldsymbol{\Omega}_i\big)\Big] \qquad (25)$$

for the case of sphere-wall contact. Note that $\boldsymbol{M}_{ij}^t$ in Eq. 24/Eq. 25 calculated with respect to the center of the sphere, so the sum of moments on each sphere with respect to its center, due to tangential loading, is simply summation of all those moment vectors. The total sum of moments should include the torsional moments (which is a function of relative rotations around an axis perpendicular to the contact plane),

$$\boldsymbol{M}_i = \sum_{j=1}^{N_c^i}\Big[\boldsymbol{M}_{ij}^t + \boldsymbol{M}_{ij}^{tor}\Big] \qquad (26)$$

where there are N_c^i contacts for sphere i. This sum should be used as the residual moment of each sphere, which in turn will be used to find the displacements which will minimize the energies. Both the residual force and moment acting on each sphere could be used to estimate the deviation from the equilibrium, e.g. by summing the square of the norms of these vectors.

3 Using Minimization of Energy to Obtain Equilibrium

The elastic potential energy associated with the elastic deformations is the sum of the energies which are due to the normal and tangential displacements (including the rotation parallel to the contact area), and the torsion. These energies are a function of the relative linear displacements and rotations. Equilibrium configuration is obtained when the following two quantities vanish on each sphere: (a) the sum of forces; (b) the sum of moments. To use the potential energy to obtain equilibrium configuration, we will minimize a functional which includes the sum of energies from all normal and tangential relative displacements, as well as those that are associated with the relative rotation of the spheres. Note that on top of the energies associated with the internal forces/moments, one needs to take in to account those which are associated with the external forces,

$$\begin{aligned}\Pi(\boldsymbol{r}_1^k, \boldsymbol{r}_2^k, ..., \boldsymbol{r}_{NN}^k, \boldsymbol{\Omega}_1^k, \boldsymbol{\Omega}_2^k, ..., \boldsymbol{\Omega}_{NN}^k) &= \frac{1}{2}\sum_{ij=1}^{N_{cs}}\left[U_{ij}^n + U_{ij}^t + U_{ij}^{tor}\right]^k \\ &+ \sum_{ij=1}^{N_{cw}}\left[U_{ij}^n + U_{ij}^t + U_{ij}^{tor}\right]^k - \sum_{i=1}^{N}\boldsymbol{F}_{i,ext}^k \cdot \boldsymbol{\delta}_i^k\end{aligned} \qquad (27)$$

where k is the iteration index, ij denotes the contact between sphere i and other spheres/boundaries j (N_{cs} such sphere-sphere contacts, N_{cw} sphere-boundary contacts), $\boldsymbol{F}_{i,ext}^k$ is the external force applied[11] (total of N spheres), and $\boldsymbol{\delta}_l$ is the displacement vector of sphere i. The energies are associated with a single contact, thus the total potential energy is the sum of the energies over all contacts. The 1/2 factor comes from the fact that summing over all contact of all spheres will result in including each sphere-sphere contact twice. Minimizing Π with respect to all the displacement components $(\boldsymbol{r}_1^k, \boldsymbol{r}_2^k, ..., \boldsymbol{r}_{NN}^k, \boldsymbol{\Omega}_1^k, \boldsymbol{\Omega}_2^k, ..., \boldsymbol{\Omega}_{NN}^k)$ is equivalent to

[11] We exclude here loading in the form of applied moments, which can be easily added.

solving the set of equations ($N \times 6$ for the 3D case, if all spheres have 6 degrees of freedom), which are sum of forces and sum of moments (vectorial equations) equal to zero.

An important observation is that for the normal components the relative displacement from the undeformed configuration can be calculated without knowledge of that configuration, while this is not the case for the tangential and rotational components. Thus, unlike the normal contact forces, where their magnitudes (and thus the energy associated with them U^n_{ij}) are known for every configuration, the tangential forces and their associated energy U^t_{ij} are not known in the undisturbed configuration, unless the undeformed configuration is also known. The fact that the energy is related to tangential displacement, which is not known poses a problem since some deformations could occur in a direction which reduces the energy, i.e., in a reverse direction to the initial tangential displacement. Without prior knowledge, any deformations will be considered to increase energy[12]. For the time being, we will ignore this problem and consider minimization of the increment of energy from the undisturbed initial state, and not of the total energy.

3.1 Incremental Formulation

The case of deformations of a prestressed pack is different than the case of deforming an undeformed pack. We now address the problem of a prestressed pack, where one needs to determine a new equilibrium configuration (displacements) starting from some other equilibrium (hereby refereed to as "undisturbed" or "prestressed"), after a small perturbation has been introduced. To obtain the new equilibrium configuration, we will first consider an infinitesimal[13] perturbation, so that the resulting displacements are infinitesimal as well. Resorting to the incremental formulation allow us to use linear constitutive relations, which will improve the numerical scheme convergence[14]. The equilibrium configuration associated with the new perturbation will be found by minimizing the change in energy from its initial equilibrium state.

Applying a sequence of such incremental changes and integrating provides an equilibrium configuration associated with the final finite change[15]. Even though at the undisturbed configuration the tangential forces (and thus moments) are unknown, by definition, the sum of forces and moments on each grain is zero, so we will consider only the increments of forces and moments as the residuals (which will be used to minimize the incremental energy). Thus, the residuals should be calculated as sum of forces/moments in excess of those in the undisturbed configuration. This approach provides the deviation from equilibrium, since the undisturbed configuration is at equilibrium, i.e. residuals are identically zero. Note that if the tangential forces in the undisturbed configuration were known, one could calculate the sum total forces as the residuals. But, since the tangential forces are not known, summing the total forces would lead to erroneous residuals.

[12]This means that the U^t_{ij} could only increase from that configuration.

[13]Infinitesimal in this context means that it is small enough for the linear theory to apply within certain accuracy.

[14]This is of great advantage when using conjugate gradient methods, which were originally developed for systems of linear equations.

[15]Note that it may be that some other equilibrium configuration with lower energy may be attained by applying the change at once, i.e. the solution might not be unique.

3.2 Linearizing the Relations

In this section we linearize the non-linear relations which are needed to calculate the forces and energies with respect to the parameters $\boldsymbol{r}_1^k, \boldsymbol{r}_2^k, ..., \boldsymbol{r}_{NN}^k, \boldsymbol{\Omega}_1^k, \boldsymbol{\Omega}_2^k, ..., \boldsymbol{\Omega}_{NN}^k$ [16]. The linearization is done by expansion of the functions (forces, moments, energies) around a reference value, which is for zero relative displacements with respect to the prestressed configuration, dropping all the terms of higher order than linear. Note that there are deformation and thus contact forces in that configuration.

This procedure is sensible only for a prestressed configuration, where for all contacts the contact area is assumed to be far enough from being singular, i.e., a set of points. However, since a granular medium contains multiple contacts, some of those might be closer to the singular limit, and thus lose contact with a small incremental change. In that case, the values of forces, moments and potential energies associated with those particular contacts should be identically zero, and not calculated using the linear formulae. For the case of new contacts which are due to the incremental change, the values should be calculated using the full nonlinear formulation, as in Section 2. Note that intuitively one can expect this situation to be uncommon, and if it will only happen with very few contacts the overall effect on the calculations might be small.

Starting with the normal components, it is necessary to linearize the forces and energy with respect to the position vectors. Noting that rotation vector does not affect the normal components, the force will be expressed as a linear function of the displacements. Note that both the direction and the magnitude of the force vector in Eq. 1 depends on the displacement, so both will be linearized by

$$\boldsymbol{P}_{ij}(\boldsymbol{\delta r}_{ij}) \approx \boldsymbol{P}_{0ij} + \boldsymbol{\delta P_{ij}} = \boldsymbol{P}_{0ij} + \bigtriangledown \boldsymbol{P}_{ij}\big|_{\boldsymbol{\delta r}_{ij}=0} \cdot \boldsymbol{\delta r}_{ij} \tag{28}$$

where $\boldsymbol{P}_{0ij}$ is obtained by using the undisturbed geometry, i.e., $\boldsymbol{r}_{0ij}$ in Eq. 1, and the gradient is defined by $\bigtriangledown \boldsymbol{P}_{ij}\big|_{\boldsymbol{\delta r}_{ij}=0} = \frac{\partial \boldsymbol{P}_{0ij}}{\partial \boldsymbol{\delta r}_{ij}}\big|_{\boldsymbol{\delta r}_{ij}=0}$. For a sphere-sphere contact, this gradient is given by

$$\bigtriangledown \boldsymbol{P}_{ij}\big|_{\boldsymbol{\delta r}_{ij}=0} = \frac{4}{3}E_{ij}^{*}\sqrt{R_{ij}}\left\{\frac{h_{0ij}^{\frac{3}{2}}}{||\boldsymbol{r}_{0ij}||}\mathbf{1} - \frac{\sqrt{h_{0ij}}}{||\boldsymbol{r}_{0ij}||^3}\left(\frac{3}{2}||\boldsymbol{r}_{0ij}|| + h_{0ij}\right)(\boldsymbol{r}_{0ij} \otimes \boldsymbol{r}_{0ij})\right\} \tag{29}$$

where $\mathbf{1}$ is the unit tensor, i.e., the second order diagonal tensor with 1 along the diagonal, and $h_{0ij} = R_i + R_j - ||\boldsymbol{r}_{0i} - \boldsymbol{r}_{0j}||$ is the undisturbed mutual approach. The dot product of this expression with $\boldsymbol{\delta r}_{ij}$ (see Eq. 28) provides the linear increment in force,

$$\boldsymbol{\delta P_{ij}} = \frac{4}{3}E_{ij}^{*}\sqrt{R_{ij}}\left\{\frac{h_{0ij}^{\frac{3}{2}}}{||\boldsymbol{r}_{0ij}||}\boldsymbol{\delta r}_{ij} - \frac{\sqrt{h_{0ij}}}{||\boldsymbol{r}_{0ij}||^3}\left(\frac{3}{2}||\boldsymbol{r}_{0ij}|| + h_{0ij}\right)(\boldsymbol{r}_{0ij} \cdot \boldsymbol{\delta r}_{ij})\boldsymbol{r}_{0ij}\right\} \tag{30}$$

For a contact between a sphere and a fixed boundary, noting that the mutual approach is already linear with respect to the displacement of the sphere (see Eq. 2), and that the

[16] Since $\boldsymbol{r}_i = \boldsymbol{r}_{0i} + \boldsymbol{\delta r_i}$, it will also be linear with respect to the displacements

direction of the vector is fixed (it is the normal to the planar boundary), the increment in force simplifies to

$$\boldsymbol{\delta P_{ij}} = -2E^{*}_{ij}\sqrt{R_{ij}h_{0ij}}(\boldsymbol{n}_j \cdot \boldsymbol{\delta r}_i)\boldsymbol{n}_j \tag{31}$$

To obtain a quadratic form (with respect to the displacements) for the change in U^n_{ij}, it will be calculated by integrating the linear force (Eq. 28) along the relative displacement (see Eq. 4)

$$\delta U^n_{ij} = \int_{\boldsymbol{r}_{ij}}^{(\boldsymbol{r}_{ij}+\boldsymbol{\delta r}_{ij})} (\boldsymbol{P}_{0ij} + \boldsymbol{\delta P_{ij}}) \cdot d\boldsymbol{r}'_{ij} \tag{32}$$

The integration could be simplified upon parameterizing the displacements as $\boldsymbol{\delta r}_{ij}(s) = s\boldsymbol{\delta r}_{ij}$ where s is a scalar which varies form 0 to 1, such that $s = 0$ and $s = 1$ are the initial (prestressed) and disturbed configuration, respectively. With this, the integration is done over $d\boldsymbol{r}'_{ij} = s\boldsymbol{\delta r}_{ij}ds$, where only $\boldsymbol{\delta r}_{ij}$ is a function of s within that integral. Taking out the constant parts and integrating over s from 0 to 1, get

$$\delta U^n_{ij} = (\boldsymbol{P}_{0ij} + \frac{1}{2}\boldsymbol{\delta P_{ij}}) \cdot \boldsymbol{\delta r}_{ij} \tag{33}$$

Note that since $\boldsymbol{\delta P_{ij}}$ is linear with $\boldsymbol{\delta r}_{ij}$, the second term in Eq. 33 is quadratic. The first term is linear with it, so the energy can be reduced (when the distance between the bodies is decreasing). This situation is different than the case of the energies that are due to other deformations, where the single quadratic term implies that the energy could only increase from the prestressed deformation. This is not true in the case of displacements in a direction opposite to the the initial ones (i.e. from the undeformed configuration), unless the tangential stresses dissipate and do not exist in the prestressed pack. This is a reasonable assumption for geological media which is formed over long periods, and consolidates long after.

The tangential force is already linear with respect to the relative tangential displacement δ^t_{ij}, which in turn is linear with the linear and angular displacements. Nevertheless, the contact area a which appears in Eq. 15 is nonlinear with the linear displacement, so it could also be linearized as

$$a_{ij} \approx \underbrace{\sqrt{R_{ij}h_{0ij}}}_{a_{0ij}} + \frac{1}{2}\sqrt{\frac{R_{ij}}{h_{0ij}}}\delta h_{ij} \tag{34}$$

However, since the second term in Eq. 34 is of higher order, the product of it with the incremental relative displacement $\delta_{t(ij)}$ can be neglected in the linear approximation. Thus, the contact area will be considered to be constant, equal to its value in the prestressed configuration, a_{0ij}, i.e. decouples the effect of the normal stresses on the tangential ones.

With this simplification, the forces, moments and energies which are associated with the tangential displacements and rotations are linear with respect to the relative disbarments (linear and rotational). With linear relationships between the tangential forces/twisting moments and the tangential displacement and rotations, the energy associated with those deformations will be quadratic with respect to them, see Eq. 18. Keep in mind that the calculated U^t_{ij} (e.g. in Eq. 18) is the increment of energy, ignoring amount stored in the undisturbed configuration. This increment will therefore be denoted by ΔU^t_{ij}.

4 Appendix: Numerical Schemes

In this section, a brief overview of the methods used to solve for the equilibrium configuration is presented, together with a note on the implementation of these methods. The simplest method which is presented in the steepest descent, while the method chosen was the conjugate gradient, which has proven to converge within finite number of iterations for linear systems.

4.1 Steepest Descent Method

The starting point of iteration is an initial configuration, guessing the linear and rotational displacements with respect to the undisturbed equilibrium state. For example, one could take the undisturbed configuration, i.e., zero displacements, as the initial guess. For the current iteration (configuration = linear displacements/rotations), calculate the corresponding relative displacements. These relative displacements enable (see Section 2) the calculation of normal and tangential forces, moments and energies associated with the relative displacements. The sum of forces and sum of moments are the residuals, which will be identically zero at the equilibrium configuration.

Minimizing the energy is done by displacing the spheres in the anti-direction of the residuals, i.e., linear displacements of α^k_{lin} times the residual force of each sphere, and angular displacements of α^k_{rot} times the corresponding residual moment, where the units of these coefficients differ from one another, to make the units consistent. Finding these two coefficients is a problem of minimization of a function (Π) with respect to two variables (α^k_{lin} and α^k_{rot}), which would be an excessive complication compared to using a single coefficient.

To use a single coefficient, one needs to make sure that the units and scales of the parameters updated by that coefficient are similar. Consider a coefficient that is relating the linear displacements (units of length [L]) and residual forces, i.e. it should be in units of [L]/[F]. Relating the rotation (dimensionless) to the moments, one needs a coefficient which has units of 1/([F][L]). Assuming that the tangential and normal forces are of the same order, since the moments are the sum of tangential forces times the sphere radius R_i, the moments are about R_i larger than the sum of forces. On the other hand, the linear displacements should be of order of rotations times R_i. To obtain a similar order, we consider the variables to be the linear displacements $\boldsymbol{\delta}_i$ and the arc length vector $R_i\boldsymbol{\Omega}_i$, and in addition we update the arc length variable by the sum of moments times the coefficient divided by R_i,

$$\begin{aligned} \boldsymbol{\delta}_i^{k+1} &= \boldsymbol{\delta}_i^k - \alpha^k \boldsymbol{f}_i^k \\ R_i\boldsymbol{\Omega}_i^{k+1} &= R_i\boldsymbol{\Omega}_i^k - \frac{\alpha^k}{R_i}\boldsymbol{M}_i^k \end{aligned} \tag{35}$$

4.2 Conjugate Gradient Method

The classical conjugate gradient method was developed for numerical solution of one of two equivalent problems: a system of linear equations

$$A\mathbf{x} = \mathbf{b} \tag{36}$$

or minimization of a quadratic criterion

$$J(\mathbf{x}) = \frac{1}{2}A\mathbf{x}\cdot\mathbf{x} - \mathbf{b}\cdot\mathbf{x} \tag{37}$$

Here b is a known column-vector of dimension N, and A is a symmetric positive-definite $N \times N$ matrix. The gradient $J'(\mathbf{x})$ of $J(\mathbf{x})$ is

$$J'(\mathbf{x}) = A\mathbf{x} - \mathbf{b} \tag{38}$$

Hence, Equation Eq. 36 is equivalent to $J'(\mathbf{x}) = 0$. The solution $\mathbf{x}_*$ to system Eq. 36 is the minimum of function Eq. 37, and *vice versa*.

Conjugate gradients method is an iterative procedure where starting from some $\mathbf{x}_0$, a step from $\mathbf{x}_n$ (n is the iteration index) to $\mathbf{x}_{n+1}$ is performed by the following formula

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \alpha_n\mathbf{p}_n \tag{39}$$

The step-size coefficient[17] α_n is selected to minimize $J(\mathbf{x}_n - \alpha_n\mathbf{p}_n)$ (the potential energy in this case) for a given $\mathbf{x}_n$ and $\mathbf{p}_n$. At the minimum,

$$\frac{d}{d\alpha}J(\mathbf{x}_n - \alpha\mathbf{p}_n)\bigg|_{\alpha=\alpha_n} = (A(\mathbf{x}_n - \alpha_n\mathbf{p}_n) - \mathbf{b})\cdot\mathbf{p}_n = (A\mathbf{x}_{n+1} - \mathbf{b})\cdot\mathbf{p}_n = 0 \tag{40}$$

Therefore,

$$\alpha_n = \frac{\mathbf{r}_n\cdot\mathbf{p}_n}{A\mathbf{p}_n\cdot\mathbf{p}_n} \tag{41}$$

where

$$\mathbf{r}_n = A\mathbf{x}_n - \mathbf{b} \tag{42}$$

is the gradient of the energy in this case, as defined in Eq. 38. Note that Eq. 39 and Eq. 40 imply that

$$\mathbf{r}_{n+1}\cdot\mathbf{p}_n = 0 \tag{43}$$

Also, from Eq. 39

$$-\alpha_n A\mathbf{p}_n = A\mathbf{x}_{n+1} - A\mathbf{x}_n = (A\mathbf{x}_{n+1} - \mathbf{b}) - (A\mathbf{x}_n - \mathbf{b}) = \mathbf{r}_{n+1} - \mathbf{r}_n \tag{44}$$

hence

$$A\mathbf{p}_n = \frac{1}{\alpha_n}(\mathbf{r}_n - \mathbf{r}_{n+1}) = \frac{1}{\alpha_n}(J'(\mathbf{x}_n) - J'(\mathbf{x}_{n+1})) \tag{45}$$

Since $\mathbf{x}_*$ is the solution to the system $A\mathbf{x} = \mathbf{b}$, Eq. 40 implies

$$(A\mathbf{x}_* - \mathbf{b})\cdot\mathbf{p}_n = 0 \tag{46}$$

Thus far, all calculations are valid for an arbitrary choice of vectors $\mathbf{p}_n$. Let the vector, $\mathbf{p}_0$, be the gradient of the criterion Eq. 37 at some initial guess $\mathbf{x} = \mathbf{x}_0$:

[17] One could possibly choose it to be different for each sphere, making it a vector and not a scalar. Selection of α in the case of a scalar, reduces to a minimization problem of a function of one variable, which is easily solved by methods such as the golden section.

$$\mathbf{p}_0 = A\mathbf{x}_0 - \mathbf{b} = J'(\mathbf{x}_0) \tag{47}$$

Note that due to Eq. 42,

$$\mathbf{p}_0 = \mathbf{r}_0 \tag{48}$$

Clearly, vector $-\mathbf{p}_0$ points in the direction of fastest rate of decay of the criterion Eq. 37. Thus, from Eq. 43,

$$\mathbf{r}_0 \cdot \mathbf{r}_1 = J'(\mathbf{x}_0) \cdot J'(\mathbf{x}_1) = 0 \tag{49}$$

Eq. 46 and Eq. 40 at $n = 0$, in particular, implies that both $\mathbf{x}_1$ and $\mathbf{x}_*$ are in the same plane orthogonal to $\mathbf{p}_0$. Therefore, one can constrain further iterations to this plane only. This means that we select a direction $\mathbf{p}_1$, which is orthogonal to $\mathbf{p}_0$. To do so, we put $\mathbf{p}_1$ equal to a projection, in some sense, of the gradient of function Eq. 37 on this plane. namely, we subtract from the gradient $\mathbf{p}_0$ with an appropriate coefficient β_1. So, put

$$\mathbf{p}_1 = J'(\mathbf{x}_1) - \beta_1 \mathbf{p}_0 \tag{50}$$

Or, equivalently,

$$\mathbf{p}_1 = (A\mathbf{x}_1 - \mathbf{b}) - \beta_1 \mathbf{p}_0 = \mathbf{r}_1 - \beta_1 \mathbf{p}_0 \tag{51}$$

The dot product $A\mathbf{p}_1 \cdot \mathbf{p}_0$ must vanish,

$$A\mathbf{p}_1 \cdot \mathbf{p}_0 = 0 \tag{52}$$

Hence,

$$\beta_1 = \frac{A\mathbf{r}_1 \cdot \mathbf{p}_0}{A\mathbf{p}_0 \cdot \mathbf{p}_0} = \frac{(A\mathbf{x}_1 - \mathbf{b}) \cdot A\mathbf{p}_0}{A\mathbf{p}_0 \cdot \mathbf{p}_0} \tag{53}$$

The coefficient β_1 has been chosen in such a way that for any coefficient α, the vector $\mathbf{x}_1 - \alpha\mathbf{p}_1$ is in the same plane defined by Eq. 46 at $n = 0$:

$$(A(\mathbf{x}_1 - \alpha\mathbf{p}_1) - \mathbf{b}) \cdot \mathbf{p}_0 = 0 \tag{54}$$

After some algebra, it can be shown that for i, j not exceeding 2, we have

$$A\mathbf{p}_i \cdot \mathbf{p}_j = 0, \quad i \neq j \tag{55}$$

$$\mathbf{r}_i \cdot \mathbf{r}_j = 0, \quad i \neq j \tag{56}$$

and

$$\mathbf{r}_i \cdot \mathbf{p}_j = 0, \quad i > j \tag{57}$$

A general step of the algorithm is as follows: After $\mathbf{x}_i$ and $\mathbf{p}_i$ have been computed for $i = 0, 1, \ldots, n$ along with the coefficients α_i and β_i for $i < n$, relationships Eq. 55–Eq. 57 hold true for appropriate i, j not exceeding n. The next iteration $\mathbf{x}_{n+1}$ is computed using Eq. 39 and Eq. 41. Next direction is computed using

$$\mathbf{p}_{n+1} = \mathbf{r}_{n+1} - \beta_{n+1}\mathbf{p}_n \tag{58}$$

where β_{n+1} is selected to provide for

$$A\mathbf{p}_{n+1} \cdot \mathbf{p}_n = 0 \tag{59}$$

That is,

$$\beta_{n+1} = \frac{A\mathbf{r}_{n+1} \cdot \mathbf{p}_n}{A\mathbf{p}_n \cdot \mathbf{p}_n} \tag{60}$$

Using relationships Eq. 55–Eq. 57, the latter equation can be modified:

$$\beta_{n+1} = \frac{\mathbf{r}_{n+1} \cdot (\mathbf{r}_n - \mathbf{r}_{n+1})}{(\mathbf{r}_n - \mathbf{r}_{n+1}) \cdot \mathbf{p}_n} = -\frac{\mathbf{r}_{n+1} \cdot \mathbf{r}_{n+1}}{\mathbf{r}_n \cdot \mathbf{p}_n} = -\frac{\mathbf{r}_{n+1} \cdot \mathbf{r}_{n+1}}{\mathbf{r}_n \cdot (\mathbf{r}_n - \beta_n \mathbf{p}_{n-1})} = -\frac{\mathbf{r}_{n+1} \cdot \mathbf{r}_{n+1}}{\mathbf{r}_n \cdot \mathbf{r}_n} \tag{61}$$

By virtue of Eq. 38,

$$\beta_{n+1} = \frac{(J'(\mathbf{x}_{n+1}) - J'(\mathbf{x}_n)) \cdot J'(\mathbf{x}_{n+1})}{(J'(\mathbf{x}_{n+1}) - J'(\mathbf{x}_n)) \cdot \mathbf{p}_n} = -\frac{||J'(\mathbf{x}_{n+1})||^2}{||J'(\mathbf{x}_n)||^2} \tag{62}$$

4.2.1 Implementation of Conjugate Gradient for Granular Media

In cases where $J(\mathbf{x})$ is an arbitrary function (i.e. not quadratic), as in the current case (the energy is related to the displacement with a power of 5/2), the conjugate gradient algorithm can be applied for its minimization in the following way. After picking an initial guess, the first step is done using the steepest descent method, Eq. 47. In this case, we choose the initial guess for the first iteration to be the undeformed configuration.

The next iterations are performed by the same scheme, selecting α_n by the steepest descent method, and computing β_{n+1} using the rightmost expression in Eq. 60. The algorithm may not work in the same manner as it works for minimization of a quadratic criterion. For example, after sufficiently many iterations, the direction $\mathbf{p}_{n+1}$ computed by Eq. 58 may point not in a direction of decay of function $J(\mathbf{x})$. In such a case, one can refresh the procedure by enforcing $\beta_{n+1} = 0$ (i.e. performing a steepest descent step). The frequency of such an operation can be determined empirically. Note that if the conjugate gradients algorithm is restarted at every iteration, it becomes equivalent to the steepest descent method.

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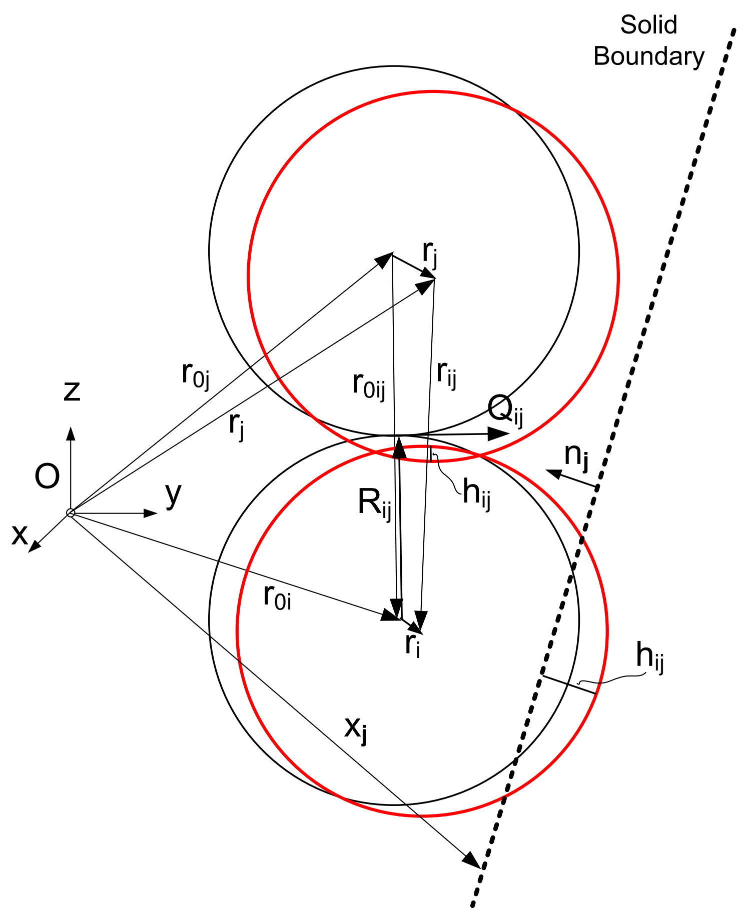

Figure 1: Relative displacements of two spheres in contact.