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TOWARDS A CONSTITUTIVE MODEL FOR CEMENTED GRANULAR MATERIALS

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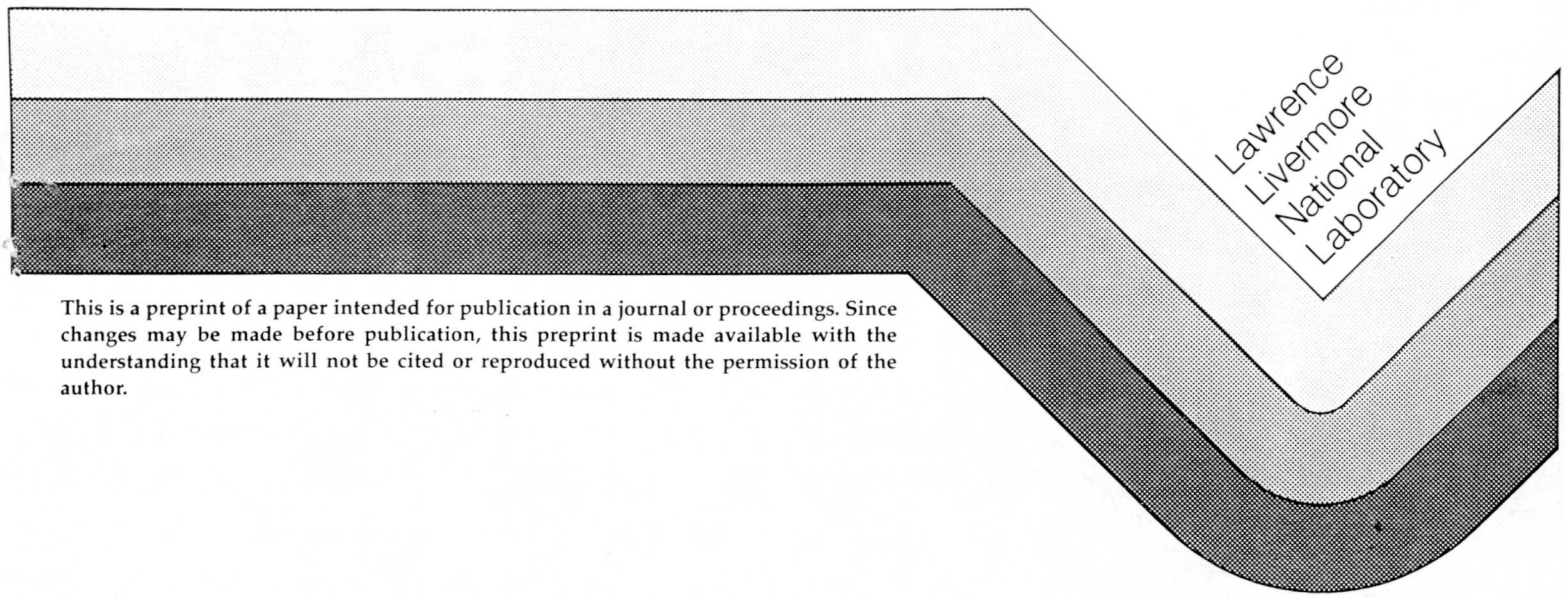

Towards a constitutive model for cemented granular materials

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1. INTRODUCTION

For several years we have been embarked on a program to understand the response of cemented granular materials to large deformations at high strain rates. A typical problem of interest is the formation of a crater in alluvium by a nuclear explosion (Margolin, et. al., 1988). Our goal is to construct a constitutive model that represents the complex behavior of such materials and yet is simple enough to use in large scale calculations based on computer programs that model solid continuum dynamics.

Our research is based on two premises. First we believe that the elastic properties -- i.e., the moduli -- of a cemented granular material depend mostly on the elastic properties of the bonding material and on the topology of the bonding, and are relatively independent of the elastic properties of the grains. Of course other properties of the material, such as bulk density, may depend mostly on the grains. Second we believe that macroscopic inelasticity in the response of a cemented granular material to loading is due mostly to one microscopic process, the fracture of the preexisting bonds.

Our research program has proceeded in several phases. The first phase was the construction of a numerical sample of a cemented granular material (Trent, 1987; Trent, 1988). The numerical sample is based on the discrete element method. In particular, we modified the TRUBAL code (Cundall, 1987) by adding elastic bonds between pairs of particles whose centers are closer than a specified distance. Although forces may still be produced by direct particle-particle contacts, the behavior of the material actually is dominated by the forces and moments produced by the shearing or stretching of the bonds as the particles rotate and get closer or further apart.

The second phase has been to verify that our numerical model accurately reproduces the inelastic behavior of real granular materials. The numerical model represents a considerable simplification of a real granular material. In particular, the only mechanism for inelasticity that we provide in our model is the fracture of bonds. It is encouraging that we can qualitatively reproduce such macroscopic behavior as plasticity in the compaction of hollow spheres as well as brittle crack growth in a flat plate (Trent and Margolin, 1989). By qualitative agreement, we mean that we preserve mathematical relationships between the physical variables, rather than achieving numerical agreement between a particular experiment and a calculation.

Although the modified TRUBAL code is well-suited to verifying the qualitative behavior of granular materials, it is unsuited for real problems with length scales of tens and hundreds of meters. We use several hundred particles in our numerical calculations, with a typical sample dimension on the order of centimeters. This number is chosen large enough to guarantee a small surface to volume ratio so that material behavior is dominated by material properties

rather than the details of the loading. Even a geometrically simple problem like cratering would require at least six orders of magnitude more particles. A calculation of this size on today's computers is not practical. Even if it were, most of the detailed output of such a calculation would be useless.

In the third phase of our research, we are attempting further simplifications by constructing an analytic model of the modified TRUBAL code. In this analytic model we will preserve our two premises, that the particles interact only through elastic bonds, and that the main source of inelasticity is fracture of the bonds. The major simplification occurs when we replace our detailed knowledge of the granular assembly, which is contained in the computer code, with a statistical model for the average grain.

The purpose of this paper is to describe the process of creating the analytic model. We will derive an expression for the effective elastic moduli expressed as integrals over the configurations of the average grain. These integrals depend on probability distributions for the number of bonds, their lengths, and their relative orientations. The form of these probability distributions will vary for different materials and depends on the process by which the material was formed. We do not discuss this point in this paper. Instead, we will make some reasonable assumptions for the probability distributions and go on to evaluate the qualitative dependencies of the effective moduli. Our final results show that the Youngs' modulus of the granular assembly should vary linearly with the area of the bond, the number of bonds per grain (i.e., the coordination number), the expected length of the bond, and the Youngs' modulus of the bonding material. Also, Poisson's ratio should be 0.25. We verify these dependencies numerically with calculations in our modified TRUBAL code.

2. ELASTIC BONDS IN THE MODIFIED TRUBAL CODE

We have modified the two-dimensional TRUBAL code by adding elastic bonds between particles whose centers are closer than some specified distance. The geometry of the bonding is specified by three parameters, α, β, and δ. These represent the width of the bond, the size of a preexisting Griffith crack within the bond, and the length of the bond. Each is made dimensionless by dividing by the particle radius, R. These parameters are illustrated graphically in Figure 1.

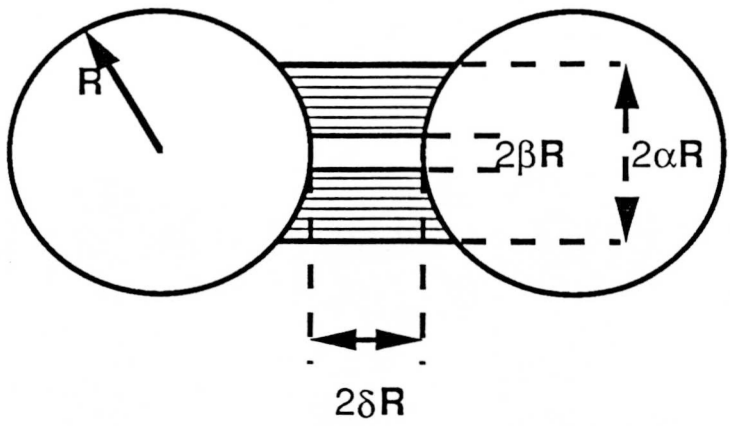

Figure 1. The dimensionless parameters α, β, and δ define the geometry of two bonded particles. In the middle of the bond is a vertical crack of width $2\beta R$.

To evaluate the restoring forces and moments between particles, we divide the bond into a set of infinitesimal strips , each of which acts as a simple spring. The effective spring constant (K) for a strip of width dA is simply given by Youngs' modulus ($E\mu$) times the infinitesimal area and divided by the length of the strip. The distance between the particles may change, producing a set of restoring forces and moments. In addition, the particles may rotate, which produces additional forces. The net force on the particles is found by summing up the individual contributions of the strips. The presence of the crack (which is vertical in figure 1) decreases the number of strips that connect the particles and so decreases the net force between the particles. In general, the crack may grow -- i.e., β can increase -- whenever the stresses within the bond are large enough. However, crack growth plays no role in the results of this paper.

3. MACROSCOPIC STRESS

The average stress tensor enclosed by a volume V is

$$\bar{\sigma}_{ij} = \frac{1}{V}\int_V \sigma_{ij}\,dV = \frac{1}{V}\left[\int_{V_p} \sigma_{ij}\,dV + \int_{V_b} \sigma_{ij}\,dV\right] \qquad (1)$$

where Vp is the volume of the particles and Vb is the volume of the bonds. We idealize the bonds by letting the total area A go to zero while the product (E A) remains finite. Our only purpose here is to simplify the mathematics by ignoring the change in length of the individual strips within the bond due to the curvature of the particle. We also assume that the surfaces of both the bonds and the particles are stress-free except at the contacts. In this case, the volume integrals in equation 1 can be transformed into surface integrals using the divergence theorem. After some manipulation, we can rewrite equation 1

$$\bar{\sigma}_{ij} = \frac{2}{V}\sum_{\text{particles}}\sum_{a} F_i^{(a)} L_j^{(a)} \qquad (2)$$

The inner sum is over the contacts of a particular particle. By contact, we mean the connection between a particle and a bond. The superscript (a) identifies the contact. **F** is the force within the bond. **L** is the vector pointing from the contact along the bond, and with magnitude equal to <u>half</u> of the length of the bond (e.g., $|\delta R|$; see figure 3). The forces within the particle have been eliminated in favor of the forces within the bond.

So far, our results apply exactly to the numerical model within the code. However they require a detailed knowledge of the configuration of particles and bonds within the material. We can simplify our equations if we replace the inner sum over the contacts about a particular particle by a sum over the contacts about an "average" particle. The outer sum over all the particles is then just the total number of particles, N, times the inner sum over the average particle.

To be more precise about what we mean by an "average" particle, let us assume that we can write down a probability distribution for the number of neighbors to which a central particle is bonded, for the lengths and orientations of the individual bonds. We denote this distribution

$$P(N_a, \mathbf{L}^{(1)}, \mathbf{L}^{(2)}, \ldots \mathbf{L}^{(N_a)})$$

where N_a is the number of neighbors. Thus the distribution P represents the probability of any possible configuration of neighbors and bonds around a particle. In these terms, equation 2 becomes

$$\bar{\sigma}_{ij} = \frac{2}{V} N < \sum_{a=1}^{N_a} F_i^{(a)} L_j^{(a)} > \qquad (3)$$

The brackets mean the distribution P is used to average over all configurations.

In principle, we can derive the probability distribution P from the code itself. In fact we have done this for the distribution of bond lengths, as well as the probability of the different coordination numbers. We assume that the bond lengths of separate bonds are uncorrelated.

The material in the modified TRUBAL code is formed by letting 270 identical particles fall under gravity and settle. Then all particles closer than a specified distance are bonded together. Figure 2 shows the cumulative number of bonds as the search distance is varied.

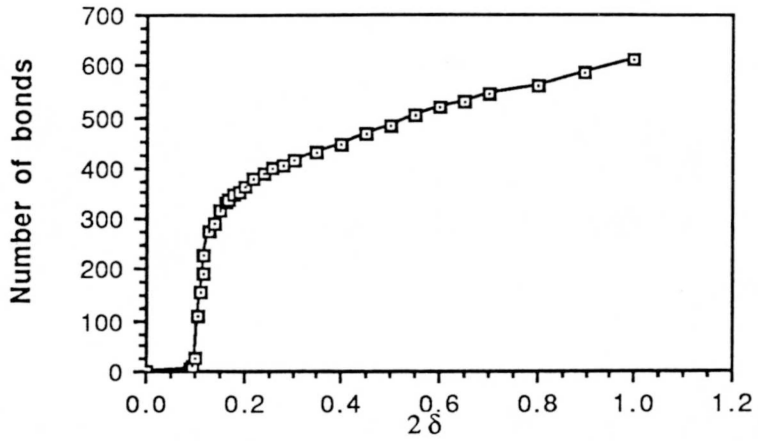

Figure 2. The cumulative number of bonds as a function of δ, which is the ratio of half the maximum separation distance to the particle radius R.

The case for the angular distributions -- i.e., for the orientations -- is more difficult, since the various orientations of the neighbors of a particle are clearly correlated in the sense that two neighbors cannot overlap. We attempted to bracket these angular distributions by evaluating two limit cases. In the first, we assume that the bonds are isotropic and uncorrelated. In the second, we assume that the bonds are evenly distributed about the central particle and so once one is known, the others are all determined. Remarkably, both assumptions lead to exactly the same result. Further, the results of comparing our theory to the numerical calculations bear out the conclusion that it is sufficient to treat the bond orientations as isotropically distributed and uncorrelated. Thus, we write

$$P(N_a, \mathbf{L}^{(1)}, \ldots \mathbf{L}^{(N_a)}) \approx P_1(N_a) \prod_{a=1}^{N_a} P_2(|L^{(a)}|) \frac{1}{2\pi} \qquad (4)$$

Both the functions P_1 and P_2 can be constructed from the graph in Figure 2.

4. THE MICROSCOPIC FORCE

We will calculate the effective moduli of the granular assembly by imposing a particular displacement of the boundaries and calculating the macroscopic stress in terms of those displacements. Suppose that we are given a specific configuration such as is shown in figure 3. We find the microscopic forces for such a configuration in terms of the bond vectors, and then average this force over all the possible configurations of the bond vectors.

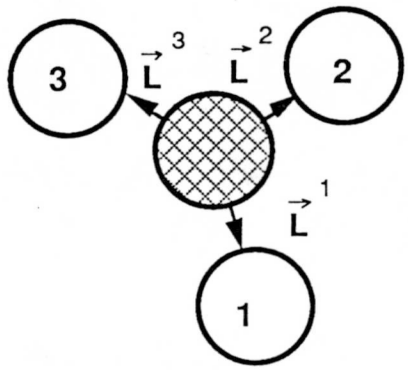

Figure 3. A specific configuration of a central particle bonded to three neighbors.

The displacement of the boundaries defines an average or macroscopic strain tensor. We shall assume that the neighboring particles are each displaced by the average strain tensor and so the magnitude of the displacement of neighbor 1 with respect to the original position of the central particle is

$$\left|\Delta x_i^{(1)}\right| = \sqrt{\Delta x_i^{(1)} \Delta x_i^{(1)}} = \frac{L_i^{(1)} L_j^{(1)} \bar{\varepsilon}_{ij}}{\left|L_i^{(1)}\right|} \tag{5}$$

We find, to first order in the strain tensor,

$$F_i^{(a)} = \frac{K}{2}\left\{\frac{L_i^{(a)} L_j^{(a)} L_k^{(a)} \bar{\varepsilon}_{jk}}{\left|L^{(a)}\right|^3} - \frac{L_i^{(a)} L_j^{(a)} \Delta x_j}{\left|L^{(a)}\right|^3}\right\} \tag{6}$$

where K is the effective spring constant and Δx_j, the displacement of the central particle, can be found from the equations of static equilibrium

$$\sum_{a=1}^{N_a} F_i^{(a)} = 0 \tag{7}$$

Once we have solved for the displacement, Δx_j , we can insert the expression for the force, equation 6, into equation 3 and so evaluate the effective moduli.

5. A COMPARISON OF ANALYTIC AND NUMERICAL RESULTS

Using the approximations for the probability distributions discussed above, we have derived the following expressions for the effective Youngs' modulus and the effective Poisson's ratio of the granular assembly (see Table 1 for notation).

$$\overline{E} = \frac{5}{8}\frac{\rho}{\rho_\mu}\frac{<L>}{R} <N_c> 2(\alpha-\beta) E_\mu$$
$$\nu = 0.25 \qquad (8)$$

The equation shows that the effective Youngs' modulus scales directly with Youngs' modulus of the bonding material, a result we derived previously based on dimensional analysis (Trent and Margolin, 1989), and is independent of Poisson's ratio of the bonding material. The effective Youngs' modulus also scales directly with the expected value of coordination number, and with the expected value of L, which is half the bond length. The final factor 2 $(\alpha - \beta)$ essentially represents the cross-sectional area of the bond possibly reduced by the presence of a crack.

The effective Youngs' modulus also depends on the ratio of macroscopic density ρ to the density of the grains ρ_μ (within the TRUBAL code, the bonds are assumed to be massless). This ratio may be eliminated in favor of the material porosity ϕ

$$\overline{E} = \frac{5}{8}(1-\phi)\frac{<L>}{R} <N_c> 2(\alpha-\beta) E_\mu \qquad (9)$$

In deriving equations 8, we made one addition simplification -- we set the displacement of the central grain $\Delta x_j = 0$ in equation 6. Heuristically, we argue that this term should be of order of the deviations of bond lengths from their average value. On the basis of figure 2, we know that most of the bonds are the same size, roughly one tenth of the particle radius, until we allow very large search distances. Thus, we expect equation 8 will be valid until the maximum search distance becomes large -- i.e., comparable to the particle radius.

Table 1. Baseline values of the input to TRUBAL for the parameter studies

Symbol	Description	Value	(units)
N	Total Number of Particles	270	
E_μ	Youngs' Modulus of Bonds	10000	MPa
ρ	Bulk density	1670	kg / m^3
ρ_μ	Grain density	2650	kg / m^3
R	Particle radius	.001	m

We have performed a parameter study on the modified TRUBAL code to verify the dependencies of equation 8. The baseline values of the input are shown in Table 1. In the calculations, we calculate the effective moduli by sending both a longitudinal and a shear wave through the sample and measuring the wave speeds, from which the moduli can be calculated (see Trent and Margolin, 1989).

In this parameter study we varied $2\delta R$, the maximum separation distance for bonding. This causes both the expected value of bond length $< L >$ and of coordination $< N_c >$ to vary. These expected values can be found from figure 2. In these calculations, we chose $\alpha = 0.5$ and $\beta = 0.025$. In figure 4 we plot the modulus versus the product $< N_c > < L >$. Equation 8 predicts this will be a straight line, which is verified by TRUBAL. Note that the agreement is best for small values of δ. We attribute this to our neglect of the displacement of the central particle in the force analysis, as explained in Section 4.

We have performed similar parameter studies to verify the dependence on cross-sectional area of the bonds, and also the prediction that Poisson's ratio should be 0.25. Poisson's ratio is remarkably constant at this value for smaller choices of the separation δ, but also shows a systematic deviation for larger values as the bond lengths approach the size of the particle radius. Lack of space precludes showing the details of these calculations here.

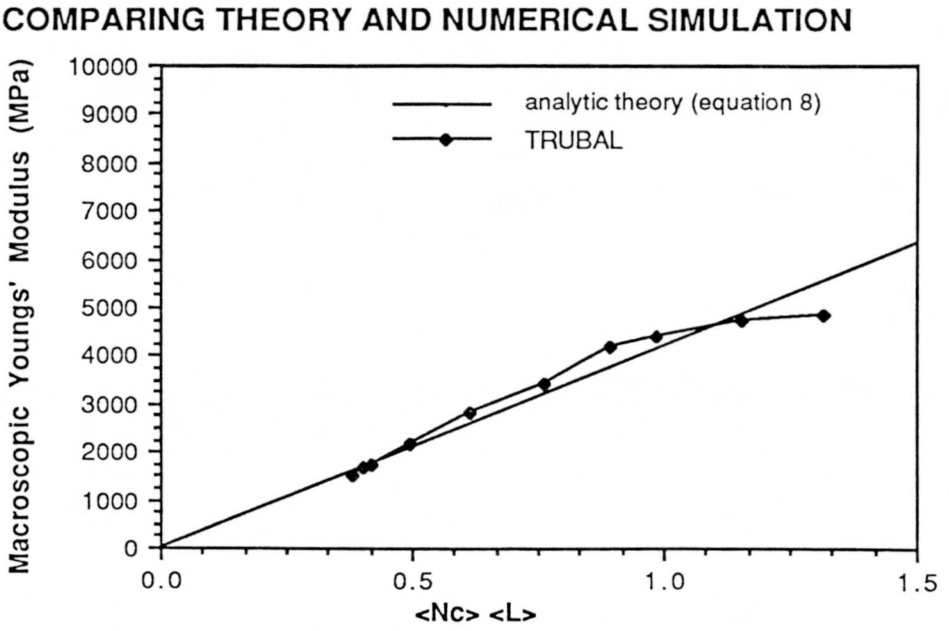

Figure 4. The variation of macroscopic Youngs' modulus as the maximum bonding distance is increased. The theory predicts that the modulus will vary linearly with the expected values of bond length and coordination number.

6. CONCLUSIONS AND FUTURE DIRECTIONS

We have derived an analytic model relating the effective moduli of a cemented granular material to the elastic properties and the topology of the bonds. The analysis is based on the idea of replacing the details of a granular assembly by a model of the average grain. We show that predictions of the analytic model compare well with the results of numerical simulation in our modified TRUBAL computer program.

Our analysis makes specific assumptions about the distribution that describes the probability of finding a bond at a given orientation or of a given length about a grain. These assumptions are reasonable for an undamaged isotropic material. However, when some bonds are damaged or broken as the result of loading, the assumption of isotropy must be discarded. We have begun work to generalize our results to predict effective moduli for materials with prescribed anisotropic damage. The generalized results, combined with a method for calculating the breaking of bonds, will provide the basis for a constitutive model for cemented granular materials suitable for large scale computing.

7. REFERENCES

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8. ACKNOWLEDGEMENT

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