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# Micromechanical Aspects of Isotropic Granular Assemblies With Linear Contact Interactions

*The paper presents a micromechanical analysis of plane granular assemblies of discs with a range of diameters, and interacting according to linear contact force-interparticle compliance relationships. Contacts are assumed to be fixed and indestructible. Macroscopically, the system is described in terms of a two-dimensional analogue of generalized Hooke's law. Explicit expressions for elastic constants in terms of microstructure are derived for dense isotropic assemblies. It is shown that Poisson's ratio for dense systems depends on the ratio of tangential to normal contact stiffnesses. The derived expression for Poisson's ratio is verified by numerically simulating plane assemblies comprising 1000 particles. The effect of density on Poisson's ratio is investigated using numerical simulations. The theory of dense plane systems is extended to dense three-dimensional systems comprising spheres. Finally, it is shown that Poisson's result $\nu = 1/4$ is recovered for spherical particles with central interactions.*

## Introduction

This study is concerned with the micromechanics of two-dimensional random isotropic assemblies of discs. The paper is limited to a detailed analysis of microscopic processes in the simplest system of this class comprising particles with a fixed system of indestructible contacts. Particles interact according to linear contact force-interparticle compliance relationships at the contacts.

From a macroscopic point of view, deformation properties of the system are described by a two-dimensional analogue of generalized Hooke's law and emphasis is placed on the relationship between macroscopic elastic parameters ($E$, $\nu$) and characteristics of microstructure such as interparticle stiffness and contact density.

Numerical simulations reported in this paper show that despite the apparent simplicity of the considered systems, their behavior is complex at the microscopic level. Results of numerical simulations are used in the current study to both guide and verify analytical developments which link microscopic and macroscopic descriptors.

Results of this study show that the principal element of complexity is local interparticle rotations which, nevertheless, become negligible in very dense systems. For these systems, an explicit relationship between Poisson's ratio and the ratio of linear contact stiffness components is derived. The latter development is presented for both plane and three-dimensional systems and Poisson's result $\nu = 1/4$ (e.g., Love, 1926) is recovered for spherical particles with central interactions.

## Description of Microstructure

**General.** Microchemical studies of granular materials require introduction of some unique physical concepts and have necessarily evolved a terminology specific to the discipline. In the soil mechanics literature the term *fabric* has been used extensively as a generic term to describe the geometry of particle packing (microstructure). In this section, characteristics of fabric relevant to mechanical description of two-dimensional assemblies of discs are introduced. Similar characteristics can be introduced for three-dimensional systems.

The assemblies under study are assumed to comprise essentially rigid particles which are joined together at indestructible compliant point contacts.

An individual particle at static equilibrium may be in contact with several neighbors. The number of contacts per particle is called the *coordination number* of the particle. Clearly each *physical* contact contributes two *contacts* to the assembly. The *average coordination number*, $\gamma$ of the assembly is:

$$\gamma = \frac{M_V}{N} \tag{1}$$

Here $M_V$ represents the total number of contacts within the assembly volume and $N$, the total number of particles.

Coordination number introduced above is an incomplete description of particle packing as it carries no information on relative particle orientations. This aspect of microstructure is often described by particle *contact normals* where a contact

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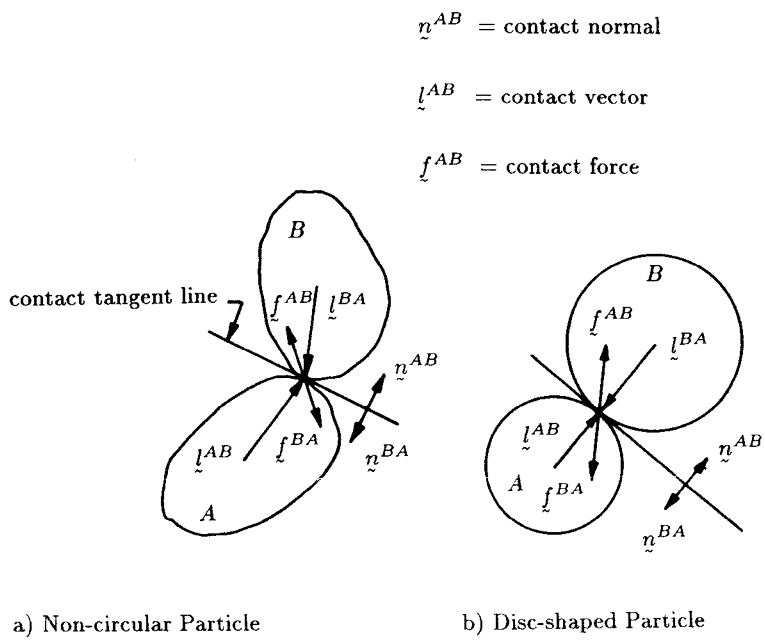


**Fig. 1 Contact normals, contact vectors, and contact forces**

normal $\mathbf{n}^c$ is the exterior directed normal to the tangent plane at the point of contact between particles. The relative frequency of contacts with different orientations of normals can be described in terms of a *contact orientation* distribution $E(\theta)$ such that $M_V E(\theta)\,\Delta\theta$ is the number of contacts with normals between $\theta$ and $\theta+\Delta\theta$ (Horne, 1965).

Description of particles of arbitrary shape requires identification of contacts in terms of *contacts vectors* (Rothenburg and Selvadurai, 1981*a*). For each contact, contact vector $\mathbf{l}^c$ is directed from the mass center of a particle to a point of contact with a neighbor. The orientational distribution of contact vector lengths implicitly contains information related to particle shape. Contact normals and contact vectors are illustrated in Fig. 1. For spherical particles (or discs) the direction of contact vectors is coincident with the direction of contact normals and the length of contact vectors is equal to particle radius.

**Microstructure of Isotropic Assemblies of Discs.** In the current study, contact normals are assumed to be distributed homogeneously through a two-dimensional system consisting of a very large number of *discs*.

Rothenburg (1980) has proposed that for two-dimensional assemblies of discs, $E(\theta)$ can be represented by a truncated even Fourier series of the form:

$$E(\theta)=\frac{1}{2\pi}\{1+a\cos 2(\theta-\theta_a)+b\cos 4(\theta-\theta_b)\} \tag{2}$$

Expression (2) satisfies the condition $E(\theta)=E(\theta-\pi)$ for assemblies of discs and when integrated over the limits $0\le\theta\le 2\pi$ gives:

$$\int_0^{2\pi} E(\theta)d\theta=1 \tag{3}$$

Terms $a$ and $b$ are called *coefficients of anisotropy* and define frequencies of contact normals in *directions of anisotropy* $\theta_a$ and $\theta_b$. It should be noted, however, that expression (2), in the strictest sense, describes an infinite, statistically homogeneous, assembly where the normalized distribution function $E(\theta)$ can be continuous. For any large but finite system of particles this relationship is a useful approximation.

In this paper, theoretical developments are restricted to *isotropic* assemblies (i.e., systems with $a=0$, $b=0$). Under these conditions:

$$E(\theta)=\frac{1}{2\pi} \tag{4}$$

Lack of orientational bias in numerically simulated assemblies was checked by calculating parameters of anisotropy from complete information on orientation of contact normals. The technique used to carry out these calculations has been described by Bathurst (1985).

In the current investigation, theoretical developments are also restricted to assemblies with a narrow range of disc sizes in which there is no bias between particle size and direction of interparticle contacts. Hence:

$$\bar{l}^c(\theta)=\bar{l}_o \tag{5}$$

Here $\bar{l}_o$ represents the *average* contact length taken from all assembly contacts.

## Theoretical Developments

**Average Stress Tensor from Averages of Contact Forces.** An average stress tensor in terms of the summation of discrete contact forces and fabric can be expressed as:

$$\bar{\sigma}_{ij}=\frac{1}{V}\sum_{c\epsilon V} f_i^c l_j^c \qquad i,j=1,2 \tag{6}$$

Terms $f_i^c$ and $l_j^c$ refer to scalar components of contact forces $\mathbf{f}^c$ and contact vectors $\mathbf{l}^c$ at contact locations (refer to Fig. 1). Equivalent expressions for three-dimensional idealized granular assemblies have been reported by Weber (1966), Dantu (1968), Rothenburg (1980), Christoffersen et al. (1981), and Bathurst (1985). Rothenburg (1980) and Rothenburg and Selvadurai (1981a) have proposed that expression (6) is a useful approximation to the stress tensor of continuum mechanics for granular assemblies comprising a large but finite number of particles. This equivalency can be understood by considering sums of force-contact vector components for many subregions of a given assembly volume. Quantities calculated from equation (6) would be expected to fluctuate from subvolume to subvolume. However, as the subdomains

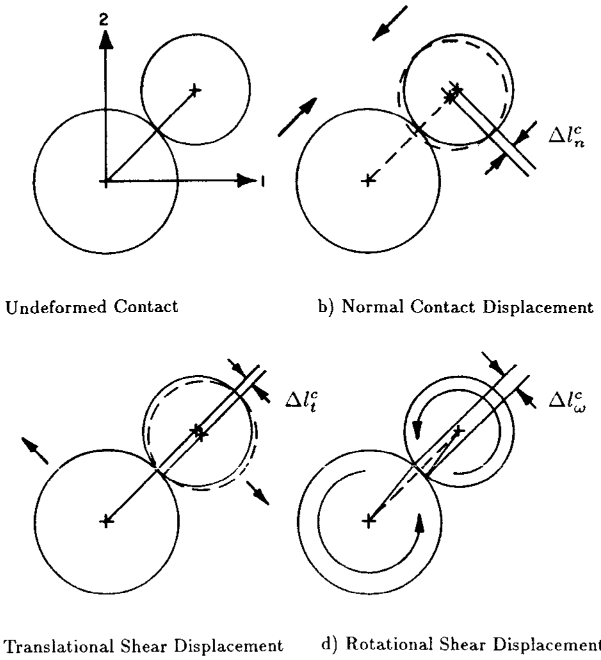


**Fig. 2 Contact displacement components**

increase in volume and number of particles within a homogeneous system, these fluctuations can be expected to become smaller and smaller. This tendency to a single representative *average stress tensor* is assured by the composition of the function where each term makes a small contribution to $f_i^c l_j^c / V$. For finite but large particle systems, the average stress tensor from discrete information is an accurate analogue to the stress tensor of continuum mechanics and in the following text they are assumed equivalent (i.e., $\sigma_{ij} = \bar{\sigma}_{ij}$).

Unfortunately, calculation of the average stress tensor using relationship (6) requires exact knowledge of contact forces and contact vector terms for all particles. Equivalent more manageable expressions can be developed by considering certain *averages* of grouped discrete information in a similar manner to the approach adopted in the previous section.

If contacts are grouped within a finite number of orientational class intervals, then group averages $\overline{f_i^c l_j^c}(\theta_g)$ can be calculated. The stress tensor relationship (6) can now be rewritten as:

$$\sigma_{ij} = \frac{M_V}{V} \sum_{\theta_g} \overline{f_i^c l_j^c}(\theta) E(\theta) \Delta\theta \tag{7}$$

Here a normalized discontinuous $E(\theta)$ is used to describe the orientational distribution of contact normals. Assuming an assembly with $\lim_{V\to\infty}$, $\lim_{M_V\to\infty}$ and $\lim_{\Delta\theta\to 0}$, relation (7) can be expressed in integral form as:

$$\sigma_{ij} = \frac{M_V}{V} \int_0^{2\pi} \overline{f_i^c l_j^c}(\theta) E(\theta) d\theta \tag{8}$$

If *isotropic* assemblies are considered, possible correlations between $\bar{l}_j^c(\theta)$ and $\bar{f}_i^c(\theta)$ are not a concern and the stress tensor expression is simplified to:

$$\sigma_{ij} = \frac{m_v \bar{l}_o}{2\pi} \int_0^{2\pi} \bar{f}_i(\theta) n_j(\theta) d\theta \tag{9}$$

Here, the term $m_v = M_V/V$ is introduced for brevity and is used to denote contact density with respect to assembly area. The above expression forms the basis of a constitutive relationship once the link between contact forces and strain is established.

**Relationship Between Average Contact Forces and Strain Tensor.** The link to average contact displacements can be made through a contact force-displacement law. A linear contact model offers mathematical simplicity and can be expressed as follows:

$$f_n^c = k_n \left( \frac{\Delta l_n^c}{l} \right)$$

$$f_s^c = k_s \left( \frac{\Delta l_t^c}{l} + \frac{\Delta l_\omega^c}{l} \right) \tag{10}$$

Here $l$ is the distance between particle centers in contact (i.e., the sum of contact vector lengths at a contact); $\Delta l_n^c / l$ is the relative normal displacement between particle centers; $(\Delta l_t^c / l + \Delta l_\omega^c / l)$ represents relative tangential displacement at a contact and consists of two terms describing relative translational displacement between particle centers and relative rotation. These terms are illustrated in Fig. 2. Parameters $k_n$ and $k_s$ in equations (10) refer to normal and tangential (shear) contact stiffnesses and $f_n^c$, $f_s^c$ the associated contact force components. A positive value for $f_s^c$ signifies a contact shear force which tends to rotate a disc in a counterclockwise direction.

Further theoretical developments are simplified if rotations $\Delta l_\omega^c$ can be neglected. The results of numerical simulations presented later in this paper show that this simplification is valid for dense systems. For these systems, the development of contact forces is entirely due to relative displacement components between particle centers. Considering that expression (9) for the stress tensor involves only *averages* of forces of similar orientations, it is reasonable to equate the latter to quantities describing *average* displacement components for similarly oriented contacts. It is useful at this point to introduce terms describing relative normal and tangential (shear) interparticle displacement components such as $\bar{\delta}_n^c(\theta)$ and $\bar{\delta}_t^c(\theta)$ averaged over groups of contacts with similar orientations:

$$\bar{\delta}_n^c(\theta) = \left(\frac{\overline{\Delta l_n^c(\theta)}}{l}\right)$$

$$\bar{\delta}_t^c(\theta) = \left(\frac{\overline{\Delta l_t^c(\theta)}}{l}\right) \tag{11}$$

Averages of forces with similar orientations can now be written as:

$$\bar{f}_n^c(\theta) = k_n \bar{\delta}_n^c(\theta)$$

$$\bar{f}_s^c(\theta) = k_s \bar{\delta}_t^c(\theta) \tag{12}$$

In order to link $\bar{\delta}_n^c(\theta)$ and $\bar{\delta}_t^c(\theta)$ with the strain tensor, it is convenient to resort to properties of the strain tensor of continuum mechanics as follows: In a uniformly strained continuum, a vector **L** connecting two arbitrary points is transformed into vectors **L** + Δ**L** in such a manner that $\Delta L_i = \epsilon_{ij} L_j$. Relative displacements in the direction normal and tangential to vector **L** can be calculated as follows:

$$\frac{\Delta L_n}{L} = \epsilon_{ij} n_i n_j$$

$$\frac{\Delta L_t}{L} = \epsilon_{ij} t_i n_j \quad i, \quad j = 1, 2 \tag{13}$$

Here **n** and **t** are coincident and orthogonal to **L**, respectively, and are defined by **n** = (cos θ, sin θ) and **t** = (− sin θ, cos θ). Expressions (13) cannot be applied on a scale comparable to the size of *grains* which physically constitute a *continuum*. However, if this is nevertheless done, it can expected that relations (13) will hold true when expressed as averages taken over an ensemble of similarly oriented points. When such points correspond to centers of particles forming contacts with similar orientations, it is reasonable to expect that:

$$\bar{\delta}_n^c(\theta) = \zeta(\epsilon_{ij} n_i n_j)$$

$$\bar{\delta}_t^c(\theta) = \zeta(\epsilon_{ij} t_i n_j) \tag{14}$$

where $\zeta$ is a constant. More detailed analysis presented by Rothenburg (1980) suggests that $\zeta < 1$. Assumptions which lead to equations (13) and link microscopic averages with similar characteristics calculated on the basis of rules of continuum mechanics are quite common (e.g., Batchelor and O'Brien, 1977). In the present paper the above relationships are verified directly on the basis of numerical simulations described later in this paper.

**Stress-Strain Relationship.** If expressions for average normal and tangential contact forces (12) are combined with equations (14) and the resulting expression for the average contact force vector is introduced into equation (9), then the following stress-strain relationship can be recovered:

$$\sigma_{ij} = A_{ijkl} \epsilon_{kl} \quad i, j, k, l = 1, 2 \tag{15}$$

where:

$$A_{ijkl} = \frac{\zeta k_n \bar{l}_o m_v}{2\pi} \int_0^{2\pi} \{ n_i n_j n_k n_l + \lambda t_i n_j t_k n_l \} d\theta \tag{16}$$

In these expressions, parameter λ is introduced as the ratio of tangential to normal contact stiffness (i.e., $\lambda = k_s / k_n$).

Direct calculation of integrals defining components of $A_{ijkl}$ results in Hooke's law for two-dimensional isotropic material with bulk and shear moduli as follows:

$$K = \frac{m_v \bar{l}_o k_n \zeta}{4}, \quad G = \frac{m_v \bar{l}_o k_n \zeta}{4} \left(\frac{1+\lambda}{2}\right) \tag{17}$$

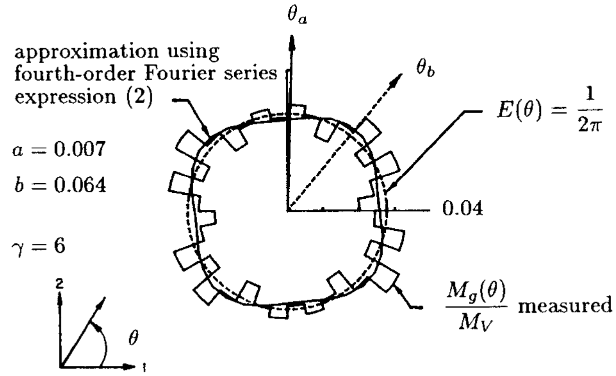


**Fig. 3 Normalized distribution of contact orientations for 1000 disc assembly**

Although the above moduli contain parameter $\zeta$ whose value is unspecified, Poisson's ratio is independent of $\zeta$ and depends on the ratio of tangential to normal contact stiffness according to:

$$\nu = \frac{1-\lambda}{3+\lambda} \tag{18}$$

## Numerical Simulation of Disc Assemblies

**General.** In the current investigation, numerical simulation of disc assemblies comprising 1000 particles was undertaken to verify fundamental relationships proposed in the preceding text. A principal advantage of numerical simulation is that it allows all *microscopic* information to be extracted from the assemblies under study. In addition, the influence of micromechanical properties such as stiffness ratio λ can be assessed more readily from these experiments than from comparable physical models (i.e., photo-elastic disc assemblies).

Numerical simulations were carried out using a program which is a modified version of the program BALL originally reported by Strack and Cundall (1978) and used by them to investigate the micromechanical behavior of *cohesionless* disc assemblies. Major modifications involved changes to internal bookkeeping to take advantage of specific computer hardware and elimination of data updating algorithms made possible by numerical assemblies comprising *fixed* contacts. The program implements a time-finite-difference scheme which solves the system of equations modelling a dynamic transient mechanical system. The mechanical system can be imagined as a network of lumped-mass-dashpot elements in which linear springs connect disc-shaped masses. Although the system is dynamic, the transient state approaches a static equilibrium condition if loading rates at the sample boundaries are kept low enough that inertial forces are always a small fraction of the average contact forces acting through the assembly. Kinetic energy is dissipated through the introduction of artificial damping, without which, the approximation to a static equilibrium condition would not be achieved.

Numerical tests were carried out from initial (undeformed) assemblies with near-isotropic microstructure. The disc radii in these tests fell within a narrow size range $0.78 \leq r/\bar{r}_o \leq 1.29$. Prior to loading, the coordination number of an assembly could be modified by searching out *near* contacts or deleting selected contacts in a random manner. Qualitatively this is equivalent to introducing small distortions in disc geometry such that interparticle contacts are created or lost while maintaining coincidence of contact normals and contact vectors.

The resulting microstructure for a typical assembly in the current study is illustrated by the polar histograms plotted in

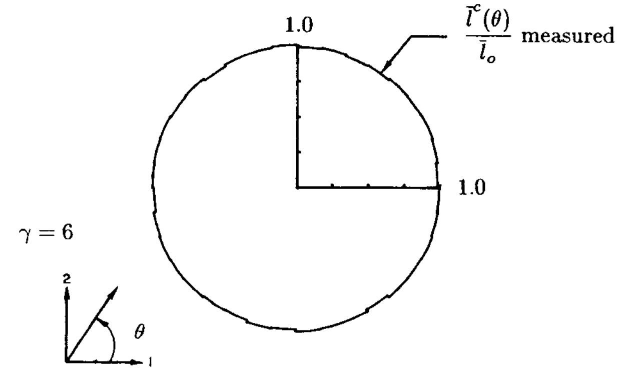


**Fig. 4 Normalized distribution of contact lengths for 1000 disc assembly**

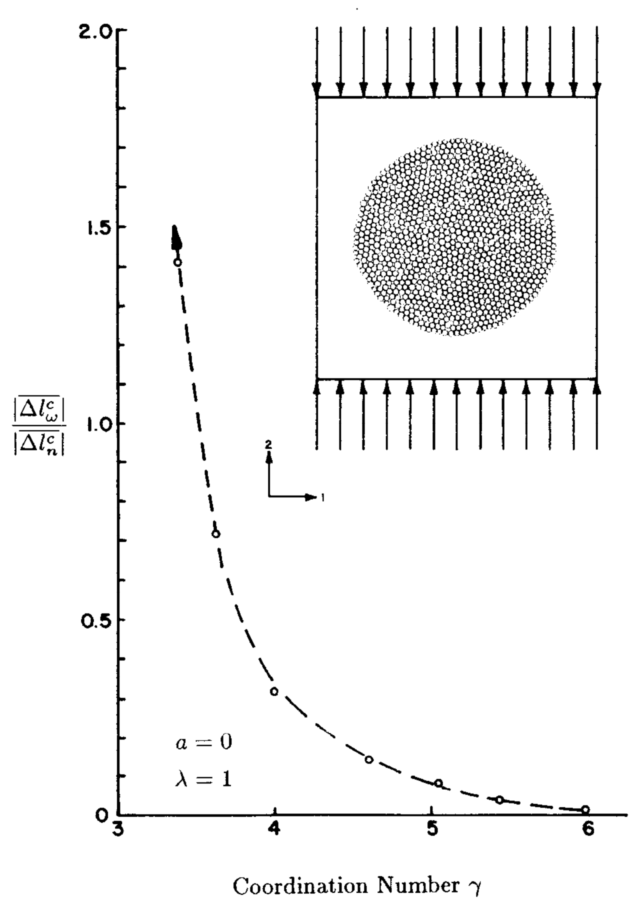


**Fig. 5 Influence of assembly coordination number on average rotational contact displacements**

Figs. 3 and 4. Figure 3 shows that the assembly is essentially isotropic with respect to the *second-order* distribution of contact normals (i.e., $a \approx 0$). Some anisotropy in higher-order microstructure is evident from the figure and can be quantified by the fourth-order coefficient of anisotropy as $b = 0.064$. Nevertheless, Bathurst (1985) has shown from the results of similar numerical experiments on *cohesionless* disc assemblies that coefficient terms greater than order two in equation (2) do not significantly influence stress quantities when *anisotropic* distributions for $E(\theta)$ are considered in equations (7) and (8). Isotropic microstructure with respect to the distribution of contact lengths is clearly evident from Fig. 4.

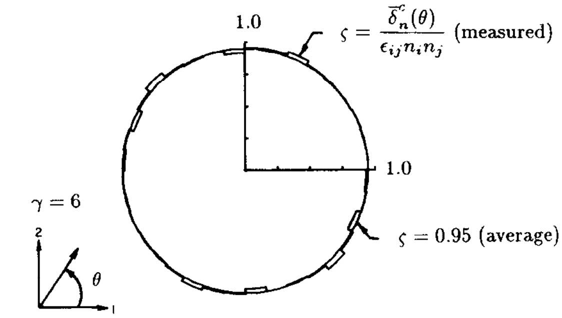


**Fig. 6(a) Stiffness reduction coefficient $\varsigma$ from distribution of average normal contact displacements $\bar{\delta}_n^c(\theta)$**

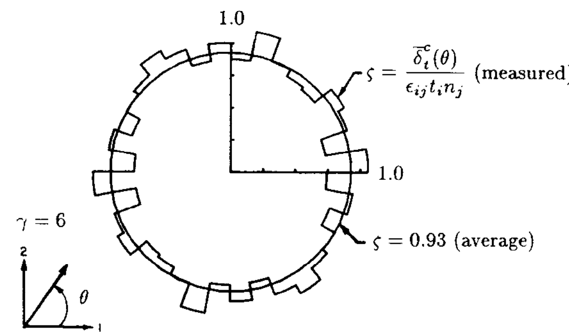


**Fig. 6(b) Stiffness reduction coefficient $\varsigma$ from distribution of average tangential contact displacements $\bar{\delta}_t^c(\theta)$**

**Test Program.** A series of numerical simulations were undertaken to verify assumptions (14) and Poisson's ratio expression in terms of interparticle stiffness ratio (18).

Assemblies comprising 1000 discs were subjected to biaxial compression by imposing at the sample boundary discrete forces approximating the stress state $\sigma_{22} > 0$, $\sigma_{11} = 0$ and $\sigma_{12} = \sigma_{21} = 0$. Under these conditions Poisson's ratio could be calculated directly by measuring the resulting principal strain ratio.

Disc interactions in this investigation were controlled by the linear force-displacement laws given in expressions (10). The ratio of interparticle stiffnesses was kept constant for all contacts but was varied between tests over the range $0 \le \lambda \le 1$. A stiffness ratio of unity represents a lower limit on the ratio of tangential to normal compliances for elastic spheres in contact according to Mindlin (1949). Truly elastic spheres or discs interact in a nonlinear manner but a linear spring model is useful for verification of theoretical concepts. It is expected that nonlinear contact interactions would lead to other qualitative effects. This topic is currently under investigation by the authors.

**Test Results.** The influence of coordination number (i.e., system density) on shear displacements generated through particle rotations can be appreciated from Fig. 5. The figure shows that the relative magnitude of $|\overline{\Delta l_\omega^c}|$ for all contacts increases dramatically for assemblies as $\gamma \to 3$. Plane assemblies with coordination number lower than 3 cannot generally be maintained in static equilibrium. For assemblies with a coordination number close to 3, average particle rotations are large, reflecting the freedom afforded interparticle deformations by low system density. Conversely, the magnitude of average particle rotations reduces to zero as the maximum coordination number of 6 is approached. In this case, particles are constrained to the point that their rotations virtually disappear.

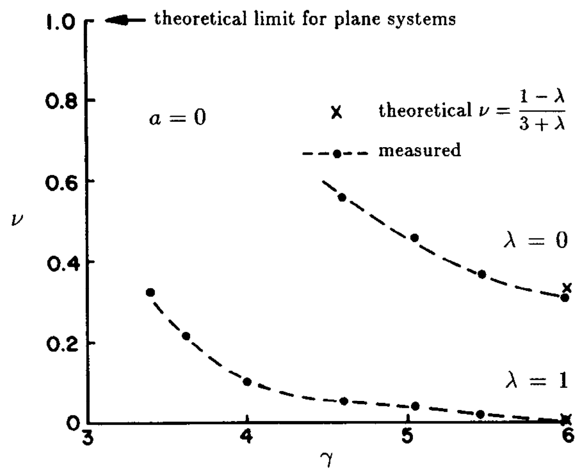


Fig. 7 Measured Poisson's ratio ν versus coordination number γ

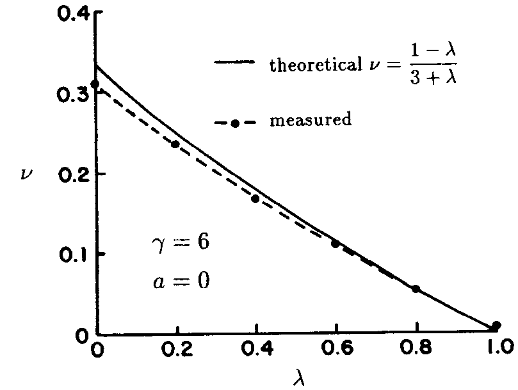


Fig. 8 Comparison of measured and theoretical values of Poisson's ratio ν against stiffness ratio λ

A major concept that allows stress-strain relationships for the considered systems to be developed is obtained in equations (14). It is through this relationship that the link between average interparticle displacements and macroscopic strain is made. Relationship (14) implies that $\zeta$ is a direction-independent constant. Figures 6(*a*) and 6(*b*) plot ratios $\bar{\delta}_n^c(\theta)/(\epsilon_{ij}n_in_j)$ and $\bar{\delta}_t^c(\theta)/(\epsilon_{ij}t_in_j)$ as polar histograms. It is clear from the figures that these ratios are direction-independent and nearly equal for both normal and tangential displacements and hence verify the fundamental assumption contained in expression (14).

The Poisson's ratio expression (18) predicts values of 0 and 1/3 for stiffness ratios 1 and 0, respectively, provided particle rotations are prohibited. The deviation from predicted values for assemblies with $3 \le \gamma \le 6$ is shown in Fig. 7. It should be noted that the predicted values of Poisson's ratio are generally lower than measured values from numerical simulations. The discrepancy is observed to increase with the magnitude of particle rotations. This component of shear deformations was essentially neglected in theoretical developments. Theoretical expressions, therefore, overpredict actual shear stiffness while correctly predicting bulk modulus. In general, this situation leads to an underestimate of Poisson's ratio. Nevertheless, Fig. 7 shows that as $\gamma \rightarrow 6$, theoretically predicted values for Poisson's ratio emerge. The data on this figure for $\lambda = 0$ is restricted to tests with $\gamma \ge 4.5$ corresponding to the range of stable numerical results. For less dense systems, the number of particles in unstable configurations was great enough to prevent the entire assembly from approaching static equilibrium within a reasonable number of calculation cycles.

The results of a series of tests with $\gamma = 6$ and $0 \le \lambda \le 1$ are given in Fig. 8. The data show that relationship (18) gives a reasonable estimate of Poisson's ratio for these systems.

## Implications to Three-Dimensional Systems

Numerical simulation of two-dimensional assemblies of discs can be thought of as an analogue to idealized assemblies of *spheres* having variable radius and interacting through linear compliant *fixed* contacts. Unfortunately, numerical simulation of these systems is prohibitively expensive for assemblies having a statistically meaningful number of particles. Nevertheless, the theoretical developments leading to the Poisson's ratio expression for two-dimensional systems are analogous to the approach which can be adopted to arrive at a similar expression for dense three-dimensional assemblies. For example, if three-dimensional assemblies of spheres with *isotropic* fabric are considered, then $E(\Omega) = 1/4\pi$, $\bar{l}^c(\Omega) = \bar{l}_o$ and the stress tensor expression become:

$$\sigma_{ij} = \frac{m_v \bar{l}_o}{4\pi} \int_\Omega \bar{f}_i^c(\Omega) n_j(\Omega) d\Omega \qquad i,j = 1, 2, 3 \tag{19}$$

Here, $d\Omega = \sin\beta d\beta d\theta$ corresponding to the unit spherical coordinate system with $0 \le \beta \le \pi$ and $0 \le \theta \le 2\pi$. Components of the normal vector $\mathbf{n}$ are related to the unit spherical coordinate system according to:

$$\begin{aligned} n_1 &= \sin\beta\sin\theta \\ n_2 &= \cos\beta \\ n_3 &= \sin\beta\cos\theta \end{aligned} \tag{20}$$

Rothenburg and Selvadurai (1981b) have shown that if particle rotations are negligible, average contact force components in relation (19) can be equated to the strain tensor according to:

$$\bar{f}_i^c(\Omega) = \zeta k_n \{\lambda \epsilon_{il} n_l + (1-\lambda)(\epsilon_{kl} n_l n_k) n_i\} \quad i, k, l = 1, 2, 3 \tag{21}$$

Substitution of equations (20) and (21) into equation (19) leads to an expression for Poisson's ratio as follows:

$$\nu = \frac{1-\lambda}{4+\lambda} \tag{22}$$

Based on experience from numerical simulation of two-dimensional systems, it is reasonable to expect that this relationship is valid for dense assemblies of spheres with a fixed system of contacts and linear contact interactions. If these assemblies are restricted to a narrow range of particle sizes, then dense assemblies would correspond to systems with $\gamma \rightarrow 12$. Equation (22) is in agreement with the value of $\nu = 1/4$ established by Poisson (e.g., Love, 1926) for random assemblies of spheres with central interactions (i.e., $\lambda = 0$).


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