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# On the stress–force–fabric relationship for granular materials

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ABSTRACT

This paper employed the theory of directional statistics to study the stress state of granular materials from the particle scale. The work was inspired by the stress–force–fabric relationship proposed by Rothenburg and Bathurst (1989), which represents a fundamental effort to establish analytical macro–micro relationship in granular mechanics. The micro-structural expression of the stress tensor $\sigma_{ij} = \frac{1}{V}\sum_{c \in V} v_i^c f_j^c$, where $f_i^c$ is the contact force and $v_i^c$ is the contact vector, was transformed into directional integration by grouping the terms with respect to their contact normal directions. The directional statistical theory was then employed to investigate the statistical features of contact vectors and contact forces. By approximating the directional distributions of contact normal density, mean contact force and mean contact vector with polynomial expansions in unit direction vector **n**, the directional dependences were characterized by the coefficients of the polynomial functions, i.e., the direction tensors. With such approximations, the directional integration was achieved by means of tensor multiplication, leading to an explicit expression of the stress tensor in terms of the direction tensors. Following the terminology used in Rothenburg and Bathurst (1989), the expression was referred to as the stress–force–fabric (SFF) relationship.

Directional statistical analyses were carried out based on the particle-scale information obtained from discrete element simulations. The result demonstrated a small but isotropic statistical dependence between contact forces and contact vectors. It has also been shown that the directional distributions of contact normal density, mean contact forces and mean contact vectors can be approximated sufficiently by polynomial expansions in direction **n** up to 2nd, 3rd and 1st ranks, respectively. By incorporating these observations and revoking the symmetry of the Cauchy stress tensor, the stress–force–fabric relationship was further simplified, while its capacity of providing nearly identical predictions of the stresses was maintained. The derived SFF relationship predicts the complete stress information, including the mean normal stress, the deviatoric stress ratio as well as the principal stress directions.

The main benefits of deriving the stress–force–fabric relationship based on the directional statistical theory are: (1) the method does not involve space subdivision and does not require a large number of directional data; (2) the statistical and directional characteristics of particle-scale directional data can be systematically investigated; (3) the directional integration can be converted into and achieved by tensor multiplication, an attractive feature to conduct computer program aided analyses.



## 1. Introduction

Granular materials often exhibit sophisticated collective behavior even though they consist of solid particles with relatively simple particle–particle interactions. This makes multi-scale investigation an important branch of granular mechanics. Particle-scale information, which was a difficult and rare source to obtain in history, has nowadays become easily accessible, mainly due to the emergence and fast growth of the discrete element method (DEM) (Cundall and Strack, 1979). The good qualitative agreement between laboratory observations and DEM simulations has made DEM a popular numerical tool for multi-scale investigations. One of the remaining challenges, as addressed in the current paper, is to extract the key statistical features from the massive amount of particle-scale information in order to advance our understanding in granular materials.

The micro-structural definition of the stress tensor is a well-established starting point of many multi-scale investigations. In case of static equilibrium, the stresses acting on the material boundary are transmitted through the internal structure and in equilibrium with the inter-particle interactions. Viewing a granular material as an assembly of granular particles with only point

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contact, the macro stress tensor could be evaluated from the tensor product of contact forces $f_i^c$ and contact vectors $v_i^c$ as:

$$\sigma_{ij} = \frac{1}{V} \sum_{c \in V} v_i^c f_j^c \tag{1}$$

in which $\sigma_{ij}$ stands for the average stress tensor over volume $V$. To be consistent with the sign convention in soil mechanics, a contact vector is defined as the vector pointing from the contact point to the particle centre. Eq. (1) links the stress tensor defined at equivalent continuum scale with inter-particle contact forces (Love, 1927; Weber, 1966; Goddard, 1977; Christoffersen et al., 1981; Rothenburg and Selvadurai, 1981; Bagi, 1996; Li et al., 2009). It has been derived rigorously for quasi-static granular materials based on the Newton's 2nd law of motion with only the uniformity and point contact assumption.

Like many other relationships addressing homogenization between macro and micro variables, the expression of Eq. (1) involves summation over a massive amount of particle-scale information as appeared on the right hand side of the equation. It is a source of complication pertinent to the fact that the particle-scale information, including both contact vectors and contact forces, are random variables, and intrinsically direction dependent (Drescher and De Josselin de Jong, 1972; Oda et al., 1982; Cundall and Strack, 1983).

The development and application of the statistical theory to process directional data has been pioneered by Kanatani (1984). His work dealt with unit vectors. Examples in the context of granular mechanics are contact normals and particle orientations. Being aware that the physical quantities, like forces, displacements, are to be represented by vectors, reflecting information on both their directions and magnitudes, Li and Yu (2011) have extended the mathematical formulations (Kanatani, 1984) to vector-valued directional data. The form of polynomial expansions in direction $\mathbf{n}$ has been followed to approximate the directional distributions. And the least square error criterion has been employed to determine the tensorial coefficients, i.e., the direction tensors. These direction tensors are macroscopic measures defined on the statistics of particle-scale directional data. They can be used as macro variables for the development of the micro–macro relationships and physical laws reflecting fundamental mechanisms. The theoretical formulations and the applied techniques have been published in a preceding paper (Li and Yu, 2011).

Directional statistical analyses are of particular importance in the study of material anisotropy, which has been recognized as an important aspect of granular material behaviors for many years (Casagrande and Carrillo, 1944; Drescher and Josselin De Jong, 1972; Oda, 1972; Oda et al., 1985). Rothenburg and Selvadurai (1981) were among the first to introduce Fourier series in the description of the directional dependence of contact normal density. Such an approximation has been shown to have the root in the directional statistical theory (Kanatani, 1984). Rothenburg and Bathurst (1989) also used Fourier series to approximate the directional distributions of mean normal contact force and mean tangential contact force with coefficients interpretable as measures of anisotropy in respective quantities. They hence derived the stress–force–fabric (SFF) relationship for two dimensional assemblies consisting of disks, and later extended the expression to two dimensional elliptical-shaped particles (Rothenburg and Bathurst, 1993) and three dimensional ellipsoidal particles with anisotropy tensors (Ouadfel and Rothenburg, 2001).

The SFF relationship proposed by Rothenberg and his co-workers formulated the macroscopic stress tensor as an explicit statistical description in terms of anisotropic parameters. It provides a micromechanical insight into the continuum-scale shear strength of granular materials. However, the basic assumptions made during their derivation have not been fully validated, mainly: (i) the contact vectors and the contact forces in each direction are statistically independent; (ii) the Fourier functions up to 2nd rank are sufficient to approximate the directional distributions of contact normal density, normal and tangential contact forces.

The main objective of this paper is to apply the mathematical theory of directional statistics to conduct the multi-scale investigation on the stress state of granular materials. In particular, we will revisit and study the validity of the key assumptions made by Rothenberg and his co-workers with the newly developed directional statistical theory. In this paper, unless indicated otherwise an Einstein summation convention is adopted for repeated subscripts.

## 2. General form of the stress–force–fabric relationship

### 2.1. Integral form of the micro-structural stress tensor

Let $\Omega$ represent the unit circle in two dimensional spaces ($D = 2$) or the unit sphere in three dimensional spaces ($D = 3$). We denote the total number of contacts in a granular assembly as $M$, and $\Delta M(\mathbf{n})$ represents the number of contacts whose normal directions fall into the stereo-angle element $\Delta\Omega$ centered at direction $\mathbf{n}$. The terms on the right hand side of Eq. (1) can be grouped according to their contact normal directions, leading to:

$$\sigma_{ij} = \frac{1}{V} \sum_{\Omega} \langle v_i f_j \rangle|_{\mathbf{n}} \Delta M(\mathbf{n}) = \frac{M}{V} \sum_{\Omega} e^c(\mathbf{n}) \langle v_i f_j \rangle|_{\mathbf{n}} \Delta\Omega \tag{2}$$

where $*|_{\mathbf{n}}$ denotes the value of variable $*$ in direction $\mathbf{n}$, and $\langle * \rangle|_{\mathbf{n}}$ denotes the average value of all terms of $*$ sharing the same contact normal direction $\mathbf{n}$. The discrete spectra of function $e^c(\mathbf{n}) = \Delta M(\mathbf{n})/\Delta\Omega$ is the probability density of contact normals. $e^c(\mathbf{n})\Delta\Omega$ represents the probability that an arbitrary selected contact has a normal direction falling within the stereo-angle element $\Delta\Omega$. When the stereo-angle increment approaches zero, we have $e^c(\mathbf{n}) = \lim_{\Delta\Omega \to 0} \Delta M(\mathbf{n})/\Delta\Omega$. It becomes a continuous function at the thermodynamic limit.

The average number of contacts per particle is $\omega = M/N$, where $N$ is the total number of particles. In the case of thermodynamic limit, $\omega$ approaches a limit, i.e., $\lim_{N \to \infty} M/N = \omega$. It is referred to as the coordination number, an index characterizing the packing density. When $\Delta\Omega \to 0$, transition leads to an expression of the stress tensor in terms of integration over all stereo-angles as:

$$\sigma_{ij} = \frac{\omega N}{V} \oint_{\Omega} e^c(\mathbf{n}) \langle v_i f_j \rangle|_{\mathbf{n}} d\Omega \tag{3}$$

where $d\Omega$ is an elementary solid angle.

Eq. (3) involves the joint product $\langle v_i f_j \rangle|_{\mathbf{n}}$ within the integration. In general, $\langle v_i f_j \rangle|_{\mathbf{n}} \neq \langle v_i \rangle|_{\mathbf{n}} \langle f_j \rangle|_{\mathbf{n}}$, where $\langle v_i \rangle|_{\mathbf{n}}$ and $\langle f_j \rangle|_{\mathbf{n}}$ denote the mean contact vector and the mean contact force along direction $\mathbf{n}$ respectively. For randomly distributed contact vectors $\mathbf{v}$ and contact forces $\mathbf{f}$, the covariance matrix:

$$\begin{aligned} \mathrm{Cov}(\mathbf{v}|_{\mathbf{n}}, \mathbf{f}|_{\mathbf{n}}) &= \left\langle (\mathbf{v}|_{\mathbf{n}} - \langle \mathbf{v} \rangle|_{\mathbf{n}}) \cdot (\mathbf{f}|_{\mathbf{n}} - \langle \mathbf{f} \rangle|_{\mathbf{n}})^T \right\rangle \\ &= \left\langle \mathbf{v}|_{\mathbf{n}} \cdot \mathbf{f}|_{\mathbf{n}}^T \right\rangle - \langle \mathbf{v} \rangle|_{\mathbf{n}} \cdot \langle \mathbf{f} \rangle|_{\mathbf{n}}^T \end{aligned} \tag{4}$$

reflects the statistical dependence in direction $\mathbf{n}$, which could be direction dependent. The statistical dependence has been investigated using the statistical dependence theory as detailed later in Section 4. It will be shown based on the particle-scale information obtained from DEM that the statistical dependence between the contact vectors and contact forces is almost isotropic, i.e.,

$$\left\langle \mathbf{v}|_{\mathbf{n}} \cdot \mathbf{f}|_{\mathbf{n}}^T \right\rangle = \varsigma \langle \mathbf{v} \rangle|_{\mathbf{n}} \cdot \langle \mathbf{f} \rangle|_{\mathbf{n}}^T \tag{5}$$