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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:

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

in which σ_{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 **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 Ω 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:

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

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, ω 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:

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

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:

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

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.,

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

where ς is a direction independent scalar. It is hence taken as an assumption to avoid unnecessary complication. With this assumption, Eq. (3) can be rewritten as:

$$\sigma = \frac{\omega N}{V}\oint_{\Omega}\varsigma e^{c}(\mathbf{n})\langle\mathbf{v}\rangle|_{\mathbf{n}}\cdot\langle\mathbf{f}\rangle|_{\mathbf{n}}^{T}d\Omega \tag{6}$$

In Eq. (6), there are scalar quantities including the coordination number ω, the particle density N/V, the statistical dependence coefficient ς and an integration over direction of the multiplication of the contact normal probability density $e^c(\mathbf{n})$, the mean contact vector $\langle\boldsymbol{v}\rangle|_{\mathbf{n}}$ and the mean contact force $\langle\mathbf{f}\rangle|_{\mathbf{n}}$.

2.2. Contact normal probability density $e^c(\mathbf{n})$

Orientations can be represented by direction vectors of unit length. For point contacts, each contact is associated with two contact normals, represented by unit normal vectors $\mathbf{n}$ and $-\mathbf{n}$, respectively. The probability density of contact normals can be approximated by an even function $E^c(\mathbf{n})$, symmetric with respect to direction $\mathbf{n}$, i.e., $E^c(\mathbf{n}) = E^c(-\mathbf{n})$. With $E^c(\mathbf{n})$ being the probability density distribution, it must satisfy:

$$\oint_{\Omega}E^{c}(\mathbf{n})d\Omega = 1 \quad \text{and } E^{c}(\mathbf{n}) \geqslant 0 \tag{7}$$

Using a polynomial in unit direction vector $\mathbf{n}$ with indeterminate coefficients (Kanatani 1984; Li and Yu, 2011), the n-th rank approximation takes the following form:

$$E^{c}(\mathbf{n}) = \frac{1}{E_0}F^{c}_{i_1 i_2\cdots i_n}n_{i_1}n_{i_2}\cdots n_{i_n} \tag{8}$$

where $E_0 = \oint_{\Omega}d\Omega$. In the two dimensional space, $E_0 = 2\pi$ and in the three dimensional space, $E_0 = 4\pi$. The rank of the approximation refers to the highest rank of the power terms in the polynomial expansion. For symmetric distributions, the rank of approximation in Eq. (8) should only be even numbers, and the direction tensor $F^c_{i_1 i_2\cdots i_n}$ is a symmetric tensor, i.e., $F^c_{i_1 i_2\cdots i_n} = F^c_{(i_1 i_2\cdots i_n)}$, () over the subscripts designates the symmetrisation of the indices. $F^c_{i_1 i_2\cdots i_n}$ is referred to as the direction tensor for contact normal density.

Making an orthogonal decomposition, Eq. (8) can be expressed equivalently as:

$$E^{c}(\mathbf{n}) = \frac{1}{E_0}\left[D_0 + D^{c}_{i_1 i_2}n_{i_1}n_{i_2} + \cdots + D^{c}_{i_1 i_2\cdots i_n}n_{i_1}n_{i_2}\cdots n_{i_n} + \cdots\right] \tag{9}$$

Each term in Eq. (9) is independent from the others. In view of its symmetry, $D^c_{i_1 i_2\ldots i_n}$ should be also symmetric with respect to subscripts $i_1, i_2, \ldots i_n$, i.e., $D^c_{i_1 i_2\ldots i_n} = D^c_{(i_1 i_2\cdots i_n)}$. Being an orthogonal decomposition, $D^c_{i_1 i_2\cdots i_n}$ is deviatoric, i.e., $D^c_{i_1\cdots i_k\cdots i_l\cdots i_n}\delta_{i_k i_l} = 0$. $D^c_{i_1 i_2\cdots i_n}$ is termed as the deviatoric direction tensor for contact normal density. The direction tensors $F^c_{i_1 i_2\cdots i_n}$ and $D^c_{i_1 i_2\cdots i_n}$ can be calculated from the given dataset of contact normals as elaborated in Appendix A1. More details are available in Li and Yu (2011).

2.3. Mean contact vector $\langle\boldsymbol{v}\rangle|_{\mathbf{n}}$

Vector is a more general form of directional data. For vector-valued directional data, we are interested in both their probability density and their mean values in each direction. This applies to both the mean contact vector $\langle\boldsymbol{v}\rangle|_{\mathbf{n}}$ and the mean contact force $\langle\mathbf{f}\rangle|_{\mathbf{n}}$.

Here we approximate the directional distribution of mean vector $\langle\boldsymbol{v}\rangle|_{\mathbf{n}}$, (which is the mean of all the contact vectors $\boldsymbol{v}$ associated with the same contact normal direction $\mathbf{n}$) with a polynomial series $\langle\boldsymbol{v}\rangle|_{\mathbf{n}}$ as a linear combination of $n_{i_1}n_{i_2}\cdots n_{i_n}$. The n-th rank approximation of the contact vector $\langle\boldsymbol{v}\rangle|_{\mathbf{n}}$ takes the following compact form:

$$V_j(\mathbf{n}) = \upsilon_0 H^{\upsilon}_{ji_1\cdots i_n}n_{i_1}n_{i_2}\cdots n_{i_n} \tag{10}$$

where $\upsilon_0 = \oint_{\Omega}\langle\boldsymbol{v}\rangle|_{\mathbf{n}}\cdot\mathbf{n}d\Omega/E_0$ is the directional average of $\langle\boldsymbol{v}\rangle|_{\mathbf{n}}\cdot\mathbf{n}$, i.e., the component of $\langle\boldsymbol{v}\rangle|_{\mathbf{n}}$ coaxial with $\mathbf{n}$. It is noted that for contact vectors the rank of the direction tensors is one order higher than that of approximation. $H^{\upsilon}_{ji_1\cdots i_n}$ is a tensor symmetric with respect to the subscripts $i_1, i_2, \ldots i_n, \ldots$ i.e., $H^{\upsilon}_{ji_1 i_2\cdots i_n} = H^{\upsilon}_{j(i_1 i_2\cdots i_n)}$, and is referred to as the direction tensor for mean contact vector. It characterizes the directional dependence of the mean contact vector $\langle\boldsymbol{v}\rangle|_{\mathbf{n}}$.

Contact vectors are defined as vectors pointing from the contact points to the particle centres. Noticing that under quasi-static condition, all the particles are in equilibrium. Eq. (1) holds true with the particle centre being a fixed reference point for each particle. It is not necessarily to be the conventional choice as its centre of mass. If the particles have centre-point symmetric geometries, we could assume that the contact vectors are anti-symmetric with respect to direction $\mathbf{n}$, i.e., $\langle\boldsymbol{v}\rangle|_{\mathbf{n}} = -\langle\boldsymbol{v}\rangle|_{-\mathbf{n}}$. The approximations should hence have only terms of odd powers of $\mathbf{n}$. Making an orthogonal decomposition, the n-th rank approximation of $\langle\boldsymbol{v}\rangle|_{\mathbf{n}}$ takes the following expansion form

$$V_j(\mathbf{n}) = \upsilon_0\left[n_j + G^{\upsilon}_{ji_1}n_{i_1} + \cdots + G^{\upsilon}_{ji_1\cdots i_n}n_{i_1}\cdots n_{i_n} + \cdots\right] \tag{11}$$

in which $G^{\upsilon}_{ji_1\cdots i_n}$ is deviatoric and symmetric with respect to the subscripts $i_1, i_2, \ldots i_n, \ldots$ i.e., $G^{\upsilon}_{ji_1 i_2\cdots i_n} = G^{\upsilon}_{j(i_1 i_2\cdots i_n)}$ and $G^{\upsilon}_{ji_1\cdots i_k\cdots i_l\cdots i_n}\delta_{i_k i_l} = 0$. $G^{\upsilon}_{ji_1\cdots i_n}$ is referred to as the deviatoric direction tensor for the mean contact vector. The methods and procedures to calculate the direction tensors $H^{\upsilon}_{ji_1\cdots i_n}$ and $G^{\upsilon}_{ji_1\cdots i_n}$ based on the given discrete dataset has been carefully elaborated (Li and Yu, 2011). It is also briefed in Appendix A2 for completeness.

2.4. Mean contact force $\langle\mathbf{f}\rangle|_{\mathbf{n}}$

According to Newton's 3rd law of motion, there are a pair of action and reaction forces at each contact point acting on the two bodies, respectively, which are of equal magnitudes and opposite directions. Hence, it is reasonable to assume the mean contact force is an anti-symmetric function with respect to direction $\mathbf{n}$, i.e., $\langle\mathbf{f}\rangle|_{\mathbf{n}} = -\langle\mathbf{f}\rangle|_{-\mathbf{n}}$. Similarly to the method used to approximate the directional distribution for mean contact vectors, the contact forces averaged over contacts sharing the same normal directions can be approximated by following the compacted form as follows:

$$F_j(\mathbf{n}) = f_0 H^{f}_{ji_1 i_2\cdots i_n}n_{i_1}n_{i_2}\cdots n_{i_n} \tag{12}$$

or by following the form of an orthogonal decomposition as follows:

$$F_j(\mathbf{n}) = f_0\left[n_j + G^{f}_{ji_1}n_{i_1} + \cdots + G^{f}_{ji_1\cdots i_n}n_{i_1}\cdots n_{i_n} + \cdots\right] \tag{13}$$

where f_0 represents the directional average of mean normal contact force $\langle f^n\rangle|_{\mathbf{n}} = \langle\mathbf{f}\rangle|_{\mathbf{n}}\cdot\mathbf{n}$, i.e., $f_0 = \oint_{\Omega}\langle\mathbf{f}\rangle|_{\mathbf{n}}\cdot\mathbf{n}d\Omega/E_0$; $H^{f}_{ji_1 i_2\cdots i_n}$ and $G^{f}_{ji_1\cdots i_n}$ are the direction tensor and the deviatoric direction tensor for mean contact force, respectively. $G^{f}_{ji_1\cdots i_n}$ is symmetric and deviatoric with respect to subscripts $i_1, i_2, \ldots i_n, \ldots$ i.e., $G^{f}_{ji_1 i_2\cdots i_n} = G^{f}_{j(i_1 i_2\cdots i_n)}$ and $G^{f}_{ji_1\cdots i_k\cdots i_l\cdots i_n}\delta_{i_k i_l} = 0$. The determination of the direction tensors from discrete directional dataset follows the same methods and procedures as those described for mean contact vectors. They are not repeated here due to space limitation.

2.5. General expressions for the stress–force–fabric relationship

Take the sufficient ranks to approximate the directional distributions of contact normal density, mean contact vector and mean contact force as even number n, odd numbers s and t, respectively.

Following the expressing given in Eqs. (8), (10), and (12), Eq. (6) can be transformed as follows:

$$\sigma_{ij} = \frac{\omega N}{V} \varsigma v_0 f_0 F^c_{k_1\cdots k_n} H^v_{il_1\cdots l_s} H^f_{jm_1\cdots m_t} \times \overline{n_{k_1}\cdots n_{k_n} n_{l_1}\cdots n_{l_s} n_{m_1}\cdots n_{m_t}} \tag{14}$$

where $\overline{*} = \oint_\Omega (*) d\Omega / E_0$ denotes the average of $*$ over directions. The identity $\overline{n_{i_1} n_{i_2}\cdots n_{i_{2n-1}} n_{i_{2n}}}$ is a constant matrix. It has been derived in Li and Yu (2011) that:

$$\overline{n_{i_1} n_{i_2}\cdots n_{i_{2n-1}} n_{i_{2n}}} = \alpha_{2n} \delta_{(i_1 i_2} \delta_{i_3 i_4} \cdots \delta_{i_{2n-1} i_{2n})} \tag{15}$$

where $\alpha_{2n} = \begin{cases} \frac{^{2n}C_n}{2^{2n}}, D = 2 \\ \frac{1}{2n+1}, D = 3 \end{cases}$, and δ_{ij} is the Kronecker delta, and ^nC_k stands for the number of k-combinations of a n-element set.

The stress tensor in Eq. (1) possesses all the properties of the Cauchy stress tensor used in continuum mechanics (Rothenburg and Selvadurai 1981). In the quasi-static condition, the moment equilibrium imposes the symmetry of the stress tensor, i.e., $\sigma_{ij} = \sigma_{ji}$. Hence, the following equation should be satisfied:

$$F_{k_1\cdots k_n} (H^v_{il_1\cdots l_s} H^f_{jm_1\cdots m_t} - H^v_{jl_1\cdots l_s} H^f_{im_1\cdots m_t}) \times \overline{n_{k_1}\cdots n_{k_n} n_{l_1}\cdots n_{l_s} n_{m_1}\cdots n_{m_t}} = 0. \tag{16}$$

By substituting the orthogonal decomposed expressions Eqs. (9), (11), and (13) into Eq. (14), we have:

$$\sigma_{ij} = \frac{\omega N}{V} v_0 f_0 \begin{bmatrix} \overline{n_i n_j} + \sum_{t=1}^{\propto} G^f_{jm_1\cdots m_t} \overline{n_i n_{m_1}\cdots n_{m_t}} + \sum_{s=1}^{\propto} G^v_{il_1\cdots l_s} \overline{n_j n_{l_1}\cdots n_{l_s}} \\ + \sum_{s,t=1}^{\propto} G^f_{jm_1\cdots m_t} G^v_{il_1\cdots l_s} \overline{n_{l_1}\cdots n_{l_s} n_{m_1}\cdots n_{m_t}} \\ + \sum_{n=2}^{\propto} D^c_{k_1\cdots k_n} \overline{n_{k_1}\cdots n_{k_n} n_i n_j} \\ + \sum_{n=2;t=1}^{\propto} D^c_{k_1\cdots k_n} G^f_{jm_1\cdots m_t} \overline{n_{k_1}\cdots n_{k_n} n_i n_{m_1}\cdots n_{m_t}} \\ + \sum_{n=2;s=1}^{\propto} D^c_{k_1\cdots k_n} G^v_{il_1\cdots l_s} \overline{n_{k_1}\cdots n_{k_n} n_{l_1}\cdots n_{l_s} n_j} \\ + \sum_{n=2;s=1;t=1}^{\propto} D^c_{k_1\cdots k_n} G^f_{jm_1\cdots m_t} G^v_{il_1\cdots l_s} \overline{n_{k_1}\cdots n_{k_n} n_{l_1}\cdots n_{l_s} n_{m_1}\cdots n_{m_t}} \end{bmatrix} \tag{17}$$

Being orthogonal decompositions, we have the coefficient tensors satisfying

$$\begin{aligned} D^c_{i_1\cdots i_n} \overline{n_{i_1} n_{i_2}\cdots n_{i_n} n_{j_1} n_{j_2}\cdots n_{j_m}} &= 0 \\ G^v_{i_0 i_1\cdots i_s} \overline{n_{i_1} n_{i_2}\cdots n_{i_s} n_{j_1} n_{j_2}\cdots n_{j_t}} &= 0 \\ G^f_{i_0 i_1\cdots i_s} \overline{n_{i_1} n_{i_2}\cdots n_{i_s} n_{j_1} n_{j_2}\cdots n_{j_t}} &= 0 \end{aligned} \tag{18}$$

when $m < n, t < s, m$ and n are even numbers, s and t are odd numbers. Following the derivation in Appendix A3, Eq. (17) can be simplified as:

$$\sigma_{ij} = \frac{\omega N}{V} \varsigma v_0 f_0 \begin{bmatrix} \overline{n_i n_j} + G^f_{jm_1} \overline{n_i n_{m_1}} + G^v_{il_1} \overline{n_{l_1} n_j} + D^c_{k_1 k_2} \overline{n_{k_1} n_{k_2} n_i n_j} \\ + \sum_{s=1}^{\propto} G^f_{jm_1\cdots m_s} G^v_{il_1\cdots l_s} \overline{n_{l_1}\cdots n_{l_s} n_{m_1}\cdots n_{m_s}} \\ + \sum_{n=2,\text{even}}^{\propto} D^c_{k_1\cdots k_n} G^f_{jm_1\cdots m_{n-1}} \overline{n_i n_{k_1}\cdots n_{k_n} n_{m_1}\cdots n_{m_{n-1}}} \\ + \sum_{n=2,\text{even}}^{\propto} D^c_{k_1\cdots k_n} G^f_{jm_1\cdots m_{n+1}} \overline{n_i n_{k_1}\cdots n_{k_n} n_{m_1}\cdots n_{m_{n+1}}} \\ + \sum_{n=2,\text{even}}^{\propto} D^c_{k_1\cdots k_n} G^v_{im_1\cdots m_{n-1}} \overline{n_j n_{k_1}\cdots n_{k_n} n_{m_1}\cdots n_{m_{n-1}}} \\ + \sum_{n=2}^{\propto} D^c_{k_1\cdots k_n} G^v_{im_1\cdots m_{n+1}} \overline{n_j n_{k_1}\cdots n_{k_n} n_{m_1}\cdots n_{m_{n+1}}} \\ + \sum_{n=2;s,t=1;|s-t|\leqslant n\leqslant s+t}^{\propto} D^c_{k_1\cdots k_n} G^v_{il_1\cdots l_s} G^f_{jm_1\cdots m_t} \\ \times \overline{n_{k_1}\cdots n_{k_n} n_{l_1}\cdots n_{l_s} n_{m_1}\cdots n_{m_t}} \end{bmatrix} \tag{19}$$

For any symmetric and deviatoric tensor $D_{i_1 i_2\cdots i_n}$, we have (Li and Yu, 2011):

$$D_{j_1 j_2\cdots j_n} \overline{n_{j_1} n_{j_2}\cdots n_{j_n} n_{i_1} n_{i_2}\cdots n_{i_n}} = \alpha_{2n} \frac{2^n}{^{2n}C_n} D_{i_1 i_2\cdots i_n} \tag{20}$$

With this relationship, the terms in Eq. (19) can be calculated individually as detailed in Appendix A4. And the stress tensor hence becomes:

$$\sigma_{ij} = \frac{\omega N}{V} \varsigma v_0 f_0 \begin{bmatrix} \alpha_2 \delta_{ij} + \alpha_2 G^f_{ji} + \alpha_2 G^v_{ij} + \frac{2}{3} \alpha_4 D^c_{ij} + \sum_{s=1}^{\propto} \alpha_{2s} \frac{2^s}{^{2s}C_s} G^f_{jl_1\cdots l_s} G^v_{il_1\cdots l_s} \\ + \sum_{n=2}^{\propto} \alpha_{2n} \frac{2^n}{^{2n}C_n} D^c_{im_1\cdots m_{n-1}} G^f_{jm_1\cdots m_{n-1}} + \sum_{n=2}^{\propto} \alpha_{2n+2} \frac{2^{n+1}}{^{2n+2}C_{n+1}} D^c_{k_1\cdots k_n} G^f_{jik_1\cdots k_n} \\ + \sum_{n=2}^{\propto} \alpha_{2n} \frac{2^n}{^{2n}C_n} D^c_{im_1\cdots m_{n-1}} G^v_{jm_1\cdots m_{n-1}} + \sum_{n=2}^{\propto} \alpha_{2n+2} \frac{2^{n+1}}{^{2n+2}C_{n+1}} D^c_{k_1\cdots k_n} G^v_{jik_1\cdots k_n} \\ + \sum_{n=2,|s-t|\leqslant n\leqslant s+t}^{\propto} \alpha_{2n} \frac{2^n}{^{2n}C_n} D^c_{k_1\cdots k_n} Q^{vf,st}_{ijk_1\cdots k_n} \end{bmatrix} \tag{21}$$

This equation expresses the stress tensor in terms of direction tensors that characterize the internal structure (fabric) and inter-particle reaction forces, and is referred to as the stress–force–fabric (SFF) relationship, following the terminology proposed by Rothenburg and Bathurst (1989).

3. Statistical features of granular materials

The expression of Eq. (21) is mathematically derived from the micro-structural expression of the stress tensor as in Eq. (1). The only assumption we have adopted is the statistical dependence between contact vectors and contact forces being isotropic. The rank of approximation can be very high. Experimental and numerical work in granular mechanics suggested that the directional distributions can be approximated with limited ranks of approximation (Oda et al., 1985; Rothenburg and Bathurst, 1989). In this section, we analyze the particle-scale information obtained from DEM. By conducting the directional statistical analyses, we could determine the rank of approximation based on the particle-scale directional data, and use the observations to simplify the general expression given as Eq. (21). With the particle scale information obtained from two dimensional numerical simulations, the analyses described in this section are limited to two dimensional cases.

Using the numerical experimental technique developed in Li et al. (2013), the elementary behavior of two dimensional granular materials subjected to various loading paths have been simulated and reported (Li and Yu, 2009, 2010). In these numerical experiments, each particle is formed by clumping two equal-sized disks together. The distance between the centres of the two disks is equal to 1.5 times the disk radius, r. The particle size was uniformly distributed within the range (0.2, 0.6 mm) in terms of equivalent diameter, and the disk thickness was $t = 0.2$ mm. The number of particles used is about 3500, and according to Rothenburg and Bathurst (1989) is sufficient to model an infinite system for purposes of force balance in two dimensional assemblies.

The mechanical interaction between two elastic disks were derived based on the contact theories (Li, 2006) and used in the simulations. In two dimensional cases, the contact law includes two linear elastic models (normal and tangential) of equal stiffnesses, and a slip model. The effect of contact moment is ignored. Both the normal and tangential particle stiffnesses were set to be 10^5 N/m. The coefficient of friction was $\mu = 0.5$. The properties of the boundary walls were set to be the same as those of the particles. The material gravity was set to be zero. Local damping was used to dissipate kinetic energy.

An isotropic specimen was prepared using the radius expansion method, and then subjected to isotropic consolidation up to confining pressure $p_c = 1000$ kPa before biaxial shearing. The void ratio at $P_c = 1000$ kPa was 0.192. The specimen preparation method and material responses to various loading have been detailed in Li et al. (2013). The material responses have been observed to be in qualitative agreement with laboratory observations, though not repeated here due to space limitation. During shearing, the major principal strain direction α_ε was fixed, the mean normal stress was kept constant, while the magnitude of deviatoric strain ε_q was increasing. Loading applied vertically is denoted by angle 90°, in terms of its deviation to the x_1 axis.

3.1. Contact normal density $e^c(\mathbf{n})$

The directional distribution of contact normal density can be approximated using the compacted form of polynomial expansions as in Eq. (8) or in the form of orthogonal decomposition as in Eq. (9) with its main statistical features reflected by the direction tensor $F^c_{i_1\cdots i_n}$ or alternatively the deviatoric direction tensor $D^c_{i_1\cdots i_n}$. The latter is used here since the deviatoric tensor can be determined independently for different ranks of approximation.

In two dimensional spaces, a symmetric and deviatoric tensor $D^c_{i_1\cdots i_n}$ only has two independent components. Denoting $D^c_{1\overbrace{1\cdots1}^{n-1}} = a_n$ and $D^c_{2\overbrace{1\cdots1}^{n-1}} = b_n$, we have the tensor components expressed as follows:

$$D^c_{11\cdots1\overbrace{22\cdots2}^{k}} = \begin{cases} (-1)^{k/2} a_n, & \text{when } k \text{ is even} \\ (-1)^{(k-1)/2} b_n, & \text{when } k \text{ is odd} \end{cases} \tag{22}$$

With $d_n = \sqrt{a_n^2 + b_n^2}$ and $\tan\phi_n = b_n/a_n$, we have $a_n = d_n\cos\phi_n$ and $b_n = d_n\sin\phi_n$. It is shown in Appendix A5 that the n-th rank power term in the orthogonal decomposition of Eq. (9) can be expressed as:

$$D^c_{i_1\cdots i_n} n_{i_1} n_{i_2}\cdots n_{i_n} = a_n\cos n\theta + b_n\sin n\theta = d^c_n\cos(n\theta - \phi^c_n) \tag{23}$$

It is a cosine function with the period $2\pi/n$, the magnitude d_n and the phase angle ϕ_n/n. With Eqs. (9) and (23), the directional distribution of the contact normal probability density $E^c(\mathbf{n})$ can be expressed as a summation over even numbers n as

$$E^c(\mathbf{n}) = \frac{1}{E_0}\left[1 + \sum_n d^c_n\cos\left(n\theta - \phi^c_n\right)\right] \tag{24}$$

Based on particle-scale information obtained from discrete element simulations, the direction tensors for contact normal density $F^c_{i_1\cdots i_n}$ and $D^c_{i_1\cdots i_n}$ were calculated following the procedure introduced in Appendix A1. They were then used to determine the magnitudes and phase angles in Eq. (24). The magnitudes of the 2nd, 4th and 6th rank orthogonal decompositions, d^c_2, d^c_4, d^c_6, are plotted in Fig. 1(a). It is shown that the magnitude of deviatoric direction tensor decreases rapidly as the rank of approximation increases. The 2nd rank orthogonal decomposition is observed to be the main contributor to the direction dependent distribution of contact normal density, while the 4th and 6th rank terms are negligible. As shear continues, the material fabric anisotropy gradually increases in order to withstand the external shearing. The phase angle of the 2nd rank approximation is $\phi_2/2$ = 90° as shown in Fig. 2(b), suggesting that the maximum probability density is co-directional with the loading direction. With the negligible magnitudes for the 4th and 6th rank terms, the values of their phase angles are of little significance and hence not plotted in the figure.

In summary, the numerical observation indicates that the directional distribution of the contact normal probability density $E^c(\mathbf{n})$ can be sufficiently approximated by up to 2nd rank power terms as:

$$E^c(\theta) = \frac{1}{2\pi}\left[1 + d^c_2\cos\left(2\theta - \phi^c_2\right)\right] \tag{25}$$

In terms of direction tensors, it is:

$$D^c_{i_1i_2} = d^c_2\begin{pmatrix} \cos\phi^c_2 & \sin\phi^c_2 \\ \sin\phi^c_2 & -\cos\phi^c_2 \end{pmatrix} \tag{26}$$

3.2. Mean contact vector $\langle\mathbf{v}\rangle|_\mathbf{n}$

The directional distributions of mean contact vector could be approximated using the compacted form as in Eq. (10) or in the form of orthogonal decomposition as in Eq. (11) with its main statistical features reflective by the direction tensor $H^v_{ji_1i_2\cdots i_n}$ or alternatively the deviatoric direction tensor $G^v_{ji_1\cdots i_n}$. In analogy to Eq. (23), the n-th power term of Eq. (11) in two dimensional spaces could be expressed as:

$$\begin{aligned} g^v_{nj} &= G^v_{ji_1\cdots i_n} n_{i_1} n_{i_2}\cdots n_{i_n} = a^v_{nj}\cos n\theta + b^v_{nj}\sin n\theta \\ &= d^v_{nj}\cos(n\theta - \phi^v_{nj}) \end{aligned} \tag{27}$$

where d^v_{nj} and ϕ^v_{nj}/n stand for the magnitudes and phase angles for the n-th rank orthogonal decomposition terms, respectively.

Denoting $A^v_n = \sqrt{d^{v2}_{n1} + d^{v2}_{n2} - 2d^v_{n1}d^v_{n2}\sin(\phi^v_{n1} - \phi^v_{n2})}/2$, $B^v_n = \sqrt{d^{v2}_{n1} + d^{v2}_{n2} + 2d^v_{n1}d^v_{n2}\sin(\phi^v_{n1} - \phi^v_{n2})}/2$, $\alpha^v_n = \arctan\left[(d^v_{n1}\sin\phi^v_{n1} - d^v_{n2}\cos\phi^v_{n2})/(d^v_{n1}\cos\phi^v_{n1} + d^v_{n2}\sin\phi^v_{n2})\right]$, $\beta^v_n = \arctan\left[(d^v_{n1}\sin\phi^v_{n1} + d^v_{n2}\cos\phi^v_{n2})/(d^v_{n1}\cos\phi^v_{n1} - d^v_{n2}\sin\phi^v_{n2})\right]$, the n-th power term becomes:

$$g^v_{nj} = G^v_{ji_1\cdots i_n} n_{i_1}\cdots n_{i_n} = A^v_n\begin{pmatrix} \cos\left(n\theta - \alpha^v_n\right) \\ \sin\left(n\theta - \alpha^v_n\right) \end{pmatrix} + B^v_n\begin{pmatrix} \cos\left(n\theta - \beta^v_n\right) \\ -\sin\left(n\theta - \beta^v_n\right) \end{pmatrix} \tag{28}$$

The expression suggests that the n-th power term in Eq. (11) can be decomposed into two components whose magnitudes being A^v_n and B^v_n, respectively. With Eqs. (11) and (28), the directional distribution of mean contact vector $\langle\mathbf{v}\rangle|_\mathbf{n}$ is expressed in terms of summation taken over odd number n as:

$$\langle\mathbf{v}\rangle|_\mathbf{n} = v_0\left[\begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} + \sum_n A^v_n\begin{pmatrix} \cos\left(n\theta - \alpha^v_n\right) \\ \sin(n\theta - \alpha^v_n) \end{pmatrix} + \sum_n B^v_n\begin{pmatrix} \cos(n\theta - \beta^v_n) \\ -\sin(n\theta - \beta^v_n) \end{pmatrix}\right] \tag{29}$$

The deviatoric direction tensor $G^v_{ji\overbrace{1111}^{n-1}}$ is:

$$G^v_{ji\overbrace{1111}^{n-1}} = G^{vA}_{ji\overbrace{1111}^{n-1}} + G^{vB}_{ji\overbrace{1111}^{n-1}} = A^v_n\begin{pmatrix} \cos\alpha^v_n & \sin\alpha^v_n \\ -\sin\alpha^v_n & \cos\alpha^v_n \end{pmatrix} + B^v_n\begin{pmatrix} \cos\beta^v_n & \sin\beta^v_n \\ \sin\beta^v_n & -\cos\beta^v_n \end{pmatrix} \tag{30}$$

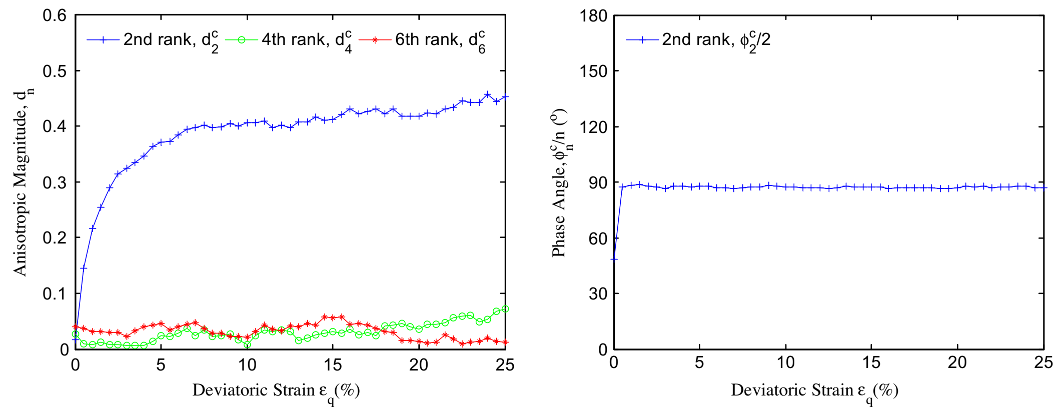
As shown in Appendix A2, we have $G_{jj} = H_{jj} - \delta_{jj} = \frac{D}{m_0}K_{jj} - \delta_{jj} = 0$, indicating $A^v_1 = 0$.

With the n-th power term of mean contact vector given in Eq. (28), its normal component g^{vn}_n in the normal direction $\mathbf{n}$ = (cosθ, -sinθ) and its tangential component g^{vt}_n in the tangential direction $\mathbf{t}$ = ($-$sinθ, cosθ) could be determined as:

$$g^{vn}_n = \mathbf{g}^v_n\cdot\mathbf{n} = A^v_n\cos\left[(n-1)\theta - \alpha^v_n\right] + B^v_n\cos\left[(n+1)\theta - \beta^v_n\right] \tag{31}$$

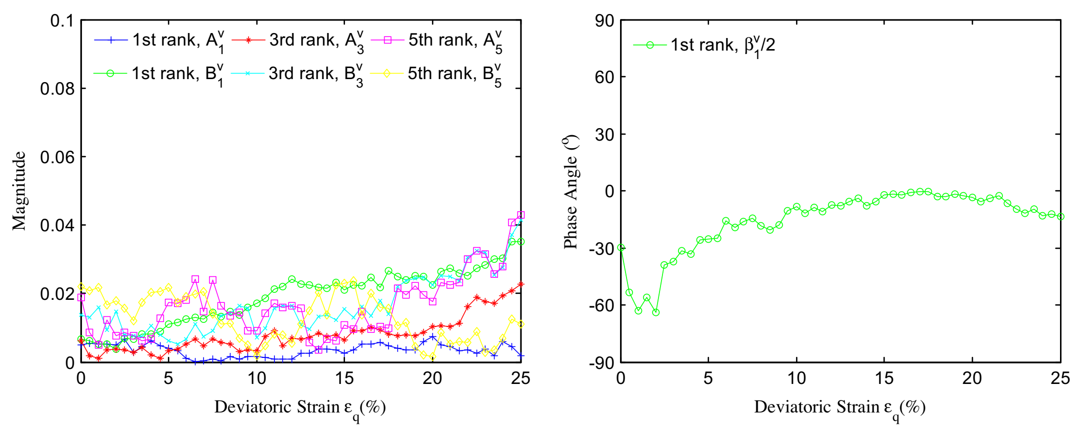
$$g^{vt}_n = \mathbf{g}^v_n\cdot\mathbf{t} = A^v_n\sin\left[(n-1)\theta - \alpha^v_n\right] - B^v_n\sin\left[(n+1)\theta - \beta^v_n\right] \tag{32}$$

The approximation of the normal and tangential components of $\langle\mathbf{v}\rangle|_\mathbf{n}$ up to n-th rank approximation becomes:



(a) Magnitude (b) Phase angle

Fig. 1. Approximation of contact normal density.



(a) Magnitude (b) Phase angle

Fig. 2. Approximation of the mean contact vector.

$$\langle v^n\rangle|_\theta = v_0\left[1+\sum_n A_n^v\cos\left[(n-1)\theta-\alpha_n^v\right]+\sum_n B_n^v\cos\left[(n+1)\theta-\beta_n^v\right]\right] \tag{33}$$

$$\langle v^t\rangle|_\theta = v_0\left[\sum_n A_n^v\sin\left[(n-1)\theta-\alpha_n^v\right]-\sum_n B_n^v\sin\left[(n+1)\theta-\beta_n^v\right]\right] \tag{34}$$

They are summation of sinusoidal terms whose magnitudes are A_n^v and B_n^v with the corresponding periods being $2\pi/(n-1)$ and $2\pi/(n+1)$, and the corresponding phase angles being $\alpha_n^v/(n-1)$ and $\beta_n^v/(n+1)$.

With the pre-determined approximation for contact normal density, $H_{ji_1i_2\cdots i_n}^v$ and $G_{ji_1i_2\cdots i_n}^v$ were calculated from particle-scale data following the procedure introduced in Appendix A2, and then used to determine the magnitudes, A_n^v, B_n^v, and phase angles, α_n^v, β_n^v in Eq. (28) accordingly. The magnitudes for 1st, 3rd, 5th rank terms A_1^v, B_1^v, A_3^v, B_3^v, A_5^v, B_5^v, are plotted in Fig. 2(a). $A_1^v\approx 0$ is observed as expected. The anisotropy in the mean contact vector is observed to be small, despite the non-circular particle shape used in the simulations. This may be due to the fact that the specimen starts with an almost isotropic distribution of particle orientation. Upon shearing, B_1^v is observed to continuously increase with the corresponding phase angle given in Fig. 2(b). The phase angle $\beta_1^v/2$ remains about 0°, suggesting the preferred direction is normal to the loading direction, as a result that as shearing continues, the particle orientations tend to be normal to the loading direction.

Considering the possibility of non-circular particle shape and potential particle orientation anisotropy, 1st rank approximation is used to approximate the mean contact vector as:

$$\langle \mathbf{v}\rangle|_{\mathbf{n}} = v_0\left[\begin{pmatrix}\cos\theta\\ \sin\theta\end{pmatrix}+B_1^v\begin{pmatrix}\cos(\theta-\beta_1^v)\\ -\sin(\theta-\beta_1^v)\end{pmatrix}\right] \tag{35}$$

In the form of direction tensors, we have one term $G_{ji_1}^v$ as

$$G_{ji_1}^v = B_1^v\begin{pmatrix}\cos\beta_1^v & \sin\beta_1^v\\ \sin\beta_1^v & -\cos\beta_1^v\end{pmatrix} \tag{36}$$

3.3. Mean contact force $\langle \mathbf{f}\rangle|_{\mathbf{n}}$

The directional distributions of mean contact force can be approximated using the compacted form as in Eq. (12) or in the form of orthogonal decomposition as in Eq. (13) with its main statistical features reflective by the direction tensor $H_{ji_1i_2\cdots i_n}^f$ or alternatively the deviatoric direction tensor $G_{ji_1\cdots i_n}^f$. The n-th power term of Eq. (13) in two dimensional spaces could be expressed as:

$$\begin{aligned} g_{nj}^f &= G_{ji_1\cdots i_n}^f n_{i_1}n_{i_2}\cdots n_{i_n} = a_{nj}^f\cos n\theta + b_{nj}^f\sin n\theta\\ &= d_{nj}^f\cos(n\theta-\phi_{nj}^f)\end{aligned} \tag{37}$$

where d^f_{nj} and ϕ^f_{nj}/n stand for the magnitudes and phase angles for the n-th rank orthogonal decomposition terms, respectively.

Denoting $A^f_n = \sqrt{d^{f2}_{n1} + d^{f2}_{n2} - 2d^f_{n1}d^f_{n2}\sin(\phi^f_{n1} - \phi^f_{n2})}/2$, $B^f_n = \sqrt{d^{f2}_{n1} + d^{f2}_{n2} + 2d^f_{n1}d^f_{n2}\sin(\phi^f_{n1} - \phi^f_{n2})}/2$, $\alpha^f_n = \arctan\left[\left(d^f_{n1}\sin\phi^f_{n1} - d^f_{n2}\cos\phi^f_{n2}\right)/\left(d^f_{n1}\cos\phi^f_{n1} + d^f_{n2}\sin\phi^f_{n2}\right)\right]$, $\beta^f_n = \arctan\left[\left(d^f_{n1}\sin\phi^f_{n1} + d^f_{n2}\cos\phi^f_{n2}\right)/\left(d^f_{n1}\cos\phi^f_{n1} - d^f_{n2}\sin\phi^f_{n2}\right)\right]$, the n-th power term becomes:

$$g^f_{nj} = G^f_{ji_1\cdots i_n} n_{i_1}\cdots n_{i_n} = A^f_n\begin{pmatrix}\cos\left(n\theta - \alpha^f_n\right)\\ \sin(n\theta - \alpha^f_n)\end{pmatrix} + B^f_n\begin{pmatrix}\cos\left(n\theta - \beta^f_n\right)\\ -\sin(n\theta - \beta^f_n)\end{pmatrix} \tag{38}$$

The deviatoric direction tensor $G^f_{ji\overbrace{1111}^{n-1}}$ is hence expressed as:

$$G^f_{ji\overbrace{1111}^{n-1}} = G^{fA}_{ji\overbrace{1111}^{n-1}} + G^{fB}_{ji\overbrace{1111}^{n-1}}$$

$$= A^f_n\begin{pmatrix}\cos\alpha^f_n & \sin\alpha^f_n\\ -\sin\alpha^f_n & \cos\alpha^f_n\end{pmatrix} + B^f_n\begin{pmatrix}\cos\beta^f_n & \sin\beta^f_n\\ \sin\beta^f_n & -\cos\beta^f_n\end{pmatrix} \tag{39}$$

and $A^f_1 = 0$. With Eqs. (13) and (39), the directional distribution of mean contact force $\langle\mathbf{f}\rangle|_\mathbf{n}$ is expressed in terms of summation taken over odd number n as:

$$\langle\mathbf{f}\rangle|_\mathbf{n} = f_0\left[\begin{pmatrix}\cos\theta\\ \sin\theta\end{pmatrix} + \sum_n A^f_n\begin{pmatrix}\cos(n\theta - \alpha^f_n)\\ \sin(n\theta - \alpha^f_n)\end{pmatrix} + \sum_n B^f_n\begin{pmatrix}\cos(n\theta - \beta^f_n)\\ -\sin(n\theta - \beta^f_n)\end{pmatrix}\right] \tag{40}$$

With the n-th power term of mean contact force given in Eq. (38), its normal component g^{fn}_n and its tangential component g^{ft}_n could be expressed as:

$$g^{fn}_n = \mathbf{g}^f_n\cdot\mathbf{n} = A^f_n\cos\left((n-1)\theta - \alpha^f_n\right) + B^f_n\cos\left((n+1)\theta - \beta^f_n\right) \tag{41}$$

$$g^{ft}_n = \mathbf{g}^f_n\cdot\mathbf{t} = A^f_n\sin\left((n-1)\theta - \alpha^f_n\right) - B^f_n\sin\left((n+1)\theta - \beta^f_n\right) \tag{42}$$

The approximation of the normal and tangential components of $\langle\mathbf{f}\rangle|_\mathbf{n}$ with up to n-th rank of approximation becomes:

$$\langle f^n\rangle|_\theta = f_0\left[1 + \sum_n A^f_n\cos\left[(n-1)\theta - \alpha^f_n\right] + \sum_n B^f_n\cos\left[(n+1)\theta - \beta^f_n\right]\right] \tag{43}$$

$$\langle f^t\rangle|_\theta = f_0\left[\sum_n A^f_n\sin\left[(n-1)\theta - \alpha^f_n\right] - \sum_n B^f_n\sin\left[(n+1)\theta - \beta^f_n\right]\right] \tag{44}$$

They are summation of sinusoidal terms whose magnitudes are A^f_n and B^f_n with the corresponding periods being $2\pi/(n-1)$ and $2\pi/(n+1)$, and the corresponding phase angles being $\alpha^f_n/(n-1)$ and $\beta^f_n/(n+1)$.

With the approximation of directional distributed contact normal density, the direction tensors for mean contact force $H^f_{ji_1i_2\cdots i_n}$ and $G^f_{ji_1i_2\cdots i_n}$ were calculated from particle-scale data, and were used to determine the magnitudes, A^f_n, B^f_n, and phase angles, α^f_n, β^f_n accordingly. The magnitudes for 1st, 3rd, 5th rank terms, A^f_1, B^f_1, A^f_3, B^f_3, A^f_5, B^f_5, are plotted in Fig. 3(a). It is observed that the magnitudes of orthogonal decomposition diminish quickly as the rank of approximation increases. Only terms relating to B^f_1, A^f_3 are considered to be significant and other terms are negligible. Their corresponding phase angles are given in Fig. 3(b). Both phase angles $\beta^f_1/2$ and $\alpha^f_3/2$ are about 90°, co-directional with the loading direction.

The results indicate that the directional distribution of mean contact force $\langle\mathbf{f}\rangle|_\mathbf{n}$ could be sufficiently approximated by up to 3rd rank of power terms as:

$$\langle\mathbf{f}\rangle|_\mathbf{n} = f_0\left[\begin{pmatrix}\cos\theta\\ \sin\theta\end{pmatrix} + B^f_1\begin{pmatrix}\cos(\theta - \beta^f_1)\\ -\sin(\theta - \beta^f_1)\end{pmatrix} + A^f_3\begin{pmatrix}\cos(3\theta - \alpha^f_3)\\ \sin(3\theta - \alpha^f_3)\end{pmatrix}\right] \tag{45}$$

In the form of direction tensors, we have two deviatoric direction tensors $G^f_{ji_1}$ and $G^f_{ji_1i_2i_3}$ as:

$$G^f_{ji_1} = B^f_1\begin{pmatrix}\cos\beta^f_1 & \sin\beta^f_1\\ \sin\beta^f_1 & -\cos\beta^f_1\end{pmatrix},\quad G^f_{ji_111} = A^f_3\begin{pmatrix}\cos\alpha^f_3 & \sin\alpha^f_3\\ -\sin\alpha^f_3 & \cos\alpha^f_3\end{pmatrix} \tag{46}$$

The rest component of $G^f_{ji_1i_2i_3}$ can be found easily as it is symmetric and deviatoric with respect to i_1, i_2, i_3.

3.4. Simplification based on the chosen limited ranks of approximation

In summary, statistical analyses based on micro-scale data for an isotropic specimen subjected to biaxial shearing suggest that it is sufficient to approximate the directional distributions of contact normal density, mean contact forces and mean contact vectors with up to 2nd, 3rd and 1st ranks of power terms as given in Eqs. (25), (35), and (45). These observations can be used to simplify Eq. (21) by keeping only direction tensors of $D^c_{i_1i_2}$, $G^v_{ji_1}$ and $G^f_{ji_1}$, $G^f_{ji_1i_2i_3}$.

With the chosen ranks of approximation and Eq. (15), we have:

$$\begin{aligned}&\sum_{n=2;s,t=1;|s-t|\leqslant n\leqslant s+t}^{\infty} D^c_{k_1\cdots k_n}G^v_{il_1\cdots l_s}G^f_{jm_1\cdots m_t}\overline{n_{k_1}\cdots n_{k_n}n_{l_1}\cdots n_{l_s}n_{m_1}\cdots n_{m_t}}\\ &= D^c_{k_1k_2}G^v_{il_1}G^f_{jm_1}\overline{n_{k_1}n_{k_2}n_{l_1}n_{m_1}} + D^c_{k_1k_2}G^v_{il_1}G^f_{jm_1m_2m_3}\overline{n_{k_1}n_{k_2}n_{l_1}n_{m_1}n_{m_2}n_{m_3}}\\ &= \tfrac{2}{3}\alpha_4 D^c_{l_1m_1}G^v_{il_1}G^f_{jm_1} + \alpha_4\tfrac{2^2}{^4C_2}D^c_{k_1k_2}G^{vf,13}_{ijk_1k_2}\end{aligned} \tag{47}$$

Following Eqs. (A27) and (A28) in Appendix A4, we have

$$G^v_{il_1}G^f_{jm_1m_2m_3}\overline{n_{l_1}n_{m_1}n_{m_2}n_{m_3}n_{p_1}n_{p_2}} = \alpha_6\frac{2^3}{^6C_3}G^v_{il_1}G^f_{jl_1p_1p_2} \tag{48}$$

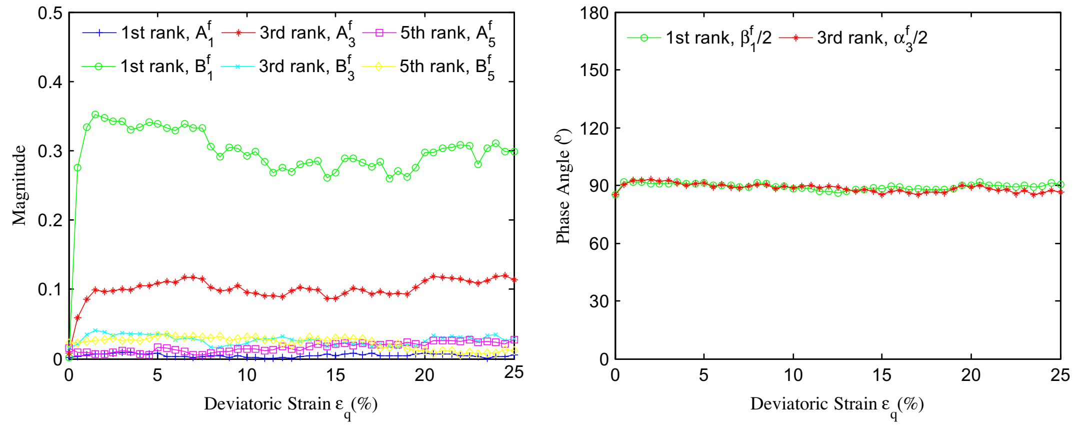
Hence Eq. (21) can be simplified as:

$$\sigma_{ij} = \frac{\omega N}{V}\varsigma v_0 f_0\left[\begin{aligned}&\alpha_2(\delta_{ij} + G^f_{ji} + G^v_{ij} + G^f_{jl_1}G^v_{il_1})\\ &+\tfrac{2}{3}\alpha_4(D^c_{ij} + D^c_{im_1}G^f_{jm_1} + D^c_{im_1}G^v_{jm_1} + D^c_{l_1m_1}G^v_{il_1}G^f_{jm_1})\\ &+\tfrac{2}{5}\alpha_6(D^c_{k_1k_2}G^f_{jik_1k_2} + D^c_{k_1k_2}G^v_{il_1}G^f_{jl_1p_1p_2})\end{aligned}\right] \tag{49}$$

Eq. (49) is valid for both two dimensional spaces and three dimensional spaces as long as the chosen ranks for approximation are considered sufficient.

3.5. Stress–force–fabric relationship in two dimensional spaces

In two dimensional spaces, Eq. (15) gives $\alpha_2 = 1/2, \alpha_4 = 3/8$, $\alpha_6 = 5/16$. The stress tensor in Eq. (49) hence becomes:



(a) Magnitude (b) Phase angle

Fig. 3. Approximation of the mean contact force.

$$\sigma_{ij} = \frac{\omega N}{2V}\varsigma v_0 f_0 \begin{bmatrix} \left(\delta_{ij} + G^f_{ji} + G^v_{ij} + G^f_{jl_1} G^v_{il_1}\right) \\ +\frac{1}{2}\left(D^c_{ij} + D^c_{ik_1} G^f_{jk_1} + D^c_{jk_1} G^v_{ik_1} + D^c_{k_1k_2} G^v_{ik_1} G^f_{jk_2}\right) \\ +\frac{1}{4}\left(D^c_{k_1k_2} G^f_{jik_1k_2} + D^c_{k_1k_2} G^v_{il_1} G^f_{jl_1k_1k_2}\right) \end{bmatrix} \tag{50}$$

The expression can be further simplified by invoking the symmetry in the Cauchy stress tensor, i.e., $\sigma_{12} = \sigma_{21}$. Notice that $D^c_{i_1i_2}$, $G^v_{ji_1}$ and $G^f_{ji_1}$ are symmetric and deviatoric tensors. With the expressions of direction tensors $D^c_{i_1i_2}$, $G^v_{ji_1}$ and $G^f_{ji_1}$, $G^f_{ji_1i_2i_3}$ given in Eqs. (26), (36), and (46) respectively, we found that:

$$G^f_{jl_1} G^v_{il_1} = B^f_1 B^v_1 \begin{pmatrix} \cos(\beta^f_1 - B^v_1) & -\sin\left(\beta^f_1 - B^v_1\right) \\ \sin\left(\beta^f_1 - B^v_1\right) & \cos\left(\beta^f_1 - B^v_1\right) \end{pmatrix} \tag{51}$$

$$D^c_{ik_1} G^f_{jk_1} = d^c_2 B^f_1 \begin{pmatrix} \cos\left(\phi^c_2 - \beta^f_1\right) & -\sin\left(\phi^c_2 - \beta^f_1\right) \\ \sin\left(\phi^c_2 - \beta^f_1\right) & \cos\left(\phi^c_2 - \beta^f_1\right) \end{pmatrix} \tag{52}$$

$$D^c_{jk_1} G^v_{ik_1} = d^c_2 B^v_1 \begin{pmatrix} \cos\left(\phi^c_2 - \beta^v_1\right) & -\sin\left(\phi^c_2 - \beta^v_1\right) \\ \sin\left(\phi^c_2 - \beta^v_1\right) & \cos\left(\phi^c_2 - \beta^v_1\right) \end{pmatrix} \tag{53}$$

$$D^c_{k_1k_2} G^f_{jik_1k_2} = 2 d^c_2 A^f_3 \begin{pmatrix} \cos\left(\phi^c_2 - \alpha^f_3\right) & -\sin(\phi^c_2 - \alpha^f_3) \\ \sin(\phi^c_2 - \alpha^f_3) & \cos(\phi^c_2 - \alpha^f_3) \end{pmatrix} \tag{54}$$

$$D^c_{k_1k_2} G^v_{ik_1} G^f_{jk_2} = d^c_2 B^v_1 B^f_1 \begin{pmatrix} \cos(\phi^c_2 - \beta^v_1 + \beta^f_1) & \sin(\phi^c_2 - \beta^v_1 + \beta^f_1) \\ \sin(\phi^c_2 - \beta^v_1 + \beta^f_1) & -\cos(\phi^c_2 - \beta^v_1 + \beta^f_1) \end{pmatrix} \tag{55}$$

$$D^c_{k_1k_2} G^v_{il_1} G^f_{jl_1k_1k_2} = 2 d^c_2 B^v_1 A^f_3 \begin{pmatrix} \cos(\phi^c_2 + \beta^v_1 - \alpha^f_3) & \sin(\phi^c_2 + \beta^v_1 - \alpha^f_3) \\ \sin(\phi^c_2 + \beta^v_1 - \alpha^f_3) & -\cos(\phi^c_2 + \beta^v_1 - \alpha^f_3) \end{pmatrix} \tag{56}$$

The joint products $D^c_{k_1k_2} G^v_{ik_1} G^f_{jk_2}$ and $D^c_{k_1k_2} G^v_{il_1} G^f_{jl_1k_1k_2}$ are found to be symmetric and deviatoric. However, $G^f_{jl_1} G^v_{il_1}, D^c_{ik_1} G^f_{jk_1}, D^c_{jk_1} G^v_{ik_1}$, $D^c_{k_1k_2} G^f_{jik_1k_2}$ could be asymmetric if the eigenvectors of $D^c_{i_1i_2}$, $G^v_{ji_1}$ and $G^f_{ji_1}$ are not co-incident. Since the stress tensor is to be symmetric, $[G^f_{jl_1} G^v_{il_1} + \frac{1}{2}(D^c_{ik_1} G^f_{jk_1} + D^c_{jk_1} G^v_{ik_1}) + \frac{1}{4} D^c_{k_1k_2} G^f_{jik_1k_2}]$ has to be symmetric. Hence,

$$B^f_1 B^v_1 \sin(\beta^f_1 - B^v_1) \\ -\frac{1}{2}\left[d^c_2 B^f_1 \sin\left(\phi^c_2 - \beta^f_1\right) - d^c_2 B^v_1 \sin\left(\phi^c_2 - \beta^v_1\right) - d^c_2 A^f_3 \sin\left(\phi^c_2 - \alpha^f_3\right)\right] \\ = 0.$$

As a result, we can write

$$G^f_{jl_1} G^v_{il_1} + \frac{1}{2}\left(D^c_{ik_1} G^f_{jk_1} + D^c_{jk_1} G^v_{ik_1}\right) + \frac{1}{4} D^c_{k_1k_2} G^f_{jik_1k_2} = C\delta_{ij} \tag{57}$$

where

$$C = \begin{bmatrix} B^f_1 B^v_1 \cos(\beta^f_1 - B^v_1) + \frac{1}{2} d^c_2 B^f_1 \cos(\phi^c_2 - \beta^f_1) \\ +\frac{1}{2} d^c_2 B^v_1 \cos(\phi^c_2 - \beta^v_1) + \frac{1}{2} d^c_2 A^f_3 \cos(\phi^c_2 - \alpha^f_3) \end{bmatrix}.$$

The stress tensor in Eq. (50) becomes:

$$\sigma_{ij} = \frac{\omega N}{2V}\varsigma v_0 f_0 \left[(1+C)\delta_{ij} + G^f_{ji} + G^v_{ij} + \frac{1}{2} D^c_{ij} + \frac{1}{2} D^c_{k_1k_2} G^v_{ik_1} G^f_{jk_2} + \frac{1}{4} D^c_{k_1k_2} G^v_{il_1} G^f_{jl_1k_1k_2}\right] \tag{58}$$

The magnitudes of orthogonal decompositions are generally limited. The anisotropic magnitude in contact vector $G^v_{ji_1}$ has been observed to be small. The contribution from the two joint product terms, $D^c_{k_1k_2} G^v_{ik_1} G^f_{jk_2}$ and $D^c_{k_1k_2} G^v_{il_1} G^f_{jl_1k_1k_2}$, are expected to be extremely small, and hence negligible. This leads to a concise form of the stress–force–fabric relationship in two dimensional spaces as:

$$\sigma_{ij} = \frac{\omega N}{2V}\varsigma v_0 f_0 \left[(1+C)\delta_{ij} + G^f_{ji} + G^v_{ij} + \frac{1}{2} D^c_{ij}\right] \tag{59}$$

It is interesting to point out that $G^f_{ji_1i_2i_3}$ do not appear directly in Eq. (59). It contributes to and only to the coefficient C though the joint product $D^c_{k_1k_2} G^f_{jik_1k_2}$. In component form, we have:

$$\begin{cases} \sigma_{11} = \frac{\omega N}{2V}\varsigma v_0 f_0 \left[(1+C) + \left(B^f_1 \cos 2\beta^f_1 + B^v_1 \cos 2\beta^v_1 + \frac{1}{2} d^c_2 \cos 2\phi^c_2\right)\right] \\ \sigma_{12} = \sigma_{21} = \frac{\omega N}{2V}\varsigma v_0 f_0 \left[B^f_1 \sin 2\beta^f_1 + B^v_1 \sin 2\beta^v_1 + \frac{1}{2} d^c_2 \sin 2\phi^c_2\right] \\ \sigma_{22} = \frac{\omega N}{2V}\varsigma v_0 f_0 \left[(1+C) - \left(B^f_1 \cos 2\beta^f_1 + B^v_1 \cos 2\beta^v_1 + \frac{1}{2} d^c_2 \cos 2\phi^c_2\right)\right] \end{cases} \tag{60}$$

With $D^c_{i_1i_2}$, $G^v_{ji_1}$ and $G^f_{ji_1}$ are symmetric and deviatoric tensors, we have the expression of the mean normal stress:

$$p = \frac{\omega N}{2V}\varsigma(1+C)v_0 f_0 \quad (61)$$

the normalized deviatoric stress tensor as:

$$\eta_{ij} = \frac{\sigma_{ij}}{p} - \delta_{ij} = \frac{1}{1+C}\left[G^f_{ji} + G^v_{ij} + \frac{1}{2}D^c_{ij}\right] \quad (62)$$

The stress ratio is mainly determined by D^c_{ij}, G^v_{ij}, G^f_{ji}, and slightly affected by C. The principal stress direction could be predicted with good confidence based on the information on the magnitudes d^c_2, B^f_1, B^v_1 and phases angles ϕ^c_2, β^f_1, β^v_1. Among them, the anisotropic magnitudes from the first two components d^c_2, B^f_1 are observed to be much larger than B^v_1, their influence is dominant.

3.6. The accuracy of the SFF relationship

With the pre-calculated direction tensors, the stress tensor can be determined from Eq. (59). The accuracy of the derived stress–force–fabric relationship was checked by comparing the prediction from Eq. (59) and the stress measured directly on the specimen boundary. The result is shown as in Fig. 4 in terms of the stress invariants $p = (\sigma_{11} + \sigma_{22})/2$, $q = \sqrt{(\sigma_{11} - \sigma_{22})^2 + 4\sigma_{12}\sigma_{21}}$ and the principal stress direction θ_a.

The coincidence of the two set of data confirms that the derived stress–force–fabric relationship as defined by Eq. (59) predicts the complete stress state with excellent accuracy. The main reason is that different from other physical models, the proposed stress–force–fabric (SFF) relationship has been mathematically derived by employing the directional statistical theory. Even though the expression of Eq. (59) seems very different from Eq. (1), they are equivalent as long as (1) the statistical dependence between the contact vectors and contact forces can be considered as isotropic; (2) it is sufficient to approximate the directional distributions of contact normal density, mean contact forces and mean contact vectors with up to 2nd, 3rd and 1st ranks of power terms of direction vector $\mathbf{n}$ as given in Eqs. (25), (35), and (45).

3.7. Comparison with Rothenburg and Bathurst's SFF relationship (1989)

There is no doubt that even though the derivation process used in this paper is different from that of Rothenburg and Bathurst (1989), the resulted SFF relationships should be the same following the same assumptions. The directional distributions used in Rothenburg and Bathurst (1989) are:

$$\begin{cases} E^c(\theta) = \frac{1}{2\pi}[1 + a_c\cos 2(\theta - \theta_a)] \\ \bar{f}^n(\theta) = f_0[1 + c_n\cos 2(\theta - \theta_a)] \\ \bar{f}^t(\theta) = -f_0 c_t \sin 2(\theta - \theta_a) \end{cases} \quad (63)$$

The mean contact vector was assumed to be isotropic.

By keeping only terms of B^f_1 and A^f_3 in Eqs. (43) and (44), the normal and tangential components of mean contact forces become:

$$\langle f^n\rangle|_\theta = f_0\left[1 + B^f_1\cos(2\theta - \beta^f_1) + A^f_3\cos(2\theta - \alpha^f_3)\right] \quad (64)$$

$$\langle f^t\rangle|_\theta = f_0\left[-B^f_1\sin(2\theta - \beta^f_1) + A^f_3\sin(2\theta - \alpha^f_3)\right] \quad (65)$$

With the assumption of $\phi^c_2 = \beta^f_1 = \alpha^f_3 = 2\theta_a$, and denoting $c_n = (B^f_1 + A^f_3)$, $c_t = (B^f_1 - A^f_3)$, $d^c_2 = a_c$, the expressions given as Eqs. (25), (64), and (65) become the same as Eq. (63), and the coefficient $C = [\frac{1}{2}d^c_2B^f_1 + \frac{1}{2}d^c_2A^f_3] = \frac{1}{2}a_c c_n$. The stress–force–fabric relationship given in Eq. (59) becomes:

$$\sigma_{ij} = \frac{\omega N}{2V}v_0 f_0\left[\left(1 + \frac{1}{2}a_c c_n\right)\delta_{ij} + \frac{1}{2}(a_c + c_n + c_t)\begin{pmatrix}\cos\theta_a & \sin\theta_a \\ \sin\theta_a & -\cos\theta_a\end{pmatrix}\right] \quad (66)$$

The general stress–force–fabric relationship Eq. (59) developed in this paper reduces to the special form given in Rothenburg and Bathurst (1989) with the assumptions of $\phi^c_2 = \beta^f_1 = \alpha^f_3 = 2\theta_a$ and the contact vector distribution being isotropic $G^v_{ij} = 0$.

4. Statistical dependence between contact vectors and contact forces

Section 2.1 assumed an isotropic statistical dependence between contact vectors and contact forces, i.e., $\langle \mathbf{v}|_\mathbf{n} \cdot \mathbf{f}|^T_\mathbf{n}\rangle = \varsigma\langle\mathbf{v}\rangle|_\mathbf{n} \cdot \langle\mathbf{f}\rangle|^T_\mathbf{n}$. Here, we will show how the assumption has been supported by statistical analyses based on the particle-scale information. The statistical dependence can be investigated by comparing the directional distribution of $\langle v_i f_j\rangle|_\mathbf{n}$, $\langle v_i\rangle|_\mathbf{n}\langle f_j\rangle|_\mathbf{n}$.

4.1. Directional distribution of $\langle v_i f_j\rangle|_n$

The method and procedure proposed by Li and Yu (2011) was generalized to study direction dependent, multi-dimensional arrays, such as $\langle v_i f_j\rangle|_\mathbf{n}$ and $\langle v_i\rangle|_\mathbf{n}\langle f_j\rangle|_\mathbf{n}$, as elaborated in the following. Taking the average of product $\langle v_i f_j\rangle|_\mathbf{n}$ as an even function with re-

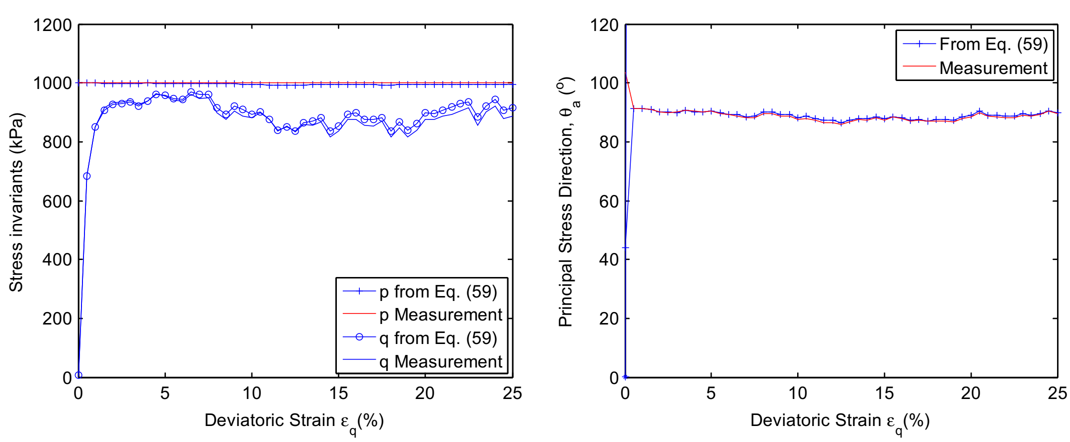


Fig. 4. The accuracy of the stress–force–fabric relationship.

spect to direction $\mathbf{n}$, the n-th rank approximation of $\langle v_i f_j\rangle|_{\mathbf{n}}$ takes the compact form (n is an even integer):

$$(V_iF_j)(\mathbf{n}) = (vf)_0^{pa} P^{pa}_{ijk_1k_2\cdots k_n} n_{k_1} n_{k_2}\cdots n_{k_n} \quad (67)$$

where $P^{pa}_{ijk_1\cdots k_n}$ stands for the direction tensor. It is symmetric with respect to subscripts $k_1,k_2,\ldots k_n$, i.e., $P^{pa}_{ijk_1k_2\cdots k_n} = P^{pa}_{ij(k_1k_2\cdots k_n)}$. The superscript suggests the sequence of operations. $\langle v_i f_j\rangle|_{\mathbf{n}}$is obtained by firstly taking the tensor product of contact vectors and contact forces and then taking the average. $(vf)_0^{pa}$ represents the directional average of dot product $\langle \mathbf{v}^T \cdot \mathbf{f}\rangle|_{\mathbf{n}}$, i.e., $(vf)_0^{pa} = \oint_\Omega \langle \mathbf{v}^T\cdot\mathbf{f}\rangle|_{\mathbf{n}}\, d\Omega/E_0$. In the form of orthogonal decomposition, we have:

$$(V_iF_j)(\mathbf{n}) = (vf)_0^{pa} \times \left[\frac{\delta_{ij}}{D} + Q^{pa}_{ij} + Q^{pa}_{ijk_1k_2} n_{k_1}n_{k_2} + \cdots + Q^{pa}_{ijk_1\cdots k_n} n_{k_1}\cdots n_{k_n} + \cdots\right] \quad (68)$$

in which $Q^{pa}_{ijk_1k_2\cdots k_n}$ is the deviatoric direction tensor. It is symmetric and deviatoric with respect to subscripts $k_1,k_2,\ldots k_n$, i.e., $Q^{pa}_{ijk_1k_2\cdots k_n} = Q^{pa}_{ij(k_1k_2\cdots k_n)}$ and $Q^{pa}_{ijk_1\cdots k_k\cdots k_l\cdots k_n}\delta_{k_kk_l} = 0$. The method to calculate the direction tensors are given as Appendix A6.

4.2. Directional distribution of $\langle v_i\rangle|_n\langle f_j\rangle|_n$

$\langle v_i\rangle|_{\mathbf{n}}\langle f_j\rangle|_{\mathbf{n}}$ can be calculated by taking multiplication of Eqs. (11) and (13). Alternatively, we could apply a similar method and procedure as detailed in Section 4.1. The approximation can take the following compact form:

$$\langle V_i\rangle(\mathbf{n})\langle F_j\rangle(\mathbf{n}) = (vf)_0^{ap} P^{ap}_{ijk_1k_2\cdots k_n} n_{k_1}n_{k_2}\cdots n_{k_n} \quad (69)$$

where the direction tensor $P^{ap}_{ijk_1\cdots k_n}$ is symmetric with respect to subscripts $k_1,k_2,\ldots k_n$, i.e., $P^{ap}_{ijk_1k_2\cdots k_n} = P^{ap}_{ij(k_1k_2\cdots k_n)}$. Here what to be investigated is $\langle v_i\rangle|_{\mathbf{n}}\langle f_j\rangle|_{\mathbf{n}}$. It is obtained by firstly taking the averages of contact vectors and contact forces respectively and then multiplying them to get the product. Hence, we use the superscripts as *ap*. $(vf)_0^{ap}$ represents the directional average of dot product $\langle\mathbf{v}\rangle|_{\mathbf{n}}{}^T\cdot\langle\mathbf{f}\rangle|_{\mathbf{n}}$, i.e., $(vf)_0^{ap} = \oint_\Omega \langle\mathbf{v}\rangle|_{\mathbf{n}}^T\cdot\langle\mathbf{f}\rangle|_{\mathbf{n}}\, d\Omega/E_0$. In the form of an orthogonal decomposition, we have:

$$\langle V_i\rangle(\mathbf{n})\langle F_j\rangle(\mathbf{n}) = (vf)_0^{ap} \times \left[\frac{\delta_{ij}}{D} + Q^{ap}_{ij} + Q^{ap}_{ijk_1k_2}n_{k_1}n_{k_2} + \cdots + Q^{ap}_{ijk_1\cdots k_n}n_{k_1}\cdots n_{k_n} + \cdots\right] \quad (70)$$

in which the deviatoric direction tensor $Q^{ap}_{ijk_1k_2\cdots k_n}$ is symmetric and deviatoric with respect to subscripts $k_1,k_2,\ldots k_n$, i.e., $Q^{ap}_{ijk_1k_2\cdots k_n} = Q^{ap}_{ij(k_1k_2\cdots k_n)}$ and $Q^{ap}_{ijk_1\cdots k_k\cdots k_l\cdots k_n}\delta_{k_kk_l} = 0$. The method to determine the direction tensors is the same as that in Section 4.1, hence is not repeated.

4.3. Observations on the statistical dependence

The statistical dependence between contact vectors and contact forces can be studied by comparing the direction distributions of $\langle v_i f_j\rangle|_{\mathbf{n}}$ and $\langle v_i\rangle|_{\mathbf{n}}\langle f_j\rangle|_{\mathbf{n}}$. With the two distributions approximated with polynomial expansions as in Eqs. (68) and (70), the two directional dependent multi-dimensional arrays $\langle v_i f_j\rangle|_{\mathbf{n}}$ and $\langle v_i\rangle|_{\mathbf{n}}\langle f_j\rangle|_{\mathbf{n}}$ can be compared in terms of their directional averages and their direction tensors of different ranks.

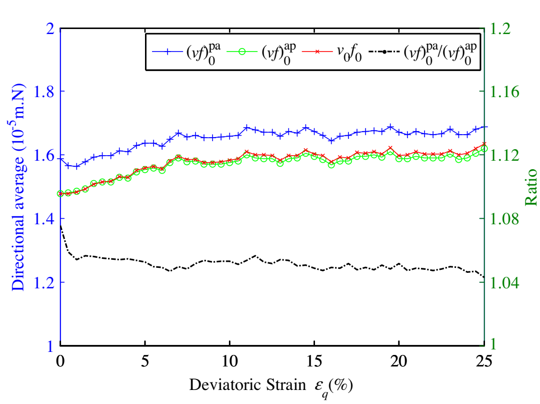
The directional averages and the 0th-rank deviatoric direction tensors for approximating $\langle v_i f_j\rangle|_{\mathbf{n}}$ and $\langle v_i\rangle|_{\mathbf{n}}\langle f_j\rangle|_{\mathbf{n}}$ are calculated from particle-scale information following the procedure introduced in Appendix A6 and plotted in Fig. 5. The value of $v_0 f_0$ is also given in Fig. 5(a) as a reference value. The difference between $(vf)_0^{pa}$ and $(vf)_0^{ap}$ shown in Fig. 5(a) suggests that statistical dependence between contact vectors and contact forces does exist. $(vf)_0^{ap}$ is observed to be close to $v_0 f_0$ as seen from the figure, indicating the contribution from joint product of higher rank anisotropic terms being negligible. The ratio of $(vf)_0^{pa}/(vf)_0^{ap}$ has also been plotted in the figure. It varies from 1.07 at beginning and decrease slightly to 1.04 at large strain levels.

The components of the deviatoric direction tensors Q^{pa}_{ij} and Q^{ap}_{ij} are given in Fig. 5(b). They are observed to be almost identical, indicating that the statistical dependence can be considered to be the same in different directions. Statistical analyses show that the magnitude of direction tensors decreases as the rank of approximation increases. Hence, higher rank approximation would be expected to be even less significant. This observation supports the assumption made in Section 2.1 that the statistical dependence between the contact vectors and contact forces is isotropic.

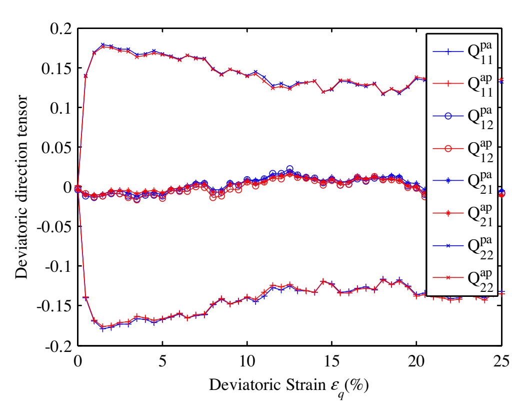
Analyses have been carried out on different specimens undergoing various loading paths. The isotropy in statistical dependence has been found as a generally valid assumption. In cases that statistical dependence is shown to be strongly direction dependent, the SFF relationship can be established using similar procedure only that higher rank terms are to be introduced to reflect its directional dependence and the results are expected to include some additional direction tensors.

5. SFF relationship in non-proportional loading

Rothenburg and Bathurst (1989)'s SFF relationship is based on the assumption that the principal directions of contact normal density, normal tangential contact force and tangential contact



(a) Directional averages



(b) Deviatoric direction tensor

Fig. 5. Statistical dependence between contact vectors and contact forces.

force are coaxial with the principal stress direction. It gives a good prediction in the mean normal stress and the stress ratio for initially isotropic specimen subjected to proportional loading. However, the coaxial assumption excludes the ability of predicting principal stress directions. Moreover, in non-proportional loading, the fabric and particle interaction may not always be co-axial (Li and Yu, 2009; Li and Yu, 2011). By characterizing the directional distributions in terms of direction tensor, the coaxial assumption is not needed. Hence, Eq. (59) is applicable in non-proportional loadings.

5.1. Discrete element simulations of non-proportional loading

Material behavior to non-proportional loading, involving rotation of either material fabric or principal stresses, has attracted much research interest over the last few decades (Arthur et al., 1980; Towhata and Ishihara, 1985; Gutierrez et al., 1991; Yoshimine et al., 1998; Li and Dafalias, 2004; Tsutsumi and Hashiguchi, 2005; Yu and Yuan, 2006; Yu, 2008).

In the effort to study the dependence of granular material behavior on initial fabric and loading paths, Li and Yu (2009) prepared two anisotropic specimens and sheared the specimens in different directions to study material anisotropy. One was prepared using the deposition method, and was referred as the initially anisotropic specimen. The other was the preloaded specimen, prepared by shearing initially anisotropic specimen monotonically up to 25% axial strain in the deposition direction, and then unloaded to isotropic stress state. The two specimens were consolidated to $p_c = 1000$ kPa, and sheared along various loading directions. Noticeable difference in non-coaxiality with and without preshearing was reported (Li and Yu, 2009). Later, numerical simulation of stress rotation has been reported (Li and Yu, 2010). The isotropic specimen was firstly sheared in the vertical direction $\alpha_\sigma = 90^\circ$ up to stress ratio $\eta = 0.8$ and then subjected to pure stress rotation with continuous rotation of principal stress direction α_σ. These two tests involved non-coincidence between the principal fabric direction, the principal stress directions and their relative rotations. Both are non-proportional loadings.

5.2. Statistical characteristics in non-proportional loading

The data from these simulations were used here for statistical analyses. Directional statistical analyses confirmed that even for non-proportional loadings the previous observations still hold true. That is to say, the magnitudes of orthogonal decomposition diminish quickly as the rank of approximation increases. The 2nd rank approximation of contact normal density d_2^c, the 1st rank and 3rd rank approximation of contact force, B_1^f and A_3^f, and the 1st rank approximation of contact vector, B_1^v were all the anisotropic terms necessary to give sufficient approximations. The 4th rank terms for contact normal density d_4^c was observed to increase gradually as shear continues, while remain limited.

5.2.1. Anisotropic specimen subjected to monotonic shearing

For the anisotropic specimens subjected to monotonic shearing, results on the specimens when subjected to fixed loading direction $\alpha_\varepsilon = 30^\circ$ were analyzed and presented here. α_ε denotes the deviation of loading direction to horizontal direction.

Figs. 6 and 7 give the magnitudes and phase angles for the initially anisotropic specimen and the preloaded specimen, respectively. Initially, the magnitude of contact normal d_2^c was about 0.22. The phase angle of contact normal $\phi_2^c/2$ was 90°, suggesting that the initial anisotropic structure had the preferred direction the same as particle deposition. As shear continued, its magnitude increased. In the meantime, its phase angle $\phi_2^c/2$ approached 30°, coaxial with the loading direction.

Different from the previous results on isotropic specimen, deviations between the phase angles of contact normal and contact forces were clearly shown in Figs. 6 and 7(b), though diminishing at large strain levels. This clear evidence suggested that the coaxiality assumption between fabric and contact forces may not be valid in non-proportional loading. The rate for the contact normal density to approach the loading direction was observed to be slower than that for contact force anisotropy. For the initially anisotropic specimen, the contact force anisotropy, both the 1st rank term and the 3rd rank term, became coaxial with loading direction upon the initiation of loading, while for the preloaded specimen, it took about 5% deviatoric strain for the 3rd rank anisotropic terms become coaxial with loading direction.

5.2.2. Isotropic specimen to stress rotation

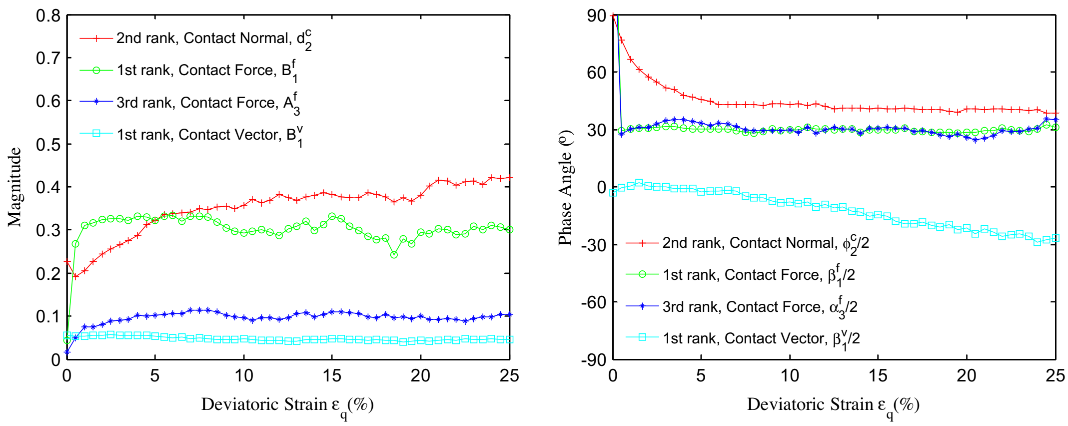
The statistical characteristics of the isotropic specimen subjected to stress rotation were plotted in Fig. 8. The anisotropy in mean contact vector was observed to be negligible, while the anisotropy in contact normal density and contact forces were significant. The phase angle of the 2nd rank contact normal density $\phi_2^c/2$, and those of contact forces, $\beta_1^f/2$ and $\alpha_3^f/2$ were plotted in Fig. 8(b). It was shown that the phase angles rotated together with the rotation of the principal stress direction. Again, the non-coaxiality between the contact normal density and the contact forces was noticeable. The differences between the phase angles were plotted in Fig. 9. The 1st rank phase angle $\beta_1^f/2$ was observed almost coincident with the principal stress direction, while the phase angles for the contact normal density $\phi_2^c/2$ and the phase angle for the 3rd rank contact force $\alpha_3^f/2$ were left behind in the range of $10^\circ \sim 20^\circ$.

5.3. The accuracy of the SFF relationship in non-proportional loading

The comparisons of the stress tensor calculated from Eq. (59) and those measured on the specimen boundary were given in Figs. 10 and 11, for the non-proportional loading, i.e., the two anisotropic specimens to monotonic loading and the isotropic specimen to stress rotation, respectively. The almost identical results confirmed the capability of Eq. (59) to provide complete and accurate prediction on the specimen stress state. The main reason is that the derivation of SFF relationship involved neither pre-assumption on the loading path nor material constitutive relationship. It is a mathematical approach. Eq. (59) provides good prediction on the material stress as long as the conditions of isotropic statistical dependence and the chosen ranks of approximation remain valid.

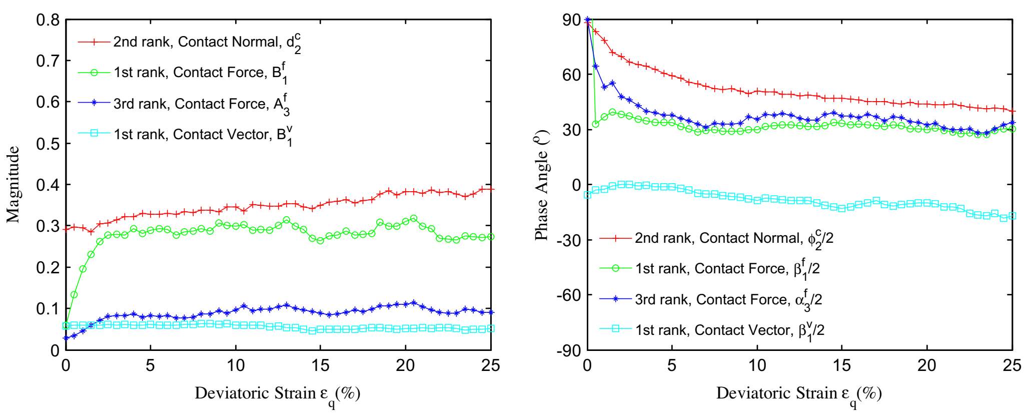
6. Benefits of using directional statistical theories

This paper concerned about the same problem as in Rothenburg and Bathurst (1989). The novelty of the present paper lies on the usage of the directional statistical theories. The directional statistical theory is a technique to interpret a set of directional data and requires no pre-requisite assumptions. The directional distributions are approximated by polynomial expansions in unit direction vector $\mathbf{n}$. The key characteristics of the set of directional data are embedded in the direction tensors, which are the coefficients determined by minimizing the least square error. This allows for the flexibility to choose the proper ranks of polynomial terms for approximation based on the characteristics of given directional data. Moreover, this approach simultaneously determines all the components of the direction tensors. It is different from the conventional scheme, in which minimization only leads to the determination of one parameter and additional assumptions are often needed.



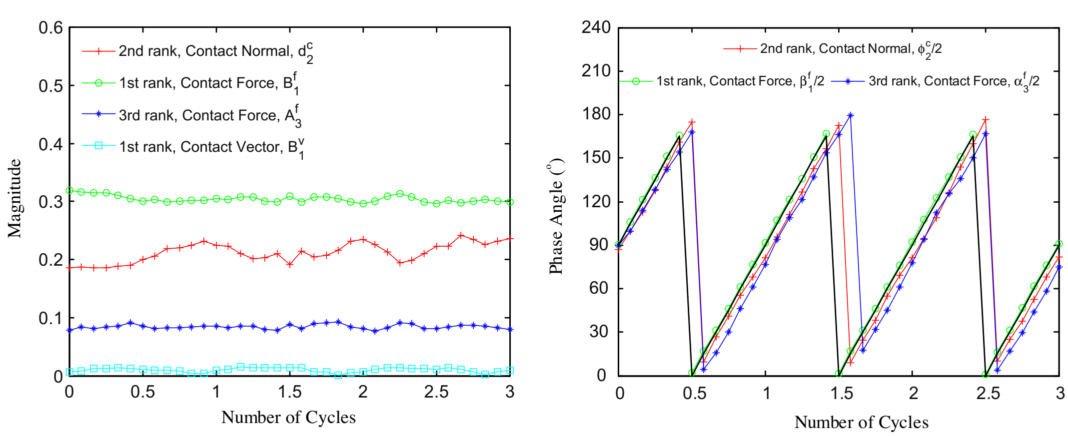
(a) Magnitude (b) Phase angle

Fig. 6. Initially anisotropic specimen to monotonic loading.



(a) Magnitude (b) Phase angle

Fig. 7. Preloaded specimen to monotonic loading.



(a) Magnitude (b) Phase angle

Fig. 8. Isotropic specimen to stress rotation.

One of the benefits by using the directional statistical theory was to validate the assumptions made during the derivation of Rothenburg and Bathurst's SFF relationship (1989). The statistical dependence between contact vectors and contact forces has been investigated and a statistical dependence between contact vectors and contact forces was demonstrated in Section 4. It was taken into account by introducing a direction independent scalar ς. Also, by employing the directional statistical theory, we can determine the coefficient tensor directly from the discrete particle-scale dataset, and hence choose the sufficient rank for approximation. In the

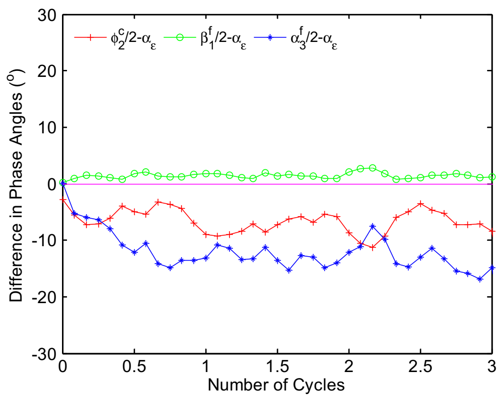
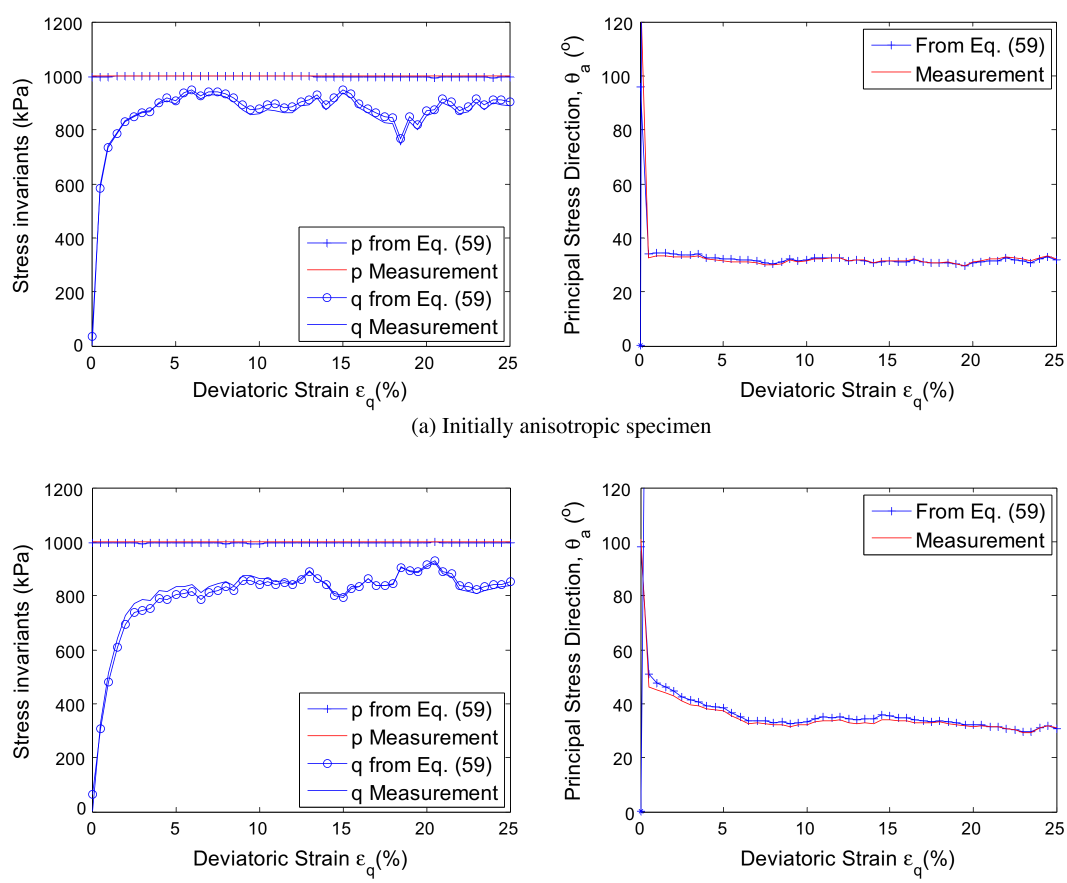


Fig. 9. Non-coaxiality among the phase angles.

present work, we choose the rank of approximation based on the discrete element simulation results. The magnitudes of the higher rank terms have been observed to be small. Observation given in Sections 3.2–3.4 supported that it is sufficient to approximate the directional distributions of contact normal density, mean contact forces and mean contact vectors with up to 2nd, 3rd and 1st power terms of direction vector $\mathbf{n}$ as given in Eqs. (25), (35), and (45). This leads to the simplified stress–force–fabric relationship as given in Eq. (59).

The derivation of the stress–force–fabric relationship is a good example demonstrating the powerful application of the directional statistical theory in granular mechanics. The conventional directional analyses start with subdividing the directional space into a number of space segments covering the entire range of orientations. Given some tolerance $\Delta\mathbf{n}$ on sampling is allowed, the directional data are grouped to be allocated into the space segments. This is the first step for further statistical analyses to study the directional probability function or the directional distributed characteristics values. In physical terms, determination of the directional distributions is possible for a system with such irregular and abundant data that the sets corresponding to each group are non-empty no matter how small the interval can be. In other words, this requires a sufficiently large amount of directional data. Otherwise, the statistical characterisation may be sensitive to the space subdivision when the data are limited. However, the data processing method employing the directional statistical theory do not involve subdivision of the whole space into small segments, and is hence subjected to no limitation of the amount of available data. The directional statistical theory provides a new approach to conduct directional analyses in granular materials. The method has the benefit of being readily applied to both two dimensional and three dimensional spaces.

Moreover, by approximating the directional distributions with polynomial expansions in direction $\mathbf{n}$, the statistical and directional characteristics of particle-scale directional data are quantified in terms of the macro-scale direction tensors. The directional integration is hence converted into tensor multiplication as shown in Section 2.5. This avoids the difficulty of conducting directional



(a) Initially anisotropic specimen

(b) Preloaded specimen

Fig. 10. Comparison for anisotropic specimens to monotonic loading.

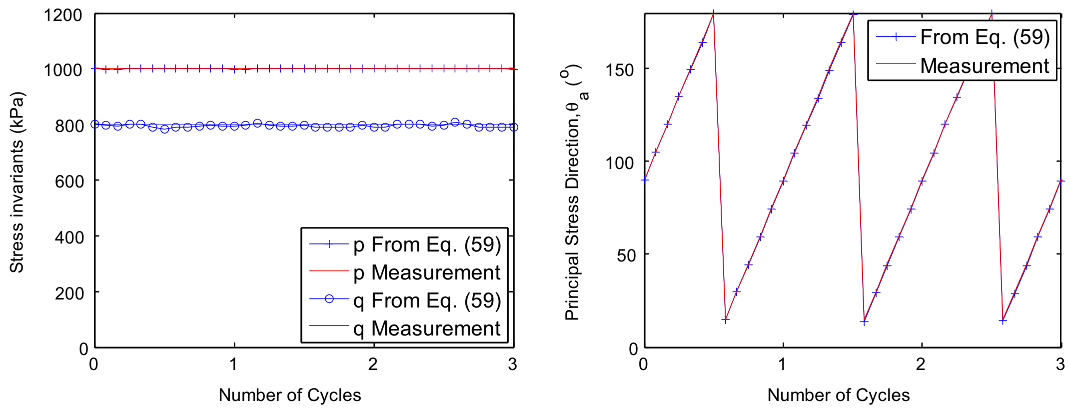


Fig. 11. Comparison for isotropic specimen to stress rotation.

integration, and eventually leads to an explicit form of the stress–force–fabric relationship as defined by Eq. (59). This approach is advantageous in conducting numerical analyses with the aid of computer programs.

7. Conclusions

The paper applied the theory of directional statistics in granular mechanics to study material stress state. The employment of the directional statistical theory makes it possible to look into the statistical dependence of contact vectors and contact forces, and to choose the appropriate ranks of approximation based on the characteristics of given directional data. Moreover, it quantifies the directional dependence in terms of direction tensors and converts the directional integration into tensor multiplication.

Based on the directional statistical theory, the general stress–force–fabric relationship has been derived as given in Eq. (21). Two dimensional granular material behaviors have been studied including both proportional loading and non-proportional loading paths. The statistical features of the contact vectors and contact forces have been investigated. Incorporating the findings into the general expression of the stress–force–fabric relationship as in Eq. (21), and imposing the symmetry in the Cauchy stress tensor, we derived the stress–force–fabric relationship in two dimensional spaces in a very concise form as in Eq. (59). 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. It explicitly expresses the stress tensor in terms of direction tensors characterizing contact normal density D^c_{ij}, contact vectors G^v_{ij} and contact forces G^f_{ji}. The parameter ς reflects the statistical dependence between contact vectors and contact forces, and the parameter C is due to the contribution from the joint products of deviatoric direction tensors.

The relationship gives good accuracy in predicting the stress state of granular materials. This is mainly because the derivation has been conducted mathematically without pre-assumptions on loading paths, material states or constitutive relationship. Although the expression (59) looks quite different from Love's initial equation, they describe the same fundamental relationship between the stress tensor, contact forces and contact vectors in a granular material. It is a predictive relationship established starting from the micro-structural stress tensor and based on the following assumptions:

(1) The statistical dependence between the contact vectors and contact forces can be considered as isotropic, i.e., the effect of the statistical dependence between contact vectors and contact forces could be taken into account by assuming $\langle \mathbf{v}|_{\mathbf{n}} \cdot \mathbf{f}|^T_{\mathbf{n}}\rangle = \varsigma\langle \mathbf{v}\rangle|_{\mathbf{n}} \cdot \langle \mathbf{f}\rangle|^T_{\mathbf{n}}$, where ς is a direction independent scalar.
(2) It is sufficient to approximate the directional distributions of contact normal density, mean contact forces and mean contact vectors with up to 2nd, 3rd and 1st ranks of power terms of direction vector **n** as given in Eqs. (25), (35).

By employing the directional statistical theory, the validity of the assumptions made by Rothenburg and Bathurst (1989) has been investigated. The statistical independence between the contact vectors and contact forces may not hold true. And the coaxiality among the directional distributions has been shown invalid in non-proportional loadings. Following the same set of assumptions, the expression derived in this paper is found to be identical with Rothenburg and Bathurst (1989)'s formulation.

The direction tensors serve as the statistical measures of the particle-scale variables so that they can be used in the development of micro-mechanics based constitutive relationship in the frame-indifferent form. The stress–force–fabric relationship developed in this paper provides a key analytical tool to understand the micromechanical origin of the shear strength of granular materials.

Acknowledgments

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Appendix A1. Calculation of the direction tensors for contact normal density

To determine the coefficient tensor $F^c_{i_1 i_2 \cdots i_n}$ from a given set of observed discrete directional data, the minimization of the square error

$$E = \oint_\Omega [E^c(\mathbf{n}) - e^c(\mathbf{n})]^2 d\Omega \rightarrow \min \tag{A1}$$

can be used as the criterion (Li and Yu, 2011). Let $\mathbf{n}^{(1)}$, $\mathbf{n}^{(2)}$, ... and $\mathbf{n}^{(N)}$ be unit vectors representing N contact normals. The average of their n-th rank tensor product is called the moment tensor of rank n and is defined as:

$$N_{i_1 i_2 \cdots i_n} = \langle n_{i_1} n_{i_2} \cdots n_{i_n} \rangle = \frac{1}{N} \sum_{\alpha=1}^{N} n_{i_1}^{(\alpha)} n_{i_2}^{(\alpha)} \cdots n_{i_n}^{(\alpha)} = \oint_\Omega n_{i_1} n_{i_2} \cdots n_{i_n} e^c(\mathbf{n}) d\Omega \tag{A2}$$

where $\langle * \rangle$ designates the sample mean, i.e., $\langle * \rangle = \sum_{\alpha=1}^{N} *^{(\alpha)}/N$; or in continuous form, $\langle * \rangle = \oint_\Omega \langle * \rangle|_\mathbf{n} e^c(\mathbf{n}) d\Omega$. The moment tensor is fully symmetric. The least square error criteria lead to:

$$N^c_{i_1 i_2 \cdots i_n} = \frac{1}{E_0} \oint_\Omega F^c_{j_1 j_2 \cdots j_n} n_{j_1} n_{j_2} \cdots n_{j_n} n_{i_1} n_{i_2} \cdots n_{i_n} d\Omega = F^c_{j_1 j_2 \cdots j_n} \overline{n_{j_1} n_{j_2} \cdots n_{j_n} n_{i_1} n_{i_2} \cdots n_{i_n}} \tag{A3}$$

where $\overline{*} = \oint_\Omega (*) d\Omega / E_0$ denotes the average of $*$ over directions.

The direction tensor $F^c_{i_1 i_2 \cdots i_n}$ and the deviatoric direction tensor $D^c_{i_1 i_2 \cdots i_n}$ can then be determined successively. The constraint of being a probability density distribution leads to $F_0 = D_0 = 1$. Starting from here, with the n-th rank moment tensor $N_{i_1 i_2 \cdots i_n}$ calculated from observed directional data and the known $(n-2)$-th rank direction tensor $F^c_{i_1 i_2 \cdots i_{n-2}}$, the n-th rank deviatoric direction tensor $D^c_{i_1 i_2 \cdots i_n}$ can be calculated as:

$$D^c_{i_1 \cdots i_n} = \frac{1}{\alpha_{2n}} \frac{(2n)!}{2^n (n!)^2} \left(N_{i_1 \cdots i_n} - F^c_{j_1 \cdots j_{n-2}} \overline{n_{j_1} \cdots n_{j_{n-2}} n_{i_1} \cdots n_{i_n}} \right) \tag{A4}$$

And the n-th rank direction tensor $F^c_{i_1 i_2 \cdots i_n}$ can be found in view of the symmetry in $F^c_{i_1 i_2 \cdots i_n}$ and $D^c_{i_1 i_2 \cdots i_n}$ as:

$$F^c_{i_1 i_2 \cdots i_n} = D^c_{i_1 i_2 \cdots i_n} + F^c_{(i_1 i_2 \cdots i_{n-2}} \delta_{i_{n-1} i_n)} \tag{A5}$$

Appendix A2. Calculation of the direction tensors for mean contact vectors

Let $\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \cdots$ and $\mathbf{v}^{(N)}$ be contact vectors associated with the observed N contact normals $\mathbf{n}^{(1)}, \mathbf{n}^{(2)}, \cdots$ and $\mathbf{n}^{(N)}$ respectively. Define the moment tensor as:

$$K^v_{j i_1 \cdots i_n} = \frac{1}{E_0} \oint_\Omega \langle \mathbf{v} \rangle|_\mathbf{n} \otimes \overbrace{\mathbf{n} \otimes \mathbf{n} \cdots \otimes \mathbf{n}}^{n} d\Omega = \frac{1}{E_0} \oint_\Omega \langle v_j \rangle|_\mathbf{n} n_{i_1} \cdots n_{i_n} d\Omega \tag{A6}$$

Minimizing the least square error

$$E = \oint_\Omega [\mathbf{V}(\mathbf{n}) - \langle \mathbf{v} \rangle|_\mathbf{n}]^T \cdot [\mathbf{V}(\mathbf{n}) - \langle \mathbf{v} \rangle|_\mathbf{n}] d\Omega \to \min \tag{A7}$$

leads to $\partial E / \partial H^v_{j i_1 i_2 \cdots i_n} = 0$ and

$$K^v_{j i_1 i_2 \cdots i_n} = v_0 H^v_{j k_1 k_2 \cdots k_n} \overline{n_{k_1} n_{k_2} \cdots n_{k_n} n_{i_1} n_{i_2} \cdots n_{i_n}} \tag{A8}$$

With the pre-determined approximation of contact normal probability density of $\mathbf{n}$, $K^v_{j i_1 i_2 \cdots i_n}$ can be calculated from discrete observations by taking the s-th rank approximation of the probability density with the form given in Eq. (8). Hence:

$$K^v_{j i_1 i_2 \cdots i_n} = \frac{1}{E_0} \oint_\Omega \langle v_j \rangle|_\mathbf{n} n_{i_1} n_{i_2} \cdots n_{i_n} E^c(\mathbf{n}) \frac{1}{E^c(\mathbf{n})} d\Omega \approx \frac{1}{E_0} \langle v_j n_{i_1} n_{i_2} \cdots n_{i_n} / E^c(\mathbf{n}) \rangle = \frac{1}{N} \sum_{\alpha=1}^{N} \left[\left(v_j n^\alpha_{i_1} n^\alpha_{i_2} \cdots n^\alpha_{i_n} \right) / \left(F^c_{k_1 k_2 \cdots k_s} n^\alpha_{k_1} n^\alpha_{k_2} \cdots n^\alpha_{k_n} \right) \right] \tag{A9}$$

The direction tensor $H^v_{j i_1 \cdots i_n}$ and the deviatoric direction tensor $G^v_{j i_1 \cdots i_n}$ can hence be determined successively. From Eqs. (10) and (A9), we have v_0 calculated from:

$$v_0 = \oint_\Omega \langle \mathbf{v} \rangle|_\mathbf{n} \cdot \mathbf{n} d\Omega \Big/ E_0 = \oint_\Omega \langle v_j \rangle|_\mathbf{n} n_j d\Omega \Big/ E_0 = K^v_{jj} \tag{A10}$$

And the direction tensor $H_{j i_1}$ and the deviatoric tensor $G_{j i_1}$ can be determined as follows:

$$H^v_{j i_1} = \frac{D}{v_0} K^v_{j i_1} \quad \text{and} \quad G^v_{j i_1} = H^v_{j i_1} - \delta_{j i_1} \tag{A11}$$

where D stands for the dimension of the space. With the moment tensor $K^v_{j i_1 i_2 \cdots i_n}$ calculated from observed directional data and the known lower rank direction tensor $H^v_{j k_1 \cdots k_{n-2}}$, the n-th rank deviatoric direction tensor $G^v_{j i_1 i_2 \cdots i_n}$ can be determined as:

$$G^v_{j i_1 \cdots i_n} = \frac{1}{\alpha_{2n}} \frac{{}^{2n}C_n}{2^n} \left(K^v_{j i_1 \cdots i_n} \Big/ v_0 - H^v_{j k_1 \cdots k_{n-2}} \overline{n_{k_1} \cdots n_{k_{n-2}} n_{i_1} \cdots n_{i_n}} \right) \tag{A12}$$

Noticing the symmetry in $H^v_{j i_1 \cdots i_n}$ and $G^v_{j i_1 \cdots i_n}$, we have the direction tensor $H^v_{j i_1 \cdots i_n}$ for the n-th rank approximation determined as

$$H^v_{j i_1 \cdots i_n} = H^v_{j(i_1 i_2 \cdots i_{n-2}} \delta_{i_{n-1} i_n)} + G^v_{j i_1 \cdots i_n} \tag{A13}$$

Appendix A3. General stress–force–fabric relationship

Being orthogonal decompositions, the coefficient tensors satisfy

$$\begin{aligned} &D^c_{i_1 \cdots i_n} \overline{n_{i_1} n_{i_2} \cdots n_{i_n} n_{j_1} n_{j_2} \cdots n_{j_m}} = 0 \\ &G^v_{i_0 i_1 \cdots i_s} \overline{n_{i_1} n_{i_2} \cdots n_{i_s} n_{j_1} n_{j_2} \cdots n_{j_t}} = 0 \\ &G^f_{i_0 i_1 \cdots i_s} \overline{n_{i_1} n_{i_2} \cdots n_{i_s} n_{j_1} n_{j_2} \cdots n_{j_t}} = 0 \end{aligned} \tag{A14}$$

when $m < n$, $t < s$, m and n are even numbers, s and t are odd numbers. Hence,

$$\sum_{t=1,\text{odd}}^{\infty} G^f_{j m_1 \cdots m_t} \overline{n_i n_{m_1} \cdots n_{m_t}} = G^f_{j m_1} \overline{n_i n_{m_1}} \tag{A15}$$

$$\sum_{s=1,\text{odd}}^{\infty} G^v_{i l_1 \cdots l_s} \overline{n_j n_{l_1} \cdots n_{l_s}} = G^v_{i l_1} \overline{n_j n_{l_1}} \tag{A16}$$

$$\sum_{k=2,\text{even}}^{\infty} D^c_{k_1 k_2 \cdots k_n} \overline{n_{k_1} n_{k_2} \cdots n_{k_n} n_i n_j} = D^c_{k_1 k_2} \overline{n_{k_1} n_{k_2} n_i n_j} \tag{A17}$$

Furthermore, since,

$$G^f_{j m_1 \cdots m_t} G^v_{i l_1 \cdots l_s} \overline{n_{l_1} \cdots n_{l_s} n_{m_1} \cdots n_{m_t}} = \begin{cases} G^v_{i l_1 \cdots l_s} (G^f_{j m_1 \cdots m_t} \overline{n_{m_1} \cdots n_{m_t} n_{l_1} \cdots n_{l_s}}) = 0, & \text{when } s < t \\ \neq 0, & \text{when } s = t \\ G^f_{j m_1 \cdots m_t} (G^v_{i l_1 \cdots l_s} \overline{n_{l_1} \cdots n_{l_s} n_{m_1} \cdots n_{m_t}}) = 0, & \text{when } s > t \end{cases} \tag{A18}$$

$$D^c_{k_1 k_2 \cdots k_n} G^f_{j m_1 \cdots m_s} \overline{n_{k_1} n_{k_2} \cdots n_{k_n} n_i n_{m_1} \cdots n_{m_s}} = \begin{cases} G^f_{j m_1 \cdots m_s} \left(D^c_{k_1 k_2 \cdots k_n} \overline{n_{k_1} n_{k_2} \cdots n_{k_n} n_i n_{m_1} \cdots n_{m_s}} \right) = 0, & \text{when } s+1 < n \\ D^c_{k_1 k_2 \cdots k_n} \left(G^f_{j m_1 \cdots m_s} \overline{n_{m_1} \cdots n_{m_s} n_{k_1} n_{k_2} \cdots n_{k_n} n_i} \right) = 0, & \text{when } s > n+1 \\ \neq 0, & \text{otherwise} \end{cases} \tag{A19}$$

$$D^c_{k_1 k_2 \cdots k_n} G^v_{i l_1 \cdots l_s} \overline{n_{k_1} n_{k_2} \cdots n_{k_n} n_j n_{l_1} \cdots n_{l_s}} = \begin{cases} G^v_{i l_1 \cdots l_s} \left(D^c_{k_1 k_2 \cdots k_n} \overline{n_{k_1} n_{k_2} \cdots n_{k_n} n_i n_{l_1} \cdots n_{l_s}} \right) = 0, & \text{when } s+1 < n \\ D^c_{k_1 k_2 \cdots k_n} \left(G^v_{i l_1 \cdots l_s} \overline{n_{l_1} \cdots n_{l_s} n_{k_1} n_{k_2} \cdots n_{k_n} n_i} \right) = 0, & \text{when } s > n+1 \\ \neq 0, & \text{otherwise} \end{cases} \tag{A20}$$

we have,

$$\sum_{s=1,\mathrm{odd};t=1,\mathrm{odd}}^{\propto} G^f_{jm_1\cdots m_t} G^v_{il_1\cdots l_s} \overline{n_{l_1}\cdots n_{l_s} n_{m_1}\cdots n_{m_t}} = \sum_{s=1,\mathrm{odd}}^{\propto} G^f_{jm_1\cdots m_s} G^v_{il_1\cdots l_s} \overline{n_{l_1}\cdots n_{l_s} n_{m_1}\cdots n_{m_s}} \tag{A21}$$

$$\begin{aligned}&\sum_{n=2,\mathrm{even};t=1,\mathrm{odd}}^{\propto} D^c_{k_1k_2\cdots k_n} G^f_{jm_1\cdots m_t} \overline{n_{k_1}n_{k_2}\cdots n_{k_n} n_i n_{m_1}\cdots n_{m_t}} \\ &= \sum_{n=2,\mathrm{even}}^{\propto} D^c_{k_1k_2\cdots k_n} G^f_{jm_1\cdots m_{n-1}} \overline{n_i n_{k_1}n_{k_2}\cdots n_{k_n} n_{m_1}\cdots n_{m_{n-1}}} \\ &+ \sum_{n=2,\mathrm{even}}^{\propto} D^c_{k_1k_2\cdots k_n} G^f_{jm_1\cdots m_{n+1}} \overline{n_i n_{k_1}n_{k_2}\cdots n_{k_n} n_{m_1}\cdots n_{m_{n+1}}}\end{aligned} \tag{A22}$$

$$\begin{aligned}&\sum_{n=2,\mathrm{even};s=1,\mathrm{odd}}^{\propto} D^c_{k_1k_2\cdots k_n} G^v_{il_1\cdots l_s} \overline{n_{k_1}n_{k_2}\cdots n_{k_n} n_{l_1}\cdots n_{l_s} n_j} \\ &= \sum_{n=2,\mathrm{even}}^{\propto} D^c_{k_1k_2\cdots k_n} G^v_{im_1\cdots m_{n-1}} \overline{n_j n_{k_1}n_{k_2}\cdots n_{k_n} n_{m_1}\cdots n_{m_{n-1}}} \\ &+ \sum_{n=2,\mathrm{even}}^{\propto} D^c_{k_1k_2\cdots k_n} G^v_{im_1\cdots m_{n+1}} \overline{n_j n_{k_1}n_{k_2}\cdots n_{k_n} n_{m_1}\cdots n_{m_{n+1}}}\end{aligned} \tag{A23}$$

As for the last term in Eq. (17), using the orthogonal decompositions, $D^c_{k_1k_2\cdots k_n} G^f_{jm_1\cdots m_t} \overline{n_{k_1}n_{k_2}\cdots n_{k_n} n_{m_1}\cdots n_{m_t}}$, $D^c_{k_1k_2\cdots k_n} G^v_{il_1\cdots l_s} \overline{n_{k_1}n_{k_2}\cdots n_{k_n} n_{l_1}\cdots n_{l_s}}$, $G^f_{jm_1\cdots m_t} G^v_{il_1\cdots l_s} \overline{n_{l_1}\cdots n_{l_s} n_{m_1}\cdots n_{m_t}}$ could be expressed in terms of a polynomial in $\mathbf{n}$ up to rank $(n+t)$, $(n+s)$, $(s+t)$ respectively as:

$$\begin{aligned}D^c_{k_1\cdots k_n} G^f_{jm_1\cdots m_t} n_{k_1}\cdots n_{k_n} n_{m_1}\cdots n_{m_t} &= \sum_{r=1,\mathrm{odd}}^{n+t} Q^{cf,nt}_{jk_1\cdots k_r} n_{k_1}\cdots n_{k_r} \\ D^c_{k_1\cdots k_n} G^v_{il_1\cdots l_s} n_{k_1}\cdots n_{k_n} n_{l_1}\cdots n_{l_s} &= \sum_{r=1,\mathrm{odd}}^{n+s} Q^{cv,ns}_{ik_1\cdots k_r} n_{k_1}\cdots n_{k_r} \\ G^v_{il_1\cdots l_s} G^f_{jm_1\cdots m_t} n_{l_1}\cdots n_{l_s} n_{m_1}\cdots n_{m_t} &= \sum_{r=2,\mathrm{even}}^{s+t} Q^{vf,st}_{ijk_1\cdots k_r} n_{k_1}\cdots n_{k_r}\end{aligned} \tag{A24}$$

The coefficient tensors are symmetric and deviatoric with respect to the subscripts k_1,k_2,…k_r. Hence, we also have:

$$D^c_{k_1k_2\cdots k_n} G^v_{il_1\cdots l_s} G^f_{jm_1\cdots m_t} \overline{n_{k_1}n_{k_2}\cdots n_{k_n} n_{l_1}\cdots n_{l_s} n_{m_1}\cdots n_{m_t}} = \begin{cases} \sum_{r=1,\mathrm{odd}}^{n+t} Q^{cf,nt}_{jk_1k_2\cdots k_r}\left(G^v_{il_1\cdots l_s} \overline{n_{k_1}n_{k_2}\cdots n_{k_r} n_{l_1}\cdots n_{l_s}}\right) = 0, & \\ \quad \text{when } s > n+t & \\ \sum_{r=1,\mathrm{odd}}^{n+s} Q^{cv,ns}_{ik_1k_2\cdots k_r}\left(G^f_{jm_1\cdots m_t} \overline{n_{k_1}n_{k_2}\cdots n_{k_r} n_{m_1}\cdots n_{m_t}}\right) = 0, & \\ \quad \text{when } t > n+s & \\ \sum_{r=2,\mathrm{even}}^{s+t} Q^{vf,st}_{ijk_1k_2\cdots k_r}\left(D^c_{k_1k_2\cdots k_n} \overline{n_{k_1}n_{k_2}\cdots n_{k_r} n_{k_1}n_{k_2}\cdots n_{k_n}}\right) = 0, & \\ \quad \text{when } n > s+t & \\ \neq 0, \quad \text{otherwise} & \end{cases} \tag{A25}$$

Substituting the above equations into Eq. (17), we have the stress tensor expressed as:

$$\sigma_{ij} = \frac{\omega N}{V} \varsigma v_0 f_0 \left[\begin{aligned}&\overline{n_i n_j} + G^f_{jm_1}\overline{n_i n_{m_1}} + G^v_{il_1}\overline{n_{l_1} n_j} + D^c_{k_1k_2}\overline{n_{k_1}n_{k_2}n_i n_j} \\ &+\sum_{s=1}^{\propto} G^f_{jm_1\cdots m_s} G^v_{il_1\cdots l_s}\overline{n_{l_1}\cdots n_{l_s} n_{m_1}\cdots n_{m_s}} \\ &+\sum_{n=2,\mathrm{even}}^{\propto} D^c_{k_1\cdots k_n} G^f_{jm_1\cdots m_{n-1}}\overline{n_i n_{k_1}\cdots n_{k_n} n_{m_1}\cdots n_{m_{n-1}}} \\ &+\sum_{n=2,\mathrm{even}}^{\propto} D^c_{k_1\cdots k_n} G^f_{jm_1\cdots m_{n+1}}\overline{n_i n_{k_1}\cdots n_{k_n} n_{m_1}\cdots n_{m_{n+1}}} \\ &+\sum_{n=2,\mathrm{even}}^{\propto} D^c_{k_1\cdots k_n} G^v_{im_1\cdots m_{n-1}}\overline{n_j n_{k_1}\cdots n_{k_n} n_{m_1}\cdots n_{m_{n-1}}} \\ &+\sum_{n=2}^{\propto} D^c_{k_1\cdots k_n} G^v_{im_1\cdots m_{n+1}}\overline{n_j n_{k_1}\cdots n_{k_n} n_{m_1}\cdots n_{m_{n+1}}} \\ &+\sum_{n=2;s,t=1;|s-t|\leqslant n\leqslant s+t}^{\propto} D^c_{k_1\cdots k_n} G^v_{il_1\cdots l_s} G^f_{jm_1\cdots m_t}\overline{n_{k_1}\cdots n_{k_n} n_{l_1}\cdots n_{l_s} n_{m_1}\cdots n_{m_t}}\end{aligned}\right] \tag{A26}$$

The coefficient direct tensors $P^{vf,st}_{ijk_1k_2\cdots k_n}$ and $Q^{vf,st}_{ijk_1k_2\cdots k_n}$ could be determined as follows. Multiplying both sides of Eq. (A24) with $n_{p_1}\cdots n_{p_q}$ and integrating, we have the moment tensor:

$$\begin{aligned}R^{vf,st}_{ijp_1p_2\cdots p_q} &= G^v_{il_1\cdots l_s} G^f_{jm_1\cdots m_t} \overline{n_{l_1}\cdots n_{l_s} n_{m_1}\cdots n_{m_t} n_{p_1}\cdots n_{p_q}} \\ &= \sum_{r=0,\mathrm{even}}^{s+t} Q^{vf,st}_{ijn_1n_2\cdots n_r} \overline{n_{n_1}n_{n_2}\cdots n_{n_r} n_{p_1}\cdots n_{p_q}} \\ &= \sum_{r=0,\mathrm{even}}^{q} Q^{vf,st}_{ijn_1n_2\cdots n_r} \overline{n_{n_1}n_{n_2}\cdots n_{n_r} n_{p_1}\cdots n_{p_q}}\end{aligned} \tag{A27}$$

With $G^v_{il_1\cdots l_s}, G^f_{jm_1\cdots m_t}$ being the deviatoric direction tensor obtained from orthogonal decompositions, we have $R^{vf,st}_{ijp_1p_2\cdots p_q} = 0$ when $q < |s-t|$, so that $P^{vf,st}_{ijn_1n_2\cdots n_r}$ and $Q^{vf,st}_{ijn_1n_2\cdots n_r}$ are both zero when $r < |s-t|$. When $q = |s-t|$, $R^{vf,st}_{ijp_1p_2\cdots p_q}$ becomes non-zero while $P^{vf,st}_{ijp_1p_2\cdots p_q} = Q^{vf,st}_{ijp_1p_2\cdots p_q}$, and:

$$R^{vf,st}_{ijp_1p_2\cdots p_q} = Q^{vf,st}_{ijn_1n_2\cdots n_q} \overline{n_{n_1}n_{n_2}\cdots n_{n_q} n_{p_1}\cdots n_{p_q}} = \alpha_{2q}\frac{2^q}{{}^{2q}C_q} Q^{vf,st}_{ijp_1p_2\cdots p_q} \tag{A28}$$

This gives us the start point to calculate $P^{vf,st}_{ijp_1p_2\cdots p_q}$ and $Q^{vf,st}_{ijp_1p_2\cdots p_q}$ successively when $q > |s-t|$. With $R^{vf,st}_{ijp_1p_2\cdots p_q}$ calculated from Eq. (A27), we have:

$$Q^{vf,st}_{ijp_1\cdots p_q} = \frac{1}{\alpha_{2q}}\frac{{}^{2q}C_q}{2^q}\left[R^{vf,st}_{ijp_1\cdots p_q} - P^{vf,st}_{ijl_1\cdots l_{q-2}} \overline{n_{l_1}\cdots n_{l_{q-2}} n_{p_1}\cdots n_{p_q}}\right] \tag{A29}$$

Noticing the symmetry in $P^{vf,st}_{ijp_1p_2\cdots p_q}$ and $Q^{vf,st}_{ijp_1p_2\cdots p_q}$, the direction tensor $P^{vf,st}_{ijp_1p_2\cdots p_q}$ for n-th rank approximation is then determined as

$$P^{vf,st}_{ijp_1p_2\cdots p_q} = P^{vf,st}_{ij(p_1p_2\cdots p_{q-2}}\delta_{p_{q-1}p_q)} + Q^{vf,st}_{ijp_1p_2\cdots p_q} \tag{A30}$$

Appendix A4. Simplification of stress–force–fabric relationship

From Eq. (15), we have:

$$\overline{n_{i_1}n_{i_2}} = \alpha_2\delta_{i_1i_2} \tag{A31}$$

Hence,

$$G^f_{jm_1}\overline{n_i n_{m_1}} = \alpha_2 G^f_{jm_1}\delta_{im_1} = \alpha_2 G^f_{ji} \tag{A32}$$

$$G^v_{il_1}\overline{n_{l_1}n_j} = \alpha_2 G^v_{il_1}\delta_{l_1j} = \alpha_2 G^v_{ij} \tag{A33}$$

Together with Eq. (20), we have:

$$D^c_{k_1k_2}\overline{n_{k_1}n_{k_2}n_i n_j} = \alpha_4\frac{2^2}{{}^4C_2}D^c_{ij} = \frac{2}{3}\alpha_4 D^c_{ij} \tag{A34}$$

$$G^f_{jm_1\cdots m_s}G^v_{il_1\cdots l_s}\overline{n_{l_1}\cdots n_{l_s}n_{m_1}\cdots n_{m_s}} = \alpha_{2s}\frac{2^s}{{}^{2s}C_s}G^f_{jl_1\cdots l_s}G^v_{il_1\cdots l_s} \tag{A35}$$

$$D^c_{k_1k_2\cdots k_n}G^f_{jm_1\cdots m_{n-1}}\overline{n_in_{k_1}n_{k_2}\cdots n_{k_n}n_{m_1}\cdots n_{m_{n-1}}} = \alpha_{2n}\frac{2^n}{{}^{2n}C_n}D^c_{im_1\cdots m_{n-1}}G^f_{jm_1\cdots m_{n-1}} \tag{A36}$$

$$D^c_{k_1k_2\cdots k_n}G^f_{jm_1\cdots m_{n+1}}\overline{n_in_{k_1}n_{k_2}\cdots n_{k_n}n_{m_1}\cdots n_{m_{n+1}}} = \alpha_{2n+2}\frac{2^{n+1}}{{}^{2n+2}C_{n+1}}D^c_{k_1k_2\cdots k_n}G^f_{jik_1\cdots k_n} \tag{A37}$$

$$D^c_{k_1k_2\cdots k_n}G^v_{jm_1\cdots m_{n-1}}\overline{n_in_{k_1}n_{k_2}\cdots n_{k_n}n_{m_1}\cdots n_{m_{n-1}}} = \alpha_{2n}\frac{2^n}{{}^{2n}C_n}D^c_{im_1\cdots m_{n-1}}G^v_{jm_1\cdots m_{n-1}} \tag{A38}$$

$$D^c_{k_1k_2\cdots k_n}G^v_{jm_1\cdots m_{n+1}}\overline{n_in_{k_1}n_{k_2}\cdots n_{k_n}n_{m_1}\cdots n_{m_{n+1}}} = \alpha_{2n+2}\frac{2^{n+1}}{{}^{2n+2}C_{n+1}}D^c_{k_1k_2\cdots k_n}G^v_{jik_1\cdots k_n} \tag{A39}$$

More effort is required for the last term. $G^f_{jm_1\cdots m_t}G^v_{il_1\cdots l_s}n_{l_1}\cdots n_{l_s}n_{m_1}\cdots n_{m_t}$ can be expressed in terms of a polynomial in $\mathbf{n}$ up to rank $(s+t)$ using the orthogonal decompositions in the form of Eq. (A24).

Noticing that,

$$D^c_{k_1k_2\cdots k_n}G^{vf,st}_{ijk_1k_2\cdots k_r}\overline{n_{k_1}n_{k_2}\cdots n_{k_n}n_{l_1}\cdots n_{l_r}} = \begin{cases} D^c_{k_1k_2\cdots k_n}\left(G^{vf,st}_{ijk_1k_2\cdots k_r}\overline{n_{k_1}n_{k_2}\cdots n_{k_n}n_{l_1}\cdots n_{l_r}}\right)=0, & \text{when } r>n \\ G^{vf,st}_{ijk_1k_2\cdots k_r}\left(D^c_{k_1k_2\cdots k_n}\overline{n_{k_1}n_{k_2}\cdots n_{k_n}n_{l_1}\cdots n_{l_r}}\right)=0, & \text{when } n>r \\ \neq 0, & \text{otherwise}\end{cases} \tag{A40}$$

we have,

$$\sum_{r=0,\text{even}}^{s+t} D^c_{k_1k_2\cdots k_n}G^{vf,st}_{ijl_1l_2\cdots l_r}\overline{n_{k_1}n_{k_2}\cdots n_{k_n}n_{l_1}\cdots n_{l_r}} = D^c_{k_1k_2\cdots k_n}G^{vf,st}_{ijl_1l_2\cdots l_n}\overline{n_{k_1}n_{k_2}\cdots n_{k_n}n_{l_1}\cdots n_{l_n}} \tag{A41}$$

Hence, when $|s-t|\leqslant n\leqslant s+t$, we have

$$D^c_{k_1k_2\cdots k_n}G^v_{il_1\cdots l_s}G^f_{jm_1\cdots m_t}\overline{n_{k_1}n_{k_2}\cdots n_{k_n}n_{l_1}\cdots n_{l_s}n_{m_1}\cdots n_{m_t}} = D^c_{k_1k_2\cdots k_n}G^{vf,st}_{ijl_1l_2\cdots l_n}\overline{n_{k_1}n_{k_2}\cdots n_{k_n}n_{l_1}\cdots n_{l_n}} = \alpha_{2n}\tfrac{2^n}{{}^{2n}C_n}D^c_{k_1k_2\cdots k_n}G^{vf,st}_{ijk_1k_2\cdots k_n} \tag{A42}$$

Substituting the above equations into the expanded form Eq. (19), the stress tensor is expressed as:

$$\sigma_{ij} = \frac{\omega N}{V}\varsigma v_0 f_0\left[\begin{array}{l}\alpha_2\delta_{ij}+\alpha_2G^f_{ji}+\alpha_2G^v_{ij}+\tfrac{2}{3}\alpha_4D^c_{ij} \\ +\sum_{s=1}^{\infty}\alpha_{2s}\tfrac{2^s}{{}^{2s}C_s}G^f_{jl_1\cdots l_s}G^v_{il_1\cdots l_s} \\ +\sum_{n=2}^{\infty}\alpha_{2n}\tfrac{2^n}{{}^{2n}C_n}D^c_{im_1\cdots m_{n-1}}G^f_{jm_1\cdots m_{n-1}} \\ +\sum_{n=2}^{\infty}\alpha_{2n+2}\tfrac{2^{n+1}}{{}^{2n+2}C_{n+1}}D^c_{k_1\cdots k_n}G^f_{jik_1\cdots k_n} \\ +\sum_{n=2}^{\infty}\alpha_{2n}\tfrac{2^n}{{}^{2n}C_n}D^c_{im_1\cdots m_{n-1}}G^v_{jm_1\cdots m_{n-1}} \\ +\sum_{n=2}^{\infty}\alpha_{2n+2}\tfrac{2^{n+1}}{{}^{2n+2}C_{n+1}}D^c_{k_1\cdots k_n}G^v_{jik_1\cdots k_n} \\ +\sum_{n=2,|s-t|\leqslant n\leqslant s+t}^{\infty}\alpha_{2n}\tfrac{2^n}{{}^{2n}C_n}D^c_{k_1\cdots k_n}Q^{vf,st}_{ijk_1\cdots k_n}\end{array}\right] \tag{A43}$$

Appendix A5. Expression of $D_{i_1\cdots i_n}n_{i_1}n_{i_2}\cdots n_{i_n}$

The value of $D_{11\cdots1\overbrace{22\cdots2}^{k}}$ given in Eq. (22) can be expressed in alternative form as

$$D_{11\cdots1\overbrace{22\cdots2}^{k}} = \frac{i^k+(-i)^k}{2}a_n + \frac{-i^k+(-i)^k}{2}ib_n \tag{A44}$$

where i is the standard imaginary unit with $i^2=-1$. With $e^{i\theta}=\cos\theta+i\sin\theta$, expansion of $D_{i_1\cdots i_n}n_{i_1}n_{i_2}\cdots n_{i_n}$ becomes:

$$\begin{aligned} D_{i_1\cdots i_n}n_{i_1}n_{i_2}\cdots n_{i_n} &= \sum_{k=1}^{n}{}^nC_k\left[\tfrac{i^k+(-i)^k}{2}a_n+\tfrac{-i^k+(-i)^k}{2}ib_n\right]\cos^{n-k}\theta\sin^k\theta \\ &= \sum_{k=0}^{n}{}^nC_k\left[\tfrac{i^k+(-i)^k}{2}a_n+\tfrac{-i^k+(-i)^k}{2}ib_n\right]\left[\tfrac{1}{2}\left(e^{i\theta}+e^{-i\theta}\right)\right]^{n-k}\left[\tfrac{i}{2}\left(e^{-i\theta}-e^{i\theta}\right)\right]^k \\ &= \tfrac{a_n}{2}\sum_{k=0}^{n}{}^nC_k\left[\tfrac{1}{2}\left(e^{i\theta}+e^{-i\theta}\right)\right]^{n-k}\left\{\left[-\tfrac{1}{2}\left(e^{-i\theta}-e^{i\theta}\right)\right]^k+\left[\tfrac{1}{2}\left(e^{-i\theta}-e^{i\theta}\right)\right]^k\right\} \\ &\quad -i\tfrac{b_n}{2}\sum_{k=0}^{n}{}^nC_k\left[\tfrac{1}{2}\left(e^{i\theta}+e^{-i\theta}\right)\right]^{n-k}\left\{\left[-\tfrac{1}{2}\left(e^{-i\theta}-e^{i\theta}\right)\right]^k-\left[\tfrac{1}{2}\left(e^{-i\theta}-e^{i\theta}\right)\right]^k\right\} \\ &= \tfrac{a_n}{2}\left[\tfrac{1}{2}\left(e^{i\theta}+e^{-i\theta}\right)-\tfrac{1}{2}\left(e^{-i\theta}-e^{i\theta}\right)\right]^n+\tfrac{a_n}{2}\left[\tfrac{1}{2}\left(e^{i\theta}+e^{-i\theta}\right)+\tfrac{1}{2}\left(e^{-i\theta}-e^{i\theta}\right)\right]^n \\ &\quad -i\tfrac{b_n}{2}\left[\tfrac{1}{2}\left(e^{i\theta}+e^{-i\theta}\right)-\tfrac{1}{2}\left(e^{-i\theta}-e^{i\theta}\right)\right]^n+i\tfrac{b_n}{2}\left[\tfrac{1}{2}\left(e^{i\theta}+e^{-i\theta}\right)+\tfrac{1}{2}\left(e^{-i\theta}-e^{i\theta}\right)\right]^n \\ &= \tfrac{a_n}{2}\left[e^{in\theta}+e^{-in\theta}\right]+i\tfrac{b_n}{2}\left[-e^{in\theta}+e^{-in\theta}\right] \\ &= a_n\cos n\theta+b_n\sin n\theta = d_n\cos(n\theta-\phi_n)\end{aligned} \tag{A45}$$

where $d_n=\sqrt{a_n^2+b_n^2}$ and $\tan\phi_n=b_n/a_n$.

Appendix A6. Calculation of the direction tensors for $\langle v_if_j\rangle|_{\mathbf{n}}$

We define the least square error as follows:

$$E=\oint_\Omega\left[(V_iF_j)(\mathbf{n})-\langle v_if_j\rangle|_{\mathbf{n}}\right]:\left[(V_iF_j)(\mathbf{n})-\langle v_if_j\rangle|_{\mathbf{n}}\right]d\Omega \tag{A46}$$

Minimizing the least square error leads to $\partial E/\partial P^{pa}_{ijk_1k_2\cdots k_n}=0$, and the expression of the moment tensor as follows:

$$\begin{aligned} R^{pa}_{ijk_1k_2\cdots k_n} &= (vf)^{pa}_0P^{pa}_{ijl_1l_2\cdots l_n}\overline{n_{l_1}n_{l_2}\cdots n_{l_n}n_{k_1}n_{k_2}\cdots n_{k_n}} \\ &= \tfrac{1}{N}\sum_{\alpha=1}^{N}\left[\left(v_if_jn^\alpha_{k_1}n^\alpha_{k_2}\cdots n^\alpha_{k_n}\right)\Big/\left(F_{l_1l_2\cdots l_n}n^\alpha_{l_1}n^\alpha_{l_2}\cdots n^\alpha_{l_n}\right)\right]\end{aligned} \tag{A47}$$

which can be calculated from discrete particle-scale information with the pre-determined approximation of contact normal density as in Eq. (8).

From Eqs. (67), (68), and (A47), we have:

$$R^{pa}_{ij}=\frac{1}{E_0}\oint_\Omega\langle v_if_j\rangle|_{\mathbf{n}}d\Omega=(vf)^{pa}_0P^{pa}_{ij}=(vf)^{pa}_0\left[\frac{1}{D}\delta_{ij}+Q^{pa}_{ij}\right] \tag{A48}$$

Hence, $Q^{pa}_{ij}=R^{pa}_{ij}/(vf)^{pa}_0-\delta_{ij}/D$. Again, we can have $P^{pa}_{ijk_1k_2\cdots k_n}$ and $Q^{pa}_{ijk_1k_2\cdots k_n}$ determined successively. With the moment tensor $R^{pa}_{ijk_1k_2\cdots k_n}$ and the known lower rank direction tensor $P^{pa}_{ijk_1k_2\cdots k_{n-2}}$, the n-th rank deviatoric direction tensor $Q^{pa}_{ijk_1k_2\cdots k_n}$ can be determined from:

$$Q^{pa}_{ijk_1\cdots k_n}=\frac{1}{\alpha_{2n}}\frac{{}^{2n}C_n}{2^n}\left[R^{pa}_{ijk_1\cdots k_n}\Big/(vf)^{pa}_0-P^{pa}_{ijl_1\cdots l_{n-2}}\overline{n_{l_1}\cdots n_{l_{n-2}}n_{k_1}\cdots n_{k_n}}\right] \tag{A49}$$

Noticing the symmetry in $P^{pa}_{ijk_1k_2\cdots k_n}$ and $Q^{pa}_{ijk_1k_2\cdots k_n}$, the direction tensor $P^{pa}_{ijk_1k_2\cdots k_n}$ for n-th rank approximation is then determined as

$$P^{pa}_{ijk_1k_2\cdots k_n}=P^{pa}_{ij(k_1\cdots k_{n-2}}\delta_{k_{n-1}k_n)}+Q^{pa}_{ijk_1k_2\cdots k_n} \tag{A50}$$

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