



Deposited via The University of Leeds.

White Rose Research Online URL for this paper:

<https://eprints.whiterose.ac.uk/id/eprint/236491/>

Version: Accepted Version

Article:

Cai, W., Wanatowski, D., Xu, P. et al. (2026) Micro-mechanical analysis of cohesionless-frictional particulate materials considering principal stress rotation induced by moving surface loads. *Acta Geotechnica*, 21 (4). pp. 1883-1898. ISSN: 1861-1125

<https://doi.org/10.1007/s11440-025-02884-5>

This is an author produced version of an article published in *Acta Geotechnica*, made available via the University of Leeds Research Outputs Policy under the terms of the Creative Commons Attribution License (CC-BY), which permits unrestricted use, distribution and reproduction in any medium, provided the original work is properly cited.

Reuse

This article is distributed under the terms of the Creative Commons Attribution (CC BY) licence. This licence allows you to distribute, remix, tweak, and build upon the work, even commercially, as long as you credit the authors for the original work. More information and the full terms of the licence here:

<https://creativecommons.org/licenses/>

Takedown

If you consider content in White Rose Research Online to be in breach of UK law, please notify us by emailing eprints@whiterose.ac.uk including the URL of the record and the reason for the withdrawal request.

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30

Micro-mechanical analysis of
cohesionless-frictional particulate materials
considering principal stress rotation induced by
moving surface loads

First Wei Cai^{1,3}, Second Dariusz Wanatowski², Third Ping Xu^{1,3*},
Fourth Hai-Sui Yu², Fifth Zhengyang Zhang^{1,3}

^{1*}School of Civil Engineering, Henan Polytechnic University, Jiaozuo,
454003, China.

²Faculty of Engineering and Physical Sciences, University of Leeds,
Leeds, LS2 9JT, UK.

³Henan Provincial Engineering Research Center for Ecological
Architecture and Environmental Construction, Henan Polytechnic
University, Jiaozuo, 454003, China.

*Corresponding author(s). E-mail(s): xuping@hpu.edu.cn;
Contributing authors: caiwei@hpu.edu.cn; D.Wan@leeds.ac.uk;
H.Yu@leeds.ac.uk; zhazheya@hpu.edu.cn;

Abstract

The principal stress rotation induced by moving surface loads has been extensively investigated, predominantly through hollow cylinder tests. In contrast to these element tests, residual stresses are generated within a structural component due to plastic strain accumulation during the loading and unloading process. Given the significant influence of residual stresses on principal stress distributions, it is essential to investigate the principal stress rotation at the structural scale rather than relying solely on element-scale analyses. In this study, a discrete element method (DEM) model was developed to simulate the mechanical response of a cohesionless-frictional particulate structure subjected to moving surface loads. The macroscopic stresses responsible for principal stress rotation were analytically derived, and their behaviour was found to be significantly affected by residual stresses during the unloading process. Furthermore, a comprehensive micro-mechanical analysis was conducted, with particular emphasis

on the evolution of fabric anisotropy. The results revealed a pronounced non-coaxiality between the principal directions of the fabric anisotropy. Finally, a stress-force-fabric (SFF) relationship was employed to validate the concept of fabric anisotropy and to establish a connection between particle-scale contact mechanics and macro-scale stresses. The influence of branch vectors on macroscopic stresses was found to be negligible under conditions involving the principal stress rotation and irregular particle morphologies.

Keywords: principal stress rotation, stress-force-fabric (SFF) relationship, fabric anisotropy, cohesionless-frictional particulate material, moving surface load

1 Introduction

In geotechnical engineering, granular materials frequently encounter complex stress states, characterised by variations in both the magnitude and direction of principal stresses. These variations, commonly referred to as principal stress rotation, are induced by factors such as earthquake loads, wave loads, and traffic loads [7, 49, 54]. The significant plastic strains observed in geotechnical structures are more likely attributed to the principal stress rotation rather than dead loads, thereby accelerating the degradation of the mechanical performance of the structure [62]. Consequently, the influence of principal stress rotation on the mechanical behaviour of granular materials has attracted increasing attention in engineering practice [48, 63]. The stress path of an element within a half-space geotechnical structure subjected to moving surface loads typically comprises vertical, horizontal, and shear components, as noted by Lekarp et al [20]. In granular materials, vertical and horizontal stresses are generally compressive, whereas the shear stress reverses direction as the load moves, resulting in a rotation of the principal stresses.

The hollow cylinder test is widely used to investigate stress paths induced by moving surface loads, including principal stress rotation [5, 13, 53]. The hollow cylinder test has demonstrated a reduction in the vertical resilient modulus [47] and an accelerated accumulation of plastic strains [31] in granular materials, both attributed to the principal stress rotation induced by equivalent moving surface loads. Furthermore, a comparative study between the conventional triaxial test and the hollow cylinder test revealed that stress paths accounting for principal stress rotation led to greater permanent deformation in clay under identical confining pressures [35]. Moreover, the intermediate principal stress significantly influences the constitutive response of granular materials subjected to stress rotation [57]. Under otherwise identical conditions, rotational shear behaviour exhibits distinct variations in pore pressure resistance and stiffness degradation characteristics under different intermediate principal stress parameters. Finally, the liquefaction susceptibility of granular materials and the correlation between cyclic stress ratio and cycles to failure are significantly influenced by the coupled effects of consolidation conditions and principal stress rotation patterns [6].

A range of methods for quantifying the microscopic structures of physical specimens has been proposed, employing advanced imaging techniques such as X-ray,

CT and stereophotogrammetry [2, 32]. However, acquiring detailed fabric information, including contact normal and contact force components, remains challenging due to the limitations of measurement instruments and the significant costs associated with physical testing. As a result, the investigation of micro-mechanical behaviour and micro-structural evolution becomes equally challenging [21]. The discrete element method (DEM), initially proposed by Cundall and Strack [9], has proven to be a powerful tool for obtaining fabric information for microscopic analysis, providing a valuable complement to macroscopic mechanical tests [14, 41, 60]. In the DEM study, a hexagonal vessel composed of six rigid walls was employed to generate specimens, facilitating the simulation of stress paths induced by moving surface loads for macro- to micro-mechanical analysis [24]. This approach was subsequently extended to three dimensions to generate polyhedral specimens, enabling a series of numerical tests with the principal stress rotation [30]. Additionally, a hollow cylindrical specimen was developed for DEM simulations to investigate the macro- and micro-mechanical behavior of granular materials. The results demonstrated that the principal stress rotation significantly influences both the scalar anisotropy coefficients and the directional distributions of fabric parameters [18]. Furthermore, the principal stress rotation intensifies the development of vertical accumulated plastic strain, particle displacements, and the degradation of the microstructure of granular assemblies [8].

In addition to element tests, numerical experiments have also been conducted to model pavement structures and analyse macroscopic stresses and permanent deformations. For example, Vallejo et al [42] utilized DEM simulations to investigate the degradation of the granular base layer in flexible pavements. Additionally, the macroscopic stress path for an element within pavements has been examined using a DEM pavement structure model [40, 56]. These studies predominantly focused on the evolution of normal stress, horizontal stress, and shear stress under moving surface loads from a macroscopic perspective. However, the influence of residual stresses induced by external loads on these macroscopic stress distributions remains predominantly unexplored. Furthermore, Peng et al [34] examined the macro-mechanical behaviour of asphalt pavement subjected to moving traffic loads, with a particular emphasis on the variation of shear stress and plastic strain distribution across the depth of the asphalt layers.

As reviewed in previous studies, the investigation of principal stress rotation has predominantly relied on hollow cylinder tests performed at the element scale. Residual stresses emerge within the structural system as a result of plastic strain developments induced by external loads. This study demonstrates that their influence on both macro- and micro-mechanical behaviour is significant. Although structural-scale testing has been implemented in some studies, its applicability is primarily limited to macro-mechanical analysis, failing to consider the investigation of micro-scale mechanisms. Relative to previous numerical studies, micro-mechanical analysis effectively utilise the capabilities of DEM simulations in characterising the principal stress rotation caused by moving surface loads. In this study, micro-parameters, including fabric anisotropy and the principal direction of anisotropy, were quantitatively analysed. It is demonstrated that fabric anisotropy generally reaches its maximum at the critical point during both loading and unloading stages, after which it gradually decreases.

Moreover, approximate coaxiality with the principal directions of fabric anisotropy is found exclusively at this critical point. Furthermore, a stress-force-fabric (SFF) relationship [23, 28, 37] was adopted to establish quantitative correlations between particle-scale contact mechanics and macroscopic stress responses. The results demonstrate that the branch vector exerts a negligible influence on macroscopic stresses in granular materials with irregular particle morphologies subjected to principal stress rotation, while the normal contact force constitutes the dominant factor governing macroscopic stress development. These findings enrich the theoretical understanding of micromechanical behaviour in granular materials and offer essential insights for optimizing engineering design.

2 Numerical implementation

2.1 Numerical structure

A square region located beneath the structural surface, referred to as Element *A*, was designated for the analysis of the stress path induced by the moving surface load (see Fig. 1). The depth of Element *A* was deliberately chosen to be small, measuring only 0.1 m, to account for the shallow distribution range of residual stresses [3, 44]. In this way, the influence of residual stresses on stress paths can be effectively analysed. Determining the size of Element *A* presents great challenges in DEM experiments. The size of Element *A* should remain small while ensuring that it contains a sufficient number of particles. In this study, Element *A* was defined as a square with dimensions of 0.15 m $\times$ 0.15 m, comprising approximately 1,400 particles. The particle number approximately aligns with the micro-mechanical investigations reported by Cai et al [4], Hosseininia [11], and Rothenburg and Bathurst [37]. The macro- and micro-mechanical results presented in Sections 3.1, 3.4, and 3.6 further validate the feasibility of the size selection.

A narrow radius range of 1 to 3 mm for circular particles was uniformly generated to ensure an adequate quantity of particles within Element *A* for subsequent micro-mechanical analysis. Geotechnical materials, encompassing soils and gravel particles, exhibit a wide range of particle size distributions, typically varying from less than 0.075 mm to over 40 mm [1]. However, fine particles were excluded to simplify numerical computations, as relatively large particles predominantly contribute to strong force chains and facilitate the transmission of macroscopic stress within a granular system [15, 43, 55]. Subsequently, irregular particles were substituted for circular ones while preserving the same volume and maintaining a uniformly distributed orientation to replicate natural gravels more accurately. Accordingly, the diameter of the circular particle was defined as the equivalent size of the irregular particle. Furthermore, as highlighted by Wang et al [50], the two-dimensional contours of real-shaped gravels can be classified into three categories: long, square, and a general contour that lies in between. Following the contour framework outlined by Cai et al [3], this study employed the general contour to generate irregular particles (see Fig. 1b), with the detailed particle generation methodology described by Wang et al [50].

The dimensions of the numerical structure (1.80 m long $\times$ 0.945 m high) were established through a sensitivity analysis to ensure the stabilization of macroscopic stress

160 within Element *A*. The detailed methodology for the preparation of the numerical
 161 structure is provided by Cai et al [3], specifically addressing residual stress evolution
 162 under post-loading conditions. Following generation, a periodic boundary condition,
 163 implemented using PFC^{2D} [16], was applied to the left and right sides of the structure.
 164 The application of the periodic boundary condition allows the left and right bound-
 165 aries to be treated as connected. The numerical structure was initially isotropically
 166 consolidated and subsequently brought to a stress-free state (i.e. the confining pres-
 167 sure $\sigma_{cp} = 0$). Finally, self-weight consolidation was performed to completion (see Fig.
 168 1a). A linear constitutive model was adopted for interparticle contacts, as it is widely
 169 used in DEM experiments to investigate the behaviour of cohesionless-frictional mate-
 170 rials [16]. With reference to Lashkari et al [19] and Wu et al [52], a particle stiffness
 171 of 10^6 N/m is implemented for equivalent particle radii ranging from 1 to 3 mm. For
 172 granular materials, the contact damping ratio typically ranges from 0.02 to 0.5 in DEM
 173 simulations. An alternative approach involves adjusting the particle damping coeffi-
 174 cient. With reference to Lashkari et al [19] and Wu et al [52], the particle damping
 175 coefficient is set to 0.7 throughout the DEM experiments. The relevant parameters of
 176 the numerical structure are summarized in Table 1.

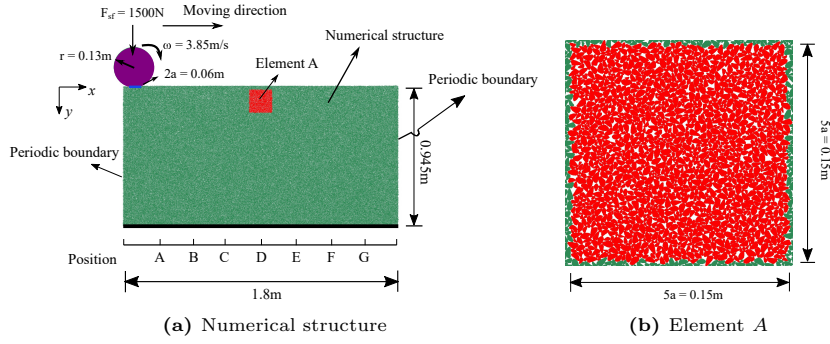


Fig. 1. Numerical structure and Element *A* subjected to the moving surface load.

Table 1

Summary of properties for the numerical structure.

Numerical structure properties	
Structure size: length $\times$ height (m)	approx. 1.80×0.945
Number of particles	approx. 105,600
Porosity	0.155
Particle properties	
Equivalent particle radius (mm)	1.0-3.0
Particle friction coefficient	0.7
Particle specific gravity	2.65
Normal stiffness of Pebble-Pebble (N/m)	1×10^6
Tangential stiffness of Pebble-Pebble (N/m)	1×10^6
Particle damping coefficient	0.7

2.2 Numerical procedure

A loading particle with a radius r of 0.13 m was positioned on the top surface of the left boundary of the numerical structure. A surface load ($F_{sf} = 1500$ N) was subsequently applied to simulate the traffic load (see Fig. 1a). Following this, the loading particle traversed the surface of the structure, moving from the left boundary to the right boundary. Consequently, the stress path in Element A could be determined for various surface positions, ranging from Position A to G , corresponding to the locations reached by the loading particle. The central position D represents the critical point for both the loading and unloading stages. After reaching Position D , the unloading stage commences and concludes at the right boundary of the structural surface. To maintain a quasi-static state, the spin velocity ω of the loading particle was kept constant at a low value of 3.85 m/s [17, 45]. Additionally, the friction coefficient of the loading particle was set to 0.7, consistent with that of the structural particles. The contact width $2a$ between the loading particle and the structural surface was maintained at approximately 0.06 m by adjusting the stiffness of the loading particle. A load pass was considered complete when the loading particle moved from the left boundary to the right boundary.

3 Numerical results and discussion

3.1 Macroscopic stress

The average stress tensor in a granular assembly can be expressed as follows [39, 51, 61]:

$$\sigma_{ij} = \frac{1}{V} \int_0^{2\pi} v_i \otimes f_{r,j} d\theta = \frac{1}{V} \sum_{N_c} v_i \otimes f_{r,j} \quad (1)$$

where V represents the volume of the assembly, and N_c denotes the total number of interparticle contacts. v_i indicates the branch vector connecting the centroids of two contacting particles, while $f_{r,j}$ represents the interparticle resultant force at a contact (see Fig. 2).

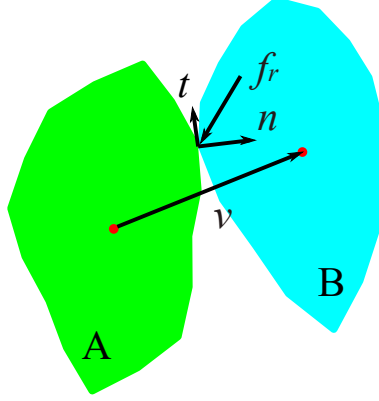


Fig. 2. Two contacting irregular particles and the associated normal contact vector (n), tangential contact vector (t), force vector (f_r) and branch vector (v).

The macroscopic stress in Element A can be calculated using Eq. (1) as the loading particle moves across Positions A to G along the structural surface (see Fig. 3). The initial stress state shows non-zero vertical and horizontal components, reflecting self-weight contributions. The vertical stress component σ_{yy} exhibits a characteristic symmetric pattern during both the loading and unloading processes. These findings align qualitatively with the theoretical work of Lekarp et al [20] and the numerical studies of Yan et al [56] on comparable structures subjected to moving surface loads. As the loading particle passes through the central position D , the shear stress components σ_{xy} and σ_{yx} undergo directional reversal, thereby inducing principal stress rotation. Unlike the findings of Lekarp et al [20], the shear stresses σ_{xy} and σ_{yx} retain non-zero values at the central position D as a result of rolling friction effects.

In contrast to the observations of Lekarp et al [20], the horizontal stress σ_{xx} demonstrates asymmetric behaviour during the load pass, which can be attributed to the accumulation of horizontal residual stress σ_{xx}^r . During the load pass, Element A experiences plastic deformation, resulting in particle reorganization and an increase in

interparticle forces, as observed by Cai et al [3]. This process gives rise to the development of residual stresses. As demonstrated by Yu [58], Yu and Wang [59], and Wang and Yu [46], residual stresses in two-dimensional half-space systems under moving surface loads exhibit a uniform distribution pattern exclusively along the horizontal direction. Owing to the contribution of horizontal residual stress σ_{xx}^r , the magnitude of σ_{xx} during the unloading phase consistently exceeds that observed during the loading phase. Figure 4 illustrates the depth-dependent residual stress field, which is quantified by comparing the stress components σ_{ij} before and after the load pass [3]. The residual stress pattern σ_{ij}^r demonstrates strong qualitative agreement with the experimental observations of Radovsky and Murashina [36] and the finite element analysis conducted by Wang and Yu [45]. Figure 4 reveals a substantial horizontal residual stress σ_{xx}^r in Element A, highlighting its significant influence on the macroscopic stress field. The presence of σ_{xx}^r induces the asymmetric behaviour observed in σ_{xx} .

Figure 5 presents the heart-shaped stress path in the deviatoric plane, expressed as $\frac{(\sigma_{yy} - \sigma_{xx})}{2}$ versus σ_{xy} , which clearly demonstrates the principal stress rotation phenomenon. Due to the presence of rolling friction and horizontal residual stress σ_{xx}^r , the heart-shaped stress path exhibits asymmetry about the horizontal axis. Furthermore, the deviatoric stress exhibits persistent deviation from its initial state, resulting in an open heart-shaped stress path.

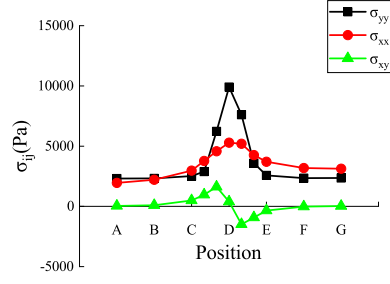


Fig. 3. Macroscopic stress path induced by the moving surface load.

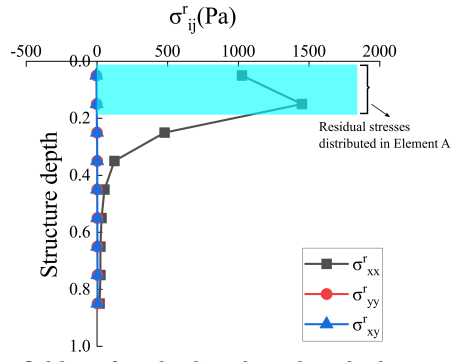


Fig. 4. Residual stress field uniformly distributed with the numerical structure depth.

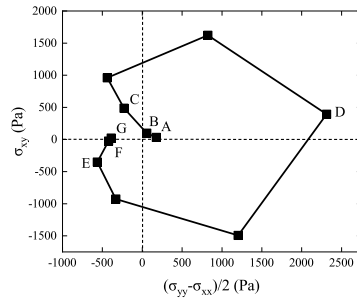


Fig. 5. Heart-shaped stress path induced by the moving surface load.

3.2 Contribution of interparticle component forces

In a cohesionless-frictional granular assembly, interparticle contacts are characterised by two force components: the normal force f_n and the tangential force f_t . The contributions of f_n and f_t to macroscopic stresses have been investigated by Li et al [22] and Zou et al [64], resulting in the following reformulation of Eq. (1):

$$\begin{aligned}\sigma_{ij} &= \frac{1}{V} \sum_{N_c} v_i \otimes f_{r,j} = \frac{1}{V} \sum_{N_c} v_i \otimes (f_{n,j} + f_{t,j}) \\ &= \frac{1}{V} \sum_{N_c} v_i \otimes f_{n,j} + \frac{1}{V} \sum_{N_c} v_i \otimes f_{t,j} \\ &= \sigma_{ij}(f_n) + \sigma_{ij}(f_t)\end{aligned}\tag{2}$$

where $\sigma_{ij}(f_n)$ and $\sigma_{ij}(f_t)$ respectively represent the contributions of f_n and f_t to the macroscopic stress σ_{ij} . f_n provides the dominant contribution to σ_{ij} , with $\sigma_{ij}(f_n)$ exhibiting patterns similar to σ_{ij} across all components (σ_{yy} , σ_{xx} , and σ_{xy}) (see Fig. 6). These findings align with the numerical results reported by Li et al [22] and Zou et al [64]. The contribution of f_t to σ_{yy} and σ_{xx} becomes significant exclusively near Position D , where it coincides with the reversal in shear stress direction. However, f_t contributes reversely to σ_{yy} and σ_{xx} , as evidenced by the negative sign of $\sigma_{xx}(f_t)$. On the other hand, the contribution of f_t is substantial for σ_{xy} , as $\sigma_{xy}(f_t)$ exhibits patterns consistent with both σ_{xy} and $\sigma_{xy}(f_n)$.

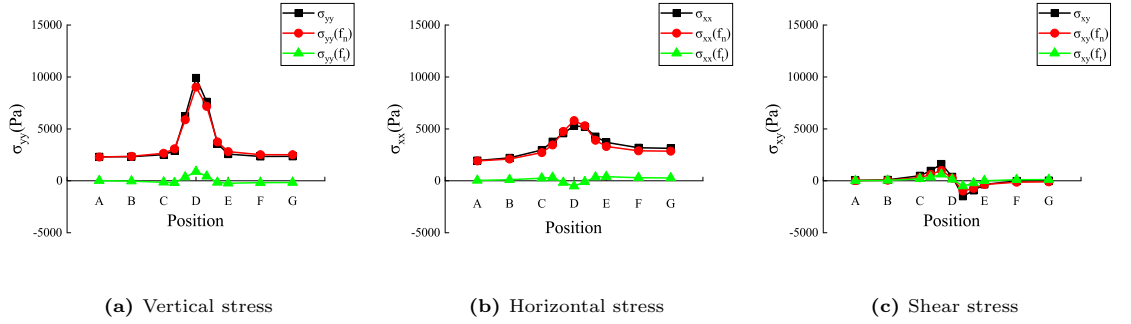


Fig. 6. Contributions of interparticle component forces to macroscopic stresses.

3.3 Micro-mechanical parameters

The probability density distribution of f_n , denoted as $PDD(f_n)$, exhibits a similar behaviour to that of $PDD(f_n/\bar{f}_0)$, both characterised by an exponential decay pattern (see Fig. 7a and Fig. 7b). $\bar{f}_0$ denotes the global average magnitude of normal contact forces. The proportion of interparticle contacts carrying relatively small forces, denoted as P_{sf} , (e.g. $f_n < 10N$, $f_n/\bar{f}_0 < 1$), accounts for the majority of interparticle contacts. At the initial stage of the loading process, the moving load is located far from the central position D of Element A , and a peak is observed simultaneously in $PDD(f_n)$. $P_{sf}(f_n)$ decreases rapidly as the moving load progresses, particularly from Position C to D during principal stress rotation, and reaches its minimum at the central position D . The growth of $\bar{f}_0$ (see Fig. 7a) exerts a dominant influence on the reduction of $P_{sf}(f_n)$ during this stage. During the unloading stage, the principal stress continues to rotate from Position D to F , accompanied by a progressive increase in the magnitude of $P_{sf}(f_n)$. However, the development of horizontal residual stress σ_{xx}^r inhibits its complete restoration to the initial state (see Fig. 4).

On the other hand, $P_{sf}(f_n/\bar{f}_0)$ exhibits a slight increase with the growing number of contacts (see Fig. 7b), corresponding to the movement of the surface load from Position B to C . Subsequently, $P_{sf}(f_n/\bar{f}_0)$ demonstrates accelerated growth as the surface load progresses from Position C , through D , to Position E . At this stage, it can be inferred that interparticle contacts transmitting relatively large forces, specifically those exceeding $\bar{f}_0$, decrease significantly. Toward the end of the load pass from Position E to F , $P_{sf}(f_n/\bar{f}_0)$ diminishes to a comparatively low magnitude. However, due to the accumulation of residual stress σ_{xx}^r , a considerable $P_{sf}(f_n/\bar{f}_0)$ persists relative to the initial state.

In contrast to $PDD(f_n)$ and $PDD(f_n/\bar{f}_0)$, the distribution of interparticle contacts for $PDD(f_t)$ and $PDD(f_t/\bar{f}_0)$ exhibits a predominant concentration at lower interparticle forces (e.g. $f_t < 5N$, $f_t/\bar{f}_0 < 0.5$) (see Fig. 7c and Fig. 7d). The evolution of $P_{sf}(f_t)$ throughout the load pass demonstrates similar characteristics to that of $P_{sf}(f_n)$. A notable reduction is observed prior to the central position D , predominantly attributed to an increase in $\bar{f}_0$, particularly evident in between Position C and D . Throughout the unloading stage, a significant increase of $P_{sf}(f_t)$ is observed with the continued principal stress rotation, primarily attributed to the elimination of contacts sustaining relatively large forces. On the other hand, a significant reduction of $P_{sf}(f_t/\bar{f}_0)$ is observed at the initial loading stage, followed by a minor reduction of $P_{sf}(f_t/\bar{f}_0)$ from Position C to D . Subsequently, an approximate restoration of $P_{sf}(f_t/\bar{f}_0)$ to the state at Position C manifests during the unloading stage, progressing from Position D to E , and ultimately to Position F .

The average normal contact force, denoted as $\bar{f}_0$, initially rises to reach its maximum value at Position D . Following this peak, $\bar{f}_0$ decreases but remains at a comparatively elevated magnitude in relation to the initial state. This phenomenon can be attributed to the existence of the residual stress component, σ_{xx}^r (see Fig. 7a). In contrast, the global average branch vector $\bar{v}_0$ exhibits a reverse pattern compared to $\bar{f}_0$ (see Fig. 7a). The coordination number, γ , is defined as the ratio between the total number of interparticle contacts (N_c) and the total number of particles (N_p). Due to the invariance of the particle count within Element A , the coordination number

294 exhibits an initial increase corresponding to the formation of additional interparti-
 295 cle contacts. Subsequently, it reaches a peak at the central position D , followed by
 296 a decrease during the unloading stage (see Fig. 7b). Relative to the initial state, the
 297 final coordination number exhibits a lower magnitude, attributed to the development
 298 of plastic deformations induced by the load pass. This observation is consistent with
 299 the numerical results reported by Cai et al [3].

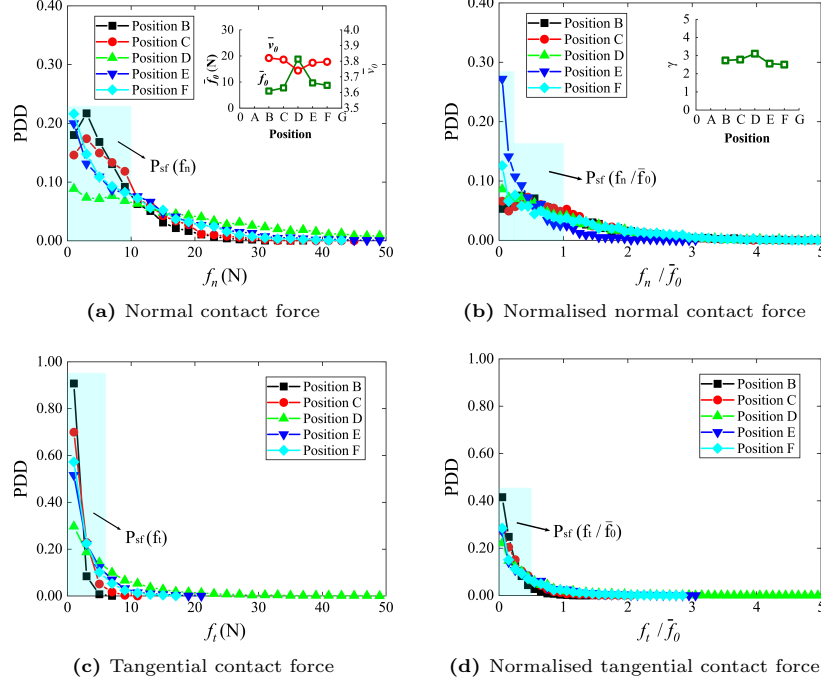


Fig. 7. Probability density distribution of contact forces and the variation of γ , $\bar{f}_0$ and $\bar{v}_0$ with the load pass.

3.4 Fabric anisotropy

Rothenburg and Bathurst [37] established a stress-force-fabric relationship for granular assemblies by employing Fourier series approximations of directional fabric distributions. This approach involved analysing the directional distribution of the fabric, including the contact normal density and average contact forces (normal component $\bar{f}_n$ and tangential component $\bar{f}_t$). By integrating these approximated distributions over all possible directions, they derived a theoretical relationship linking microscopic particle interactions to macroscopic stress states. The stress tensor expression for a granular assembly presented in Eq. (1) can be reformulated as follows [18, 29]:

$$\sigma_{ij} = \frac{N_c}{V} \int_0^{2\pi} E(\theta) \bar{v}_i(\theta) \bar{f}_{r,j}(\theta) d\theta = \frac{N_c}{V} \sum_{N_\theta} E(\theta) \bar{v}_i(\theta) \bar{f}_{r,j}(\theta) \Delta\theta \quad (3)$$

where N_c denotes the total number of interparticle contacts within the granular assembly, while N_θ represents the number of discrete angular intervals. The terms $\bar{v}_i(\theta)$ and $\bar{f}_{r,j}(\theta)$ indicate the average branch vector and average contact force, respectively, acting on contacts whose normal directions lie within the interval $\theta \in [\theta - \Delta\theta/2, \theta + \Delta\theta/2]$, denoted as $[\theta]$. Let $\Delta N_c(\theta)$ denote the number of interparticle contacts with normal directions confined within $[\theta]$. The contact normal density function $E(\theta)$ can be determined through the following expression:

$$E(\theta) = \frac{\Delta N_c(\theta)}{N_c \Delta\theta} \quad (4)$$

The average contact force acting on contacts oriented within $[\theta]$ can be decomposed into two components, the average normal force $\bar{f}_n(\theta)$ and average tangential force $\bar{f}_t(\theta)$, which are expressed as follows:

$$\bar{f}_{r,i}(\theta) = \bar{f}_n(\theta) n_i + \bar{f}_t(\theta) t_i \quad (5)$$

The directional distribution of the contact normal density and interparticle component forces can be approximated by the 2nd-rank Fourier series function as follows [12, 37]:

$$\begin{cases} E(\theta) = \frac{1}{2\pi} [1 + a_c \cos 2(\theta - \theta_c)] \\ \bar{f}_n(\theta) = \bar{f}_0 [1 + a_n \cos 2(\theta - \theta_n)] \\ \bar{f}_t(\theta) = \bar{f}_0 [a_w - a_t \sin 2(\theta - \theta_t)] \end{cases} \quad (6)$$

where the non-dimensional coefficients a_c , a_n , a_t and a_w quantify the anisotropy of contact normal density and corresponding contact forces. Simultaneously, the terms θ_c , θ_n and θ_t represent the major principal direction associated with the respective anisotropies. Equation (6) has been validated for isotropic assemblies under monotonic loading conditions, where the assumption of coaxiality is satisfied, such that

$\theta_c = \theta_n = \theta_t$ [37]. In contrast, the applicability of 2nd-rank Fourier series for approximating the directional fabric distribution has been demonstrated for anisotropic granular assemblies subjected to loading paths involving the principal stress rotation [25]. While maintaining minimal influence on micro-mechanical behaviour, this simplification facilitates subsequent characterisation of fabric anisotropy. However, under such loading conditions, the assumption of coaxiality between principal directions of contact normal density anisotropy and contact force anisotropy is no longer valid. Therefore, the non-coaxiality of the principal directions of anisotropy is explicitly considered in this study.

The initial structure undergoes self-weight consolidation and, as a result, exhibits anisotropic characteristics. In the initial state, the directional distribution of contact normals exhibits a preferential vertical orientation, resulting in non-zero initial values for a_c and θ_c . The anisotropy of the contact normal density, a_c , initially decreases gradually as the moving load approaches the central position D (see Fig. 8a), attributed to the gradual increase of the horizontal stress σ_{xx} induced by the moving load (see Fig. 3). The increase of horizontal stress σ_{xx} diminishes the preferential vertical orientation of contact normals, consequently reducing the magnitude of a_c . However, as the moving load approaches Position D , the vertical stress σ_{yy} becomes dominant in determining a_c , thereby enhancing the preferential vertical orientation. Consequently, the magnitude of a_c exhibits a rapid increase. Subsequently, during the unloading path, the influence of σ_{yy} on a_c diminishes more rapidly than that of σ_{xx} , resulting in a progressive decrease in a_c . Furthermore, the horizontal residual stress σ_{xx}^r exerts an influence on a_c . Therefore, the magnitude of a_c during the unloading stage is reduced compared to that observed during the loading path. Finally, as the moving load departs from Position D , specifically progressing from Position F to G , its influence gradually diminishes. Nevertheless, σ_{xx}^r continues to influence a_c , maintaining its magnitude at a relatively low level.

During the load movement from Position A to B , while σ_{yy} remains approximately constant, σ_{xx} increases until approaching the magnitude of σ_{yy} . Simultaneously, the shear stress σ_{xy} remains zero (see Fig. 3). In response to the nearly isotropic macroscopic stress field present in Element A , the magnitude of a_n is observed to decrease, reaching a significantly low value (Fig. 8b). As the surface load progressively traverses toward the central position D , a monotonic increase in the magnitude of a_n is observed (Fig. 8b). This phenomenon arises from the enhanced anisotropy in macroscopic stress fields, driven by the widening differential between σ_{xx} and σ_{yy} components, coupled with an increasing magnitude of the shear stress component σ_{xy} . At the central position D , where the maximum differential is observed, a_n exhibits a decreasing trend, which can be attributed to the observed reduction in the shear stress component σ_{xy} (see Fig. 3). Subsequently, a nearly constant reduction of a_n is observed until Position F throughout the unloading phase. Toward the end of the unloading stage from Position E to G , a_n , in contrast to a_c , exhibits a greater magnitude compared to that observed during the initial loading stage, which can be attributed to the development of residual stress σ_{xx}^r .

As a result of self-weight consolidation, the macroscopic shear stresses σ_{xy} and σ_{yx} are nearly negligible in the initial state, thereby rendering the magnitudes of a_t and a_w

insignificant (see Fig. 8c). Following the application of surface loading on the structure, a_t gradually increases, reaching its peak between Position C and D , where σ_{xy} grows rapidly, subsequently followed by a sharp decrease (see Fig. 3). At the central position D , a valley value of a_t is observed, corresponding to the reduction in shear stress (see Fig. 3). Departing from the valley value, a_t decreases rapidly with the reduction of shear stresses. The other parameter characterising the anisotropy of tangential contact forces, a_w , consistently remains small. However, its sign transitions to negative, and its magnitude exhibits a slight increase during the load pass. The influence of a_w on macroscopic stresses will be analysed in detail in the subsequent section.

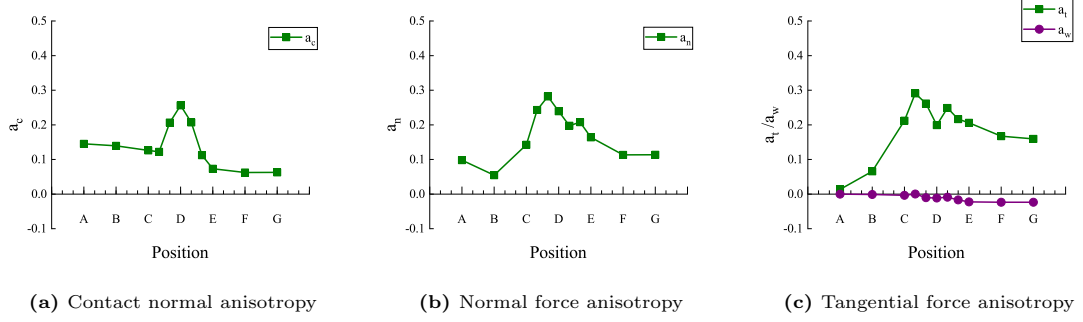


Fig. 8. Variation of the anisotropy of contact normals and contact forces with the load pass.

As the surface load approaches the central position D , an initial increase in θ_c is observed, attributed to the growth of σ_{xx} (see Fig. 9). In this study, the vertical direction is defined as 90 degrees. Therefore, the increase in θ_c indicates that the principal direction of the anisotropy of contact normal densities transitions from near-vertical to horizontal in a counterclockwise direction. As the moving load progresses from Position C to D , the rapid increase in σ_{yy} (see Fig. 3) results in a decrease in θ_c near Position D , indicating a reorientation of the principal direction of anisotropy toward the vertical direction. As the moving load traverses from Position D to E , the influence of σ_{yy} diminishes significantly, resulting in a clockwise deviation of θ_c from the vertical direction, gradually reverting toward the horizontal direction. Subsequently, during the movement of the surface load from Position E to F , the reduction in σ_{xx} leads to an increase in θ_c , causing the principal direction to shift back toward the vertical direction. Finally, during the concluding stage of the load pass from Position F to G , given the negligible magnitude of σ_{xx} and σ_{yy} , the dominant σ_{xx}^r prevents θ_c from returning to its initial state. As demonstrated in Fig. 10a depicting the directional distribution of the contact normal density, a distinct variation in θ_c is observed between Positions C and E .

The initial principal orientation of normal contact force anisotropy, θ_n , predominantly aligns with the vertical direction attributed to the self-weight consolidation. During the movement of the surface load from distal positions to the central position D , θ_n exhibits a progressive increase from approximately 90 degrees (see Fig.

9), demonstrating a systematic rotation of the principal stress direction from near-vertical to horizontal alignment. As the surface load approaches Position D , θ_n rapidly decreases toward 90 degrees. This behaviour can be attributed to the significant increase in σ_{yy} , which causes the principal direction to shift back toward the vertical orientation. The shift in the principal direction of the anisotropy is reflected in the directional distribution of contact forces, as shown in Fig. 10b. During the subsequent unloading stage, σ_{xx} primarily influences the evolution of θ_n , resulting in the principal direction of anisotropy gradually rotating clockwise toward the horizontal orientation (see Fig. 9 and Fig. 10b). Following the unloading stage, θ_n stabilises at a constant value close to zero, indicating a near-horizontal orientation for θ_n , which is attributed to the accumulation of σ_{xx}^r .

At the onset of the load pass, the principal direction of the anisotropy of tangential contact forces, θ_t , is observed to be approximately 140 degrees (see Fig. 9). As the surface load progresses toward Position B , θ_t exhibits an initial increase, with only negligible variations in shear stresses (see Fig. 3), indicating a counter-clockwise rotation of the principal direction of the anisotropy. Subsequently, a decrease in θ_t is observed with the development of shear stresses, accompanied by a clockwise rotation of the principal direction of the anisotropy, as evidenced by the directional distribution of tangential contact forces (see Fig. 10c). Finally, toward the end of the load pass from Position E to G , θ_t approaches zero, and the principal direction of the anisotropy aligns with the near-horizontal direction.

As previously discussed, the asymmetric evolution of fabric anisotropy and its principal direction during the load pass is mechanistically linked to corresponding asymmetries in macroscopic horizontal stress, primarily induced by the residual stress component σ_{xx}^r . The principal directions of anisotropy for the contact normal density and contact forces are generally non-coaxial. Overall, at the macroscopic scale, the divergence of fabric anisotropy principal directions is primarily induced by principal stress rotation in the present study, as demonstrated in Li and Yu [26]. From a micro-mechanical standpoint, particle rotation induced by loading path variations constitutes the primary mechanism underlying this divergence. When the surface load is sufficiently distant from the central Position D (i.e., when moving from Position A to B), its effect on particle rotation becomes negligible, leading to $\theta_c \approx \theta_n$. With the surface load approaching Position D , the induced substantial particle rotations cause a significant divergence increase between θ_c and θ_n . However, as the moving load is in close proximity to the central position D , the principal directions of fabric anisotropy become approximately coaxial, exhibiting minimal disparity (see Fig. 9). Specifically, at the central position D , the coaxial principal direction is oriented approximately 90 degrees, aligning with the vertical orientation. Coaxiality is exclusively observed at Position D , where the loading direction of Element A coincides with the initial vertical consolidation direction. With minimal shear stress observed at Position D (see Fig. 3), rolling friction demonstrates insignificant effect on fabric anisotropy evolution, maintaining undisturbed coaxiality of fabric anisotropy principal directions. After passing Position D and receding, the surface load induces significant $\theta_c - \theta_n$ divergence through σ_{xx}^r influence.

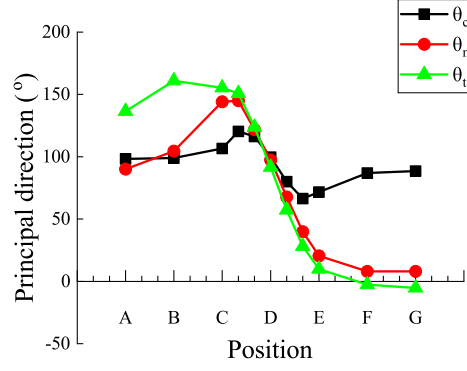


Fig. 9. Variation of the principal direction of the anisotropy with the load pass.

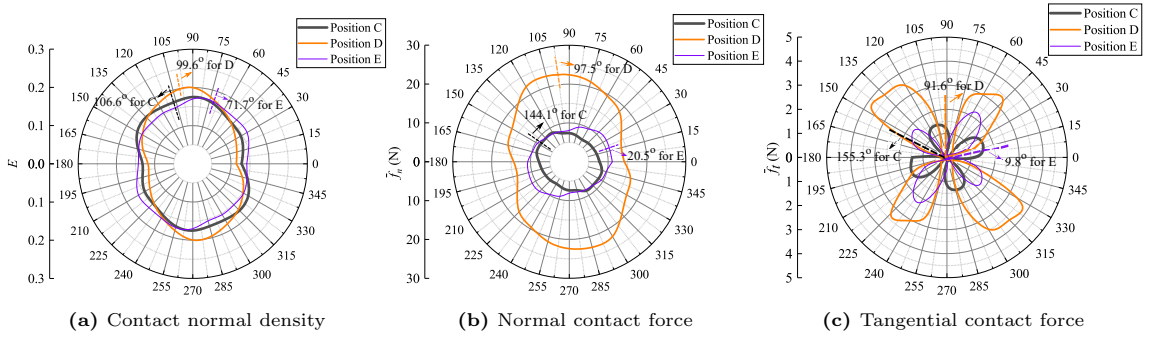


Fig. 10. Directional distribution of the contact normal density, normal and tangential contact forces.

3.5 Branch vector anisotropy

Compared to Eq. (3), a more general stress-force-fabric relationship was proposed as follows [27, 33]:

$$\sigma_{ij} = \frac{N_c}{V} \int_0^{2\pi} E(\theta) \overline{v_i f_{r,j}}(\theta) d\theta = \frac{N_c}{V} \sum_{N_\theta} E(\theta) \overline{v_i f_{r,j}}(\theta) \Delta\theta \quad (7)$$

while a simplified relationship is commonly utilised in macroscopic stress calculations as follows [11, 38]:

$$\sigma_{ij} = \frac{N_c \bar{v}_0}{V} \int_0^{2\pi} E(\theta) f_r(\theta) n_i n_j d\theta = \frac{N_c \bar{v}_0}{V} \sum_{N_\theta} E(\theta) f_r(\theta) n_i n_j \Delta\theta \quad (8)$$

451 where $\bar{v}_0$ denotes the global average branch vector. As mentioned by Li and Yu [25, 29],
 452 and Khakpour and Mirghasemi [18], even for an anisotropic specimen involving the
 453 principal stress rotation, the assumption $\overline{v_i f_{r,j}} = \bar{v}_i \bar{f}_{r,j}$ is both feasible and broadly
 454 applicable in micro-mechanical studies. The assumption in Eq. (8) implies that the
 455 directions of the contact normal and the branch vector are coaxial, which is considered
 456 reasonable for circular particles. However, in this study, the irregular particle mor-
 457 phology leads to a significant deviation from coaxiality between the contact normal
 458 direction and branch vector orientation, as illustrated in Fig. 2. With reference to Hos-
 459 seininia [11], the average branch vector acting on contacts in the normal direction $[\theta]$,
 460 denoted as $\bar{v}_i(\theta)$, can be decomposed into two component average branch vectors, the
 461 normal component $\bar{v}_n(\theta)$ and the tangential component $\bar{v}_t(\theta)$. As a consequence,

$$\bar{v}_i(\theta) = \bar{v}_n(\theta)n_i + \bar{v}_t(\theta)t_i \quad (9)$$

462 Following the mathematical framework established for characterising the direc-
 463 tional distributions of average contact normals and contact forces in Eq. (6), the
 464 average branch vector components in both normal and tangential directions are sim-
 465 ilarly represented using the 2nd-rank Fourier series functions, as demonstrated in
 466 previous studies [11, 12]:

$$\begin{cases} \bar{v}_n(\theta) = \bar{v}_0 [1 + a_{ln} \cos 2(\theta - \theta_{ln})] \\ \bar{v}_t(\theta) = \bar{v}_0 [a_{lw} - a_{lt} \sin 2(\theta - \theta_{lt})] \end{cases} \quad (10)$$

467 where $\bar{v}_0$ retains the same meaning as defined in Eq. (8). The terms a_{ln} , a_{lt} , and a_{lw}
 468 represent the anisotropy of the average normal and tangential branch vectors, while θ_{ln}
 469 and θ_{lt} denote the principal directions associated with the corresponding anisotropy.

470 As the surface load progresses to Position *C*, a_{ln} and a_{lt} begin to increase slightly,
 471 eventually stabilising after reaching Position *E* (see Fig. 11a). In general, the magni-
 472 tudes of a_{ln} and a_{lt} remain very small, with a_{ln} particularly negligible, having a value
 473 of less than 0.05. This is supported by the nearly isotropic directional distribution of
 474 the average normal branch vector (see Fig. 12a). a_{lw} remains close to zero through-
 475 out the load pass, with its sign reversing after the central position *D*. The principal
 476 directions of the anisotropy of branch vectors, θ_{ln} and θ_{lt} , exhibit values approaching
 477 zero, indicating an almost horizontal orientation. Furthermore, their variations with
 478 respect to the load pass demonstrate negligible significance (Fig. 11b), as evidenced
 479 by the directional distribution patterns of the average normal and tangential branch
 480 vectors (Fig. 12).

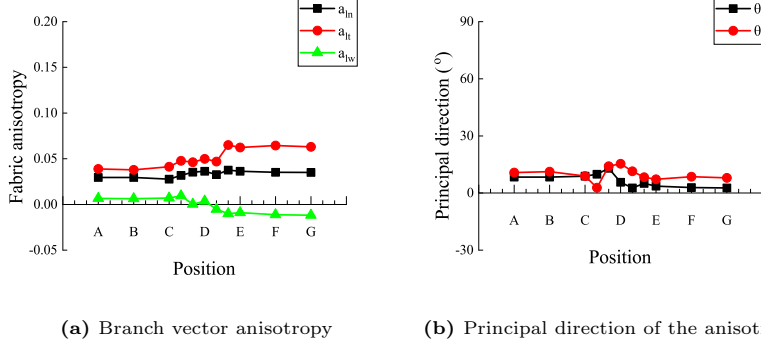


Fig. 11. Variation of the branch vector anisotropy and the principal direction of the anisotropy with the load pass.

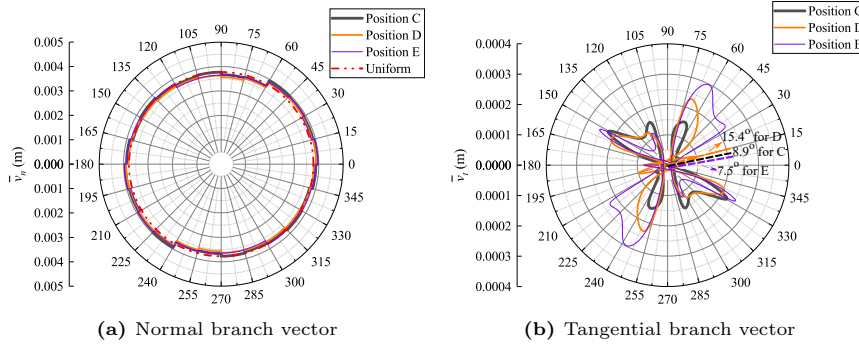


Fig. 12. Directional distribution of normal and tangential branch vectors.

3.6 Stress-force-fabric (SFF) relationship

This study examines an anisotropic structure composed of irregular particles, which is generated through an initial isotropic consolidation followed by self-weight consolidation (see Section 2.1). This numerical structure is subjected to the principal stress rotation induced by the moving surface load. The principal directions of anisotropy for both contact normal densities and contact forces exhibit a distinct non-coaxial alignment, as illustrated in Fig. 9. Consequently, the influence of non-coaxiality cannot be disregarded in the calculation of macroscopic stresses. Furthermore, the influences of the term a_w and the average branch vector $\bar{v}_i(\theta)$ on the stress calculation will be addressed in the following study.

The macroscopic stress σ_{ij} can be simply calculated by substituting Eq. (5) into Eq. (3) as follows:

$$\sigma_{ij} = \frac{N_c \bar{v}_0}{V} \int_0^{2\pi} [\bar{f}_n(\theta) n_i n_j + \bar{f}_t(\theta) t_i n_j] E(\theta) d\theta \quad (11)$$

where $\bar{f}_n(\theta)$ and $\bar{f}_t(\theta)$ are determined using Eq. (6). Initially, macroscopic stresses calculated using Eq. (1) and Eq. (11) are compared to validate the SFF relationship. In general, σ_{ij} calculated through the SFF relationship, denoted as $\sigma_{ij}(sff)$, demonstrates marginally higher values compared to those obtained from Eq. (1), denoted as $\sigma_{ij}(forCont)$. However, a consistent evolution trend is observed throughout the load pass in both cases, as illustrated in Fig. 13. The characteristics of $\sigma_{ij}(sff)$ accord well with those of $\sigma_{ij}(forCont)$. The root mean square errors (RMSEs) for σ_{yy} , σ_{xx} , and σ_{xy} are calculated as 1090, 783, and 246 Pa, respectively, with corresponding coefficients of determination (R^2) of 0.812, 0.809, and 0.907, respectively. Furthermore, a comparison of σ_{ij} with and without the consideration of the term a_w , denoted as $\sigma_{ij}(sff)$ and $\sigma_{ij}(sff/a_w)$, respectively, is conducted based on Eq. (11) (see Fig. 14). The results reveal no significant variation, demonstrating that the influence of a_w on σ_{ij} is negligible under the investigated conditions.

The expression for σ_{ij} , accounting for the influence of $\bar{v}_i(\theta)$, denoted as $\sigma_{ij}(\bar{v}_i(\theta))$, can be derived by substituting Eq. (5) and Eq. (9) into Eq. (3), as follows:

$$\sigma_{ij} = \frac{N_c}{V} \int_0^{2\pi} [\bar{v}_n(\theta)\bar{f}_n(\theta)n_in_j + \bar{v}_t(\theta)\bar{f}_n(\theta)t_in_j + \bar{v}_n(\theta)\bar{f}_t(\theta)n_it_j + \bar{v}_t(\theta)\bar{f}_t(\theta)t_it_j] E(\theta)d\theta \quad (12)$$

where $\bar{v}_n(\theta)$ and $\bar{v}_t(\theta)$ can be determined through Eq. (10). The influence of $\bar{v}_i(\theta)$ on σ_{ij} has been studied, as illustrated in Fig. 14, which reveals only negligible deviation between $\sigma_{ij}(\bar{v}_i(\theta))$ and $\sigma_{ij}(sff)$. This conclusion is in agreement with the results obtained for ellipsoid-packed assemblies, as reported by Ouadfel and Rothenburg [33]. Furthermore, as discussed in Section 3.5, the anisotropy terms associated with branch vectors, a_{ln} , a_{lt} , θ_{ln} and θ_{lt} , exhibit negligible magnitudes, while the normal branch vector demonstrates an approximately isotropic directional distribution. Consequently, the consideration of $\bar{v}_i(\theta)$ as a non-dimensionless term, $\bar{v}_0$, as stated in Eq. (8) and Eq. (11), is feasible under the present conditions.

The contributions of the normal and tangential contact forces to $\sigma_{ij}(sff)$ have been analysed, as illustrated in Fig. 15. These contributions are generally consistent with the discussions presented in Section 3.2 (see Fig. 6). f_n contributes positively to $\sigma_{yy}(sff)$, denoted as $\sigma_{yy}(sff-f_n)$, exhibiting a synchronized variation pattern with $\sigma_{yy}(sff)$ throughout the load pass. The contribution of f_t , denoted as $\sigma_{yy}(sff-f_t)$, appears insignificant, except for a relatively apparent influence near the central position D . Compared to $\sigma_{yy}(sff-f_t)$, the contribution of f_t to $\sigma_{xx}(sff)$, denoted as $\sigma_{xx}(sff-f_t)$, exhibits an inverse relationship, with a negative contribution observed near Position D . In contrast, the contribution of f_t to $\sigma_{xy}(sff)$ is non-negligible and exhibits a trend analogous to that observed for $\sigma_{xy}(sff)$. In conclusion, f_n contributes more significantly to $\sigma_{ij}(sff)$ in comparison with f_t .

The SFF relationship facilitates stress state characterisation in granular materials via particle-scale investigations. Furthermore, the SFF relationship demonstrates direct correlation with fabric anisotropy, enabling the construction of multiscale constitutive relations from macroscopic to microscopic levels. Moreover, fabric anisotropy exhibits direct correlation with shear strength of granular materials [26, 37], while

533 being significantly influenced by particle morphology and other particle physical char-
 534 acteristics [10, 12]. Consequently, the SFF relationship provides a critical framework
 535 for investigating the connection between shear strength and particle-scale physical
 536 properties in future studies.

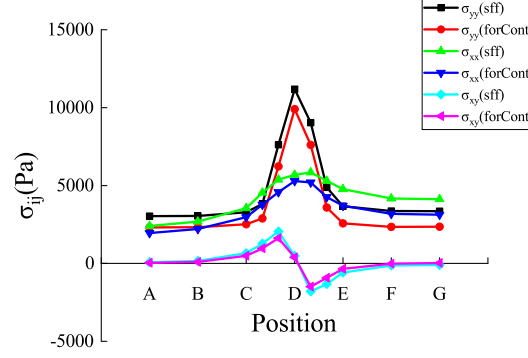


Fig. 13. Comparison between macroscopic stresses calculated using the SFF relationship and Eq. (1).

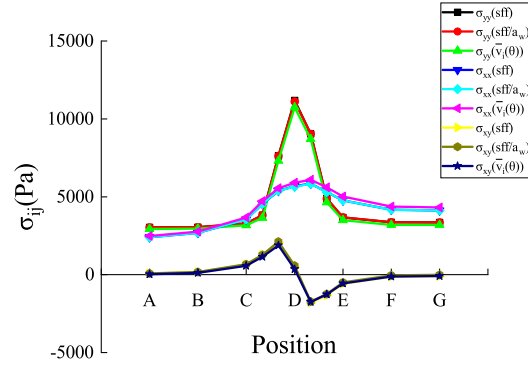


Fig. 14. Comparison between macroscopic stresses calculated by the SFF relationship, in terms of considering a_w and $\bar{v}_i(\theta)$ or not

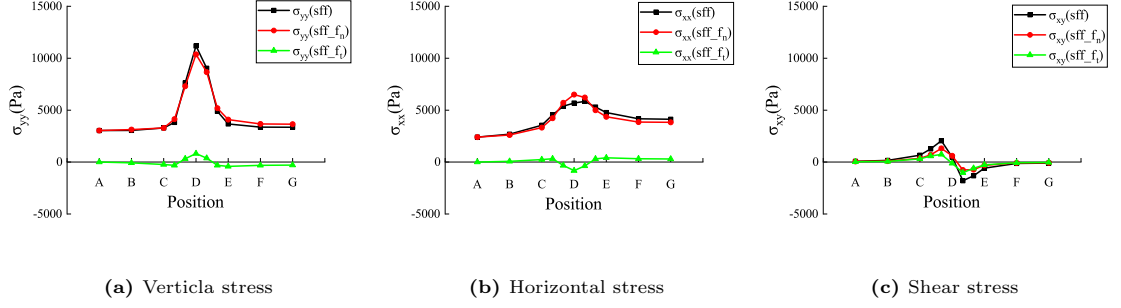


Fig. 15. Contributions of interparticle component forces to macroscopic stresses calculated using SFF relationships.

4 Concluding remarks

The principal stress rotation in a structure composed of irregular particles subjected to moving surface loads was investigated through DEM numerical simulations. Subsequent analysis of the residual stress σ_{xx}^r induced by the external loads provided insights into both macro- and micro-mechanical behaviours. During the unloading stage, the horizontal macroscopic stress σ_{xx} demonstrates a significant increase compared to the loading stage, in contrast to the behaviour observed in vertical and shear stresses. This phenomenon is primarily attributed to the accumulation of residual stress σ_{xx}^r . After a single load pass, the residual stress σ_{xx}^r induces contrasting effects, as it increases the global average normal contact force $\bar{f}_0$ while simultaneously decreasing the average branch vector $\bar{v}_0$. The majority of interparticle contacts are characterised by relatively small forces, and exhibits significant variation in response to changes in macroscopic stresses.

The anisotropy coefficients characterising contact normal densities and contact force components, denoted as a_c , a_n , a_t , and a_w , were systematically investigated. Under variations in macroscopic stresses, the terms a_c , a_n , and a_t exhibit an increasing trend, attaining their maximum values near the central position D , followed by a gradual decrease. Notably, σ_{xx}^r exhibits a reverse influence on a_c and a_n toward the end of the load pass. The variation in a_w is observed to be insignificant, as confirmed by the calculated macroscopic stresses using the SFF relationship. On the other hand, the principal directions of the fabric anisotropy, θ_c , θ_n , and θ_t , maintain a non-coaxial orientation throughout the load pass. However, near the central position D , approximate coaxiality is observed, occurring at an angle close to 90 degrees.

Non-coaxiality generally exists between branch vectors and contact normals, attributed to the irregularity of particles within the numerical structures. Nevertheless, the anisotropy coefficients for branch vectors remain relatively small, exhibiting minimal variation throughout the load pass. Simultaneously, small variations are observed in the principal directions of the anisotropy, as reflected in the directional distribution of branch vectors and further validated by the macroscopic stresses calculated using the SFF relationship. On the other hand, the stress estimated using the SFF relationship

slightly exceeds the actual macroscopic stress. The normal contact force predominantly contributes to the macroscopic stresses, exerting a particularly significant influence on the vertical and horizontal stress components.

In summary, unlike previous studies, the development of residual stresses within the structure was explicitly considered, resulting in the observed asymmetric distribution of σ_{xx} throughout the load pass. Furthermore, the micro-mechanisms associated with principal stress rotation induced by moving surface loads were quantitatively analysed in this study. The results indicate that the development of macroscopic stresses is consistent with the evolution of fabric anisotropy. Finally, based on the SFF relationship, it is demonstrated that branch vectors have a negligible influence on macroscopic stresses, while the normal contact force constitutes the primary contributor to macroscopic stress development. These findings provide valuable insights for researchers to better understand the micro-scale behaviour of granular materials and for engineers to optimize designs in practical engineering applications.

It is important to acknowledge the limitations of this study and propose constructive improvements for future investigations. While two-dimensional DEM simulations have yielded valuable insights into principal stress rotation phenomena [24, 40], this 2D simplification fundamentally limits full three-dimensional stress field characterisation, thereby omitting the intermediate principal stress which has been demonstrated to potentially influence shear strength behaviour of granular materials [57]. Furthermore, neglecting lateral displacement components may lead to underestimated predictions of permanent deformation in future studies.

Supplementary information. Not applicable

Acknowledgments. This work was supported by the Henan Province International Science and Technology Cooperation Cultivation Project (252102520021), the National Natural Science Foundation of China (52478250), and the Fundamental Research Funds for the Universities of Henan Province (NSFRF240303). These financial supports are gratefully acknowledged.

Author contributions. W. (Wei Cai): Methodology, Validation, Formal Analysis, Original Draft. D. (Dariusz Wanatowski): Methodology, Validation, Reviewing and Editing. P. (Ping Xu): Validation, Software. H.-S. (Hai-Sui Yu): Reviewing and Editing. Z. (Zhengyang Zhang): Reviewing and Editing.

Data availability. The data that support the findings of this study are available from the corresponding author upon reasonable request.

Declarations

Conflict of interest. The authors declare no competing interests.

References

- [1] AASHTO (1993) AASHTO Guide for Design of Pavement Structures. American Association of State Highway and Transportation Officials, Wash., D.C.

- 606 [2] Alshibli KA, Hasan A (2008) Spatial variation of void ratio and shear band thick-
607 ness in sand using x-ray computed tomography. *Géotechnique* 58(4):249–257.
608 <https://doi.org/10.1680/geot.2008.58.4.249>
- 609 [3] Cai W, Xu P, Zhang RH (2024) Micro-mechanical analysis for residual stresses
610 and shakedown of cohesionless-frictional particulate materials under moving sur-
611 face loads. *Numer Analyt Meth Geomech* 48(17):4136–4153. [https://doi.org/10.
612 1002/nag.3837](https://doi.org/10.1002/nag.3837)
- 613 [4] Cai W, Xu P, Zhang RH (2024) Micro-mechanical analysis of residual stresses in
614 cohesive-frictional particulate materials under moving surface loads. *Comp Part*
615 *Mech* 11(6):2601–2618. <https://doi.org/10.1007/s40571-024-00740-z>
- 616 [5] Chai JC, Miura. N (2002) Traffic-load-induced permanent deformation of road
617 on soft subsoil. *J Geotech Geoenviron Eng* 128(11):907–916. [https://doi.org/10.
618 1061/\(ASCE\)1090-0241\(2002\)128:11\(907\)](https://doi.org/10.1061/(ASCE)1090-0241(2002)128:11(907))
- 619 [6] Chen G, Ma W, Qin Y, et al (2021) Liquefaction susceptibility of saturated coral
620 sand subjected to various patterns of principal stress rotation. *J Geotech Geoen-*
621 *viron* 147(9):04021093. [https://doi.org/10.1061/\(ASCE\)GT.1943-5606.0002590](https://doi.org/10.1061/(ASCE)GT.1943-5606.0002590)
- 622 [7] Cui X, Li X, Hao J, et al (2022) Dynamic response of unsaturated poroelastic
623 ground underlying uneven pavement subjected to vehicle load. *Soil Dyn Earthq*
624 *Eng* 156:107164. <https://doi.org/10.1016/j.soildyn.2022.107164>
- 625 [8] Cui X, Li X, Du Y, et al (2024) Macro-micro numerical analysis of granular mate-
626 rials considering principal stress rotation based on DEM simulation of dynamic
627 hollow cylinder test. *Constr Build Mater* 412:134818. [https://doi.org/10.1016/j.
628 conbuildmat.2023.134818](https://doi.org/10.1016/j.conbuildmat.2023.134818)
- 629 [9] Cundall PA, Strack ODL (1979) A discrete numerical model for granular assem-
630 blies. *Géotechnique* 30(3):331–336. <https://doi.org/10.1680/geot.1980.30.3.331>
- 631 [10] Hosseininia ES (2012) Discrete element modeling of inherently anisotropic granu-
632 lar assemblies with polygonal particles. *Particuology* 10(5):542–552. [https://doi.
633 org/10.1016/j.partic.2011.11.015](https://doi.org/10.1016/j.partic.2011.11.015)
- 634 [11] Hosseininia ES (2013) Stress-force-fabric relationship for planar granular materi-
635 als. *Géotechnique* 63(10):830–841. <https://doi.org/10.1680/geot.12.P.055>
- 636 [12] Hosseininia ES (2015) A micromechanical study on the stress rotation in granular
637 materials due to fabric evolution. *Powder Technol* 283:462–474. [https://doi.org/
638 10.1016/j.powtec.2015.06.013](https://doi.org/10.1016/j.powtec.2015.06.013)
- 639 [13] Huan X, Lin G, Yuan-Qiang C (2016) Deformation behaviors of sandy subgrade
640 soil under traffic load-induced stress path. *Chin J Geotech Eng* 38(4):662–669

- [14] Huang X, Hanley KJ, O'Sullivan C, et al (2014) Exploring the influence of inter-particle friction on critical state behaviour using DEM. *Numer AnalYT Meth Geomech* 38(12):1276–1297. <https://doi.org/10.1002/nag.2259>
- [15] Huang YL, Li JM, Teng YC, et al (2017) Numerical simulation study on macroscopic mechanical behaviors and micro-motion characteristics of gangues under triaxial compression. *Powder Technol* 320:668–684. <https://doi.org/10.1016/j.powtec.2017.08.002>
- [16] Itasca (2019) Particle Flow Code in Two Dimensions (Version 6.0). Itasca Consult. Gr., Inc., Minn.
- [17] Juspi S (2007) Experimental validation of the shakedown concept for pavement analysis and design. PhD thesis, University of Nottingham, the United Kingdom
- [18] Khakpour M, Mirghasemi AA (2023) Macro-micro mechanical study of principal stress rotation in granular materials using DEM simulations of hollow cylinder test. *Powder Technol* 425:118580. <https://doi.org/10.1016/j.powtec.2023.118580>
- [19] Lashkari A, Khodadadi M, Binesh SM, et al (2019) Instability of particulate assemblies under constant shear drained stress path: DEM approach. *Int J Geomech* 19(6):04019049. [https://doi.org/10.1061/\(ASCE\)GM.1943-5622.0001407](https://doi.org/10.1061/(ASCE)GM.1943-5622.0001407)
- [20] Lekarp F, Isacsson U, Dawson A (2000) State of the art. i: Resilient response of unbound aggregates. *J Transp Eng* 126(1):66–75. [https://doi.org/10.1061/\(ASCE\)0733-947X\(2000\)126:1\(66\)](https://doi.org/10.1061/(ASCE)0733-947X(2000)126:1(66))
- [21] Li B, Huang MS (2016) Discrete element simulation for torsional shear test by hollow cylinder apparatus. *Rock Soil Mech* 37(4):1161–1170. <https://doi.org/10.16285/j.rsm.2016.04.031>
- [22] Li T, Jiang M, Li L (2021) DEM analysis of mechanical behavior of unsaturated silt under strain-controlled constant stress ratio compression tests. *Int J Geomech* 21(10):04021197. [https://doi.org/10.1061/\(ASCE\)GM.1943-5622.0002177](https://doi.org/10.1061/(ASCE)GM.1943-5622.0002177)
- [23] Li X, Yu HS (2009) Influence of loading direction on the behavior of anisotropic granular materials. *Int J Eng Sci* 47(11-12):1284–1296. <https://doi.org/10.1016/j.ijengsci.2009.03.001>
- [24] Li X, Yu HS (2010) Numerical investigation of granular material behaviour under rotational shear. *Géotechnique* 60(5):381–394. <https://doi.org/10.1680/geot.2010.60.5.381>
- [25] Li X, Yu HS (2011) Applicability of stress-force-fabric relationship for non-proportional loading. *Comput Struct* 89:1094–1102. <https://doi.org/10.1016/j.compstruc.2010.12.004>

- 677 [26] Li X, Yu HS (2011) Applicability of stress-force-fabric relationship for non-
678 proportional loading. *Comput Struct* 89:1094–1102. [https://doi.org/10.1016/j.
679 compstruc.2010.12.004](https://doi.org/10.1016/j.compstruc.2010.12.004)
- 680 [27] Li X, Yu HS (2011) Tensorial characterisation of directional data in micromechan-
681 ics. *Int J Solids Struct* 48(14-15):2167–2176. [https://doi.org/10.1016/j.ijsolstr.
682 2011.03.019](https://doi.org/10.1016/j.ijsolstr.2011.03.019)
- 683 [28] Li X, Yu HS (2013) On the stress-force-fabric relationship for granular materi-
684 als. *Int J Solids Struct* 50(9):1285–1302. [https://doi.org/10.1016/j.ijsolstr.2012.
685 12.023](https://doi.org/10.1016/j.ijsolstr.2012.12.023)
- 686 [29] Li X, Yu HS (2015) Particle-scale insight into deformation noncoaxiality of gran-
687 ular materials. *Int J Geomech* 15(4):04014061. [https://doi.org/10.1061/\(ASCE\)
688 GM.1943-5622.0000338](https://doi.org/10.1061/(ASCE)GM.1943-5622.0000338)
- 689 [30] Li X, Yang D, Yu HS (2016) Macro deformation and micro structure of 3d granular
690 assemblies subjected to rotation of principal stress axes. *Granul Matter* 18(3):53.
691 <https://doi.org/10.1007/s10035-016-0632-2>
- 692 [31] Li X, Yang Y, Wang J, et al (2022) Deformation of pavement subgrade sub-
693 jected to traffic loads considering multi-direction principal stress rotation. *Soil
694 Dyn Earthq Eng* 162:107480. <https://doi.org/10.1016/j.soildyn.2022.107480>
- 695 [32] Oda M, Kazama H (1998) Microstructure of shear bands and its relation to
696 the mechanism of dilatancy and failure of dense granular soils. *Géotechnique*
697 48(4):465–481. <https://doi.org/10.1680/geot.1998.48.4.465>
- 698 [33] Ouadfel H, Rothenburg L (2001) ‘stress-force-fabric’ relationship for assemblies
699 of ellipsoids. *Mech Mater* 33(4):201–221. [https://doi.org/10.1016/S0167-6636\(00\)
700 00057-0](https://doi.org/10.1016/S0167-6636(00)00057-0)
- 701 [34] Peng Y, Chen YB, Xu YR, et al (2023) Discrete element modelling of mechanical
702 response of crumb rubber-modified asphalt pavements under traffic loads. *Int J
703 Pavement Eng* 24(2). <https://doi.org/10.1080/10298436.2022.2068546>
- 704 [35] Qian J, Du Z, Lu X, et al (2019) Effects of principal stress rotation on stress-
705 strain behaviors of saturated clay under traffic-load-induced stress path. *Soils
706 Found* 59(1):41–55. <https://doi.org/10.1016/j.sandf.2018.08.014>
- 707 [36] Radovsky BS, Murashina NV (1996) Shakedown of subgrade soil under repeated
708 loading. *Transport Res Rec* 1547:82–88. <https://doi.org/10.3141/1547-12>
- 709 [37] Rothenburg L, Bathurst RJ (1989) Analytical study of induced anisotropy in ide-
710 alized granular materials. *Géotechnique* 39(4):601–614. [https://doi.org/10.1680/
711 geot.1989.39.4.601](https://doi.org/10.1680/geot.1989.39.4.601)

- [38] Rothenburg L, Bathurst RJ (1992) Micromechanical features of granular assemblies with planar elliptical particles. *Géotechnique* 42(1):79–95. <https://doi.org/10.1680/geot.1992.42.1.79>
- [39] Rothenburg L, Bathurst RJ (1996) Micromechanical definition of the strain tensor for granular materials. *J Appl Mech* 63(3):706–711. <https://doi.org/10.1115/1.2823353>
- [40] Si C, Zhou X, You Z, et al (2019) Micro-mechanical analysis of high modulus asphalt concrete pavement. *Constr Build Mater* 220:128–141. <https://doi.org/10.1016/j.conbuildmat.2019.06.019>
- [41] Vairaktaris E, Theocharis AI, Dafalias YF (2020) Correlation of fabric tensors for granular materials using 2D DEM. *Acta Geotech* 15(3):681–694. <https://doi.org/10.1007/s11440-018-0755-1>
- [42] Vallejo LE, Lobo-Guerrero S, Hammer K (2006) Degradation of a granular base under a flexible pavement: DEM simulation. *Int J Geomech* 6(6):435–439. [https://doi.org/10.1061/\(ASCE\)1532-3641\(2006\)6:6\(435\)](https://doi.org/10.1061/(ASCE)1532-3641(2006)6:6(435))
- [43] Voivret C, Radja F, Delenne JY, et al (2009) Multiscale force networks in highly polydisperse granular media. *Phys Rev Lett* 102(17):178001. <https://doi.org/10.1103/PhysRevLett.102.178001>
- [44] Wang J (2011) Shakedown analysis and design of flexible road pavements under moving surface loads. PhD thesis, University of Nottingham, the United Kingdom
- [45] Wang J, Yu HS (2013) Residual stresses and shakedown in cohesive-frictional half-space under moving surface loads. *Geomech and Geoengin* 8(1):1–14. <https://doi.org/10.1080/17486025.2012.759281>
- [46] Wang J, Yu HS (2021) Shakedown analysis and its application in pavement and railway engineering. *Comput Geotech* 138:104281. <https://doi.org/10.1016/j.compgeo.2021.104281>
- [47] Wang J, Zhou Z, Hu X, et al (2019) Effects of principal stress rotation and cyclic confining pressure on behavior of soft clay with different frequencies. *Soil Dyn Earthq Eng* 118:75–85. <https://doi.org/10.1016/j.soildyn.2018.12.013>
- [48] Wang J, Yang Y, Yu HS, et al (2023) Influence of consolidation shear stress magnitude and orientation on stress-strain behavior of sand under traffic loading. *Int J Geomech* 23(2):04022285. <https://doi.org/10.1061/IJGNAL.GMENG-7418>
- [49] Wang Y, Fu H, Cai Y, et al (2022) Seismic subsidence of soft subgrade with considering principal stress rotation. *Int J Civ Eng* 20(7):827–837. <https://doi.org/10.1007/s40999-022-00709-0>

- [50] Wang Y, Xiao H, Ling X, et al (2023) 2D ballast particle contour generation based on the random midpoint displacement algorithm. *Comput Part Mech* 10(4):729–745. <https://doi.org/10.1007/s40571-022-00526-1>
- [51] Wei J (2021) DEM exploration of confining stress effect in cyclic liquefaction of granular soils. *Comput and Geotech* 136:104214. <https://doi.org/10.1016/j.compgeo.2021.104214>
- [52] Wu QX, Zheng JJ, Yang ZX (2023) Effects of initial fabric anisotropy on the undrained rotational shear responses of granular material using discrete element simulations. *Acta Geotech* 18(10):5175–5194. <https://doi.org/10.1007/s11440-023-01927-z>
- [53] Xiao J, Juang CH, Wei K, et al (2014) Effects of principal stress rotation on the cumulative deformation of normally consolidated soft clay under subway traffic loading. *J Geotech Geoenviron Eng* 140(4):04013046. [https://doi.org/10.1061/\(ASCE\)GT.1943-5606.0001069](https://doi.org/10.1061/(ASCE)GT.1943-5606.0001069)
- [54] Xiao Y, Zhang Z, Chen L, et al (2018) Modeling stress path dependency of cyclic plastic strain accumulation of unbound granular materials under moving wheel loads. *Mater Des* 137:9–21. <https://doi.org/10.1016/j.matdes.2017.10.024>
- [55] Xu D, Tang Z, Zhang L (2019) Interpretation of coarse effect in simple shear behavior of binary sand-gravel mixture by DEM with authentic particle shape. *Constr Build Mater* 195:292–304. <https://doi.org/10.1016/j.conbuildmat.2018.11.059>
- [56] Yan Z, Liang J, Bai Y, et al (2021) Response of asphalt pavement structure layer and particle movement velocity based on particle flow theory. *J Constr Eng M* 147(12):04021170. [https://doi.org/10.1061/\(ASCE\)CO.1943-7862.0002199](https://doi.org/10.1061/(ASCE)CO.1943-7862.0002199)
- [57] Yang ZX, Li XS, Yang J (2007) Undrained anisotropy and rotational shear in granular soil. *Géotechnique* 57(4):371–384. <https://doi.org/10.1680/geot.2007.57.4.371>
- [58] Yu HS (2005) Three-dimensional analytical solutions for shakedown of cohesive-frictional materials under moving surface loads. *Proc R Soc A: Math, Phys Eng Sci* 461:1951–1964. <https://doi.org/10.1098/rspa.2005.1445>
- [59] Yu HS, Wang J (2012) Three-dimensional shakedown solutions for cohesive-frictional materials under moving surface loads. *Int J Sol Struct* 49(26):3797–3807. <https://doi.org/10.1016/j.ijsolstr.2012.08.011>
- [60] Zhang T, Zhang C, Yang Q, et al (2020) Inter-particle friction and particle sphericity effects on isotropic compression behavior in real-shaped sand assemblies. *Comput Geotech* 126:103741. <https://doi.org/10.1016/j.compgeo.2020.103741>

- 784 [61] Zhou W, Yang SH, Liu JY, et al (2022) Effect of inter-particle friction on
785 3D accordance of stress, strain, and fabric in granular materials. *Acta Geotech*
786 17(7):2735–2750. <https://doi.org/10.1007/s11440-021-01371-x>
- 787 [62] Zhu JF, Zhao HY, Jeng DS (2019) Dynamic characteristics of a sandy seabed
788 under storm wave loading considering the effect of principal stress rotation. *Eng*
789 *Geol* 259:105132. <https://doi.org/10.1016/j.enggeo.2019.05.009>
- 790 [63] Zhu JF, Zhao HY, Jeng DS (2019) Effects of principal stress rotation on
791 wave-induced soil response in a poro-elastoplastic sandy seabed. *Acta Geotech*
792 14(6):1717–1739. <https://doi.org/10.1007/s11440-019-00809-7>
- 793 [64] Zou YX, Ma G, Zhao SW, et al (2023) Particle shape transforms the driving of
794 shear stress in granular materials. *Powder Technol* 416:118235. <https://doi.org/10.1016/j.powtec.2023.118235>
795