



Swansea University
Prifysgol Abertawe



Cronfa - Swansea University Open Access Repository

This is an author produced version of a paper published in :
Jisuan Lixue Xuebao/Chinese Journal of Computational Mechanics

Cronfa URL for this paper:
<http://cronfa.swan.ac.uk/Record/cronfa30128>

Paper:

Feng, Y., Zhao, T., Katao, C. & Zhou, W. (2016). Stochastic discrete element modelling of rough particles-a random normal interaction law. *Jisuan Lixue Xuebao/Chinese Journal of Computational Mechanics*, 33(4), 629-636.
<http://dx.doi.org/10.7511/jslx201604032>

This article is brought to you by Swansea University. Any person downloading material is agreeing to abide by the terms of the repository licence. Authors are personally responsible for adhering to publisher restrictions or conditions. When uploading content they are required to comply with their publisher agreement and the SHERPA RoMEO database to judge whether or not it is copyright safe to add this version of the paper to this repository.
<http://www.swansea.ac.uk/iss/researchsupport/cronfa-support/>

Stochastic discrete element modelling of rough particles—a random normal interaction law

FENG Yun-tian^{*1}, ZHAO Ting-ting¹, KATO Jun¹, ZHOU Wei²

(1. Zienkiewicz Centre for Computational Engineering, College of Engineering, Swansea University, Swansea, SA2 8PP, UK;

2. School of Water Resource and Hydropower, Wuhan University, Wuhan 430072, China)

Abstract: Particles are assumed smooth in classical discrete element modelling, but real particles have random rough surfaces which may influence their mechanical properties. It is necessary therefore to quantitatively improve the conventional discrete element model particles by taking their surface roughness into consideration. In this work, a new random normal contact law is established for particles that have random rough surfaces. The contact law, based on the classic Greenwood and Williamson (GW) model, is derived by both theoretical derivation and numerical simulation. A Newton-Raphson based numerical solution procedure is proposed to obtain the total contact force for a given overlap and a set of rough surface parameters. Some related computational issues key to improve computational efficiency and accuracy are addressed. Instead of a complicated integral expression involved in the GW model, the curve fitted empirical formula of the random contact law retains the closed form and simplicity of the Hertz model, with only one added parameter, σ , the standard deviation of the surface roughness, and therefore can be readily incorporated into the current discrete element modelling framework.

Key words: surface roughness; contact law; discrete element method; stochastic DEM; numerical model

1 Introduction

The discrete element method (DEM)^[1] is a computational technique that is well suited to simulate the response of systems of particle assemblies^[2]. DEM has been applied successfully in simulating and predicting the performance of many processes involving granular solids and discontinuous materials, especially in granular flows, powder mechanics and rock mechanics. Its basic idea is to model the elements as rigid discrete particles. In order to obtain the response as a whole system, the interaction forces between the contacting elements are introduced based on some appropriate physical interaction laws.

The basic particles commonly used in DEM

are all assumed to have smooth surfaces. However real materials contain geometric irregularities at both macroscopic and microscopic levels. The discrete element modelling of irregularities of real materials has mostly been focused on the macroscopic level. Complicated geometric shapes are often represented by bonding together some basic entities^[3-8]. However surface irregularities at the microscopic level, also called the surface roughness, are more difficult to be considered, although they may have strong influence on the phenomena of contact, friction, wear and lubrication^[9]. Up to now, very few attempts have been reported to address this problem. The current contact laws in DEM method, such as the linear contact model and the Hertz contact model, are intended for contact between smooth particles. It is therefore necessary to quantitatively improve the classical DEM by taking the surface roughness into consid-

Received by: 2016-05-15; Revised by: 2016-06-15.

Corresponding authors: FENG Yun-tian* (1963-), Male, Dr. Professor
(E-mail: y. feng@swansea. ac. uk).

eration. It is important to provide random interaction laws that can be readily applied in DEM to estimate the contact forces between rough particles.

The earliest and most recognized statistical treatment of rough surfaces is the Greenwood and Williamson (GW) model^[10], in which a rough surface is described as an assembly of asperities whose properties are obtained from a given statistical height distribution, and then the Hertz contact solution is applied to each asperity to obtain an overall contact pressure distribution. This method can be viewed as a single scale method since the statistical parameters used to represent rough surfaces are scale-dependent. An early attempt of using multiple scale methods is developed by Archard^[11]. Archard models the asperities of rough surface as protuberance upon protuberance. Another statistical approach, where a fractal curve/surface is adopted to describe a rough surface is introduced by Majumdar et al^[12]. This fractal based approach can be regarded as multiple scaled because of the inherent multiscale invariant characteristics of most fractal curves and surfaces.

For the contact between two rough curved bodies, the first analytical study is conducted by Greenwood et al^[14] who employ the GW asperity contact model together with the bulk surface deformation for circular point contact. More recent works have extended the GW approach to the elasto-plastic deformation regime^[15-17]. Ali et al^[18] apply the same method of line contact^[13] in the elliptical point contact. They present different results of contact behaviour of curved rough surfaces based on different contact models and also provide the predictive formulas that can be used for the prediction of the maximum contact pressure, contact dimensions, contact compliance, real area of contact and pressure distribution. However the formulas contain many parameters and coefficients, making them less ready to be adopted in DEM.

2 The GW model

A rough surface consists of a myriad of asperities or peaks that restrict the real contact area. Due to its complex profile of a rough surface, a general analytical technique is to model the real surface as a profile, which has a statistical distribution of asperities, e. g. the Gaussian distribution or the exponential distribution. Greenwood et al^[10] adopt this statistical approach to mathematically represent rough surfaces, and by further combining with the Hertz elastic theory, derive solutions for the contact problem of rough surfaces.

Several assumptions are made in the GW model; the height profile of a rough surface is assumed to a Gaussian distribution; the summits of the asperities are spherical with constant curvature; each individual asperity deforms separately; and the bulk surface deformation below the individual asperity is negligible. Fig. 1 shows the profile of an actual rough surface and its description in the GW model.

2.1 Characteristics of rough surfaces

The topographical characteristics of rough surfaces which are closely connected with their behaviour under contact pressure are discussed. The characteristics of a rough surface are based on the profile which is the line of a cross section in a direction perpendicular to the surface as shown in Fig. 2. From this profile, surface roughness parameters are determined by scrutinizing a set of points $z(x_i)$, ($i = 1, \dots, M$) which gives the height from the mean line in the sample length interval L .

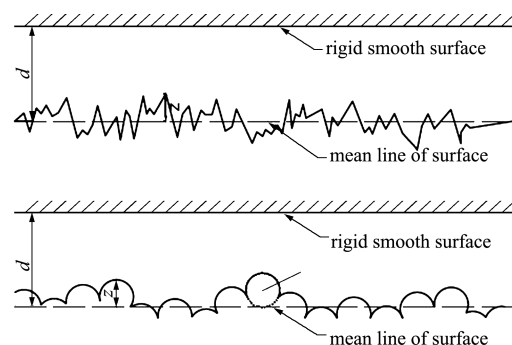


Fig. 1 Profile of an actual rough surface (top) and simplified description in the GW model

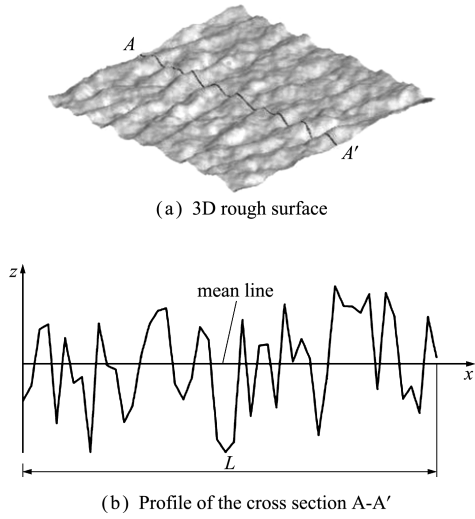


Fig. 2 Topography of a rough surface

Root mean squareroughness σ : This parameter, also called RMS, is the standard deviation of the height distribution of a surface from its mean line

$$\sigma = \sqrt{(1/L) \int_0^L z_s^2(x) dx} \quad (1)$$

Probability density function φ : The probability density function represents the distribution spectrum of a profile height and can be expressed by plotting the density of the profile height shown in Fig. 3.

In the GW model, it is assumed that the height distribution is close to the following normal or Gaussian probability

$$\varphi(z) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-z^2/2\sigma^2) \quad (2)$$

2.2 Contact of nominally flat rough surfaces

Firstly, consider the contact problem of two nominally flat rough surfaces which are assumed to have RMS roughness values σ_1 and σ_2 respectively. The problem can be further reduced to the contact of a rigid smooth flat surface with a de-

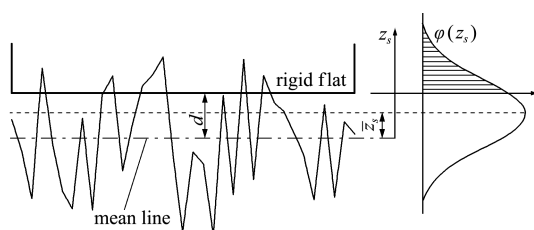


Fig. 3 Profile heights and probability density of summits

formable rough flat surface which has the equivalent RMS roughness $\sigma^2 = \sigma_1^2 + \sigma_2^2$. The height profile of the rough surface is given by the summit height z_s , the mean summit height \bar{z}_s , and probability function $\varphi(z_s)$ as shown in Fig. 3.

As mentioned above, all the summits are assumed to have the same radius β and there are N summits in the nominal surface area. Since the overlap between an asperity which exceeds the separation d and the flat surface can be written by $\delta = z_s - d$, the contact force g of a summit of height $z_s > d$ is defined by

$$g(z_s) = \frac{4}{3} E\beta^{1/2} (z_s - d)^{3/2} \quad (3)$$

Then the total contact force of the nominal surface area is

$$P(d) = \frac{4}{3} EN\beta^{1/2} \int_d^\infty (z_s - d)^{3/2} \varphi(z_s) dz_s \quad (4)$$

2.3 Contact of two rough spheres

When the above GW theory is applied to the contact problem of two rough spheres, the only difference from the contact of two rough flat surfaces is in the geometric aspect. Because of the spherical profile, the separation between the two spheres will be a function of r , the distance from the centre of the contact area. The contact problem between two rough spheres is equivalent to the contact between a deformable smooth sphere of radius R and a nominally rigid flat rough surface having a Gaussian distribution of asperities heights σ_s , where R and σ can be obtained by the radii and roughness parameters of the two spheres using the following two relationships:

$$\frac{1}{R} = \frac{1}{R_1} + \frac{1}{R_2}, \quad \sigma^2 = \sigma_{s1}^2 + \sigma_{s2}^2 \quad (5)$$

in which subscripts 1 and 2 indicate the surface numbers. As shown in Fig. 4, the overlap of the sphere with the asperity at r is given by

$$\delta(r) = z_s + z_0 - w_b(r) - r^2/2R \quad (6)$$

in which z_s is the height of the asperity and $w_b(r)$ is the (bulk) deformation of the sphere.

Then the effective contact pressure distribution over the entire contact area can be expressed as

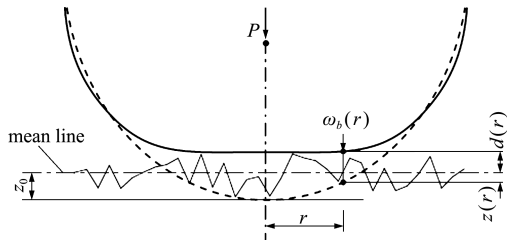


Fig. 4 Contact between a smooth sphere and a nominal flat rough surface

$$p(r) = \frac{4}{3} EN\beta^{1/2} \int_{w_b(r)+r^2/2R}^{\infty} \left[z_s - \frac{r^2}{2R} - w_b(r) \right]^{3/2} \times (1/\sigma\sqrt{2\pi}) e^{-(z_s-z_0)^2/2\sigma^2} dz_s \quad (7)$$

where N and β denote the asperity density and radius respectively; z_0 is the overlap between the undeformed configuration of the sphere and the mean line; and $w_b(r)$ is the deformation of the sphere that can be obtained from the solution for the axisymmetric deformation of an elastic half-space subject to the pressure $p(r)$ as follows

$$w_b(r) = \frac{4}{\pi E} \int_0^a [t/(t+r)] p(t) \mathbf{K}(k) dt \quad (8)$$

where $\mathbf{K}(k)$ is the first kind complete elliptic integral with the elliptic modulus $k=2(rt)^{1/2}/(r+t)$, and a is the radius of the contact area. Then by integrating the pressure distribution (7) over the contact radius a , the total contact force P_{rough} between the sphere and the rough plat surface with overlap z_0 can be obtained by

$$P_{\text{rough}}(z_0) = 2\pi \int_0^a r p(r) dr \quad (9)$$

Eqs. (7~9) provide the complete solution for the contact of two rough spheres, leading to a random interaction law between the overlap $\delta=z_0$ and the contact force P_{rough} for a pair of rough spheres with the given geometric, material and surface roughness properties. Note that there are three roughness parameters N, β and σ in Eq.(7), but there are only two independent variables σ and $N\beta^{1/2}$ instead.

Nevertheless, due to the inter-dependence between the pressure $p(r)$ and the deformation $w(r)$, and also to the non-integrable part involving the Gaussian distribution, as shown in Eqs. (7,8), an explicit expression between the overlap δ and the contact force P_{rough} cannot be established. Thus, numerical solutions have to be

sought to obtain the interaction law.

3 Numerical solutions and computational issues

3.1 Numerical solutions of the pressure and deformation distributions and the contact force

Because Eqs. (7,8) are coupled to implicitly define the pressure distribution $p(r)$ in terms of the deformation of the sphere $w_b(r)$ over the contact area, both equations are needed to be solved simultaneously by the Newton-Raphson method to obtain a numerical solution. Note that the contact radius a may not be known precisely *in priori* because the rough surface extends the contact radius from a smooth Hertz contact case, but a sufficiently large value can be estimated based on the given overlap $\delta=z_0$ and the roughness σ .

Firstly, the interval of the contact area $[0, a]$ is discretised into m discrete points $r_m = [r_1, r_2, \dots, r_m]^T$. These points are taken to be the integration points of a chosen numerical integration quadrature, and the corresponding weights are assumed to be $s_m = [s_1, s_2, \dots, s_m]^T$. Then Eq. (7) can be discretized as

$$p_i = \mu \int_{d_i}^{\infty} (z_s - d_i)^{3/2} \varphi(z_s) dz_s \equiv \mu g(w_i) \quad (10)$$

where $\mu = \frac{4}{3} EN\beta^{1/2}$, $\varphi(z_s) dz_s$

$$d_i = r_i^2/2R + w_i, \quad g(w_i) = \int_{d_i}^{\infty} (z_s - r_i^2/2R - w_i)^{3/2}$$

and Eq. (8) becomes

$$w_i = (4/\pi E) \sum_{j=1}^m s_j \alpha_{ij} p_j \quad (11)$$

where coefficients

$$\alpha_{ij} = [r_j/(r_j + r_i)] \mathbf{K}(k_{ij}), \quad k_{ij} = 2(r_i r_j)^{1/2}/(r_i + r_j)$$

Thus the equation which must be satisfied at discrete point i is given by

$$F_i(p_1, \dots, p_m) = p_i - \mu g(w_i) = 0 \quad (12)$$

Since this equation has to be satisfied at all the discrete points, $i = 1, \dots, m$, it leads to a non-linear system of equations in vector format

$$\mathbf{F}(\mathbf{p}) = \mathbf{p} - \mu \mathbf{g}(\mathbf{w}) = 0 \quad (13)$$

To solve this system of equations in terms of \mathbf{p} by the Newton-Raphson method, the function \mathbf{F} is expanded by the Taylor series in the neighbour-

hood of \mathbf{p} with an increment $\delta\mathbf{p}$

$$\mathbf{F}(\mathbf{p} + \delta\mathbf{p}) = \mathbf{F}(\mathbf{p}) + \mathbf{J} \cdot \delta\mathbf{p} + O(\delta\mathbf{p}^2) \quad (14)$$

where \mathbf{J} is the Jacobian matrix of the vector \mathbf{F}

$$\mathbf{J} = \nabla\mathbf{F}, \quad J_{ij} = \partial F_i / \partial p_j \quad (15)$$

By ignoring the 2nd order and higher terms, the increment $\delta\mathbf{p}$ can be obtained as

$$\delta\mathbf{p} = -\mathbf{J}^{-1}\mathbf{F}(\mathbf{p}) \quad (16)$$

The final solution \mathbf{p} is achieved when the iterative process converges starting from a trial solution. Then the total contact force can be obtained by numerically integrating the converged discrete pressure distribution \mathbf{p} over the entire contact area

$$P_{\text{rough}}(z_0) = 2\pi \sum_{j=1}^m s_j r_j p_j \quad (17)$$

3.2 Computational issues

There are several numerical issues involved in the above numerical procedure that may have some significant impact on the overall computational efficiency and accuracy and thus need to be discussed in detail.

3.2.1 Numerical integrations

There are three integrals involved in Eqs. (7~9) that need to be evaluated numerically. Although many numerical integration quadratures can be used, the Gaussian quadrature is adopted in the current work due to its high algebraic accuracy. As the two integrals in Eqs. (7, 8) have the same integral domain which is the contact area, the same set of Gaussian points and weights is used. This is also the requirement of the numerical solution outlined in the previous subsection.

The integral in (7) or (10) has a different integral domain and thus should be evaluated using a different number of Gaussian points. Although the upper bound of the domain should be infinity in theory, a limited value based on the given roughness σ can be adopted instead.

3.2.2 Evaluation of the Jacobian matrix \mathbf{J}

The Jacobian \mathbf{J} needs to be evaluated at each Newton-Raphson iteration. It is however difficult to obtain the analytical expression for \mathbf{J} . In this work, a finite difference approximation to \mathbf{J} is employed. Let \mathbf{J}_j be the j -th column of \mathbf{J} and $\mathbf{e}_j = [0, \dots, 1, \dots, 0]^T$ be a unit vector with only the j -

component be unity. Then

$$\mathbf{J}_j = \frac{1}{\Delta} [\mathbf{F}(\mathbf{p} + \mathbf{e}_j \Delta) - \mathbf{F}(\mathbf{p})] \quad (j=1, \dots, m) \quad (18)$$

where Δ is a small value.

3.2.3 Determination of coefficients α_{ij}

The coefficients α_{ij} in (11) play a crucial role in the current numerical solution procedure. An efficient approach to determine their values are described below.

Introducing a ratio $\lambda_{ij} = r_i / r_j$, α_{ij} can now be expressed in a slightly different form

$$\alpha_{ij} = \frac{1}{1 + \lambda_{ij}} \mathbf{K}(k_{ij}), \quad k_{ij} = 2\lambda_{ij}^{1/2} / (1 + \lambda_{ij}) \quad (19)$$

As λ_{ij} is fixed for a given m of the integration quadrature regardless of the contact radius \underline{a} , α_{ij} are also fixed. Also note that $k_{ij} = k_{ji}$, thus $\mathbf{K}(k_{ij}) = \mathbf{K}(k_{ji})$. Since it is computationally intensive to compute the value of the elliptic function $\mathbf{K}(k)$, utilising this symmetrical property can halve the computational costs involved in evaluating α_{ij} .

However, one technical difficulty occurs when evaluating the diagonal terms α_{ii} since $\lambda_{ii} = k_{ii} = 1$ and $\mathbf{K}(1)$ is infinity. This singularity problem is resolved by utilising the Hertz theory: for a given Hertz pressure distribution $p_{H_z}(\mathbf{r}) = p_0(1 - r^2/\underline{a}^2)^{1/2}$ over the contact region $[0, \underline{a}]$, the deformation is given by the Hertz deformation $w_{H_z}(\mathbf{r}) = w_0(1 - r^2/2\underline{a}^2)$. So it is required that α_{ii} should be determined in such a manner so that for the given Hertz pressure distribution $p_{H_z}(\mathbf{r})$, the calculated w_i from (11) should be equal to $w_{H_z}(r_i)$

$$w_{H_z}(r_i) = (4/\pi E) \sum_{j=1}^m s_j \alpha_{ij} p_{H_z}(r_j) \quad (20)$$

which leads to

$$\alpha_{ii} = \frac{1}{s_i p_{H_z}(r_i)} \left[\frac{\pi E}{4} w_{H_z}(r_i) - \sum_{j=1, j \neq i}^m s_j \alpha_{ij} p_{H_z}(r_j) \right] \quad (21)$$

In summary, all the coefficients α_{ij} are solely determined by the number of integration points m for the chosen integration quadrature and thus can be pre-calculated when m is given and used for any overlap and surface roughness. This feature, together with the property $\mathbf{K}(k_{ij}) = \mathbf{K}(k_{ji})$, significantly increases the computational efficiency of

the preceding numerical solution procedure. The specific approach to determining the diagonal terms α_{ii} not only eliminates the singularity problem, but also maintains the numerical accuracy of the integration quadrature.

4 A random contact interaction law for DEM

A contact law in DEM establishes the explicit relationship between the contact force, the overlap and other characteristics of the two contacting particles. Most commonly used interaction laws used in DEM are explicit and simple functions of the overlap and other contact characteristics. However, the GW model leads to a very complicated but essentially implicit relationship between the overlap and the total contact force, and therefore cannot be directly employed in DEM. In order to obtain the random normal interaction law that can be used in DEM, an explicit relationship between the total force P and the overlap δ needs to be defined from the numerical results which build the bridge between the GW model and the interaction law in DEM.

A series of numerical simulations with different values of roughness σ and overlap δ between the sphere and the rough flat surface is carried out, in which the range of σ is $0 \sim 0.1$ and the range of δ is $-0.001 \sim 0.1$. All the other parameters are set to be 1. The simulation results are shown in Fig. 5.

4.1 Reduction of roughness parameters

It is of practical importance that the resulting $P \sim \delta$ relationship should have a simple closed form with the minimum number of added parameters. It is obvious that the $P \sim \delta$ relationship

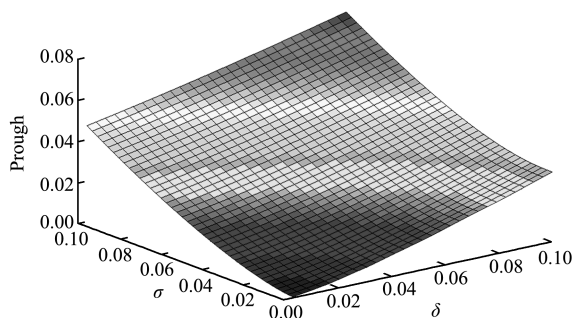


Fig. 5 Numerical simulation results

should degenerate to the Hertz law when $\sigma = 0$.

However, to treat $N\beta^{1/2}$ as an independent parameter in addition to σ will violate this requirement as different values of $N\beta^{1/2}$ would lead to different $P \sim \delta$ curves at $\sigma = 0$. To resolve this issue, $N\beta^{1/2}$ is calibrated in the following manner. When σ is sufficiently small, the rough surface can be regarded as a smooth surface and thus should have the same $P \sim \delta$ relationship as the Hertz law. However, Fig. 6 depicts a clear difference between P_{smooth} and P_{rough} (with $N\beta^{1/2} = 1$, and assuming that $\sigma = 10^{-6}$ is sufficiently small).

Our numerical calculation shows that the condition $P_{\text{rough}}(\sigma = 0) = P_{\text{smooth}}$ can be enforced if $N\beta^{1/2}$ takes the following value:

$$N\beta^{1/2} = P_{\text{smooth}}/P_{\text{rough}} = 0.49R^{-1/2}\delta^{-1} \quad (22)$$

The correctness of this formula can be further verified by the following theoretical analysis.

In Eq. (7), the non-integrable part involving the Gaussian distribution can be simplified when σ is small. Note that the Gaussian distribution reduces to the Dirac Delta function when $\sigma \rightarrow 0$:

$$\delta(t) = \lim_{\sigma \rightarrow 0} (1/\sqrt{2\pi}\sigma) e^{-t^2/2\sigma^2} \quad (23)$$

Thus when $\sigma \rightarrow 0$, the pressure distribution $p(r)$ in Eq. (7) reduces to

$$p(r) = \frac{4}{3}EN\beta^{1/2}[z_0 - r^2/2R - \omega_b(r)]^{3/2} \quad (24)$$

An explicit expression for $p(r)$ is not possible because of the inter-dependence between $p(r)$ and $\omega_b(r)$. However, artificially setting $\omega_b(r) = 0$ leads to an explicit but approximate expression for $p(r)$

$$p(r) = \frac{4}{3}EN\beta^{1/2}(z_0 - r^2/2R)^{3/2} \quad (25)$$

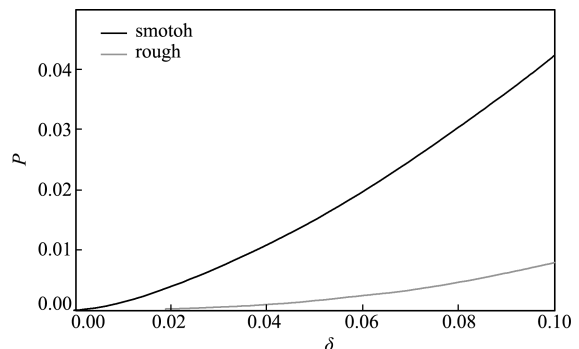


Fig. 6 $P \sim \delta$ relationships of smooth surface and rough surface ($\sigma = 10^{-6}$, $N\beta^{1/2} = 1$)

The total contact force is obtained by substituting Eq. (25) into Eq. (9) as (note that $\delta = z_0$):

$$P_{\text{rough}} = 2.76EN\beta^{1/2}R\delta^{5/2} \quad (26)$$

The flat rough surface can be considered as a smooth surface when $\sigma \rightarrow 0$. The contact force between the sphere and the smooth surface can be calculated by the Hertz law

$$P_{\text{smooth}} = (4/3)ER^{1/2}\delta^{3/2} \quad (27)$$

The condition $P_{\text{rough}} = P_{\text{smooth}}$ gives rise to Eq. (22).

The relationship (22) is useful to reduce the number of roughness parameters in the expression for $p(r)$. There are three roughness parameters N, β and σ in Eq. (7). By incorporating Eq. (22) into Eq. (7), the final expression for the total force contains only one roughness parameter σ , making the new interaction law much simpler.

4.2 Curve fitted empirical formula

In order to obtain the random normal interaction law that can be used in DEM, an explicit relationship between the total force P and the overlap δ needs to be defined from the numerical results via curve-fitting. It is also desirable that the random interaction law retains the closed form and simplicity of the Hertz model.

Based on the numerical results obtained above and by applying nonlinear least squares curve fitting, a predictive formula for calculating the normal contact force between two rough spheres is derived. The fitted formulas are presented in the Tab. 1 where both σ and δ are normalised by R and thus non-dimensional. The R-squared values are 0.99, indicating a very high accurate fitting obtained. When $\sigma = 0$, the formula recovers the Hertz law as required. The resulting random normal contact law retains the closed form and simplicity of the Hertz model and has only one added roughness parameter σ .

Tab. 1 Random normal contact law

	Empirical formula (σ and δ are normalised by R)	R-squared
$\delta > 0$	$P_{\text{rough}} = ER^2[(4/3 + 0.45\sigma)\delta^{(3/2+5.90\sigma)} + 1.53\delta^{0.13}\sigma^{1.30} + 1.5\sigma^{2.4}]$	0.99
$\delta = 0$	$P_{\text{rough}} = 1.5ER^2\sigma^{2.4}$	0.99
$\delta < 0$	$P_{\text{rough}} = ER^2[0.36\sigma(-\delta)^{(0.06-0.82\sigma)} + 1.5\sigma^{2.4}]$	0.99

5 Conclusion

In this work, a new random normal contact law has been established for particles that have random rough surfaces based on the classic Greenwood and Williamson model. For a given overlap δ and a roughness σ , a Newton-Raphson based iterative solution procedure has proposed to calculate the contact pressure and the total force. The key elements in this procedure include the use of the Gaussian quadrature to evaluate three integrals, a finite-difference approximate to the Jacobian matrix, and determination of the coefficients α_{ij} and particularly the diagonal terms α_{ii} . These features not only significantly increase the computational efficiency of the preceding numerical solution procedure, but also maintain the high accuracy of the numerical solutions.

On the basis of the numerical results obtained and by applying nonlinear least squares curve fitting, an explicit predictive formula for calculating the normal contact force between two rough spheres has been derived. The fitted formula recovers the Hertz law when $\sigma = 0$. More importantly it retains the closed form and simplicity of the Hertz model and has only one added roughness parameter σ . Thus it can be readily incorporated into the DEM modelling framework.

References:

- [1] Cundall P A, Strack O D L. A discrete numerical model for granular assemblies [J]. *Geotechnique*, 1979, **29**(1):47-65.
- [2] Owen D R J, Feng Y T, de Souza Neto E A, et al. The modelling of multi-fracturing solids and particulate media [J]. *International Journal for Numerical Methods in Engineering*, 2004, **60**(1):317-340.
- [3] Jensen R P, Bosscher P J, Plesha M E, et al. DEM simulation of granular media-structure interface: effects of surface roughness and particle shape [J]. *International Journal for Numerical and Analytical Methods in Geomechanics*, 1999, **23**(6):531-47.
- [4] Wang L, Park J Y, Fu Y. Representation of real particles for DEM simulation using X-ray tomography [J]. *Construction and Building Materials*, 2007, **21**(2):338-46.

- [5] Lu M, McDowell G R. The importance of modelling ballast particle shape in the discrete element method [J]. *Granular Matter*, 2007, **9**(1-2): 69-80.
- [6] Ferrellec J F, McDowell G R. A simple method to create complex particle shapes for DEM [J]. *Geomechanics and Geoengineering: An International Journal*, 2008, **3**(3): 211-6.
- [7] Garcia X, Latham J P, Xiang J, et al. A clustered overlapping sphere algorithm to represent real particles in discrete element modelling [J]. *Geotechnique*, 2009, **59**(9): 779-84.
- [8] Shamsi M M M, Mirghasemi A A. Numerical simulation of 3D semi-real-shaped granular particle assembly [J]. *Powder Technology*, 2012, **221**: 431-46.
- [9] Barber J R, Ciavarella M. Contact mechanics [J]. *International Journal of Solids and Structures*, 2000, **37**(1): 29-43.
- [10] Greenwood J A, Williamson J B P. Contact of nominally flat surfaces [J]. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 1966, **295**(1442): 300-319.
- [11] Archard J F. Elastic deformation and the laws of friction [J]. *In Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 1957, **243**(1233): 190-205.
- [12] Majumdar A, Bhushan B. Role of fractal geometry in roughness characterization and contact mechanics of surfaces [J]. *Journal of Tribology*, 1990, **112**(2): 205-16.
- [13] Beheshti A, Khonsari M M. Asperity micro-contact models as applied to the deformation of rough line contact [J]. *Tribology International*, 2012, **52**: 61-74.
- [14] Greenwood J A, Tripp J H. The elastic contact of rough spheres [J]. *Journal of Applied Mechanics*, 1967, **34**(1): 153-159.
- [15] Cohen D, Kligerman Y, Etsion I. The effect of surface roughness on static friction and junction growth of an elastic-plastic spherical contact [J]. *Journal of Tribology*, 2009, **131**(2): 021404.
- [16] Gelinck E R M, Schipper D J. Deformation of rough line contacts [J]. *Journal of Tribology*, 1999, **121**(3): 449-454.
- [17] Li L, Etsion I, Talke F E. Elastic-plastic spherical contact modeling including roughness effects [J]. *Tribology Letters*, 2010, **40**(3): 357-363.
- [18] Beheshti A, Khonsari M M. On the contact of curved rough surfaces: contact behavior and predictive formulas [J]. *Journal of Applied Mechanics*, 2014, **81**(11): 111004.

粗糙颗粒的随机离散元模拟——随机法向接触定律

冯云田^{*1}, 赵婷婷¹, 加藤淳¹, 周伟²

(1. 斯旺西大学 辛克维奇计算工程中心, 英国斯旺西 SA2 8PP; 2. 武汉大学 水利水电学院, 武汉 430072)

摘要: 真实颗粒的力学性质会受到其随机粗糙表面的影响, 然而在传统离散元模拟中通常假设颗粒具有光滑表面, 因此有必要在定量考虑颗粒表面粗糙度的基础上改进离散元的接触模型。本文基于经典 Greenwood-Williamson (GW) 模型通过理论分析和数值模拟提出了一种可以考虑颗粒表面粗糙度的法向接触定律; 开发了基于 Newton-Raphson 迭代的数值计算方法, 通过输入颗粒重叠量和一系列表面粗糙系数计算总接触力; 讨论了改进计算方法效率和准确性的相关问题。相对于 GW 模型中接触关系的复杂积分表示, 拟合得到新随机接触定律的表达式具有类似 Hertz 定律的简单结构, 只包含一个表征颗粒表面粗糙度标准偏差的新增参数, σ , 可以方便的引入当前离散元模拟程序中进行计算。

关键词: 表面粗糙度; 接触定律; 离散元; 随机离散元; 数值模型

中图分类号: O34

文献标志码: A

文章编号: 1007-4708(2016)04-0629-08

收稿日期: 2016-05-15; **修改稿收到日期:** 2016-06-15.

作者简介: 冯云田* (1963-), 男, 博士, 教授

(E-mail: y. feng@swansea. ac. uk);

赵婷婷 (1989-), 女, 博士生;

加藤淳 (1979-), 男, 博士, 高级工程师;

周伟 (1975-), 男, 博士, 教授.