Development of a random particle generator for the distinct lattice spring model

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Abstract. Particles in a regular arrangement will always be simplistically used in the discrete numerical analysis to represent materials ranging from steels to geomaterials (e.g., rock and concrete). As for those heterogeneous materials, this simplification violates reality more or less. In this work, a random particle model generator is developed to provide a computational model for the Distinct Lattice Spring Model (DLSM). The generator covers the determination of particles within polygons and the linkage formation between particles. Firstly, the computational domain represented by an implicit description is initially discretized into polygons based on the Centroidal Voronoi diagrams and then optimized by the topology optimization algorithm. Subsequently, the random particles are located within the polygons by using the minimal inner tangent circle, in which the centroid of the polygons are regarded as the particle centre and determined by the simplex method. Based on the Delaunay triangulation algorithm, the particles will be initially linked together. To avoid the long-range interaction between particles that could fail to predict the elastic response, the initial linkage will be re-detected by a second contact detection law. Compared with the particle model in a regular arrangement, the irregularity along the model boundary in an arbitrary computational domain can be eliminated by the random particle model. Prior to fracture problems, the elastic response of the random particle model under the framework of the DLSM is numerically verified by the beam bending problem. In the following, the crack propagation of the quasi-brittle materials is investigated by using a modified cohesive damage-plasticity model (m-CDPM), in which the linear elastic, nonlinear and softening stages are included. As for the crack path preference occurring in the regular particle model, it can be alleviated by the random particle model. Besides, the applicability of the random particle model associated with the m-CDPM on fracture problems is investigated by two numerical examples including the semi-circular bending and tension-shear tests.

1. Introduction
Nowadays, numerical analysis as a favourable tool is popularly used by researchers in all walk of life. Compared with the theoretical analysis and laboratory tests, numerical analysis prevails since it features repeatability and low cost [1]. There exist several numerical methods, which can be classified into the continuum-based and discontinuum-based method [2]. The continuous assumption in the continuum-based method makes it not suitable for fracture problems. Fortunately, the discontinuum-based method breaks through this limitation, in which the computational domain is discretized into particles or polygons (polyhedrons) and the dynamic equation will be iteratively solved to reproduce the macro mechanical responses. As a representative, the discrete element method (DEM) [4] makes use of particles to simulate most materials. However, the drawback is the tedious and complicated parameter calibration between macro elastic constants (e.g., elastic modulus and Poisson ratio) and micro ones.
(e.g., spring stiffness). As another solution, the lattice spring model (LSM) was initially proposed by Hrennikoff [5] to investigate the elastic and fracture problems of a disordered media, where only a fixed Poisson ratio can be reproduced. After decades of development, the DLSM [6] as one of its derivatives has attracted most researchers interest. Compared with the DEM, parameter calibration is no longer required in the DLSM. Moreover, the least square method is introduced to evaluate the shear deformation, which removes the rigid rotation and improves the computational efficiency. However, particles in a regular arrangement are always adopted [6], which violates reality more or less for those heterogeneous materials. Although random particle models have been used in the DEM, it is still unknown in the DLSM.

Generally, two methods are always used to generate the random particle model. The first one is the dynamic stacking method [8], in which a lot of moving particles will be thrown into a container, and their positions and sizes change as the particles collide with each other until it reaches to the equilibrium state. However, contact detection is time-consuming. Besides, the geometric filling method is another choice [10]. In this method, the computational domain will be firstly meshed into arbitrary polygons (polyhedrons). Subsequently, the random particle model will be generated by filling these polygons or placing the particles at the vertices. In view of high efficiency of this method, this work takes a general-purpose polygonal mesh generator proposed by Talischi et al. [12] as a candidate to generate the random particle model. After that, the crack propagation will be investigated to highlight its superiority over the regular particle model.

The remainder of this work is organized as follows: a two-dimensional incremental version of the DLSM will be briefly described followed by the introduction of the m-CDPM in Section 2. Subsequently, a random particle model generator will be proposed to serve the DLSM in Section 3. Next, numerical examples will be conducted to verify the correctness of the random particle model under the framework of the DLSM and to investigate the crack propagation of the quasi-brittle materials. In the end, some conclusions are drawn.

2. The model

In this section, a brief introduction of the 2D incremental DLSM and its associated m-CDPM will be both presented, which will be as a numerical tool to investigate the rock fracturing subsequently demonstrated in Section 4. More details on the model description can be accessed in the Ref [13].

2.1. 2D incremental DLSM

The DLSM was initiated by Zhao et al. (2011) [6] in a total form for dynamic fracturing, in which the model domain is discretized into a mass of mass points in a regular arrangement linked by the spring pairs (e.g., normal spring and shear spring), and the processive breakage of springs can be regarded as the material fracture. However, the initial DLSM is unsuitable for those plastic models in an incremental form. Under the circumstances, an incremental DLSM was tailored to cater for the m-CDPM. For simplification, this work takes the two-dimensional case as an example.

Different from the total version of the DLSM, the relative velocity as a substitute for the relative displacement is used to update the force in the incremental DLSM. Given the velocity of the particles, the relative velocity can be computed by:

\[ \mathbf{u}_{ij} = \mathbf{u}_j - \mathbf{u}_i \]  

where \( \mathbf{u}_{ij} \) is the relative velocity, \( \mathbf{u}_i \) and \( \mathbf{u}_j \) are the velocity of particle \( i \) and \( j \), respectively. By taking the orthogonal decomposition, the normal relative velocity vector can be written as:

\[ \mathbf{u}_{ij}^n = (\mathbf{u}_{ij} \cdot \mathbf{n}) \mathbf{n} \]  

where \( \mathbf{n} \) is the normal unit vector pointing from particle \( i \) to particle \( j \). Different from the DEM, the shear component in the DLSM is evaluated by the least square method to avoid the redundant energy
caused by the rigid rotation, therefore, reducing the rotational degree of freedom and enhancing the computational efficiency. Therefore, the relative shear velocity can be expressed as:

\[ \hat{\mathbf{u}}_y = \mathbf{e}^{bond}_{ij} \mathbf{n} - \left( \mathbf{e}^{bond}_{ij} \mathbf{n} \right) \mathbf{n}/l_{ij} \]  

(3)

where \( \mathbf{n} \) is the shear unit vector, \( l_{ij} \) is the spring length and \( \mathbf{e}^{bond}_{ij} \) is the local strain rate, which can be evaluated by:

\[ \mathbf{e}^{bond}_{ij} = \frac{\dot{\mathbf{e}}_{ij} + \dot{\mathbf{e}}_{ij}}{2} \]  

(4)

Once the relative velocities are determined, the normal and shear force can be respectively updated by:

\[ F_{ij}^{n,t \Delta t} = \begin{cases} F_{ij}^{n,t} + k_n u_{n} \Delta t, & u_{n} < u_{n}^* \text{ and } \left| u_{n} \right| < \left| u_{n}^* \right| \\ 0, & u_{n} \geq u_{n}^* \text{ or } \left| u_{n} \right| \geq \left| u_{n}^* \right| \end{cases} \]  

(5)

\[ F_{ij}^{s,t \Delta t} = \begin{cases} F_{ij}^{s,t} + k_s u_{s} \Delta t, & u_{s} < u_{s}^* \text{ and } \left| u_{s} \right| < \left| u_{s}^* \right| \\ 0, & u_{s} \geq u_{s}^* \text{ or } \left| u_{s} \right| \geq \left| u_{s}^* \right| \end{cases} \]  

(6)

where, \( k \) is the stiffness of the spring, \( u \) is the displacement, \( \Delta t \) is the time step, subscripts \( n \) and \( s \) are the corresponding components in the normal and shear directions, respectively, and the superscript * is the ultimate state.

Another merit of the DLSM is the automatic parameter calibration between macro elastic constants and micro spring stiffness, which are described as:

\[ k_n = \frac{E}{\alpha^{2D} (1-\nu)} \]  

(7)

\[ k_s = \frac{(1-3\nu)E}{\alpha^{2D} (1-\nu^2)} \]  

(8)

where \( E \) is the elastic modulus, \( \nu \) is the Poisson ratio and \( \alpha^{2D} \) is a dimensionless coefficient related to the model domain area.

2.2. The m-CDPM

The CDPM proposed by Nguyen et al. (2017) [14] aims to describe the mechanical behavior of the quasi-brittle or soft rock materials within the whole process, which covers the linearly elastic and nonlinear response in the pre-peak stage and the plastic and damage response caused by the crack initiation and crack propagation in the post-peak stage. Considering the plastic deformation and the damage, the force update in Eqs. (5) and (6) should be rewritten as

\[ f_n = \begin{cases} k_n^0 (1-D) \left( u_n - u_n^p \right), & \text{Under tension} \\ k_n^0 \left( u_n - u_n^p \right), & \text{Under compression} \end{cases} \]  

(9)

\[ f_s = k_s^0 (1-D) \left( u_s - u_s^p \right) \]  

(10)

where \( k_n^0 \) is the initial spring stiffness without damage, \( D \) is the damage variable, \( u_n^p \) is the plastic deformation. Here, the damage of the spring stiffness will be considered only under the tension state. To associate the damage variable with plastic deformation, a smooth exponential form is adopted, which can be expressed as:

\[ D = 1 - e^{-\left( \frac{u_n - u_n^p}{\nu_n - u_n^p} \right)} \]  

(11)

where \( \nu \) is the softening parameter that controls the post-peak response. Similar to the Mohr-Coulomb criterion, a hyperbolic form is used as the yield function, which can be described as:
\[ F(f_c, f_s, D) = \beta^2 f_s^2 - \left[ f_c^0 (1-D) - f_s \tan \varphi \right]^2 + \left[ f_c^0 (1-D) - f_s^0 (1-D) \tan \varphi \right]^2 \]  \hfill (12)

where \( f_c^0 \) and \( f_s^0 \) are the cohesion and tension strength, \( \varphi \) is the frictional angle, and \( \beta \) is a constant, which can be defined as:

\[ \beta = \sqrt{\frac{2 f_c^0 f_s^0 \tan \varphi - (f_s^0 \tan \varphi)^2}{f_s^2}} \]  \hfill (13)

To clarify, the yield surface is depicted in Fig. 1(b). It can be seen that the yield surface controlled by the cohesion, tension strength and friction angle shrinks as the damage evolves. To evaluate the plastic deformation, a non-associate flow rule is selected, and the potential function can be written as:

\[ G(f_c, f_s, D) = f_s^0 - \left[ f_c^0 (1-D) - f_s \tan \psi \right]^2 + \left[ f_c^0 (1-D) - f_s^0 (1-D) \tan \psi \right]^2 \]  \hfill (14)

where \( \psi \) is the dilatancy angle. At this point, the incremental plastic deformation can be calculated as:

\[ \delta u^p = \delta \lambda \frac{\partial G}{\partial \mathbf{F}} \]  \hfill (15)

where \( \delta \lambda \) is a multiplier, which can be calculated by using the first-order Taylor’s expansion of the yield function.

**Figure 1.** A schematic diagram of the modified cohesive damage-plasticity model, (a) mechanical behaviour under pure normal loadings, (b) evolutionary yield surface.

However, there are two open questions for coupling the CDPM into the DLSM. One is the CDPM is unsuitable for the negative stiffness, which could be encountered in the DLSM when the Poisson ratio is greater than 1/3 for plane stress problem. Although the natural lattice structure could make it possible to mimic the hardening stage when it reaches the plastic state, the CDPM cannot control the material nonlinearity. To overcome these two problems, a so-called hyper-elastic stage was introduced to modify the CDPM, in which a critical effective displacement was defined as:

\[ \bar{\delta} = \gamma \frac{f_c^0}{k_u} \]  \hfill (16)

where \( \gamma \) is a dimensionless coefficient that controls the initiation of the nonlinearity, whose degree is ruled by the degradation of the spring stiffness, which is defined as:

\[ k_s = \begin{cases} \alpha k_u, & \delta > \bar{\delta} \\ k_u, & \delta \leq \bar{\delta} \end{cases} \]  \hfill (17)

\[ k_s = \begin{cases} \eta k_u, & \delta > \bar{\delta} \\ k_u, & \delta \leq \bar{\delta} \end{cases} \]  \hfill (18)

where the \( \alpha \) and \( \eta \) are the dimensionless coefficients. In this work, \( \alpha \), \( \eta \) and \( \gamma \) are recommended as 0.8, 0.25 and 0.8, respectively. Once the effective displacement exceeds its critical value, the stiffness will be modified, and the negative stiffness will also be avoided, in which the effective displacement was defined as:
\[
\delta = \begin{cases} 
\sqrt{u_n^2 + u_r^2}, & u_n > 0 \\
|u_n|, & u_n \leq 0
\end{cases} \tag{19}
\]

To make it clear, the mechanical response under the pure normal loading is described in Fig. 1(a) as an example. It should be noted that the hyper-elastic stage representing the material nonlinearity covers the nonlinearity caused by the hardening stage in morphology.

3. Random particle model generator

In the previous study on the DLSM, the particle model is always be placed in a regular arrangement, which violates reality more or less if it is used for rock-like materials. In this section, a random particle model generator, including the particle packing and the linkage formation, will be proposed based on the polygonal discretization and Delaunay triangulation, which could provide the computational model for the DLSM to represent the material heterogeneity.

As a computational domain, it will be firstly represented in an implicit form followed by the polygonal meshing by using the Centroidal Voronoi diagrams. Subsequently, the topology optimization is used to generate a relatively uniform or non-uniform mesh, which could be a certain user-defined law. More details on the polygonal discretization and its optimization can be referred to the Ref. [12].

![Figure 2. Particle determination inside a polygon.](image)

In this work, the random particle model is generated by filling the particles represented by the inner tangent circle into each polygon. It is assumed that a needed polygonal mesh is prepared, the particle center that coincided with the centroid of the polygon and its radius are the priority for the filling. Taking Fig. 2 as an example, the polygon can be represented by head to tail vectors in a counterclockwise closed form. In this sense, the centroid of the polygon can be calculated by the simplex method, which is mathematically expressed as:

\[
c = (x_c, y_c) = \frac{1}{6A} \sum_{i=0}^{N-1} \left( (p_i + p_{i+1}) \times |p_i \times p_{i+1}| \right) \tag{20}
\]

where \( p \) is the vertex position, \( N \) is the number of vertexes, and \( A \) is the polygonal area, which can be calculated by:

\[
A = \frac{1}{2} \sum_{i=0}^{N-1} |p_i \times p_{i+1}| \tag{21}
\]

The radius can be determined by minimizing the perpendicular distance between the centroid and each edge of the polygon, which can be calculated by:

\[
L_i = \frac{|(c - p_i) \times (p_j - p_{i+1})|}{|p_j - p_{i+1}|} \tag{22}
\]

\[
R = \min \left( L_0, L_1, \cdots L_N \right) \tag{23}
\]

Once the particles are filled into the polygons, the linkage between particles is necessary to be formed as the lattice structure to make the constitutive model workable. Here, the Delaunay triangulation algorithm is used to initially link particles together (Fig. 3(b)). To avoid the long-range interaction that could fail to correctly describe the elastic deformation [15], a second contact detection is used. In this sense, the linkage only works if the surface distance between two particles is less than a fixed value, which can be described as:
\[ |c_i - c_j| - R_i - R_j < 1.2 \bar{R} \]  

(24)

where $\bar{R}$ is the average radius of all particles. For example, a cube model with the random particles (Fig. 3(c)) and its lattice structure (Fig. 3(d)) are generated based on the polygonal mesh (Fig. 3(a)) and Delaunay triangulation (Fig. 3(b)).

**Figure 3.** A cube model generation process from the polygonal discretization to random particle model, (a) polygonal discretization, (b) triangulation, (c) random particle model, (d) lattice structure.

Fortunately, the random particle generator also inherits the advantage of the mesh discretization that can represent a smooth boundary. As an example, a comparison of a disc with an eccentric circle model between the random particle model and the regular particle model is made in Fig. 4. As a result, the irregularity along the boundary in a regular arrangement could be avoided by the random particle model.

**Figure 4.** An example of a disc with an eccentric circle model, (a) polygonal discretization, (b) random particle model, (c) regular particle model.

4. Numerical Examples

In this section, three numerical examples are conducted to verify the feasibility of the random particle model under the framework of the DLSM and the advantage of the random particle model on rock fracturing, which covers the beam bending problem for the validation of the elastic response and the semi-circular bending and tension-shear test for rock fracturing.

4.1. Beam bending problem

To verify whether the random particle model can reproduce the correct elastic response under the framework DLSM, a beam bending problem as an example is numerically simulated, and its geometry and boundary conditions are described in Fig. 5, in which the bottom corners are supported by roller bearings, and a 10 N load is applied at the middle point of the beam. The elastic constants are elastic modulus 1 GPa and Poisson ratio 0.2. As for the computational model, the particle models in the regular and random arrangement with the same number of particles are separately generated, the average particle size is taken as 1 mm.

**Figure 5.** The geometry and boundary conditions for the beam bending problem.
The numerical results are shown in Fig. 6, in which Fig. 6 (a) and (b) depict the displacement contour in $y$ direction multiplied by 10 times for the convenience of comparison, and the same deformation in appearance can be observed. To make a quantitative analysis, the displacement of the measuring line in $y$ direction is measured, and the analytical solution as a reference is also compared with the numerical results as shown in Fig. 6(c). It can be seen that both regular and random structure can predict the correct elastic results, which demonstrates the feasibility of the random particle model in the DLSM.

Figure 6. A comparison among analytical result and numerical results predicted by the regular model and random model, (a) displacement contour in $y$ direction ($x10$) predicted by the regular model, (b) displacement contour in $y$ direction ($x10$) predicted by the random model, (c) displacement curves.

4.2. Semi-circular bending

In this part, a semi-circular bending test is selected to investigate the fracture anisotropy of the lattice spring model. Actually, this numerical example with the regular particle model was conducted in our previous work [13]. As an extension, the random particle model is used to dig out its advantage on rock fracturing. Fig. 7 shows its geometry and boundary conditions, and the macro material parameters include an elastic modulus of 450 MPa, Poisson ratio of 0.2, tension strength and cohesion of 0.6 MPa, fracture energies for mode I and II of 11.56 N/m, friction angle of 32$^\circ$ and dilatancy angle of 9$^\circ$ [14]. Moreover, its calibrated parameters are listed in Table 1, and Ref. [13] can be accessed for more information on the calibration process.

Figure 7. The geometry and boundary conditions for the semi-circular bending.

Table 1. Model parameters for the SCB

| Calibrated model parameters | Value |
|----------------------------|-------|
| Tensile force/Cohesion $f_t^u$, $f_c^u$ | 704 N |
| Normal/shear softening parameter $u_s^*$, $u_t^*$ | 0.0106 mm |
| Maximum normal/shear displacement $u_s^*$, $u_t^*$ | 0.0138 mm |
| Frictional angle $\phi$ | 32 |
| Dilatancy angle $\psi$ | 9 |
Since the regular particle model has a feature of eight-fold symmetry, only four counterclockwise rotation on the regular particle model are included, e.g., 0, 15, 30, 45 degrees, whose numerical results are shown in Fig. 8(a)-(d), it can be seen that the crack of the regular models rotated by 0 and 45 degrees propagates along the prefabricated crack due to its bilateral symmetry, while the crack path of the regular models rotated by 15 and 30 degrees deviates from the upward direction.

Due to the non-symmetry of the random particle model, rotation is not considered. Here, two random particle models, whose resolution are consistent with the particle size in a regular arrangement, are generated to assess its performance on the crack propagation. From Fig. 8(e) and (f), it can be seen that the crack path preference will be alleviated by the random particle model. Moreover, the irregularity of the boundary in the regular particle model is avoided. Besides, the load-displacement curves of these numerical results are plotted in Fig. 8(g) and compared with the experimental data. Although the same calibrated parameters with the regular particle model are used in the random particle model, reasonable results can still be captured.

4.3. Tension-shear test

To further investigate the random particle model for rock fracturing, a mixed-mode fracture problem named tension-shear test is numerically simulated, whose dimensions and loading conditions are shown in Fig. 9. Referring to the study of Wei et al., (2021) [13], the macroscopic material constants take an elastic modulus of 32 GPa, Poisson ratio of 0.2, a tensile strength of 3.0 MPa, a mode-I fracture energy of 0.11 N/mm, a cohesion of 3.0 MPa, a mode-II fracture energy of 0.11 N/mm, a friction angle of 20° and a dilatancy angle of 9°. The calibrated parameters are listed in Table 2, in which the calibration procedure can be referred to Ref. [13].

| Table 2. Model parameters for the tension-shear test |
|-----------------------------------------------|
| Calibrated model parameters                  |
| Tensile force/Cohesion $f_c^*, f_c$           | 1560 N |
| Normal/shear softening parameter $u_s^*, u_s^*$ | 0.027 mm |
| Maximum normal/shear displacement $u_s^*, u_s^*$ | 0.027 mm |
| Frictional angle $\phi$                      | 20    |
| Dilatancy angle $\psi$                       | 9     |

Fig. 10 shows the numerical results of different methods and constitutive models. Similar to DLSM with the regular particle model (Fig. 10(a)) and the material point method (MPM) [18], the DLSM with random particle model (Fig. 10(b)) can still reproduce the correct crack path compared with the experimental test. Besides, the DLSM with a random particle model can reproduce the material.
nonlinearity and the softening feature shown in Fig. 10(c) and (d). Quantitatively, the DLSM with random particle model predicts a lower load for the tensile boundary, while a better result of the shear load-displacement relationship can be observed. Compared with the result of the regular DLSM, the random DLSM can provide smoother load-displacement curves. Besides, an improper parameter selection for the random particle model maybe is a reason for a lower predictive load. For example, the same parameter calibration procedure with the regular particle model is used in the random particle model. Even so, it still can be concluded that it is successful to use the random particle model to predict the rock fracturing by the m-CDPM.

**Figure 9.** The geometry, boundary conditions and measuring point locations for the tension-shear test.

**Figure 10.** A comparison of numerical results of different methods and models, (a) and (b) fracture patterns, (c) and (d) load-displacement curves
5. Conclusions
In this work, a random particle model generator as a substitute for the regular particle model in the original DLSM is developed to investigate the crack propagation of quasi-brittle materials. Based on the Centroidal Voronoi diagrams and the topology optimization algorithm, the computation domain will be discretized into polygons in a user-defined arrangement (default as a uniform style). And, the random particle model is generated by filling each polygon with a particle, where the centroid of the polygon determined by the simplex method coincides with the particle centre and the minimal inter tangent circle is our target particle location. In terms of the Delaunay triangulation algorithm, the linkage between particles will be initially formed. Besides, the linkage will be re-detected by a second detection law to avoid the long-range interaction. Based on the random particle model, several numerical examples are performed, and some conclusions are drawn out.

- The computational model with a smooth boundary can be generated by the random particle model compared with the regular particle model.
- The elastic response of the random particle model is numerically verified by a beam bending problem. Compared with the analytical solution, the random particle model can give a better prediction than the regular particle model under the same resolution.
- The crack path preference along the regular particle model can be relieved by the random particle model.
- The mechanical response and fracture pattern can be both captured under the mode-I and mixed-mode fracture problem by using the m-CDPM. And smooth load-displacement curves are obtained than that of the regular particle model. However, a low predictive load can be observed since the same parameters with the regular particle model are used. Therefore, a proper parameter calibration procedure for the random particle model should be focused on in our future work.

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