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ON USING QUASI-RANDOM LATTICES FOR SIMULATION OF ISOTROPIC MATERIALS

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Abstract. Elastic properties of three-dimensional lattices are usually anisotropic. This fact limits the range of applicability of lattice models in solid mechanics problems. In the present paper, we propose a simple three-dimensional lattice model with isotropic elastic properties. A quasi-random lattice is generated by randomly displacing particles of the face-centered cubic lattice. Then particles are connected by linear and angular springs such that initially forces in all springs are equal to zero. It is shown numerically that the resulting quasi-random lattice has isotropic elastic properties, provided that amplitudes of random displacements are sufficiently large. Poisson's ratio of the lattice depends on number of angular springs per particle and stiffnesses of these springs. In the present model, values of Poisson's ratio belong to the interval [0;0.41]. The model can be used, in particular, for simulation of deformation and brittle fracture of rocks in hydraulic fracturing.

Keywords: particle dynamics; quasi-random lattice; face-centered cubic lattice; effective elastic properties; isotropy; molecular dynamics.

1. Introduction

Discrete mechanical models are widely used for simulation of deformation and fracture of materials at different length scales [1,2]. In these models, a material is represented as a set of interacting particles (e.g. material points or rigid bodies). Then mechanical properties of the material are determined by its structure (particle positions) and interparticle interactions.

Specifying initial positions of particles (structure of the material) can be a challenge [1]. The simplest arrangement of particles is a perfect lattice. If crystals are concerned, lattices arise naturally. For other materials, lattices are used as coarse-grained models [3-5]. Advantage of lattice models is that, in many cases, relations between microscopic and macroscopic properties of the material can be derived analytically [4,6-9]. Therefore calibration of model parameters (e.g. parameters of interparticle interactions) is relatively straightforward. At the same time, symmetry of lattices significantly influence their mechanical properties. In particular, elastic properties of three-dimensional lattices are usually anisotropic (see e.g. [1, 9, 10,11]). Influence of lattice symmetry on fracture processes is even more pronounced. Therefore for simulation of isotropic materials, more complicated irregular packings of particles should be used.

A natural way for simulation of isotropic materials is generation of random (amorphous) [5,12-14] or polycrystalline structures [15]. For example, algorithms for generation of random close-packings of spheres are proposed, in papers [13,14]. Creation of polycrystalline materials is discussed in paper [15]. However, implementation of algorithms [13-15] is relatively time-consuming, especially in three-dimensional case. Therefore, more efficient and simple algorithms are required.

In the present paper, we present a simple discrete model with isotropic elastic properties. Quasi-random lattice is generated. Particles in the lattice are connected by linear and angular springs. It is shown that proper choice of parameters of the model allows to simulate isotropic materials with prescribed elastic moduli.

2. Generation of the quasi-random lattice

The quasi-random lattice is generated as follows. Initially, the particles form a perfect face-centered cubic lattice (FCC). Radius vectors of the particles have form

$$\boldsymbol{R}_{nmk} = a(n\,\boldsymbol{e}_1 + m\,\boldsymbol{e}_2 + k\,\boldsymbol{e}_3), \qquad a = \frac{d}{\sqrt{2}}, \tag{1}$$

where $n, m, k, \frac{n+m+k}{2}$ are integers, $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$ are orthogonal unit vectors, $2a$ is the lattice spacing.

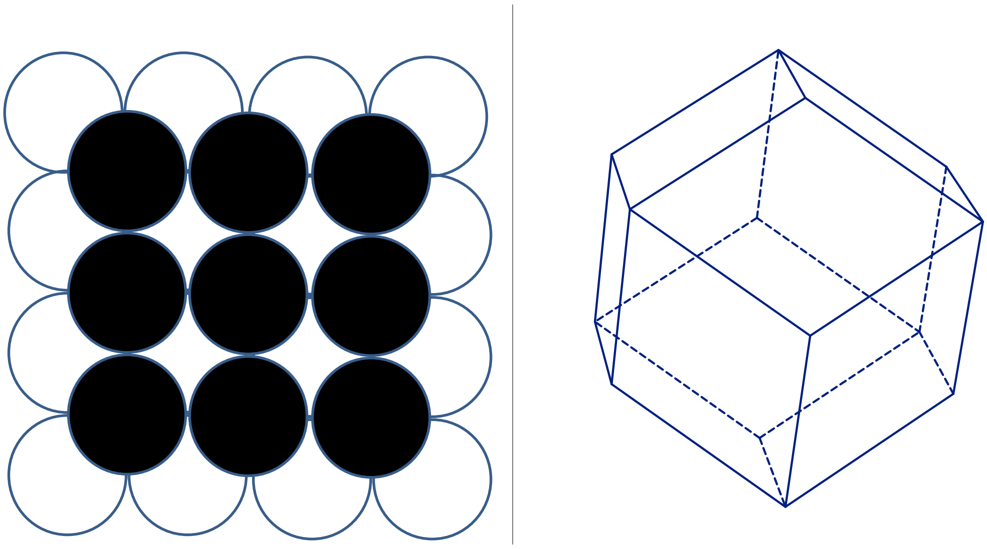

Fig. 1. Two layers of particles (left) and a unit cell (right) of the FCC lattice.

Particles are randomly displaced from their positions given by formula (1). Amplitudes of random displacements are chosen according to the following algorithm. The minimum distance, d_{min}, between the particles is specified. For each particle, the corresponding unit cell is constructed. The particle is connected to 12 nearest neighbors by line segments. Then planes, orthogonal to segments, and passing through their centers are drawn. The unit cell is a body bounded by these planes. In the case of FCC, the unit cell has a shape of rhombic dodecahedron (see figure 1). The unit cell is compressed by the following factor:

$$k_{dev} = 1 - \frac{d_{min}}{d} \tag{2}$$

Random displacements of particles are chosen such that the following three conditions are satisfied. Firstly, the particle belong to the compressed unit cell. Secondly, the particle is outside the sphere, inscribed into the compressed cell. Thirdly, the particle is outside the cube such that midpoints of its edges coincide with middle points of sides of the compressed unit cell. Thus, particle positions belong to the volume given by the difference between the compressed unit cell and union of the inscribed sphere and the cube.

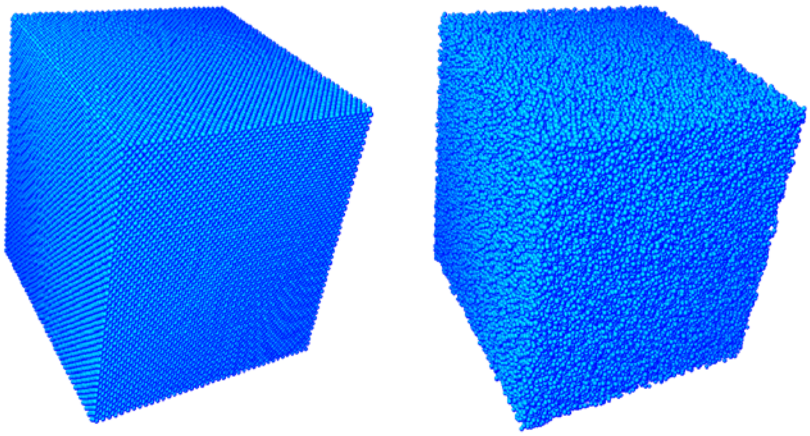

Fig. 2. Regular FCC lattice (k_{dev} = 0, left) and quasi-random lattice (k_{dev}=0.7, right).

Thus, amplitude of particle displacements is determined by parameter k_{dev}. For $k_{\mathrm{dev}} = 0$, particles form a perfect FCC lattice. For $0 < k_{\mathrm{dev}} < 1$, particle positions are random. At the same time, particles remain in their unit cells. Therefore, the lattice is referred to as the quasi-random.

Interparticle interactions are described by linear springs. Two particles are connected by the spring, if the distance between them is less than a_{cut}. Equilibrium length of the spring is equal to the initial distance between particles. Therefore initially forces in all springs are equal to zero. Force $\boldsymbol{F}_{ij}$ acting between particles i, j is calculated as

$$\boldsymbol{F}_{ij} = c_{ij}\left(R_{ij} - d_{ij}\right)\boldsymbol{e}_{ij}, \tag{3}$$

where $\boldsymbol{e}_{ij} = \frac{\boldsymbol{R}_{ij}}{R_{ij}}$, $\boldsymbol{R}_{ij} = \boldsymbol{R}_j - \boldsymbol{R}_i$, c_{ij} is the bond stiffness, d_{ij} is the equilibrium bond length. The bond stiffness is inversely proportional to bond length, i.e.

$$c_{ij} = c_L \frac{d}{d_{ij}}, \tag{4}$$

where c_L is characteristic value of the bond stiffness, d is the characteristic distance between neighboring particles, given by formula (1).

Thus, elastic properties of the quasi-random lattice depend on four parameters: c_L, d, a_{cut}, k_{dev}. In the following sections, we show that fitting these parameters yields isotropic material with prescribed elastic properties.

3. Isotropy of the quasi-random lattice

In the present section, we show that a proper choice of random displacements of particles (k_{dev}) allows to create a material with isotropic elastic properties.

Elastic properties of the quasi-random lattice are calculated numerically as follows. By construction, the lattice is orthotropic and it has cubic symmetry. Therefore two test problems are sufficient for calculation of elastic properties. In the first problem, the cubic sample under periodic boundary conditions is subjected to uniform uniaxial strain, ε_{11}. Normal stresses in the direction of stretching, σ_{11}, and in the orthogonal direction, σ_{22}, are calculated. Then coefficients of the stiffness tensor C_{11}, C_{12} are calculated as

$$C_{11} = \frac{\sigma_{11}}{\varepsilon_{11}}, \qquad C_{12} = \frac{\sigma_{22}}{\varepsilon_{11}} \tag{5}$$

In the second problem, the cubic sample is subjected to uniform shear deformation, ε_{12}. Corresponding shear stresses are calculated. Then the stiffness coefficient is as follows

$$C_{44} = \frac{\sigma_{12}}{2\,\varepsilon_{12}} \tag{6}$$

Thus, the test problems yield components C_{11}, C_{12}, C_{44} of the stiffness tensor.

Anisotropy of the material is characterized by the following parameter [10]:

$$\eta = \frac{2C_{44}}{C_{11}-C_{12}} \tag{7}$$

The anisotropy parameter η is equal to 1 for isotropic materials. Since η is dimensionless, then it depends only on dimensionless parameters of the model $k_{\rm dev}$ and a_{cut}/d. The value of $a_{cut} = 1.9d$ was chosen using trial and error approach in the problem of crack propagation. This value ensures that strength of the lattice is isotropic. Therefore it is sufficient to consider the dependence of η on $k_{\rm dev}$. Parameters of numerical simulations are summarized in table 1.

Table 1. Numerical parameters used for calculation of elastic properties. Here $\beta_{cr} = \sqrt{c_L m}$, m is particle's mass. Leapfrog integration scheme is used.

Interaction radius (a_{cut})	1.9 d
Size of the computational domain	28 d
Initial deformation ($\varepsilon_{11} = \varepsilon$, $\varepsilon_{12} = \varepsilon/2$)	$\varepsilon = 10^{-4}$
Viscous friction coefficient	$1.0 \cdot \beta_{cr}$
Time step	$0.02\,\pi \left(\frac{d_{\min}}{d}\right)^{1/2} \sqrt{\frac{m}{c_L}}$

Resulting dependence of the anisotropy parameter, η, on the amplitude of random displacements of particles ($k_{\rm dev}$) is shown in figure 3. As expected, the anisotropy parameter decreases for sufficiently large $k_{\rm dev}$. Isotropy of elastic properties is reached at $k_{\rm dev} \approx 0.67$.

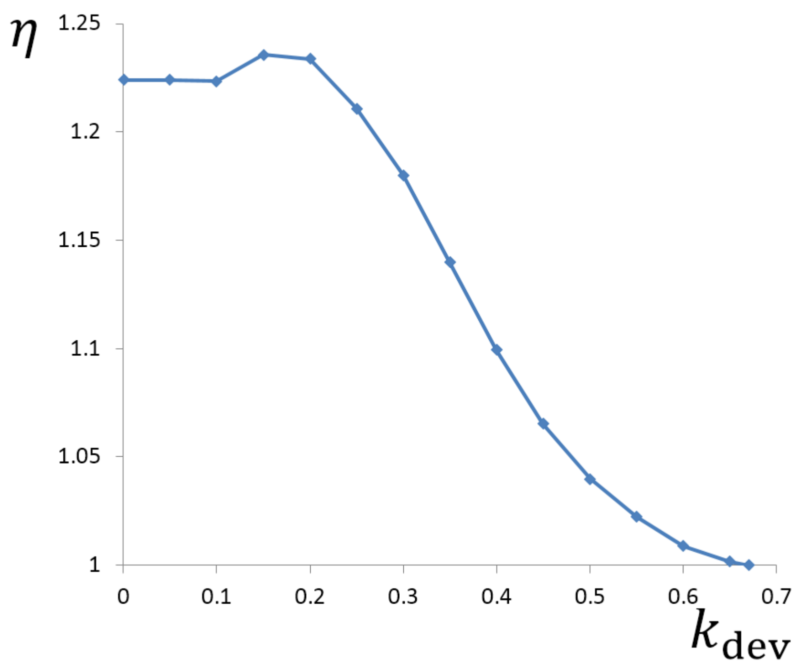

Fig. 3. Dependence of the anisotropy parameter on the amplitude of random displacements of particles ($a_{cut} = 1.9\ d$). Points show the results averaged over 10 realizations.

4. Changing Poisson's ratio of the quasi-random lattice

Elastic properties of the isotropic material, described in the previous section, are characterized by Young's modulus and Poisson's ratio. Proper choice of bond stiffnesses, c_L, allows to fit any value of Young's modulus. At the same time, Poisson's ratio of this material is fixed. Numerical simulations show that it is equal to 0.255. In the present section, we show that adding three-particle interactions (angular springs) allows to change Poisson's ratio in the interval from 0 to 0.414.

Potential energy of the spring connecting pairs of particles i, j and i, k reads

$$\Pi = \frac{1}{2} c_\varphi (\varphi - \varphi_0)^2, \qquad (8)$$

where c_φ is the stiffness of angular spring, φ is the angle between the bonds, φ_0 is the initial value of φ. Forces acting on particles i, j, k, caused by the spring, are the following

$$\boldsymbol{F}_j = \frac{c_\varphi}{R_{ij}} \Delta\boldsymbol{\varphi} \times \boldsymbol{e}_{ij}, \quad \boldsymbol{F}_k = -\frac{c_\varphi}{R_{ik}} \Delta\boldsymbol{\varphi} \times \boldsymbol{e}_{ik},$$

$$\Delta\boldsymbol{\varphi} = (\varphi - \varphi_0) \frac{\boldsymbol{e}_{ij} \times \boldsymbol{e}_{ik}}{|\boldsymbol{e}_{ij} \times \boldsymbol{e}_{ik}|}, \quad \boldsymbol{F}_i = -\boldsymbol{F}_j - \boldsymbol{F}_k, \qquad (9)$$

where $\boldsymbol{e}_{ij} = \frac{\boldsymbol{R}_{ij}}{R_{ij}}$, $\boldsymbol{R}_{ij} = \boldsymbol{R}_j - \boldsymbol{R}_i$, $\boldsymbol{R}_i$ is radius vector of particle i.

Angular springs are added using the following algorithm. For particle number i, all neighbors are found such that for each neighbor, j, the inequalities $L_{\min} < R_{ij} < a_{\text{cut}}$ are satisfied. Then all different triples i, j, k are formed such that distances R_{ij}, R_{ik}, and R_{ik} are all greater than $L_{\min}$. For each of these triples, three angular springs (in all three angles) are introduced. Stiffness of the angular spring between pairs i, j and i, k depends on lengths R_{ij}, R_{ik} as follows

$$c_\varphi = c_{\varphi 0} \left(\frac{\min(R_{ij}, R_{ik})}{d} \right)^2 \qquad (10)$$

For now on, the model has two additional dimensionless parameters $c_{\varphi 0}/(c_L\, d^2)$ and $L_{\min}/d$. These parameters are used in order to change Poisson's ratio of the quasi-random lattice. Dependence of Poisson's ratio on stiffness of the angular spring for fixed $L_{\min} = 1.7d$ is shown in figure 4.

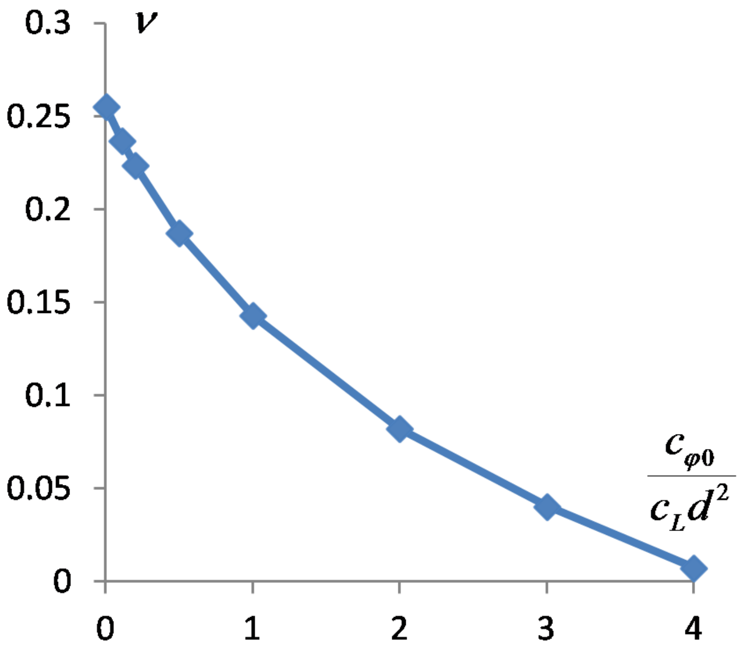

Fig. 4. Dependence of Poisson's ratio on angular stiffness $c_{\varphi 0}/(c_L\, d^2)$.

It is seen that increasing the angular stiffness, we change Poisson's ratio in the interval from 0.255 (for $c_{\varphi 0} = 0$) to 0 (for $c_{\varphi 0} \approx 4 c_L d^2$).

In order to achieve Poisson's ratios larger than 0.255, angular springs with negative stiffness should be used. Then we fix $c_{\varphi 0} = -0.11 c_L\, d^2$ and change the ratio $L_{\min}/d$. The ratio controls the average number of angular springs per particle. For $L_{\min} = a_{\text{cut}} = 1.9d$, angular springs are absent. The dependence of Poisson's ratio on $L_{\min}/d$ is shown in figure 5.

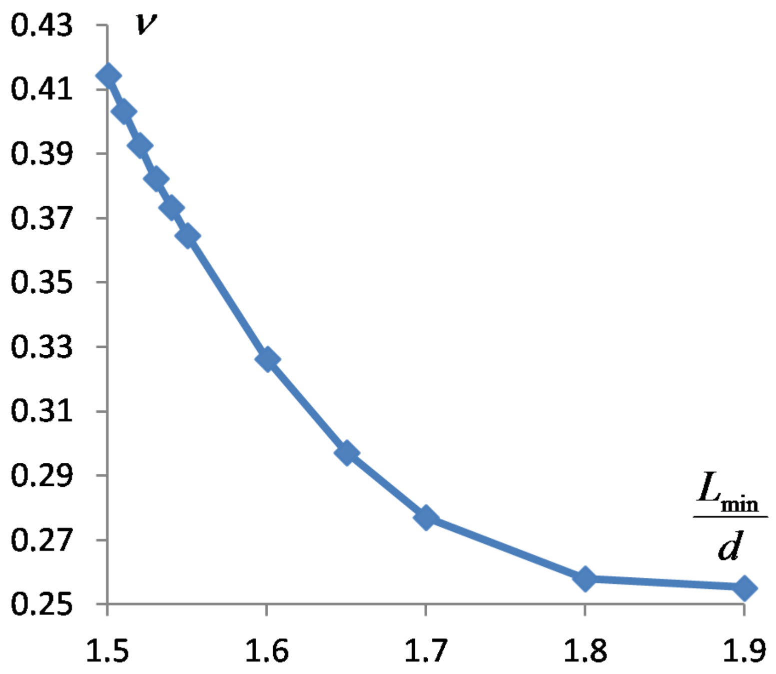

Fig. 5. Dependence of the Poisson's ratio on number of angular springs per particle, controlled by parameter $L_{\min}/d$.

Thus changing the number of angular springs per particle (parameter $L_{\min}/d$), values of Poisson's ratio up to 0.414 can be reached.

5. Conclusions

An algorithm for generation of three-dimensional quasi-random lattices was presented. Particle positions were generated by randomly displacing nodes of the face-centered cubic lattice. It was shown that elastic properties of the quasi-random lattice are isotropic, provided that the amplitude of random displacements is sufficiently large. In order to control both Young's modulus and Poisson's ratio of the material, the particles were connected by linear and angular springs. Choosing stiffness of linear springs, any value of Young's modulus can be fitted. Angular springs allows to change Poisson's ratio in the interval [0; 0.414], which is sufficient in many applications. Simulation of incompressible materials ($\nu = 0.5$) remains a challenge.

The presented model can be generalized in order to simulate brittle fracture. A criterion for bond breakage should be added. Then preliminary calculations show that if elastic properties of the quasi-random lattice are isotropic, then its strength is also isotropic. Therefore, the model can be used, for example, for simulation of crack propagation in isotropic materials. In particular, hydraulic fracturing in naturally fractured reservoirs [16] can be simulated. However, detailed discussion of crack propagation is beyond the scope of the present paper.

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