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A local constitutive model with anisotropy evolution for homogeneous 2D biaxial deformation modes

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Abstract Granular materials in a biaxial box setup are simulated using the Discrete Particle Method. Both isotropic compression and pure shear experiments are performed to obtain the material parameters required for the simple local constitutive model proposed by Luding et al. With these parameters the model is capable of quantitatively reproducing the results obtained from simulations.

Keywords Granular materials · isotropic compression · simple shear · constitutive model

1 Introduction

Introduction is not yet written, plan is to combine experiments, simulations and theory (references to for example Behringer and Radjai)

2 Molecular Dynamics

2.1 Discrete Particle Model

Granular materials are modeled as grains which deform under stress. However realistic modeling of the deformations of the particles is usually much too complicated. Therefore particle deformation is modeled as a normal interaction force, where the magnitude of the force is proportional to the overlap Δ of two circular particles. When all forces f_i^p acting on particle p, either from other particles, from boundaries or from external sources are known, the modeling of granular material is reduced to the integrations of Newton's equations of motion for all particles:

$$m_p \ddot{x}_i^p = f_i^p \tag{1}$$

where m_p is the mass of particle p and x_i^p the location of particle p. In this paper two types of forces are introduced, interaction forces between particles and background damping. So Newton's law is extended to:

$$m_p \ddot{x}_i^p = \sum_{q \in P} f_i^{pq} - \gamma_b \dot{x}_i^p \tag{2}$$

with P the collection of all particles, f_i^{pq} the force due to the interaction between particle p and q and γ_b the background friction. The background damping is added to prevent the system from reaching a steady state, where all particles have a velocity, but there is no change in the interaction forces.

2.2 Interaction Model

Consider two particles at locations x_i^p and x_i^q respectively. The vector connecting the two particles is called the branch vector: (see Fig 1)

$$l_i^{pq} = x_i^q - x_i^p \tag{3}$$

The two particles p and q interact only if they are in contact, so that their overlap:

$$\Delta^{pq} = (r^p + r^q) - |l^{pq}| \tag{4}$$

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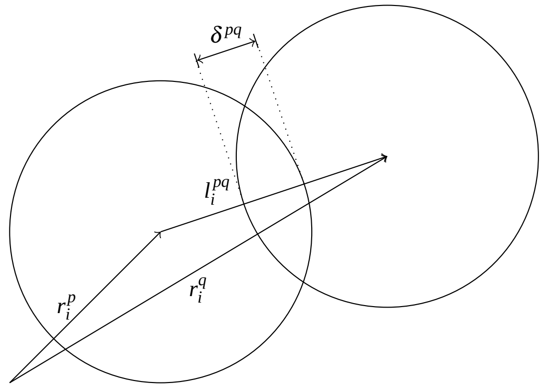
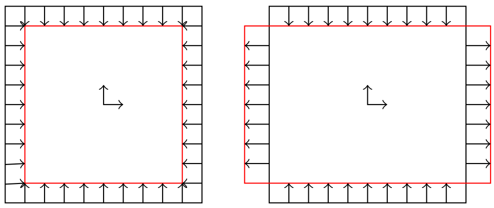


Fig. 1 Two particles in contact



(a) Isotropic compression (b) Pure Shear

Fig. 2 The two deformation modes

is positive. In this case the Particles exert a force on each other. This force consist of the terms. The first term is proportional to the overlap and is used to model particle deformation. The second term is proportional to the relative velocity and is used to model the loss of energy due to particle deformations.

$$f_i^{pq} = \begin{cases} -\left(k\Delta^{pq} + \gamma_p \dot{\Delta}^{pq}\right) n_i^{pq} & \text{if } \Delta^{pq} > 0 \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

with k the spring constant, γ_p the particle-particle friction and n_i^{pq} the unit normal pointing from particle p to particle q. Also the contact pair is added to the list of all contacts C.

2.3 Model system

The experiment used in this research is the biaxial box setup. All boundary conditions are periodic to avoid boundary effects. In a typical simulation the distance between the periodic boundaries is changed to simulate compression or expansion. This deformation is performed slowly according to a half cosine function, in order to avoid shocks and inertia effects. Moreover two main deformation modes are used, the isotropic compression (Fig 2(a)), where all boundaries have the same relative motion ($\varepsilon_{xx} = \varepsilon_{yy}$) and the pure shear (Fig 2(b)), where the volume of the sample is kept constant, while the boundaries are moved in opposite direction ($\varepsilon_{xx} = -\varepsilon_{yy}$).

Table 1 Simulation parameters

Parameter	Value	Explanation
k	10000 Nm^{-1}	Contact stiffness
γ_b	0.0294 Nsm^{-1}	Background friction
γ_w	10.0 Nsm^{-1}	Wall friction
γ_p	0.2938 Nsm^{-1}	Inter particle friction
p^0	100 Nm^{-1}	Initial pressure
ρ	20 kgm^{-2}	Particle density

2.4 Parameters

The parameters used in this study are shown in table 1. Initial conditions are generated using 1000 particles with radii r^p randomly drawn from a homogeneous distribution between $r^{min} = 3.7\cdot 10^{-3}$ m and $r^{max} = 7.4\cdot 10^{-3}$ m. Resulting in a two-particle eigenfrequency of 4.8 s^{-1} for the smallest particles. The time step used in the Verlet algorithm is chosen as a fiftieth of the half period vibration time:

$$\Delta t = \frac{\pi}{50\sqrt{\frac{k}{m}}} \approx 1.3\cdot 10^{-5}\ \mathrm{s} \tag{6}$$

The inter particle friction is chosen such that the coefficient of restitution for the smallest particles equals 0.8. The background damping is chosen to be an order of magnitude smaller then the inter particle friction to achieve rapid equilibration, without have to much influence on the stresses.

2.5 Initial configuration

Initially, the particles are randomly distributed in a huge box. Then the box is compressed where the movement of the two walls is dependent on the stress in the domain.

$$m_w \ddot{L_x} = -\gamma_w \dot{L_x} + \left(\sigma_{xx} - p^0\right) L_y \tag{7}$$
$$m_w \ddot{L_y} = -\gamma_w \dot{L_y} + \left(\sigma_{yy} - p^0\right) L_x \tag{8}$$

Because of the three different methods of damping available in the system (particle-particle damping, background damping and wall damping), the system will relax to a steady isotropic situation.

3 Constitutive Model

In this section a short overview of the used constitutive model is given. For more information the reader is referred to the work of Magnanimo and Luding [1, 2]. The model starts from the incremental Hooke's Law:

$$\delta\sigma_{ij} = C_{ijkl}\,\delta\varepsilon_{kl} \tag{9}$$

Whenever the major and minor symmetries of the stiffness tensor C are considered, the system can be rewritten into (for 2D systems):

$$\begin{bmatrix}\delta\sigma_{11}\\ \delta\sigma_{22}\\ \delta\sigma_{12}\end{bmatrix} = \begin{bmatrix}C_{1111} & C_{1122} & C_{1112}\\ C_{1122} & C_{2222} & C_{1222}\\ C_{1112} & C_{1222} & C_{1212}\end{bmatrix}\begin{bmatrix}\delta\varepsilon_{11}\\ \delta\varepsilon_{22}\\ \delta\varepsilon_{12}\end{bmatrix} \tag{10}$$

However in the bi-axial geometry with periodic boundary conditions, the stress and strain tensor only have diagonal components:

$$\begin{bmatrix}\delta\sigma_{11}\\ \delta\sigma_{22}\end{bmatrix} = \begin{bmatrix}C_{1111} & C_{1122}\\ C_{1122} & C_{2222}\end{bmatrix}\begin{bmatrix}\delta\varepsilon_{11}\\ \delta\varepsilon_{22}\end{bmatrix} \tag{11}$$

Now the stresses and strains can be decomposed into an (isotropic) volumetric and a (pure shear) deviatoric part ($\overline{\overline{\varepsilon}} = \overline{\overline{\varepsilon}}^V + \overline{\overline{\varepsilon}}^D$ and $\overline{\overline{\sigma}} = \overline{\overline{\sigma}}^V + \overline{\overline{\sigma}}^D$), with:

$$\begin{aligned}\overline{\overline{\varepsilon}}^V &= \left(\frac{\varepsilon_{xx}+\varepsilon_{yy}}{2}\right)\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} = \varepsilon^v\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\\ \overline{\overline{\sigma}}^V &= \left(\frac{\sigma_{xx}+\sigma_{yy}}{2}\right)\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} = \sigma^v\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\end{aligned} \tag{12}$$

$$\begin{aligned}\overline{\overline{\varepsilon}}^D &= \overline{\overline{\varepsilon}} - \overline{\overline{\varepsilon}}^V = \gamma\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} = \left(\frac{\varepsilon_{xx}-\varepsilon_{yy}}{2}\right)\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\\ \overline{\overline{\sigma}}^D &= \overline{\overline{\sigma}} - \overline{\overline{\sigma}}^V = \tau\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} = \left(\frac{\sigma_{xx}-\sigma_{yy}}{2}\right)\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\end{aligned} \tag{13}$$

Leading to:

$$\begin{bmatrix}\delta\sigma^v\\ \delta\tau\end{bmatrix} = \begin{bmatrix}2B & A\\ A & 2G\end{bmatrix}\begin{bmatrix}\delta\varepsilon^v\\ \delta\gamma\end{bmatrix} \tag{14}$$

Where the bulk modules B, the shear modulus G and the anisotropy A are defined as:

$$B = \frac{C_{1111}+C_{2222}+2C_{1122}}{4} \tag{15}$$

$$A = \frac{C_{1111}-C_{2222}}{2} \tag{16}$$

$$G = \frac{C_{1111}+C_{2222}-2C_{1122}}{4} \tag{17}$$

Two small modifications to the standard model are made, a non-linear stress evolution and a varying anisotropy, which are both explained in the following sections.

3.1 Non-linear stress evolution

The first modification is a non-linear stress evolution. From DEM simulations it is observed that for increasing shear strains, the stress increments decrease until the stress saturates in the critical state regime. This is modeled by multiplying the incremental shear strain with the stress anisotropy S:

$$\begin{bmatrix}\delta\sigma^h\\ \delta\tau\end{bmatrix} = \begin{bmatrix}2B & A\\ A & 2G\end{bmatrix}\begin{bmatrix}\delta\varepsilon^v\\ S\delta\gamma\end{bmatrix} \tag{18}$$

Where the stress anisotropy is defined as:

$$S = 1 - \frac{\tau}{\sigma^h}\frac{\operatorname{sign}(\delta\gamma)}{s^d_{max}} \tag{19}$$

Where $s^d_{max} = \left(\frac{\tau}{\sigma^h}\right)_{max}$ is the absolute maximum allowable deviatoric stress ratio in the material.

3.2 Varying anisotropy

The second modification is to assume a non constant anisotropy A, but one who is described by an evolution equation dependent on the shear stress:

$$\frac{dA}{d\gamma} = -\beta_A \Phi\left(A_{max} + \operatorname{sign}(\delta\gamma)A\right) \tag{20}$$

With A_{max} the absolute maximum allowable anisotropy in the material and β_s a parameter that determines how fast the anisotropy changes and thus how fast saturation is approached. The importance of the parameter Φ is still an ongoing investigation, several arguments exist for setting it equal to S as well as for leaving it to 1. In this paper is is set to 1 everywhere. If $\delta\gamma$ does not change sign, equation 20 can be solved analytically:

$$A = -\operatorname{sign}(\delta\gamma)A_{max}\left(1 - e^{-\beta_A|\gamma|}\right) + e^{-\beta_A|\gamma|}A_0 \tag{21}$$

With A_0 the initial anisotropy.

4 Results

From the simulation data fabric, stresses and stiffnesses are calculated using:

$$\sigma_{ij} = \frac{k}{L_x L_y}\sum_{c\in C}\Delta^c_i l^c_j \tag{22}$$

$$C_{ijkl} = \frac{k}{L_x L_y}\sum_{c\in C}\left(r^{c^{p1}} + r^{c^{p2}}\right) l^c_i n^c_j n^c_k n^c_l \tag{23}$$

Where C is the collection of all contacts and $p1$ and $p2$ are the two interaction particles.

4.1 Isotropic compression

The results of simulations on isotropic compression are displayed in Fig. 3. The volumetric stress scales linear with the volumetric strain, which allows us to calculate the bulk modules B used in the model from the slope of the curve ($2B = 10421$ N/m). The shear stress remains roughly constant during the compression, indicating an initial isotropic situation ($A = 0$ and $S = 1$). Some small deviations from zero shear stress are observed due to non-affine motion of the particles.

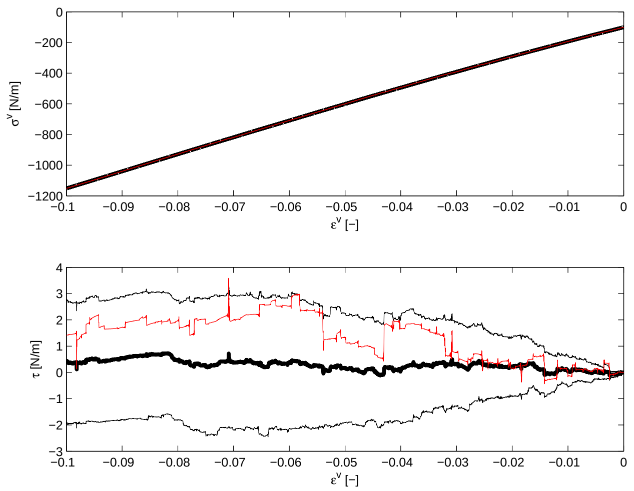


Fig. 3 Volumetric and shear stress as a function of volumetric strain for the isotropic compression simulations. The red line is a typical single simulation result, the thick black line the average of 100 realizations, and the thin black lines the average plus or minus the standard deviation. The volumetric stress (top figure) is in this case a linear function of the volumetric strain with a slope of $2B = 10421$ N/m, whereas the shear stress (bottom figure) stays almost constant at 0 N/M

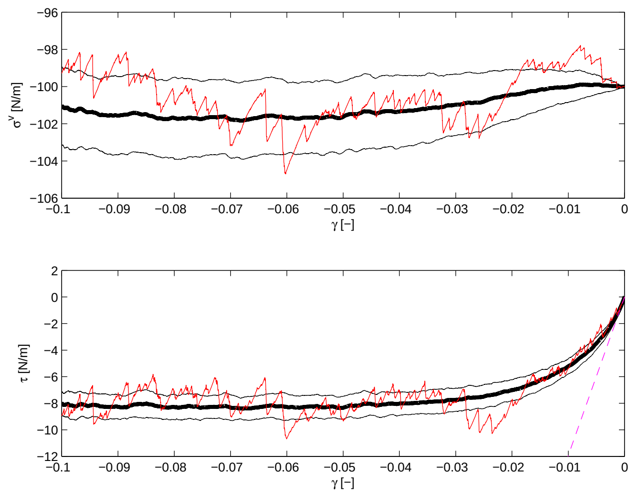


Fig. 4 Volumetric and shear stress as a function of shear strain for the pure shear simulations (in this case horizontal compression and vertical extension) . The red line is a typical single simulation result, the thick black line the average of 100 realizations, and the thin black lines the average plus or minus the standard deviation. The volumetric stress (top figure) is roughly constant during the simulation, while the shear stress (bottom figure) decreases quite rapidly initially and settles at a level of -8 N/m. The dotted magenta line indicates the initial slope of $2G = 1193$ N/m. (see also Fig. 5)

4.2 Pure Shear

The results of simulations on pure shear are visible in Fig. 4. A decrease in deviatoric stress is visible, until the system reaches the critical regime at a deviatoric strain of approximately $\gamma = 0.03$ and a stress level of $\tau = -8$ N/m indicating that the maximum allowable deviatoric stress ratio in the constitutive model should be $s^d_{max} = 0.08$. A zoom of the results for small stress is visible in Fig. 5. From this picture we can obtain the initial slopes of both stresses. For the volumetric stress this slope is zero, indicating an initially isotropic material (just as from the isotropic compression case). For the deviatoric stress this slope is equal to the term $2GS_0 = 1193$ N/m in the constitutive model, with $S_0 = 1$.

The only two remaining parameters in the model are the maximum anisotropy A_{max} and the parameter β_A which determines the growth rate of the anisotropy. An estimate of these parameters can be obtained from looking at the evolution of the stiffness during the shear deformation. This is done by looking at the normalized anisotropy level:

$$\frac{A}{2B} = \frac{C_{1111} - C_{2222}}{C_{1111} + C_{2222} + 2C_{1212}} \tag{24}$$

A plot of this anisotropy is shown in Fig. 6. In this graph the exponential behavior of the anisotropy becomes clear. The green line shows an exponential fit to equation 21 with $A_{max}/2B = 0.026$ and $\beta_A = 72.4$.

Now all parameters are determined (see Table 2 for the values) the model is able to predict the stress quite well as can be seen in Fig. 7.

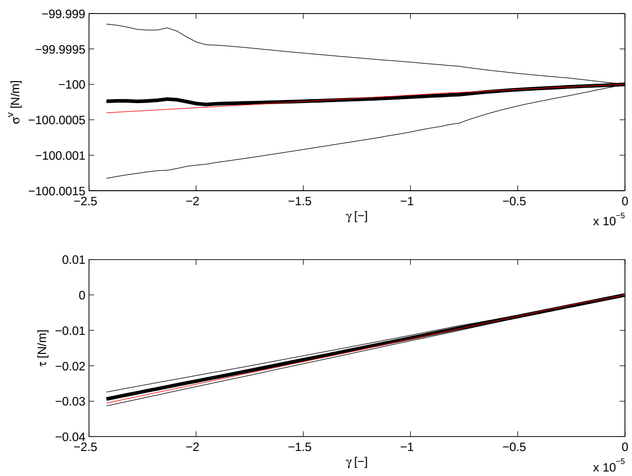


Fig. 5 Zoom of figure 4 for small shear strain to show the initial slopes. For the volumetric stress the slope is $A \approx 0$ N/m and for the shear stress the slope is $2GS = 1193$ N/m

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Table 2 Model parameters

Parameter	Explanation	Value
B	Bulk modulus	5210 N/m
G	Shear modulus	597 N/m
β_A	Anisotropy growth parameter	72.4
A_0	Initial anisotropy	0
A_{max}	Maximum anisotropy	271

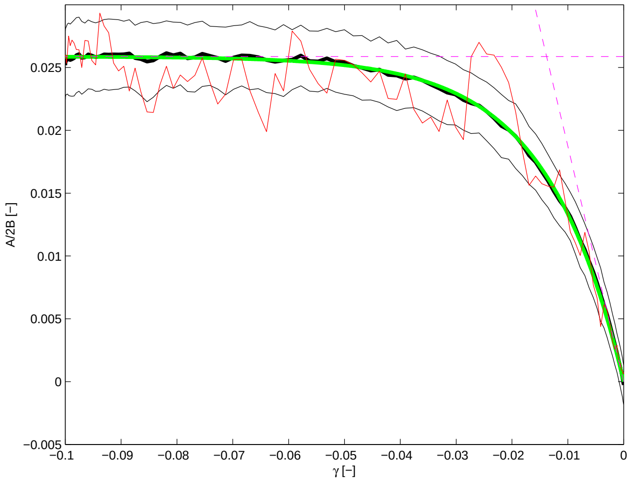

Fig. 6 Anisotropy divided by the bulk modulus as a function of shear strain for the pure shear simulations. The red line is a typical result, the thick black line the average of 100 realizations, the thin black lines the average plus or minus the standard deviation and the green line is an exponential fit to equation 21. The initial slope is indicated by the right part of the magenta dashed line and equals $-\frac{A_{max}\beta_A}{2B} = 1.88$. The left part of the line indicates the saturation level of $A_{max}/2B = 0.026$.

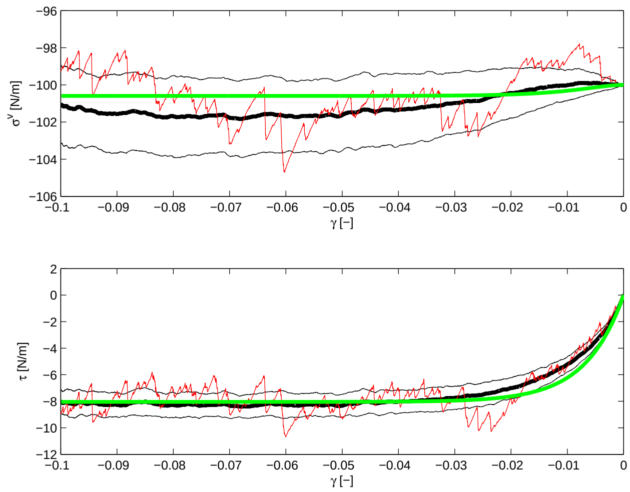

Fig. 7 The same as Fig. 4, only now the green line indicates the model predictions. Good agreement is achieved for both stresses.

5 Conclusion

In this paper granular materials are simulated using normal springs as the interaction model. Isotropic compression and simple shear simulations are performed to obtain the parameters required for the constitutive model proposed by Luding et al. [1]. With these parameters the model is capable of quantitatively reproducing the results obtained from the simulations.

References

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