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

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Abstract

A local constitutive model for granular materials with anisotropy is proposed and applied to various biaxial box deformation modes. The simplified version of the model (in the coordinate system of the biaxial box) involves only scalar values for hydrostatic and shear stresses, for the isotropic and shear strains as well as the new parameter, the (scalar) anisotropy modulus.

A non-linear constitutive evolution equation, for both shear stress and anisotropy, during deviatoric (shear) deformation is based on observations gained from Discrete Element Method (DEM) simulations. While parameters like the bulk modulus are set to constant, for the sake of simplicity, the model involves a yield stress and a maximal anisotropy as well as the corresponding deviatoric shear-rate pre-factors for incremental stress and incremental anisotropy modulus.

In this study, the self-consistency of the model is discussed before it is applied to various biaxial deformation modes. Constant anisotropy is compared to evolving anisotropy, where the sign accounts for the direction (vertical or horizontal). Generalization to arbitrary orientation and possible non-coaxial strain, stress and fabric tensors is not attempted in this study.

1 Introduction

Dense granular materials show peculiar mechanical properties quite different from classical fluids or solids [1, 2]. These phenomena involve dilatancy, yield stress and history dependence – among many others. The reason is the inherent discrete structure of particulate packings that is far from understood [3–11]. Particularly, if a granular packing is subject to isotropic compression the shear stress remains close to zero and the major control parameters are the volume fraction and the pressure. However, under shear deformation, not only shear stress builds up until it reaches a yield-limit, but also the anisotropy of the contact network develops, as related to the creation and destruction of contacts and force-chains, see e.g. [12–16] and also Ref. [9] and references therein. These phenomena are at the origin of the interesting behavior of granular media, in particular their “memory”, i.e., their history dependence The contact structure, its evolution and especially its anisotropy are neglected in many continuum models of particulate matter.

In order to better understand and model the deformation behavior of particle systems, the Discrete Element Method is a very useful tool [7, 11, 16–18]. From the analysis of such simulations, when using consistent averaging procedures [18–24], useful relations can be derived between the fabric, strain and stress tensors. The collective behavior of the particles can then be described by a homogenized model, using macroscopic definitions and formulations of these tensors. The homogenized model has advantages since it can be implemented in a FEM software to observe the deformation mechanisms in arbitrary (inhomogeneous) loading conditions.
Most of the existing models describe the constitutive behavior of granular materials but one important ingredient missing is the anisotropy and possible non-coaxiality of the macroscopic tensors. Only few theories, see e.g. [11, 16, 18, 25–27] and references therein, involve an anisotropy state variable or non-coaxiality; even less deal with both anisotropy and rotations [24,28–31]. The DEM simulations reveal that considerable anisotropy develops in the system during deformation. This is an essential part of the constitutive model because it contains the information how the different modes of deformation have affected the mechanical state of the system during the deformation. In this sense, the anisotropy is a history parameter.

In the following, a constitutive model that is based on observations from DEM simulations will be presented in its simplest form. Anisotropy is included in the model through the evolution of the stiffness tensor components in a prescribed manner. The (classical) isotropic and shear moduli are set constant, at first, in order to be able to focus on the effect of anisotropy exclusively.

2 Model System and Theory

The model system is shown schematically in Fig. 1 as used for the DEM simulations in Ref. [18]. In this system, the strain $\varepsilon_{22}$ in the $y$ direction and the normal stress $t = \sigma_{11}$ in the $x$ direction are prescribed. (Below we refer to this bi-axial deformation as mode 3). All bi-axial deformation modes, as specified below, can be described in a strain tensor with only diagonal components in the global coordinate system:

$$[\varepsilon] = \begin{bmatrix} \varepsilon_{11} & 0 \\ 0 & \varepsilon_{22} \end{bmatrix},$$  \hspace{1cm} (1)

which, naturally, are the eigenvalues of the strain tensor. This coordinate system is the natural choice and identical to the tensor-eigensystem, and thus identical to the bi-axial system walls, if there is no wall friction involved.

The stress that develops in the system also consists of the diagonal terms only (with components given in the global coordinate system):

$$[\sigma] = \begin{bmatrix} \sigma_{11} & 0 \\ 0 & \sigma_{22} \end{bmatrix}.$$  \hspace{1cm} (2)

Initially, an isotropic stress is applied to the system to confine the particles. The initial strain and stress conditions therefore are given as:

$$[\varepsilon_0] = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \hspace{0.5cm} [\sigma_0] = \begin{bmatrix} \sigma_0 & 0 \\ 0 & \sigma_0 \end{bmatrix},$$  \hspace{1cm} (3)

where $\sigma_0$ is the initial (isotropic) hydrostatic stress applied.

Figure 1: Illustration of the bi-axial model system used for the DEM simulations. The vertical displacement $\varepsilon_{22}(t)$ and the horizontal stress $\sigma_{11} = t = \sigma_0$ are prescribed.
One very important point for the model is the selection of a sign convention for strain and stress. In the present work, the general convention is positive (+) for dilatation, extension and negative (–) for compression, contraction. According to this definition, when the top boundary is moved inwards/downwards \( \varepsilon_{22} \) (the prescribed strain) will have a negative value whereas \( \varepsilon_{11} \), moving outwards, will be positive.

The strain can be decomposed into an isotropic part and a deviatoric part:

\[
\varepsilon = \varepsilon^V + \varepsilon^D. \tag{4}
\]

The isotropic part is given as

\[
\varepsilon^V = \frac{\varepsilon_{11} + \varepsilon_{22}}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \varepsilon^v I = \frac{1}{D} \text{tr}(\varepsilon) I, \tag{5}
\]

with dimension \( D \), so that the volume change is \( \text{tr}(\varepsilon) = 2\varepsilon^v \) in the following. (Note that the abbreviation \( \text{tr}(\varepsilon) = \varepsilon^\text{vol} \) is used in many other studies, however, we adopt the alternative definition that involves the division by dimension — similar to the definition of the pressure (isotropic stress \( \sigma^h \)) below). Accordingly the deviatoric part is:

\[
\varepsilon^D = \varepsilon - \varepsilon^V = \frac{\varepsilon_{11} - \varepsilon_{22}}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \frac{\varepsilon_{11} - \varepsilon_{22}}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \gamma I^D, \tag{6}
\]

where \( \gamma \) is the scalar that describes the pure shear deformation as \( \gamma = \frac{\varepsilon_{11} - \varepsilon_{22}}{2} \) and \( I^D \) is the traceless unit-deviator in 2D. The unit-deviator has the eigenvalues, +1 and –1, with the eigendirections \( \hat{n}(+1) = \hat{x} \) and \( \hat{n}(-1) = \hat{y} \), where the hats denote unit vectors.

As seen in Eq. (5) the isotropic part can be expressed fully using only one scalar, independent of the coordinate system chosen. This defines the isotropic strain and hence the amount of volume change. Positive and negative \( 2\varepsilon^v \) correspond to volume increase and decrease, respectively.

The same type of interpretation is not possible for the deviatoric part in general. According to the coordinate system that is chosen, the sign of the shear deformation changes, e.g., when the \( x \) and \( y \) directions are exchanged. Equivalently, when the deviatoric (shear) strain \( \gamma \) changes sign, the deformation is reversed. An additional point concerning the strain terms is therefore the selection of the coordinate system and the type of deformation. If the coordinate system chosen is rotated from the biaxial orientation or the prescribed deformation is different from Eq. (1), one has off-diagonal terms, as discussed below. In order to keep the model as simple as possible, we restrict ourselves to biaxial deformations and the biaxial orientation of the coordinate system.

### 2.1 Alternative formulation for arbitrary orientation

To further elaborate this issue, we compare the two possible representations of the deviatoric part of a symmetric tensor. The first one is to define a positive scalar and let an orientation tensor completely take care of the direction:

\[
\varepsilon^D = \varepsilon^d D(\phi_c), \quad \text{with: } \varepsilon^d = \frac{\left| \varepsilon_{11} - \varepsilon_{22} \right|}{2} = |\gamma|, \tag{7}
\]

and the oriented unit-deviator:

\[
D(\phi_c) = R(\phi_c) \cdot I^D \cdot R^T(\phi_c). \tag{8}
\]

with the angle between the horizontal and the positive eigen-direction of the deviator: \( \phi_c \in [0, \pi] \) (due to symmetry, \( \phi_c + \pi = \phi_c \)).

In the second case, which is not generally applicable, one allows the sign of the scalar value \( \gamma \) to be positive or negative and brackets the orientation angles:

\[
\varepsilon^D = \gamma D(\phi_c), \quad \text{with: } \gamma = \frac{\varepsilon_{11} - \varepsilon_{22}}{2}, \tag{9}
\]
\[ D(\varphi_\varepsilon) = R(\varphi_\varepsilon) \cdot I^D \cdot R^T(\varphi_\varepsilon). \] (10)

and \( \varphi_\varepsilon \in \left[ 0, \frac{\pi}{2} \right] \), since \( \varphi_\varepsilon + \frac{\pi}{2} = \varphi_\varepsilon \) but \( \gamma(\varphi_\varepsilon + \frac{\pi}{2}) = -\gamma(\varphi_\varepsilon) \).

Thus, in the general case, the magnitude of shear is represented by the positive scalar \( \varepsilon^d > 0 \) and the orientation by \( D(\varphi_\varepsilon) \). A reversal of strain direction then is indicated by a transition of \( \varphi_\varepsilon \rightarrow \varphi_\varepsilon + \frac{\pi}{2} \). However, in the biaxial system, it is possible to use \( \gamma \) and distinguish between the two possible directions \( \varphi_\varepsilon = 0 \) and \( \varphi_\varepsilon = \frac{\pi}{2} \) by the sign of \( \gamma \). This latter convention is adopted below, since the eigen-system does not rotate.

With the selection of the deformation and the coordinate system as described above, it is possible to define a rotation, which makes it possible to represent the shear strain with one scalar only. Since simple shear takes place at 45 degrees relative to the principal basis, one has:

\[ \varepsilon^S = R \left( \frac{\pi}{4} \right) \cdot \varepsilon^D \cdot R^T \left( \frac{\pi}{4} \right), \]

which gives:

\[ \varepsilon^S = \begin{bmatrix} 0 & \frac{\sigma_{22} - \sigma_{11}}{2} \\ \frac{\sigma_{11} - \sigma_{22}}{2} & 0 \end{bmatrix} = \gamma D \left( \frac{\pi}{4} \right). \] (12)

Eq. (12) shows that shear strain deformations (for the biaxial box geometry) can also be described with one scalar \( \gamma \), since the orientation is hidden in the directed unit-deviator.

The same definitions can be applied to the stress tensor as well. The decomposition in this case is for the hydrostatic stress and the deviatoric stress:

\[ \sigma = \sigma^H + \sigma^D. \] (13)

The hydrostatic part is given as

\[ \sigma^H = \frac{\sigma_{11} + \sigma_{22}}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \frac{1}{3} \text{tr}(\sigma) I. \] (14)

and, accordingly, the deviatoric part becomes:

\[ \sigma^D = \sigma - \sigma^H = \begin{bmatrix} \frac{\sigma_{11} - \sigma_{22}}{2} \\ 0 \end{bmatrix} = \sigma^d D(\phi_\varepsilon) = \tau I^D, \]

with \( \tau = \frac{\sigma_{11} - \sigma_{22}}{2} \).

In this case when the same rotation as above is performed, one obtains the magnitude of the shear stress:

\[ \sigma^S = R \left( \frac{\pi}{4} \right) \cdot \sigma^D \cdot R^T \left( \frac{\pi}{4} \right) = \begin{bmatrix} 0 & \frac{\sigma_{22} - \sigma_{11}}{2} \\ \frac{\sigma_{11} - \sigma_{22}}{2} & 0 \end{bmatrix} = \tau D \left( \frac{\pi}{4} \right), \]

where, according to their definition, both \( \gamma \) and \( \tau \) can be positive or negative.

### 2.2 Evolution equation for the anisotropy

Finally, the additional tensor (that will be used for the calculations in the next section) is the anisotropy modulus tensor, \( a^D \) (second order). This tensor originates in the stiffness tensor and defines the directions and the magnitude of the anisotropy. Using the same definitions as above, it can also be reduced to a scalar value, \( A \), since in the biaxial system anisotropy also evolves in only two directions:

\[ a^D = A I^D, \] with: \( A = \frac{C_{11} - C_{22}}{2} \),

where \( C_{11} \) and \( C_{22} \) are defined below.

In summary, for the biaxial system, the tensors \( \varepsilon^D, \sigma^D, \) and \( a^D \) can be represented by the scalars \( \gamma, \tau, \) and \( A \), respectively, while the orientation is fixed to \( I^D \). Change of sign corresponds to reversal of deformation, stress, or anisotropy, respectively.
### Governing equations

As in a general constitutive relation of anisotropic elasticity, the relation between stress and strain increments is:

$$\delta \sigma = C : \delta \varepsilon$$  \hfill (18)

where $C$ is the (rank four) stiffness tensor of the system. Since in the biaxial box we deal with two components of stress and strain only, the following reduction can be performed:

$$\begin{bmatrix} \delta \sigma_{11} \\ \delta \sigma_{22} \end{bmatrix} = \begin{bmatrix} C_{1111} & C_{1122} \\ C_{2211} & C_{2222} \end{bmatrix} \cdot \begin{bmatrix} \delta \varepsilon_{11} \\ \delta \varepsilon_{22} \end{bmatrix}.$$  \hfill (19)

For simplicity in notation, the components of the stiffness will be referred to with reduced indices according to Eq. (19), i.e., $C_{11} \equiv C_{1111}$, $C_{22} \equiv C_{2222}$, and $C_{12} \equiv C_{1122} = C_{21} \equiv C_{2211}$.

As shown in the previous section, the incremental evolution of the hydrostatic stress is then given as a scalar equation using Eq. (19):

$$\delta \sigma^h = \frac{\delta \sigma_{11} + \delta \sigma_{22}}{2} = \frac{C_{11} + C_{22} + 2C_{12}}{2} \delta \varepsilon^v + \frac{C_{11} - C_{22}}{2} \delta \gamma.$$  \hfill (20)

Similarly, the equation for incremental shear stress evolution is:

$$\delta \tau = \frac{\delta \sigma_{11} - \delta \sigma_{22}}{2} = \frac{C_{11} - C_{22}}{2} \delta \varepsilon^v + \frac{C_{11} + C_{22} - 2C_{12}}{2} \delta \gamma.$$  \hfill (21)

These equations serve as the basic governing equations of the model. As abbreviations, the following three scalars (moduli) are defined [18, 22]:

$$E = \frac{C_{11} + C_{22} + 2C_{12}}{2}, \quad G = C_{12}, \quad A = \frac{C_{11} - C_{22}}{2},$$  \hfill (22)

and the parameter combination $B = E - 2G$ is introduced. From the equations it is also apparent that $(E/2)$ is the bulk modulus due to Eq. (5), $B$ is the shear modulus, and $A$ is the anisotropy modulus that couples bulk stress to shear strain and shear stress to isotropic strain:

$$\delta \sigma^h = E \delta \varepsilon^v + A \delta \gamma.$$  \hfill (23)

Similarly, the equation for incremental shear stress evolution is:

$$\delta \tau = A \delta \varepsilon^v + B \delta \gamma.$$  \hfill (24)

They can be used in different ways utilizing the anisotropy or non-linearity in the formulations, which will be discussed below. In all cases assumed here, however, one should note that $C_{12} = C_{21}$ holds, so that a single anisotropy modulus $A$ is the only new parameter when compared to isotropic materials.

#### 3.1 Model without anisotropy

For the system to be isotropic, the stiffness in all directions should be the same. Hence, in the isotropic system $C_{11} = C_{22}$ must hold, so that $A = 0$. When anisotropy starts developing, this equivalence condition is lost, as discussed in the following subsection.

In the isotropic case, the second term in Eq. (23) and the first term in Eq. (24) vanish and one arrives at the equations:

$$\delta \sigma^h = E \delta \varepsilon^v$$  \hfill (25)

$$\delta \tau = B \delta \gamma.$$  \hfill (26)
It is clear, in this case, that the hydrostatic stress only depends on the isotropic strain and similarly the shear stress only depends on the shear strain. For constant $E$ and $B$, this special case is thus purely linear with isotropic and deviatoric components decoupled.

Note that both $E$ and $B$ will develop with respectively applied isotropic or deviatoric (shear) deformations. But since this is not the focus of this study, we only use constant $E$ and $B$ in the following.

### 3.2 Model with evolution of anisotropy

When there is anisotropy in the system, i.e., $C_{11} \neq C_{22}$, the complete version of Eqs. (23) and (24) must be used. Even though $A$ is defined as the scalar anisotropy modulus, in the general case, it is actually a tensorial quantity with a certain orientation. However, in the biaxial system, similar to the strain and stress, it can be reduced to a scalar quantity, which can have both positive and negative values. Positive in our convention means that the horizontal stiffness is larger than the vertical one, and negative implies the opposite.

From Discrete Element Method simulations [18] of an initially isotropic system, with $A_0 = 0$, during deformation, anisotropy builds up to a limit $A_{\text{max}}$. This a-posteriori rectified the assumption of constant $E$ and $B$, to first order, since these two quantities change much less than $A$ for mode 3 deformations, as discussed below. It is also observed that the anisotropy develops only due to shear strain and not due to isotropic strain. Therefore, the evolution of $A$ can be described as:

$$\frac{\partial A}{\partial \gamma} = -\beta_A \text{sign}(A_{\text{max}}) (A_{\text{max}} - A) \quad , \quad \frac{\partial A}{\partial \varepsilon^v} = 0 \quad , \quad \text{(27)}$$

with $A_{\text{max}} = -|A_{\text{max}}| \gamma/|\gamma| = -A^m \gamma/|\gamma| = -A^m \text{sign}(\gamma)$, with positive maximal anisotropy, $A^m$, i.e., the sign of $A_{\text{max}}$ is determined by the direction of shear. \(^1\) Note that Eq. (27) can also be written as

$$\frac{\partial A}{\partial |\gamma|} = \beta_A (A_{\text{max}} - A) \quad ,$$

or

$$\frac{\partial A}{\partial \gamma} = \beta_A \text{sign}(\gamma) (A_{\text{max}} - A) = \beta_A (-A^m - \text{sign}(\gamma)A) = -\beta_A (A^m + \text{sign}(\gamma)A) \quad ,$$

which actually are all equivalent to the form originally proposed in Refs. [18, 22], where only vertical compression and thus positive $\gamma$ was considered. \(^2\) The integrated form of Eq. (27) (using the exponential technique for ODE’s) is calculated as:

$$A = A_{\text{max}} - (A_{\text{max}} - A_0) \exp (-\beta_A |\gamma|) \quad . \quad \text{(28)}$$

This form of the evolution equation represents the fact that anisotropy starts at $A_0$ and then approaches exponentially fast to its maximum for large $\gamma$. For isotropic initial configuration, $A_0 = 0$, the growth is linear for small deformations $\gamma$, where the parameter $\beta_A$ determines how fast the anisotropy changes and thus also how fast saturation is approached. Typical values for these parameters – from DEM simulations – are $\beta_A \approx 80$, observed at small shear strain, and $A_{\text{max}} \approx 0.2E$, observed at large strain.

#### 3.2.1 Interpretation of the model

When $A_0 = 0$ the stress evolution equations (23) and (24) take the simple linear elastic form as shown in Eqs. (25) and (26). The hydrostatic stress grows linearly with isotropic strain and the

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1. Assume horizontal compression, which corresponds to $\gamma/|\gamma| < 0$, that leads to an increase of horizontal stiffness and thus a positive $A_{\text{max}}$. Compressively, compression in vertical direction leads to a negative $A_{\text{max}}$ – while tension in horizontal or vertical direction lead to negative and positive $A_{\text{max}}$, respectively.

2. The incremental anisotropy, here, is only defined for bi-axial deformation modes, i.e., for $\phi_v = 0$ (horizontal extension and vertical compression deviatoric strain) or $\phi_v = \pi/2$ (horizontal compression and vertical extension). A more general representation has still to be found.
shear stress is proportional to the shear strain. However, the underlying physics changes since anisotropy can develop to $A \neq 0$.

The presence of the $A$ term creates a cross-link between the two types of deformations, shear and isotropic. This is best visualized considering a pure shear deformation, i.e., $\varepsilon^v = 0$. In this case, for $A \neq 0$, the hydrostatic stress will start developing although the deformation is isochoric. This can be viewed differently as well: The build-up of compressive stresses during isochoric shear deformation is due to the anisotropy modulus in Eq. (23). In a closed boundary system this means that the material wants to expand but it is confined by the boundaries. Therefore, the governing equations predict that shear deformation will cause expansion of the anisotropic system. The explanation for this phenomenon is the interlocking of particles in the initial configuration. The system can not deform easily unless it is relaxed. The relaxation means that the system is creating more voids and hence is expanding.

The second equation (24) predicts that under purely isotropic compressive strain, the shear stress will increase. This will be realized considering the sign of the term involving $\varepsilon^v$. Compression and extension will lead to positive and negative changes of $\tau$, respectively. This result is plausible as it ensures symmetry in the system. If the stiffness is not isotropic, under compression, stress will develop differently in different directions. This will lead to principal stresses different from each other, hence shear stresses.

### 3.2.2 Energy, work, stability

Another important issue is the instability of the particulate system. This can be analyzed numerically using the system of equations introduced earlier. The stability condition for materials is [32]:

$$\delta^2 W = \delta \sigma : \delta \varepsilon \geq 0,$$

which is equivalent in this case to:

$$\delta \varepsilon : C : \delta \varepsilon \geq 0.$$

For Eq. (30) to have a solution, $C$ must be positive-definite. This implies that at the onset of instability, $C$ will not be positive-definite anymore. In this case it can be checked by considering the matrix form given in Equation (19). For the $C$ matrix to be singular its determinant must vanish, i.e., $\det C = 0$. Evaluating this analytically gives:

$$C_{11} C_{22} - C_{12}^2 = 0$$

$$\Rightarrow (E - A - G)(E + A - G) - G^2 = 0$$

$$\Rightarrow E^2 - 2EG - A^2 = EB - A^2 = 0.$$

Using Eq. (31), the value of $A$ that will cause the system to be unstable can be found. For a typical case where $B = E/2$ for instance the system will be unstable when $A$ reaches a value of $E/\sqrt{2} \approx 0.71E$. Note, that this is not (yet) consistent with typically observed values of $A_{\text{max}} \approx 0.2E$.

### 3.3 Non-linear stress evolution

It is observed from DEM simulations, in bi-axial deformation mode 3, that the response of the system to deformation is not always linear. As the amount of strain gets larger, the stress increments decrease until a level where the stress saturates. In Refs. [18, 22], the evolution equation that leads to saturation under vertical compression and horizontally prescribed stress, is expressed as:

$$\frac{\partial s_d}{\partial \gamma} = \beta_s \text{sign}(\gamma) (s_d^{\text{max}} - s_d)$$

where $s_d$ is the stress deviator ratio, given by:

$$s_d = \frac{\sigma_{11} - \sigma_{22}}{(\sigma_{11} + \sigma_{22})} = \frac{\tau}{\sigma^h},$$

$$7$$
and \( s_{d}^{\text{max}} = -|s_{d}^{\text{max}}| \gamma/|\gamma| = -s_{d}^{m} \gamma/|\gamma| = -s_{d}^{m} \text{sign}(\gamma) \), with positive maximum deviatoric stress ratio \( s_{d}^{m} \). There are two reasons to use \( s_{d} \) (instead of \( \tau \)). First, it is very similar to the Mohr-Coulomb plastic yield criterion, \( \mu \equiv s_{d}^{m} \), and second, as empirical observation, \( s_{d}^{m} \) does not much depend on the confining stress – which suggests that it is a material parameter (or at least a zero-order starting point).

The derivative of \( s_{d} \) with respect to \( \gamma \) reads

\[
\frac{\partial s_{d}}{\partial \gamma} = \frac{\partial}{\partial \gamma} \left( \frac{\tau}{\sigma^{h}} \right) = \frac{1}{\sigma^{h}} \left( \frac{\partial \tau}{\partial \gamma} - \frac{\tau}{\sigma^{h}} \frac{\partial \sigma^{h}}{\partial \gamma} \right),
\]

which, when inserting Eq. (32) and resolving with respect to \( \partial \tau / \partial \gamma \), leads to

\[
\frac{\partial \tau}{\partial \gamma} = \sigma^{h} \beta_{s} \text{sign}(\gamma) (s_{d}^{\text{max}} - s_{d}) + \frac{\tau}{\sigma^{h}} \frac{\partial \sigma^{h}}{\partial \gamma} = B (1 - s_{d}/s_{d}^{\text{max}}) + s_{d} A,
\]

after the second term of Eq. (23) is inserted.

Starting from an isotropic sample, for very small strain, with \( A_{0} = \tau_{0} = 0 \), we identify \( B = \sigma^{h} \beta_{s} s_{d}^{m} \) or \( \beta_{s} = B/(\sigma^{h} s_{d}^{m}) \), where the dependence on isotropic stress, \( \sigma^{h} \), is not fully consistent with observations from DEM simulations, see the discussion around Eq. (22) in Ref. [18], and requires further study to understand the hidden explicit dependence of \( B \) or \( s_{d}^{m} \) on the hydrostatic stress.

On the other hand, for very large strain, one has \( s_{d} \to s_{d}^{\text{max}} \), i.e., the first term in Eq. (35) vanishes so that

\[
\frac{\partial \tau}{\partial \gamma} = s_{d}^{\text{max}} \frac{\partial \sigma^{h}}{\partial \gamma} = s_{d}^{\text{max}} A^{\text{max}}
\]

remains, while \( \partial s_{d}/\partial \gamma \to 0 \). Relying on the above observations, and requiring a “critical state flow” regime where all derivatives with respect to \( \delta \gamma \) vanish after large enough deviatoric strain (with conserved volume \( \delta \varepsilon^{v} = 0 \)), a phenomenological extension of the linear model described in Eqs. (23) and (24) is proposed. In order for the deviator stress to vanish at large strain, the simplest possibility is to disregard the last term in Eq. (35), so that Eq. (24) is modified by a factor that vanishes when \( s_{d} \) reaches its maximum \( s_{d}^{\text{max}} \):

\[
\delta \tau = A \delta \varepsilon^{v} + B \left( 1 - \frac{s_{d}}{s_{d}^{\text{max}}} \right) \delta \gamma = A \delta \varepsilon^{v} + B S \delta \gamma,
\]

using the abbreviation \( S = (1 - s_{d}/s_{d}^{\text{max}}) \). With this equation, another parameter is introduced in the model, namely the macroscopic coefficient of friction, \( s_{d}^{\text{max}} \). The results of the DEM simulations [18], for example, show values \( s_{d}^{\text{max}} \approx 0.4 \), dependent strongly in the contact coefficient of friction of the material, but only weakly dependent on the confining stress, see Refs. [18, 22].

### 3.4 Improved self-consistent non-linear Model

Inserting the new deviatoric modulus, \( \partial \tau / \partial \gamma = BS \), from Eq. (36) into Eq. (34), shows the inconsistency of the model in Eq. (36), i.e.,

\[
\frac{\partial s_{d}}{\partial \gamma} = \frac{1}{\sigma^{h}} \left( BS \right) \left( 1 - \frac{s_{d}}{s_{d}^{\text{max}}} \right) - \frac{\tau}{\sigma^{h}} \frac{\partial \sigma^{h}}{\partial \gamma} = \frac{1}{\sigma^{h}} (BS - s_{d} A),
\]

does not vanish for large deviatoric strain – in conflict with the critical state flow assumption. The consistency of the model can be restored by also correcting the second term in Eq. (23), analogously to the deviatoric modulus, by the factor \( S \), so that the complete constitutive model reads:

\[
\delta \sigma^{h} = E \delta \varepsilon^{v} + A S \delta \gamma,
\]

\[
\delta \tau = A \delta \varepsilon^{v} + B S \delta \gamma,
\]
\[ \delta A = \beta A \text{sign}(\gamma) (A_{\text{max}} - A) \delta \gamma, \]  
(40)

with three field quantities \( \sigma^h, \tau, \) and \( A \) and five material model parameters: the bulk and shear moduli \( E, B, \) the macroscopic coefficient of friction, \( s_{d_{\text{max}}}^{\text{max}}, \) as well as the evolution rate of anisotropy from an isotropic original state, \( \beta_A, \) and the maximal anisotropy \( A_{\text{max}}. \) Furthermore, the initial conditions \( \sigma_0, S_0 \) and \( A_0 \) are required, where the abbreviation \( S = (1 - s_d/s_d^{\text{max}}) \) was used.

How to measure the material model parameters will be discussed below and in future studies.

### 3.4.1 Check of consistency

Inserting the deviatoric modulus, \( \partial \tau / \partial \gamma = BS \), from Eq. (39), and the anisotropic modulus \( \partial \sigma^h / \partial \gamma = AS \), from Eq. (38), into Eq. (34), shows the consistency of the model, i.e.,

\[ \frac{\partial s_d}{\partial \gamma} = \frac{1}{\sigma^h} \left( B \left( 1 - \frac{s_d}{s_d^{\text{max}}} \right) - \tau \frac{\partial \sigma^h}{\partial \gamma} \right) = \frac{1}{\sigma^h} (B - s_d A) S, \]  
(41)

does vanish for large deviatoric strain.

Combining Eq. (32) with (41) leads to

\[ \beta s \sigma^h s_{d_{\text{max}}}^{\text{max}} = (B - s_d A), \]

which, starting from an isotropic sample, for very small strain, with \( A_0 = \tau_0 = 0, \) again leads to \( B_0 = \sigma^h_0 / s_{d_{\text{max}}}^{\text{max}} \) or \( \beta = B_0 / (\sigma^h_0 s_{d_{\text{max}}}^{\text{max}}), \) as before. For very large strain, one has \( s_d \rightarrow s_d^{\text{max}}, \) i.e., \( S \rightarrow 0, \) so that, according to Eq. (41), one has \( \partial s_d / \partial \gamma \rightarrow 0. \) Furthermore, since \( A \rightarrow A_{\text{max}}, \) one also has:

\[ \beta s \sigma^h s_{d_{\text{max}}}^{\text{max}} = B_0 = (B_{\text{max}} - s_{d_{\text{max}}}^{\text{max}} A_{\text{max}}), \]

which (unfortunately) is inconsistent again, unless \( B \neq B_0, \) i.e., the modulus \( B \) requires an evolution equation by itself, that must fulfill the consistency relation: \( B_{\text{max}} = B_0 + s_{d_{\text{max}}}^{\text{max}} A_{\text{max}}. \) Since typically \( s_{d_{\text{max}}}^{\text{max}} A_{\text{max}} \ll B_0, \) we assume \( B \approx B_0 = \text{const.} \) in the following.

### 3.4.2 Alternative anisotropy evolution model

Whether Eq. (40) has to be modified in a way similar to the second terms in Eqs. (38) and (39), which would lead to:

\[ \delta A = \beta_A \text{sign}(\gamma) (A_{\text{max}} - A) S \delta \gamma, \]  
(42)

will be discussed elsewhere. Since it is not necessary to achieve \( \partial A / \partial \gamma \rightarrow 0 \) for large deviatoric strains, we disregard this option and continue using Eq. (40) instead.

### 3.5 Energy, work, stability for the non-linear model

Again, examining the stability condition by considering the matrix form given in Eq. (19), which actually is equivalent to the split hydrostatic/deviatoric form:

\[
\begin{bmatrix}
\delta \sigma^h \\
\delta \tau
\end{bmatrix} =
\begin{bmatrix}
E & AS \\
A & BS
\end{bmatrix}
\begin{bmatrix}
\delta \varepsilon^h \\
\delta \gamma
\end{bmatrix},
\]  
(43)

leads to the condition \((EB - A^2)S = 0,\) which can be fulfilled by either having the term in brackets vanish, or by \( S \rightarrow 0, \) as it happens for large shear strain anyway.
4 Results

In this section, a series of tests will be performed, using the proposed constitutive model in different variants. The goal is to demonstrate the behavior of the model for different modes of deformation, as shown in Table 1.

Mode 0 is purely isotropic, while mode 2 is purely deviatoric, i.e., volume conserving, which both take especially simple forms. Modes 1 and 3 are mixed modes, which are often applied experimentally. The uni-axial test is the superposition of an isotropic and a deviatoric test, whereas the bi-axial tests involve mixed stress- and strain-control instead of completely prescribed strains.

In our examples, the strain component $\varepsilon_{22}$ is prescribed while either the isotropic stress $\sigma_h$ or the horizontal stress component $\sigma_{11}$ are also prescribed, which makes, e.g., the horizontal strain component $\varepsilon_{11}$ an unknown variable. Many further possible deformation modes are not discussed here.

<table>
<thead>
<tr>
<th>Mode</th>
<th>1-dir. $\varepsilon$</th>
<th>2-dir. $\varepsilon''$</th>
<th>$\gamma$</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 (isotropic)</td>
<td>$\varepsilon_0$</td>
<td>$\varepsilon_0$</td>
<td>0</td>
<td>$\varepsilon_0 &gt; 0$ dilatation, $\varepsilon_0 &lt; 0$ compression</td>
</tr>
<tr>
<td>1 (uniaxial)</td>
<td>$\varepsilon_1$</td>
<td>0</td>
<td>$\frac{\varepsilon_1}{2}$</td>
<td>horizontal, $\varepsilon_1 &gt; 0$ tension, $\varepsilon_1 &lt; 0$ compression</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>$\varepsilon_1$</td>
<td>$\frac{\varepsilon_1}{2}$</td>
<td>vertical, $\varepsilon_1 &gt; 0$ tension, $\varepsilon_1 &lt; 0$ compression</td>
</tr>
<tr>
<td>2 (deviatoric)</td>
<td>$\varepsilon_2$</td>
<td>$-\varepsilon_2$</td>
<td>0</td>
<td>pure shear, $\varepsilon_2 &gt; 0$ positive, $\varepsilon_2 &lt; 0$ negative</td>
</tr>
<tr>
<td>3 (bi-axial)</td>
<td>$\sigma_{11} = \sigma_0$</td>
<td>$\varepsilon_{22}$</td>
<td>?</td>
<td>horizontal stress- and vertical strain-control</td>
</tr>
</tbody>
</table>

Table 1: Summary of various deformation modes that can be imposed on the system. The term 1-dir. is the abbreviation for x- or 1-direction. The symbols $\varepsilon_\alpha$ with $\alpha = 0, 1, 2, 3$ indicate the magnitude of strain of the respective mode and should not be confused with eigen-values or a-like.

In the following, different cases of the constitutive model will be discussed, starting from isotropy and constant anisotropy $A$ and furthermore using different variants of the non-linear, anisotropic model.

4.1 Isotropy $A = 0$

The isotropic special case is realized by setting $A = A^{\max} = \beta_A = 0$, which de-couples the evolution equations for the isotropic and deviatoric stresses and allows for a straightforward integration given the constants $E$, $B$, and $s_{\alpha}^{\max}$, with initial conditions $\sigma_0$ and $S_0 = \tau_0/\sigma_0$.

4.2 Constant Anisotropy $A = A_0$

In this subsection the cases where $A$ is constant are discussed, which implies that the anisotropy of the system is not changing with the deformation. Isotropy is a special case belonging to this class. For the sake of simplicity, in the constitutive mode Eqs. (38) and (39), we set $S = 1$; variations in $S$ will be discussed in the next subsection.

*Note that this subsection is relevant for very small deformations of systems with initial values of $E_0$, $B_0$, $A_0$ and $S_0$. With other words, this subsection describes the stress-strain response of the model for infinitesimal deformations from an arbitrary initial configuration.*
4.2.1 Linear Model, Mode 0 and constant $A = A_0$

The first example shows the effects of pure isotropic deformation (mode 0) on the shear stress. The prescribed deformation consists of $\varepsilon_{11} = \varepsilon_{22} = \varepsilon_0/2$ and $\varepsilon_v = \varepsilon_0 < 0$, i.e., compression. The stresses that develop during the deformation are shown in Figure 2.

Figure 2: The development of shear and hydrostatic stresses under isotropic compression (mode 0) for fixed $A$. The parameters used are $\sigma_0 = -100$ Pa, $E = 20000$ Pa, $B = E/2$, and $A = A_0 = E/5$.

The results of the compression test leads to increasing negative isotropic stress. Furthermore, even though there is no shear deformation in the system, $\gamma = 0$, the shear stress $\tau$ changes for $A \neq 0$. For this example system, recall that positive $A$ corresponds to a larger horizontal than vertical stiffness. Therefore, the (deviatoric) shear stress-response, $\tau$, also must be negative, i.e., the horizontal stress (negative) increases stronger than the vertical stress (negative).

In the case of negative $A < 0$, the isotropic stress remains unchanged, but the shear stress, $\tau$, changes sign, i.e., the vertical stress (negative) increases stronger than the horizontal stress (negative) and thus $\tau > 0$.

When the system is expanded, i.e., $\varepsilon_0 > 0$, the stresses will develop in the opposite (positive) direction – the isotropic stress will increase, while the deviatoric stress increases to positive values too, i.e., the horizontal stress increases stronger than the vertical stress, leading to positive shear stress $\tau$.

Best Practice Tipp 1: Applying an infinitesimal purely isotropic deformation (mode 0) to a sample thus allows to measure the modulus $E$ and the initial anisotropy of the sample, $A_0$.

4.2.2 Linear model, Mode 2 and constant $A = A_0$

The next example shows a case where the prescribed deformation is pure shear (mode 2), with $\varepsilon_{11} = -\varepsilon_{22} = \varepsilon_2 > 0$, i.e., for compression in vertical and expansion in horizontal direction. In Figure 3 the development of the deviatoric stress ($\equiv \tau$) and the hydrostatic stress are shown.

Even though there is no isotropic strain involved, the model leads to an increase of the hydrostatic stress, i.e., a reduction of the compression. This is due to $A$, so that the horizontal stress increases faster (tensile) than the vertical stress decreases (compressive). If the volume would not be prescribed as constant, the constitutive model would lead to dilatancy, i.e., increase of volume of the anisotropic system due to pure shear deformation.

Inversion of the sign of $A$ does not affect the shear stress, but leads to a system with stiffer response in vertical direction and, correspondingly, to a sign reversal of the hydrostatic stress and therefore...
compaction instead of dilatancy. Reversal of the shear direction, but keeping $A > 0$, just inverts all signs for both strain and stress.

Best Practice Tipp 2: Applying an infinitesimal purely deviatoric deformation (mode 2) to a sample thus allows to measure the modulus $B$ and the initial anisotropy, $A_0$. Note that, as shown below, according to our model, the initial anisotropy depends also on the initial condition of $S_0$.

4.2.3 Comparison of mode 0 and mode 2 for constant $A = A_0$

Comparison of the two cases, mode 0 and mode 2, reveals an important characteristics of the model. There exists a coupling symmetry or, in other words, the cross-link between shear (deviatoric) and isotropic strains works in both directions: shear strain causes a change in hydrostatic stress and isotropic strain causes a change in shear (deviatoric) stress – if anisotropy is present.

4.2.4 Linear model, Mode 1 for constant $A = A_0$ (and $S = S_0 = 1$)

Applying uni-axial deformation (mode 1), with strain $\delta \varepsilon_1$ to the system in horizontal or vertical direction leads to

$$\delta \sigma^h = (E/2)\delta \varepsilon_1 \pm (A/2)\delta \varepsilon_1 = (E \pm A)\delta \varepsilon_1^v = (\pm E + A)\delta \gamma_1 ,$$  \hspace{1cm} (44)

and

$$\delta \tau = (A/2)\delta \varepsilon_1 \pm (B/2)\delta \varepsilon_1 = (A \pm B)\delta \varepsilon_1^v = (\pm A + B)\delta \gamma_1 ,$$  \hspace{1cm} (45)

respectively, where the positive/negative, $\pm$, corresponds to horizontal/vertical deformation with corresponding shear strain $\delta \gamma_1 > 0$ or $\delta \gamma_1 < 0$. Inserting our choice of parameters, $A = E/5$ and $B = E/2$, yields:

$$\delta \sigma^h = (1/2 \pm 1/10)E \delta \varepsilon_1 ,$$  \hspace{1cm} (46)

and

$$\delta \tau = (1/10 \pm 1/4)E \delta \varepsilon_1 .$$  \hspace{1cm} (47)

Note that for the simplest uni-axial (mode 1) deformation experiments, typically only the stress in one direction (deformation direction) can be measured. Therefore, by addition or subtraction of Eqs. (44) and (45), the relations

$$\delta \sigma_{11} = (E/2 + B/2 + A)\delta \varepsilon_{11} ,$$  \hspace{1cm} (48)
and

\[ \delta \sigma_{22} = \left( \frac{E}{2} + \frac{B}{2} - A \right) \delta \varepsilon_{22}, \] (49)

can be used – if the horizontal or vertical stresses are measured for the respective horizontal or vertical deformation direction.

For these cases, when the deformation direction is reversed, \( \delta \varepsilon_1 \to -\delta \varepsilon_1 \), one obtains the same moduli (due to sign inversion of the stress response). The model with constant \( A \) thus does not show non-linearity under reversal of deformation direction. On the other hand, when the anisotropy direction is reversed, \( A \to -A \), the apparent moduli for horizontal or vertical deformation are exchanged in Eqs. (48) and (49).

If the experiment also allows to measure the stress perpendicular to the uni-axial deformation direction, one has the relations

\[ \delta \sigma_{11} = \left( \frac{E}{2} - \frac{B}{2} \right) \delta \varepsilon_{22}, \] (50)

and

\[ \delta \sigma_{22} = \left( \frac{E}{2} - \frac{B}{2} \right) \delta \varepsilon_{11}, \] (51)

i.e., three apparent moduli can be measured to determine the three unknowns \( E, B, \) and \( A \). The fourth unknown \( S_0 \) will be introduced in the next sub-subsection. Note that in practice uni-axial experiments are usually not flexible enough to provide all four measurement results. From DEM simulations, however, one can easily obtain the three moduli, given the system is initially isotropic in stress, \( S_0 = 1 \).

*Best Practice Tipp 3.1: The uni-axial deformation mode does not provide direct access to the constitutive model parameters – however, various combinations can be obtained for different tests, dependent on the direction of deformation and initial anisotropy. In particular, combinations like \( E \pm B/2 \) and \( A \) can be measured.*

---

**Figure 4:** (Left) The horizontal and vertical stresses under vertical uni-axial deformation, mode 1, plotted as function of the negative vertical strain (such that compression appears positive). (Right) shear and hydrostatic stresses from the same data, also plotted against (negative) vertical strain. The data are for fixed \( A \), with \( \sigma_0 = -100 \) Pa, \( E = 20000 \) Pa, \( B = E/2 \), and \( A = A_0 = E/5 \) and \( S_0 = 1 \). The apparent moduli, i.e., the slopes of the curves in the left panel are \(-(E/2+B/2\cdot-A)\) = \(-11000\) Pa for the vertical stress, see Eq. (49), and \(-(E/2-B/2)\) = \(-5000\) Pa for the horizontal stress, see Eq. (50). The slopes in the right panel are \(-8000\) Pa and \(+3000\) Pa, as can be read off from Eqs. (44) and (45), for the hydrostatic and the deviatoric stress, respectively.

Examples of the linear model for uni-axial compression, mode 1, and how to obtain the apparent moduli from the previous set of equations, are given in Figs. 4 and 5. In the following subsection, the same system will be examined with initial anisotropy \( S < 1 \).
Figure 5: The development of shear and hydrostatic stresses under horizontal (Left) and vertical (Right) uni-axial deformation, mode 1, for fixed $A$, with $\sigma_0 = -100$ Pa, $E = 20000$ Pa, $B = E/2$, and $A = A_0 = E/5$ and $S_0 = 1$. In the right panel, for vertical uni-axial compression, in contrast to Fig. 4, the hydrostatic and deviatoric stresses are plotted against the isotropic and deviatoric strains, respectively. The corresponding slopes $E - A = 16000$ Pa and $B - A = 6000$ Pa can also be read off from Eqs. (44) (2nd term) and (45) (third term). In the left panel, for horizontal uni-axial compression, the slopes are $E + A = 24000$ Pa and $B + A = 14000$ Pa.

4.2.5 Linear model, Mode 1 for constant $A = A_0$ (and $S = S_0 \neq 1$)

Applying uni-axial deformation (mode 1), with strain $\delta \varepsilon_1$ to the (deviatorically) pre-stressed system (with $S_0 \neq 1$), in horizontal or vertical direction, leads to

$$\delta \sigma^h = (E/2)\delta \varepsilon_1 \pm (A/2)S_0\delta \varepsilon_1 ,$$

and

$$\delta \tau = (A/2)\delta \varepsilon_1 \pm (B/2)S_0\delta \varepsilon_1 ,$$

respectively. This leads to the modified relations for the simplest uni-axial test

$$\delta \sigma_{11} = (E/2 + BS_0/2 + A/2 + AS_0/2)\delta \varepsilon_{11} ,$$

and

$$\delta \sigma_{22} = (E/2 + BS_0/2 - A/2 - AS_0/2)\delta \varepsilon_{22} ,$$

which can be used if the horizontal and vertical stresses are measured for the respective horizontal and vertical deformation directions. If the experiment also allows to measure the stress perpendicular to the uni-axial deformation direction, one has the independent relations

$$\delta \sigma_{11} = (E/2 - BS_0/2 + A/2 - AS_0/2)\delta \varepsilon_{22} ,$$

and

$$\delta \sigma_{22} = (E/2 - BS_0/2 - A/2 + AS_0/2)\delta \varepsilon_{11} ,$$

i.e., four relations for the four unknowns $E$, $B$, $A$, and $S_0$.

Best Practice Tipp 3.2: The uni-axial deformation mode does not provide direct access to the constitutive model parameters – however, various combinations can be obtained in different realizations, dependent on the direction of deformation and initial anisotropy. In particular combinations like $E \pm BS_0/2$ and $A(1 \pm S_0)/2$ can be measured.
4.2.6 Comment on direction reversal of uni-axial deformation

Now a final remark about the non-linearity under direction reversal. Like above for $S = 1$, for constant $A$ and $S = S_0 < 1$, there is no non-linearity due to reversal of deformation-direction. However, as will be discussed in the following subsection, for $A$ and $S$ developing as functions of the applied strain history, the non-linearity in the model shows up.

More specific, assume the special case, where the sample was compressed deviatorically in horizontal direction (long enough, $\gamma \ll 0$) such that the final, critical state with $A = A_{\text{max}} = A^m > 0$, and $s_{d,c}^{\text{max}} = -s_d^m < 0$ was reached. Measuring uni-axially the horizontal stiffness under further horizontal compression implies $A_0 = A^m$ and $S_0 = 0$ so that Eq. \((54)\) leads to the apparent modulus $C_{1111} = (E + A^m)/2$ ($= 3E/5$ for our parameters with $A^m = E/5$).

On the other hand, after stop and measuring uni-axially the horizontal stiffness under the (opposite) horizontal deformation (i.e., tension) implies sign reversal of strain and (due to the definitions of $A_{\text{t}}$ and $s_{d,t}$, see Eq. \((27)\), and $s_{d,t}^{\text{max}} = s_d^m$, see Eq. \((32)\)) implies $A = A_0 = -A^m$ and $S_0 = 2$ (at the instant of direction reversal), which leads to the apparent modulus $C_{1111}^\text{rev} = E/2 + B - 3A^m/2$ ($= 7E/10$ for our parameters). In general, the modulus under reversal, $C_{1111}^\text{rev}$, is different from the apparent modulus $C_{1111}$ under further uni-axial compression, which allows to quantify the strength of non-linearity via $\Psi^\text{rev} = C_{1111}^\text{rev}/C_{1111} = (E+2B-3A^m)/(2E-A^m)$ ($= 7/6$ for our parameters). For $\Psi^\text{rev} > 1$ one has an increased stiffness under strain reversal whereas for $\Psi^\text{rev} < 1$, the stiffness would decrease under strain reversal. Since the former is usually observed in experiments and simulations, we can define an upper limit for $|A| \leq A \Psi := B/2$, for which $\Psi^\text{rev} \equiv 1$.

4.2.7 Mode 3 for constant $A = A_0$

The last example for constant $A$ is the actual bi-axial model system, i.e., mode 3 with constant horizontal stress. In this case only $\varepsilon_{22}$ is prescribed as compressive (negative) and $\varepsilon_{11}$ is calculated using the constraint condition $\sigma_{11} = \sigma_0$.

![Figure 6: The development of stresses during the biaxial deformation (mode 3) of the system, plotted against the negative vertical strain. (Left) Horizontal and vertical stress and (Right) hydrostatic and deviatoric stress for a system with fixed $A$, with $\sigma_{11} = \sigma_0 = -100\, \text{Pa}$, $E = 20000\, \text{Pa}$, $B = E/2$, and $A = 0.2E$.](image)

Figure 6 shows the components of the stress tensor as well as the shear and hydrostatic stresses. The horizontal stress remains constant, as prescribed, and, for our choice of parameters, the shear stress increases with slope $C_3$ while the isotropic stress decreases with slope $-C_3$.\(^{3}\) As expected, $\sigma_{11}$ remains equal to the prescribed normal stress during the deformation while $\sigma_{22}$ evolves according

\(^{3}\)The anti-symmetry in isotropic and deviatoric stress for mode 3 is due to the prescribed constant horizontal stress $\sigma_{11} = \sigma_0$, which implies $\delta \sigma_{11} = 0$. The constant $C_3 = C_{2222}/2$ as discussed below.
to the constitutive relations, i.e., it decreases to higher compressive stress magnitude (negative). Since $A$ is constant, the model leads to a linear increase of stress magnitude to values much larger than the confining stress.

Inserting the definitions into the constitutive model

$$\delta \sigma^h = \delta \sigma_{22}/2 = E(\delta \varepsilon_{11} + \delta \varepsilon_{22})/2 + A(\delta \varepsilon_{11} - \delta \varepsilon_{22})/2 = E\delta \varepsilon^v + A\delta \gamma,$$  

$$\delta \tau = -\delta \sigma_{22}/2 = A(\delta \varepsilon_{11} + \delta \varepsilon_{22})/2 + B(\delta \varepsilon_{11} - \delta \varepsilon_{22})/2 = A\delta \varepsilon^v + B\delta \gamma,$$

and setting $\delta A = 0$, allows to solve for the unknowns

$$\delta \varepsilon_{11} = -\frac{(E - B)}{(E + B + 2A)} \delta \varepsilon_{22} = -\nu_P \delta \varepsilon_{22},$$

and

$$\delta \sigma_{22} = \frac{[EB - A^2]}{(E + B + 2A)} \delta \varepsilon_{22} = C_{2222} \delta \varepsilon_{22},$$

where the first equation defines the Poisson ratio $\nu_P$ and the second equation directly provides the modulus $C_{2222}$ for the bi-axial compression mode. The Poisson ratio allows to relate the isotropic to the deviatoric strains via: $\varepsilon^v = -\frac{1 - \nu_P}{1 + \nu_P} \gamma$. Inserting our choice of parameters, $A = E/5$ and $B = E/2$, yields $\nu_P = 5/19$, and $C_{2222} = 46E/95$, which corresponds to the (negative) slope of $\sigma_{22}$ in Fig. 6.

Best Practice Tipp 4.1: The bi-axial deformation mode does not provide direct access to the constitutive model parameters – however, other quantities like a Poisson ratio and one modulus can be obtained.

In Figure 7 both the evolution of the strains and the scaled stresses is shown, where the latter are defined as:

$$s_v = \frac{\sigma_{11} + \sigma_{22}}{2\sigma_0} - 1, \quad \text{and} \quad s_d = \frac{\sigma_{11} - \sigma_{22}}{(\sigma_{11} + \sigma_{22})}.$$  

In the left panel, we observe a continuous decrease of volume, $\delta \varepsilon_v < 0$ (negative slope of the red curve), with slope $-(1 - \nu_P)/2 = 7/19$, due to the relation $\varepsilon_v = (1 - \nu_P)\varepsilon_{22}/2$. The vertical strain is continuously decreasing while the horizontal strain increases – but more slowly – which leads to a net decrease of volume (compaction). For the same reasons, the shear strain continuously increases according to $\gamma = -(1 + \nu_P)\varepsilon_{22}/2$, with slope $12/19$.

From the right panel, we observe that the isotropic stress is continuously increasing (consistent with the isotropic compaction) according to $s_v = \sigma_{22}/(2\sigma_0) = C_5\varepsilon_{22}/\sigma_0$. The deviatoric stress ratio, on the other hand, approaches the value $s_d^{\text{max}} = -1$, due to the continuous increase of $\sigma_{22}$.

4.3 Model with evolution of anisotropy $A$

From discrete element simulations it is observed that $A$ evolves during the deformation according to the proposed function in Eq. (40) – before shear band formation, as long as the system is homogeneous. The model proposed in this study in Eqs. (38), (39), and (40), is therefore implemented for evolving $A$ – to be compared with DEM simulations in a future study. Here, results will be shown for the biaxial box deformation mode 3, i.e., for vertical compression and with fixed horizontal stress.

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*Note that our positive $A = E/5$ corresponds to a material that is stiffer in horizontal than in vertical direction. Inserting $A = -E/5$ corresponds to a material that is stiffer in vertical directions. This leads to $\nu_P = 5/11$, i.e., a considerably larger Poisson ratio than for positive $A$, while $A = 0$ leads to a value in between. The volume change is given by $\varepsilon_v = (1 - \nu_P)\varepsilon_{22}/2$, so that $A = E/5, 0$, and $-E/5$ lead to $\{1 - \nu_P\} = 0.736842, 0.6666$, and $0.545454$, respectively. The higher the stiffness in compression direction, the smaller the volume change for given compression.*
4.3.1 Biaxial mode 3 with vertical compression

In the first example the maximal anisotropy is \( A^m = E/5 \), like the constant \( A \) before, however, the anisotropy \( A \) is now free to change, starting from \( A_0 = 0 \), if not explicitly mentioned. The other parameters in the simulation are: \( \sigma_0 = -100 \) Pa, \( E = 20000 \) Pa, \( B = E/2 \), \( \beta_A = 82 \), and \( s_{md} = 0 \).

Figures 8 and 9 show initially the same behavior as for constant \( A = A_0 = 0 \) (data not shown). The behavior starts, as expected, being linear, isotropic and evolves towards being saturated, anisotropic. In Fig. 8 (Left), the horizontal stress remains constant, as prescribed, and the vertical stress increases towards a maximum within about 5% of vertical strain. In Fig. 8 (Right), the isotropic stress increases towards higher (negative) compressive values, while the shear stress takes positive values, and both stresses saturate. In Fig. 9 (Left), the isotropic strain indicates the initial compression and then saturates at around 2% of vertical strain, while the deviatoric strain increases continuously with increasing slope during the initial deformation and constant slope later on. The continuously increasing shear strain is due to the horizontal extension and vertical compression, which both enter \( \gamma \) positively.

In Fig. 9 (Right), the non-dimensional shear stress ratio, \( s_d \), decreases and saturates at \( s_d^{max} = -0.4 \), as prescribed. Notably, the isotropic stress ratio also saturates, at a positive value \( s_v^{max} \), which was not prescribed, but is due to the constant horizontal stress \( \sigma_{11} = \sigma_0 \), which together with the prescribed \( s_d^{max} \) does not allow the isotropic stress to change anymore beyond \( s_v^{max} = -\left(1/s_d^{max} + 1\right)^{-1} = \frac{2}{3} \).

When plotting the isotropic stress against isotropic strain and the deviatoric stress against deviatoric strain in Fig. 10 (Left), volume decrease is accompanied by a decrease in isotropic stress, while the deviatoric stress saturates at some deviatoric strain around 5%. The evolution of anisotropy \( A \) is displayed in Fig. 10 (Right), and shows saturation at \( A^{max} = -E/5 \) around 7% of strain. The negative \( A \) means that the horizontal stiffness is smaller than the vertical stiffness, which is plausible due to the vertical compression and the horizontal extension.

The forces \( -f_1 \) and \( -f_2 \) on the walls – compressive forces are negative, which makes the displayed forces positive – are shown in Fig. 11 (Left). The force \( -f_1 = -\sigma_{11}L_y \) on the side-walls (that are stress-controlled) decreases due to the decrease in height \( L_y \). On the other hand, the force \( -f_2 = -\sigma_{22}L_x \) first increases due to the rapid change in vertical \( \delta \) and then increases slower since the vertical stress has saturated and only the width of the system \( L_x \) is slowly increasing.

The second-order mechanical work, as defined in Eq. (30), is shown in Fig. 11 (Right), and displays a rapid decay from large values down to zero in the anisotropy saturation regime.
Figure 8: The development of diagonal stresses (Left) and the isotropic and shear stresses (Right) during the biaxial deformation of the system, mode 3, with vertically prescribed compression and constant horizontal stress, $\sigma_0 = -100$ Pa, for evolving $A$, and maximal stress-anisotropy, using the standard parameters as given in the main text, together with the new parameters $\beta_A = 82$, $A^m = E/2$, and $s_d^m = 0.4$.

Figure 9: The development of shear and isotropic strains (Left) and of the non-dimensional stress-ratios, $s_d$ and $s_v$, (Right), from the same simulation as in Fig. 8.

Figure 10: The development of isotropic and deviatoric stress plotted against isotropic and deviatoric strain (Left), during mode 3 vertical compression, with constant horizontal confining stress, for evolving $A$ (Right).
Figure 11: The development of forces during the biaxial deformation of the system, mode 3, for evolving $A$ (Left). The development of second-order mechanical work (Right) from the same system.

4.3.2 Biaxial mode 3 with vertical extension

The second example is identical to the first example, only reversing the vertical strain direction to extension, starting from $A_0 = 0$, with $A^m = E/5$, $\sigma_0 = -100$ Pa, $E = 20000$ Pa, $B = E/2$, $\beta_A = 82$, and $s^m_d = 0.4$.

Figures 12 and 13 show initially the same behavior as for constant $A = A_0 = 0$ (data not shown). The behavior starts, as expected, being linear, isotropic and evolves towards being saturated, anisotropic. Besides the opposite sign of strain, due to extension, the saturation is reached at considerably smaller strains around 1-2%. In Fig. 12 (Left), the horizontal stress remains constant, as prescribed, and the vertical stress decreases in magnitude towards its minimum. In Fig. 12 (Right), the isotropic stress decreases towards lower (still negative) compressive values, while the shear stress takes negative values.

Figure 12: The development of diagonal stresses (Left) and the isotropic and shear stresses (Right) during the biaxial deformation of the system, mode 3, with vertically prescribed extension and constant horizontal stress, $\sigma_0 = -100$ Pa, for evolving $A$, and maximal stress-anisotropy, using the standard parameters as given in the main text, together with the new parameters $\beta_A = 82$, $A^m = E/2$, and $s^m_d = 0.4$.

In Fig. 13 (Left), the isotropic strain indicates the initial dilation and then saturates at around 1-2% of vertical strain, faster than under vertical compression, while the deviatoric strain decreases continuously with increasing slope during the initial deformation and constant slope later on. The
continuously decreasing shear strain is due to the horizontal compression and vertical extension, which both enter $\gamma$ negatively. In Fig. 13 (Right), the non-dimensional shear stress ratio, $s_d$, increases and saturates at $s_d^{\text{max}} = 0.4$, as prescribed. The isotropic stress ratio also saturates, at a negative value $s_v^{\text{max}} = -(1/s_d^{\text{max}} + 1)^{-1} = -\frac{4}{7}$, which was not prescribed.

When plotting the isotropic stress against isotropic strain and the deviatoric stress against deviatoric strain in Fig. 14 (Left), volume increase is accompanied by an increase in isotropic stress, while the deviatoric stress becomes negative and saturates at a smaller deviatoric strain than under compression. The evolution of anisotropy $A$ is displayed in Fig. 14 (Right), and shows saturation at $A^{\text{max}} = E/5$ around 7% of strain, like for compression. The positive $A$ means that the horizontal stiffness is larger than the vertical stiffness, which is plausible due to the vertical extension and the horizontal compression.

Best Practice Tipp 4.2: The compression mode 3 leads to saturated shear stress, like the extension mode 3, where the former is considerably slower than the latter (with about 5% of strain vs. 1-2% to reach saturation). Starting from an initial isotropic system ($A_0 = 0$), the equivalent moduli (initial slope of the stress strain curve) are identical (note the different range of isotropic stress under compression and extension). The anisotropy develops with the same rate and reaches saturation at about 7% of strain for the chosen model parameters.

These observations wait for experimental validation.
5 Summary and Conclusion

In the biaxial system – where the eigen-vectors of all tensors are either horizontal or vertical – a new constitutive model, as based on DEM simulations in Ref. [18, 22], is presented in Eqs. (38), (39), and (40). It involves the hydrostatic and deviatoric stresses, together with one anisotropy modulus that evolves during deviatoric deformations of the system and thus represents a history/memory parameter.

The five macroscopic field quantities are the hydrostatic stress, the shear stress, the anisotropy modulus, the isotropic strain and the shear strain. The model involves only three moduli: the classical bulk modulus \( E/2 \), a shear modulus, \( B \), and the anisotropy modulus \( A \), whose sign indicates the direction of anisotropy in the present formulation. Due to the anisotropy, \( A \), the model involves a cross coupling of the two types of strains and stresses, namely isotropic and shear (deviatoric). As opposed to isotropic materials, shear strain can cause dilatation and hence compressive stresses. Similarly, a pure isotropic strain can cause shear stresses and thus shear deformation in the system. The shear stress evolution with shear strain is proportional to \( B \), while the anisotropy grows proportional shear strain and a new parameter \( \beta_A \).

The model also leads to a critical state regime, where the stresses and the anisotropy modulus do not change anymore, given constant \( E \) and \( B \). The critical state is described by the maximal anisotropy \( A^m \) and the maximal deviatoric stress ratio \( s_d^m \), which is equivalent to a macroscopic friction coefficient in Mohr-Coulomb type constitutive relations, and thus represents a yield-stress limit.

5.1 Micro-Macro Mechanics and Constitutive Relations

The flow of granular materials is controlled by the micro-mechanics of the disordered structure of the material. On the macroscopic level of description, one history parameter is introduced that accounts for the micro-mechanical anisotropy evolution of the system. This single new parameter is the only extension as compared to classical continuum theories. Furthermore, all tensors are split into their scalar components, which is possible only in the bi-axial system. In more general situations, the tensors can be split into their (scalar) moduli and a non-dimensional unit-deviator (“director”) that involves the orientation of the tensor eigen-system. In two dimensions (2D) this is particularly simple, since each tensor direction is uniquely defined by one angle.

In contrast to elasto-plastic models, the present evolution of stress and anisotropy is smooth: both \( s_d \) and \( A \) approach their critical state regime exponentially fast, which means a linear regime for small strain and a critical state regime for large strain, without any discontinuities of the derivatives. Strain reversal, on the other hand, leads to a non-linear stress evolution – again due to the presence of the anisotropy – with different loading and un-loading stiffnesses.

Note that the model does not show softening – softening was not inserted, but shows up as an artefact when, e.g., the inconsistent variant of the model is used (data not shown). Disregarding softening is on purpose, since the model is only locally valid (or for homogeneous systems), whereas softening and other effects are (to our knowledge) observed for inhomogeneous systems only. Softening – in our philosophy – should NOT be inserted into a (simple) local model, since it will be the result of the collective behavior of the material in a particular experiment with its boundary conditions.

The condition when the system becomes instable has also been derived analytically and is fulfilled automatically in the critical state regime: The existence of anisotropy in the model causes instability when it becomes larger than a certain value that is a function of the bulk and shear moduli.

\(^5\)Future formulations will take into account arbitrary orientations of stress, anisotropy and strain.

\(^6\)The latter is a simplification, where evolution equations for \( E \) and \( B \) will be introduced elsewhere [33]. Their change is often smaller than the variation of the new modulus, \( A \).
However, interestingly, such large anisotropy was never observed in DEM simulations, which leaves the question about the particulate origin of the instability open.

5.2 From Constant to Evolving Anisotropy

To better understand the model, a series of simulations has been performed for special cases: Some analytical predictions can be made for constant anisotropy in the system. As expected, linear relations between strains and stresses are observed, in line with the coupling via the (constant) anisotropy mentioned above. The constant anisotropy also reflects the system behavior with evolving anisotropy for very small strains. For larger strains the non-linear behavior sets in with a particular interplay between isotropic and deviatoric components, which are cross-coupled by the anisotropy. The evolving anisotropy of the structure, $A$, and of the stress, $s_d$, lead to non-linear effects as the critical state regime and the change of stiffness under strain-reversal.

5.3 Future Work

The next step is the formulation of the model for arbitrary orientations of the stress-, strain- and anisotropy-tensors, but keeping the number of parameters fixed. This is a requirement for a possible Finite Element Method implementation of the model, in order to study arbitrary boundary conditions other than bi-axial systems.

After this is achieved, the model can be generalized to three dimensions (3D), where (at least) one additional anisotropy parameter (tensor) is expected to be present in arbitrary deformation histories. Otherwise, the spirit of the model will not be different in 3D.

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