DEVELOPMENT OF DISCRETE ELEMENT APPROACH TO MODELING HETEROGENEOUS ELASTIC-PLASTIC MATERIALS AND MEDIA

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Abstract. A general approach to realization of models of elasticity and plasticity of isotropic materials within the framework of discrete element method (DEM) is proposed in the paper. It is based on building many-body potentials/forces of discrete element interaction, which provide response of element ensemble correctly conforming to the response of simulated solids. Developed formalism makes possible realization of various rheological models in the framework of DEM to study deformation and fracture of solid-phase media of various nature.

1 INTRODUCTION

An important direction in deformable solid mechanics is development of numerical methods and their application to problems connected with deformation and fracture of heterogeneous materials. A perspective and intensively developed representative of numerical methods in mechanics is a group of particle methods. At the present time this term is collective one as it includes very different numerical methods that belong both to "conventional" representatives of the discrete approach in mechanics (PM, DEM, MCA) and to meshless algorithms for numerical solution of equations of continuum (for example, particle-in-cell method [1], SPH [2], SPAM [3] and so on). Moreover, nowadays some modern realizations of conventional numerical methods (such as particle-finite element method [4]) are also referred to as particle methods. The following consideration will concern "conventional" particle methods.

In the framework of "conventional" particle methods simulated material is considered as an ensemble of interacting particles (elements) having finite size and predefined initial shape that can change as a consequence of loading. Evolution of an ensemble is defined by solution of the system of Newton-Euler motion equations:

$$\begin{aligned} m_i \frac{d^2 \vec{R}_i}{dt^2} &= \sum_{j=1}^{N_i} \left(\vec{F}_n^{ij} + \vec{F}_\tau^{ij} \right) \\ \hat{J}_i \frac{d^2 \vec{\theta}_i}{dt^2} &= \sum_{j=1}^{N_i} \vec{M}_{ij} \end{aligned} \tag{1}$$

where $\vec{R}_i$ and $\vec{\theta}_i$ are radius-vector and rotation angle of the particle i, m_i and $\hat{J}_i$ are particle mass and moment of inertia, $\vec{F}_n^{ij}$ and $\vec{F}_\tau^{ij}$ are forces of central (normal) and tangential interaction of considered element i with neighbor j, $\vec{M}_{ij}$ is momentum of force, N_i is a number of neighbors (conventionally only nearest neighbors of element i are taken into account). It is seen from (1) that "macroscopic" (integral) properties of ensemble of elements are defined by the structure and parameters of potential (potential forces) of element interaction.

The best known representative of this group of particle methods is the discrete element method (DEM) [5,6]. At the present time DEM is widely used to study behavior of granular (loose) and weakly bonded media including features of their rheology, deformation and fracture pattern, mixing effects and so on [5-7]. Nevertheless, until recently, potentialities of application of DEM to study mechanical phenomena in consolidated medium were limited, as a rule, by porous brittle materials [5,6]. These limitations are concerned with insufficient development of mathematical models of interaction of discrete elements. In particular, overwhelming majority of models within the framework of DEM is based on use of pair-wise (two-particle) potentials/forces of element interaction. Such simplification can lead to a series of artificial manifestations (effects) of response of the ensemble of elements that are not inherent to modelled medium. Most important of them are:

- strongly pronounced dependence of macroscopic mechanical properties of ensemble of discrete elements on packing type (close, square, stochastic,…);
- inability to realize arbitrary desired ratio between macroscopic elastic moduli (shear and bulk moduli, Young modulus and Poisson ratio and so on);
- **problems in correct simulation of irreversible strain accumulation in ductile materials, whose plasticity is provided by mechanisms of crystal lattice scale;**
- etc.

These disadvantages are of principle for simulation of consolidated low porous materials. In this connection one of fundamental problems in DEM is formulation of interaction potentials/forces, which provide response of element ensemble conforming to response of consolidated solids with various rheological properties (elastic-plastic, visco-elastic-plastic and so on). It is clear that such potentials/forces have to have many-body form.

2 GENERAL FORMALISM OF MANY-PARTICLE INTERACTION

Authors propose a general approach to building many-body forces of discrete element interaction to simulate deformation and fracture of consolidated heterogeneous media. The structural form of these forces is analogous to interatomic forces calculated on the basis of embedded-atom method. In the framework of embedded-atom model [8] the general expression for potential energy of atom i contains a pair interaction potential ϕ as a function of distance r_{ij} between atoms i and j and a "density-dependent" embedding function F (here it depends on electron charge density $\bar{\rho}_i$):

$$E_i(R) = \sum_{j \neq i} \phi(r_{ij}) + \sum_i F(\bar{\rho}_i)$$

where $\overline{\rho}_i = \sum_{j\neq i}\rho_j(r_{ij})$ is a sum of contributions of neighbors j to local value of density at the location of atom i.

By analogy with this expression the following general form of notation of the expression for the force $\vec{F}_i$ acting on discrete element i from surroundings is proposed:

$$m_i\frac{d^2\vec{R}_i}{dt^2} = \vec{F}_i = \sum_{j=1}^{N_i}\vec{F}^{ij}_{pair} + \vec{F}^{i}_{\Omega} \tag{2}$$

This force is written as a superposition of pair-wise constituents $\vec{F}^{ij}_{pair}$ depending on spatial position/displacement of element i with respect to nearest neighbor j and of volume-dependent constituent $\vec{F}^{i}_{\Omega}$ connected with combined influence of nearest surroundings of element.

When simulating locally isotropic media with various rheologies the volume-dependent contribution $\vec{F}^{i}_{\Omega}$ can be expressed in terms of pressure P_i in the volume of discrete element i as follows [9]:

$$\vec{F}^{i}_{\Omega} = -A\sum_{j=1}^{N_i}P_iS_{ij}\vec{n}_{ij} \tag{3}$$

where S_{ij} is square of area of interaction (contact) of elements i and j, $\vec{n}_{ij}$ is a unit vector directed along the line between mass centres of considered elements, A is a parameter.

In such formulation the right part of the expression (2) can be reduced to the sum of forces of interaction of pairs of elements and divided into central ($\vec{F}^{ij}_{n}$) and tangential ($\vec{F}^{ij}_{\tau}$) constituents:

$$\vec{F}_i = \sum_{j=1}^{N_i}\left(\vec{F}^{ij}_{pair} - AP_iS_{ij}\vec{n}_{ij}\right) = \sum_{j=1}^{N_i}\left[\left(F^{ij}_{pair,n}\left(h_{ij}\right) - AP_iS_{ij}\right)\vec{n}_{ij} + F^{ij}_{pair,\tau}\left(l^{ij}_{shear}\right)\vec{t}_{ij}\right] = \sum_{j=1}^{N_i}\left(\vec{F}^{ij}_{n} + \vec{F}^{ij}_{\tau}\right) \tag{4}$$

where $F^{ij}_{pair,n}$ and $F^{ij}_{pair,\tau}$ are central and tangential components of pair-wise interaction force that depend on the values of element-element overlap h_{ij} and relative shear displacement l^{ij}_{shear} (l^{ij}_{shear} is calculated taking into account rotation of both elements) [5,6]. Note that although the right part of the expression (4) formally confirms to notation of element interaction in conventional models (1) [5-7], their fundamental distinction consists in many-body form of central interaction of discrete elements in the proposed model.

It is seen from (4) that an important problem of building many-particle interaction is definition of local value of pressure (P_i) in the volume of discrete element. Authors propose to use an approach to calculation of pressure P_i (or, what is the same – of mean stress) in the volume of the element i that is based on the computation of components of average stress tensor in the volume of the element [6].

The case of plane motion of three-dimensional objects (quasi-two-dimensional approximation) is considered in the paper. In this approximation the expression for average stresses in terms of central (F^{ij}_{n}) and tangential (F^{ij}_{τ}) interaction forces can be written as follows [6]:

$$\overline{\sigma}^i_{\alpha\beta} = \frac{1}{V_i}\sum_{j=1}^{N_i} q_{ij}\left[F_n^{ij}\cos\theta_{ij,\alpha}\cos\theta_{ij,\beta} \pm F_\tau^{ij}\cos\theta_{ij,\alpha}\sin\theta_{ij,\beta}\right] \tag{5}$$

where $\alpha,\beta = x,y$ (XY is a plane of motion); V_i is a current value of the volume of element i; q_{ij} is a distance from mass centre of element i to the central point of area of interaction (contact area) with neighbour j; $\theta_{ij,\alpha}$ is an angle between the line connecting mass centres of interacting elements i and j and axis α of laboratory system of coordinates (Figure 1). Components $\overline{\sigma}^i_{xz}$ and $\overline{\sigma}^i_{yz}$ are identically zero in the framework of considered quasi-two-dimensional approximation and definition of $\overline{\sigma}^i_{zz}$ depends on constitutive equations of considered medium. Note that values of $\overline{\sigma}^i_{xy}$ and $\overline{\sigma}^i_{yx}$ coincide only in static equilibrium state of ensemble of discrete elements, while they can slightly differ at the stage of establishing static equilibrium. Therefore their mean value ($\left(\overline{\sigma}^i_{xy}+\overline{\sigma}^i_{yx}\right)/2$) is used in the proposed model (hereinafter it is called as $\overline{\sigma}^i_{xy}$).

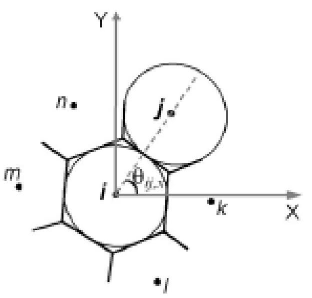

Figure 1: An example of definition of angle $\theta_{ij,\alpha}$ between line connecting mass centers of discrete elements in the pair *i-j* and α-axis of laboratory system of coordinates (α=X is considered here). The center of coordinate system is translated to the mass center of the element *i*.

Calculated in this way the stress tensor components can be used to determine the pressure in the volume of discrete element:

$$P_i = -\overline{\sigma}^i_{mean} = -\frac{\overline{\sigma}^i_{xx}+\overline{\sigma}^i_{yy}+\overline{\sigma}^i_{zz}}{3} \tag{6}$$

Note that calculated values of average stress tensor components can be used to determine other tensor invariants as well, for example stress intensity:

$$\overline{\sigma}^i_{\text{int}} = \frac{1}{\sqrt{2}}\sqrt{\left(\overline{\sigma}^i_{xx}-\overline{\sigma}^i_{yy}\right)^2+\left(\overline{\sigma}^i_{yy}-\overline{\sigma}^i_{zz}\right)^2+\left(\overline{\sigma}^i_{zz}-\overline{\sigma}^i_{xx}\right)^2+6\left(\overline{\sigma}^i_{xy}\right)^2} \tag{7}$$

It follows form (1), (4), (5) that the central problem in the framework of proposed approach to building many-body interaction of discrete element is to determine expressions for F_n^{ij} and F_τ^{ij}, which provide necessary rheological characteristics of mechanical response of ensemble of elements. Analysis of relationships (1), (4), (5) leads to the conclusion that expressions for interaction forces could be directly reformulated from constitutive equations of considered medium (equations of state). Below is a derivation of such expressions for locally isotropic elastic-plastic materials.

3 DESCRIPTION OF ELASTIC-PLASTIC MEDIUM WITH DEM FORMALISM

For convenience hereinafter parameters of interaction of discrete elements will be considered in reduced units.

In particular, values of central and tangential relative displacements of elements of the pair *i-j* are distributed among them and normalized to element sizes:

$$\Delta\varepsilon_{ij} = \frac{\Delta r_{ij}}{\left(d_i + d_j\right)/2} = \frac{\Delta q_{ij}}{d_i/2} + \frac{\Delta q_{ji}}{d_j/2} = \Delta\varepsilon_{i(j)} + \Delta\varepsilon_{j(i)}$$
$$\Delta\gamma_{ij} = \frac{\Delta l^{ij}_{shear}}{r_{ij}} = \frac{V^{ij}_{shear}\Delta t}{r_{ij}} = \Delta\gamma_{i(j)} + \Delta\gamma_{j(i)} \tag{8}$$

where symbol Δ hereinafter indicates increment of corresponding parameter during one time step Δt, r_{ij} is the distance between mass centers of discrete elements *i* and *j* (Figure 2), q_{ij} and q_{ji} are the distances from mass centers of elements *i* and *j* to the center of area of interaction ($q_{ij}+q_{ji}=r_{ij}$), d is size of element, V^{ij}_{shear} is a velocity of relative shear displacement of elements (it is calculated taking into account rotation of both elements [6]). Space variables $\varepsilon_{i(j)}$ and $\gamma_{i(j)}$ hereinafter will be called as central and shear strains of discrete element *i* in the pair *i-j*.

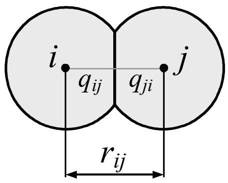

Figure 2: Parameters of spatial relation of the pair of discrete elements *i* and *j*: distance between mass centers (r_{ij}) and distances from mass centers of element to the center of area of interaction (q_{ij} and q_{ji}).

So, in the general case strains of elements *i* and *j* in the pair *i-j* differ from each other. As shown below, the rule of strain distribution in the pair is inseparable linked with the expression for element interaction forces.

Forces of central (F_n^{ij}) and tangential (F_τ^{ij}) interaction of discrete elements *i* and *j* will be considered in specific units:

$$F_n^{ij} = \sigma_{ij} S_{ij}$$
$$F_\tau^{ij} = \tau_{ij} S_{ij} \tag{9}$$

Specific values (σ_{ij} and τ_{ij}) of interaction forces will be called as central and tangential pair stresses. In accordance with (4), the general form of expressions for the central and tangential interaction forces in specific units can be written as follows:

$$\sigma_{ij} = \sigma_{ij}^{pair}\left(\varepsilon_{ij}\right) - AP_i = \sigma_{ij}^{pair}\left(\varepsilon_{ij}\right) + A\overline{\sigma}^i_{mean} \tag{10}$$

$$\tau_{ij} = \tau_{ij}^{pair}\left(\gamma_{ij}\right)$$

The proposed below model of elastic-plastic interaction of discrete elements will be formulated in terms of reduced values of interaction parameters.

3.1 Description of linearly-elastic medium

Stress-strain state of isotropic linearly elastic medium is described on the basis of generalized Hooke's law. The following notation of this law will be used in the paper:

$$\sigma_{\alpha\alpha} = 2G\varepsilon_{\alpha\alpha} + (1 - 2G/K)\sigma_{mean} \qquad (11)$$
$$\tau_{\alpha\beta} = G\gamma_{\alpha\beta}$$

where $\alpha,\beta = x,y,z$; $\sigma_{\alpha\alpha}$ and $\varepsilon_{\alpha\alpha}$ are diagonal components of stress and strain tensors; $\tau_{\alpha\beta}$ and $\gamma_{\alpha\beta}$ are off-diagonal components; $\sigma_{mean} = \left(\sigma_{xx} + \sigma_{yy} + \sigma_{zz}\right)/3$ is mean stress; K is bulk modulus; G is shear modulus.

It can be seen that the form and the matter of expressions (11) for diagonal and off-diagonal stress tensor components are analogous to expressions (10) describing normal and tangential interaction of discrete elements. This leads to the simple idea to write down expressions for force response of automaton i to the impact of the neighbor j by means of direct reformulation of Hooke's law relationships:

$$\sigma_{ij} = 2G_i\varepsilon_{i(j)} + \left(1 - 2G_i/K_i\right)\overline{\sigma}_{mean}^{i} \qquad (12)$$
$$\tau_{ij} = 2G_i\gamma_{i(j)}$$

where G_i and K_i are shear and bulk elastic moduli of material filling the element i, $\varepsilon_{i(j)}$ and $\gamma_{i(j)}$ are central and shear strains of element i in the pair i-j, mean stress $\overline{\sigma}_{mean}^{i}$ is calculated using (6).

Proposed relationships (12) for force of element response to the impact of the neighbor j are not arbitrary. Thus, by substituting relations (6) in (4) easy to show that proposed expressions for respond force automatically provide implementation of Hooke's law for components of average stress ($\overline{\sigma}_{\alpha\beta}^{i}$) and strain ($\overline{\varepsilon}_{\alpha\beta}^{i}$) tensors in the volume of element i. Note that $\overline{\varepsilon}_{\alpha\beta}^{i}$ are determined by analogy with (5) in terms of strains $\varepsilon_{i(k)}$ and $\gamma_{i(k)}$ of the element i in pairs i-k.

Proposed relationships (12) make it possible to calculate central and tangential interaction of discrete elements, whose ensemble simulates isotropic elastic medium. Taking into account the need to implement Newton's third law for interacting pairs of discrete element ($\sigma_{ij}=\sigma_{ji}$ and $\tau_{ij}=\tau_{ji}$) and the need to distribute relative displacement of elements in the pair the expressions for specific interaction forces can be written as follows:

$$\Delta\sigma_{ij} = \Delta\sigma_{ji} = 2G_i\Delta\varepsilon_{i(j)} + \left(1 - \frac{2G_i}{K_i}\right)\Delta\overline{\sigma}_{mean}^{i} = 2G_j\Delta\varepsilon_{j(i)} + \left(1 - \frac{2G_j}{K_j}\right)\Delta\overline{\sigma}_{mean}^{j} \qquad (13)$$
$$\Delta\varepsilon_{i(j)}\, d_i/2 + \Delta\varepsilon_{j(i)}\, d_j/2 = \Delta r_{ij}$$

and

$$\Delta\tau_{ij} = \Delta\tau_{ji} = 2G_i\Delta\gamma_{i(j)} = 2G_j\Delta\gamma_{j(i)}$$
$$\Delta\gamma_{i(j)}\, {d_i}/{2} + \Delta\gamma_{j(i)}\, {d_j}/{2} = V_{shear}^{ij}\Delta t \tag{14}$$

Here, relations for calculating the central and tangential interaction forces are written in increments (in hypoelastic form).

It should be noted that in two-dimensional formulation of the problem approximations of plane stress or plane strain state are widely used. A similar approach is used in described model:

$$\Delta\bar{\sigma}_{zz}^i = \frac{1 - {2G_i}/{K_i}}{2 + {2G_i}/{K_i}}\left(\Delta\bar{\sigma}_{xx}^i + \Delta\bar{\sigma}_{yy}^i\right) \quad \textit{plane strain}$$
$$\Delta\bar{\sigma}_{zz}^i = 0 \qquad \textit{plane stress} \tag{15}$$

Testing results (including comparison with results obtained using the commercial software ANSYS/LS-DYNA) showed that ensemble of discrete elements that interact according to (4)-(6), (8), (9), (13)-(15), demonstrates a “macroscopically” isotropic response, even with the regular packing of elements of the same size. Note that achieving isotropic response of regularly packed elements is a fundamental problem in conventional models of DEM that use approximation of two-particle interaction.

3.2 Description of elastic-plastic medium

An important advantage of proposed approach to building many-body interaction of discrete elements is a capability to realize various models of elasticity and plasticity within the framework of DEM. In particular, a model of plastic flow (incremental plasticity) with the criterion of Mises was implemented to simulate deformation of isotropic elastic-plastic media.

For this purpose, radial return algorithm of Wilkins [10] was adopted to discrete element approach. Typically, this algorithm is formulated in terms of the stress deviator (Figure 3):

$$\hat{D}'_\sigma = \hat{D}_\sigma M \tag{16}$$

where

$$\hat{D}_\sigma = \begin{vmatrix} \sigma_x - \sigma_{cp} & \tau_{yx} & \tau_{zx} \\ \tau_{xy} & \sigma_y - \sigma_{cp} & \tau_{zy} \\ \tau_{xz} & \tau_{yz} & \sigma_z - \sigma_{cp} \end{vmatrix}$$

Being written in terms of stress, for components of average stress tensor in the volume of discrete element i it has the following form:

$$\left(\bar{\sigma}_{\alpha\alpha}^i\right)' = \left(\bar{\sigma}_{\alpha\alpha}^i - \bar{\sigma}_{mean}^i\right)M_i + \bar{\sigma}_{mean}^i$$
$$\left(\bar{\sigma}_{\alpha\beta}^i\right)' = \bar{\sigma}_{\alpha\beta}^i M_i \tag{17}$$

where $\alpha,\beta = x,y,z$ and $\alpha\neq\beta$; $\left(\bar{\sigma}^i_{\alpha\alpha}\right)'$ and $\left(\bar{\sigma}^i_{\alpha\beta}\right)'$ are corrected (returned) average stress tensor components; $\bar{\sigma}^i_{\alpha\alpha}$ and $\bar{\sigma}^i_{\alpha\beta}$ are stress tensor components, which result from solution of elastic problem (13)-(15) at the current time step; $M_i = \sigma^i_{pl} / \bar{\sigma}^i_{\text{int}}$ is current value of the coefficient M for discrete element i; σ^i_{pl} is current radius of von Mises yield circle for the element i; $\bar{\sigma}^i_{\text{int}}$ is calculated on the basis of (7) after solving elastic problem at the current time step.

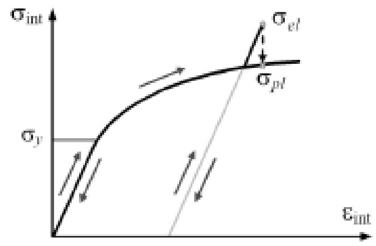

Figure 3: Schematic representation of functioning of radial return algorithm of Wilkins. Here σ_{el} is stress intensity after elastic problem solution at the current time step.

The main problem in realization of the algorithm of Wilkins within the framework of DEM is formulation of correcting relations for element interaction forces that provide for implementation of necessary conditions of the algorithm [10]. By analogy with the elastic problem the expressions for correction of specific central and tangential forces of response of the element i were derived by direct reformulation of relations (17) for average stress:

$$\sigma'_{ij} = \left(\sigma_{ij} - \bar{\sigma}^i_{mean}\right) M_i + \bar{\sigma}^i_{mean}$$
$$\tau'_{ij} = \tau_{ij} M_i \tag{18}$$

where σ'_{ij} and τ'_{ij} are corrected specific forces.

It is easy to show that substitution of (18) in expression (5) for average stress tensor automatically provides reduction of its components to yield circle for the element i. This demonstrates the correctness of the proposed model.

It is necessary to note that in the general case values of reduced specific forces of response of element i (σ'_{ij} and τ'_{ij}) to the impact of neighbor j differ from those of element j (σ'_{ji} и τ'_{ji}). In view of the need for implementation of Newton's third law correction of specific interaction force in the pair i-j has to be done with use of "united and matched" coefficient M_k:

$$\sigma'_{ij} = \left(\sigma_{ij} - \sigma^k_{mean}\right) M_k + \sigma^k_{mean}$$
$$\tau'_{ij} = \tau_{ij} M_k \tag{19}$$

where $k=i$ or $k=j$ depending on the rule of matching of specific forces. We propose to use the minimum one of $\{M_i, M_j\}$ as the coefficient M_k:

$$M_k = \min\{M_i, M_j\} \tag{20}$$

where

$$k = i, \quad if\ M_i < M_j$$
$$k = j, \quad if\ M_i > M_j \tag{21}$$

Such "individual" approach to correction of forces of interaction of the element i with different neighbours j can result in divergence from rigorous satisfaction of the necessary conditions ($\left(\overline{\sigma}_{mean}^i\right)' = \overline{\sigma}_{mean}^i$ and $\left(\overline{\sigma}_{\text{int}}^i\right)' = M_i \overline{\sigma}_{\text{int}}^i$ [10]) of the algorithm of Wilkins. Nevertheless testing results demonstrate that divergence from precise fulfillment of these conditions is quite small even for pairs of dissimilar elements, the elastic constants (G и K) and hardening curves of which differ considerably.

It should be also noted that in considered two-dimensional formulation of the problem the peculiarities of the algorithm of Wilkins for approximations of plane stress or plane strain state are taken into account [10,11]:

$$\left(\overline{\sigma}_{zz}^i\right)' = \left(\overline{\sigma}_{zz}^i - \overline{\sigma}_{mean}^i\right) M_i + \overline{\sigma}_{mean}^i \qquad \textit{plane strain}$$
$$\left(\overline{s}_{zz}^i\right)' = \overline{s}_{zz}^i \frac{b_i M_i^{iter}}{b_i M_i^{iter} + \left(1 - M_i^{iter}\right)}, \quad \left(\overline{\sigma}_{zz}^i\right)' = \overline{\sigma}_{zz}^i \qquad \textit{plane stress} \tag{22}$$

where $\overline{s}_{zz}^i$ is a Z-component of the average stress deviator tensor, $b_i = \left(1 + 4G_i/K_i\right)$, M_i^{iter} is a stress correction coefficient that is calculated on the basis of M_i with use of iterative method of Newton [11].

Testing results have shown that proposed model of elastic-plastic interaction of discrete elements provides good agreement of spatial distribution of stresses and strain in the ensemble of discrete elements modeling elastic-plastic medium with corresponding analytical solutions as well as with results of numerical simulation by means of commercial software ANSYS/LS-DYNA.

4 DISCRETE ELEMENT MODELS OF FRACTURE AND COUPLING

A fundamental advantage of DEM as a numerical technique is its inherent capability of direct simulation of material fracture (including multiple fracture and mixing of fragments) and coupling (cohesion) of fragments. This capability is taken into account by means of change of the state of the pair of discrete elements ("linked" pair ↔ "unlinked" pair, Figure 4a). Within the framework of conventional models of two-particle interaction of elements pair-wise force or deformation criteria of fracture are used. They are expressed in terms of critical values of central and tangential forces or relative displacements [6]. Potentialities of the developed approach to building many-body interaction of discrete elements make it possible to apply various multiparametric "force" fracture criteria (Huber-Mises-Hencky, Drucker-Prager and so on) as criteria of interelement bond breaking.

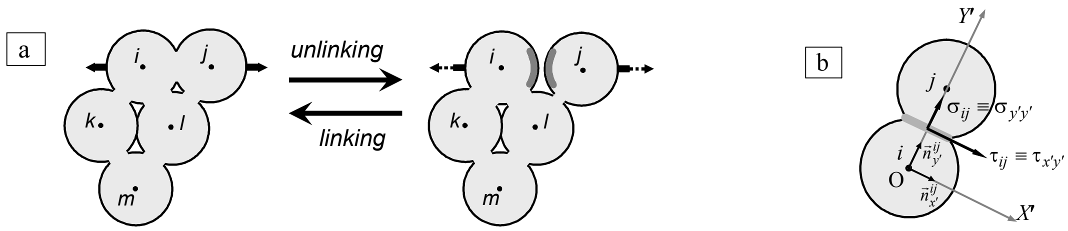

Figure 4: a) schematic representation of switching between *linked* (at the left) and *unlinked* (at the right) states of the pair of discrete elements *i* and *j*; b) instantaneous local coordinate system concerned with current spatial position of interacting pair *i-j*.

Authors proposes the following method of calculating these criteria for pairs of "linked" discrete elements *i* and *j*. It is based on determination of local values of stress tensor components at the area of interaction of considered pair *i-j* (hereinafter denote this tensor as $\sigma^{ij}_{\alpha'\beta'}$) in the local coordinate system *X′Y′* of the pair (Figure 4b). Indeed, in the coordinate system *X′Y′* in accordance with (5) values of components $\bar{\sigma}_{y'y'}$ and $\bar{\sigma}_{x'y'}$ for elements *i* and *j* are identically equal to each other and numerically equal to specific forces of central (σ_{ij}) and tangential (τ_{ij}) interaction of the elements:

$$\begin{aligned}\bar{\sigma}^{i}_{y'y'} \equiv \bar{\sigma}^{j}_{y'y'} \equiv \bar{\sigma}^{i}_{\alpha'y'} n_{\alpha'} = f^{ij}_{y'} = \sigma_{ij} \\ \bar{\sigma}^{i}_{x'y'} \equiv \bar{\sigma}^{j}_{x'y'} \equiv \bar{\sigma}^{i}_{\alpha'x'} n_{\alpha'} = f^{ij}_{x'} = \tau_{ij}\end{aligned} \tag{23a}$$

where $\alpha'=x',y'$; $n_{\alpha'}$ are direction cosines; $f^{ij}_{\alpha'}$ are projections of specific value of interaction force vector (stress vector at the area of interaction of elements *i* and *j*). It is evident that these values of stress tensor components can be assigned to the area of element interaction ($\sigma_{ij} = \sigma^{ij}_{y'y'}$ and $\tau_{ij} = \sigma^{ij}_{x'y'}$). At the same time, other components ($\bar{\sigma}_{x'x'}$ and $\bar{\sigma}_{z'z'}$) of average stress tensor in the local coordinate system *X′Y′* are different for elements *i* and *j*. Therefore corresponding components of tensor $\sigma^{ij}_{\alpha'\beta'}$ at the area of interaction of the elements can be calculated on the basis of "lever rule":

$$\begin{aligned}\sigma^{ij}_{x'x'} = \frac{\bar{\sigma}^{i}_{x'x'} q_{ji} + \bar{\sigma}^{j}_{x'x'} q_{ij}}{r_{ij}} \\ \sigma^{ij}_{z'z'} = \frac{\bar{\sigma}^{i}_{z'z'} q_{ji} + \bar{\sigma}^{j}_{z'z'} q_{ij}}{r_{ij}}\end{aligned} \tag{23b}$$

where $\bar{\sigma}^{i}_{\alpha'\beta'}$ and $\bar{\sigma}^{j}_{\alpha'\beta'}$ are components of average stress tensor in the volume of elements *i* and *j* in the local coordinate system of the pair.

Components $\sigma^{ij}_{\alpha'\beta'}$, thus defined, are used to calculate necessary invariants of stress tensor which then can be used to calculate current value of applied criterion of pair fracture. In particular, below the conditions of bond breaking in the pair *i-j* with use of Huber-Mises-Hencky and Drucker-Prager criteria are shown:

$$\begin{aligned} &\sigma_{\text{int}}^{ij} > \sigma_c && \textit{Huber – Mises – Hencky criterion} \\ &\sigma_{\text{int}}^{ij}\, 0.5(a+1) + \sigma_{mean}^{ij}\, 1.5(a-1) > \sigma_c && \textit{Drucker – Prager criterion} \end{aligned} \tag{24}$$

where σ_c is corresponding threshold value for considered pair (value characterizing strength of chemical bond), a is a ratio of material compressive strength to tensile strength, σ_{int}^{ij} and σ_{mean}^{ij} are calculated by analogy with (6)-(7).

Distinctive features of interaction of "unlinked" (i.e. contacting) elements *i* and *j*, among other things, are the lack of resistance to tension (pair is considered as interacting only when $\sigma_{ij} \le 0$) and limited value of the force of tangential interaction. Maximum allowed value of tangential force in "unlinked" pairs is determined by the model of friction of surfaces of interacting elements (Amonton's law of friction, model of Dieterich [12] and so on).

In many problems (in particular, modeling of friction pairs [13]) it is important to take into account a possibility of coupling of interacting elements (onset of cohesion in the pairs of previously "unlinked" elements). For this purpose, authors proposed some simple criteria of formation of "linked" pairs as a result of contact interaction (compression + friction) of "unlinked" elements. Examples of such criteria are: i) specific value of central force under compression ($\sigma_{ij} \le 0$, $|\sigma_{ij}| > \sigma_{bond}$ where σ_{bond} is threshold value for bonding); ii) pair strain under compression ($\varepsilon_{ij} \le 0$, $|\varepsilon_{ij}| > \varepsilon_{bond}$); iii) friction work in considered pair taking into account the value of central interaction force (σ_{ij}) i.e. the value of compression.

5 CONCLUSIONS

- A solution to the problem of modeling the consolidated elastic-plastic media by ensemble of discrete elements is proposed in the paper. This solution is based on use of many-particle interaction forces and on determination of volume-dependent constituent of interaction via calculation of components of average stress tensor in the volume of discrete elements. Final relations for central and tangential interaction forces are derived from constitutive rheological equations for modeled medium.
- An important advantage of the proposed expressions for element interaction is a possibility of implementation of various models of elastoplasticity or viscoelastoplasticity (which are conventionally written in terms of stress/strain tensor components) in terms of element interaction force and displacement increments. In particular, the authors realized plastic flow theory with von Mises yield criterion within the framework of DEM.
- Another important advantage of the developed formalism is a possibility to directly apply conventional multiparametric fracture criteria (Huber-Mises-Hencky, Drucker-Prager, Mohr-Coulomb etc.) as criteria of interelement bond breakage. The use of these criteria is very important for correct modeling of fracture of complex heterogeneous materials of various nature.
- At the present time described models of interaction of discrete elements are approved and widely applied to study response (including fracture) of heterogeneous materials at different scales from nanoscopic to macroscopic one. Advantages of the approach to description of elastic-plastic interaction of discrete elements makes possible

correct simulation of phenomena and processes, whose study by conventional numerical methods of continuum mechanics is difficult. The problems of this type include, for example, study of physical and mechanical processes in contact patches of technical and natural frictional pairs [13,14].

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