Vector-based model of elastic bonds for simulation of granular solids

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A model (further referred to as the V model) for the simulation of granular solids, such as rocks, ceramics, concrete, nanocomposites, and agglomerates, composed of bonded particles (rigid bodies), is proposed. It is assumed that the bonds, usually representing some additional gluelike material connecting particles, cause both forces and torques acting on the particles. Vectors rigidly connected with the particles are used to describe the deformation of a single bond. The expression for potential energy of the bond and corresponding expressions for forces and torques are derived. Formulas connecting parameters of the model with longitudinal, shear, bending, and torsional stiffnesses of the bond are obtained. It is shown that the model makes it possible to describe *any* values of the bond stiffnesses *exactly*; that is, the model is applicable for the bonds with arbitrary length/thickness ratio. Two different calibration procedures depending on bond length/thickness ratio are proposed. It is shown that parameters of the model can be chosen so that under small deformations the bond is equivalent to either a Bernoulli-Euler beam or a Timoshenko beam or short cylinder connecting particles. Simple analytical expressions, relating parameters of the V model with geometrical and mechanical characteristics of the bond, are derived. Two simple examples of computer simulation of thin granular structures using the V model are given.

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I. INTRODUCTION

The discrete (or distinct) element method (DEM) [1] is widely used for the computer simulation of solid and free-flowing granular materials. Similarly to classical molecular dynamics [2,3], in the framework of DEM the material is represented by a set of many interacting rigid body particles (granules). The equations of the particles' motion are integrated numerically. In free-flowing materials the particles interact *via* contact forces, dry and viscous friction forces, electrostatic forces, etc. Computer simulation of deformation and fracture of granular solids, such as rocks [4], concrete [5], ceramics [6,7], particle compounds [8], agglomerates [9], nanocomposites [10], etc., is even more challenging. Particles in granular solids are usually connected together by some additional bonding material such as cement [4,5] or glue [6–10]. The example of composite material consisting of PbS nanoparticles bonded together by a copolymer is shown in Fig. 1 (for details, see Ref. [10]). The copolymer (bonding material) resists the relative translation and rotation of neighboring PbS particles. In DEM simulations bonding material is usually taken into account implicitly using the concept of so-called bonds [4,7,9,11]. Neighboring particles are connected by the bonds that resist stretching/compression, shear, bending, and torsion. The bonds cause forces and torques acting on the particles along with contact forces [12]. The mass of the bonding material is usually neglected [4,7,9,11]. The assumption does not influence static properties of the granular material. The influence on the dynamic properties is not so straightforward and should be considered separately. However, let us note that in many practical applications [4,7,9,10] the mass of bonding material is much smaller than the mass of the particles (see, for example, Fig. 1). Therefore, the mass of bonding material can be neglected.

According to the review, presented in Ref. [11], only a few models proposed in the literature allow a description of all possible deformations of the bond accurately. The bonded-particle model (BPM), proposed in Ref. [4], is widely used for simulation of deformation and fracture of solids, in particular, rocks [13,14] and agglomerates [9]. For example, the impact of a granule with a rigid wall is considered in Ref. [9]. Several drawbacks of the BPM, in particular, in the case of coexistence of bending and torsion of the bond, are discussed in Ref. [11]. It is noted that the main reason for the drawbacks is the incremental algorithm, used in the framework of the BPM. Also it should be noted that the BPM contains only two independent parameters, describing bond stiffnesses, while, in general, the bond has four independent stiffnesses (longitudinal, shear, bending, and torsional). A Timoshenko beam connecting particles' centers is used as a model of a bond in Ref. [15]. The model has a clear physical meaning and is applicable for thin, long bonds under small deformations. However, it has low accuracy for the description of short bonds, connecting particles' surfaces. For example, the model [15] is not accurate in the case shown in Fig. 1. Also the generalization of the model for the case of large nonlinear deformations of the bond is not straightforward. The approach, based on decomposition of relative rotation of particles, is proposed in Ref. [11]. Forces and torques are represented as functions of angles, describing the relative rotation of the particles. It is shown that the method in Ref. [11] is more accurate from the computational point of view than the incremental procedure of the BPM. Though the formalism proposed in Ref. [11] is correct from a mathematical point of view, it has a drawback. It is evident from the paper that if particles rotate in the same direction and there is no relative translation, then forces and torques are equal to zero. The reason is that the forces and torques, proposed in Ref. [11], depend only on relative position and orientation of the particles, while, in general, the dependence on the orientation of the particles with respect to the bond should also be taken into account.

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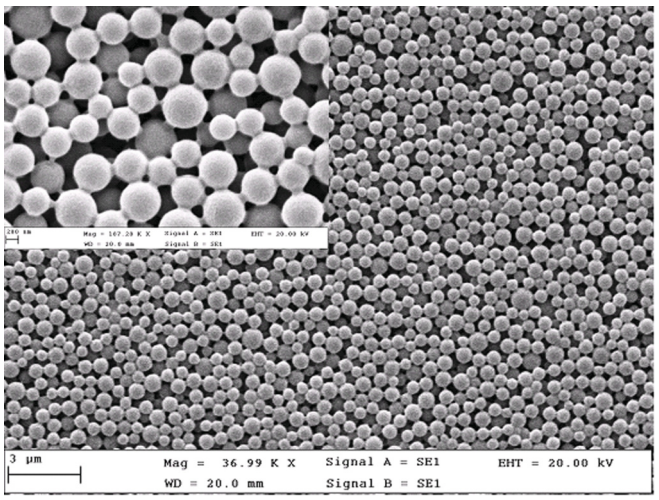

FIG. 1. Scanning electron microscope images of composite consisting of PbS nanoparticles bonded by a copolymer. From Ref. [10].

Another approach for description of interactions between both material points [2] and rigid bodies [3] is used in classical molecular dynamics. Forces and torques, acting between particles, are derived from the potential energy. Linear interactions between rigid body particles in crystalline solids are discussed in detail in Refs. [16,17]. Different types of nonlinear interactions are proposed in Refs. [3,18] and [19,20] for molecular liquids and crystalline solids, respectively.

In the present paper a vector-based model (further referred to as the V model) of elastic bonds in solids is developed using a combination of approaches, proposed in Refs. [16] and [3,18]. Equations describing interactions between two rigid bodies in the general case are summarized. The general expression for the potential energy of the bond is represented *via* vectors rigidly connected with bonded particles. The vectors are used for description of different types of bond deformation. The expression for potential energy corresponding to tension/compression, shear, bending, and torsion of the bond is proposed. Forces and torques acting between particles are derived from the potential energy. Two approaches for calibration of V model parameters for bonds with different length/thickness ratios are presented. Simple analytical formulas connecting geometrical and elastic characteristics of the bond with parameters of the V model are derived. The main aspects of numerical implementation of the model are discussed. Two examples of computer simulations using the V model are given.

II. PAIR POTENTIAL INTERACTIONS BETWEEN RIGID BODIES: THE GENERAL CASE

Let us consider the approach for the description of pair potential interactions between rigid bodies in the general case [3,17,18]. In the literature the formalism is referred to as moment interactions [16,17,19–21]. In the present paper moment interactions are applied for description of elastic bonds between particles in granular solids.

Consider a system consisting of two interacting rigid body particles, marked by indexes i and j. In the general case particles interact *via* forces and torques depending on their relative position, relative orientation, and orientation with respect to the vector connecting the particles. Let us introduce the following designations: $\mathbf{F}_{ij}$ and $\mathbf{M}_{ij}$ are force and torque, respectively, acting on particle i from particle j. Torque $\mathbf{M}_{ij}$ is calculated with respect to the center of mass of particle i. In Ref. [17] it is shown that $\mathbf{F}_{ij}$ and $\mathbf{M}_{ij}$ satisfy Newton's third law, its analog for torques, and equation of energy balance,

$$\begin{aligned} &\mathbf{F}_{ij} = -\mathbf{F}_{ji}, \quad \mathbf{M}_{ij} + \mathbf{M}_{ji} - \mathbf{r}_{ij} \times \mathbf{F}_{ij} = 0, \\ &\dot{U}_{ij} = \mathbf{F}_{ij} \cdot \dot{\mathbf{r}}_{ij} - \mathbf{M}_{ij} \cdot \boldsymbol{\omega}_i - \mathbf{M}_{ji} \cdot \boldsymbol{\omega}_j, \end{aligned} \tag{1}$$

where $\mathbf{r}_{ij} \stackrel{\text{def}}{=} \mathbf{r}_j - \mathbf{r}_i$; $\mathbf{r}_i, \mathbf{r}_j$ are radius vectors of particles i and j; $\boldsymbol{\omega}_i, \boldsymbol{\omega}_j$ are angular velocities; U_{ij} is the internal energy of the system.

Assume that the interactions between particles are potential and that the internal energy U_{ij} depends on particles' relative position, relative orientation, and orientation with respect to $\mathbf{r}_{ij}$. Relative position of the particles can be described by vector $\mathbf{r}_{ij}$. Therefore, U_{ij} should be a function of $\mathbf{r}_{ij}$. In order to introduce the dependence of U_{ij} on particles' orientation the approach, initially proposed for liquids in Ref. [18] and applied for solids in Ref. [20], is used. Let us describe the orientation of particle i via the set of vectors $\{\mathbf{n}_i^k\}_{k\in\Lambda_i}$, rigidly connected with the particle, where Λ_i is a set of indexes. Hereinafter the lower index corresponds to a particle's number, while the upper index corresponds to a vector's number. The maximum amount of vectors is not limited and does not influence the general considerations. Since orientations of the particles are determined by vectors $\{\mathbf{n}_i^k\}_{k\in\Lambda_i}$, $\{\mathbf{n}_j^m\}_{m\in\Lambda_j}$, it follows that internal energy has the form

$$U_{ij} = U\left(\mathbf{r}_{ij}, \left\{\mathbf{n}_i^k\right\}_{k\in\Lambda_i}, \left\{\mathbf{n}_j^m\right\}_{m\in\Lambda_j}\right). \tag{2}$$

Let us derive the relation between forces, torques, and potential energy U_{ij}. Substituting formula (2) into equation of energy balance (1) and assuming that forces $\mathbf{F}_{ij}$ and torques $\mathbf{M}_{ij}$ are independent on linear and angular velocities of the particles, one can show that

$$\begin{aligned} &\mathbf{F}_{ij} = -\mathbf{F}_{ji} = \frac{\partial U}{\partial \mathbf{r}_{ij}}, \quad \mathbf{M}_{ij} = \sum_{k\in\Lambda_i} \frac{\partial U}{\partial \mathbf{n}_i^k} \times \mathbf{n}_i^k, \\ &\mathbf{M}_{ji} = \sum_{m\in\Lambda_j} \frac{\partial U}{\partial \mathbf{n}_j^m} \times \mathbf{n}_j^m. \end{aligned} \tag{3}$$

If the internal energy (2) is known, then forces and torques are calculated using formulas (3). Note that function U must satisfy the material objectivity principle. That is, it must be invariant with respect to rigid body rotation. If the objectivity principle is satisfied, then forces and torques, calculated using formulas (3), satisfy Newton's third law for torques automatically. Therefore, U must be a function of some invariant arguments. For instance, the following invariant values can be used: $r_{ij}, \mathbf{e}_{ij} \cdot \mathbf{n}_i^k, \mathbf{e}_{ji} \cdot \mathbf{n}_j^m, \mathbf{n}_i^k \cdot \mathbf{n}_j^m, |\mathbf{e}_{ij} \times \mathbf{n}_i^k|, |\mathbf{n}_i^k \times \mathbf{n}_j^m|$, etc., where $\mathbf{e}_{ij} \stackrel{\text{def}}{=} \mathbf{r}_{ij}/r_{ij}, k \in \Lambda_i, m \in \Lambda_j$. In practice the first four expressions from the list are sufficient as the remaining invariants can be represented via their combination. These expressions have simple geometrical meaning. The first one is a distance between the particles. The second and the third invariants ($\mathbf{e}_{ij} \cdot \mathbf{n}_i^k$ and $\mathbf{e}_{ji} \cdot \mathbf{n}_j^m$) describe the orientation of particles i and j with respect to vector $\mathbf{r}_{ij}$. The fourth invariants

$\mathbf{n}_i^k \cdot \mathbf{n}_j^m$ describe the relative orientation of the particle. Thus, in the general case the potential of interaction between rigid bodies is represented in the following form:

$$U_{ij} = U\left(r_{ij}, \left\{\mathbf{e}_{ij}\cdot\mathbf{n}_i^k\right\}_{k\in\Lambda_i}, \left\{\mathbf{e}_{ji}\cdot\mathbf{n}_j^m\right\}_{m\in\Lambda_j}, \left\{\mathbf{n}_i^k\cdot\mathbf{n}_j^m\right\}_{k\in\Lambda_i, m\in\Lambda_j}\right). \tag{4}$$

In general, sets Λ_i, Λ_j may contain any number of vectors. However, from computational point of view it is desirable to minimize this number.

III. VECTOR-BASED MODEL OF A SINGLE BOND

Let us use moment interactions for the description of the elastic deformation of the bond. Note that, in general, the particle can be bonded with any number of neighbors. However, the behavior of the bonds is assumed to be independent. Therefore, for simplicity, only two bonded particles i and j are considered. Assume that the bond connects two points that belong to the particles. The points lie on the line connecting the particles' centers in the initial (undeformed) state. For example, the points can coincide with particles centers. Let us denote distance from the points to the particles' centers of mass as R_i and R_j, respectively (see Fig. 2). For example, in the case shown in Fig. 2, the points lie on the particles' surfaces and values R_i and R_j coincide with the particles' radii. Let us introduce orthogonal unit vectors $\mathbf{n}_i^1, \mathbf{n}_i^2, \mathbf{n}_i^3$ and $\mathbf{n}_j^1, \mathbf{n}_j^2, \mathbf{n}_j^3$, rigidly connected with particles i and j, respectively. The lower indexes correspond to particles' numbers; the upper indexes correspond to vectors' numbers. Assume that in the undeformed state the following relations are satisfied:

$$\mathbf{n}_i^1 = -\mathbf{n}_j^1 = \mathbf{e}_{ij}, \quad \mathbf{n}_i^2 = \mathbf{n}_j^2, \quad \mathbf{n}_i^3 = \mathbf{n}_j^3. \tag{5}$$

Following the idea described in the previous paragraph, let us represent the potential energy of the bond as a function of vector $\mathbf{D}_{ij} \stackrel{\text{def}}{=} \mathbf{r}_{ij} + R_j\mathbf{n}_j^1 - R_i\mathbf{n}_i^1$ and vectors $\mathbf{n}_i^k, \mathbf{n}_j^m, k,m = 1,2,3$. Vector $\mathbf{D}_{ij}$ connects the "bonded" points with radius vectors $\mathbf{r}_i + R_i\mathbf{n}_i^1, \mathbf{r}_j + R_j\mathbf{n}_j^1$ (see Fig. 2). Let us consider the following form for potential energy of the bond:

$$\begin{aligned} U &= U_L(D_{ij}) + U_B\left(\mathbf{n}_i^1\cdot\mathbf{n}_j^1, \mathbf{d}_{ij}\cdot\mathbf{n}_i^1, \mathbf{d}_{ji}\cdot\mathbf{n}_j^1\right) \\ &\quad + U_T\left(\left\{\mathbf{n}_i^k\cdot\mathbf{n}_j^k, \mathbf{d}_{ij}\cdot\mathbf{n}_i^k, \mathbf{d}_{ji}\cdot\mathbf{n}_j^k\right\}_{k=2,3}\right), \\ D_{ij} &= |\mathbf{D}_{ij}|, \quad \mathbf{d}_{ij} = \mathbf{D}_{ij}/D_{ij}. \end{aligned} \tag{6}$$

Note that potential energy (6) satisfies the objectivity principle. That is, it is invariant with respect to rotation of the system as a rigid body. Let us describe the relation between functions U_L, U_B, U_T and different kinds of deformation of the bond, shown in Fig. 3. Function U_L describes stretching/compression, function U_B describes bending and shear of the bond. Arguments $\mathbf{d}_{ij}\cdot\mathbf{n}_i^1, \mathbf{d}_{ji}\cdot\mathbf{n}_j^1$ change in the case of bending and shear. Argument $\mathbf{n}_i^1\cdot\mathbf{n}_j^1$ changes only in the case of bending and is invariant with respect to shear. Function U_T changes in the case of both torsion and bending. The following expressions for functions U_L, U_B, U_T from formula (6) are proposed in the present paper:

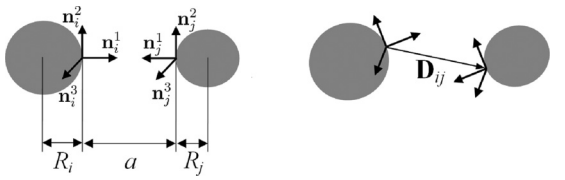

FIG. 2. Two bonded particles in the undeformed state (left) and deformed state (right). Here and below a is an equilibrium distance.

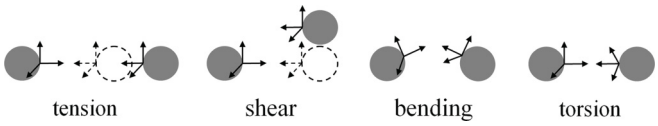

FIG. 3. Different kinds of deformation of the bond and corresponding change in vectors, connected with the particles. Dashed lines show the initial states of the particles.

$$\begin{aligned} U_L(s) &= \frac{B_1}{2}(s-a)^2, \\ U_B(s_1,s_2,s_3) &= -\frac{B_2}{2}s_1^2 - \frac{B_3}{2}\left(s_2^2+s_3^2\right), \\ U_T(\{s_{1k},s_{2k},s_{3k}\}_{k=2,3}) &= -\frac{B_4}{4}\sum_{k=2,3}(s_{1k}+s_{2k}s_{3k})^2 \\ &\quad \times \left(1+s_{2k}^2\right)\left(1+s_{3k}^2\right), \end{aligned} \tag{7}$$

where a is an equilibrium length of the bond (see Fig. 2); $B_m, m = 1,\ldots,4$, are parameters of the model. Functions (7) are the simplest with independent longitudinal, shear, bending, and torsional stiffnesses (see Sec. IV A). Note that the number of parameters of the V model is equal to the number of bond stiffnesses. Further it is shown that the behavior of the bond under small deformations can be described exactly by fitting parameters of the model. For brittle materials, such as rocks [4], it is sufficient as critical deformations are usually small. On the other hand, it is shown below that the V model has reasonable behavior at finite deformations (see Sec. VI). Thus, very flexible structures can be considered as well. Also the V model can be generalized for the nonlinear case, changing expressions for U_L, U_B, U_T and introducing new parameters into the potential. The generalization can be important, in particular, for simulation of polymer bonds [7]. Note that analogous generalization of existing models, such as the BPM [4], is not so straightforward.

Let us derive expressions for force $\mathbf{F}_{ij}$ and torque $\mathbf{M}_{ij}$. Using formulas (3) and (7), one obtains

$$\begin{aligned} \mathbf{F}_{ij} &= B_1(D_{ij}-a)\mathbf{d}_{ij} - \frac{B_3}{D_{ij}}\mathbf{d}_{ij}\cdot\left(\mathbf{n}_i^1\widetilde{\mathbf{n}}_i^1 + \mathbf{n}_j^1\widetilde{\mathbf{n}}_j^1\right) \\ &\quad + \frac{1}{D_{ij}}\sum_{k=2,3}\left(\frac{\partial U_T}{\partial s_{2k}}\widetilde{\mathbf{n}}_i^k - \frac{\partial U_T}{\partial s_{3k}}\widetilde{\mathbf{n}}_j^k\right), \\ \mathbf{M}_{ij} &= R_i\mathbf{n}_i^1\times\mathbf{F}_{ij} - \mathbf{n}_i^1\cdot\left[B_2\mathbf{n}_j^1\mathbf{n}_j^1 + B_3\mathbf{d}_{ij}\mathbf{d}_{ij}\right]\times\mathbf{n}_i^1 \\ &\quad + \sum_{k=2,3}\left(\frac{\partial U_T}{\partial s_{1k}}\mathbf{n}_j^k + \frac{\partial U_T}{\partial s_{2k}}\mathbf{d}_{ij}\right)\times\mathbf{n}_i^k. \end{aligned} \tag{8}$$

Here and below $\widetilde{\mathbf{n}}_i^k = \mathbf{n}_i^k - \mathbf{n}_i^k\cdot\mathbf{d}_{ij}\mathbf{d}_{ij}$. The expressions for partial derivatives $\partial U_T/\partial s_{mk}, m = 1,2,3, k = 2,3$ are the

following:

$$\frac{\partial U_T}{\partial s_{1k}} = -\frac{B_4}{2}(s_{1k} + s_{2k}s_{3k})\left(1 + s_{2k}^2\right)\left(1 + s_{3k}^2\right),$$
$$\frac{\partial U_T}{\partial s_{2k}} = -\frac{B_4}{2}(s_{1k} + s_{2k}s_{3k})\left(1 + s_{3k}^2\right) \times \left(s_{3k} + s_{1k}s_{2k} + 2s_{3k}s_{2k}^2\right),$$
$$\frac{\partial U_T}{\partial s_{3k}} = -\frac{B_4}{2}(s_{1k} + s_{2k}s_{3k})\left(1 + s_{2k}^2\right) \times \left(s_{2k} + s_{1k}s_{3k} + 2s_{2k}s_{3k}^2\right), \quad k = 2,3. \tag{9}$$

Thus, formulas (8) and (9) are used for calculation of forces and torques, acting on the bonded particles. Note that in contrast to incremental procedure [4], the V model allows us to calculate forces and torques at every moment of time (time step) independently.

Note that the V model can be applied to both two- and three-dimensional problems. In two dimensions function U_T describing torsion can be set equal to zero.

IV. PARAMETER CALIBRATION

A. Bond stiffnesses

Let us choose parameters of the V model $B_m, m = 1, \ldots, 4$ in order to describe *any* given elastic properties of the bond in the case of small deformations exactly. Following the idea, proposed in Ref. [17], let us introduce stiffnesses of the bond. Consider the force $\mathbf{F}_{ij}$ and torque

$$\mathbf{M} \stackrel{\text{def}}{=} \mathbf{M}_{ij} - \left(R_i\mathbf{n}_i^1 + \mathbf{D}_{ij}/2\right) \times \mathbf{F}_{ij}, \tag{10}$$

calculated with respect to the center of the bond, defined by vector $\mathbf{r}_i + R_i\mathbf{n}_i^1 + \mathbf{D}_{ij}/2$. According to the results of Ref. [17], under small deformations $\mathbf{F}_{ij}$ and $\mathbf{M}$ can be represented in the form

$$\mathbf{F}_{ij} = \mathbf{A} \cdot \big(\mathbf{u}_j - \mathbf{u}_i - (R_i\boldsymbol{\varphi}_i + R_j\boldsymbol{\varphi}_j) \times \mathbf{d}_{ij} + \tfrac{1}{2}\mathbf{D}_{ij} \times (\boldsymbol{\varphi}_i + \boldsymbol{\varphi}_j)\big),$$
$$\mathbf{M} = \mathbf{G} \cdot (\boldsymbol{\varphi}_j - \boldsymbol{\varphi}_i), \tag{11}$$

where $\mathbf{A}$, $\mathbf{G}$ are stiffness tensors; $\mathbf{u}_i$, $\boldsymbol{\varphi}_i$ are displacement and a vector indicating a small rotation of particle i. In the case of transversally symmetrical bonds, considered in the present paper, the stiffness tensors have form

$$\mathbf{A} = c_A\mathbf{d}_{ij}\mathbf{d}_{ij} + c_D(\mathbf{E} - \mathbf{d}_{ij}\mathbf{d}_{ij}),$$
$$\mathbf{G} = c_B(\mathbf{E} - \mathbf{d}_{ij}\mathbf{d}_{ij}) + c_T\mathbf{d}_{ij}\mathbf{d}_{ij}, \tag{12}$$

where $\mathbf{E}$ is a unit tensor. The values c_A, c_D, c_B, c_T are further referred to as longitudinal, shear, bending, and torsional stiffness, respectively. One can see from formulas (11) and (12) that the stiffnesses completely determine the behavior of the bond in the case of small deformations.

Let us derive the relations between parameters of potential (7) and bond stiffnesses. First consider the expression (8) for force $\mathbf{F}_{ij}$ in the case of pure tension:

$$\mathbf{F}_{ij} = B_1(D_{ij} - a)\mathbf{e}_{ij} = B_1(|r_{ij} - R_i - R_j| - a)\mathbf{e}_{ij}. \tag{13}$$

Therefore, according to formula (11) longitudinal stiffness of the bond c_A is equal to B_1. Let us determine the relation between shear stiffness c_D and parameter B_3. Consider the following deformation of the bond. Assume that position of particle i is fixed and particle j has a displacement $u_j\mathbf{k}$, where $\mathbf{k}$ is orthogonal to the line connecting particles in the undeformed state. Orientations of both particles are fixed. In this case the first formula from (11) has the form

$$\mathbf{F}_{ij} \cdot \mathbf{k} = c_D u_j. \tag{14}$$

Let us expand the expression (8) for $\mathbf{F}_{ij}$ into a series, assuming that $|u_j/a| \ll 1$ and neglecting the second order terms. In this case the projection of $\mathbf{F}_{ij}$ on vector $\mathbf{k}$ has form (14). Omitting the derivation let us present the final expression for c_D:

$$c_D = \frac{2B_3}{a^2}. \tag{15}$$

Let us obtain analogous relation for bending stiffness of the bond c_B. Assume that vector $\mathbf{D}_{ij}$ remains fixed in the equilibrium state, while the particles are rotated by vectors of small turn $\boldsymbol{\varphi}_i, \boldsymbol{\varphi}_j$. In this case vectors $\mathbf{n}_i^k, \mathbf{n}_j^m$ in the current (deformed) configuration can be calculated as follows:

$$\mathbf{n}_p^k \approx \mathbf{n}_p^k(0) + \boldsymbol{\varphi}_p \times \mathbf{n}_p^k(0), \quad k = 1,2,3, \quad p = i, j. \tag{16}$$

Here zero denotes initial configuration, for example, $\mathbf{n}_i^1(0) = -\mathbf{n}_j^1(0) = \mathbf{e}_{ij}(0)$. This deformation corresponds to bending the bond. Substituting (8) and (16) into (10) and leaving the first order terms only, one obtains

$$\mathbf{M} \approx \left[\left(\frac{B_3}{2} + B_2\right)(\mathbf{E} - \mathbf{d}_{ij}\mathbf{d}_{ij}) + B_4\mathbf{d}_{ij}\mathbf{d}_{ij}\right] \cdot (\boldsymbol{\varphi}_j - \boldsymbol{\varphi}_i). \tag{17}$$

The expressions for bending stiffness c_B and torsional stiffness c_T follows from the comparison of formula (17) with the second formula from (11). As a result the expressions relating the parameters of the V model to bond stiffnesses have the form

$$c_A = B_1, \quad c_D = \frac{2B_3}{a^2}, \quad c_B = \frac{B_3}{2} + B_2, \quad c_T = B_4. \tag{18}$$

It follows from formulas (18) that choosing parameters $B_m, m = 1, \ldots, 4$ one can fit any values of the stiffnesses. Therefore, the linear elastic behavior of the bond can be described exactly. Note that no assumptions about bond's length/thickness ratio are made.

Thus, if stiffnesses of the bond are known, then the calculation of V model parameters is straightforward. In principle, the stiffnesses can be measured, performing the experiments on tension, shear, bending, and torsion for the system of two bonded particles. In this case, formulas (18) are sufficient for calibration. However, if the body, for example, agglomerate [9], contains many bonds with different geometrical characteristics, then experimental calibration is practically impossible. Therefore, an additional model connecting the stiffnesses with geometrical and physical characteristics of the bond, such as bond length, shape, cross section area, elastic moduli of bonding material, etc., is required. Evidently the behavior of the bond strongly depends on bond's length/thickness ratio. Therefore, models used for calculation of the stiffnesses should

be different for the different ratios. Two procedures for long and short bonds are proposed below.

B. Calibration for long bonds: The Bernoulli-Euler and Timoshenko beam theories

Assume that bonds are relatively long (length/thickness ratio is larger than unity). In this case, elastic beam, connecting particles, can be used as a model of the bond [15]. Comparison of the V model with the results of Bernoulli-Euler and Timoshemko beam theories [22] is used as a theoretical basis for calibration. Note that in contrast to Ref. [15], in the framework of the V model the bonds, connecting, for example, particle surfaces, can be considered. This fact is important for simulation of solids, composed of glued particles, for example, composites [7,10].

Let us derive the relation between parameters of the V model and massless Bernoulli-Euler beam connecting particles (the beam connects points with radius vectors $\mathbf{r}_i + R_i\mathbf{n}_i^1$ and $\mathbf{r}_j + R_j\mathbf{n}_j^1$). Assume that the beam has equilibrium length a, constant cross section, and isotropic bending stiffness. The expressions for longitudinal, shear, bending, and torsional stiffnesses of a Bernoulli-Euler beam are derived in Ref. [21]:

$$c_A = \frac{EA}{a}, \quad c_D = \frac{12EJ}{a^3}, \quad c_B = \frac{EJ}{a}, \quad c_T = \frac{GJ_p}{a}, \tag{19}$$

where E, G, A, J, and J_p are Young's modulus, shear modulus, cross section area, moment of inertia, and polar moment of inertia of the cross section respectively. For example, for the beam with circular cross section

$$J = \frac{\pi d_b^4}{64}, \quad J_p = 2J, \quad A = \frac{\pi d_b^2}{4}, \tag{20}$$

where d_b is a diameter of the beam. Using formulas (18) and (19) one obtains the expressions, connecting parameters of the V model with characteristics of the beam

$$B_1 = \frac{EA}{a}, \quad B_2 = -\frac{2EJ}{a}, \quad B_3 = -3B_2, \quad B_4 = \frac{GJ_p}{a}. \tag{21}$$

Formula (21) can be used for calibration of the parameters in the case of long bonds. If the parameters are determined by formula (21), then under small deformations the V model is equivalent to a Bernoulli-Euler beam connecting particles. Note that in this case values $\tilde{B}_m \stackrel{\text{def}}{=} B_m a, m = 1, \ldots, 4$, do not depend on the equilibrium bond length a. Therefore, $\tilde{B}_m$ are the same for bonds with different length, but equal cross section and elastic properties. Using this fact one can reduce the number of parameters, stored in RAM, in computer simulations of systems with bonds of different length.

The Bernoulli-Euler model provides simple theoretical basis for calibration. However, if length and thickness of the bond are comparable, then this model is no longer applicable [22]. In this case more accurate models are required. Calibration using a Timoshenko model [22] is described below.

Consider a Timoshenko beam of length a and constant cross section with spherical inertia tensor. Let us derive the expressions, connecting parameters of the beam with its stiffnesses. Longitudinal and torsional stiffnesses are determined by formulas (19). Without loss of generality the derivation of expressions for shear and bending stiffnesses is carried out in the two dimensional case. Consider pure shear of the beam. The corresponding system of equilibrium equations and boundary conditions for the beam has the form [22]

$$w''(s) = \theta'(s), \quad \theta''(s) + \frac{\kappa A}{2J(1+\nu)}[w'(s) - \theta(s)] = 0, \tag{22}$$

$$w(0) = 0, \quad \theta(0) = 0, \quad w(a) = u_j, \quad \theta(a) = 0, \tag{23}$$

where ν is Poisson's ratio of material of the bond; $w(s)$ and $\theta(s)$ are the deflection and angle of rotation for the cross section with coordinate s; κ is dimensionless shear coefficient [22]. Shear coefficients for rods with different cross sections are derived, in particular, in Ref. [23].

Solving the system of partial differential equations (22) with boundary conditions (23) one obtains an expression for the magnitude of the shear force Q, acting in the beam, and shear stiffness:

$$Q = \kappa GA(w' - \theta) = c_D u_j, \quad c_D = \frac{12\kappa AEJ}{a[\kappa Aa^2 + 24J(1+\nu)]}. \tag{24}$$

Let us consider bending of the beam under the following boundary conditions:

$$w(0) = 0, \quad \theta(0) = \varphi_i, \quad w(a) = 0, \quad \theta(a) = \varphi_j. \tag{25}$$

Solving the system of equations (22) with boundary conditions (25) and calculating the magnitude of the torque M, acting in the middle of the beam, one obtains

$$M = EJ\theta'\left(\frac{a}{2}\right) = \frac{EJ}{a}(\varphi_j - \varphi_i). \tag{26}$$

Formula (26) gives the expression for the bending stiffness of the bond. Thus, the stiffnesses of a Timoshenko beam has form

$$c_A = \frac{EA}{a}, \quad c_D = \frac{12\kappa AEJ}{a[\kappa Aa^2 + 24J(1+\nu)]}, \quad c_B = \frac{EJ}{a}, \quad c_T = \frac{GJ_p}{a}. \tag{27}$$

Finally, using formulas (27) one obtains the relation between parameters of the V model and the Timoshenko beam:

$$B_1 = \frac{EA}{a}, \quad B_2 = -\frac{2EJ[\kappa Aa^2 - 12J(1+\nu)]}{a[\kappa Aa^2 + 24J(1+\nu)]}, \quad B_3 = \frac{6\kappa AEJa}{\kappa Aa^2 + 24J(1+\nu)}, \quad B_4 = \frac{GJ_p}{a}. \tag{28}$$

Note that in the limit $\kappa \to \infty$ formulas (28) exactly coincide with analogous formulas (21), obtained using Bernoulli-Euler beam theory. If formula (28) is used for the calibration, then for small deformation the V model is equivalent to Timoshenko beam connecting particles.

C. Calibration for short bonds

Generally speaking, the approach for calibration described above is applicable for relatively long and thin bonds with length/thickness ratio larger than unity. In the case of short bonds, shown, for example, in Fig. 1, the models based

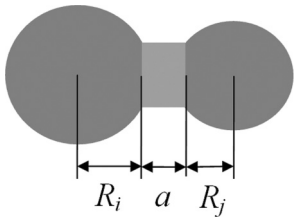

FIG. 4. Particles connected by a short cylinder.

on elasticity theory should be used for calibration. Let us consider a simple qualitative model, based on elasticity theory. Assume that particles are connected by a short cylinder with equilibrium length a as is shown in Fig. 4. Note that, in general, parameters R_i, R_j are not equal to particles' radii (the particles can even be in contact with each other). Let us derive the relations between the parameters of the bond and its stiffnesses. Longitudinal stiffness c_A is, by definition, the proportionality coefficient between force and elongation of the bond. In the case of tension the force $\mathbf{F}_{ij}$ is caused by the normal stress σ, acting in the bond. The following relation is satisfied:

$$\mathbf{F}_{ij} \cdot \mathbf{e}_{ij} = \int_{(A)} \sigma dA, \tag{29}$$

In the case of a short bond, rigidly attached to the particles, the strain state of the bond is approximately uniaxial with the strain equal to $(u_j - u_i)/a$, where u_i, u_j are particles' displacements. Then the normal stress σ can be represented using Hooke's law $\sigma \approx (\lambda + 2\mu)(u_j - u_i)/a$, where λ, μ are the Lamé coefficients for the bond. Substituting this formula into Eq. (29) one obtains

$$\begin{aligned} \mathbf{F}_{ij} \cdot \mathbf{e}_{ij} &= \frac{(\lambda + 2\mu)A}{a}(u_j - u_i) \\ &= \frac{(1-\nu)EA}{(1+\nu)(1-2\nu)a}(u_j - u_i), \end{aligned} \tag{30}$$

Therefore, the longitudinal stiffness of the bond has the form

$$c_A = \frac{(1-\nu)}{(1+\nu)(1-2\nu)}\frac{EA}{a}. \tag{31}$$

One can see that longitudinal stiffness (31) differs from the first formula from (27) by a factor of $(1-\nu)/[(1+\nu)(1-2\nu)]$. Note that for nearly incompressible bonding materials the difference is crucial.

Let us derive the expression for the shear stiffness c_D. Consider pure shear of the bond. Assume that position of particle i is fixed and particle j has a displacement $u_j\mathbf{k}$, where $\mathbf{k}$ is orthogonal to the line connecting particles in the undeformed state. Orientations of both particles are fixed. In this case the force $\mathbf{F}_{ij}$ is caused by shear stresses τ acting inside the bond. Integrating the stresses over the cross section let us represent $\mathbf{F}_{ij} \cdot \mathbf{k}$ in the following form:

$$\mathbf{F}_{ij} \cdot \mathbf{k} = \int_{(A)} \tau dA. \tag{32}$$

Assume that the stress distribution over the cross section is uniform and $\tau \approx Gu_j/a$. Substituting this formula into formula (32) and comparing the result with formula (14) one obtains the following expression for shear stiffness:

$$c_D = \frac{GA}{a}. \tag{33}$$

One can see that the expression for shear stiffness (33) and the second formula from (27), derived using Timoshenko beam theory, are qualitatively different. However, it is notable that the formulas coincide in the limit of vanishing length/thickness ratio, if shear coefficient $\kappa = 1$. Analogous derivations for bending and torsional stiffnesses of the bond lead to the following results:

$$c_B = \frac{(1-\nu)}{(1+\nu)(1-2\nu)}\frac{EJ}{a}, \quad c_T = \frac{GJ_p}{a}. \tag{34}$$

Finally, using formulas (18) and (34) one obtains expressions, connecting the parameters of the V model with bond characteristics:

$$\begin{aligned} B_1 &= \frac{(1-\nu)EA}{(1+\nu)(1-2\nu)a}, \quad B_2 = G\left[\frac{2(1-\nu)}{1-2\nu}\frac{J}{a} - \frac{Aa}{4}\right], \\ B_3 &= \frac{GAa}{2}, \quad B_4 = \frac{GJ_p}{a}. \end{aligned} \tag{35}$$

Thus, in the case of short bonds formulas (35) can be used to calibrate the V model.

V. NUMERICAL IMPLEMENTATION OF THE V MODEL

Let us describe the numerical procedure for simulation of solids using the V model. Consider the system of N particles, connected by bonds. Other types of interactions are not considered in the present paragraph. The system of motion equations has the classical form

$$m_i\ddot{\mathbf{r}}_i = \sum_{j\neq i}\mathbf{F}_{ij}, \quad \Theta_i\dot{\boldsymbol{\omega}}_i = \sum_{j\neq i}\mathbf{M}_{ij}, \tag{36}$$

where m_i, Θ_i are the mass and the moment of inertia of the particle (for simplicity, it is assumed that all particles have spherical inertia tensor). If particles i and j are bonded, then force $\mathbf{F}_{ij}$ and torque $\mathbf{M}_{ij}$, caused by the bond, are calculated using formulas (8). Otherwise, they are equal to zero. The system (36) is solved together with the kinematic equations connecting linear and angular velocities with positions and orientations of the particles. For example, let us determine the turn of particle i from initial orientation to current one by rotational tensor $\mathbf{P}_i$. Then kinematic formulas are

$$\dot{\mathbf{r}}_i = \mathbf{v}_i, \quad \dot{\mathbf{P}}_i = \boldsymbol{\omega}_i \times \mathbf{P}_i. \tag{37}$$

Numerical integration of Eqs. (36) and (37) gives current positions and orientations of the particles at every time step.

As was discussed, forces and torques between particles i and j are calculated using vectors $\mathbf{n}_i^k, \mathbf{n}_j^k, k = 1,2,3$, connected with the particles. The vectors are introduced according to formula (5) at moment t_*, when the bond is created, and corotate with the particles. Consider the simplest approach for calculation of their current coordinates. Let us introduce the basis, consisting of orthogonal unit vectors $\mathbf{x}_i^m, m = 1,2,3$, rotating with particle i. Then current orientation of vectors $\mathbf{x}_i^m$ is determined as follows:

$$\mathbf{x}_i^m(t) = \mathbf{P}_i(t) \cdot \mathbf{x}_i^m(0). \tag{38}$$

Let us use coordinates of vectors $\mathbf{n}_i^k, k = 1,2,3$ in the comoving basis $\mathbf{x}_i^m, m = 1,2,3$ for calculation of current orientation of the vectors $\mathbf{n}_i^k, k = 1,2,3$. Then at each time step vectors $\mathbf{x}_i^m, m = 1,2,3$ are rotated using Eq. (38) and vectors $\mathbf{n}_i^k$ are determined using their coordinates $\mathbf{n}_i^k \cdot \mathbf{x}_i^m, m,k = 1,2,3$, stored in RAM:

$$\mathbf{n}_i^k = \sum_{m=1}^{3} \left(\mathbf{n}_i^k \cdot \mathbf{x}_i^m\right)\mathbf{x}_i^m. \tag{39}$$

Note that $\mathbf{n}_i^k \cdot \mathbf{x}_i^m, k,m = 1,2,3$ does not depend on time and therefore can be calculated only at $t = t_*$. The described procedure allows us to avoid rotation of all vectors, connected with the particle, using Eq. (38).

Consider the calculation of forces and torques caused by the bonds. At every time step one should go over all the bonds and calculate corresponding forces and torques. Therefore in computer code, written in object-oriented programming language, it is convenient to introduce a class "Bond." In general, the element of this class contains the following parameters: pointers to bonded particles, initial length of the bond a, parameters $B_m, m = 1, \ldots, 4$, and coordinates of vectors $\mathbf{n}_i^k, \mathbf{n}_j^k, k = 1,2,3$ in the comoving coordinate systems. For storage of the bonds it is also convenient to introduce a class for bond list. For example, in C++ language it can be implemented using std::map.

Thus, the algorithm for computer simulation using the V model is the following. At every time step, do the following.

(1) Create new bonds if required. Calculate parameters of the bonds. Add created bonds to the list.

(2) Check if the particles are bonded using list of the bonds. For each pair of bonded particles, get bond parameters and calculate current vectors $\mathbf{n}_i^k, \mathbf{n}_j^k$, $k = 1,2,3$, and length of the bond D_{ij}.

(3) Calculate forces and torques between the particles using (8).

(4) Calculate linear and angular velocities at the next time step.

(5) Calculate positions and orientations of the particles and coordinates for vectors $\mathbf{x}_i^k, k = 1,2,3$ at the next time step.

VI. EXAMPLES

In general, using the V model one can simulate mechanical behavior of any solid consisting of (or represented by) bonded particles. However, accurate description of the bonds is especially important for computer simulation of thin rodlike [24] or shell-like granular structures [25]. The structures are widely used in the chemical industry and pharmaceutics. In particular, the review on synthesis and application of shell-like polymer particles is given in Ref. [25]. In the present paper simulation of mechanical behavior of the simplest thin structures is carried out in order to test the applicability of the V model. Modeling of more complex and realistic structures is a subject for future work.

For simplicity, assume that all particles have the same mass m and radius R. The bonds connect particles' centers and have circular cross section with diameter d_b. The Bernoulli-Euler model is used for the calibration. Let us represent all values via three dimensional parameters: equilibrium bond length a [26], particle mass m, and longitudinal stiffness of the bond c_A. In computer code these parameters can be set equal to unity. All other parameters are represented via a,m,c_A and dimensionless values. In particular, the following dimensionless parameters are used:

$$\begin{aligned} &\frac{Ea}{c_A} = \frac{4}{\pi}\left(\frac{a}{d_b}\right)^2, \quad \frac{A}{a^2} = \frac{\pi}{4}\left(\frac{d_b}{a}\right)^2, \quad \frac{J}{a^4} = \frac{\pi}{64}\left(\frac{d_b}{a}\right)^4, \\ &\frac{B_1}{c_A} = 1, \quad \frac{B_2}{c_A a^2} = -\frac{1}{8}\left(\frac{d_b}{a}\right)^2, \quad \frac{B_3}{c_A a^2} = \frac{3}{8}\left(\frac{d_b}{a}\right)^2, \\ &\frac{B_4}{c_A a^2} = \frac{1}{16(1+\nu)}\left(\frac{d_b}{a}\right)^2. \end{aligned} \tag{40}$$

One can see that in this case the dimensionless parameters of the bond depends only on Poisson's ratio ν and the ratio d_b/a.

A. Quasistatical and dynamical buckling of a discrete beam

Consider the simplest thin structure, a notably straight discrete beam, directed along the x axis and consisting of N bonded particles. Assume that the bonds connect particles' centers. First let us simulate quasistatical buckling of the beam under compression using the following procedure. Initial velocities of the particles are randomly distributed in the circle with radius v_0. Initial angular velocities are set equal to zero. Every T_* time units the uniform deformation ε_* is applied to the discrete beam. After every deformation equations of particles motion (36) are integrated using leap-frog algorithm [3]. Translational degrees of freedom of the ends of the discrete beam remain fixed. The procedure is repeated until buckling. During the simulation compressive force acting in the beam is calculated and averaged with period T_*. The following values of the parameters are used:

$$\begin{aligned} &N = 10, \quad \frac{R}{a} = 0.4, \quad \frac{\Theta}{ma^2} = 64 \times 10^{-3}, \quad \frac{v_0}{v_*} = 10^{-6}, \\ &\frac{\Delta t}{T_0} = 10^{-2}, \quad \frac{d_b}{a} = 0.2, \quad \nu = 0.2, \quad \frac{B_1}{c_A} = 1, \\ &\frac{B_2}{c_A a^2} = -5 \times 10^{-3}, \quad \frac{B_3}{c_A a^2} = 15 \times 10^{-3}, \\ &\frac{B_4}{c_A a^2} = 2.08 \times 10^{-3}, \quad \varepsilon_* = -10^{-7}, \quad \frac{T_*}{T_0} = 10, \end{aligned} \tag{41}$$

where Θ is particle's moment of inertia; Δt is a time step; $T_0 = 2\pi\sqrt{m/c_A}$ is a period of small vibrations of one particle on the spring with stiffness c_A; $v_* = a\sqrt{c_A/m}$ is a velocity of long waves in one-dimensional chain, composed of particles with mass m, connected by springs with stiffness c_A and equilibrium length a.

As a result the following value of critical compressive force is obtained: $f/(c_A a) = 3.19 \times 10^{-4}$. The resulting value is only 4% higher than the static Euler critical force $f_E/(c_A a) = \pi^2 EJ/(c_A a^3) = 3.05 \times 10^{-4}$. Note that in the framework of the Bernoulli-Euler model the critical force depends on the length and bending stiffness of the beam. Therefore, the bending stiffness of the discrete beam, composed of particles, within 4% accuracy coincides with the bending stiffness of the Bernoulli-Euler beam.

Consider the dynamical buckling of the same discrete beam. In addition to the V model, linear viscous forces

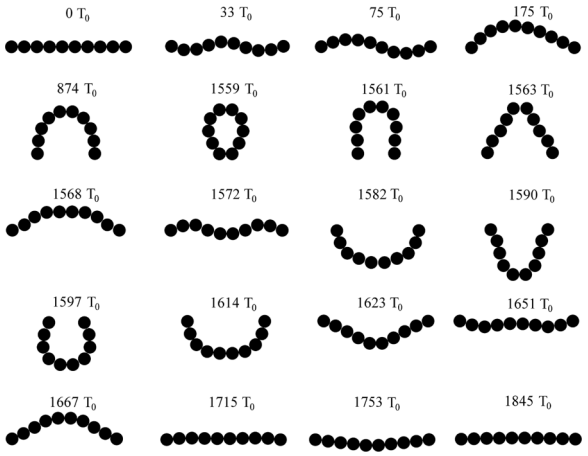

FIG. 5. Dynamical buckling of the discrete beam. Numbers in the figure are corresponding moments of time. Particles radii equal to $0.5a$ are used for visualization.

proportional to particles velocities are introduced. Denote viscosity coefficient as b. Initial velocities of the particles are randomly distributed inside the sphere with radius v_0. In order to simplify visualization of the results z components of the velocities for all particles are set equal to zero [27]. Initial angular velocities are equal to zero. Let the ends of the beam move toward each other with constant velocities v_e until the distance between the ends becomes equal to a (see Fig. 5; $t/T_0 = 1559$). Then x components of the velocities of the beam ends are released and $y-,z-$ components remain equal to zero. The following values of dimensionless parameters are used in addition to parameters (41): $v_e/v_* = 10^{-3}, b/b_0 = 26 \times 10^{-4}$, where $b_0 = 2\sqrt{mc_A}$ is a critical value of friction for a two particle system. The motion of the discrete beam is shown in Fig. 5. One can see the buckling and postbuckling behavior of the discrete beam. At time $t/T_0 = 33$ shape of the discrete beam corresponds to the third buckling mode of Bernoulli-Euler beam. The excitation of higher-order modes of instability is typical for fast dynamical buckling. At the moment $t/T_0 = 1559$ x components of velocities of the beam ends are released and the beam performs strongly nonlinear free vibrations, converging to its initial straight configuration ($t/T_0 > 1845$). Therefore, there is no plastic deformation.

Thus, the V model allows us to simulate large elastic deformations of discrete rods including large displacements and rotations of the particles. In the case of small deformations considered above, the behavior of the discrete beam is in a good agreement with Bernoulli-Euler beam theory.

B. Discrete half-spherical shell under the action of point force

Let us simulate the dynamical buckling of the discrete half-spherical shell under the action of constant point force, acting along the axis of central symmetry. The shell can be considered as the simplest model of porous polymer particles, described in the review [25]. Let us generate relatively uniform distribution of particles on the half-sphere [28]. First, the circle with radius R_c of the half-sphere is created. The number of particles lying on the circle is calculated as the nearest integer value to $2\pi R_c/a$. These particles are uniformly distributed on the circle and remain fixed during creation of the initial

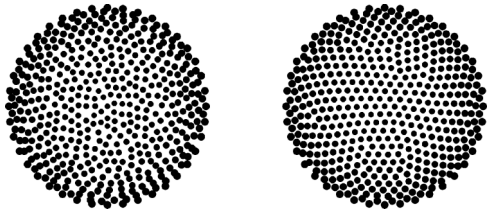

FIG. 6. The initial (left) and final (right) distributions of the particles on the half-sphere. Bottom view. Particles of radii $0.125a$ are used for the visualization.

configuration. The other particles are generated randomly on the half sphere. The restriction that particles cannot be closer than $0.4a$ to each other is used. Note that in this case a is a length scale of the problem. In general it is not equal to equilibrium bond length. The resulting random distribution of the particles is shown in Fig. 6 (left). Then the dynamics of translational motion of the particles interacting via repulsive force $\mathbf{F}^r_{ij}$ only is simulated. The forces are calculated according to the following formula:

$$\mathbf{F}^r_{ij} = -f_0\left(\frac{a}{r_{ij}}\right)^8 \mathbf{r}_{ij}. \tag{42}$$

The restriction $r_i = R_c$, $i = 1,\ldots,N$ is applied during the simulation. The following values of the parameters are used for the simulation:

$$N = 458, \quad N_s = 15 \times 10^3, \quad \frac{v_0}{v_*} = 0, \quad \frac{\Delta t}{T_0} = 10^{-2}, \quad \frac{a_{\text{cut}}}{a} = 2.1, \quad \frac{f_0}{c_A} = 10^{-2}, \quad \frac{b}{b_0} = 26 \times 10^{-5}, \tag{43}$$

where a_{cut} is a cutoff radius; N_s is a number of time steps. The initial and final distributions of the particles are shown in Fig. 6. One can see that the resulting distribution of the particles is much more uniform than the initial one.

After creation of the initial configuration the near-neighbor particles are bonded. For the sake of simplicity it is assumed that bonds connect particle centers. The equilibrium length for each bond is set equal to the distance between centers of the particles. Therefore, there is no residual stress in the initial state of the discrete shell. Also, it is assumed that parameters of the V model $B_m, m = 1,\ldots,4$ are the same for all bonds. Dynamical buckling of the shell under the action of constant point force of magnitude f_s is considered. The force is applied along the axis of central symmetry of the shell until complete buckling occurs. In the given example the force vanishes at $t/T_0 = 3000$. Components of displacements of the boundary particles along the symmetry axis are set equal to zero. In order to avoid self-penetration of the shell contact Hertz forces $\mathbf{F}^H_{ij}$ are introduced. The forces are calculated using the formula

$$\mathbf{F}^H_{ij} = \begin{cases} -\frac{c_H}{\sqrt{a}}(2R - r_{ij})^{\frac{3}{2}}\mathbf{e}_{ij}, & r_{ij} < 2R, \\ 0, & r_{ij} \geqslant 2R, \end{cases} \tag{44}$$

where c_H is a contact stiffness of the particle. Particle radius R is chosen so that $2R$ is smaller than the minimum distance between particles in the initial configuration. The following

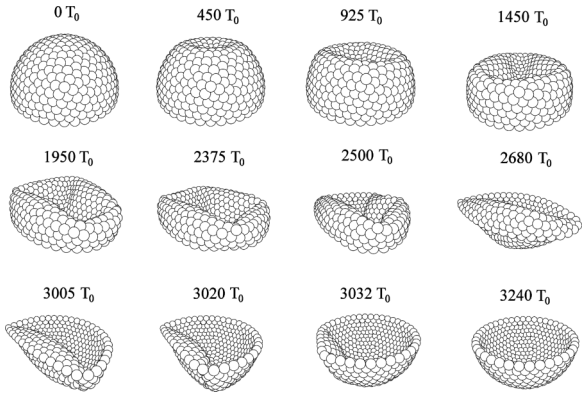

FIG. 7. Buckling of the discrete half-spherical shell under point force load. Particle radii equal $0.5a$ are used for visualization.

values of the parameters are used for the simulation:

$$N = 458, \quad \frac{R}{a} = 0.35, \quad \frac{\Theta}{ma^2} = 49 \times 10^{-3}, \quad \frac{v_0}{v_*} = 10^{-6},$$
$$\frac{\Delta t}{T_0} = 10^{-2}, \quad \frac{b}{b_0} = 26 \times 10^{-4}, \quad \frac{d_b}{a} = 0.2, \quad \nu = 0.2,$$
$$\frac{c_H}{c_A} = 1, \quad \frac{f_s}{c_A a} = 10^{-2}, \quad \frac{B_1}{c_A} = 1, \quad \frac{B_2}{c_A a^2} = -5 \times 10^{-3},$$
$$\frac{B_3}{c_A a^2} = 15 \times 10^{-3}, \quad \frac{B_4}{c_A a^2} = 2.08 \times 10^{-3}. \tag{45}$$

The results of the simulation are shown in Fig. 7. Buckling and postbuckling behavior of the shell are presented. In the places where the shell folds, the bonds undergo extremely large rotations and deformation. For example, large deformations occur at moment $t/T_0 = 2680$ (see Fig. 7). However, large deformations do not lead to any instability or other unphysical behavior of the V model.

Thus, one can conclude that the V model is applicable for computer simulation of discrete shells under large displacements, rotations, and deformations.

VII. RESULTS AND DISCUSSIONS

In the present paper a new model for elastic bonds in solids is proposed. Vectors rigidly connected with particles are used for description of bond deformation. The expression for potential energy of the bond as a function of the vectors is proposed. Corresponding forces and torques acting between bonded particles are calculated from a potential energy function. This approach guarantees that the forces and torques are conservative and the bonds are perfectly elastic. Dissipative terms can also be added if required. Expressions connecting parameters of the V model with longitudinal, shear, bending, and torsional stiffnesses of the bond are derived in the case of small deformations. It is shown that appropriate choices of the parameters allow us to describe *any* values of all the bond stiffnesses *exactly*. Two different calibration procedures depending on bond length/thickness ratio are proposed. In the case of beamlike bonds the comparison with Bernoulli-Euler and Timoshenko beam theories are used for calibration. It is shown that parameters of the V model can be chosen so that under small deformations the bond is equivalent to either Bernoulli-Euler or Timoshenko beam connecting particles. Note that in the framework of the V model the bond may connect any two points belonging to the particles and lying on the line connecting particle centers in the initial state (in particular, particles' centers or points lying on the surfaces). The model for calibration in the case of short bonds is proposed. In all the cases simple expressions, connecting parameters of the V model with geometrical and mechanical characteristics of the bond, are derived. Two examples of computer simulations using the V model are given. The most challenging structures, notably one layer thin discrete rods and shells, are considered. Computer simulations of dynamical buckling of the straight discrete beam and half-spherical shell are carried out. It is shown that the V model is applicable for description of large elastic deformations of solids composed of bonded particles.

Simulation of fracture is not considered in the present paper. However, the V model permits formulating fracture criteria for the bond. For example, the criterion, proposed in Ref. [4], can be directly implemented in the framework of the V model.

ACKNOWLEDGMENTS

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[26] In the case of discrete shell considered below, the bonds have different lengths. Thus, a is a length scale of the problem.
[27] Otherwise, the buckling is performed in several planes and the visualization is not so straightforward.
[28] Note that the problem of setting the initial distribution of the particles problem is similar to the mesh-generation problem in the framework of, for example, the finite element method.