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Scalar form of dynamic equations for a cluster of bodies

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Abstract. The dynamic equations for an arbitrary cluster comprising rigid spheres or assemblies of spheres (subclusters) encountered in granular-type systems are considered. The system is treated within the framework of multibody dynamics. It is shown that for an arbitrary cluster topology the governing equations can be given in an explicit scalar from. The derivation is based on the D'Alembert principle, on inertial coordinate system for each body and direct utilization of the path matrix describing the topology. The scalar form of the equations is important in computer simulations of flow of granular-type materials. An illustrative example of a three-body system is given.

Key words: discrete systems; governing equations; granular materials.

1. Introduction

Granular materials are discrete systems of interconnected bodies. The significant feature of these systems is the variability of the connectivity between the bodies (its topology) during the system motion. This factor makes a major impact on the time-efficiency of computer simulations of the dynamics of granular materials.

The changes in the system topology are due to the changes in the number of interfaces between the bodies in the process of motion and they take place at the discrete points in time. The occurrence of either a new interface or disappearance of the existing one is called an event. Between the two consecutive events the topology remains invariable. The simulation efficiency is affected by the need 1) to analyze a new topology after each event, 2) to generate a new system of equations corresponding to the new topology, 3) to find the new solution of the governing equations, and 4) to find the time of the next event.

Thus, it is clear that the efficiency could be greatly improved if an explicit relationship between the topology and the structure of the equations was established. The generation of the governing equations based on explicit utilization of the path matrix describing the system topology and the Lagrangian approach was done by the author for a system of disks (Vinogradov 1991) and spheres (Vinogradov 1992). In addition to relating topology and equations, the differential equations were derived in a symbolic scalar form. Such form of the equations has other benefits in simulations since it allows 1) mapping of the equations on a linked dynamic data structure, and 2) incorporating an approach whereby a system state is updated rather than recalculated anew each time the topology changes (Sun, *et al.* 1994).

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The granular materials are treated within the framework of the theory of multi-rigid body systems. In the last three decades, the research in the area of multibody dynamics was directed, basically, at two objectives: 1) to develop general computer-oriented methods of analysis of large systems, and 2) to find the most efficient algorithms for specific classes of systems. Different approaches (Newton-Euler's, Lagrangian, D'Alembert, Kane's, recursive), different coordinate systems for the bodies (inertial and relative), and different ways of handling the system topology (incidence and path matrices) were tried. Overviews of the subject made at different times and from different perspectives can be found in (Jerkovsky 1978, Neuman and Murray 1985, Huston 1991, Thomas 1991).

In this paper, the development is based on the D'Alembert principle, inertial coordinate system for the individual bodies, and direct utilization of the path matrix. Such an approach allows one to obtain the differential equations in an explicit scalar form and has been applied recently by the author to a generic manipulator (Vinogradov 1995).

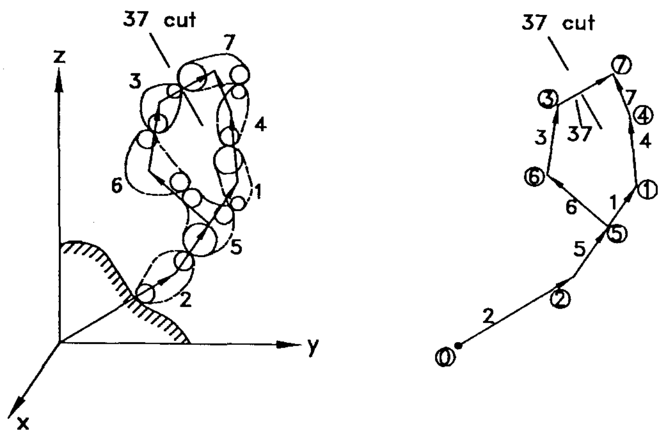
In should also be noted that the path matrix was used in the dynamics of multibody systems before, but in a different context. Wittenburg (1977) used it, within the framework of the relative coordinate formulation, to find explicity the resultant of all inertial joint forces acting on a body. Jerkovsky (1978) used the path matrix to convert inertial coordinates into relative coordinates and thus to transform an uncoupled system expressed in an intertial frame to a coupled one in relative coordinates. Ho (1977) call his approach a "direct path method", whereas, in fact, he uses the incidence matrix to identify a path from a base body to any other body.

In the following, first the model of the physical system is described, then the governing equations are derived, and finally an illustrative example of a three-sphere system is given.

2. Model of the system

In this paper, a granular material is modelled by an arbitrary system of irregularly shaped bodies made out of rigid spheres and arranged in a cluster. The bodies may roll and slide relative to each other, but they neither break apart nor make new contacts; in other words, the number of interfaces between the bodies remains the same, which is to say that the system is considered within the time interval between two events during the simulation. It is also assumed that the external forces acting on each body are known.

Each body in a cluster is made out of spheres of variable sizes and the shape of a body is irregular (or random). The irregularity of the body's shape may be the result of either an attempt to simulate the shape of real physical objects or of clustering of spheres during the motion. In the first case, some preassigned bonding forces are assumed, while in the second case, the body is kept together by external forces during the time interval between two events. The bodies belonging to the second type were called quasi-rigid bodies in (Vinogradov and Springer 1990). In the following, no distinction is made between the two types of bodies, since it is assumed that the geometrical integrity of each body remains unchanged during some time interval. It is also assumed that any two contiguous bodies interface each other at a common for two spheres point. In the case of more than two contact points, the bodies either form a new quasi-rigid body or a relative motion between the two is governed by some ball-and-socket type joint. The former case should be eliminated from our consideration since all bodies were assumed to be geometrically invariable, whereas the second case is a particular one of



(a) (b)

Fig. 1 A multibody granular-type system a) and corresponding directed graph b).

a more general one point contact assumed here.

Let us consider a cluster which comprises N bodies numbered from 1 to N in a random fashion. An example of a multibody system is shown in Fig. 1a. A directed graph associated with this system is shown in Fig. 1b. On the graph the vertex numbers, shown in small circles, are the body numbers, and the arcs correspond to the vectors connecting the centers of mass of the bodies. The arc is assigned the number of the vertex to which it converges. One body serves as a reference body and is called the root body (in Fig. 1a it is the body 2). The motion of the system is described in the inertial coordinate system (x, y, z), and each body is also referenced in this system.

A path between the centers of mass of any two adjoining bodies i and j in a tree is characterized by the vector (see Fig. 2a)

$$\boldsymbol{s}_j=\boldsymbol{u}_i(\psi_i,\ \theta_i)+c_j(\alpha_j,\ \beta_j)+e_j(\psi_j,\ \theta_j,\ \phi_j) \tag{1}$$

where $\boldsymbol{u}_i$ (ψ_i, θ_i) is the vector connecting the center mass of the body i with the center of the sphere interfacing the following body j along the path, $\boldsymbol{e}_j(\psi_j,\ \theta_j,\ \phi_j)$ is the vector connecting the center of the sphere interfacing the preceding body along the path to the body j with the center of mass of body j, and $c_j(\alpha_j,\ \beta_j)$ is called here the connecting vector, since it connects the centers of two interfacing spheres of the two contiguous bodies.

It should be noted that the specific system of generalized coordinates used in the following does not impose any limitations on the application of the method. It is only important that they are given in the inertial coordinate system. Here, for a specific local imbedded coordinate system shown in Fig 2, the vector u_i depends on two Euler angles ψ_i, θ_i (since the self-rotation of the i body around the z_i axis does nor affect the position of the vector $\boldsymbol{u}_i$, and the angle of self-rotation, ϕ_i, should be taken into account only in the rotary motion of the body i), the vector $\boldsymbol{e}_j$ depends on all three Euler angles ψ_j, θ_j, ϕ_j, and the vector c_j characterizes the constant distance between the two bodies and it depends on two spherical coordinates (angles) (α_j, β_j), given in the intertial coordinate system. The Euler angles are difined in Fig. 2b, where ON is the intersection of the moving (x_j, y_j) and stationary (x, y) planes.

Thus, the vector $\boldsymbol{s}_j$ connecting the two contiguous bodies is a function of seven independent

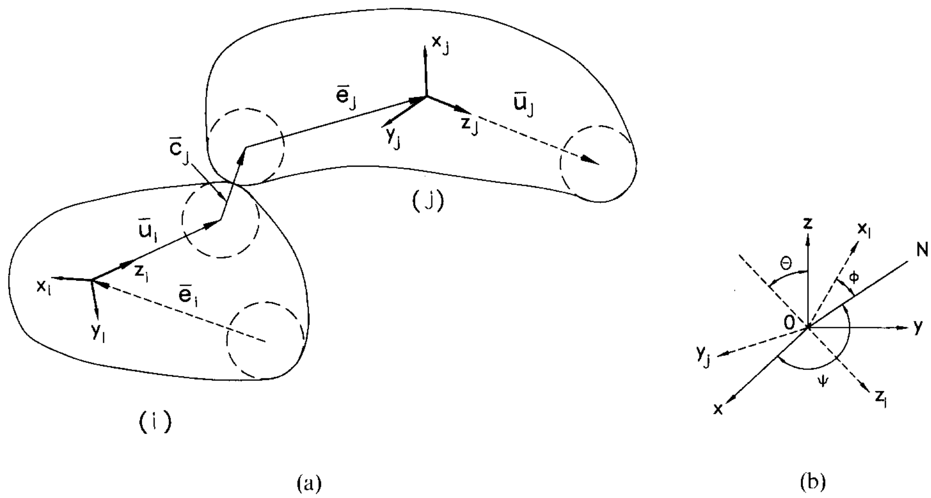


Fig. 2 Vectors connecting centers of mass of two adjoining bodies along the path a) and definition of Euler angles b).

angles which are taken as the generalized coordinates, i.e., $s_j=s_j(x_j)$, where $x_j=(\psi_i,\ \theta_i,\ \alpha_j,\ \beta_j,\ \psi_j,\ \theta_j,\ \phi_j)^T$.

A matrix $P=[p_{ij}]$, which is called the path matrix (Roberson and Schwertassek 1988), is associated with the directed graph and, in general, has the following meaning: $p_{ij}=1$, if the arc i is on the way from the root to the vertex j; $p_{ij}=-1$, if the arc i is on the way from the vertex to the root; and $p_{ij}=0$, otherwise.

Since the topology of the system is assumed to be invariable during some time interval, which means that the spheres interfacing adjoining bodies remain in contact during this time, the geometrical constraints are satisfied if the magnitudes of the connecting vectors c_j remain constant. Thus the two adjoining bodies may only roll and slide relative to each other. In the described system the constraints maintaining the invariability of the system are automatically satisfied. As a result, the system is described by a minimal set of differential equations.

3. Differential equations

For a system of N bodies the following equation associated with the generalized coordinate q_v follows from the D'Alembert principle

$$\sum_{k=1}^{N} \frac{\partial \boldsymbol{r}_k{}^T}{\partial q_v}(\boldsymbol{F}_k-m_k\ddot{\boldsymbol{r}}_k)+\frac{\partial \omega_k{}^T}{\partial \dot{q}_v}(\boldsymbol{M}_k-\dot{\boldsymbol{L}}_k)=0 \tag{2}$$

where m_k, $\boldsymbol{r}_k$, ω_k, $\boldsymbol{F}_k$, $\boldsymbol{M}_k$ and $\boldsymbol{L}_k$ are respectively, the mass, the position vector of the center of mass, the angular velocity vector, the external force, the external moment, and the absolute angular momentum with respect to the center of mass, all associated with the body k. The superscript T here and in the following denotes the transposition sign.

The time rate of change of the angular momentum is

$$\dot{\boldsymbol{L}}_k=\boldsymbol{I}_k\dot{\omega}_k+\tilde{\omega}_k\boldsymbol{I}_k\omega_k \tag{3}$$

where I_k=central interia matrix, and $\tilde{\omega}_k$=skew−symmetric matrix associated with the vector ω_k, which has components

$$\begin{aligned}\omega_{x_k} &= \psi_k \sin\theta_k \sin\phi_k + \dot{\theta}_k \cos\phi_k \\ \omega_{y_k} &= \psi_k \sin\theta_k \cos\phi_k - \dot{\theta}_k \sin\phi_k \\ \omega_{z_k} &= \dot{\phi}_k + \psi_k \cos\theta_k\end{aligned} \tag{4}$$

In Eq. (2) the component

$$T_{q_v} = -\sum_{k=1}^{N} \left(m_k \frac{\partial \boldsymbol{r}_k{}^T}{\partial q_v} \ddot{\boldsymbol{r}}_k + \frac{\partial \omega_k{}^T}{\partial \dot{q}_v} \dot{\boldsymbol{L}}_k \right) \tag{5}$$

characterizes the inertial forces and can be called the generalized intertial force. Similarly,

$$Q_{q_v} = \sum_{k=1}^{N} \left(\frac{\partial \boldsymbol{r}_k{}^T}{\partial q_v} \boldsymbol{F}_k + \frac{\partial \omega_k{}^T}{\partial \dot{q}_v} \boldsymbol{M}_k \right) \tag{6}$$

is the generalized force.

The difficulty of deriving motion equations is always associated with constraints. In this case the constraints are embodied in the translational component of the generalized inertial force and the force-vector in the expression for the generalized force. The corresponding terms associated with moments and angular velocity vectors are not coupled and can be easily found using Eqs. (3) and (4). For this reason, in the following only the translational component of the generalized inertial force, which called here for simplicity "the generalized inertial force", and the generalized force-vector are considered.

Firstly, the expressions for the generalized inertial forces are derived by introducing the position vector $\boldsymbol{r}_k$, and finding its derivatives.

The position vector $\boldsymbol{r}_k$ can be given in the following form

$$\boldsymbol{r}_k = \boldsymbol{P}_k{}^T \boldsymbol{s} \tag{7}$$

where $\boldsymbol{P}_k$ is the kth column of the path matrix $\boldsymbol{P}$, and $\boldsymbol{s} = [\boldsymbol{s}_j]_{N \times 1}$. Note that the elements of the matrix $\boldsymbol{P}$ must be considered as factors corresponding to each vector $\boldsymbol{s}_j$. Note also that although the numbering of the bodies may not be ordered, the components in $\boldsymbol{s}$ are arranged in an ordered set.

Representing the position vector through the path matrix allows one to derive the differential equations in a scalar form, and also it allows one to directly map equations onto a data structure, since linked data structure reflects the topology of the physical system (Sun, *et al.* 1994).

The translational velocity of the body k, found from Eq. (7), is

$$\dot{\boldsymbol{r}}_k = \boldsymbol{P}_k{}^T \dot{\boldsymbol{s}} \tag{8}$$

where $\dot{\boldsymbol{s}} = [\dot{\boldsymbol{s}}_j]_{N \times 1}$, and the dot, here and in the following denotes the time derivative in the inertial frame.

Taking into account Eq. (1), the velocity vector $\dot{\boldsymbol{s}}_j$ can be written in the from

$$\dot{\boldsymbol{s}}_j = \boldsymbol{a}_j{}^T \dot{x}_j \tag{9}$$

where

$$\boldsymbol{a}_j = (\boldsymbol{u}_{i,\psi},\ \boldsymbol{u}_{i,\theta},\ \boldsymbol{c}_{j,\alpha},\ \boldsymbol{c}_{j,\beta},\ \boldsymbol{e}_{j,\psi},\ \boldsymbol{e}_{j,\theta},\ \boldsymbol{e}_{j,\phi}) \tag{10}$$

and, in the latter, the two indexes in a subscript separated by a coma indicate a partial derivative, e.g., $\boldsymbol{u}_{i,\psi}=\partial \boldsymbol{u}_i/\partial \psi_i$. Note also that the index of the variable always coincides with the index of the differentiated vector.

Taking into account Eq. (9), the velocity vector can now be written in the form

$$\dot{\boldsymbol{r}}_k=\boldsymbol{P}_k^T\boldsymbol{A}\dot{\boldsymbol{x}} \tag{11}$$

where $\boldsymbol{A}$ is a diagonal block matrix, $\boldsymbol{A}=diag[\boldsymbol{a}_j^T]_{NxN}$, and $\dot{\boldsymbol{x}}=[\dot{\boldsymbol{x}}_j]_{1xN}$.
The translational accelerations are equal to

$$\ddot{\boldsymbol{r}}_k=\boldsymbol{P}_k^T\left(\frac{\partial \boldsymbol{A}}{\partial t}\dot{\boldsymbol{x}}+\boldsymbol{A}\ddot{\boldsymbol{x}}\right) \tag{12}$$

After taking the time derivative of $\boldsymbol{A}$ in the latter, the product $\frac{\partial \boldsymbol{A}}{\partial t}\dot{\boldsymbol{x}}$ can be written in the from

$$\frac{\partial \boldsymbol{A}}{\partial t}\dot{\boldsymbol{x}}=\boldsymbol{B}\dot{\boldsymbol{x}}^2 \tag{13}$$

where it is denoted

$$\dot{\boldsymbol{x}}^2=[\dot{\boldsymbol{x}}_j^2]_{Nx1} \tag{14}$$

$$\boldsymbol{B}=diag[\boldsymbol{b}_j^T]_{NxN} \tag{15}$$

$$\boldsymbol{b}_j^T=(\boldsymbol{u}_{i,\psi\psi},\ 2\boldsymbol{u}_{i,\psi\theta},\ \boldsymbol{u}_{i,\theta\theta},\ \boldsymbol{c}_{j,\alpha\alpha},\ 2\boldsymbol{c}_{j,\alpha\beta},\ \boldsymbol{c}_{j,\beta\beta},\ \boldsymbol{e}_{j,\psi\psi},\ 2\boldsymbol{e}_{j,\psi\theta},\ \boldsymbol{e}_{j,\theta\theta},\ 2\boldsymbol{e}_{j,\psi\phi},\ 2\boldsymbol{e}_{j,\theta\phi},\ 2\boldsymbol{e}_{j,\phi\phi}) \tag{16}$$

$$\dot{\boldsymbol{x}}_j^2=(\dot{\psi}_i^2,\ \dot{\psi}_i\dot{\theta}_i,\ \dot{\theta}_i^2,\ \dot{\alpha}_j^2,\ \dot{\alpha}_j\dot{\beta}_j,\ \dot{\beta}_j^2,\ \dot{\psi}_j^2,\ \dot{\psi}_j\dot{\theta}_j,\ \dot{\theta}_j^2,\ \dot{\psi}_j\dot{\phi}_j,\ \dot{\theta}_j\dot{\phi}_j,\ \dot{\phi}_j^2)^T \tag{17}$$

Let us consider now the partial derivative in Eq. (5). Taking into account that $\frac{\partial \boldsymbol{r}_k^T}{\partial q_v}=\frac{\partial \boldsymbol{s}^T}{\partial q_v}\boldsymbol{P}_k$ (see Eq. (7)) and Eq. (12), the first term in the brackets in Eq. (5) takes the form

$$m_k\frac{\partial \boldsymbol{r}_k^T}{\partial q_v}\ddot{\boldsymbol{r}}_k=m_k\frac{\partial \boldsymbol{s}^T}{\partial q_v}\boldsymbol{P}_k\boldsymbol{P}_k^T(\boldsymbol{B}\dot{\boldsymbol{x}}^2+\boldsymbol{A}\ddot{\boldsymbol{x}}) \tag{18}$$

The partial derivatives of the vector $\boldsymbol{s}^T$ with respect to various generalized coordinates are

$$\frac{\partial \boldsymbol{s}^T}{\partial \psi_i}=\left(\boldsymbol{0},\ \cdots,\ \frac{\partial \boldsymbol{s}_i^T}{\partial \psi_i},\ \cdots,\ \boldsymbol{0},\ \cdots,\ \frac{\partial \boldsymbol{s}_j^T}{\partial \psi_i},\ \cdots,\ \boldsymbol{0}\right) \tag{19}$$

$$\frac{\partial \boldsymbol{s}^T}{\partial \alpha_j}=\left(\boldsymbol{0},\ \cdots,\ \frac{\partial \boldsymbol{s}_j^T}{\partial \alpha_j},\ \cdots,\ \boldsymbol{0}\right) \tag{20}$$

$$\frac{\partial \boldsymbol{s}^T}{\partial \psi_j}=\left(\boldsymbol{0},\ \cdots,\ \frac{\partial \boldsymbol{s}_j^T}{\partial \psi_j},\ \cdots,\ \frac{\partial \boldsymbol{s}_l^T}{\partial \psi_j},\ \cdots,\ \boldsymbol{0}\right) \tag{21}$$

$$\frac{\partial \boldsymbol{s}^T}{\partial \phi_j}=\left(\boldsymbol{0},\ \cdots,\ \frac{\partial \boldsymbol{s}_j^T}{\partial \phi_j},\ \cdots,\ \boldsymbol{0}\right) \tag{22}$$

The derivatives for the generalized coordinates θ_i and θ_j are obtained from Eqs. (19) and (21) by substituting θ for ψ with the corresponding indexes. In Eq. (19) the variable ψ_i is present in both vectors $\boldsymbol{s}_i$ and $\boldsymbol{s}_j$, where i is the number of the body which precedes the body j along the path. Similarly, in Eq. (21), l is the number of the body which follows the body j along the path. The form of the derivatives in Eqs. (19)-(22) is due to the choice of the generalized coordinates in the inertial system and the structure of the connecting vectors (see Eq. (1))

Let us denote the product of two vectors in Eq. (18) as follows

$$\boldsymbol{P}_k \boldsymbol{P}_k^T = \boldsymbol{G}^k = [g_{nm}^k]_{NxN} \tag{23}$$

where $g_{nm}^k = p_{nk} p_{mk}$, and $\boldsymbol{G}^k$ is a symmetric matrix, as it is the product of a vector and its transpose.

Premultiplying $\boldsymbol{G}^k$ by $\dfrac{\partial \boldsymbol{s}^T}{\partial q_j}$, as in Eq. (18), results in either one or two transposed vectors, depending on the specific generalized coordinate q_v, and the indexes of these vectors are determined by the positions of the non-zero elements in Eqs. (19)-(22).

To be specific, let us consider now the case when $q_v = \psi_i$, as in Eq. (19). The translational component of the inertial force in Eq. (5), after using Eqs. (18), (19) and (23), and collecting similar terms in the sum, results in the following expression

$$T_{\psi_i} = \sum_{k=1}^{N} m_k \frac{\partial \boldsymbol{r}_k^T}{\partial \psi_i} \ddot{\boldsymbol{r}}_k = \left(\frac{\partial \boldsymbol{s}_i^T}{\partial \psi_i} \gamma_i^T + \frac{\partial \boldsymbol{s}_j^T}{\partial \psi_i} \gamma_j^T \right) \dot{\boldsymbol{x}}^2 + \left(\frac{\partial \boldsymbol{s}_i^T}{\partial \psi_i} \zeta_i^T + \frac{\partial \boldsymbol{s}_j^T}{\partial \psi_i} \zeta_j^T \right) \tag{24}$$

where γ_i^T, γ_j^T, ζ_i^T, and ζ_j^T are

$$\gamma_i^T = [M_{il} \boldsymbol{b}_l^T]_{1xN} \tag{25}$$

$$\gamma_j^T = [M_{jl} \boldsymbol{b}_l^T]_{1xN} \tag{26}$$

$$\zeta_i^T = [M_{il} \boldsymbol{a}_l^T]_{1xN} \tag{27}$$

$$\zeta_j^T = [M_{jl} \boldsymbol{a}_l^T]_{1xN} \tag{28}$$

and

$$M_{il} = \sum_{k=1}^{N} m_k g_{il}^k = \sum_{k=1}^{N} m_k p_{ik} p_{lk} \tag{29}$$

is the generalized mass associated with the body i and equals to the sum of all masses lacated on the branch of the tree originating at the body i and away from the root body. Similarly for the $\boldsymbol{M}_{jl}$.

The second partial derivative in Eq. (5). describing the self-rotation of the body, is non-zero only when $j=k$. The corresponding terms in the differential equation can be found using Eqs. (3) and (4).

The force component of the generalized force, the first term in Eq. (6), is found, using Eq. (7) for $\boldsymbol{r}_k$, to be as follows

$$Q_{\psi_i} = \sum_{k=1}^{N} \frac{\partial \boldsymbol{r}_k^T}{\partial \psi_i} \boldsymbol{F}_k = \frac{\partial \boldsymbol{s}_i^T}{\partial \psi_i} \boldsymbol{Q}_i + \frac{\partial \boldsymbol{s}_j^T}{\partial \psi_i} \boldsymbol{Q}_j \tag{30}$$

where

$$\boldsymbol{Q}_i = \sum_{k=1}^{N} p_{ik} \boldsymbol{F}_k \tag{31}$$

is the sum of all external forces acting on bodies located on the branch originating at the body i and away from the root body. For the force $\boldsymbol{Q}_j$ the expression is similar except that the index j is used in place of i.

Equations for the forces T_{α_j} and Q_{α_j}, taking into account Eq. (20), have the same forms as Eqs. (24) and (30)

$$T_{\alpha_j}=\frac{\partial s_j^T}{\partial \alpha_j}(\gamma_j^T \dot{x}^2+\zeta_j^T \ddot{x}) \tag{32}$$

$$Q_{\alpha_j}=\frac{\partial s_j^T}{\partial \alpha_j} Q_j \tag{33}$$

Equations for θ_i, ψ_j and θ_j are similar to Eqs. (24) and (30), and may be obtained by substituting the above coordinates for ψ_i. The equation for β_j is obtained from Eqs. (32) and (33) by substituting β_j for α_j. Substitution of Eqs.(24) and (30) into Eq. (2) results in a differential equation associated with the generalized coordinate ψ_i. Similarly for all other coordinates.

The derived differential equations can be further simplified and finally written in an explicit scalar form. Since the procedure involved is straightforward, only an outline for the generalized coordinate ψ_i is given here (more details are given in the example which follows).

The simplification is based on the fact that forms of vectors in Eq. (1) are known in their respective coordinate systems (Euler for $\boldsymbol{u}_i$ and $\boldsymbol{e}_j$ or spherical for $\boldsymbol{c}_j$). Taking that into account, (e.g., in Eq. (24)), then $\frac{\partial s_i^T}{\partial \psi_i}=\frac{\partial e_i^T}{\partial \psi_i}$ and $\frac{\partial s_j^T}{\partial \psi_i}=\frac{\partial u_i^T}{\partial \psi_i}$ (see Eq. (1)), and thus that these derivatives and the derivatives in Eqs. (10) and (16) are known functions, the procedure for obtaining the scalar form of equations becomes algorithmic. This will be further illustrated in the example.

4. Constraint equations

The constraint equations follow from the requirement of constant distance between any two interfacing bodies i and j across the cut. The cord vector $\boldsymbol{s}_{ij}=(\boldsymbol{u}_i, \boldsymbol{c}_{ij}, \boldsymbol{e}_j)^T$ is equal to (see Fig. 1 where $\boldsymbol{s}_{ij}=\boldsymbol{s}_{37}$)

$$\boldsymbol{s}_{ij}=\boldsymbol{r}_j-\boldsymbol{r}_i \tag{34}$$

Taking into account Eq. (7) for the position vectors, the latter can be written in the from

$$\boldsymbol{s}_{ij}=(\boldsymbol{P}_j-\boldsymbol{P}_i)^T\boldsymbol{s} \tag{35}$$

Eq. (35) represents three algebraic relationship between the generalized coordinates. For a given topology the algebraic equations are thus easily generated.

5. Example

A simple system of three spheres in contact with each other and moving around the "grounded" sphere (see Fig. 3a) is considered to illustrate the application of the derived equations. The inertial system of coordinate is located at the center of the grounded sphere.

The topology is described by a directed graph shown in Fig. 3b, and the associated path matrix is as follows

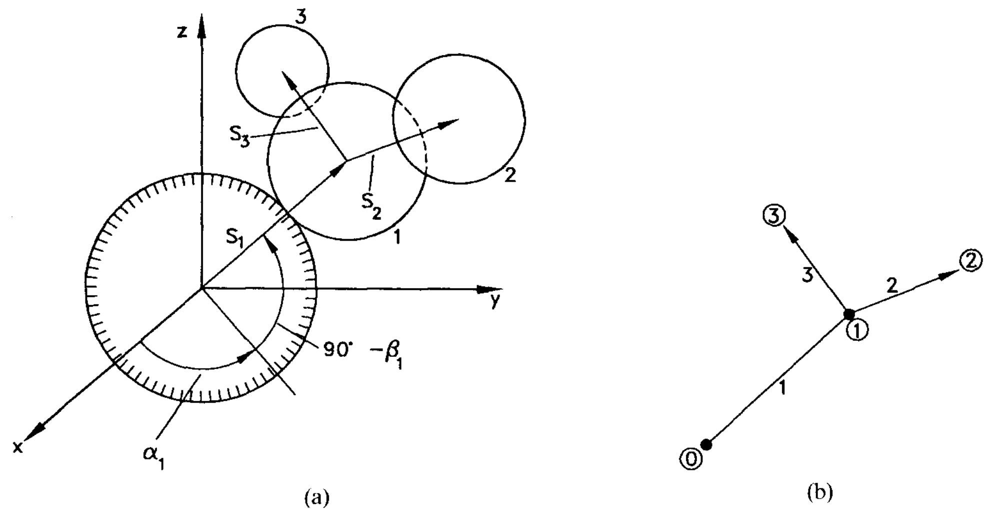


Fig. 3 A system of three spheres a) and corresponding graph b).

$$\boldsymbol{P}=\begin{vmatrix} 1 & 1 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix} \tag{36}$$

The vectors connecting the centers of mass are in this case the connecting vectors c_i ($i=1, 2, 3$). The corresponding unit vectors are

$$\varepsilon_i=(\sin\beta\cos\alpha,\ \sin\beta\sin\alpha,\ \cos\beta)_i^T \tag{37}$$

For the generalized coordinate α_i the inertial force is

$$T_{\alpha_i}=-c_{i,\alpha}(\zeta_i^T\ddot{\boldsymbol{x}}+\gamma_i^T\dot{\boldsymbol{x}}^2)\quad i=1,\ 2,\ 3 \tag{38}$$

and the generalized force is

$$Q_{\alpha_i}=c_{i,\alpha}^T(\boldsymbol{F}_1+\boldsymbol{F}_2+\boldsymbol{F}_3)\quad i=1,\ 2,\ 3 \tag{39}$$

where

$$\ddot{\boldsymbol{x}}=[\ddot{\boldsymbol{x}}_j]\quad j=1,\ 2,\ 3 \tag{40}$$

$$\dot{\boldsymbol{x}}_2=[\dot{\boldsymbol{x}}_j^2]\quad j=1,\ 2,\ 3 \tag{41}$$

$$\ddot{\boldsymbol{x}}_j=(0,\ 0,\ \ddot{\alpha}_j,\ \ddot{\beta}_j,\ 0,\ 0,\ 0)^T \tag{42}$$

$$\dot{\boldsymbol{x}}_j^2=(0,\ 0,\ 0,\ \dot{\alpha}_j^2,\ \dot{\alpha}_j\dot{\beta}_j,\ \dot{\beta}_j^2,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0)^T \tag{43}$$

$$\zeta_i^T=[M_{ij}\boldsymbol{a}_j^T]\quad j=1,\ 2,\ 3 \tag{44}$$

$$\gamma_i^T=[M_{ij}\boldsymbol{b}_j^T]\quad j=1,\ 2,\ 3 \tag{45}$$

$$\boldsymbol{a}_j^T=c_j(\boldsymbol{0},\ \boldsymbol{0},\ \varepsilon_{j,\alpha},\ \varepsilon_{j,\beta},\ \boldsymbol{0},\ \boldsymbol{0},\ \boldsymbol{0}) \tag{46}$$

$$\boldsymbol{b}_j^T=c_j(\boldsymbol{0},\ \boldsymbol{0},\ \boldsymbol{0},\ \varepsilon_{j,\alpha\alpha},\ \boldsymbol{2}\varepsilon_{j,\alpha\beta},\ \varepsilon_{j,\beta\beta},\ \boldsymbol{0},\ \boldsymbol{0},\ \boldsymbol{0},\ \boldsymbol{0},\ \boldsymbol{0},\ \boldsymbol{0}) \tag{47}$$

$$M_{ij}=\sum_{k=1}^{3} m_k p_{ik} p_{jk} \quad j=1,\ 2,\ 3 \tag{48}$$

and c_j is the magnitude of the vector c_j. For the generalized coordinate β, Eqs. (38) and (39) are obtained by substituting β in place of α.

The scalar form of the governing equations is obtained by taking first and second order partial derivatives of the unit vectors, Eq. (37), making corresponding multiplications in Eqs. (38) and (39). Note that form of the derivatives and their products is index-independent, a fact which makes the procedure algorithmically efficient. The multiplication of vectors can be performed in a symbolic form.

Neglecting the self-rotation of the spheres, the differential equations for the generalized coordinates α_1, β_1, α_2 and β_2 are as follows

$$\begin{gathered}-m_1 c_1^2 \eta_{11}^{\alpha} \ddot{\alpha}_1 - m_2 c_1 c_2 (\eta_{12}^{\alpha} \ddot{\alpha}_2 + \eta_{12}^{\beta} \ddot{\beta}_2) - m_3 c_1 c_3 (\eta_{13}^{\alpha} \ddot{\alpha}_3 + \eta_{13}^{\beta} \ddot{\beta}_2) \\ -m_1 c_1^2 \mu_{11}^{\alpha\beta} \dot{\alpha}_1 \dot{\beta}_1 - m_2 c_1 c_2 (\mu_{12}^{\alpha} \dot{\alpha}_2^2 + 2\mu_{12}^{\alpha\beta} \dot{\alpha}_2 \dot{\beta}_2 + \mu_{12}^{\beta} \dot{\beta}_2^2) - m_3 c_1 c_3 (\mu_{13}^{\alpha} \dot{\alpha}_3^2 + 2\mu_{13}^{\alpha\beta} \dot{\alpha}_3 \dot{\beta}_3 + \mu_{13}^{\beta} \dot{\beta}_3^2) = Q_{\alpha_1}\end{gathered} \tag{49}$$

$$\begin{gathered}-m_1 c_1^2 \ddot{\beta}_1 - m_2 c_1 c_2 (\eta_{22}^{\alpha} \ddot{\alpha}_2 + \eta_{22}^{\beta} \ddot{\beta}_2) - m_3 c_1 c_3 (\eta_{23}^{\alpha} \ddot{\alpha}_3 + \eta_{23}^{\beta} \ddot{\beta}_3) \\ -m_1 c_1^2 \mu_{21}^{\alpha} \dot{\alpha}_1^2 - m_2 c_1 c_2 (\mu_{22}^{\alpha} \dot{\alpha}_2^2 + \mu_{22}^{\alpha\beta} \dot{\alpha}_2 \dot{\beta}_2 + \mu_{22}^{\beta} \dot{\beta}_2^2) - m_3 c_1 c_3 (\mu_{23}^{\alpha} \dot{\alpha}_3^2 + \mu_{23}^{\alpha\beta} \dot{\alpha}_3 \dot{\beta}_3 + \mu_{23}^{\beta} \dot{\beta}_3^2) = Q_{\beta_1}\end{gathered} \tag{50}$$

$$\begin{gathered}-m_2 c_2 [c_1 (\eta_{31}^{\alpha} \ddot{\alpha}_1 + \eta_{31}^{\beta} \ddot{\beta}_1) + c_2 \eta_{32}^{\alpha} \ddot{\alpha}_2 + \\ c_1 (\mu_{31}^{\alpha} \dot{\alpha}_1^2 + 2\mu_{31}^{\alpha\beta} \dot{\alpha}_1 \dot{\beta}_1 + \mu_{31}^{\beta} \dot{\beta}_1^2) + \mu_{32}^{\alpha\beta} \dot{\alpha}_2 \dot{\beta}_2] = Q_{\alpha_2}\end{gathered} \tag{51}$$

$$\begin{gathered}-m_2 c_2 [c_1 (\eta_{41}^{\alpha} \ddot{\alpha}_1 + \eta_{41}^{\beta} \ddot{\beta}_1) + c_2 \ddot{\beta}_2 + \\ c_1 (\mu_{41}^{\alpha} \dot{\alpha}_1^2 + 2\mu_{41}^{\alpha\beta} \dot{\alpha}_1 \dot{\beta}_1 + \mu_{41}^{\beta} \dot{\beta}_1^2) + c_2 \mu_{42}^{\alpha} \dot{\alpha}_2^2] = Q_{\beta_2}\end{gathered} \tag{52}$$

In Eqs. (49)-(52) it is denoted

$$\begin{gathered}\eta_{11}^{\alpha}=\sin^2\beta_1,\ \ \eta_{12}^{\alpha}=\sin\beta_1 \sin\beta_2 \cos(\alpha_2-\alpha_1),\ \ \eta_{12}^{\beta}=\sin\beta_1 \cos\beta_2 \sin(\alpha_2-\alpha_1), \\ \eta_{13}^{\alpha}=\sin\beta_1 \sin\beta_3 \cos(\alpha_3-\alpha_1),\ \ \eta_{13}^{\beta}=\sin\beta_1 \cos\beta_3 \sin(\alpha_3-\alpha_1)\end{gathered} \tag{53}$$

$$\begin{gathered}\mu_{11}^{\alpha\beta}=\sin 2\beta_1, \\ \mu_{12}^{\alpha}=\sin\beta_1 \sin\beta_2 \sin(\alpha_1-\alpha_2),\ \ \mu_{12}^{\alpha\beta}=\sin\beta_1 \cos\beta_2 \cos(\alpha_1-\alpha_2),\ \ \mu_{12}^{\beta}=\sin\beta_1 \sin\beta_2 \sin(\alpha_1-\alpha_2), \\ \mu_{13}^{\alpha}=\sin\beta_1 \sin\beta_3 \sin(\alpha_1-\alpha_3),\ \ \mu_{13}^{\alpha\beta}=\sin\beta_1 \cos\beta_3 \cos(\alpha_1-\alpha_3),\ \ \mu_{13}^{\beta}=\sin\beta_1 \sin\beta_3 \sin(\alpha_1-\alpha_3)\end{gathered} \tag{54}$$

$$\begin{gathered}\eta_{22}^{\alpha}=-\cos\beta_1 \sin\beta_2 \sin(\alpha_1-\alpha_2),\ \ \eta_{22}^{\beta}=\cos\beta_1 \cos\beta_2 \cos(\alpha_1-\alpha_2)+\sin\beta_1 \sin\beta_2, \\ \eta_{23}^{\alpha}=-\cos\beta_1 \sin\beta_3 \sin(\alpha_1-\alpha_3),\ \ \eta_{23}^{\beta}=\cos\beta_1 \cos\beta_3 \cos(\alpha_1-\alpha_3)+\sin\beta_1 \sin\beta_3,\end{gathered} \tag{55}$$

$$\begin{gathered}\mu_{21}^{\alpha}=-0.5\ \sin 2\beta_1, \\ \mu_{22}^{\alpha}=-\cos\beta_1 \sin\beta_2 \cos(\alpha_1-\alpha_2),\ \ \mu_{22}^{\alpha\beta}=-\cos\beta_1 \cos\beta_2 \sin(\alpha_1-\alpha_2), \\ \mu_{22}^{\beta}=-\cos\beta_1 \sin\beta_2 \cos(\alpha_1-\alpha_2)+\sin\beta_1 \cos\beta_2, \\ \mu_{23}^{\alpha}=-\cos\beta_1 \sin\beta_3 \cos(\alpha_1-\alpha_3),\ \ \mu_{23}^{\alpha\beta}=-\cos\beta_1 \cos\beta_3 \sin(\alpha_1-\alpha_3),\end{gathered}$$

$$\mu_{23}^{\beta}=-\cos\beta_1\sin\beta_3\cos(\alpha_1-\alpha_3)+\sin\beta_1\cos\beta_3, \tag{56}$$

$$\eta_{31}^{\alpha}=\sin\beta_1\sin\beta_2\cos(\alpha_2-\alpha_1),\ \ \eta_{31}^{\beta}=\cos\beta_1\sin\beta_2\sin(\alpha_2-\alpha_1),\ \ \eta_{32}^{\alpha}=\sin^2\beta_2 \tag{57}$$

$$\mu_{31}^{\alpha}=\sin\beta_1\sin\beta_2\sin(\alpha_2-\alpha_1),\ \ \mu_{31}^{\alpha\beta}=\cos\beta_1\sin\beta_2\cos(\alpha_2-\alpha_1),$$
$$\mu_{31}^{\beta}=\sin\beta_1\sin\beta_2\sin(\alpha_2-\alpha_1),\ \ \mu_{22}^{\alpha\beta}=0.5\ \sin2\beta_2 \tag{58}$$

$$\eta_{41}^{\alpha}=-\sin\beta_1\cos\beta_2\sin(\alpha_2-\alpha_1),\ \ \eta_{41}^{\beta}=\cos\beta_1\cos\beta_2\cos(\alpha_2-\alpha_1)+\sin\beta_1\sin\beta_2, \tag{59}$$

$$\mu_{41}^{\alpha}=-\sin\beta_1\cos\beta_2\cos(\alpha_2-\alpha_1),\ \ \mu_{41}^{\alpha\beta}=-\sin\beta_1\cos\beta_2\sin(\alpha_2-\alpha_1),$$
$$\mu_{41}^{\beta}=-\sin\beta_1\cos\beta_2\cos(\alpha_2-\alpha_1)+\cos\beta_1\sin\beta_2,\ \ \mu_{42}^{\alpha}=-0.5\sin2\beta_2 \tag{60}$$

$$Q_{\alpha_1}=-c_1(F_{1x}+F_{2x}+F_{3x})\sin\alpha_1\sin\beta_1+c_1(F_{1y}+F_{2y}+F_{3y})\cos\alpha_1\sin\beta_1 \tag{61}$$

$$Q_{\beta_1}=c_1(F_{1x}+F_{2x}+F_{3x})\cos\alpha_1\cos\beta_1$$
$$+c_1(F_{1y}+F_{2y}+F_{3y})\sin\alpha_1\cos\beta_1-c_1(F_{1z}+F_{2z}+F_{3z})\sin\beta_1 \tag{62}$$

$$Q_{\alpha_2}=-c_2(F_{2x}\sin\alpha_2+F_{2y}\cos\alpha_2)\sin\beta_2 \tag{63}$$

$$Q_{\beta_2}=c_2(F_{2x}\cos\alpha_2\cos\beta_2+F_{2y}\sin\alpha_2\cos\beta_2-F_{2z}\sin\beta_2) \tag{64}$$

and

$$F_i=(F_{ix},\ F_{iy},\ F_{iz})^T\quad i=1,\ 2,\ 3 \tag{65}$$

For the generalized coordinates α_3 and β_3 the differential equations are the same as for α_2 and β_2 if the index 3 is substituted in place of 2. Note that the structure of the equations reflects the topology through the expressions for the generalized masses (Eq. 48).

6. Conclusions

It is shown in the paper that for a system of irregularly shaped interconnected bodies made out of spheres the differential-algebraic equations can be derived in an explicit scalar form. The structure of the equations reflects the topology of the system and they are give in terms of the coefficients of the path matrix. This allows the mapping of the equations on a linked data structure, and thus, in principle, avoids matrix operations while solving them. In addition, it allows for the development of more efficient algorithms for updating the system state. The results obtained are important in computer simulations of dynamics of systems with variable topology, such as granular materials.

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