The Use of Zero-Mass Particles in Analytical and Multi-Body Dynamics: Sphere Rolling on An Arbitrary Surface

Zero-mass particles are, as a rule, never used in analytical dynamics, because they lead to singular mass matrices. However, recent advances in the development of the explicit equations of motion of constrained mechanical systems with singular mass matrices permit their use under certain circumstances. This paper shows that the use of such particles can be very efficacious in some problems in analytical dynamics that have resisted easy, general formulations, and in obtaining the equations of motion for complex multi-body systems. We explore the ease and simplicity that suitably used zero-mass particles can provide in formulating and simulating the equations of motion of a rigid, non-homogeneous sphere rolling under gravity, without slipping, on an arbitrarily prescribed surface. Computational results comparing the significant difference in the motion of a homogeneous sphere and a non-homogeneous sphere rolling down an asymmetric arbitrarily prescribed surface are obtained, along with measures of the accuracy of the computations. While the paper shows the usefulness of zero-mass particles applied to the classical problem of a rolling sphere, the development given is described in a general enough manner to be applicable to numerous other problems in analytical and multi-body dynamics that may have much greater complexity. [DOI: 10.1115/1.4052002]

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1 Introduction

Particles whose mass is zero, referred in this paper as zero-mass particles, are almost never used in classical nonrelativistic mechanics since from a physical standpoint no forces can be applied to them, and hence their accelerations cannot be uniquely found. While photons have zero mass and carry energy and momentum in special relativity, in nonrelativistic mechanics, the addition of such zero-mass particles to any unconstrained mechanical system causes the entire mass matrix of that system to become singular, and since the mass matrix is then noninvertible, the accelerations of the system to the given forces cannot be found. However, advances in the development of the explicit equations of motion of constrained mechanical systems with singular mass matrices permit their use under certain circumstances. This paper shows that the use of such particles can be very efficacious in some problems in analytical dynamics that have resisted easy, general formulations and in obtaining the equations of motion for complex multi-body systems. We explore the ease and simplicity that suitably used zero-mass particles can provide in formulating and simulating the equations of motion of a rigid, non-homogeneous sphere rolling under gravity, without slipping, on an arbitrarily prescribed surface. Computational results comparing the difference in the motion of a homogeneous sphere and a non-homogeneous sphere rolling down an asymmetric arbitrarily prescribed surface are obtained, along with measures of the accuracy of the computations. While the paper shows the usefulness of zero-mass particles applied to the classical problem of a rolling sphere, the development given is described in a general enough manner to be applicable to numerous other problems in analytical and multi-body dynamics.

A useful approach in the development of the explicit equations of motion for general, multi-body mechanical systems is to use a simple three-step procedure. The first step involves the setting down of the equations of motion of the unconstrained system, wherein the coordinates that describe the position of the system are all assumed to be independent of each other; the second step involves the setting down of the kinematical and dynamical constraints; and the third involves obtaining the equations of motion of the constrained system, using the relations developed in the previous two steps. This final step, which gives the explicit equations of motion for the constrained system, can be taken by directly using the fundamental equation of constrained motion. While this three-step procedure was first established some time ago [1–5], the explicit equation of motion obtained through its use required that the mass matrix of the unconstrained system be positive definite—a circumstance that usually occurs in analytical dynamics. A decade later, this requirement was relaxed, and an explicit equation of motion for constrained systems whose unconstrained equations of motion have semi-positive definite mass matrices was developed [6,7]. The most common way in which such singular mass matrices can arise in complex multi-body systems is when a constrained mechanical system is described through the use of more coordinates than the minimum number needed. The use of such additional coordinates can greatly simplify the modeling task, provide clarity and ease of description of the multi-body dynamics, and yield general formulations for systems that have often been difficult to obtain. The three-step procedure described earlier is important in ensuring that a proper description of complex multi-body systems can be systematically obtained [8]. It provides a framework for the proper use of zero-mass particles to facilitate the derivation of the equations of motion for such systems. A further refinement and simplification of the approach proposed in Ref. [7] that also considerably improves computational efficiency is provided in Ref. [9].
This paper uses the abovementioned three-step procedure to describe the motion of a non-homogeneous, rigid sphere rolling under gravity, without slipping, on an arbitrarily prescribed (rough) surface. We make explicit use of one or more zero-mass particles to formulate its equations of motion. We show that the use of such zero-mass particles greatly facilitates the mathematical description of the dynamical system thereby permitting a simple, general formulation of the problem. While we show the usefulness of zero-mass particles in this paper for handling the problem of a sphere rolling on an arbitrarily prescribed surface, their use is described in a general enough manner so as to be applicable to numerous other problems in analytical and multi-body dynamics.

The dynamics of a rigid sphere rolling under gravity without slipping on a surface is one of the classical problems of mechanics in which nonholonomic constraints play an important role, and in which the standard Lagrangian formalism is difficult to apply to readily simulate the dynamical behavior when the surface is arbitrarily prescribed. One of the first contributions to this problem was published by Lindelöf in 1895 [10], in which it seemed that cases [11,12]. In this work, Chaplygin derived the integrals of motion of a sphere rolling on an arbitrarily prescribed surface, their use is described in a general enough manner so as to be applicable to numerous other problems in analytical and multi-body dynamics.

2 Formulation of Problem

2.1 Description of the Unconstrained System. We begin with an unconstrained system [8] described by a rigid non-homogeneous sphere S of radius r and mass m whose center, O, is located at \((x_o, y_o, z_o)\) and whose center of mass, C, is located at \((x_C, y_C, z_C)\) in the XYZ inertial frame of reference (see Fig. 1). The vector from the center of the sphere, O, to the point C is denoted by \(p\). The principal axes of inertia of the sphere that go through the point C are denoted by \(x, y, z\) as shown; they form a body-fixed right-handed coordinate frame of reference. The moments of inertia of the sphere about these respective body-fixed principal axes of inertia are denoted by \(I_1, I_2, I_3\) and the \(3 \times 3\) moment of inertia matrix is denoted by \(J = \text{Diag}(I_1, I_2, I_3)\). In order to get away from singularities while describing the rotational motion of the sphere S, we shall use the quaternion 4-vector \((4 \times 1\) column vector) \(w = [w_o, w_1, w_2, w_3]^T\) to describe its orientation [17]. Hence, the position and orientation of the sphere are described by the seven-component column vector of coordinates \(q_S^o := [x_o, y_o, z_o, u_0, u_1, u_2, u_3]^T = [w_o^T, u^T]^T\), where \(w_o^T := [x_o, y_o, z_o]^T\). The reason we choose the coordinates of O in our description of the system is that the coordinates of O and those of the point of contact between S and \(\Gamma\) are most convenient for writing the constraints that the sphere is subjected to when it rolls without slipping on \(\Gamma\).

Though we are interested primarily in the dynamics of the sphere S, we begin by conceiving the unconstrained system as being composed of two members: the sphere S and a particle P that has zero mass located at an arbitrary point \((\alpha_1, \alpha_2, \alpha_3)\) (see Fig. 1). Thus, the 10-vector \((10 \times 1\) column vector) \(q := [x_0, y_0, z_0, w_0, u_0, v_0, u_1, u_2, u_3, \alpha_1, \alpha_2, \alpha_3]^T := [w_0^T, u^T, \alpha^T]^T\) (1) describes the position (configuration) of the ‘unconstrained’ system consisting of the sphere S and the zero-mass particle P, where we have denoted \(\alpha = [\alpha_1, \alpha_2, \alpha_3]^T\). By unconstrained we mean that the components of the configuration vector \(\alpha\) are assumed to be independent of one another. The components of the column vectors \(w_o\) and \(\alpha\) are measured in the inertial frame of reference XYZ.
The equations of motion of this unconstrained system subjected to the downward force of gravity can now be easily written down. Since the sphere $S$ and the particle $P$ are not connected in any way, their equations of motion can be separately written. The potential energy of the sphere $S$ is given by $V = m g z_c$; its kinetic energy of translation is given by $T_{trans} = \frac{m}{2} \left[ \dot{w}_o^T \dot{w}_o + 2 \dot{w}_o^T \dot{S} \rho + \rho^T S^T \dot{S} \rho \right]$, and its kinetic energy of rotation is given by $T_{rot} = \frac{1}{2} \omega^T I \omega$, where the 3-vector $\omega = [\omega_x, \omega_y, \omega_z]^T$ is the absolute angular velocity of the sphere $S$ whose components along the body-fixed coordinate frame $\hat{x} \hat{y} \hat{z}$ are, respectively, $\omega_x$, $\omega_y$, and $\omega_z$.

We note that the term $\omega^T S \dot{S}$ in Eq. (3) can be expressed as

$$\omega^T S \dot{S} = \omega^T S^T \dot{S} = \rho^T \hat{o} = \rho^T \hat{o} = \rho^T \rho$$

Using relations (2) and (3), the kinetic energy of the unconstrained sphere $S$ is obtained as

$$T(\dot{w}_o, u, \dot{u}) = T_{trans} + T_{rot} = \frac{m}{2} \left[ \dot{w}_o^T \dot{w}_o + 2 \dot{w}_o^T \dot{S} \rho + \rho^T S^T \dot{S} \rho \right] + 2 \dot{u}^T E \dot{E} \dot{u}$$

and its potential energy is given by

$$V(\dot{w}_o, u) = m g z_c = m g [\dot{z}_o + S z]$$

where $S z$ is the third row of the rotation matrix $S$.

The Lagrangian $L = (T(\dot{w}_o, u, \dot{u}) - V(\dot{w}_o, u))$ for the unconstrained sphere $S$ can be used to obtain its equation of motion using the usual Lagrange equation

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_i} \right) - \frac{\partial L}{\partial q_i} = 0$$

under the assumption that all the components of the seven-vector $q_i$ are independent of one another.

Using the expression for the kinetic energy in Eq. (5), we obtain

$$\frac{\partial T}{\partial \dot{w}_o} = m \ddot{w}_o + m S \dot{S} \rho = m \dot{w}_o + m C_1 \dot{u} = m \dot{w}_o + m C_1 u$$

since $\dot{S} \rho = C_1 \dot{u}$ and

$$T(\ddot{w}_o, u, \ddot{u}) = \frac{m}{2} \left[ \dot{w}_o^T \dot{w}_o + 2 \dot{w}_o^T \dot{S} \rho + \rho^T S^T \dot{S} \rho \right] + 4 \dot{u}^T E \dot{E} \dot{u}$$

with

$$C_2 = \dot{C}_1$$

Thus, we obtain using the second equality in Eq. (8).

$$\frac{d}{dt} \left( \frac{\partial T}{\partial \dot{w}_o} \right) = m \dddot{w}_o + m C_1 \ddot{u} + m C_2 \dot{u} \dot{w}_o, \quad \frac{\partial T}{\partial \dot{w}_o} = 0$$

and

$$\frac{d}{dt} \frac{\partial V}{\partial \dot{w}_o} = m g[0, 0, 1]^T$$

We note that the term $\rho^T \rho$ in Eq. (3) can be expressed as

$$\rho^T \rho = \rho^T \hat{o} = \rho^T \rho = \rho^T \rho$$

where the skew-symmetric matrices $\hat{o}$ and $\hat{\rho}$ are obtained from their respective components (see Eqs. (2) and (3)) and are given by

$$\hat{o} = \begin{bmatrix} 0 & -\omega_z & \omega_y \\ \omega_z & 0 & -\omega_x \\ -\omega_y & \omega_x & 0 \end{bmatrix} \quad \text{and} \quad \hat{\rho} = \begin{bmatrix} 0 & -\rho_3 & \rho_2 \\ \rho_3 & 0 & -\rho_1 \\ -\rho_2 & \rho_1 & 0 \end{bmatrix}$$

In Eq. (12), we have made use of the fact that $\hat{o} = S^T \hat{o}. $ Using relations (12) and (2) in the expression for the kinetic energy $T(\dot{w}_o, u, \dot{u})$ given in Eq. (5), we obtain

$$\frac{d}{dt} \left( \frac{\partial T}{\partial \dot{w}_o} \right) = m \dddot{w}_o + m C_1 \ddot{u} + m C_2 \dot{u} \dot{w}_o = m C_1 \dddot{w}_o + m C_1 \ddot{u} \dot{w}_o + 4 \dot{u}^T E \dot{E} \dot{u}$$

so that

$$\frac{d}{dt} \left( \frac{\partial T}{\partial \dot{u}} \right) = m C_1 \dddot{w}_o + 4 \dot{u}^T E \dot{E} \dot{u} + 4 \dot{E} \dot{E} \dot{u}$$

since $\dot{E} \dot{u} = 0$. Also, using the second equality in relation (14), we obtain

$$\frac{d}{dt} \left( \frac{\partial T}{\partial u} \right) = m C_1 \dddot{w}_o + 4 \dot{u}^T E \dot{E} \dot{u} = m C_1 \dddot{w}_o - 4 \dot{E} \dot{E} \dot{u}$$

since $\dot{E} \dot{u} = -\dot{E} u$ and
\[ \frac{\partial V}{\partial u} = mg \frac{\partial (S_p \rho)}{\partial u} = 2mg \begin{bmatrix} -u_2 \rho_1 + u_1 \rho_2 + u_0 \rho_3 \\ u_2 \rho_1 + u_0 \rho_2 - u_1 \rho_3 \\ -u_0 \rho_1 + u_3 \rho_2 - u_3 \rho_3 \\ u_1 \rho_1 + u_2 \rho_2 + u_3 \rho_3 \end{bmatrix} = 2mg \rho_0 \] (18)

where \( S_p \), as before, is the third row of the matrix \( S \) given in Eq. (4).

Thus, the equations of motion of the unconstrained sphere \( S \) become

\[ M_S \ddot{q}_S = \begin{bmatrix} ml & mC_1 & 0 \\ mC_1^T & 4E^TJE & 0 \\ 0 & 0 & M_p \end{bmatrix} \begin{bmatrix} \dot{\omega}_0 \\ \dot{\bar{u}} \\ \ddot{\bar{a}} \end{bmatrix} \]
\[ = \begin{bmatrix} -mC_2 \dot{\bar{u}} - mg[0, 0, 1]^T \\ -8E^T J E \ddot{\bar{u}} - 2mgp \\ 0 \end{bmatrix} := Q_U(q_s, \dot{q}_s, t) \] (19)

where \( M_p \) is a 7 \times 7 symmetric matrix. We note from Eq. (19) that the translational motion is coupled to the rotational motion and that the matrix \( 4E^TJE \) is singular.

The equation of motion of the zero-mass particle \( P \) is trivial to write down. Its mass being zero, no force can be applied to it, and hence, its equation of motion is simply

\[ M_p \ddot{\bar{a}} = 0 \] (20)

where \( M_p \) is a 3 \times 3 zero matrix.

Using Eqs. (19) and (20), we obtain the unconstrained equation of motion of the system composed of the sphere \( S \) and the particle \( P \)

\[ M_U \ddot{\bar{q}} := \begin{bmatrix} ml & mC_1 & 0 \\ mC_1^T & 4E^TJE & 0 \\ 0 & 0 & M_p \end{bmatrix} \begin{bmatrix} \dot{\omega}_0 \\ \dot{\bar{u}} \\ \ddot{\bar{a}} \end{bmatrix} \]
\[ = \begin{bmatrix} -mC_2 \dot{\bar{u}} - mg[0, 0, 1]^T \\ -8E^T J E \ddot{\bar{u}} - 2mgp \\ 0 \end{bmatrix} := Q_U(q_s, \dot{q}_s, t) \] (21)

where \( M_U \) is a 10 \times 10 block diagonal matrix. The subscript \( U \) denotes quantities related to the so-called unconstrained equation of motion of the system described in Fig. 1. We note that the matrix \( M_p \) is zero and that the matrix \( M_U \) is singular.

### 2.2 Description of the Constraints

Having obtained the unconstrained equations of motion, we now constrain the sphere \( S \) to roll without slipping on the surface \( \Gamma \), and we constrain the zero-mass particle \( P \) to lie on \( \Gamma \) and always be co-located with the point of contact between the sphere \( S \) and the surface \( \Gamma \) (see Fig. 2). The surface \( \Gamma(x, y, z) = 0 \) is described in terms of the inertial coordinates \( X, Y, Z \). It is because these constraints are most easily expressible in terms of the coordinates of the point of contact that lies on \( \Gamma \) that we add the coordinates of the point mass particle \( P \) to our dynamical system, thereby facilitating the development of the equations of motion of the desired dynamical system [1–5], which we shall obtain in explicit form in the following step in Sec. 2.3. We begin by listing out all the constraints.

(a) **Surface Constraint:** We begin by binding the zero-mass particle \( P \), which so far is located at an arbitrary point \((\alpha_1, \alpha_2, \alpha_3)\) in space, to lie on the surface \( \Gamma \) that is described by the equation

\[ \Gamma_3 := \Gamma(\alpha_1(t), \alpha_2(t), \alpha_3(t)) = 0 \] (22)

We shall denote the components (in the XYZ frame) of the gradient of \( \Gamma \) by the three-vector (3 \times 1 column vector) \( k \) so that

\[ k := \left( \frac{\partial \Gamma}{\partial \alpha_1}, \frac{\partial \Gamma}{\partial \alpha_2}, \frac{\partial \Gamma}{\partial \alpha_3} \right)^T \] (23)

and we shall henceforth assume that the sign of the expression \( \Gamma \) in the equation \( \Gamma = 0 \) (see Eq. (22)) is so chosen that the third component of the gradient vector is positive and points in the (upward) Z-direction. Taking the second derivative with respect to time of the equation \( \Gamma = 0 \) that is on the right-hand side of Eq. (22) yields the relation

\[ k \dddot{\alpha} + k \dddot{\alpha} = 0 \] (24)

which can be immediately recast, noting our definition of the column vector \( \dot{q} \) in Eq. (1), as

\[ A_1 \dddot{\dot{q}} = b_1 \] (25)

where

\[ A_1 = \begin{bmatrix} 0 & 1 & 1 \end{bmatrix}, \quad b_1 = -\dddot{\mathbf{k}} \dot{\mathbf{k}} - \dddot{\mathbf{k}} \frac{\partial \mathbf{k}}{\partial \mathbf{\alpha}} \dot{\mathbf{\alpha}} \] (26)

It should be noted that the coordinates \((\alpha_1, \alpha_2, \alpha_3)\) of the zero-mass particle, \( P \), that moves on the surface \( \Gamma \) change with time, \( t \), as the sphere \( S \) rolls on it. Hence, the unit normal to the surface \( \Gamma \) at \((\alpha_1(t), \alpha_2(t), \alpha_3(t))\) is given by the three-component column vector

\[ n(\alpha_1(t), \alpha_2(t), \alpha_3(t)) = \frac{\nabla \Gamma}{\| \nabla \Gamma \|} = \frac{k}{k^T k} \] (27)

(b) **Tangency Constraint:** This constraint that binds the particle \( P \) to the point of contact between the sphere \( S \) and the surface \( \Gamma \) is simply given by

\[ q_S := \alpha + \mathbf{m} - \mathbf{w}_0 = 0 \] (28)

where the column vector \( n \) is given in Eq. (27). Differentiating the equation on the right-hand side of Eq. (28) twice with respect to time yields the relation

\[ \dddot{\mathbf{a}} + \dddot{\mathbf{n}} \mathbf{\dot{a}} - \dddot{\mathbf{w}}_0 = 0 \] (29)

which can similarly be expressed as

\[ A_2 \dddot{\dot{q}} = b_2 \] (30)

Finding the second derivative of \( n \) with respect to time is tedious and the Appendix gives the explicit expressions for the 3 \times 10 matrix \( A_3 \) and the 3 \times 1 column vector \( b_2 \).

(c) **Rolling No-Slip Constraint:** This constraint requires that there is no slip between the sphere \( S \) and the surface \( \Gamma \) as the sphere rolls over the surface. Hence, the velocity of the center of the sphere in the inertial frame of reference is given by the relation

\[ q_{S3} := \dot{\mathbf{w}}_0 + \dddot{\mathbf{n}} \mathbf{\dot{w}} = 0 \] (31)

where the rotation matrix \( S \) given in Eq. (4) is used to transform the components of the vector \( \mathbf{n} \times \mathbf{o} \) from the body frame to the inertial frame, and \( \dddot{\mathbf{w}}_0 \) is the 3 \times 3 skew-symmetric matrix obtained, as before, from the components of the column vector \( n \) in Eq. (27). Differentiating the equation on the right-hand side of Eq. (31) once with respect to time and noting Eq. (2), we obtain

\[ \dddot{\mathbf{w}}_0 + 2\dddot{\mathbf{n}} \mathbf{\dot{S}} \mathbf{\dot{E}} \mathbf{\ddot{w}} = -2r\dddot{\mathbf{S}} \mathbf{\dot{E}} \mathbf{\ddot{w}} - 2r\dddot{\mathbf{S}} \mathbf{\dot{E}} \mathbf{\ddot{w}} = -2r \mathbf{n} \mathbf{\dot{S}} \mathbf{\dot{E}} \mathbf{\ddot{w}} \] (32)

The first term on the right-hand side of the first equality in Eq. (32) can be shown to be zero since we have

\[ 2r \dddot{\mathbf{S}} \mathbf{\dot{E}} = 2r \mathbf{S} \mathbf{\dot{S}}^T \mathbf{\dot{E}} = 2r \mathbf{\dot{S}} \mathbf{\dot{S}} \mathbf{\dot{E}} = \mathbf{\dot{S}} \mathbf{\ddot{S}} \mathbf{\dot{w}} = 0. \]

These equalities follow from the relations \( \mathbf{S} \mathbf{S}^T = \mathbf{I}, \mathbf{S} \mathbf{\dot{S}} = \mathbf{\dot{S}}, 2 \mathbf{\dot{E}} = \mathbf{\dot{o}}, \) and \( \mathbf{\ddot{w}} = 0. \) Equation (32) can again be easily expressed as

\[ A_3 \dddot{\dot{q}} = b_3 \] (33)
where
\[ A_3 = [I_{3 \times 3} | 2r \dot{n} SE | 0_{3 \times 1}] \] and \( b_3 = -2r \dot{n} SE \dot{u} \) \hspace{1cm} (34)

(d) Quaternion Constraint: For the four-vector \( u(t) \) to represent a physical rotation at each instant of time, we need the ensure that its norm is unity, so that
\[ q_4: = u^T u - 1 = 0 \] \hspace{1cm} (35)

Differentiating the right-hand equation in Eq. (35) twice with respect to time yields the relation
\[ A_4 \ddot{q} = b_4 \] \hspace{1cm} (36)

where
\[ A_4 = [0_{3 \times 3} | u^T | 0_{3 \times 1}] , \quad \text{and} \quad b_4 = -\dot{u}^T \dot{u} = -(\dot{u}_0^2 + \dot{u}_1^2 + \dot{u}_2^2 + \dot{u}_3^2) \] \hspace{1cm} (37)

The abovementioned four sets of constraints \( q_i, i = 1, 2, 3, 4 \), can thus be collectively expressed as
\[ A \ddot{q} = \begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{bmatrix} \ddot{q} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix} = b \] \hspace{1cm} (38)

where \( A \) is now an \( 8 \times 10 \) matrix and \( b \) is an \( 8 \)-vector (\( 8 \times 1 \)) with the \( A_i \) and \( b_i \) explicitly obtained earlier. We note in passing that these constraints are not all independent of one another and that the matrix \( A \) does not have full rank. Also, the elements of the matrix \( A \) and the vector \( b \) are relatively easy to obtain, since all that needs to be done is to differentiate with respect to time the sets of constraint equations \( q_i, i = 1, 2, 3, 4 \).

(e) Additional Consistent Constraints: One of the advantages of using the three-step conceptual approach to obtain the equations of motion of the constrained system—here, the sphere \( S \) rolling without slipping on the surface \( \Gamma \)—is that if one knows a priori any integrals of motion of the system they can be included in the constraints. In this instance, we know that the total energy of the sphere is conserved. Using Eqs. (6) and (14), we then find that the energy, \( E(t) \), at any time \( t \) is given by
\[ E(t) = T(\dot{w}_0, \dot{u}, \dot{\hat{u}}) + V(\dot{w}_0, \dot{u}) = \frac{m}{2} [w_0^T \dot{w}_0 + 2w_0^T C_1 \dot{u}] + 2\dot{u}^T E^T J E \dot{u} + m g [z_o + S_3 \rho] = E(0) \] \hspace{1cm} (39)

which upon differentiation once with respect to time yields the relation
\[ A_E \ddot{q} = b_E \] \hspace{1cm} (40)

where
\[ A_E = [m \dot{w}_0^T + m \dot{u}^T C_1^T | m \dot{w}_0^T C_1 + 4 \dot{u}^T E^T J E | 0_{3 \times 1}] , \quad \text{and} \quad b_E = -[m \dot{w}_0^T C_2 \dot{u} + m g z_o + m g S_3 \rho] \] \hspace{1cm} (41)

We could, if we wanted to, add this additional constraint as an additional row to the set of constraints given in Eq. (38) to obtain the description of the constrained system, as we will show in Sec. 2.3.

2.3 Description of the Constrained System. Having obtained Eq. (21) for the unconstrained system and the constraint equations (38), the equation of motion of the constrained system is given explicitly by [6]
\[ \ddot{q} = \left[ (I - A^* A) M_U \right] \ddot{b} + \left[ \frac{Q_U}{b} \right] \] \hspace{1cm} (42)

where \( X^+ \) denotes the Moore–Penrose (MP) inverse of the matrix \( X \) [3, 18]. We note that for the acceleration to be unique—and this must be the case for a physical system described by classical mechanics—a necessary and sufficient condition is that [6]
\[ \text{Rank}([M_U | A^T]) = \text{Number of components in column vector } q \] \hspace{1cm} (43)

This (full) rank condition on the matrix on the left-hand side of relation (43) serves as a check on whether the constrained system has been modeled appropriately [6]. Equation (42) is true even when the constraints are not functionally independent and the matrix \( A \) does not have full rank. The addition of constraints that are consistent with those described therefore does not limit the use of these relations. This aspect of the general approach described here in modeling the dynamics of the rolling sphere becomes useful when dealing with more complex dynamical systems [8].

When relation (43) is satisfied, an alternate way of obtaining the acceleration \( \ddot{q} \) of the constrained system is to consider an equivalent dynamical system with the augmented mass matrix \( \hat{M}_U \) given by
\[ \hat{M}_U = M_U + \kappa^2 A^T A > 0 \] \hspace{1cm} (44)

where \( \kappa \) is any real non-zero number [7, 9]. The acceleration of the constrained system (when relation (43) is satisfied) is then given explicitly by the fundamental equation [3, 9] as
\[ \ddot{q} = \hat{M}_U^{-1} Q_U + \hat{M}_U^{-1} A^T (\hat{M}_U^{-1} A)^T (b - \hat{M}_U^{-1} Q_U) \] \hspace{1cm} (45)

As before, Eq. (45) is true even when the constraints are not functionally independent and the matrix \( A \) does not have full rank.

It should be noted that Eqs. (42) and (45) are the explicit equations of motion for the same sphere constrained to roll without slipping on an arbitrarily prescribed surface, \( \Gamma(X, Y, Z) = 0 \), and they each yield the same acceleration \( \ddot{q} \).

3 An Alternative Formulation of the Problem Using Two Zero-Mass Particles

We notice that a major amount of effort is expended in the development of the unconstrained equations of motion. The complexity in getting them is principally caused by the fact that while the translational kinetic energy of the sphere \( S \) is simply \( E_{\text{trans}} = (m/2)(\dot{x}_C^2 + \dot{y}_C^2 + \dot{z}_C^2) \), we want to use the coordinates of the center of the sphere \( O \) instead of those of its center of mass \( C \) in our formulation, since the constraints are most easily expressed in terms of the location of the sphere’s center \( O \). This leads to
considerable algebra (see Eqs. (7)–(19)) resulting finally in the coupled set of equations for the unconstrained sphere S obtained in Eq. (19).

In retrospect then, one could greatly simplify the task of writing the unconstrained equations of motion of the sphere S, by including the coordinates of its center of mass C in its dynamical description. However, in order to conveniently express the constraints, we also need the coordinates of O to be included in the dynamical description. To accomplish this with some ease, we use an additional zero-mass particle Q located at an arbitrary point in space, which we will later constrain to be always coincident with the center O of the sphere. Our three-step procedure for obtaining the equations of motion then appears as follows.

### 3.1 Description of the Modified Unconstrained System

We take our unconstrained system to consist of three components: (1) the sphere S, whose description is provided by the coordinates $w_C = [x_C, y_C, z_C]^T$ and quaternion 4-vector $w$; (2) the zero-mass particle P at an arbitrary location $a$ in the XYZ frame, and (3) a second zero-mass particle Q located at an arbitrary point in space $w_Q = [\beta_1, \beta_2, \beta_3]^T$ (see Fig. 3). The description of this three-component, multi-body dynamical system, in which the three bodies are taken to be totally unconnected is given, at each instant of time, by the augmented 13 component configuration vector

$$q_{13} := [\beta_1, \beta_2, \beta_3, u_0, u_1, u_2, u_3, a_1, a_2, a_3, x_C, y_C, z_C]^T; \quad \text{Eq. (46)}$$

Besides the additional coordinates $w_C$, added to the vector $q_{13}$, the crucial difference between the vector $q$ in Eq. (1) and the vector $q_{13}$ in relation (46) is that whereas the first three coordinates $x_C, y_C, z_C$ in the vector $q$ refer to those of the center O of the sphere S, the first three coordinates $\beta_1, \beta_2, \beta_3$ of the augmented vector $q_{13}$ refer to the coordinates of a zero-mass particle located at an arbitrary point $w_Q$ in space.

The unconstrained equations of motion for this three-component system, in which we assume that each of the generalized coordinates are independent of one another, are now trivial to write down. Since the kinetic energy and the potential energy of the sphere S are given by

$$T(q, \dot{q}, \ddot{q}_C) = T_{trans} + T_{rot} = \frac{m \dot{w}_C^T \ddot{w}_C}{2} + 2u^T E^T J E u$$

and

$$V(w_C) = m g z_C$$

respectively, its unconstrained equation of motion is given by the following simple set of equations:

$$\ddot{w}_C = \begin{bmatrix} 4E^T J E & 0 \\ 0 & m I \end{bmatrix} \begin{bmatrix} \ddot{u} \\ \ddot{w}_C \end{bmatrix} = \begin{bmatrix} -8E^T J E u \\ -mg[0, 0, 1]^T \end{bmatrix}$$

in which the translational and rotational motions, unlike in Eq. (19), are now uncoupled.

The equations of motion of the zero-mass particles P and Q, as before, are simply

$$M_P \ddot{a} = 0 \quad \text{and} \quad M_Q \ddot{w}_Q = 0$$

respectively, where $M_P$ and $M_Q$ are each $3 \times 3$, zero matrices, since no force can be applied to them. Thus, the equation of motion of this three-component, multi-body, unconstrained system is then

$$\ddot{q}_{13} := \begin{bmatrix} M_Q & 0 & 0 & 0 \\ 0 & 4E^T J E & 0 & 0 \\ 0 & 0 & M_P & 0 \\ 0 & 0 & 0 & m I \end{bmatrix} \begin{bmatrix} \ddot{u} \\ \ddot{a} \\ \ddot{w}_C \end{bmatrix} = \begin{bmatrix} -8E^T J E u \\ -mg[0, 0, 1]^T \end{bmatrix}$$

The augmented configuration 13-vector that now includes the coordinates of the zero-mass particle Q is denoted by $q_{13}$, and the $13 \times 13$ augmented mass matrix is denoted by $M_{UU}$.

A comparison of Eqs. (5)–(19) with Eqs. (47)–(50) shows the ease with which the unconstrained equations of motion of the system are now obtained. As seen, the addition of a second zero-mass particle makes the equations of motion of the system trivial to write. The matrix $M_{UU}$ of the unconstrained system is now block diagonal and Eq. (51) is uncoupled. It is much easier to write, and simpler, than Eq. (21) that was obtained earlier. The mass matrix $M_{UU}$ is singular though, since the matrices $M_P, M_Q,$ and $4E^T J E$ are singular matrices.

### 3.2 Description of the Constraints

Since the constraints, as we saw earlier, can be easily expressed in terms of the coordinates of the center O of the sphere and the point of contact, our intention in adding the zero-mass particles P and Q to the unconstrained dynamical system, is, in this step, to now:

1. constrain the particle P, as before, so that it lies on I and is always the point of contact between the sphere S and I, and
2. constrain the particle Q so that it always coincides with the center O of the sphere, thereby forcing the particle Q located at $w_Q = [\beta_1, \beta_2, \beta_3]^T$ to be co-located (coincide) with O (see Fig. 4).

In addition to these two sets of constraints, we may add any other constraints that the dynamical system may be known to satisfy. To model the sphere S rolling without slipping on the surface I, we therefore need the same four sets of constraints $q_{13, i} = a_i, i = 1, 2, 3, 4,$ that we obtained in Sec. 2.2. These eight constraints can be expressed in terms of our new description of the system using the vector $q_{13}$ as (the subscript “a” stands for the augmented configuration vector)

$$\begin{bmatrix} A_1 | A_2 | A_3 | A_4 | \end{bmatrix} \begin{bmatrix} q_{13} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

$$\text{Eq. (52)}$$
where the explicit expressions for the $A_i$'s and $b_i$'s are provided in Sec. 2.2. In addition, we need to add constraints that cause the zero-mass particle $Q$ to coincide with the point $O$. This can be done by simply requiring that relation (3) be true so that

$$
\varphi_2 = w_o + \dot{S}_p - \dot{w}_C = 0 \tag{53}
$$

which upon differentiation twice with respect to time yields

$$
\ddot{\varphi}_2 + \ddot{S}_p - \ddot{w}_C = 0 \tag{54}
$$

Noting that $\dot{S}_p = C_1 \dot{u}$ where $C_1$ is given in Eq. (9), Eq. (54) simplifies to

$$
\ddot{\varphi}_2 + C_1 \ddot{u} - \ddot{w}_C + C_2 \dot{u} = 0 \tag{55}
$$

which can be expressed as

$$
A_3 \ddot{q}_a = b_3 \tag{56}
$$

where

$$
A_3 = [I \ C_1 \ {0_{3 \times 3}} \ -I] \quad \text{and} \quad b_3 = -C_2 \dot{u} \tag{57}
$$

The five sets of constraints $\varphi_i$, $i = 1, 2, 3, 4, 5$, thus yield the augmented relation

$$
A_4 \ddot{q}_a = b_4 \tag{58}
$$

in which the matrices $A_4$, $i = 1, 2, 3, 4, 5$, are stacked one below the other as are the elements $b_4$, $i = 1, 2, 3, 4, 5$ in the column vector $b_a$. The matrix $A_4$ that specifies all these constraints is now $11 \times 13$.

We note that we could add as many more constraints as we wish, as long as they are all consistent; they need not be independent. For example, we can add the constraint that the distance between the center $O$ of the sphere and the point $C$ is a constant $l$ equal to the magnitude of the vector $\rho$. This would yield the relation

$$
\varphi_3 = (w_o - w_C)^T (w_o - w_C) = l^2 \tag{59}
$$

which upon differentiation twice with respect to time would yield

$$
(w_o - w_C)^T \ddot{(w_o - w_C)} = (\ddot{w}_o - \ddot{w}_C)^T (\dot{w}_o - \dot{w}_C) \tag{60}
$$

so that

$$
A_5 = [(w_o - w_C)^T \ 0_{1 \times 4} \ 0_{1 \times 3}] \ - \ (w_o - w_C)^T \quad \text{and} \quad b_5 = -(\ddot{w}_o - \ddot{w}_C)^T (\dot{w}_o - \dot{w}_C) \tag{61}
$$

In modeling complex systems, the facility of listing as many constraints as one can think of without worrying about which of them may be functionally dependent is an important convenience afforded by the three-step approach used here; this is especially useful when there are several nonholonomic constraints.

As before, one could also add the constraint that the energy, $E(t)$, at any time $t$, equals $E(0)$, to the stack of constraints given in Eq. (58). Noting that the energy is given by a much simpler expression than before as

$$
E(t) = T(u, \dot{u}, \dot{w}_C) + V(w_C) = \frac{2m\dot{w}_C^2}{2} + 2a\dot{u}^2 J E \dot{u} + m g z_C \tag{62}
$$

and differentiating it once with respect to time, we get the relation

$$
A_E \dot{q}_a = b_E \tag{63}
$$

where

$$
A_E = [0_{1 \times 3} \ 4a\dot{u}^2 J E \ 0_{1 \times 3} \ m \dot{w}_C^2] \quad \text{and} \quad b_E = -m g z_C \tag{64}
$$

Comparing Eqs. (39)–(41) with Eqs. (62)–(64), we note the considerable simplicity that accrues with the additional zero-mass particle $Q$ in our formulation of the problem.

The third and final step of our procedure calls for obtaining the constrained equations of motion.

### 3.3 Description of the Constrained System

The explicit equations of motion of the constrained system are obtained, as we did in Sec. 2, by using Eq. (42) or (44) and (45), but now with $\dot{M}_U$ and $\dot{Q}_U$ given in Eq. (51) and $A_a$ and $b_a$ given in Eq. (58), instead of $M_U$, $Q_U$, $A$, and $b$.

### 4 Numerical Example

Consider a solid sphere of radius $r = 6$ cm. The sphere is placed on an unsymmetrical surface whose equation is given by the polynomial

$$
\Gamma(X, Y, Z) := Z - \sum_{i=1}^{\infty} h_i X^i = 0 \tag{65}
$$

in which the coefficients $h_1 = 0.65$, $h_2 = -3$, $h_3 = -6.7$, and $h_4 = 20.5$. The shape of the surface is shown in Fig. 5.

At the initial time, the sphere is located touching the surface $\Gamma$ with $\alpha(0) = -0.65$ m, $\alpha(0) = 0.1$ m; it has no angular velocity (spin) about an axis normal to the surface. The initial velocity components of the point O located at the center of sphere are taken to be $\dot{x}_o = 0.2$ m/s and $\dot{y}_o = -0.3$ m/s. The origin of the body-fixed $\hat{i}\hat{j}\hat{k}$ coordinate frame is at the center of the uniform sphere. At time $t = 0$, these body-fixed $\hat{i}$, $\hat{j}$, and $\hat{k}$ axes are taken to be along the $X$, $Y$, and $Z$ directions, respectively, of the inertial frame $\hat{X}\hat{Y}\hat{Z}$ axes. Hence, the quaternion $\mathbf{u}(t=0) = [1, 0, 0, 0]^T$. Using these initial conditions, the other initial conditions are all determined using the constraint equations.

For illustrating our numerical results, the model developed in Sec. 2 with one zero-mass particle P is used. In addition to the four sets of constraints given Eq. (38), we have added the energy conservation constraint given in Eqs. (40) and (41). Similar
numerical results are obtained when using the augmented model of Sec. 3 which uses the two zero-mass particles P and Q. The results for this case are not shown here for brevity.

Figure 6 shows the motion of a uniform density titanium sphere with density $d = 4500 \text{ kg/m}^3$. The value of $g$ is taken to be $9.81 \text{ m/s}$. The matrix $M_U$ and the vector $Q_U$ are explicitly obtained from Eq. (21), and the matrix $A$ and the vector $b$ are explicitly obtained by using Eqs. (26), (30), (34), (37), and (41). Using a value of $\kappa^2 = 0.02$ in the numerical procedure, we obtain $\hat{M}_U$ from Eq. (44). The explicit equations of motion of the sphere rolling on the surface are then obtained by substituting $\hat{M}_U$, $Q_U$, $A$, and $b$ into Eq. (45).

The computations are done on the MATLAB platform, and a modified variable-step (4,5)-Runge–Kutta integrator is used with a relative error tolerance of $10^{-11}$ and an absolute error tolerance of $10^{-15}$.

That the matrix $[M_U | A^T]$ has full rank is numerically checked throughout the integration, which is carried out for a duration of 10 s. The solid blue line shows the motion of the center of the sphere. The dashed red line shows the motion of the point of contact between the sphere and the surface $\Gamma$. Since the coordinates of the point of contact are contained in the generalized coordinates that describe the system’s configuration at each instant of time, integration of the equations of motion of the dynamical system directly yields the motion of this point as the sphere rolls on the surface $\Gamma$.

Errors in the satisfaction of the constraints $\phi_i = 0$, $i = 1, 2, 3, 4$, given in Eqs. ((22)), (28), (31), and (35) are shown in Fig. 7. We observe that these errors are all of the same order of magnitude as the error tolerances used in the numerical integration of the equations of motion.

More generally, one could, as we did for the point of contact between the sphere and the surface,

(i) “paste” a zero-mass particle at any point on the sphere (or a dynamical system),
(ii) include its coordinates as part of the configuration vector that describes the dynamical system,
(iii) provide the appropriate constraints for the system, including those on the zero-mass particle,
(iv) use the equations of constrained motion for singular mass matrices [6–9], and
(v) thereby directly obtain the motion at that point.

We next consider the motion of the same solid sphere (radius 6 cm) to be non-uniform in its density with half of it made from titanium (density $d_1 = 4500 \text{ kg/m}^3$) and half made of vanadium (density $d_2 = 5494 \text{ kg/m}^3$). The origin of the body-fixed $\hat{x}\hat{y}\hat{z}$ coordinate system is now at the center of mass of the non-uniform sphere and not at its center. The body-fixed $\hat{x}$-axis is chosen to lie along the line of axisymmetry of the non-uniform sphere, its positive direction pointing away from the lighter hemisphere. The center of mass therefore lies on this axis. Being a line of axisymmetry, a principal axis of moment of inertia of the sphere (with the origin at the center of mass of the sphere) also lies along this axis. The other two principal axes of moment of inertia lie in a plane perpendicular to the $\hat{x}$ axis; they are chosen initially to be along the inertial $Y$- and $Z$-axis forming a right-handed triad. Thus, at time $t = 0$, as before, the quaternion $u(t=0) = [1, 0, 0, 0]^T$. The same initial conditions are provided to the non-uniform sphere as were provided to the uniform sphere, and the numerical procedures and error tolerances
5 Conclusions

This paper shows that zero-mass particles can be useful in increasing the ease with which models for complex multi-body systems can be formulated and their explicit equations of motion obtained. Their use causes the number of coordinates involved in describing the mechanical system to be greater than the minimum number needed. Such additional coordinates are not commonly used in modeling complex systems because they lead to descriptions that have singular mass matrices, and these matrices being noninvertible, cannot be handled in the standard manner in Lagrangian mechanics. However, recent advances in our understanding of constrained motion in analytical dynamics allow us to utilize singular mass matrices when appropriate constraints are imposed on the additional coordinates. It is this advance in analytical and multi-body dynamics on which the effective use of these zero-mass particles hinges.

In modeling of complex multi-body systems and obtaining their equations of motion, it appears best to follow the three-step strategy of (a) writing the unconstrained equations of motion of the system; (b) writing the constraints; and (c) obtaining the explicit constrained equation of motion [8]. The third step is obtained directly from the first two by using the explicit fundamental equation of constrained motion. Hence, it is the first two steps that are usually problematic in the description of complex multi-body systems. The use of zero-mass particles can play a significant role in easing the description of these two steps. This is demonstrated by considering the problem of a sphere rolling under gravity on an arbitrary surface without slipping.

For the rolling sphere, in order to be able to write the constraints in an easy and simple manner, we need the coordinates of two points—the location of the center of the sphere, and the location of the point of contact between the sphere and the arbitrarily prescribed surface. While the coordinates of the center of the sphere can be included in the set of generalized coordinates, those of the point of contact are usually not. The addition of a zero-mass particle at the point of contact in the description of our system, which then naturally expands the set of generalized coordinates, makes writing down these constraints trivial, as shown. However, this leads to a singular mass matrix. This zero-mass particle is constrained to coincide with the point of contact between the sphere and the surface, and the point of contact is thereby included in the dynamical description of the multi-body system now consisting of the sphere and the zero-mass particle. Application of the explicit fundamental equation of constrained motion using an augmented mass matrix gives the equations of motion of the multi-body system. Upon integration, the system’s motion is obtained, and the path traced out on the (arbitrary) surface by the point of contact between the sphere and the surface, as the sphere rolls over it, is thus obtained simply and directly though this dynamical formulation. This approach is further widened in the section that follows by considering the multi-body system made up of the sphere and two zero-mass particles. This further simplifies writing of the unconstrained equations of motion as well as the constraints.

Zero-mass particles can thus also be useful in easing the description of the unconstrained system. For the rolling sphere, we observe that the kinetic energy of the unconstrained system can be trivially written by using the coordinates of the center of mass of the sphere. In Sec. 3, we therefore additionally include the coordinates of the center of mass of the sphere in our dynamical description. However, this then calls for the use of two zero-mass particles in the description of the unconstrained system, because we also need the coordinates of the center of the sphere in order to write the constraints in a simple manner, as the sphere rolls on the surface. One of the particles, as before, is later constrained to be the point of contact between S and Γ while the other zero-mass particle is constrained to coincide with the center of the sphere. Expanding the set of generalized coordinates by including two additional zero-mass points to describe the dynamical system now permits both the unconstrained equation of motion of the system and the constraints to be trivially written down. The unconstrained equations of motion are again singular. Addition of the constraints, in terms of this expanded set of generalized coordinates, allows the equations of motion of the constrained system—the sphere rolling on the surface without slip—to be obtained explicitly through application of the fundamental equation of constrained motion.

More generally, in the dynamics of complex multi-body systems, constraints play a very significant and near-central role. Often these constraints can be most easily written in terms of the coordinates of one or more points that are not part of the set that has the minimum number of generalized coordinates needed to describe the
configuration of a multi-body system. To use additional coordinates that can conveniently convey information about the system’s constraints, one can “label” such points by placing zero-mass particles at these locations and including them in the dynamical description of the system, as shown in the example of a rolling sphere in this paper. This can greatly ease not only the description of the constraints but also the development of the unconstrained equations of motion, as illustrated.

At other times, one may be interested in simply finding the motion of one or more specific points (locations) in a complex mechanical system. Such points can be similarly “labeled” by placing zero-mass particles, like post-in stickers, at those specific locations and directly incorporating these points into the description of the dynamical configuration of the multi-body system. At these labeled points, one can simply

(i) “paste” zero-mass particles at desired locations in a mechanical system (more generally, in any dynamical system),
(ii) include their coordinates as part of the configuration vector that describes the dynamical system and write the equations of motion pertaining to them, which is trivial, but which leads to a system with a singular mass matrix,
(iii) provide appropriate constraints, including those on the zero-mass particles, and
(iv) obtain the constrained equations of motion of the dynamical system using the explicit equations of motion developed in Refs. [6,7,9].

The resulting equations are easily amenable to computation, and they directly yield the motion (displacements, velocities, and accelerations) at the labeled locations where the zero-mass particles are placed in the dynamical system.

Appendix

In this appendix, we obtain the matrix \( A_2 \) and the vector \( b_2 \). The gradient vector to the surface \( \Gamma \) has components in the XYZ inertial frame given by

\[
\hat{k} = \begin{bmatrix} \partial \Gamma / \partial \alpha_1 & \partial \Gamma / \partial \alpha_2 & \partial \Gamma / \partial \alpha_3 \end{bmatrix}^T
\]

with the sign of \( \Gamma(\alpha_1, \alpha_2, \alpha_3) \) chosen so that the last component of \( \hat{k} \) is positive. The unit normal \( n \) to the surface therefore has components given by \( n = k / \sqrt{k^T k} \) so that

\[
\hat{n} = \frac{1}{\sqrt{k^T k}} \frac{\hat{k}}{\partial \alpha} - \frac{\hat{k}}{\partial \alpha} \frac{k^T k}{(k^T k)^{3/2}}, \quad \text{and} \quad \hat{n} = \frac{\hat{k}}{\partial \alpha}
\]

where

\[
\Delta = \frac{1}{\sqrt{k^T k}} \begin{bmatrix} I_3 - \frac{\hat{k} \hat{k}^T}{k^T k} \end{bmatrix}, \quad \delta = \frac{1}{(k^T k)^{3/2}} \left[ \frac{3(k^T k)^2}{k^T k} \right], \quad \text{and} \quad \hat{k} = \frac{\hat{k}}{\partial \alpha}
\]

Hence, the constraint \( \hat{n} + \hat{\omega} \hat{n} = 0 \) can be written as \( A_2 \hat{q} = b_2 \) where

\[
A_2 = \begin{bmatrix} -I_{3 \times 3} | 0_{1 \times 3} | I + rA \frac{\partial \delta}{\partial \alpha} \end{bmatrix}, \quad \text{and} \quad b_2 = -r \left[ \Delta \frac{d}{dt} \left( \frac{\hat{k}}{\partial \alpha} \right) + k \delta - \frac{2k^T k}{(k^T k)^{3/2}} \right]
\]

References