Role of Maggi's Equations in Computational Methods for Constrained Multibody Systems

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This paper presents a unified theoretical basis for a class of methods that generate the governing equations of constrained dynamical systems by eliminating the constraints. By using Maggi's equations in conjunction with a common projective theory from numerical analysis, it is shown that members of the class are precisely characterized by the basis they choose for the null-space of the variational form of the constraints. For each method considered, the specific basis chosen for the null-space of the variational constraints is derived, as well as a dual basis for the orthogonal complement. The latter basis is of particular interest since it is shown that its knowledge theoretically enables one to generalize certain methods of the class to calculate constraint forces and torques. Practical approaches based on orthogonal transformations to effect this strategy are also outlined. In addition, since the theory presented herein stresses a common, fundamental structure to the various methods, it is especially useful as a means of comparing and evaluating individual numerical algorithms. The theory presented makes clear the relationship between certain numerical instabilities that have been noted in some methods that eliminate a priori constraint contributions to the governing equations by selecting an independent subset of unknowns. It is also briefly indicated how this formalism can be extended, in principle, to the wider class of nonlinear nonholonomic constraints.

Introduction

THE need for general and efficient numerical techniques for constrained mechanical systems is well established. Studies concerning computational methods for constrained dynamical systems have arisen in the modeling of mechanism dynamics[1-3] and in the simulation of spacecraft.[4-6] Furthermore, extensive growth is expected in techniques for the optimization of mechanism dynamics[7] and for large space structure simulation and control.[8]

One means of classifying the diverse methods that have been developed in this field categorizes the techniques as to whether they employ a minimal or redundant coordinate set. This issue has been the focus of much discussion in the past, particularly in comparing the relative merits of various techniques.[9-12] Lagrangian methods in which the constraint forces are explicitly represented by multipliers[13,14] and Newton-Euler methods that retain interbody forces and torques are typical of the redundant formulations. On the other hand, Kane's technique[11] and Newton-Euler methods that analytically eliminate the constraint forces via graph theory[15] are examples of formalisms that can be employed to obtain a "minimal" number of unknowns.

Although it would seem desirable to use the least number of unknowns possible in formulating any particular problem, the choice regarding minimal or redundant coordinates in dynamics is not always clear-cut. As most succinctly put by Schwertassek and Roberson,[16]

> Minimal sets of equations are more difficult to derive, more complicated in form, possibly faster to solve, but might not yield directly all the desired information about the systems (e.g., constraint forces and torques). Descriptions with redundant equations are more easily derived, generally simpler in form, slower to solve, but provide additional information.

A close examination of the formalism of Wittenburg[15] can leave little doubt as to the complexity of some minimal methods. Likewise, Kane's method as described in Ref. 25, although minimal, does not provide a means of constraint force evaluation that is as systematic as Lagrangian approaches.

Within the past few years, several related methods have arisen that first pose the constrained dynamics problems in terms of a redundant set of unknowns and subsequently reduce the system to minimal order for solution. Thus, these methods seek to combine the simplicity of redundant formulations with the numerical efficiency of minimal techniques. The first such techniques that have appeared in the literature attempt to circumvent the numerical difficulties sometimes noted when implicit integration schemes are applied to mixed systems of algebraic and differential equations. The method of coordinate partitioning suggested by Wehage and Haug[17] uses a Lagrangian formulation and Gaussian elimination to select a subset of the original unknowns, consequently eliminating the multipliers. As a result of poor conditioning in some submatrices required in the method, Mani[18] employs singular-value decomposition instead of Gaussian elimination to select an independent subset of unknowns. The resulting technique is shown to have better stability characteristics. Kim and Vanderploeg[19] further improve on the numerical efficiency of Mani's work by introducing "null-space updating" based on QR decomposition.

As opposed to these Lagrangian-based methods, another set of algorithms has been developed using Kane's equations as the theoretical foundation. Singh[9] and Huston[10] suggest modifications to Kane's method based on singular-value decomposition and eigenvector decomposition, respectively. Both approaches pose the governing equations in terms of Kane's equations without considering the constraints, and then reduce the system numerically to a smaller set for solution. More recently, Wang and Huston[20] derived a formulation based on Kane's method that includes "undetermined multipliers," such as in Lagrange's equations. The multiplicative terms are eliminated numerically through the use of "orthogonal complement" arrays. In Ref. 31, Wampler et al. derives an "explicit" formulation, based on Kane's method, that is appropriate for symbolically, or numerically, generating a constraint-free system of equations.

One potential difficulty in assimilating and evaluating this class of methods as a whole may be attributed to the fact that

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pertinent research in the spacecraft and mechanism dynamics fields has been, to some degree, mutually isolated. This observation has been noted by other authors.[3] The lack of an overall viewpoint can be particularly disconcerting to those interested in a "global" perspective of computational techniques for constrained dynamical systems. For example, the authors are interested in the development of computational algorithms appropriate for concurrent multiprocessors. In this context, the details involved in deriving the governing equations via Newton's equations, Lagrange's equations, or Kane's technique are not nearly as important as determining the fundamental structure and numerical processes underlying a wide variety of specific methods.

In this paper, it is shown that the class of computational methods described earlier[9–11,17–20,31] may be characterized concisely in terms of Maggi's equations. The theoretical unification of these distinct techniques is accomplished by reexamining Maggi's equations in terms of modern linear operator theory. It is demonstrated that each method performs the following fundamental numerical steps:

1) The equations governing each of the constraint-free, or "relaxed," substructures are formed and then assembled into a set of system equations.

2) The equations of the "released" system are required to be orthogonal to a specific subspace for solution, particularly the null-space of the variational constraints. This step is equivalent to requiring that the projection of the system equations onto the null-space of the variational constraints is zero.

3) Constraint forces may be evaluated, if desired, by projecting the system equations onto the orthogonal complement of the null-space of the constraints.

It is shown, in fact, that the algebraic manipulation carried out in each technique to produce a reduced system of equations simply amounts to selecting a different basis for the null-space of the constraints and its orthogonal complement.

Several practical benefits are derived from the theory presented. Foremost among the advantages of the representation is that the theory emphasizes the common structure of these problems. For example, although the methods based on Lagrange's equations may all perform the constraint force calculations outlined in step 3 above, Kane's technique and the "Kane-based methods" in Refs. 9, 10, and 31 do not explicitly represent the constraint force contributions in their minimal formulations and, consequently, cannot present a general strategy for their solution. In fact, Singh[9] advocates using a Lagrangian formulation if constraint forces are desired. On the other hand, Wampler et al.[31] suggest that a redundant formulation is questionable unless constraint forces are required. Although Wang and Huston[20] remedy this situation by bringing the constraint force contributions into evidence, the relationship of the undetermined multipliers to those appearing in a Lagrangian approach is not made clear. Furthermore, no general plan of attack is suggested for their calculation. It is shown herein that these methods all may be generalized to calculate constraint forces in a systematic fashion using a unified theory that exploits the fundamental structure of the problem.

The remainder of this paper is organized into three sections. The next section reviews Maggi's equations and their relation to projective methods in operator theory. The following section briefly outlines the relationship of the methods in Refs. 9, 10, and 17–19 to Maggi's equations. Finally, the last section summarizes some important benefits derived from the unified theory.

Maggi's Equations

Maggi's equations were first presented in 1896, and then again in 1901. Although the method is conspicuously absent from most texts in the English language, Neimark and Fufaev[21] summarize the essentials of the theory. Until quite recently, the method has not been amenable to actual calculations and primarily has been of academic interest only. However, as shall be shown in this section, the advent of digital computers now permits a wide variety of practical numerical implementations of the approach. Because of the apparent lack of familiarity with the technique, this section briefly develops the method.

Let S be a system of v particles, each of whose position $\boldsymbol{r}$ relative to an inertial frame of reference is a function of N generalized coordinates q_k, $K = 1, \ldots, N$ and the time t. Simply stated, the principle of virtual work requires that the difference in the virtual work of the applied forces and the virtual work of the inertial forces must vanish for all virtual displacements consistent with the constraints. Likewise, as a consequence of Newton's second law of motion for each particle, the virtual work of the constraint forces must vanish independently.

$$\int dm\boldsymbol{a} \cdot \delta\boldsymbol{r} = \int d\boldsymbol{f} \cdot \delta\boldsymbol{r} \tag{1a}$$

$$\int d\boldsymbol{R} \cdot \delta\boldsymbol{r} = 0 \tag{1b}$$

In the preceding expressions, $d\boldsymbol{f}$ is the resultant of all forces acting on a particle p, excluding constraint forces $d\boldsymbol{R}$, and all integrations are carried out over the entire system of particles. The quantities dm, $\boldsymbol{a}$, and $\delta\boldsymbol{r}$ are the mass, acceleration, and virtual displacement of a particle p. Because one can express the contemporaneous variation of $\boldsymbol{r}$ as a linear combination of the variations in the generalized coordinates δq_k,

$$\delta\boldsymbol{r} = \boldsymbol{e}_k \delta q_k$$

where

$$\boldsymbol{e}_k \equiv \frac{\partial \boldsymbol{r}}{\partial q_k} \tag{2}$$

Equation (1a) can be rewritten in the following familiar form:

$$\int (dm\boldsymbol{a} - d\boldsymbol{f}) \cdot \boldsymbol{e}_k \delta q_k = 0 \tag{3a}$$

or

$$\{E_k(T) - Q_k\}\delta q_k = 0 \tag{3b}$$

where

$$E_k(T) \equiv \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial T}{\partial \dot{q}_k}\right) - \frac{\partial T}{\partial q_k}$$

$$T \equiv \int \frac{1}{2} dm\boldsymbol{v} \cdot \boldsymbol{v}$$

$$Q_k \equiv \int d\boldsymbol{f} \cdot \boldsymbol{e}_k$$

and the summation convention has been used in Eqs. (2) and (3). For unconstrained problems, the variations δq_k are independent and their respective coefficients in Eqs. (3) must be identically zero for $k = 1,\ldots,N$. With respect to constrained problems, Eqs. (3) have limited direct application since δq_k are not independent.

However, it is possible to create independent virtual displacements, thus resulting in a useful set of equations similar to Eqs. (3). For holonomic systems, and a large class of nonholonomic systems, constraints on the system can be expressed in terms of D equations that are linear in the differentials of the generalized coordinates as

$$a_{lk}\, \mathrm{d}q_k + b_l\, \mathrm{d}t = 0, \qquad l = 1, \ldots, D \tag{4}$$

In order that the virtual displacements $\delta \boldsymbol{r}$ are consistent with the constraints, it is necessary that the variations in the generalized coordinates δq_k satisfy

$$a_{lk}\delta q_k = 0 \tag{5}$$

Equation (5) can be alternately represented in terms of a $D \times N$ matrix $\boldsymbol{a}$ and an N vector $\delta \boldsymbol{q} = [\delta q_1,...,\delta q_N]^T$.

$$\boldsymbol{a}\delta \boldsymbol{q} = 0 \tag{6}$$

Equations (5) and (6) now can be interpreted as requiring that the N vector $\delta \boldsymbol{q}$ lie in the null-space of $\boldsymbol{a}$, or that $\delta \boldsymbol{q}$ be orthogonal to the range of $\boldsymbol{a}^T$.

$$\delta \boldsymbol{q} \in \text{null-space } (\boldsymbol{a}) \tag{7a}$$

$$\delta \boldsymbol{q} \perp \text{range } (\boldsymbol{a}^T) \tag{7b}$$

The range of $\boldsymbol{a}^T$ is equal to the span of the columns of $\boldsymbol{a}^T$, and is consequently of dimension D if the constraints are independent. Since null-space $(\boldsymbol{a})$ and range $(\boldsymbol{a}^T)$ are orthogonal subspaces, the dimension of null-space $(\boldsymbol{a})$ is $I = N - D$. Deferring, for the moment, the discussion of their calculation, let $[\boldsymbol{A}_1,...,\boldsymbol{A}_I]$ be any basis for the null-space of $\boldsymbol{a}$ and let $[\boldsymbol{p}_1,...,\boldsymbol{p}_d]$ be any basis for the range of $\boldsymbol{a}^T$. The vector $\delta \boldsymbol{q}$ may lie anywhere within the span of $[\boldsymbol{A}_1,...,\boldsymbol{A}_I]$. In other words, it is true that

$$\delta \boldsymbol{q}_k = A_{ki}\delta\theta_i, \qquad i = 1,...,I \tag{8a}$$

$$\delta \boldsymbol{q} = \boldsymbol{A}\delta\boldsymbol{\theta} \tag{8b}$$

where $\delta\theta_i$ are arbitrary coefficients and $\boldsymbol{A} = [\boldsymbol{A}_1,...,\boldsymbol{A}_I] = [A_{ki}]$ is an $N \times (N - D)$ matrix.

Substituting Eq. (8) into Eq. (3b), a form of virtual work emerges that is well suited for constrained systems. Using the fact that each $\delta\theta_i$ is arbitrary, one obtains Maggi's equations.

$$\{E_k(T) - Q_k\}A_{ki}\delta\theta_i = 0 \tag{9a}$$

$$\{E_k(T) - Q_k\}A_{ki} = 0, \qquad i = 1,...,N - D \tag{9b}$$

In effect, Eqs. (9) reflect the fact that the virtual work due to each of the independent, admissible virtual displacements $\delta \boldsymbol{r}_i$, $i = 1,...,N - D$, obtained from Eqs. (8) and (2),

$$\delta \boldsymbol{r} = \boldsymbol{e}_k\delta q_k$$

$$\delta \boldsymbol{r}_i = \boldsymbol{e}_k A_{ki}\delta\theta_i \tag{10}$$

summed over the system, be zero.

For ease of comparison to other methods, as in Refs. 9 and 17, it is useful to express Eq. (10) in operator form as

$$\boldsymbol{A}^T\{\boldsymbol{E}(T) - \boldsymbol{Q}\} = 0 \tag{11}$$

The above $N - D$ equations, together with the D constraints in Eq. (4), comprise a system of N equations in terms of N unknowns, and are sufficient to solve for the displacements, velocities, and accelerations of the system. An illustrative account of the actual details of implementing Eqs. (4) and (11) in a numerical simulation can be found in Ref. 9.

Supposing that Eq. (11) has been solved either analytically or numerically at a particular time t, the decomposition of R^N into span $\{\boldsymbol{A}_I\}$ and span $\{\boldsymbol{p}_D\}$ is also useful because it is possible to solve for constraint forces from the base vectors $[\boldsymbol{p}_1,...\boldsymbol{p}_D]$. Because the constraint forces perform zero virtual work, the formulations until now have not explicitly contained the constraint forces $d\boldsymbol{R}$. One can always insist that

$$\boldsymbol{E}(T) - \boldsymbol{Q} - \boldsymbol{Q}^{(r)} = 0 \tag{12a}$$

$$\boldsymbol{Q}^{(r)} = [Q_1^{(r)},...,Q_N^{(r)}]^T \tag{12b}$$

where

$$Q_k^{(r)} = \int d\boldsymbol{R} \cdot \boldsymbol{e}_k$$

and $d\boldsymbol{R} \equiv$ total constraint force on particle P, so that $dm\boldsymbol{a} = d\boldsymbol{f} + d\boldsymbol{R}$. Moreover, Eq. (1b) requires that the N vector $\boldsymbol{Q}^{(r)}$ be orthogonal to $\delta \boldsymbol{q}$. In other words, the N vector $\boldsymbol{Q}^{(r)}$ must be a member of the range $(\boldsymbol{a}^T)$, the orthogonal complement of the range $(\boldsymbol{A})$. It follows that, for some D vector γ,

$$\boldsymbol{Q}^{(r)} = \boldsymbol{p}\gamma \tag{13}$$

Making use of the identity in Eq. (13), it is possible to express Eqs. (12) in either of two ways.

$$\boldsymbol{E}(T) - \boldsymbol{Q} - \boldsymbol{a}^T\boldsymbol{\lambda} = 0 \tag{14a}$$

$$\boldsymbol{E}(T) - \boldsymbol{Q} - \boldsymbol{p}\gamma = 0 \tag{14b}$$

These two equations are clearly equivalent, as the columns of $\boldsymbol{p}$ are any basis for the range of $\boldsymbol{a}^T$. The two representations coincide when $[\boldsymbol{p}_1,...,\boldsymbol{p}_D]$ are chosen to be the columns of $\boldsymbol{a}^T$. Derivations that follow are carried out in the generic basis $\{\boldsymbol{p}_D\}$, a description well suited to numerical techniques that automatically generate a basis for the range $(\boldsymbol{a})^T$ that does not coincide with the columns of $(\boldsymbol{a}^T)$. Assuming that Eq. (11) has been solved and that the original unknowns $\boldsymbol{q}$ and their derivatives $\dot{\boldsymbol{q}}$ and $\ddot{\boldsymbol{q}}$ have been reconstructed, the unknown constraint contributions are simply the unique minimizers of the N-vector norm

$$\boldsymbol{Q}^{(r)} = \boldsymbol{p}\gamma = \underset{X \in \text{ range } (\boldsymbol{p})}{\text{minimizer}} \| \boldsymbol{E}(T) - \boldsymbol{Q} - \boldsymbol{X} \| \tag{15a}$$

or

$$\gamma = \underset{\xi \in R^D}{\text{minimizer}} \| \boldsymbol{E}(T) - \boldsymbol{Q} - \boldsymbol{p}\xi \| \tag{15b}$$

Equations (11) and (15) suggest a simple "geometric" interpretation to the problem of solving constrained dynamics problems that has been widely used in applied linear algebra. Equation (11) may be interpreted as a statement of orthogonality. It requires that the N vector $\boldsymbol{E}(T) - \boldsymbol{Q}$ be perpendicular to the null-space $(\boldsymbol{a})$. In other words, the projection of $\boldsymbol{E}(T) - \boldsymbol{Q}$ onto the null space of the variational constraints is zero. Likewise, when Eqs. (15) require that $\boldsymbol{Q}^{(r)}$ is the vector that lies in the range $(\boldsymbol{a}^T)$ that is closest to $\boldsymbol{E}(T) - \boldsymbol{Q}$, it implies that $\boldsymbol{Q}^{(r)}$ is the orthogonal projection of $\boldsymbol{E}(T) - \boldsymbol{Q}$ onto range $(\boldsymbol{a}^T)$, the complementary space to null-space $(\boldsymbol{a})$:

$$\boldsymbol{Q}^{(r)} = \boldsymbol{P}_{a^T}\{\boldsymbol{E}(T) - \boldsymbol{Q}\} \tag{16}$$

These relationships are depicted symbolically in Fig. 1. Carefully note that the orthogonality statement in Eq. (11) requires that the "abstract angle" θ in Fig. 1 must be zero

$$\tan\theta = \frac{\boldsymbol{P}_A[\boldsymbol{E}(T) - \boldsymbol{Q}]}{\boldsymbol{P}_{a^T}[\boldsymbol{E}(T) - \boldsymbol{Q}]} = 0 \tag{17}$$

where $\boldsymbol{P}_A$ and $\boldsymbol{P}_{a^T}$ are the orthogonal projections onto the null-space of $\boldsymbol{a}$ and the range of $\boldsymbol{a}^T$, respectively.

The solution of Eqs. (15) and (16) is given, in theory, by the normal equations

$$\gamma = (\boldsymbol{p}^T\boldsymbol{p})^{-1}\boldsymbol{p}^T\{\boldsymbol{E}(T) - \boldsymbol{Q}\} \tag{18}$$

A strategy similar to this approach in the literature on constrained dynamics is derived via algebraic considerations in Ref. 28. However, it is neither recommended nor usually required to form the "generalized inverse" depicted in Eq. (18).[22] Instead, orthogonal factorizations are employed in solving the minimization problem in Eqs. (15). If θ is an

orthogonal transformation, i.e., $\theta^T\theta = I$, then θ is an isometry. In other words, the transformation θ is norm-preserving so that

$$\| E(T) - Q - Q^{(r)} \| = \| \theta\{E(T) - Q - Q^{(r)}\} \| \tag{19}$$

A judicious choice of θ can greatly simplify the form of the norm shown above, and lead to a straightforward solution procedure. Typical choices of θ are derived from the QR and SV decompositions.[22]

Equations (15), (16), and (19) provide a complete description of the solution for the constraint forces. When the calculations are performed via orthogonal transformations, and not the normal equations, the solution exhibits well-known stability characteristics. However, Eqs. (15) and (16) are too general to permit a detailed comparison of methods that choose different bases in A and p. An alternative description of Maggi's equations given in Ref. 23, although not computationally efficient, depicts information regarding the bases selected for p and A in a compact form. In addition, the formalism displays enough information to reconstruct the projection operator P_{a^T} explicitly. In fact, when mutually orthogonal bases are chosen for A and p, Maggi's equations generate the same expressions obtained in the least-squares solution of Eq. (19).

Papastavridis[23] generates the governing relations via Maggi's equations by first supplementing the constraint matrix a to form a full-rank $N \times N$ matrix $\hat{a}$.

$$\hat{a} = \begin{bmatrix} a \\ \hline a' \end{bmatrix} \begin{matrix} \}D \\ \}I = N - D \end{matrix} \tag{20}$$

Next, the inverse $\hat{A} = \hat{a}^{-1}$ can be calculated and partitioned in the following manner:

$$\hat{A} = [A' \quad A] \tag{21a}$$

$$\begin{bmatrix} a \\ \hline a' \end{bmatrix} [A' \quad A] = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{21b}$$

$$\hat{a}\hat{A} = 1 \tag{22}$$

By inspection, it is clear that the columns of a^T and A' are reciprocal bases for the range (a^T). Likewise, if the columns of a'^T and A span the same space, they are dual bases for the null-space (a). By multiplying Eq. (12a) by $\hat{A}^T$, one obtains the governing relations

$$(A')^T\{E(T) - Q\} = \lambda \tag{23a}$$

$$(A)^T\{E(T) - Q\} = 0 \tag{23b}$$

Upon comparing Eqs. (23) and (16), one can see that the projection onto the range (a^T) is easily constructed from the dual basis $(A')^T$ when a^T and A' span the same space.

$$P_{a^T} = a^T(A')^T \tag{24}$$

The precise relationship defining the dual basis $[A'_1,...,A'_D]$ of $[a_1^T,...,a_D^T]$ can be extracted from Eq. (21), and is simply

$$A'^T a^T = aA' = I \tag{25}$$

But if we choose $p = a^T$ in Eq. (18), it is clear that $(A')^T$ is equal to the coefficient matrix $(aa^T)^{-1}a$ since there is exactly one dual basis corresponding to $[a_1^T,...,a_D^T]$ and

$$\{(aa^T)^{-1}a\}a^T = I = (A')^T a^T \tag{26}$$

Thus, in this case, the normal equation's solution reduces to Eqs. (23).

In cases where the dual bases comprising the matrices $\hat{a}$ and A can be derived analytically, the notation in Ref. 23 is concise in its representation of the solution. A knowledge of $\hat{a}$ and $\hat{A}$ conveys both the specific basis chosen to reduce the constrained system to minimal order, as well as the projection operator selected to calculate constraint forces. It will be shown presently that the theory is sufficiently detailed to provide an excellent means of tabulating computational alternatives that have appeared in recent literature.

Related Methods

Kane's Method

Kane's method is a collection of steps, which, when followed, can yield the smallest possible set of governing equations for a constrained dynamical system. It will now be shown that Kane's method can be considered as an analytical procedure for choosing the null-space basis $[A_1,...,A_I]$ in Eq. (11). The following steps summarize the approach:

1) Choose N generalized coordinates q_k, $k = 1,...,N$, sufficient to represent every configuration of the system. These coordinates may be redundant through choice, or will exceed the number of degrees of freedom of the system when the system is constrained.

2) Choose N quantities U_k, $k = 1,...,N$, the "generalized speeds," defined in terms of the generalized holonomic velocities $\dot{q}$ according to

$$U_k = Y_{kl}\dot{q}_l + Z_k \tag{27a}$$

or as

$$U = Y\dot{q} + Z \tag{27b}$$

This definition is valid only if one can solve for each $\dot{q}_k$ uniquely in terms of U_k. That is, the matrix Y must be invertible. If $Y^{-1} \equiv y$, one has

$$\dot{q}_l = y_{lk}U_k + z_l \tag{28a}$$

or

$$\dot{q} = yU + z \tag{28b}$$

3) Express all constraints on the system in terms of D equations of the form

$$\begin{aligned} U_d &= W_{di}U_i - \phi_d \\ [I \quad -W]U + \phi &= 0 \\ cU + \phi &= 0 \end{aligned} \tag{29}$$

These constraints arise either because the system is nonholonomic or by differentiating holonomic constraints due to redundant coordinates q_k. Another useful representation of these constraints is achieved by partioning the N vector U into an $I = (N - D)$ vector of "independent" generalized speeds U^I and a D vector of "dependent" generalized speeds U^D.

$$\begin{aligned} U &= \begin{bmatrix} U^D \\ U^I \end{bmatrix} = \begin{bmatrix} W \\ I \end{bmatrix} U^I + \begin{bmatrix} \phi \\ 0 \end{bmatrix} \\ &= CU^I + \theta \end{aligned} \tag{30}$$

The matrix W is $D \times I$, the matrix $= C$ is $N \times I$, and I is an $I \times I$ identity matrix. Note that $cC = 0$, just as $aA = 0$ in Eqs. (21).

4) By virtue of the definitions in Eqs. (28) and (30), the velocity of every particle in the system can be expressed as

$$v = v_i U_{i+D} + v_t, \qquad i = 1,...,I \tag{31}$$

The preceding summation only includes elements of the independent generalized speeds U^I. In the absence of constraints,

the summation runs from 1 to N. The quantities $\boldsymbol{v}_i$ are defined to be the "partial velocities" of particle p.

5) Lastly, Kane postulates the governing dynamical equations

$$F_i + F_i^* = 0, \qquad i = 1,...,I \tag{32}$$

where F_i and F_i^* are defined via integration over all of the particles.

$$F_i = \int d\boldsymbol{f} \cdot \boldsymbol{v}_i \tag{33a}$$

$$F_i^* = -\int d\boldsymbol{m}\boldsymbol{a} \cdot \boldsymbol{v}_i \tag{33b}$$

Although Kane's terminology is quite different, his method can be derived in terms of the more common virtual work expressions of the preceding section. If Eqs. (28) and (30) are substituted into

$$\boldsymbol{v} = \boldsymbol{e}_k \dot{q}_k + \frac{\partial \boldsymbol{r}}{\partial t} = \boldsymbol{e}_k (y_{k1} U_l + z_k) + \frac{\partial \boldsymbol{r}}{\partial t}$$

$$= \boldsymbol{e}_k y_{k1} C_{1i} U_{i+D} + v_t \tag{34}$$

then the partial velocities may be obtained by inspection as

$$\boldsymbol{v}_i = \boldsymbol{e}_k y_{kl} C_{li} \tag{35}$$

Upon inserting the preceding partial velocities into Eq. (32) and rearranging the summations, Kane's governing equations are just

$$\int (d\boldsymbol{m}\boldsymbol{a} - d\boldsymbol{f}) \boldsymbol{e}_k y_{kl} C_{li} = 0 \tag{36}$$

or

$$\{E_k(T) - Q_k\} y_{kl} C_{li} = 0$$

or

$$\boldsymbol{C}^T \boldsymbol{y}^T \{\boldsymbol{E}(T) - \boldsymbol{Q}\} = 0$$

The similiarity between Eqs. (36) and (9) is immediately apparent. To prove that Kane's method may be considered a null-space generating method, it only remains to show that the range ($\boldsymbol{yC}$) is indeed the null-space of the constraints. If the constraints are given in Kane's notation as in Eq. (29), the corresponding constraints in the notation of the preceding section are

$$\boldsymbol{cU} + \boldsymbol{\phi} = 0 \tag{37a}$$

$$\boldsymbol{cY}\dot{\boldsymbol{q}} + (\boldsymbol{cZ} + \boldsymbol{\phi}) = 0 \tag{37b}$$

so that

$$\boldsymbol{a} = \boldsymbol{cY} = [\boldsymbol{I} \;\; -\boldsymbol{W}]\boldsymbol{Y} \tag{38}$$

But the columns of the matrix $\boldsymbol{A} = \boldsymbol{yC}$ clearly constitute a basis for the null-space of the variational constraints since

$$\boldsymbol{aA} = \boldsymbol{cYyC} = \boldsymbol{cC} = 0 \tag{39}$$

Alternatively, the analytic nature of this formulation enables the solution procedure to be represented by the method described in Ref. 23. In this case, by combining Eqs. (29) and (36), one obtains the dual bases that may be used to calculate the reduced equations as well as the constraint forces in Eqs. (23). These bases are depicted in Table 1. It should be pointed out, however, that it is not meant to suggest in Table 1 that the matrices $\boldsymbol{y}$ and $\boldsymbol{Y}$ need to be formed in a practical implementation of Kane's method or its related variations. As will be illustrated, the dual bases can be utilized in this case without forming $\boldsymbol{y}$ or $\boldsymbol{Y}$.

Coordinate Partitioning

Generalized coordinate partitioning[17] is a computational method that uses Gaussian elimination with full pivoting on the $D \times N$ constraint matrix $\boldsymbol{a}$ to select a subset of $I = N - D$ independent generalized velocities $\dot{\boldsymbol{q}}^I$ and D dependent velocities $\dot{\boldsymbol{q}}^D$. If $\boldsymbol{a}$ has full row rank, then it is always possible to partition $\boldsymbol{a}$ into $[\boldsymbol{a}^D \;\; \boldsymbol{a}^I]$ such that $\boldsymbol{a}^D$ is a $D \times D$ nonsingular matrix.

$$\boldsymbol{a}\dot{\boldsymbol{q}} + \boldsymbol{b} = [\boldsymbol{a}^D \;\; \boldsymbol{a}^I] \begin{bmatrix} \dot{\boldsymbol{q}}^D \\ \dot{\boldsymbol{q}}^I \end{bmatrix} + \boldsymbol{b} \tag{40}$$

$$\boldsymbol{A} = \begin{bmatrix} -(\boldsymbol{a}^D)^{-1}\boldsymbol{a}^I \\ \boldsymbol{I} \end{bmatrix} \tag{41}$$

With this choice of independent velocities $\dot{\boldsymbol{q}}^I$, the columns of the matrix $\boldsymbol{A}$ are a basis for the null-space of the constraints. Furthermore, premultiplication of Lagrange's equations by $\boldsymbol{A}^T$ as in Eq. (11) yields precisely the governing equations obtained by Wehage and Haug in Eq. (26) of Ref. 17. As in Kane's method, the analytical nature of this strategy permits a closed-form expression of the dual bases in Eqs. (21), which

Table 1 Example bases

Reference	Decomposition	$\hat{\boldsymbol{a}}$	$\hat{\boldsymbol{A}}$
Wehage 1982	Gaussian elimination	$\left[\begin{array}{c\|c} \boldsymbol{a}^D & \boldsymbol{a}^I \\ \hline 0 & \boldsymbol{I} \end{array}\right]$	$\left[\begin{array}{c\|c} (\boldsymbol{a}^D)^{-1} & -(\boldsymbol{a}^D)^{-1}\boldsymbol{a}^I \\ 0 & \boldsymbol{I} \end{array}\right]$
Mani 1984	Singular value	$\left[\begin{array}{c} \boldsymbol{a} \\ \hline \boldsymbol{U}_2^T \end{array}\right]$	$\left[\begin{array}{c\|c} \boldsymbol{U}_1 \left[\frac{1}{\sigma}\right] \boldsymbol{V}^T & \boldsymbol{U}_2 \end{array}\right]$
Kim 1986	QR decomposition $\boldsymbol{a}^T = \boldsymbol{QR}$	$\left[\begin{array}{c} \boldsymbol{a} \\ \hline \boldsymbol{Q}_2^T \end{array}\right]$	$\left[\begin{array}{c\|c} \boldsymbol{Q}_1(\boldsymbol{aQ}_1)^{-1} & (\boldsymbol{I} - \boldsymbol{Q}_1(\boldsymbol{aQ}_1)^{-1}\boldsymbol{a})\boldsymbol{Q}_2 \end{array}\right]$
Singh 1985	SV decomposition $\boldsymbol{c}^T = \hat{\boldsymbol{U}}\hat{\boldsymbol{\Sigma}}\hat{\boldsymbol{V}}$	$\left[\begin{array}{c} \boldsymbol{c} \\ \hline \hat{\boldsymbol{U}}_2^T \end{array}\right] \boldsymbol{Y}$	$\boldsymbol{y}\left[\begin{array}{c\|c} \hat{\boldsymbol{U}}_1 \left[\frac{1}{\sigma}\right] \hat{\boldsymbol{V}}^T & \hat{\boldsymbol{U}}_2 \end{array}\right]$
Kane/Huston 1987		$\left[\begin{array}{c\|c} \boldsymbol{I} & -\boldsymbol{W} \\ \hline 0 & \boldsymbol{I} \end{array}\right] \boldsymbol{Y}$	$\boldsymbol{y}\left[\begin{array}{c\|c} \boldsymbol{I} & \boldsymbol{W} \\ 0 & \boldsymbol{I} \end{array}\right]$

are displayed in Table 1. It should also be noted that premultiplication by $(A')^T$ for the method by Wehage and Haug in Table 1 generates identical expressions for the Lagrange multipliers in Eq. (24) of Ref. 17.

Mani's Method

Although Gaussian elimination has been used quite effectively in some simulations utilizing coordinate partitioning,[27] one deficiency in the method has been noted in Ref. 18. The choice of a fixed set of independent coordinates may lead to poorly conditioned matrices that must be factored. On inspecting the null-space matrix A in Eq. (41), one can observe that the columns of A span the null-space of $\boldsymbol{a}$ only as long as $(\boldsymbol{a}^D)^{-1}$ exists. Since the matrix $\boldsymbol{a} = [\boldsymbol{a}^D \ \boldsymbol{a}^I]$ is time varying, in general, one cannot guarantee that this inverse is well defined for the entire time span of interest.

Mani addresses this problem by utilizing the singular-value decomposition of $\boldsymbol{a}^T$,

$$\boldsymbol{a}^T = [U_1 \ U_2]\Sigma V^T \tag{42}$$

where

$$U = [U_1 \ U_2] \quad \text{is an } N \times N \text{ orthogonal matrix} \tag{43a}$$

$$\Sigma = \begin{bmatrix} \sigma \\ 0 \end{bmatrix} \quad \text{is an } N \times D \text{ diagonal matrix} \tag{43b}$$

and V is a $D \times D$ orthogonal matrix. The diagonal terms σ are the singular values of the constraint matrix. In terms of the theory presented earlier, the integration process carried out by Mani is equivalent to choosing the dual bases as depicted in Table 1. It should be noted that the actual algorithm outlined in Ref. 18 is quite complicated in that the singular-value decomposition is carried out on an "as needed" basis at certain time steps, and the constraint violation is corrected by employing Newton-Raphson iteration.

Null-space Updating

A more recent technique is based on the QR decomposition of the constraint matrix $\boldsymbol{a}$.[19] In this decomposition, the $N \times D$ matrix $\boldsymbol{a}^T$ is expressed as the product of an $N \times N$ orthogonal matrix $\boldsymbol{Q}$ and a $D \times N$ upper-triangular matrix $\boldsymbol{R}$. It is a characteristic of the decomposition that the matrix $\boldsymbol{Q}$ can be partitioned into two matrices $\boldsymbol{Q}_1$ and $\boldsymbol{Q}_2$, where the columns of $\boldsymbol{Q}_1$ are a basis of the range of $\boldsymbol{a}^T$ and the columns of $\boldsymbol{Q}_2$ are a basis for the null-space of $\boldsymbol{a}$,

$$\boldsymbol{a}^T = \boldsymbol{QR} = [\boldsymbol{Q}_1 \quad \boldsymbol{Q}_2] \begin{bmatrix} R \\ 0 \end{bmatrix} \tag{44}$$

where $\boldsymbol{Q}$ is an $N \times N$ orthogonal matrix and $\boldsymbol{R}$ an $N \times D$ upper-triangular matrix.

In Ref. 19, $\boldsymbol{Q}_1$ and $\boldsymbol{Q}_2$ are used to create two other matrices $\hat{\boldsymbol{Q}}_1$ and $\hat{\boldsymbol{Q}}_2$ which, although not orthogonal, still satisfy Maggi's equations.

$$\hat{\boldsymbol{Q}}_1 = \boldsymbol{Q}_1(\boldsymbol{aQ}_1)^{-1} \tag{45a}$$

$$\hat{\boldsymbol{Q}}_2 = [I - \boldsymbol{Q}_1(\boldsymbol{aQ}_1)^{-1}\boldsymbol{a}]\boldsymbol{Q}_2 \tag{45b}$$

Choosing $\hat{\boldsymbol{Q}}_2$ as the matrix A and premultiplying Lagrange's equations by A^T again produces the reduced governing equation in Eq. (33) of Ref. 19.

The calculation of Lagrange multipliers in Ref. 19 is also a special case of the general method in the preceding section of this paper. Choosing the columns of $\hat{\boldsymbol{Q}}_1$ as the basis of the range of $\boldsymbol{a}^T$, Eq. (18) allows one to calculate the Lagrange multipliers referred to this basis.

$$\gamma = (\hat{\boldsymbol{Q}}_1^T\hat{\boldsymbol{Q}})_1^{-1}\hat{\boldsymbol{Q}}_1^T\{\boldsymbol{E}(T) - \boldsymbol{Q}\}$$

$$= (\boldsymbol{aa}^T)\hat{\boldsymbol{Q}}_1^T\{\boldsymbol{E}(T) - \boldsymbol{Q}\} \tag{46}$$

One can now change basis from γ to λ by the normal equations $\lambda = (\boldsymbol{aa}^T)^{-1}\boldsymbol{a}\hat{\boldsymbol{Q}}_1\gamma$. Making this replacement above gives the equations used to calculate the Lagrange multipliers in Ref. 19.

$$\lambda = \hat{\boldsymbol{Q}}_1^T\{\boldsymbol{E}(T) - \boldsymbol{Q}\} \tag{47}$$

The dual bases appropriate for this method are shown in Table 1. Again, Eq. (47) can be derived in short order by simply extracting the dual basis A' from Table 1 for Kim's method.

Singh/Huston's Method

As another example of computational applications, Singh and Likins[9] present a modification of Kane's method based on singular-value decomposition that is similar to Mani's work. In this approach, Kane's equations are first generated for the unconstrained system, i.e., for $\boldsymbol{C} = \boldsymbol{I}$ in Eq. (25). As in Mani's method, the singular-value decomposition is

$$\boldsymbol{c}^T = \hat{\boldsymbol{U}}\hat{\Sigma}\hat{\boldsymbol{V}}^T \tag{48}$$

where $\hat{\boldsymbol{U}}$, $\hat{\Sigma}$, and $\hat{\boldsymbol{V}}$ are defined in the manner analogous to that shown in Eq. (42), is then used to obtain a basis $[\hat{\boldsymbol{U}}_2]$ for the null-space of the coefficient matrix $\boldsymbol{c}$ in Eq. (29). It is subsequently shown that the reduced governing equations are

$$\hat{\boldsymbol{U}}_2^T\{\boldsymbol{F} + \boldsymbol{F}^*\} = 0 \tag{49}$$

Comparing Eqs. (9), (12), and (26) with the preceding, one can alternatively express the equations derived by Singh and Likins as

$$\hat{\boldsymbol{U}}_2^T\boldsymbol{y}^T\{\boldsymbol{E}(T) - \boldsymbol{Q} - \boldsymbol{a}^T\boldsymbol{\lambda}\} = 0 \tag{50}$$

These equations are identical to those derived in Ref. 20 for a very specific choice of basis for the null-space of the constraints. Since the columns of $\hat{\boldsymbol{U}}_2$ are a basis for the null-space of $\boldsymbol{c}$, it is clear that $\boldsymbol{A} = \boldsymbol{y}\hat{\boldsymbol{U}}_2$ is a basis for the null-space of $\boldsymbol{a}$. Consequently, it is apparent that this method simply chooses a different basis for the null-space of $\boldsymbol{a}$ in the method of virtual work. As with all the previous methods, this approach also may be succinctly represented in terms of the dual bases it uses for the null-space of the variational constraints and its orthogonal complement. These choices are found in Table 1.

Advantages of the Unified Theory

Several benefits can be derived from the theory discussed in the section regarding Maggi's equations. In one sense, all of the advantages of the approach stem from the fact that the description given enhances one's ability to compare and contrast specific techniques. For instance, in this section, it is shown that the features of Lagrange's equations that make constraint force calculation possible may be found in other reduced formulations, if they are perceived in a "unified" context. It is also demonstrated that certain ill-conditioning noted in coordinate partitioning methods is predicted by the unified theory, and has been found, in some implementations of Kane's method. As a final example, it is illustrated that the method provides a foundation for numerical methods suitable for a wider class of constraints.

Constraint Force Calculation

One benefit of the general null-space decomposition theory presented earlier is that it enables calculation of Lagrange multipliers from Kane's equations after the reduced system of equations has been solved. Neither Kane's method[25] nor its recent modifications[9,10,31] have suggested an equivalent means of calculating the eliminated constraint forces. Furthermore, the development that follows extends the work in Ref. 20 in two important respects. Although the derivation in Ref. 20 is limited to rigid bodies, no such assumption is made in this

paper. Second, although Ref. 20 establishes a form for Kane's equations that retains multiplicative "undetermined multipliers," the relationship between these terms and the multipliers in a Lagrangian formulation is not explored.

From Eqs. (14) and (36), Kane's equations for the "released" system, i.e., with $C = I$, are

$$y^T\{E(T) - Q - a^T\lambda\} = 0 \tag{51a}$$

$$F + F^* - y^T a^T \lambda = 0 \tag{51b}$$

As a consequence, the constraint force contribution can be calculated from

$$y^T a^T \lambda = P_{y^T a^T}(F + F^*) \tag{52}$$

In this equation, F and F^* are the generalized active forces and generalized inertia forces for the unconstrained system, i.e., with $C = I$. However, if one is given the constraints in terms of the generalized speeds, as shown in Eq. (29), the solution can be expressed exclusively in terms of matrices available in Kane's formulation as

$$\lambda = \min_{\xi \in R^D} \| F + F^* - c^T \xi \| \tag{53a}$$

$$c^T \lambda = P_{c^T}(F + F^*) \tag{53b}$$

As noted earlier, specific forms for the projection $P_{c^T} \equiv$ projection onto the range of c^T can be derived from the normal equations, or from the dual basis for Kane's method in Table 1.

Following derivations along the same lines, Lagrange multipliers also are readily calculated in Singh's approach. It is still true that

$$\lambda = \min_{\xi \in R^D} \| F + F^* - c^T \xi \| \tag{54}$$

However, in this method, the singular-value decomposition of c has been calculated already. Using the fact that an orthogonal transformation is an isometry, the solution of Eq. (54) can be calculated via standard techniques in numerical methods.[22]

$$\lambda = \hat{V}[1/\sigma]\hat{U}_1^T\{F + F^*\} \tag{55}$$

It is important to note that all of the information required to evaluate the constraint forces is readily available and no further matrix decomposition need be performed. This same result can be derived simply by inspecting the dual basis for Singh's method in Table 1. Equations (53) and (55) illustrate the fact mentioned earlier that the dual bases shown in Table 1 can be utilized in practical implementations without explicitly forming the matrices y and y.

Explanation of Singularities

A second advantage of the unified theory may be attributed to the ease with which the class of methods can be compared. In this example, Singh[9] noted certain "numerical instabilities" in a general implementation of Kane's method, but offer no quantitative explanation for their origin. By comparing the basis implicitly chosen in Kane's method to that selected in the method of Ref. 17, however, the nature of the singularities is brought to light.

In Kane's method, it is assumed that the constraint matrix c has the form

$$c = [I \quad -W] \tag{56}$$

This requirement is equivalent to stipulating that one can partition a constraint matrix $c = [c^D \,|\, c^I]$ so that c^D is invertible, whence

$$cU + \phi = 0 \tag{57a}$$

$$[c^D \,|\, c^I]U + \phi = 0 \tag{57b}$$

$$[I \,|\, (c^D)^{-1}c^I]U + (c^D)^{-1}\phi = 0 \tag{57c}$$

Consequently, $W = -(c^D)^{-1}c^I$ and the basis of the null-space of the constraints is just

$$A_{\text{Kane}} = y \begin{bmatrix} -(c^D)^{-1}c^I \\ I \end{bmatrix} \tag{58}$$

Recalling for a moment the basis utilized in Ref. 17,

$$A_{\text{Wehage}} = \begin{bmatrix} -(a^D)^{-1}a^I \\ I \end{bmatrix} \tag{59}$$

the remarkable similarity in form in Eqs. (58) and (59) is immediately apparent. As noted earlier, Ref. 18 explains the numerical difficulties associated with Wehage's method in terms of the poor conditioning of $(a^D)^{-1}$. The preceding clarifies that a general formulation of Kane's method may suffer the same fate if the condition of $(c^D)^{-1}$ becomes poor. The fact has been documented elsewhere (see, for example, Ref. 31).

Nonlinear Nonholonomic Constraints

A third advantage derives from one's ability to extend the theory easily to (first-order) nonlinear nonholonomic constraints, i.e., nonintegrable constraints of the form

$$F_i(q, \dot{q}, t) = 0, \qquad i = 1, \ldots, D \tag{60}$$

Carefully note that these constraints differ from those shown in Eqs. (4) and (29), in that they are not required to be linear in the generalized velocities.

The *physical* and *analytical* aspects of these constraints have already been examined over the past 75 years (see, for example, Refs. 29 and 30 and references cited therein). As of yet, however, very little research on their *computational* treatment has appeared on the open literature. Such an extension is, however, straightforward, in principle, within the theory described herein. Following the derivations carried out earlier in this paper and the developments outlined in Refs. 29 and 30, one need only replace the constraint matrix a from Eq. (4) by the Jacobian matrix of partial derivatives

$$a_{ik} = \frac{\partial F_i}{\partial \dot{q}_k} \tag{61}$$

With this new definition of the constraint matrix a, one can follow the same computational steps outlined in Eqs. (5–16) to obtain the following governing equations:

$$A^T\{E(T) - Q\} = 0 \tag{62a}$$

$$Q^{(r)} = a^T\lambda = P_{a^T}[E(T) - Q] \tag{62b}$$

where $aA = 0$.

The authors hope to examine in detail this nontrivial area in future publications.

Hybrid Methods

Finally, the theory presented herein suggests interesting "hybrid" methods that can be obtained from combining methods shown in Table 1. For example, the method of null-space updating described in Ref. 19 need not be limited only to Lagrangian formulations. By inspection of Table 1, it is clear that a null-space updating formulation of Kane's equations is obtained by choosing the dual bases

$$\hat{a} = \begin{bmatrix} c \\ \hline Q_2^T \end{bmatrix} Y \tag{63}$$

and

$$\hat{A} = y[\tilde{Q}_1(c\tilde{Q}_1)^{-1}(I - \tilde{Q}_1(c\tilde{Q}_1)^{-1}c)\tilde{Q}_2] \tag{64}$$

where

$$c = \tilde{Q}\tilde{R} = [\tilde{Q}_1\tilde{Q}_2]\tilde{R} \tag{65}$$

is the QR decomposition of the matrix c. Of course, as mentioned earlier, a practical implementation of Eqs. (63–65) does not require actual formation and calculation of Y and y.

As another example, it seems that Kim[19] is well aware that evaluating the bases at each time step

$$\hat{a} = \begin{bmatrix} a \\ \hline Q_2^T \end{bmatrix} \quad \text{and} \quad \hat{A} = [Q_1(aQ_1)^{-1}Q_2] \tag{66}$$

are perfectly reasonable choices of dual bases, although perhaps not as computationally efficient as null-space updating. The corresponding bases for a Kane-based algorithm can then be extracted from

$$\hat{a} = \begin{bmatrix} c \\ \hline \tilde{Q}_2^T \end{bmatrix} Y \quad \text{and} \quad \tilde{A} = y[\tilde{Q}_1(c\tilde{Q}_1)^{-1}\tilde{Q}_2] \tag{67}$$

Conclusions

The difficulty in systematically accommodating a wide variety of constraints in simulations of system dynamics has given rise to a variety of numerical methods that eliminate the constraints automatically. A thorough review of these methods has been presented in this paper. By using Maggi's equations and a projective interpretation from numerical analysis, the equivalence of these methods has been proven. In fact, it is shown that each method differs only in its selection of a basis for the null-space of the variational constraints and its orthogonal complement. For each method considered, the appropriate bases have been derived explicitly, and provide a convenient means of evaluating and comparing the individual methods.

The theory presented also suggests generalizations to some of the methods under consideration. It has been shown that those methods that currently do not calculate constraint forces may do so—often with little additional work—by utilizing the projection onto the orthogonal complement of the null-space of the variational constraints.

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