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SYMPLECTIC METHODS FOR CONSERVATIVE MULTIBODY SYSTEMS

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ABSTRACT. Besides preserving the energy, the flow of a conservative multibody system possesses important geometric (*symplectic*) invariants. Symplectic discretization schemes that mimic the corresponding feature of the true flow have been shown to be effective alternatives to standard methods for many conservative problems. For systems of rigid bodies, the development of such schemes can be complicated or costly to implement, depending on the choice of problem formulation. In this article, we demonstrate that a special formulation of the multibody system (based on a particle representation) together with a symplectic discretization for constrained problems borrowed from molecular dynamics offers an efficient alternative to standard approaches. Numerical experiments illustrating this approach are described.

1. INTRODUCTION

In this paper, we consider efficient numerical integrators for systems of rigid bodies interconnected by various types of mechanical joints and subject to the forces of nature. Important applications include "dynamic models" [17] of undamped and mildly damped mechanisms and manipulators [38, 23].

Symplectic schemes have been found to be effective for diverse problems such as astronomical many-body systems [36] and molecular dynamics simulations [22]. We are particularly interested in two aspects of symplectic integrators: first, all other things being equal, they appear to provide realistic simulations on longer time intervals than nonsymplectic schemes, and second, the condition for being symplectic is connected to other important properties such as norm-preservation and angular momentum-preservation. All symplectic schemes are necessarily volume preserving. In some cases, as in our example of spinning top (Section 6), conservation of integrals proves critical to successful numerical simulation.

In standard treatments of classical mechanics [2], a rigid body is viewed as a collection of point masses with fixed interparticle distances. The natural description of the body as a system of cartesian coordinates for the locations of the point masses is typically replaced by a minimal coordinate representation, for example based on the introduction of quaternions. The idea of using cartesian ("natural") coordinates for the simulation of multibody systems was first discussed by [37, 6], with the aim of improving efficiency in real-time multibody simulation.

Our approach is based on a procedure we term *particulation* in which a given rigid body is replaced by a system of point particles while preserving its dynamical properties. Some tools for constructing such particle representations were first presented by Edward Routh in his classic 1905 treatise [32]. We describe a somewhat generalized version of his procedure, discuss the imposition of constraints, and show an equivalence under discretization of two particulations of the same body. Our technique is also related to the "cartesian approach" [10, 27] of modeling rigid polyatomic molecules. The principle contribution of this article is the recognition that the particle representation offers a simple, efficient means to symplectic discretization of rigid body dynamics.

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We have also applied these techniques to treat systems of rigid bodies, showing explicitly how to handle forces of interaction and how various types of mechanical joints can be effectively modelled by quadratic length-type constraints. We touch on this briefly here, but more details can be found in [4].

To discretize the equations of motion, we use the RATTLE [1] variant of the SHAKE [34] discretization from constrained molecular dynamics, an efficient semi-explicit staggered method for the constrained equations that is both symplectic and angular momentum preserving. As an alternative to using the standard Gauss-Seidel iteration of [34] to solve the discretized equations, we have indicated in [5], in the context of molecular dynamics integration, how sparse matrix techniques can be applied to minimize the required computation.

For purposes of demonstration and evaluation, the techniques are implemented in an easy to use Matlab ToolBox **MDLab** which can be employed to study the particle formulation and various discretization schemes. We describe several experiments, including a spinning top and a seven bar chain.

An alternative to our elementary formulation in cartesian coordinates would be to develop algorithms for the motion of a rigid body formulated in $\mathbf{R}^3 \times SO(3)$ that are symplectic and/or integral conserving. This approach is discussed elsewhere in this volume (see, e.g. the article by Lewis and Simo), as well as in recent work of MacLachlan and Scovel [24]. Also in this volume, Reich discusses variations on the particulation approach and some connections between the two points of view.

2. Hamiltonian Systems, Symplectic Discretization, and Multibody Dynamics

A conservative system is one which posesses an energy functional H which is constant along trajectories. Hamilton's equations of motion are then

$$\begin{aligned} \dot{q} &= \frac{\partial H}{\partial p} \\ \dot{p} &= -\frac{\partial H}{\partial q} \end{aligned}$$

or,

$$\frac{d}{dt}\begin{pmatrix} q \\ p \end{pmatrix} = J\nabla H, \qquad J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}.$$

We can define the *flow map*[1] $\Phi_H^t : \mathbf{R}^{2n} \to \mathbf{R}^{2n}$ by

$$\frac{d}{dt}\Phi_H^t = J(\nabla H) \circ \Phi_H^t$$

The solution to the Hamiltonian system with initial values $(q(t_0), p(t_0)) = (q_0, p_0)$ is just

$$\begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = \Phi_H^t \begin{pmatrix} q_0 \\ p_0 \end{pmatrix}.$$

The flow of a Hamiltonian system preserves the 2-form $dq \wedge dp = \sum dq^i \wedge dp^i$, the outer product of differentials. A mapping with this strong property is said to be *canonical* or *symplectic*. It can be shown that a necessary and sufficient condition for a mapping Φ to be symplectic is that the Jacobian Φ' satisfy

$$(\Phi')^T J \Phi' = J.$$

We will be interested in one-step discretizations i.e. methods which can be expressed in the form

$$\begin{pmatrix} q_{n+1} \\ p_{n+1} \end{pmatrix} = \Psi^h \begin{pmatrix} q_n \\ p_n \end{pmatrix}$$

for some mapping $\Psi^h : \mathbf{R}^{2n} \to \mathbf{R}^{2n}$. A symplectic discretization is one that preserves the same canonical 2-form: $dq_{n+1} \wedge dp_{n+1} = dq_n \wedge dp_n$. The "fundamental theorem" of symplectic discretizations is simply stated as follows: if the solution to a Hamiltonian system is approximated by a certain symplectic scheme with a single stepsize h, then there exists a formal series in powers of h for a perturbed Hamiltonian $\bar{H}(h)$ such that excluding rounding error, the flow map corresponding to $\bar{H}(h)$, $\Phi_{\bar{H}(h)}$, satisfies $\Phi_{\bar{H}(h)}^h = \Psi^h$ [39, 18]. The convergence of the formal series only occurs in a weak sense in the limit as $h \to 0$. Although little work has been undertaken on practical interpretations and limitations of this theoretical result, it

[1] We are using a superscript lowercase "t" to indicate time here, whereas transpose will be signified by a superscript uppercase "T".

does appear to imply a remarkable global stability of the energy for long term symplectic integrations, and this behavior is one reason for the recent surge in interest in symplectic schemes.

Another motivation for looking at symplectic schemes is that the strong conditions imposed by requiring symplecticity often also guarantee conservation of various integrals of the flow. A general discussion of symplectic discretization schemes can be found in [35].

2.1. Constrained Multibody Systems. In typical cases, the state of the system will be restricted to a submanifold of $\mathbf{R}^{2N}$ by algebraic constraints. In this paper, we will assume that our system only posesses holonomic position constraints of the form $g(q) = 0$, where $g : \mathbf{R}^N \to \mathbf{R}^m$ is a smooth map with a full rank Jacobian in the neighborhood of its zero-set $g^{-1}(0)$. One can then consider the modified Hamiltonian $\hat{H} = H + \lambda^T g$ augmented by multipliers λ determined by the constraints:

$$\begin{aligned} \dot{q} &= \frac{\partial \hat{H}}{\partial p} = \frac{\partial H}{\partial p} \\ \dot{p} &= -\frac{\partial \hat{H}}{\partial q} = -\frac{\partial H}{\partial q} - \frac{\partial g}{\partial q}^T \lambda \\ 0 &= g(q). \end{aligned}$$

The many-body Hamiltonian H has the form $H(p,q) = \frac{1}{2} p^T M^{-1} p + V(q)$ and arises when a system of point particles moves in potential V. M is a diagonal matrix containing the masses of the particles. If constraints are placed on positions of the particles only, then we arrive at Hamiltonian equations of the form

$$\dot{q} = M^{-1} p \tag{1}$$

$$\dot{p} = -\nabla_q V - g'(q)^T \lambda \tag{2}$$

$$0 = g(q). \tag{3}$$

In the traditional approach [26], the equations of motion of a system of rigid bodies are treated by introduction of some generalized coordinate system. Using the positions of the centers of mass and the three Euler angles describing the rotation of each body about its center of mass to parameterize the motion results in canonical equations with the augmented (constrained) Hamiltonian

$$H = \frac{1}{2} p^T \bar{M}^{-1} p + \tilde{V}(q) + \tilde{g}(q)^T \lambda \tag{4}$$

where p, q are the new coordinates involving positions of each body and orientation in space, $\bar{M} = \bar{M}(q) = \mathrm{diag}(M, \tilde{I})$, with M a diagonal mass matrix and $\tilde{I}$ the inertial tensor which is a function of the Euler angles, and $\tilde{V}$ is V expressed in the new coordinate system. This formulation may have singular points (of $\tilde{I}$) which make it unsuitable for general numerical investigation [12]. The problem can be overcome with another choice of the generalized coordinates [12, 29], but a similar form of the equations of motion is obtained if other typical choices are employed [7]. Importantly, the mass matrix $\bar{M}$ is now position-dependent, unlike in the case of a system of particles in cartesian coordinates, and the Hamiltonian has become nonseparable.

2.2. Discretization of the Constrained Equations of Motion. The equations (1)-(3) and the corresponding equations on the Hamiltonian (4) are systems of differential-algebraic equations (DAEs). Various techniques exist for handling these sorts of equations. For example, a traditional approach is to parameterize the constraint manifold to obtain ODE systems in local charts (e.g. using some automatic technique such as coordinate partitioning [33]). This technique can be performed while also preserving the canonical structure, and results in Hamiltonian systems of ODEs in the parameters which can then be discretized by symplectic schemes. However, as pointed out in [21], these techniques, although symplectic, do not result in a numerical solution that is the iteration of one and the same symplectic map, hence the fundamental theorem of symplectic discretization cannot be applied. Numerical experiments show a substantial drift in energy.

An alternative approach is to develop an extension of the vector field from the constraint manifold into the space $\mathbf{R}^{2N}$ which preserves the constraints as invariants of the flow and which reduces along the constraints to the original problem. This can be done via constraint differentiation, as discussed in [28, 11]. At first glance this technique appears to introduce some additional complexity over other formulations, while also typically producing a "drift" from the constraint manifold. However, it can be shown that certain combined choices of extension and discretization can eliminate the drift up to roundoff error, at least for quadratic constraints [20]. Moreover, the extensions can be viewed as partial analytical solution of the constrained problem, enabling the use of simplified techniques such as functional iteration for solving the discrete equations at each time step.

Another popular type of extension is commonly referred to as the penalty method [29, 6, 7]. In practical terms, rigid constraints are maintained by altering the vector field so that there is a strong resisting force to those motions that violate the constraints. In [29, 7], Hamiltonian formulations of the constrained equations of motion were integrated using this technique but without consideration of the symplectic and integral structures of the flow. A symplectic approach based on the penalty method could be constructed, but an important difficulty lies in the fact that the resulting differential equations will generally be made very stiff by these artificial forces, and the numerical solution of such problems will be unnecessarily complicated. In the Baumgarte approach, on the other hand, the extension is constructed in order that the constraint manifold is turned into an attracting set for the dynamics of the unconstrained problem. Here the chief problem lies in the proper selection of those artificial parameters that will determine the dynamical properties of the extension, but for underlying conservative dynamics, no such choice of a dissipative system can be appropriate.

Still another type of extension is based on the theory of constrained Hamiltonians of P. Dirac: an extended Hamiltonian vector field is constructed by considering the augmented Hamiltonian $\hat{H} = H + \lambda^T g + \mu^T g' H_p$ and choosing the multipliers so that $g = 0$ and $g' H_p = 0$ become (weak) invariants of the flow. This formulation was examined in [21], but is probably too costly to implement in its simplest form.

Instead of the above methods, we advocate the direct discretization of the constrained equations of motion. A simplified discrete problem results from treating the motion as that of a system of particles. For the constrained many-body Hamiltonian, we can use the following constrained variant of the leap-frog discretization:

$$q_{n+1} = q_n + hM^{-1}p_{n+1/2} \tag{5}$$

$$p_{n+1/2} = p_n - (h/2)\nabla_q V(q_n) + g'(q_n)^T \lambda_n \tag{6}$$

$$g(q_{n+1}) = 0 \tag{7}$$

$$p_{n+1} = p_{n+1/2} - (h/2)\nabla_q V(q_{n+1}) + g'(q_{n+1})^T \mu_{n+1} \tag{8}$$

$$g'(q_{n+1})M^{-1}p_{n+1} = 0. \tag{9}$$

This is the RATTLE [1] variant of the SHAKE discretization [34]; in this form, the solution of the discrete equations will automatically satisfy both the position and momentum constraints. It is straightforward to show under mild smoothness assumptions that these equations have a unique solution at each step provided the stepsize h is chosen sufficiently small. Starting from given data q_n, p_n (from the previous step), equations (5)-(7), which are a system of $2N + m$ equations, can be reduced to an m-dimensional nonlinear algebraic problem to be solved for λ_n. Next, (8)-(9) are seen to be a linear system for p_{n+1}, μ_{n+1}. The variables λ_n and μ_n are not propagated from step to step.

In molecular dynamics, SHAKE discretization is a common means for freezing chemical bonds; it was first shown to be convergent (2nd order accurate) and symplectic in [22], in both traditional and RATTLE formulations. Moreover, the scheme automatically preserves the angular momentum [40, 30]. In [24], the SHAKE discretization was applied in a somewhat different way to model the motion of the N-dimensional rigid body.

As a seemingly natural alternative, one might attempt to solve the reduced system (4) by a symplectic discretization. Jay [19] has shown that the constrained analogues of the Lobatto IIIa-b partitioned Runge-Kutta methods are symplectic for general Hamiltonians. Applied to $H = \frac{1}{2}p^T \bar{M}(q)^{-1}p + \tilde{V}(q) +$

$\tilde{g}(q)^T\lambda$, we have

$$\begin{aligned}
q_{n+1} &= q_n + \frac{h}{2}(\bar{M}(q_n)^{-1} + \bar{M}(q_{n+1})^{-1})p_{n+1/2} \\
p_{n+1/2} &= p_n - \frac{h}{2}\nabla_q \tilde{V}(q_n) - \frac{h}{4}\,\nabla_q(p^T\bar{M}(q)^{-1}p)\big|_{(q_n,p_{n+1/2})} - \frac{h}{2}\tilde{g}'(q_n)^T\lambda_n \\
0 &= \tilde{g}(q_{n+1}) \\
p_{n+1} &= p_{n+1/2} - \frac{h}{2}\nabla_q \tilde{V}(q_{n+1}) - \frac{h}{4}\,\nabla_q(p^T\bar{M}(q)^{-1}p)\big|_{(q_{n+1},p_{n+1/2})} - \frac{h}{2}\tilde{g}'(q_{n+1})^T\mu_{n+1} \\
0 &= \tilde{g}'(q_{n+1})\bar{M}^{-1}p_{n+1}.
\end{aligned}$$

These equations (which reduce to RATTLE for many-body Hamiltonians) are fully implicit, requiring the solution of a system of nonlinear equations of dimension $2N+m$ at each step (for q_{n+1}, $p_{n+1/2}$ and λ_n). Applied to the standard coordinates, direct symplectic discretization thus appears to be inordinately complex and computationally expensive.

Equations (5)-(9), on the other hand, are explicit in both q and p, and can be solved by efficient sparse-matrix techniques developed in [5] for molecular dynamics problems. We will discuss this numerical implementation briefly in §5, but we first describe how the many-body formalism provides a general, practical foundation for conservative multibody systems.

3. Particulation

The three dimensional rigid body has six degrees of freedom: three rotational and three translational. For any such body, an equivalent body representation can be developed using a collection of artificial massive particles whose relative positions are held fixed. We refer to each point along with its assigned mass as a *particle* and call the process of assigning particles to the bodies *particulation*. In effect, we are replacing arbitrary rigid bodies by rigid artificial "molecules." Our approach is analogous to—but slightly generalizes—a technique described in Routh [32].

Let B be a rigid body with mass M, center of mass q_{cm} and inertia tensor $I = (I_{ij})$. To model B we assign to the ith particle a mass m_i and a position $q_i = (x_i, y_i, z_i)^T$, $i = 1, 2, ..., k$ in order to preserve the total mass ($\sum m_i = M$), center of mass ($\frac{1}{M}\sum m_i q_i = q_{cm}$), the moments of inertia

$$\sum m_i(y_i^2 + z_i^2) = I_{1,1}, \qquad \sum m_i(x_i^2 + z_i^2) = I_{2,2}, \qquad \sum m_i(x_i^2 + y_i^2) = I_{3,3}$$

and the products of inertia

$$-\sum m_i x_i y_i = I_{1,2}, \qquad -\sum m_i x_i z_i = I_{1,3}, \qquad -\sum m_i y_i z_i = I_{2,3}$$

There are a total of 10 conditions to be met, with $4k$ free parameters.

A straightforward approach to placing the masses is to begin by diagonalizing the inertia tensor $I = (I_{ij})$, yielding the *axes of inertia* u_1,u_2,u_3. By placing three pairs of particles of equal mass symmetrically about the origin along the axes of inertia, we can reduce the number of unknowns to six: the masses and their distances from the origin. Moreover, this can be reduced even further by demanding either that all masses be of the same size or all be placed at the same distance from the origin. This leads to models with six mass particles, whereas four are sufficient to match any given inertial tensor. On the other hand, it is possible to reduce the equations for the six particles to equations for the motion of the center of mass and one particle from each pair.

A more elegant solution is the following particulation in four point particles (i.e. replacement by tetrahedral molecules). We assume that the body is oriented and located so that I is diagonal and the center of mass is the origin. Define four vectors, ξ_i, $i = 1, 2, 3, 4$ as follows: $\xi_1 = [x_1\sqrt{m_1}, x_2\sqrt{m_2}, x_3\sqrt{m_3}, x_4\sqrt{m_4}]^T$, $\xi_2 = [y_1\sqrt{m_1}, y_2\sqrt{m_2}, y_3\sqrt{m_3}, y_4\sqrt{m_4}]^T$, $\xi_3 = [z_1\sqrt{m_1}, z_2\sqrt{m_2}, z_3\sqrt{m_3}, z_4\sqrt{m_4}]^T$, and $\xi_4 = [\sqrt{m_1}, \sqrt{m_2}, \sqrt{m_3}, \sqrt{m_4}]$.

Next observe that

$$\xi_4^T\xi_1 = \sum_{i=1}^{4} m_i x_i$$

so orthogonality of ξ_4 and ξ_1 is equivalent to saying that the x-coordinate of the center of mass is zero. Similarly, $\xi_4^T\xi_2 = \xi_4^T\xi_3 = 0$ when the center of mass is the origin. Furthermore, we have relations

$$\xi_1^T\xi_2 = \sum_{i=1}^4 m_i x_i y_i, \qquad \xi_1^T\xi_3 = \sum_{i=1}^4 m_i x_i z_i, \qquad \xi_2^T\xi_3 = \sum_{i=1}^4 m_i y_i z_i$$

implying ξ_1, ξ_2, and ξ_3 are mutually orthogonal precisely when the products of inertia vanish. Thus the particulation conditions reduce to orthogonality of the vectors ξ_i, $i = 1,2,3,4$ together with the linear equations

$$\begin{aligned} ||\xi_2||^2 + ||\xi_3||^2 &= I_1 \\ ||\xi_1||^2 + ||\xi_3||^2 &= I_2 \\ ||\xi_1||^2 + ||\xi_2||^2 &= I_3 \\ ||\xi_4||^2 = M \end{aligned}$$

for the squared lengths of ξ_i. To find a solution, compute the squared lengths d_i of the ξ_i from:

$$\begin{bmatrix} d_1^2 \\ d_2^2 \\ d_3^2 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}^{-1} \begin{bmatrix} I_1 \\ I_2 \\ I_3 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} I_2 + I_3 - I_1 \\ I_1 + I_3 - I_2 \\ I_1 + I_2 - I_3 \end{bmatrix}.$$

(By the "triangle inequality" [2], the solution is necessarily positive.)

Now select ξ_4 with squared length M (e.g. $m_i = M/4$, $i = 1,2,3,4$), and compute a Householder QR [16] decomposition of the 4×1 matrix ξ_4. The second through fourth columns of Q will be an orthonormal basis for the orthogonal complement of span$\{\xi_4\}$. Define ξ_1, ξ_2, ξ_3 by scaling the last three columns of Q by the computed lengths d_i. Finally, solve for the particle positions.

Although we have illustrated the procedure for a body with $n = 4$ particles, nothing changes for $n > 4$ except that the orthogonal complement of span$\{\xi_4\}$ has dimension $(n-1) > 3$, the result being additional freedom in the choice of the three vectors orthogonal to ξ_4.

In many cases, as when forces of interaction between bodies act on contact points of a body, we may wish to specify some k of the particle positions:

$$\begin{bmatrix} x_i \\ y_i \\ z_i \end{bmatrix} = \begin{bmatrix} \bar{x}_i \\ \bar{y}_i \\ \bar{z}_i \end{bmatrix}$$

for $i = 1 \ldots k$. Denoting the three chosen vectors from span$\{\xi_4\}^\perp$ as η_1,η_2 and η_3 we observe that the x-coordinates of the particles are given by

$$\begin{aligned} x &= \mathrm{diag}(\sqrt{m_1} \ldots \sqrt{m_n})^{-1}\xi_1 \\ &= \mathrm{diag}(\sqrt{m_1} \ldots \sqrt{m_n})^{-1} d_1\eta_1. \end{aligned}$$

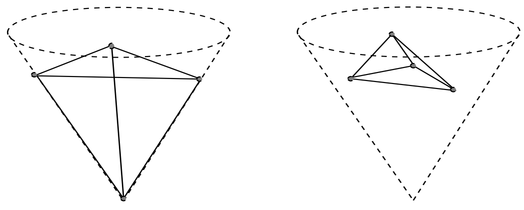
Similarly for the y and z-coordinates. Our task is to find vectors $\eta_j \in$ span$\{\xi_4\}^\perp$ for which the resulting coordinates satisfy the constraints. We can find $\eta_1 = \frac{\hat{\eta}_1}{||\hat{\eta}_1||}$ by solving the underdetermined linear system

$$\begin{bmatrix} A_1 \\ \xi_4^T \end{bmatrix} \hat{\eta}_1 = \begin{bmatrix} \bar{x} \\ 0 \end{bmatrix}$$

where $\bar{x}$ is the vector of the k specified x-coordinates and A_1 is the $k \times n$ matrix consisting of the first k rows of the matrix $d_1\mathrm{diag}(\sqrt{m_1} \ldots \sqrt{m_n})^{-1}$. Setting $\xi_1 = d_1\eta_1$ we find $\xi_2 = d_2\eta_2$ and $\xi_3 = d_3\eta_3$ by successively finding the normalized solutions of the systems

$$\begin{bmatrix} A_2 \\ \xi_1^T \\ \xi_4^T \end{bmatrix} \hat{\eta}_2 = \begin{bmatrix} \bar{y} \\ 0 \\ 0 \end{bmatrix} \qquad \text{and} \begin{bmatrix} A_3 \\ \xi_1^T \\ \xi_2^T \\ \xi_4^T \end{bmatrix} \hat{\eta}_3 = \begin{bmatrix} \bar{z} \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

In some cases, one might simply elect to impose certain constraints on the particle positions or mass distribution, adding additional particles as needed in order for the system of equations to have an acceptable solution. The resulting system of (possibly underdetermined) linear and quadratic equations



a) Conical body particulated to preserve symmetry

b) Conical body particulated using minimization scheme

FIGURE 1. Two particulations of the cone.

can be solved by a generalized Newton iteration [8] to obtain the particulated body. We use the theory of convex sets to note the following general result about the relationship of m_i and q_i to q_{cm}.

Theorem 3.1. *A point r is in the interior of a finitely generated convex set C_m with (minimal) generating set $\{r_1, r_2, \ldots, r_m\}$ if and only if $\exists \alpha_i \in (0,1)$ such that $\sum \alpha_i r_i = r$ and $\sum \alpha_i = 1$.*

The proof is an adaptation of the well know barycentric coordinates theorem [31].

For our application, the theorem and the center of mass condition above imply that $m_i > 0, \forall i$ exactly when q_{cm} is inside the polyhedral convex set generated by the q_i. Further, if q_{cm} is on or outside the polyhedron, $m_i \leq 0$ for some i. While negative masses may be nonphysical, they pose no problem for the analysis here. (They might cause difficulties for the numerical solution of the discretized equations, however.)

As an example, consider a top as the solid generated by revolving the line $z = 2x, 0 \leq x \leq 1$ about the z axis. Assuming unit mass density, we can integrate over the conical volume to obtain $M = \frac{2\pi}{3}$, $r = [00\frac{3}{2}]^T$, and the inertial constants $I_z = \frac{\pi}{3}, I_x = I_y = \frac{17\pi}{10}$, and all products of inertia equal to zero. We model the cone with four particles. The sixteen parameters giving positions and masses are determined by imposing the 10 conditions above. We resolve all but one of the remaining degrees of freedom by requiring that one particle coincide with vertex of the cone, and that the three particles which are not fixed have equal mass. So constrained, the solution of the underdetermined system shares the symmetry properties of the original body (Figure 1a).

Alternatively, we could choose some objective function to minimize subject to the ten constraints. (For a survey of constrained minimization techniques, see [13].) To illustrate, for the conical body above we minimized the summed squared distances of four uniformly massive particles from the center of mass resulting in the particulation of Figure 1b.

3.1. Regularity. A particulation consists of a set of point positions and point masses, along with a vector of constraints of the form $g_i(q) = 0$. We assume that the constraint set is solvable. A system of $n \geq 3$ particles in $\mathbf{R}^3$ has $3n$ degrees of freedom. The rigid body has six degrees of freedom. Each constraint removes one degree of freedom, thus if such a system is to be made rigid, $3n - 6$ rigid length constraints will be needed. On the other hand, for the system of equations to be well-posed and to enable the use of standard techniques to solve the discrete equations, we must have that the jacobian g' of the constraint equations $g = 0$ be full rank. When these two conditions are satisfied we say that the particulation is *regular*.

An example of an irregular particulation is the complete graph on five nodes, since the nine constraints shown in Figure 2 already make the structure rigid. Another example is the case of three particles connected by rods of lengths a,a and $2a$, hence defining a degenerate triangle.

3.2. Planar Bodies. In certain types of mechanical applications, the rigid bodies may be planar, e.g. rigid plates. If the body lies in the xy plane, its moments will satisfy $I_1 + I_2 = I_3$ [2]. This is a necessary and sufficient condition, thus all particulations of a planar body must also be planar. In $\mathbf{R}^2$, a system of n particles is made rigid by the imposition of $2n - 3$ constraints. If we consider a particulation which is rigid in the plane, and then view it as an object in $\mathbf{R}^3$, it will no longer be rigid if $n > 3$, since $3n - 6 \geq 2n - 3$, $n > 3$. This means that additional constraints must be added if $n > 3$ in order to rigidify the body. However, such a particulation will then become a degenerate three dimensional body

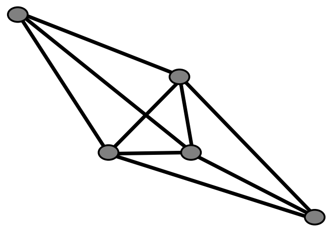


FIGURE 2. A five particle body.

and thus will be irregular. Hence *the only particulations of planar bodies which are regular in* $\mathbf{R}^3$ *are those consisting of a single mass point, a pair of masses linked by a rigid rod, and a triangle.* We can of course specialize the derivation for the tetrahedral particulation given above to the planar case.

In molecular dynamics, many molecules including the important heme group in myoglobin [25] and benzene [10] are *nearly* rigid and planar. Such molecules might on occasion be replaced by artificial three particle models to simplify dynamics, although to represent an improvement over standard techniques [27], an efficient physical basis for distributing the many-body potentials over the artificial particles would need to be found.

In cases where nonplanar but nearly planar structure is important to the dynamics of the system, the price will be ill-conditioning of the nonlinear systems which must be solved at each timestep. An open question is to determine how one could obtain the optimal particulation of a given rigid body (i.e. one which effectively minimizes the ill-conditioning of the nonlinear systems).

3.3. Equivalent Particulations: Reductions. Any two particulations of a rigid body yielding identical inertial tensors, centers of mass, and total mass will result in identical continuous-time dynamics. It is natural to ask if and when the corresponding property will be observed for the numerical dynamics. A priori, there is no reason to expect that two equivalent particulations will yield identical numerical solutions.

We first need a basis for comparison. Suppose that we are given a particulation consisting of four or more points $q = (q_1, q_2, \dots)$ not lying in a plane, and hence forming a basis for $\mathbf{R}^3$. The location of the center of mass at any time is defined by $\frac{1}{M}\sum m_i q_i = q_{cm}$ and each of the three axes of inertia u_i can be computed as linear combinations of the vectors $r_i = q_i - q_{cm}$.

Thus we can write in short, for some matrix A,

$$w(t) := \begin{pmatrix} q_{cm}(t) \\ u_1(t) \\ u_2(t) \\ u_3(t) \end{pmatrix} = Aq(t).$$

Now if $\hat{q}(t)$ is the position vector corresponding to any other particulation of the same rigid body, we can write, similarly,

$$w(t) = \hat{A}\hat{q}(t)$$

for some matrix $\hat{A}$. What this means is that $R(q, \hat{q}) := Aq - \hat{A}\hat{q}$ vanishes along the simultaneous motion of *both* particulations. Indeed, if p and $\hat{p}$ are the corresponding momenta of the two systems, we have

$$\frac{d}{dt}R(q, \hat{q}) = A\dot{q} - \hat{A}\dot{\hat{q}} = AM^{-1}p - \hat{A}\hat{M}^{-1}\hat{p}$$

defining this expression as $S(p, \hat{p})$, we see that $S = 0$ is a *linear integral invariant* of the flow of the combined system; such invariants are maintained by all of the common classes of discretization schemes, including, for example, Multistep, Runge-Kutta and Partitioned Runge-Kutta methods. It can also be seen that the linear secondary invariant $R = 0$ will also be maintained up to a weak instability.

We summarize with a theorem:

Theorem 3.2. *Assuming the discretized equations are solved exactly, equivalent particulations of the same nonplanar rigid body result in identical dynamics as long as the discretization scheme preserves linear first integrals.*

This discussion indicates an alternate set of coordinates: we could instead track the motion of the center of mass together with that of the three axes of inertia. Another way to view this is that we employ the particulation mentioned above consisting of three pairs of particles of equal mass placed symmetrically about the center of mass along the axes of inertia, but we then reduce the equations of motion to equations for the center of mass and three of the particles. Yet another choice would be to take two points on the body, and define, as in [37], a pair of arbitrary vectors fixed in the body and emanating from the two points, and then develop equations of motion in the resulting set of four basis elements.

4. Systems of rigid bodies

Arbitrarily complex systems of rigid bodies can, in principle, be treated with a particle-based approach. The basic questions are (i) how to incorporate various standard types of interactions between the bodies and (ii) how to distribute an applied force acting on the body to the system of particles. We treat the second issue here; in [4], it was shown that the at least the common holonomic joints of multibody dynamics can be represented in the particulated formulation in terms of algebraic constraints retaining the form of quadratic length constraints.

Given a force $\mathbf{F}$ acting on a body at the point given by a radial vector r from the center of mass, it is natural to choose a particulation which includes a particle at r. If such a particulation is not convenient, $\mathbf{F}$ must be distributed throughout the particulated body. To see how this is done, we decompose $\mathbf{F}$ into components parallel and perpendicular to r, say $\mathbf{F}_t$ and $\mathbf{F}_R$. Explicitly,

$$\mathbf{F}_T = \frac{rr^T}{||r||^2}\mathbf{F}$$

and

$$\mathbf{F}_R = \mathbf{F} - \mathbf{F}_T.$$

These are the translational and rotational components of $\mathbf{F}$. The torque about the center of mass is then given by $N = r \times \mathbf{F}_R$.

For a particulation with k particles, each with radial vector r_i, the distributed forces $\mathbf{F}_i$ must satisfy the following relations

$$\begin{aligned} N &= \sum_{i=1}^{k} r_i \times \mathbf{F}_i \\ \mathbf{F}_T &= \sum_{i=1}^{k} \frac{r_i r_i^T}{||r_i||^2}\mathbf{F}_i. \end{aligned}$$

5. Structure of the Nonlinear Equations at a Timestep

In this section, we consider the form of the discretized equations of motion when particulation is used to describe the system. We may assume that the constraint equations $g(q) = 0$ are just quadratic length constraints of the form $(r_i - r_j)^T(r_i - r_j) - L_{ij}^2 = 0$ which represent rods of length L_{ij} between particles i and j.

We briefly describe the techniques we propose for solving the nonlinear equations at each step of SHAKE discretization. In [5] these techniques are developed more fully in the context of molecular dynamics. In terms of q, the discrete equations are:

$$\begin{aligned} q_{n+1} &= q_n + hM^{-1}(p_n - (h/2)\nabla_q V(q_n) + g'(q_n)^T\lambda_n) \\ g(q_{n+1}) &= 0. \end{aligned}$$

For simplicity, we introduce the following notation

$$\begin{aligned} Q &= q_{n+1} \\ G &= g'(q_n) \\ \lambda &= h\lambda_n \\ \bar{Q} &= q_n + hM^{-1}(p_n - (h/2)\nabla_q V(q_n)). \end{aligned}$$

$\bar{Q}$ denotes the quantities on the right hand side which are known at a particular integration step. We may then write the equations as

$$\begin{aligned} Q &= \bar{Q} + M^{-1}G^T\lambda \\ g(Q) &= 0 \end{aligned}$$

or as a system in λ only

$$\tilde{g}(\lambda) = g(\bar{Q} + M^{-1}G^T\lambda) = 0.$$

Applying the Newton-Raphson iteration, we obtain

$$\lambda^{k+1} = \lambda^k - \tilde{g}'(\lambda^k)^{-1}\tilde{g}(\lambda^k)$$

where

$$\tilde{g}' = g'(\bar{Q} + M^{-1}G^T\lambda^k)M^{-1}G^T.$$

5.1. Symmetric Newton iteration. Each iteration of the nonlinear solver requires the solution of a system of linear equations with the form given above. G and g' are the matrix of partial derivatives of the constraint equation evaluated at different stages of the iteration, hence they have identical nonzero structure but different entries. Since M^{-1} is diagonal, the jacobian of the system of nonlinear equations $g'M^{-1}G^T$ is thus *structurally symmetric* (the nonzero entries occur symmetrically). An alternative approach is to use the symmetric positive definite approximate Jacobian

$$GM^{-1}G^T.$$

In the presence of only rod constraints, the elements of the matrix are [5]

$$\begin{aligned} (GM^{-1}G^T)_{ll} &= \frac{L_{ij}^2}{m_i + m_j} \\ (GM^{-1}G^T)_{lm} &= \frac{\pm L_{ij}L_{jk}cos(\theta_{lm})}{m_j} \end{aligned}$$

where rod l joins nodes i and j, rod m joins nodes j and k, and θ_{lm} denotes the angle between rods l and m.

Hence the diagonal entries are constant and the off diagonal entries (l, m) vary with the angle θ_{lm} between constraints l and m. For a particulated rigid body, these angles are constant. In systems of particulated bodies, the matrix consists of constant diagonal blocks corresponding to the bodies, coupled by nonconstant entries due to the changing angles between bodies. This suggests that for small motions between bodies the matrix may be held for several time steps, with updates only as needed. A key observation is that the structure of the matrix $GM^{-1}G^T$ depends only on the constraint equations. Further, nearly all of the entries depend solely on the (constant) distances between constrained particles and angles between constraints. Hence not only is the sparsity structure known in advance, but also the structure of entries which are constant throughout the integration. Any preprocessing required for the solution of the linear systems by sparse techniques, including special methods which take advantage of the constant entry structure, need be performed only once. Some examples of joints and the resulting sparsity patterns can be found in [4]. Further sparse matrix techniques for the symmetric linear systems are discussed in [5].

6. Numerical Experiments

A Matlab toolkit MDLab [3] has been developed to assist in the study of particulated models, symplectic discretizations, and efficient techniques for solving the discretized equations. The software is available by anonymous ftp (kitcs/MDLab.tar) from ftp.math.ukans.edu.

We have performed a wide range of experiments on small multibody systems using MDLab. Below, we study a pair of representative problems and compare the performance of two second order integrators: SHAKE and the two-step backward difference formula BDF2, a popular nonsymplectic method for solving ODEs [14] and DAEs [9]. BDF2 was applied to the reduced-index formulation of equations (1)-(3) as in [15]. We verified correctness of our implementations and appropriateness of parameters such as stepsize and tolerance by monitoring the observed order of the integrators (two for both methods) and the constraint residuals (both position and velocity constraints were maintained to a small multiple of machine epsilon in all experiments).

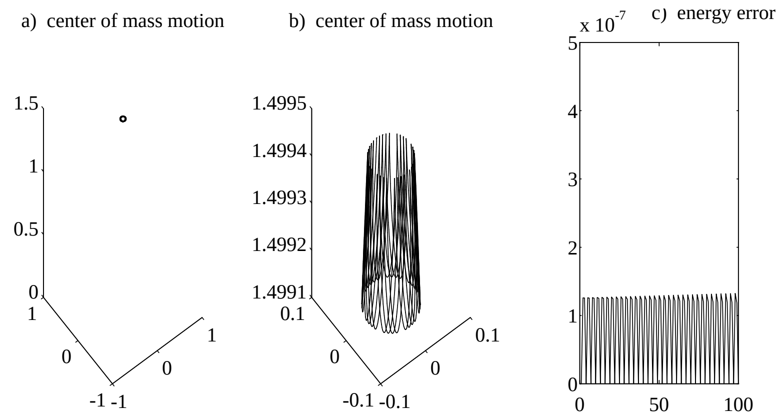


FIGURE 3. Leap-Frog Solution of Top on $[0, 100]$, $h = .05$.

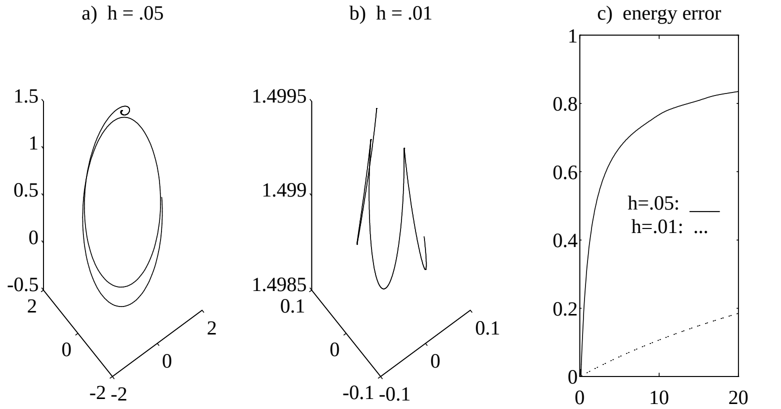


FIGURE 4. BDF2 Solution of Top on $[0, 20]$.

6.1. Lagrange's Top. We consider the conical body of Figure 1a as a top with the one vertex fixed, acting in a gravitational field. We particulate the top using four particles, one fixed at the vertex, and six rod constraints. An initial angular velocity was realized as consistent linear velocities of the three non-fixed points. No damping forces are considered, hence the system is conservative. The system was integrated with time steps of length $h = .05$ with SHAKE and BDF2. Figure 3 shows the relative energy error of the computed solution and the trajectory of the center of mass of the top for the SHAKE numerical solution. Over the interval [0,100], the motion can be seen to be stable. Precession and nutation, well known small scale motions from classical dynamics [26, 2], are well resolved for this value of h.

Figure 4 shows the relative energy error and the trajectory of the center of mass for the BDF2 solution with the time steps ($h = .05$) and ($h = .01$) over the interval $[0, 20]$. Energy loss is significant. Moreover, the plunge of the center of mass at $h = .05$ would correspond to contact of the side of the top with the ground, i.e. the top topples. In our experience, step sizes smaller by at least a factor of five are required to partially resolve the center of mass motion. Energy loss and slowed precession for $h = .01$ are still clearly evident.

We do not propose that the lack of symplecticity of BDF2 is, alone, the reason for the failure. Rather, we suspect that it is SHAKE's near-conservation of energy and the conservation of angular momentum that is important here. The presence of a noncentral gravitational force implies that angular momentum is not conserved. However, it is easy to see that in this example the third component of angular momentum *is* conserved since the gravitational force only acts in this direction. It seems that this conserved quantity is largely responsible for the regular motion of the center of mass, so it is critical that

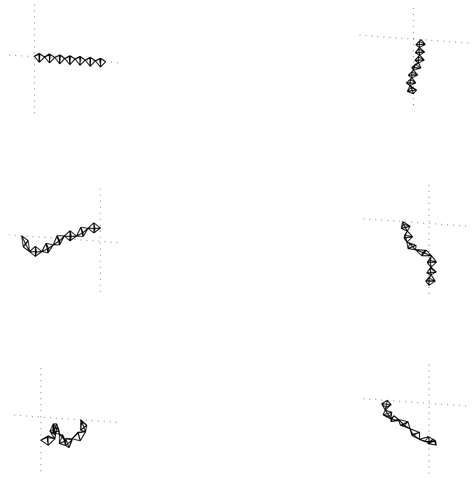


FIGURE 5. Motion of the 7-bar chain.

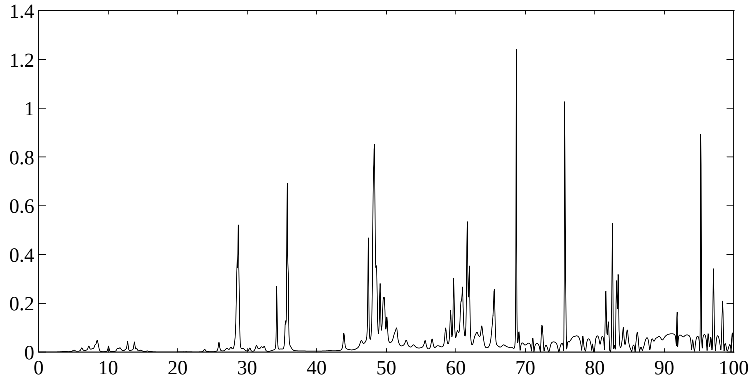


FIGURE 6. 7-bar chain: relative energy error

an angular momentum-conserving numerical scheme such as leapfrog/SHAKE be employed for numerical simulations.

6.2. Seven bar chain. As a second example, we modelled a three dimensional seven bar chain with the ends of the chain constrained to slide along a pair of given fixed perpendicular axes in the xz plane (i.e. connected to the axes by prismatic joints). Our model used seven identical cylindrical bodies of uniform unit mass density moving in the presence of gravity. We particulate the cylinders with five particles, as in Figure 2.

From an initial linear configuration along the horizontal axis, the chain is allowed to swing in gravity. Using the SHAKE method, 2000 time steps of size $h = .05$ were computed to integrate over the interval [0,100]. Snapshots of the computed motion at various points in the interval $[0, 50]$ are shown in Figure 5. Figure 6 shows the energy of the system throughout the integration. This numerical experiment illustrates the property of symplectic methods suggested by the "fundamental theorem" stated in the introduction. Despite substantial variations from the exact energy, the approximate dynamics behave reasonably on long time intervals, i.e. as the solution of a some perturbed Hamiltonian system. Note particularly the sudden drastic changes in the energy at certain points during the integration. These correspond to shocks in the motion of the chain (i.e. like the "crack of a whip"). Although it seems surprising that the integrator partially recovers from these severe shocks, this example points up deficiencies in our understanding of the "nearby Hamiltonian" and also the need for variable stepsize symplectic integrators with good properties.

7. Conclusion

We have shown that the particle formulation provides an strong foundation for symplectic integration of the equations of motion for conservative multibody systems. Of course realistic comparisons with existing nonsymplectic techniques will have to await a careful implementation of the particulation technique in the considerable framework of a multibody simulator.

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