Regularized, Stabilized, Variational Methods for Multibodies.

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Abstract

A time-discrete formulation of the variational principle of mechanics is used to construct a novel first order, fixed time step integration method for multibody systems subject to mixed constraints. The new stepper, coined Spook, includes physics motivated constraint regularization and stabilization terms. The stepper is proved to be stable for the case of linear constraints, for non-zero regularization and stabilization parameters. For fixed stabilization value, the regularization can be made arbitrarily small, corresponding to arbitrarily stiff penalty forces. The "relaxed" constraint formulation permits a separation of time scales so that stiff forces are treated as relaxed constraints. Constraint stabilization makes the stiff forces modeled this way strictly dissipative, and thus, the stepper essentially filters out the high oscillations, but is rigorously symplectic for the rest of the motion. Spook solves a single linear system per time step and is insensitive to constraint degeneracies for non-zero regularization. In addition, it keeps the constraint violations within bounds of $O(h^2)$, where h is the time step. Because it is derived from the discrete variational principle, the stepping scheme globally preserves the symmetries of the physical system. The combination of these features make Spook a very good choice for interactive simulations. Numerical experiments on simple multibody systems are presented to demonstrate the performance and stability properties.

1. Introduction

Integration methods that preserve the qualitative aspects of given sets of differential equations have captured the interest of numerical analysts over the last decade [13]. This investigative effort has shed much light on the mystery of surprisingly well behaved low order formulae widely used in the physical sciences, such as the Verlet [25], Shake, and Rattle methods of molecular dynamics [20], or the Newmark method in structural dynamics, to name just a few.

The recently developed theory of the *discrete least action* principle [22] provides an explanation for this good behavior. Indeed, all the aforementioned integration methods can be derived from the discrete least action principle. In turn, this means that they are guaranteed to be symplectic and to uniformly preserve all physical invariants withing bounds related to the time step. It is one thing to preserve energy, say, locally within $O(h^p)$, for step of size h and a method of order p, so that $|E_{k+1} - E_k| = O(h^p)$ at each step k. But it is yet more reassuring to have the global bound $|E_k - E(0)| = O(h^p)$ for all steps $k = 1, 2, \ldots$, where $E(0)$ is the known energy of the system. For the simplistic looking Verlet stepping scheme for instance, momentum is *exactly* preserved at machine precision, as long as the local stability requirements are met, irrespective of the time step. In addition, for closed physical systems with fixed energy, preservation of symmetries implies a *shadowing property*, meaning that computed trajectories intersect the analytical solution once per step [11, 15]. Therefore, the discrete samples of the trajectory might not be very accurate but they never

deviate far from the exact motion, another good property. If one takes the view that the most fundamental aspects of physical motion are the symmetries, the discrete least action principle is the appropriate technique to use for constructing new integration schemes for physical systems.

Particularly in the context of real-time interactive applications, such as simulator training systems for instance, the time constraints on computations are uniformly stringent. In addition, inputs signals are not known in advance and the system configuration can be changed at arbitrary times. In consequence, low order, single step, strongly stable, fixed step size integration methods are best suited, and the discrete least action principle is the best tool to construct them.

This is the route followed in the present article in which a novel stepping scheme is constructed for constrained mechanical systems. In particular, the issues of constraint stabilization, constraint degeneracy, time scale separation are addressed directly. The same ideas were also applied to dry frictional contact problems in my PhD thesis [18] but due to space limitations, this is not covered in the present article.

Mechanical integrators are constructed directly from a discretization of a time integral of the Lagrangian, expressed in terms of discrete time samples of the systems generalized coordinates. For the low order methods, the stepping equation are three-terms recurrence relations which are in fact the necessary stationarity conditions dictated by the least action principle for conservative systems, or the Fourier-d'Alembert principle of vanishing virtual work for non-conservative ones. The latter principle expresses the equations of motion in weak form. In turn, the weak form provides a straight forward strategy for discretizing discontinuous phenomena such as frictional impacts and contacts, though this is not done here.

The rest of the paper is organized as follows. In § 2, the discrete least action principle is introduced and applied to mechanical systems with finite degrees of freedom. Both conservative and non conservative systems are covered, as well as both holonomic and nonholonomic kinematic constraints. In § 3, the novel physics based constraint regularization and stabilization scheme is presented. This is then linearized in § 4 to produce the Spook stepping scheme. The linear stability is investigated in § 5. The results of numerical experiments are presented in § 6. Conclusions and summary remarks are collected in § 7.

2. Discrete mechanics

Consider a finite-dimensional mechanical system with configuration space Q, generalized coordinates $q : \mathbb{R} \mapsto Q$, and generalized velocities $q : \mathbb{R} \mapsto TQ$, where TQ is the tangent bundle of Q. Introduce the mass matrix $M(q)$ so the kinetic energy $T : TQ \mapsto \mathbb{R}$ is a positive definite quadratic form $T(q, \dot{q}) = \frac{1}{2}\dot{q}^T M(q)\dot{q}$, and is positive definite. Finally, introduce the continuously differentiable potential energy $V : Q \mapsto \mathbb{R}$. The Lagrangian is then

$$\mathcal{L}(q, \dot{q}) = T(q, \dot{q}) - V(q) = \frac{1}{2}\dot{q}M(q)\dot{q} - V(q), \qquad (1)$$

and the action of a given trajectory $(q(t), \dot{q}(t)), t \in [t_0, t_1]$ is the functional

$$S[q] = \int_{t_0}^{t_1} \mathrm{d}s\mathcal{L}(q(s), \dot{q}(s)). \qquad (2)$$

The principle of least action [19] then states that for any infinitesimal variation δq satisfying all the constraints on the system and such that $\delta q(t_0) = \delta q(t_1) = 0$, then, $\delta S[q] = 0$. This means that $S[q]$ is stationary for the physical trajectory $q(t)$.

For a system subject to non-conservative or polygenic forces $f(q, \dot{q}, t)$, the Fourier-d'Alembert principle of virtual work applies, namely

$$\delta S[q] + \int_{t_0}^{t_1} \mathrm{d}s f^T \delta q(s) \leq 0, \qquad (3)$$

where the inequality holds in case Q is closed and bounded and $q(t)$ touches the boundary for $t \in [t_0, t_1]$. A particularly important form of polygenic forces can be written as

$$f(q, \dot{q}) = -\frac{\partial \mathfrak{R}(q, \dot{q})}{\partial \dot{q}}, \qquad (4)$$

where $\mathfrak{R} : Q \times TQ \mapsto \mathbb{R}$ is a generalized Rayleigh dissipation function. A simple example of that is the viscous drag force $f = -\gamma D\dot{q}$ where D is a constant square, symmetric, positive semi-definite real matrix. This corresponds to $\mathfrak{R} = \frac{\gamma}{2}\dot{q}^T D\dot{q} \geq 0$.

The general least action principle leads to the Euler-Lagrange equations of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{q}^T} - \frac{\partial \mathcal{L}}{\partial q^T} = f(q, \dot{q}, t), \qquad (5)$$

which is a set of nonlinear second order differential equations which can be solved with general methods. Observe here that (3) is a weak form of the equations of motion which can be used to analyze nonsmooth phenomena.

Instead of using a standard numerical method on (3), it is possible to discretize the action directly in terms of discrete samples along the trajectory, namely, $q_k = q(kh), k = 0, 1, \ldots, N$, where $h > 0$ is the fixed time step. Introduce the discrete Lagrangian

$$\mathbb{L}_d(q_0, q_1, h) = \int_0^h \mathrm{d}s\mathcal{L}(q(s), \dot{q}(s)), \qquad (6)$$

and the discrete action

$$\mathbb{S}_d(q_0,\ldots,q_N,h)=\sum_{k=0}^{N-1}\mathbb{L}_d(q_k,q_{k+1},h). \qquad (7)$$

The discrete action is then a multivariate function $\mathbb{S}_d(q_0,\ldots,q_N,h) : \otimes^{N+1}Q \mapsto \mathbb{R}$. For a conservative, a stationary point over the discrete trajectory $(q_0,q_1,\ldots,q_N)$ must have vanishing partial derivatives with respect to each of the discrete sample points q_k, which means

$$\begin{aligned}\frac{\partial \mathbb{S}_d(q_0,\ldots,q_N,h)}{\partial q_k}&\\ =\frac{\mathbb{L}_d(q_{k-1},q_k,h)}{\partial q_k}+\frac{\mathbb{L}_d(q_k,q_{k+1},h)}{\partial q_k}&\\ =D_1\mathbb{L}_d(q_{k-},q_k,h)+D_2\mathbb{L}_d(q_k,q_{k+1},h)=0, \qquad (8)&\end{aligned}$$

where D_k is the operator yielding the partial derivative with respect to the kth argument. For a system subject to polygenic forces, first write

$$\begin{aligned}\int_{t_k}^{t_{k+1}}\mathrm{d}s f^T\delta q=&\\ \delta q_k^T f^{(+)}(k,k+1)+\delta q_{k+1}^T f^{(-)}(k,k+1). \qquad (9)&\end{aligned}$$

Then, the discrete Fourier-d'Alembert principle is

$$\begin{aligned}\Big(\frac{\partial \mathbb{S}_d(q_0,\ldots,q_N,h)}{\partial q_k}+&\\ f^{(+)}(k-1,k)^T+f^{(-)}(k,k+1)^T\Big)\delta q_k=0, \qquad (10)&\end{aligned}$$

and after transposing, this reads

$$\begin{aligned}D_1^T\mathbb{L}_d(q_k,q_{k+1},h)+D_2^T\mathbb{L}_d(q_{k-1},q_k,h)&\\ +f^{(+)}(k-1,k)+f^{(-)}(k,k+1)=0. \qquad (11)&\end{aligned}$$

Observe now that either (8) or (11) are discrete stepping equations defining a map $\Phi : Q\times Q\mapsto Q\times Q$ so that $(q_k,q_{k+1})=\Phi(q_{k-1},q_k)$. The map Φ is called a either a variational or a discrete mechanical integrator [22]. The main benefit of this integration strategy is that the discrete trajectory is in fact symplectic. In addition, a discrete form of Noether's theorem applies to the discrete variational principle which means that physical symmetries are preserved by the discrete trajectories. For fixed time integration step, energy is not preserved exactly but oscillates within bounds of $O(h^2)$ of the energy of the continuous system. Because global invariants are preserved by the discrete integrators, the trajectory produced are more faithful to the physics, even at low integration order, than general methods with higher local accuracy but without global error bounds, such as standard Runge-Kutta or multistep methods [13].

There are several choices for defining $\mathbb{L}_d(q_k,q_{k+1},h)$ and $f^{(\pm)}$ but for the present paper, the following choices are made when there is a need to be specific

$$\begin{aligned}q=q_0,\qquad \dot{q}=\frac{1}{h}(q_1-q_0)=v_1,&\\ \mathbb{L}_d(q_0,q_1,h)=\frac{1}{2h}(q_1-q_0)^T M(q_0)(q_1-q_0)-hV(q_0)&\\ f^{(+)}(0,1)=0&\\ f^{(-)}(0,1)=hf(q_1,\frac{1}{h}(q_1-q_0),0). \qquad (12)&\end{aligned}$$

Adding holonomic and nonholonomic constraints to this analysis is straight forward [22, 8]. Given holonomic constraints of the form $g(q)=0$ and Pfaffian-form nonholonomic constraints $a(q,\dot{q})=A(q)\dot{q}=0$, the extensions read

$$\begin{aligned}D_1^T\mathbb{L}_d(q_k,q_{k+1},h)+D_2^T\mathbb{L}_d(q_{k-1},q_k,h)+&\\ hG_k^T\lambda+hA_k^T\alpha+f^{(+)}(k-1,k)+f^{(-)}(k,k+1)=0&\\ g(q_{k+1})=0&\\ A_{k+1}(q_{k+1}-q_k)=0. \qquad (13)&\end{aligned}$$

This result is easily understood as an application of the theory of constrained multivariate extrema.

Stepping formulae directly or closely related to (13) include SHAKE [24] and RATTLE [1]. These are in fact extensions of the Verlet [25] stepping scheme which is common in molecular dynamics [20]. Such schemes have been all but common in multibody dynamics except for some recent applications in computer graphics [12].

The constrained stepping equations (13) form a nonlinear system of equations which has to be solved to yield the updated kinematic state (q_{k+1},q_k), as well as the constraint forces, λ,α. Questions remain as to how much numerical precision is needed in solving (13) to preserve stability and the qualitative aspects of mechanical integrators. This is addressed to some extent in the next section.

3. Constraint regularization and stabilization

It is well-known that kinematic constraints of the form $g(q)=0$ are in fact the limit of strong penalty terms of the form $U_\epsilon=\frac{1}{2\epsilon}g^Tg$, as $\epsilon\to 0$. Likewise, non-holonomic constraints can be understood as the limit of Rayleigh dissipation terms of the form $\frac{1}{2\gamma}\dot{q}^TA^T(q)A(q)\dot{q}$, as $\gamma\to 0$. The theory behind this fact is called *constraint realization*[23, 16, 17, 6, 7]. What is also well known is that introducing penalty forces without taking appropriate precaution against high frequency, low amplitude oscillations, leads to numerical catastrophe. For holonomic constraints, de-

tailed analysis [23] demonstrates that though the trajectories $(q_\epsilon, \dot{q}_\epsilon)$ of the penalized system do converge uniformly to the trajectories of the constrained system, $(q, \dot{q})$, say, but the penalized constraint forces λ_ϵ can fail to converge to the constraint forces λ.

The remedy to these problems is to use implicit time integration for the constraint forces and to introduce sufficient damping to guarantee stability. The result is a "relaxed" constrained system for which accuracy requirements on the solution of the nonlinear stepping equations (13) is dramatically reduced.

Consider first the case of holonomic constraints $g(q) = 0$ with Jacobian $G = \partial g/\partial q$. Introduce the Lagrangian term

$$\mathcal{L}_\epsilon(q, \dot{q}, \lambda, \dot{\lambda}) = \frac{\epsilon}{2}\|\lambda\|^2 + \lambda^T g(q). \tag{14}$$

Considering λ as a dynamical variable, the Euler-Lagrange equations of motion of the augmented system $\mathcal{L}(q, \dot{q}) + \mathcal{L}_\epsilon(q, \dot{q}, \lambda, \dot{\lambda})$ are

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{q}^T} - \frac{\partial \mathcal{L}}{\partial q^T} - G^T\lambda = 0 \\ \epsilon\lambda + g(q) = 0, \end{aligned} \tag{15}$$

and the standard constrained equations are recovered in the limit where $\epsilon \to 0$. To discretize this, put

$$\begin{aligned} \int_0^h \mathrm{d}s \left(\epsilon\lambda^2 + \lambda^T g(q)\right) = \\ \frac{h\epsilon}{8}\|\lambda_0 + \lambda_1\|^2 + \frac{h}{4}(\lambda_0 + \lambda_1)^T(g_0 + g_1), \end{aligned} \tag{16}$$

where $g_k = g(q_k)$. In the variational integration framework, this discretization corresponds to the implicit midpoint rule. After applying the discrete principle of least action and relabelling $\lambda = \frac{1}{4}(\lambda_{k+1} + 2\lambda_k + \lambda_{k-1})$, the discrete Euler-Lagrange equations read

$$\begin{aligned} D_1^T\mathbb{L}_d(q_k, q_{k+1}, h) + D_2^T\mathbb{L}_d(q_{k-1}, q_k, h) \\ + hG_k^T\lambda = 0 \\ \epsilon\lambda + \frac{1}{4}(g_{k+1} + 2g_k + g_{k-1}) = 0. \end{aligned} \tag{17}$$

In the limit where $\epsilon \to 0$, provided $g_0 = g_1 = 0$, the standard variational constrained equations are recovered. As shown further below however, this stepping scheme is at least linearly stable for $\epsilon > 0$. The λ variables are now regarded as the coordinates of a ghost point particle with zero mass. A short analysis reveals that if they did have finite mass, it would have to be negative to preserve physical stability, hence the term "ghost".

For nonholonomic constraints $a(q, \dot{q}) = A(q)\dot{q} = 0$, introduce the Rayleigh function

$$\mathfrak{R}\ a(q, \dot{q}, \alpha, \dot{\alpha}) = -\left(\frac{\gamma}{2}\|\dot{\alpha}\|^2 + \dot{\alpha}^T a(q, \dot{q})\right), \tag{18}$$

producing the force terms

$$\begin{aligned} f_q &= -\frac{\mathfrak{R}}{\partial \dot{q}^T} = -A^T\dot{\alpha}, \\ f_\alpha &= -\frac{\mathfrak{R}}{\partial \dot{\alpha}^T} = \gamma\dot{\alpha} + A(q)\dot{q}. \end{aligned} \tag{19}$$

This form of Rayleigh dissipation function has not been found in the literature. The reason for using $\dot{\alpha}$ instead of α itself, is that α can be treated like a ghost variable, subjected to the dissipative force $f_\alpha = -\partial\mathfrak{R}/\partial\dot{\alpha}^T$.

With the choices

$$f_q^{(-)}(0, 1) = A_0(\alpha_1 - \alpha_0), \tag{20}$$

$$f_q^{(+)}(0, 1) = 0, \tag{21}$$

$$f_\alpha^{(-)}(0, 1) = \gamma(\alpha_1 - \alpha_0) + A_1(q_1 - q_0), \tag{22}$$

$$f_\alpha^{(+)}(0, 1) = 0, \tag{23}$$

the discrete Euler-Lagrange equations become

$$\begin{aligned} D_1^T\mathbb{L}_d(q_k, q_{k+1}, h) + D_2^T\mathbb{L}_d(q_{k-1}, q_k, h) + A_k^T\alpha = 0 \\ \gamma\alpha + A_{k+1}(q_{k+1} - q_k) = 0, \end{aligned} \tag{24}$$

after defining $\alpha = \alpha_{k+1} - \alpha_k$, and the previously known variational stepping nonholonomic stepping scheme [8] is recovered in the limit where $\gamma \to 0$.

Combining these two results, holonomic constraints $g(q) = 0$ can be stabilized by introducing the dissipation term

$$\mathfrak{R}_g(q, \dot{q}, \lambda, \dot{\lambda}) = -\tau\left(\frac{\epsilon}{2}\|\dot{\lambda}\|^2 + \dot{\lambda}G(q)\dot{q}\right). \tag{25}$$

Reusing the definitions provided in (20–23), the resulting discrete Euler-Lagrange equations are now

$$\begin{aligned} D_1^T\mathbb{L}_d(q_k, q_{k+1}, h) + D_2^T\mathbb{L}_d(q_{k-1}, q_k, h) + hG_k^T\lambda = 0 \\ \epsilon\lambda + \frac{1}{4}(g_{k+1} + 2g_k + g_{k-1}) + \frac{\tau}{h}G_{k+1}(q_{k+1} - q_k) = 0, \end{aligned} \tag{26}$$

with the definition $\lambda = \frac{1}{4}(\lambda_{k+1} + 2\lambda_k + \lambda_{k-1}) + \frac{\tau}{h}(\lambda_{k+1} - \lambda_k)$. The reason for this labelling is that λ_k itself is not necessary to step the system forward and the aggregate variable is more convenient.

4. The Spook stepper

Consider a systems with constant mass matrix $M(q) = M$ with n degrees of freedom so $q, \dot{q} \in \mathbb{R}^n$. Add smooth, slowly varying potential energy $V(q)$. Subject this system to a combination of m_h holonomic constraints of the form $g_i(q) = 0, i = 1, \ldots, m_h$ with $m_h \times n$ Jacobians $G = \partial g/\partial q$, and m_n nonholonomic constraints $a_i(q), i = 1, \ldots, m_n$ so $a(q) = A(q)\dot{q} - w(t) = 0$, where $A(q)$ is a smooth $m_n \times n$ matrix, and $w : \mathbb{R} \mapsto \mathbb{R}^{m_n}$

is a smooth driving term. Add smooth non-potential forces discretized so that $f^{(-)}(k,k+1) = 0$ in (9). Then, choose a time step $h > 0$, as well as m_h pairs of positive scalars $\epsilon_i, \tau_i > 0, i = 1, \ldots, m_n$, and a further set of m_n of positive scalars $\gamma_i > 0, i = 1, \ldots, m_n$. Assemble these scalars in the following diagonal matrices

$$\begin{aligned}
\Gamma &= \frac{1}{h}\,\mathrm{diag}(\gamma_1, \gamma_2, \ldots, \gamma_{m_n}),\\
\Sigma &= \frac{4}{h^2}\,\mathrm{diag}(\frac{\epsilon_1}{1+4\frac{\tau_1}{h}}, \frac{\epsilon_2}{1+4\frac{\tau_2}{h}}, \ldots, \frac{\epsilon_{m_h}}{1+4\frac{\tau_{m_h}}{h}}),\\
\Upsilon &= \mathrm{diag}(\frac{1}{1+4\frac{\tau_1}{h}}, \frac{1}{1+4\frac{\tau_2}{h}}, \ldots, \frac{1}{1+4\frac{\tau_{m_h}}{h}}),
\end{aligned} \tag{27}$$

Starting from the discretization provided in (12), and using the linear approximation of the constraints

$$\frac{1}{4}(g_{k+1} + 2g_k + g_{k-1}) \approx g_k + \frac{h}{4}G_k v_{k+1} - \frac{h}{4}G_k v_k, \tag{28}$$

the stepping equations become

$$\begin{bmatrix} M & -A_k^T & -G_k^T \\ A_k & \Gamma & 0 \\ G_k & 0 & \Sigma \end{bmatrix} \begin{bmatrix} v_{k+1} \\ \alpha \\ \lambda \end{bmatrix} = \begin{bmatrix} r \\ s \\ t \end{bmatrix},$$

$$\text{where} \quad \begin{bmatrix} r \\ s \\ t \end{bmatrix} = \begin{bmatrix} Mv_k - h\nabla V_k + hf^{(+)}(k-1,k) \\ w_k \\ -\frac{4}{h}\Upsilon g_k + \Upsilon G_k v_k \end{bmatrix}. \tag{29}$$

Note that with suitably chosen perturbation parameters, the system matrix is never singular which means that for this formulation, constraint degeneracy is not an issue. In addition, it is now possible to model all stiff forces as "relaxed" constraints. In that respect, potential forces lead naturally to relaxed holonomic constraints, and polygenic forces lead to relaxed nonholonomic constraints.

The case of three dimensional rigid bodies is special since then, the mass matrix $M(q)$ is configuration dependent. It is possible to produce corrections to the main Spook stepper defined in (29) using the variational formulations. When this is done, matrix M is replaced by a time dependent $\tilde{M}_k = M_k + O(h^2)$, and the forcing terms are also modified to account for the gyroscopic forces. This is discussed further in my thesis [18] and a complete specification is part of future work.

The matrix appearing on the left hand side of (29) is positive definite but non-symmetric, and it can easily be transformed to a symmetric but indefinite matrix of the type processed efficiently by well-known sparse matrix packages, such as Umfpack [9], for instance. Experience shows that it is a better idea to use Umfpack directly on the large matrix instead of forming the symmetric, positive definite Schur complement matrix

$$\begin{bmatrix} A & G \end{bmatrix} M^{-1} \begin{bmatrix} A^T \\ G^T \end{bmatrix} + \begin{bmatrix} \Gamma & 0 \\ 0 & \Sigma \end{bmatrix}, \tag{30}$$

since the latter can get quite dense in comparison to the original matrix.

5. Linear stability

Several schemes have been suggested for constraint stabilization in mechanical systems [5, 3, 2]. In addition to these, there are regularization schemes for treating the differential-algebraic equations of constrained multibody systems [14]. Though the simplest and most common stabilization scheme [5] does work in some cases, there is no optimal choice of stabilization parameters [2]. Other stabilization schemes [3, 2] are stable but are not motivated from physics and require additional processing. The standard regularization method for differential algebraic equations [14] amounts to replacing constraint equations $g(q) = 0$ with $\epsilon\dot{\lambda} + g(q) = 0$, which is non physical, or replacing (14) with $-\epsilon/2\|\dot{\lambda}\|^2 + \lambda^T g(q)$, leading to $\epsilon\ddot{\lambda} + g(q) = 0$, and thus adding unnecessary second order dynamics to the system. This is clearly not justified from the point of view of constraint realization theory.

The regularization and stabilization scheme of § 3 is motivated by physics however and does reduce to known methods in the limit where the parameters ϵ and τ vanish. It remains to show that the new stepping scheme is indeed stable.

To this end, consider a mechanical system with constant, real, symmetric, and positive definite mass matrix M, of dimension $n \times n$. Set the potential to $V(q) = 0$. Add constant linear homogeneous holonomic constraints of the form $g(q) = Gq = 0$, where G is an $m \times n$ real matrix. In reference to (26), redefine λ to absorb one factor of h, and introduce the nonnegative parameters $\theta = \tau/h$, $\psi = 1/(1+4\theta)$, and $\sigma = (4/h^2)\psi\epsilon$. Discretizing the basic Lagrangian as in (12), and introducing the discrete velocity $p_k = (1/h)(q_k - q_{k-1})$, the equations of motion now read

$$\begin{aligned}
q_{k+1} - hp_{k+1} &= q_k\\
Mp_{k+1} - G^T\lambda &= Mp_k\\
\frac{h}{4}\psi^{-1}\sigma\lambda + \frac{1}{4}G(q_{k+1} + 2q_k + q_{k-1}) &\\
+ h\theta G p_{k+1} &= 0.
\end{aligned} \tag{31}$$

After defining $x_k = Gq_k$, $y_k = hGp_k$, $S = GM^{-1}G^T$ and $S_\sigma = S + \sigma I$, where I is the identity matrix of suitable dimension, eliminating λ from the system (31)

yields the reduced stepping equations

$$x_{k+1} - y_{k+1} = x_k$$
$$y_{k+1} = -4\psi S S_\sigma^{-1} x_k + (I - 4\theta\psi S S_\sigma^{-1}) y_k. \tag{32}$$

Now, it is possible to use the polar decomposition to produce a factorization $G = URP^T$ so that U is an $m \times m$ orthonormal matrix, P is a $n \times n$ permutation matrix, and R is a $m \times n$ matrix with the same rank as G. With this factorization, $(U^T G q)^T = (u_1, u_2, \ldots, u_r, 0, \ldots, 0)$. In addition, since $S = GM^{-1}G^T$ is symmetric and positive semidefinite, then, so is $\tilde{S} = U^T S U$ and so, there is an orthonormal matrix V, with $VV^T = I$, such that $V\tilde{S}V^T = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_r, 0, 0, \ldots)$. Finally, since matrices S and S_σ differ by a scalar multiple of the identity, they commute with each other and are simultaneously diagonalized by the orthogonal transform UV. Thus, changing variables in (32) to $u = UVx$ and $v = UVy$, the stepping equations become

$$Bz_{k+1} = Az_k, \quad z = \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} UV & 0 \\ 0 & UV \end{bmatrix}$$
$$B = \begin{bmatrix} I & -I \\ I & 0 \end{bmatrix}, \quad A = \begin{bmatrix} I & 0 \\ -4\psi\Gamma & (I - 4\theta\psi\Gamma) \end{bmatrix}$$
$$\Gamma = \mathrm{diag}(\frac{\lambda_1}{\lambda_1+\sigma}, \frac{\lambda_2}{\lambda_2+\sigma}, \ldots, \frac{\lambda_r}{\lambda_r+\sigma}, 0, \ldots, 0). \tag{33}$$

The stationary recurrence defined in (33) can be written as $z_{k+1} = B^{-1}Az_k$ and this is stable provided all the eigenvalues of the matrix $B^{-1}A$ are within the unit circle in the complex plane. Because of the block diagonal structure of matrices A and B, the $2m$ eigenvalues of $B^{-1}A$ come in pairs, $\mu_\pm^{(i)}$, $i = 1, 2, \ldots, m$. Straightforward computations yield

$$\mu_\pm^{(i)} = 1 - 2\gamma^{(i)}\psi(\theta+1) \pm 2\sqrt{(\gamma^{(i)}\psi(1+\theta))^2 - \gamma^{(i)}\psi},$$
$$\text{for} \quad i = 1, 2, \ldots, r, \quad \text{and}$$
$$\mu_\pm^{(i)} = 1, \quad \text{for} \quad i = r+1, \ldots, m. \tag{34}$$

Simple analysis yields

$$|\mu_\pm^{(i)}| < 1, \quad \text{when } i < r, \text{ , and}$$
$$\mu_\pm^{(i)} = 1, \quad \text{when } i > r, \epsilon > 0, \text{ and } \theta > 0. \tag{35}$$

With the choice of coordinates, $u_k^{(i)} = v_k^{(i)} = 0$ for $i > r$ and $k = 0, 1, 2, \ldots$. Therefore, $\|x_k\| = \|Gq_k\| \to 0$ and $\|y_k\| = \|hGp_k\| \to 0$ as $k \to \infty$ and so the linear homogeneous system is stable. We have thus proved the following.

Theorem 5.1. *For a discrete mechanical system with configuration space $Q = \mathbb{R}^n$, constant $n \times n$ mass matrix M that is real, symmetric and positive definite, subjected to m-dimensional linear homogeneous constraints $g(q) = Gq$, where matrix G is an $m \times n$ matrix of rank $r \leq m$, the regularized and stabilized stepping scheme of (26) is stable provided $\epsilon > 0$ and $\tau > 0$.*

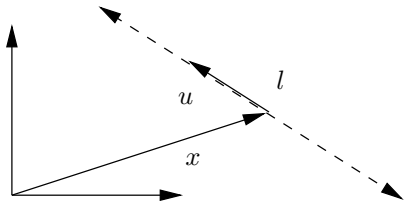

Figure 1: A two dimensional rigid rod.

Theorem 5.1 means in particular that the linearized stepping scheme can process degenerate constraints. There is strong numerical evidence that linear stability is preserved when the perturbation parameters ϵ and τ in (26) take different values for each individual constraint. However, analysis has not yielded strong enough bounds on the spectrum of the corresponding stepping matrix $B^{-1}A$ of (33) yet. Likewise, there are numerical indications that nonlinear stability is not guaranteed for cases where the constraint Jacobian varies quickly, i.e., when the curvature of the constraints is high.

6. Numerical experiments

The framework described above requires additional elements to correctly process three dimensional rigid bodies with non-homogeneous inertia tensors. To avoid these issues for the moment, consider the motion of a rigid rod as shown in Fig. 1. The coordinates for this consist of Cartesian coordinates for the center of mass $x \in \mathbb{R}^n$, and a unit vector $u \in \mathbb{R}^n$, with the constraint that $\|u\| = 1$. If the rod has length l and mass m, the inertia tensor is diagonal with value m for the first n entries, and $l^2/12$ for the remaining ones. Interconnected systems of these rods can be easily constructed in a scripting language such as Octave [10] or Matlab™, making it easy to use UMFPACK to process the linear algebra efficiently. The example considered here is that of a ladder of which one corner is attached to the origin, as shown in Fig. 2. This configuration has appeared in the literature previously [4] to test a strategy for constraint stabilization. This is provides an interesting test case for SPOOK. With the labelling provided in Fig. 2, the connections between the rods is as follows. Rods 1 and 2 have their tails fixed at the origin. Then, rod j is connected by its tail to the head of rod $j-3$ when $\mod(j, 3) = 2$, and to rod $j-2$ otherwise. Finally, rod j is connected head to head with rod $j+1$ for $j = 3k, k = 1, 2, \ldots, N$. If the total number of links is N, there are $n = 4 + 3(N-1)$ rigid rods in the system, $4N+1$ connection constraints between

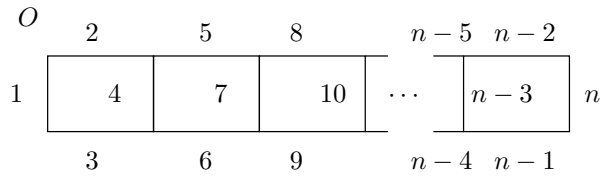

Figure 2: A square chain of rigid rods.

pairs of rods or between a rod and the origin, and n unit constraints to keep $\|u_i\| = 1$. Among the $4N + 1$ constraints, the number of closed kinematic loops is N. For the illustrations that follow, all links have mass 10 and length 1. Other runs were performed with variable masses and link lengths and the stability results were similar to what is reported here, as long as the mass ratios are less than 1000, approximately. Beyond that point, stability problems do surface. The target time step is kept at $h = 1/60$ in most cases, except when analyzing error convergence as in Fig. 6. This is because interactive applications that drive 3D graphics display are often tuned to that frequency. The stepper was found to be stable on this problem for h as large as $h = 1/20$ for $N = 20$.

The other parameters chosen here for the simulations are regularization $\epsilon = 10^{-8}$, and constraint stabilization $\tau/h = 2$. Experience with SPOOK stepper indicates that these parameters are good defaults for a wide range of problems, and rarely need to be tuned. Of course, when masses become very large and their inverses become comparable to ϵ, the regularization parameter must be reduced. A few steps of a simulation are shown in Fig. 3 where $N = 20$. This is a moderate problem size involving 427 variables in two dimensions.

An interesting aspect of the present problem is that as the ladder falls, whiplash develops at the end links after a few oscillations and some velocities become very large. Other fixed time step integration strategies such as Runge-Kutta fourth order with Baumgarte stabilization or plain SHAKE break down completely when whiplash occurs. As explained before, variable time-step is not convenient for real-time simulations and robustness against short burst of high velocity is therefore desirable. In fact, the plain linear version of SPOOK using (29) works best. Performing Newton-Raphson iterations does not improve the solution significantly in most cases, and when the velocities are too big, e.g., during whiplash, the "refined" solution was found to be worse than the linear approximation. This was evident from a sudden, large increase in energy.

The idea of using the ladder problem is to check that SPOOK can process this problem at fixed step, using a relatively large time step, but without loosing stability, even though local errors might be significant. In addition, many methods for handling loop closures in mechanical systems have complexity $O(m^2)$ where m is the number of loops. This is in fact what was reported of MEXXAX [21] in previous work [4]. In that last article, the regularization technique was found to have linear complexity in both the total number of constraints and in the number of closed loop constraints. The same result is achieved here as seen from Fig. 7, in which the time taken by linear system solver is plotted as a function of system size. Thanks to the quality of UMFPACK, this is linear as it should.

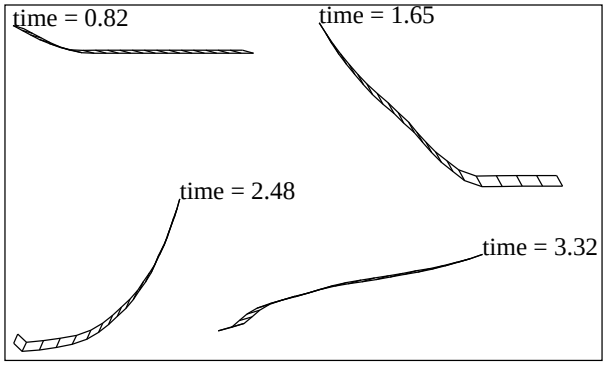

Figure 3: Animation of a rod with $N = 20$.

The energy does dissipate in this problem as seen in Fig. 4 for a chain of $N = 10$ links and another with $N = 100$ links. The reason for that is that constraint violations are damped. This damping is most severe when the chain passes the vertical position and gravity forces stretches all vertical links. However, constraint violation is kept within tight bounds as shown in Fig. 5, even for large system. It is true that for the ladder problem, with the formulation given above, most constraints are in fact linear, except for the unit length ones. On problems with predominantly nonlinear constraints, such as the simple pendulum for instance, the errors can be significantly larger.

Overall, the quality of the solution delivered by SPOOK is comparable to what was observed with other integrators. The numerical cost is less, however, since only one linear system is solved at each step. Stability is also good enough to use large constant step size. The error made on the constraint violation appears to be $O(h^2)$ as seen from Fig. 6.

7. Conclusion

The discrete variational principle provides excellent numerical integrator formulae for physical systems which globally preserve the fundamental symmetries. In addition, the technique for constructing new integration formulae is straight forward and *additive*, making it possible to mix and match different discretizations for different terms. In particular, separating fast oscillatory forces and strong damping forces from the rest of the physics is easy to achieve as described in § 3.

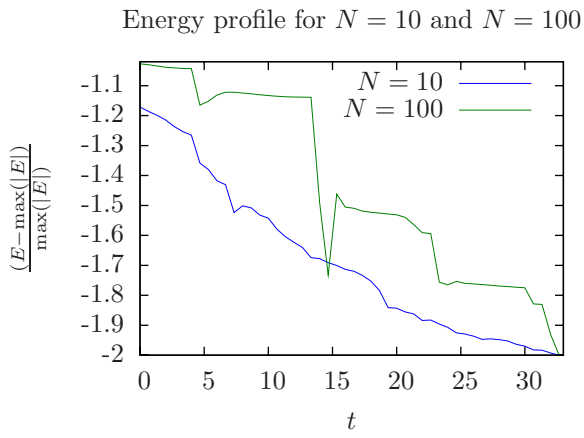

Figure 4: The energy as a function of time for $N = 10$ and $N = 100$.

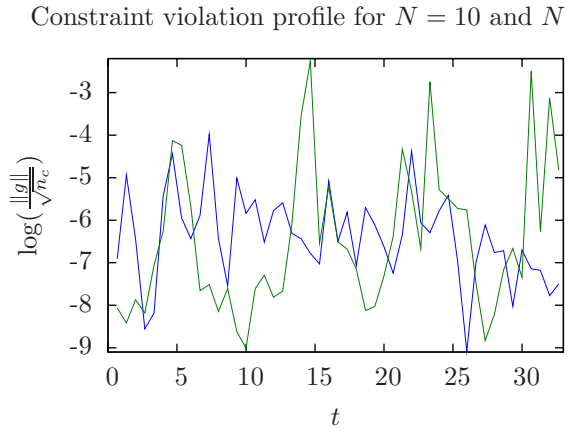

Figure 5: The root mean square norm of constraint violations for $N = 10$ and $N = 100$.

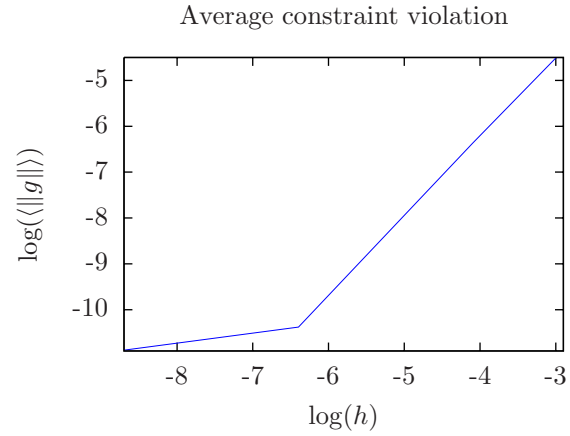

Figure 6: Average constraint violation $\langle\|g\|\rangle$ as function of time step size h.

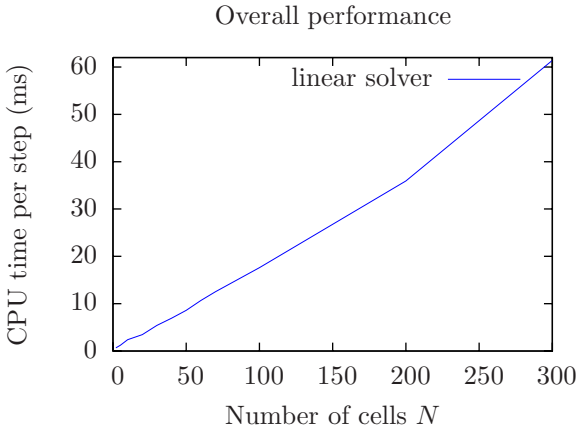

Figure 7: Overall performance of the stepper as a function of N. Average CPU time per step, in ms.

This is exactly what was done in the construction of Spook and it is very satisfying to see that indeed, it can integrate constrained mechanical systems reliably with very little tuning, as illustrated in § 6. This is not a general result for differential algebraic equations, however, since the constraint regularization technique presented here is limited strictly to the algebraic conditions appearing in mechanical systems.

At this time, Spook has not been implemented within a generic multibody dynamics library and it remains to be seen how robust it is on problems with strongly nonlinear constraints. Also not included in the present article are the subtle modifications required to treat the gyroscopic forces of generic three dimensional rigid bodies. Future work will address these issues.

8. Acknowledgements

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