Symplectic Integrators and the Dynamics of the Rigid Body

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Using the rigid body as a model problem, several methods of numerically integrating Hamiltonian systems will be illustrated. First, a brief exposition of the dynamics of the rigid body will be given, followed by several methodologies for integrating the system of equations. Specifically, the methods developed by Professor Juan Simo (Stanford) to conserve fundamental properties of the physical system will be treated in detail.

I. The Rigid Body

The rigid body (B) is a special case of a continuum subject to the constraint of rigidity, i.e.

$$\|\underset{\sim}{X}_A - \underset{\sim}{X}_B\| = \|\underset{\sim}{\Phi}(\underset{\sim}{X}_A, t) - \underset{\sim}{\Phi}(\underset{\sim}{X}_B, t)\| \quad \forall \underset{\sim}{X}_A, \underset{\sim}{X}_B, \forall t$$

where X_i is the position of a material particle (with label X_i) in a fixed reference configuration and the function $\Phi(X,t)$ describes the motion or flow of the particle throughout time. This constraint severely restricts the allowable motions of the body, in fact the function Φ must be of the following form...

$$\underset{\sim}{\Phi}(\underset{\sim}{X}, t) := \Lambda(t)\underset{\sim}{X} + \underset{\sim}{q}(t)$$

where $\Lambda(t)$ is an element of proper (or improper depending what configuration is taken as a reference) orthogonal second order tensors, which will be denoted as SO(3), and q(t) is an element of the Euclidean vector space R(3). Since the orthogonality condition on Λ reduces its dimensionality from 9 to 3, the motion of the infinite number of particles which comprise B can be parametrized by 6 real numbers. Call Q := SO(3) X R(3) the configuration space of the rigid body.

A first description of the dynamics can be obtained from Euler's Laws ... balance of linear momentum

$$\dot{G} = F \qquad \text{with} \qquad G := \int_{\mathcal{B}} \rho \dot{\underset{\sim}{x}}\, dV$$

balance of angular momentum

$$\dot{\Pi} = M \qquad \text{with} \qquad \Pi := \int_{\mathcal{B}} \underset{\sim}{x} \times \rho \dot{\underset{\sim}{x}}\, dV$$

where x := $\Phi(X,t)$ and F is the total externally applied force and M is the total externally applied moment (about the origin, a fixed point). Since it is possible to write the velocity field as the sum the velocity of the center of mass and a velocity relative to the center of mass due to rotation of the body, the dynamics of rotation of the body can be decoupled from those describing

its translation.

$$\dot{x} = \dot{\Lambda}\bar{x} + \dot{q} = \dot{\Lambda}\Lambda^T(x-q) + \dot{q} = \dot{\Lambda}\Lambda^T r + v_{cm} \quad \text{with} \quad r := x - x_{cm}$$

and since Ω, the (spatial) angular velocity tensor, is necessarily skew-symmetric it can be associated with a (spatial) angular velocity vector, ω, by...

$$\Omega c = \omega \times c \quad \forall\, c \text{ constant} \qquad (\text{so} \quad \omega_i = -\tfrac{1}{2}\epsilon_{ijk}\Omega_{jk})$$

so the balances become

$$m\dot{v}_{cm} = F \qquad \text{and} \qquad \dot{\Pi}_{cm} := \dot{\overline{J\omega}} = M_{cm}$$

where M denotes the total moment about the center of mass of the body and J, the inertia tensor.

$$J := \int_{\mathcal{B}} r \cdot r\, I - r \otimes r\, \rho dV = E \cdot I - E \qquad \text{where} \quad E := \int_{\mathcal{B}} r \otimes r\, \rho dV$$

(Also note that, for a rigid body, ignoring thermal effects the balance of energy is a direct result of the balance of linear momentum and that the balance of mass is trivially satisfied.) Now it is also possible to describe the kinematics using the pullbacks of Ω and ω: the body angular velocity tensor, $\Gamma := \Lambda^T\Omega\Lambda$ and body angular velocity vector $\gamma := \Lambda^T\omega$. The corresponding balance of angular momentum is...

$$\dot{\Pi} = \dot{\overline{\Omega J_o \Omega^T \Lambda \gamma}} = \dot{\overline{\Lambda J_o \gamma}} = \dot{\overline{\Lambda \Upsilon}} = \dot{\Lambda}\Lambda^T \Lambda J_o \gamma + \Lambda J_o \dot{\gamma} = \Lambda(\Gamma\Upsilon + \dot{\Upsilon}) = M$$

$$\rightarrow \quad \gamma \times \Upsilon + \dot{\Upsilon} = \Lambda^T M$$

using the fact that the material time derivative of J_o, the pullback of J, is zero and defining Υ as the pullback of Π. This desciption is useful for numerical methods where the mesh is convected with the motion of the body.

Since, once again, a decomposition exists for the kinetic energy...

$$T = \bar{T} + T^* = \tfrac{1}{2} v_{cm} \cdot m v_{cm} + \tfrac{1}{2} \omega \cdot J\omega$$

$$T^* = \tfrac{1}{2}\omega \cdot J\omega = \tfrac{1}{2}\gamma \cdot J_o \gamma = \tfrac{1}{2}\,\mathrm{tr}\,\Omega E \Omega^T = \tfrac{1}{2}\,\mathrm{tr}\,\dot{\Lambda} E_o \dot{\Lambda}^T$$

and noting that the dynamics associated with the position of the center of mass , i.e. those of a particle, are simple and soluble relative to those describing the rotation, Lagrange's and subsequently Hamilton's equations will only be developed for the latter. If the Lagrangian is taken to be identical with the rotational kinetic energy of the rigid body, ignoring conservative and non-conservative forces at the moment, and using that the rotational configuration space can be parametrized by 3 real numbers, at least locally, Lagranges equations become..

$$T^* = \frac{1}{2} \Lambda_i \cdot E_0 \Lambda_j \dot{q}^i \dot{q}^j \quad , \quad \Lambda_i := \frac{\partial \Lambda}{\partial q^i}$$

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} - \frac{\partial L}{\partial q^i} = \dot{\overline{\Lambda_i E_0 \Lambda_j \dot{q}^j}} - \Lambda_{ij} E_0 \Lambda_k \dot{q}^j \dot{q}^k = \dot{\overline{\pi \cdot \omega_i}} - \pi \cdot \dot{\omega}_i = \pi \cdot \omega_i = 0$$

(using the Euler equation derived from the varitional principle with no constraint on the form of the variations.) The $q^i, i = 1..3$ could be choosen, for example and for different reasons, to be Euler angles or unit quaternions (the fourth component being depenedent). (Quaternions have the desirable property of mapping all of SO(3) without singularities, unlike Euler angles, but, unfortunately, the map is not invertible.) Now, by using the Riemannian metric induced SO(3) by the kinetic energy, geometric interpretations of Lagrange's equations can be made. Most important of these is: Λ_i and λ_i represent elements of TSO(3), i.e. tangents, for the tensor and vector representations, respectively. For instantance, if the q^i 's are choosen to be Euler angles then the λ_i 's are the corresponding (non-orthogonal) Euler basis.

In addition to the traditional formulation on the tangent bundle, it is also possible to write Lagranges equations for the rigid body on so(3), the Lie algebra associated with the Lie group SO(3). This alegbra is composed of skew-symmetric linear transformations with the commutator acting as the bracket; these tensors can be identified with vectors by the relation already given for Ω and ω, where the bracket naturally becomes the ordinary vector cross-product. (It will be useful to note that there exist mappings, such as the exponental and the cayley transformations, that take the algebra into the group.) The Lie algebra approach has a direct connection to the traditional one by the fact that elements of the tangent space, $T_\Lambda SO(3)$, are obtained by right (for spatial representation) or left (for body) action of members of the algebra on the elements of the group.

A simple way of obtaining the new form of Lagrange's equation can be derived from the variational principle...

$$\delta \int L = 0 \rightarrow \frac{d}{dt}\frac{\partial L}{\partial \gamma} - \frac{\partial L}{\partial \gamma} \times \gamma = 0$$

by noticing that ...

$$\delta \Omega = \delta \Lambda^T \dot{\Lambda} + \Lambda^T \delta \dot{\Lambda} = \dot{\Sigma} - \Sigma\Gamma + \Gamma\Sigma \quad , \quad \Sigma := \Lambda^T \delta \Lambda$$

(where Σ is the pullback of an element TSO(3)) and consequently constraining the variations of Ω to be ...

$$\delta\gamma = \dot{\varepsilon} + \omega \times \varepsilon$$

Similar expressions can be obtained using the spatial form of all the quantities.

Now, by using the Legendre transform: TSO(3) $\mapsto T^*SO(3)$ a Hamiltonian can be constructed from the Lagrangian parametrized by q^i 's and their rates...

$$p_i = \frac{\partial L}{\partial \dot{q}_i} = \dot{\Lambda} \mathbb{I}_0 \Lambda_i \rightarrow H = p_i \dot{q}^i - L = \frac{1}{2} p_i (\Lambda_i \mathbb{E}_0 \Lambda_j)^{-1} p_j = T^*$$

and from the Lie algebra form...

$$\Gamma_i = \frac{\partial L}{\partial \dot{\gamma}_i} = J_0 \gamma_i \rightarrow H = \pi_i \gamma_i - L = \frac{1}{2} \pi \cdot J^{-1} \pi = T^*$$

which both coincide with the naive concept of the Hamiltonian, as expected. (Note this Hamiltonian is invariant under the group SO(3)). Now, given the fact that Ω is not simply the material time derivative of Λ, it is not surprising that the Hamilton's equations (the second is basically conservation of angular moment, the first being an identity given by the Legendre transform)...

$$\begin{cases} \dot{\Lambda} = \Lambda\Gamma \\ \dot{\Upsilon} = -\Gamma\Upsilon \end{cases}$$

do not follow directly from a cannonical two-form. (Since this two-form is not readily availible it is hard to write the symplectic version Hamilton's equations: $i_X\Omega = dH$; however, it is possible to write the equations in Poisson bracket form simply by defining a non-canonical bracket...

$$\{F,H\}_{PB} := -\Upsilon\cdot(\nabla_\Upsilon F \times \nabla_\Upsilon H) \quad \rightarrow \quad \dot{F} = \{F,H\}_{PB}$$

In the dynamics described, a rigid body in the absence of external forces, the motion conserves two quantities: H, the Hamiltonian, due to the fact Lagrange's equations imply that the kinectic energy is constant, and Π, the angular momentum, which follows from Euler's second law. Given these 'integral invariants' it is possible to find coordinates which are only functions of these quanties (a process similar to how holonomic constraints are dealt with in Lagrangian dynamics, which in effect collects solutions into equivalence classes based on initial values of the invariants) to reduce $T^*SO(3)$ to a space isomorphic to the 2-torus. Another result of having four (i.e. a scalar and a vector) integral invariants is: the system is completely integrable. (For distinct principle moments of inertia, Jacobi elliptic functions are necessary, simpler means are used to treat bodies with non-distinct moments.) The property of integrability is destoyed by introducing a potential which breaks the symmetry, as in the heavy top (which only has one component of Π preserved, relative to a fixed basis).

II. Integration Schemes

There are many ways of constructing numerical schemes to solve initial value problems, such as the system of first-order equations derived from the Hamiltonian formalism, most involve taking the differential equations into difference equations and integrating though time by discrete steps. These methods can differ in many ways: they can give the quantities at a future time as an explicit function of the current ones or the relation can be implicit or a combination of the two (e.g. predictor-corrector methods); they can accomplish the update in a single algebraic step or require multiple steps; they can work solely with the fields of interest or they can involve these quantities' derivatives. Most importantly, at least for Hamiltonian systems,

methods can be constructed preserve the various quantities that characterize the structure of the physical system; these include the integral invariants, the Hamiltonian being one, and the symplectic two-form. This two-form characterizes and gives structure to the space where Hamilton's equations naturally reside: the symplectic manifold; the relation between this two-form and Hamilton's equations is akin to the role the metric plays in Lagrange's equations when they are viewed as taking place on a Riemannian manifold.

Integration schemes that leave the two-form unaltered are called symplectic in the sense that they induce a symplectic transformation from the current state to the future one. Infinitesimally, or in general for any linear symplectic manifold, this is expressed as..

$$\mathbb{J} = L\,\mathbb{J}\,L^{T}$$

where JJ is the representation of the two-form on the cannonical basis and L is the linear operator associated with the symplectic transformation; (in general for a manifold...

$$\Omega_{1_z}(v,w) = \Omega_{2_{\varphi(z)}}\left(T_z\varphi \cdot v, T_z\varphi \cdot w\right) \qquad \varphi : 1 \mapsto 2$$

Many systems of interest, including those induced by a finite element simplification of the configuration space, lie in the category of symplectic vector spaces. However, the rigid body with a configuration manifold composed of orthogonal linear transformations is not one of them.

Since the composition of any collection of symplectic is still symplectic, it is possible to build up the flow any system by a sequence of symplectic transformations that advance the flow through time. One scheme particular to Hamiltonian systems, namely generating functions, is capable of creating symplectic transformations which lend themselves to the integration of the Hamiltonian vector field. Difference schemes can be extracted from these transformations by finding a generating function, approximating it upto the desired accuracy and then finding difference representations of the necessary derivatives. Fundamentally, this approach has its basis in the fact that generating functions provide solutions to the Hamilton-Jacobi equation and thus a solution for the flow. There are other less 'natural', in the sense of preserving the two-form, schemes for Hamitonian systems, but all methods of

devising integration schemes are limited by the following theorem by Zhong and Marsden: given an algorythm for a system whose conserved quantities only depend on H, the Hamiltonian:

> If [the] algorithm is [to be] symplectic, and [conserves] H exactly, then it is the time advance map for the exact hamiltonian system up to a reparametrization of time. In other words symplectic algorithms cannot preserve energy for nonintegrable systems.

So, in general, the integration scheme must follow the exact flow in order to be symplectic and conserve the Hamiltonian. This stipulation makes useable symplectic algorythms rare since energy conservation, besides being a basic balance law, is usually associated with stablity, at least in the sense of energy norm.

Professor Simo takes a different approach to creating integrators suitable for the dynamics of the rigid body; he concentrates on conserved quanties (in this case angular momentum and energy) first, then taylors the algorythm, if possible, to preserve the symplectic form. In a discrete environment, a clarification must be made about what 'conserve' means; it is usually defined as preserving the quantity from time step to discrete time step (and not necessarily in between). Professor Simo's early developments produced integrators which conserved angular momentum intrinscally and where forced to conserve energy by a corrector step which left the angular mometum unaltered; this step projected the predicted solution on to surface (in configuration space) of constant energy. He was able to achieve this process through a couple of different methods, most of which are fairly standard in numerical analysis. It is not surprising that he would seek to maintain angular momentum and energy before attempting imbue his algorythms with other properties, since conservation of these quantities are direct results of the balance laws of classical continuum mechanics. In addition to developing his own schemes, Professor Simo surveyed traditional families of integrators for their symplectic members. He found that the midpoint/centered Euler member of the Runge-Kutta family,

$$\begin{cases} q_{n+1} - q_n = \Delta t\, H_{,p}(p_{n+1/2}) = \left(\Delta t\, M^{-1} p_{n+1/2}\right) \\ p_{n+1} - p_n = -\Delta t\, H_{,q}(q_{n+1/2}) = \left(\Delta t\, V(q_{n+1/2})\right) \end{cases}$$

which is actually also a member of one of the classes of integrators he

developed (and is related to the Crank-Nicholson version of linear multi-step methods) is symplectic, energy and momentum preserving. In fact this implicit algorythm, whose symplectic nature had been discovered earlier (e.g. Feng Kan), is second order accurate and unconditional stable. Note, care must be taken, in that $f(t_{n+1/2})$ only corresponds to the combination $1/2f(t_n) + 1/2f(t_{n+1})$ on linear manifolds. Simo also found that the only symplectic member of the Newmark family, standard integrators for second order systems (e.g. those found in classical continuum mechanics) is the explicit central difference method:

$$\begin{cases} q_{n+1} = q_n + \Delta t^2 \left[\frac{1}{2} a_n\right] \\ v_{n+1} = v_n + \Delta t \left[\frac{1}{2} a_n + \frac{1}{2} a_{n+1}\right] \\ a_{n+1} = -M^{-1} \nabla V(q_{n+1}) \end{cases}$$

In Simo's later work, he exploits an idea he touched on in earlier work: the existence of a Lie algebra (so(3)) associated with the Lie group SO(3) and closed form mappings from the algebra to the group. The beauty of the availibility of a Lie algebra is that it is a linear space, connected to the tangent bundle of SO(3) in the fashion previously described; this makes it adaptible to a scheme that replaces what by necessity is a multiplictive update on the group by a more tractible additive one on the algebra. Simo, in keeping with his earlier developments, begins with a scheme...

$$\begin{cases} \Lambda_{n+1} - \Lambda_n = \Lambda_{n+\alpha} \Theta & \alpha \in [0,1] \\ \Upsilon_{n+1} - \Upsilon_n = -\Theta \Pi_{n+(1-\alpha)} \end{cases}$$

that has four imbedded parameters: α and the skew matrix Θ, and bears a strong resemblance to the undiscretized Euler equations. These parameters are taylored to create a momentum and energy conserving integrator. First he shows that momentum conservation is implicit in the scheme (i.e. the flow or the map of the spatial momentum is constant):

$$\Pi_{n+1} - \Pi_n = \Lambda_{n+1} \Upsilon_{n+1} - \Lambda_n \Upsilon_n = -\Lambda_{n+\alpha} \Theta \Pi_{n+(1-\alpha)} + \Lambda_{n+\alpha} \Theta \Upsilon_{n+(1-\alpha)} = 0$$

Now, to restrict that the linear transformation of Λ_n keeps Λ_{n+1} in SO(3). By solving for Λ_{n+1}...

$$\begin{cases} \Lambda_{n+1} - \Lambda_n T_\alpha(\Theta) = 0 \\ T_\alpha(\Theta) \Upsilon_{n+1} - \Upsilon_n = 0 \end{cases}$$

and reconizing that α must be 1/2 (as in the midpoint method) and T_α : $so(3) \mapsto SO(3)$ must be the Cayley tranformation. So the rotation, Λ, is updated by right translation and the momenta, Υ is updated by left translation:

$$\begin{cases} \Lambda_{n+1} = \Lambda_n \, cay(\theta) \\ \Upsilon_{n+1} = cay(\theta)\, \Upsilon_n \end{cases} \qquad cay[\bullet] := \left(1 + \tfrac{1}{2}\theta\right)\left(1 - \tfrac{1}{2}\theta\right)^{-1}$$

Conservation of energy is his next aim and through manipluation and substitution he obtains:

$$H_{n+1} - H_n = \tfrac{1}{2}\,\Pi_{n+1} \cdot J_0^{-1}\Upsilon_{n+1} - \tfrac{1}{2}\,\Upsilon_n \cdot J_0^{-1}\Upsilon_n = \left(\Upsilon_{n+1} - \Upsilon_n\right) \cdot \Omega_{n+1/2}$$
$$= \Upsilon_{n+1/2} \times \theta \cdot \Omega_{n+1/2}$$

which suggests that θ, the vector associated with Θ, must be parallel to the body angular velocity γ at time $t_{n+1/2}$. Therefore the update is of the form:

$$\theta = \kappa(\theta)\, \frac{\Delta t}{2}\, J^{-1}\left(\Upsilon_{n+1} - \Upsilon_n\right)$$

So he is left with a functional $\kappa(\Theta)$ which acts as a geometric multiplier. The hopes are to satisfy the conditions for symplecticity, which are most readily availible in infinitesimal Possion version (i.e. inverse of the two-form), by chosing this function. He shows that is actually possible for the free rigid body, which is not so surprising since the system is completely integrable; however, when the algorythm is extended to accomodate a nonzero potental, preservation of the symplectic form is traded for conservation of energy (the methodcannot follow the flow of the exact Hamiltonian). In fact he makes the interesting observation that kinetic energy is conserved, only potential energy is left unbound; this could be tied with a property of the action associated with these Hamiltonians.

References

1) Arnold, V. I. Mathematical methods of classical mechanics 2nd ed. Graduate texts in mathematics 60; New York : Springer-Verlag, 1989.

2) Marsden, J.; Ratiu, R. ; Introduction to mechanics and symmetry : a basic exposition of classical mechanical systems. Texts in applied mathematics 17; New York : Springer-Verlag, c1994.

3) Simo, JC: Wong, KK ; Unconditionally Stable Algorythms for Rigid Body Dynamics that Exactly Preserve Energy and Momentum. International Journal for Numerical Methods in Enginnering, 1991 JAN, V31 N1:19-52.

4) Simo JC; Tarnow, N; Wong, KK.; Exact Energy-Momentum Conserving Algorythms and Symplectic Schemes for Nonlinear Dynamics. Computer Methods in Applied Mechanics and Engineering, 1992 oct, V100 N1:63-116.

5) Lewis, D: Simo, JC; Conserving Algorythms for the Dynamics of Hamiltonian Systems on Lie groups. Journal of Nonlinear Science, 1994 MAY-JUN, V4 N3:253-299.

6) Zhong, Ge; Marsden, J.; Lie-Poisson Hamilton-Jacobi theory and lie-poisson integrators. Physics Letters A, 1988 Nov 7, v133, n1:134-139

7) Marsden, J.; Weinstein, A. Reduction of Symplectic Manifolds with Symmetry Reports on Mathematical Physics, 1974, v5,n1:121-130

8) Kang, F.; Difference Schemes for Hamiltonian Formalism and Symplectic Geometery Journal of Computational Mathematics, 1986 July, v4 N3:279-289

9) Channell, P.; Scovel C.; Symplectic Integration of Hamiltonian Systems Nonlinearity, 1990, V3 231-259

10) Mukres, J.; Topology: a First Course Prentice-Hall, 1975

11) Shoemake, K.; Animating Rotation with Quaternion Curves; Computer graphics, 1985, v19 n3:245-254

12) Tait, PG; An elementary treatise on quaternions, Oxford, Clarendon Press, 1867.

13) Burden, R.: Faires, J.; Numerical Analysis, 4th ed. Boston, PWS-KENT 1989

14) Casey, J.; A Treatment of Rigid Body Dynamics; ASME journal of Applied Mechanics, (1983) v50: 905-906

15) Casey, J.: Lam, VC; On the Reduction of the Rotational Equations of Rigid Body Dynamics, Meccanica, (1987) v22:41-42

16) Casey, J.; A Geometric Perspective on Lagrange's equations in the Context of Rigid Continua, ZAMP, 1994 May 16