An Exactly Conservative Integrator for the n-Body Problem

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Abstract. The two-dimensional n-body problem of classical mechanics is a non-integrable Hamiltonian system for $n > 2$. Traditional numerical integration algorithms, which are polynomials in the time step, typically lead to systematic drifts in the computed value of the total energy and angular momentum. Even symplectic integration schemes exactly conserve only an approximate Hamiltonian. We present an algorithm that conserves the true Hamiltonian and the total angular momentum to machine precision. It is derived by applying conventional discretizations in a new space obtained by transformation of the dependent variables. We develop the method first for the restricted circular three-body problem, then for the general two-dimensional three-body problem, and finally for the planar n-body problem. Jacobi coordinates are used to reduce the two-dimensional n-body problem to an $(n-1)$-body problem that incorporates the constant linear momentum and center of mass constraints. For a four-body choreography, we find that a larger time step can be used with our conservative algorithm than with symplectic and conventional integrators.

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1. Introduction

The n-body problem is the study of the motion of n arbitrary particles in space according to the Newtonian law of gravitation. When $n = 2$ (the Kepler problem), the problem has a well-known analytic solution, but Poincaré has shown that the system is in general non-integrable for $n > 2$. To approximately solve these cases, one often attempts to discretize the equations of motion and study the evolution of the system numerically. However, discretization of a system of differential equations typically leads to a loss of accuracy; first integrals of the motion may no longer be preserved and the phase portrait may become inaccurate. This often necessitates the use of small time steps, so that many iterations will be required. In this article, we demonstrate that *conservative integration* can be used to obtain an accurate picture of the dynamics even with a relatively large time step.

Conservative integration was introduced by Shadwick, Bowman, and Morrison [1, 2, 3]. These authors argued that a more robust and faithful evolution of the dynamics can be obtained by explicitly building in knowledge of the analytical structure of the equations; in this case, by preserving the known first integrals of the motion. They illustrated the method applied to a three-wave truncation of the Euler equations, the Lotka–Volterra problem, and the Kepler problem. In this work, we extend the method to the equations of motion of n bodies in space, first to the circular restricted three-body problem, then to the general three-body problem, and finally to the full n-body case. For simplicity we only consider two-dimensional motion (a reasonable assumption for all of the planets in the solar system except for Pluto); extending this work to three dimensions should be straightforward.

2. Conservative Integration

The equations describing the motion of the solar system form a conservative system: the friction that heavenly bodies sustain is so small that virtually no energy is lost. Both the total energy and total angular momentum are conserved. We argue that a robust integration algorithm should preserve both of these invariants.

One way to accomplish this is to transform the dependent variables to a new space where the energy and other conserved quantities are linear functions of the transformed variables, apply a traditional integration algorithm in this space, and then transform back to get new values for each variable [1, 2]. This approach is motivated by the following trivial lemma.

Lemma 1 *Let $\boldsymbol{x}$ and $\boldsymbol{c}$ be vectors in $\mathbb{R}^n$. If $\boldsymbol{f} : \mathbb{R}^{n+1} \to \mathbb{R}^n$ has values orthogonal to $\boldsymbol{c}$, so that $I = \boldsymbol{c}\cdot\boldsymbol{x}$ is a linear invariant of the first-order differential equation $d\boldsymbol{x}/dt = \boldsymbol{f}(\boldsymbol{x}, t)$, then each stage of the explicit m-stage discretization*

$$\boldsymbol{x}_j = \boldsymbol{x}_0 + \tau \sum_{k=0}^{j-1} b_{jk} \boldsymbol{f}(\boldsymbol{x}_k, t + a_j\tau), \qquad j = 1, \ldots, m, \tag{1}$$

also conserves I, where τ is the time step and $b_{jk} \in \mathbb{R}$.

Proof. For $j = 1, \ldots, m$, we have $\boldsymbol{c} \cdot \boldsymbol{x}_j = \boldsymbol{c} \cdot \boldsymbol{x}_0 + \tau \sum_{k=0}^{j-1} b_{jk} \boldsymbol{c} \cdot \boldsymbol{f}(\boldsymbol{x}_k, t + a_j \tau) = \boldsymbol{c} \cdot \boldsymbol{x}_0$. $\diamond$

A conservative integration algorithm can be constructed by writing any conventional integration algorithm of the form (1), for which specific values of a_j and b_{jk} are known, in a transformed space. For example, consider the *second-order predictor–corrector* (2-stage) scheme for evolving the system of ordinary differential equations $d\boldsymbol{x}/dt = \boldsymbol{f}(\boldsymbol{x}, t)$,

$$\tilde{\boldsymbol{x}} = \boldsymbol{x}_0 + \tau \boldsymbol{f}(\boldsymbol{x}_0, t), \tag{2a}$$

$$\boldsymbol{x}(t + \tau) = \boldsymbol{x}_0 + \frac{\tau}{2}[\boldsymbol{f}(\boldsymbol{x}_0, t) + \boldsymbol{f}(\tilde{\boldsymbol{x}}, t + \tau)], \tag{2b}$$

where we now write $\tilde{\boldsymbol{x}}$ and $\boldsymbol{x}(t+\tau)$ instead of $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$, respectively. In the *conservative predictor–corrector algorithm*, one seeks a transformation $\boldsymbol{\xi} = \boldsymbol{T}(\boldsymbol{x})$ of the dependent variable $\boldsymbol{x}$ such that the quantities to be conserved can be expressed as linear functions of the new variables ξ_i, $i = 1, \ldots, n$. Then, keeping (2a) as the predictor, in the transformed space one applies the corrector

$$\boldsymbol{\xi}(t + \tau) = \boldsymbol{\xi}_0 + \frac{\tau}{2}[\boldsymbol{T}'(\boldsymbol{x_0}) \boldsymbol{f}(\boldsymbol{x}_0, t) + \boldsymbol{T}'(\tilde{\boldsymbol{x}}) \boldsymbol{f}(\tilde{\boldsymbol{x}}, t + \tau)], \tag{3}$$

where $\boldsymbol{\xi}_0 = \boldsymbol{T}(\boldsymbol{x}_0)$ and $\boldsymbol{T}'$ is the derivative of $\boldsymbol{T}$. The new value of $\boldsymbol{x}$ is obtained by inverse transformation, $\boldsymbol{x}(t + \tau) = \boldsymbol{T}^{-1}(\boldsymbol{\xi}(t + \tau))$. Often the inverse transformation involves radicals, and if the argument of the radical becomes negative, it is possible to use a finite number of time-step reductions to integrate the system through this region [2]; this approach is particularly advantageous when the time step is chosen adaptively. Another way to deal with noninvertible transformations is to switch to a conventional (e.g. predictor–corrector) integrator for that one time step. If the inverse transformation involves several branches (e.g. because of a square root), the correct branch can be distinguished with sufficient accuracy using the conventional predictor solution. The error analysis for a second-order predictor–corrector algorithm is described in Appendix A. Higher-order conservative integration algorithms are readily obtained in the same way, by coupling the first $m - 1$ "predictor" stages from (1) with the final conservative corrector stage

$$\boldsymbol{\xi}(t + \tau) = \boldsymbol{\xi}_0 + \tau \sum_{k=0}^{m-1} b_{mk} \boldsymbol{T}'(\boldsymbol{x_k}) \boldsymbol{f}(\boldsymbol{x}_k, t + a_j \tau). \tag{4}$$

According to Iserles [4], a major drawback of traditional non-conservative integration is that numbers are often "thrown into the computer." Mathematical models are often discretized according to algorithms that have little to do with the original problem. Iserles argued that one should develop computational algorithms that reflect known structural features of the problem under consideration (e.g. see [5, 6]). The conservative predictor–corrector is an example of such an integrator. In the examples given by [1, 3], the transformation $\boldsymbol{T}$ is tailored to the system at hand; there is obviously no generic transformation that can be used to integrate an arbitrary conservative system.

It is interesting to compare conservative integration (which conserves the value of the Hamiltonian) with symplectic integration (which conserves phase-space volume; see Refs. [7], [8], [9], [10], and [11]). According to Ge and Marsden (1988), if an integrator is both symplectic and conservative, it must be exact. Normally we do not have the luxury of an exact discretization at our disposal. The drawback then with conservative integration is that the Hamiltonian phase-space structure will not be preserved, just as for symplectic integration the total energy will not be conserved. Which method is preferable depends on the physical structure of the problem being investigated.

Another important advantage of conservative integration algorithms is that, unlike typical symplectic integration schemes, they are explicit. Although in some cases the inverse of the transformation T may be defined by an implicit equation that requires iteration to solve (using the predicted value as an accurate initial guess), this is really nothing more than a special function evaluation; the time-stepping scheme itself, being causal, is explicit.

With conservative integration, one can preserve all of the known invariants of the n-body problem conserved exactly, even for large time steps. This can lead to a more accurate picture of the motion of the bodies [1, figure 9] for the same computational effort. In the next section, we motivate the extension of the method of conservative integration to the n-body problem by briefly revisiting the treatment of the Kepler problem in Ref. [1].

3. Kepler Problem

The Kepler problem describes the motion of two bodies with masses m_1 and m_2 located at positions $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$, respectively. The dynamics can be reduced to an equivalent one-body problem, the behaviour of a single particle of mass $m = m_1 m_2/(m_1 + m_2)$ at the position $\boldsymbol{r} = \boldsymbol{r}_2 - \boldsymbol{r}_1$ under the influence of a central gravitational force. This force may be expressed as the gradient of the potential function $V = -k/r$, where $k = Gm_1m_2$ and G is the universal gravitational constant. The equations of motion can be written in terms of the radial velocity v_r and the polar coordinate angle θ of the particle,

$$\frac{dr}{dt} = v_r, \tag{5a}$$

$$\frac{dv_r}{dt} = \frac{\ell^2}{m^2 r^3} - \frac{1}{m}\left(\frac{\partial V}{\partial r}\right), \tag{5b}$$

$$\frac{d\theta}{dt} = \frac{\ell}{mr^2}, \tag{5c}$$

where ℓ is the (constant) total angular momentum. It is convenient to rewrite the equations in terms of the linear momentum $p = mv_r$ and the angular momentum ℓ:

$$\frac{dr}{dt} = \frac{\partial H}{\partial p} = \frac{p}{m}, \tag{6a}$$

$$\frac{dp}{dt} = -\frac{\partial H}{\partial r} = \frac{\ell^2}{mr^3} - \frac{\partial V}{\partial r}, \tag{6b}$$

$$\frac{d\theta}{dt} = \frac{\partial H}{\partial \ell} = \frac{\ell}{mr^2}, \tag{6c}$$

$$\frac{d\ell}{dt} = -\frac{\partial H}{\partial \theta} = 0, \tag{6d}$$

where the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{\ell^2}{2mr^2} + V(r), \tag{7}$$

is also conserved.

3.1. Integration

To set the framework for extending two-body conservative integrators to the n-body problem, we slightly generalize the presentation in Ref. [1] to make the constant ℓ a variable that is formally integrated, but which remains constant.

The predictor step of the conservative integrator is given by (2a), where $\boldsymbol{x} = (r, \theta, p, \ell)$. To derive the corrector, the vector (r, p, ℓ) is transformed to (ξ_1, ξ_2, ξ_3), where

$$\xi_1 = -\frac{k}{r}, \tag{8a}$$

$$\xi_2 = \frac{p^2}{2m} + \frac{\ell^2}{2mr^2}, \tag{8b}$$

$$\xi_3 = \ell. \tag{8c}$$

On differentiating these equations with respect to time and exploiting the fact that both $H = \xi_1 + \xi_2$ and $L = \xi_3$ are conserved, one finds

$$\dot{\xi}_1 = \frac{kp}{mr^2}, \tag{9a}$$

$$\dot{\xi}_2 = -\dot{\xi}_1, \tag{9b}$$

$$\dot{\xi}_3 = 0. \tag{9c}$$

After applying (3), the inverse transformation

$$r = -\frac{k}{\xi_1}, \tag{10a}$$

$$\ell = \xi_3, \tag{10b}$$

$$p = \mathrm{sgn}(\tilde{p})\sqrt{2m\xi_2 - \frac{\ell^2}{r^2}} \tag{10c}$$

is used to update the values of the original variables at the new step. See Ref. [1] for details on how the invariance of the Runge–Lenz vector $\boldsymbol{A} = \boldsymbol{v} \times \boldsymbol{\ell} + V\boldsymbol{r}$ is exploited to evolve θ.‡

Before generalizing the integrator of Shadwick *et al.* to the n-body problem, it is instructive to consider first the special case of the restricted three-body problem.

‡ There is a typographical error in Eq. (54b) of Ref. [1]; it should read

$$v_r(t+\tau) = \mathrm{sgn}(\widetilde{v_r})\sqrt{v_r^2 + \frac{\ell^2}{m^2}\left(\frac{1}{r^2} - \frac{1}{r^2(t+\tau)}\right) - 2\,\frac{\Delta}{m}}. \tag{11}$$

4. Restricted Three-Body Problem

Suppose that two bodies of masses m_1 and m_2, called the primaries, revolve around their center of mass in circular orbits. The *circular restricted three-body problem* describes the motion of a third body, with a mass m_3 that is negligible compared to m_1 and m_2, at coordinates (x, y) in the plane of motion of the other two bodies. The third body does not influence the motion of the other two. The derivation of the equations of motion for the restricted problem is described in [13]. The Hamiltonian is given by

$$H = \frac{1}{2}\left(\dot{x}^2 + \dot{y}^2\right) - \frac{1}{2}\left(y^2 + x^2\right) - \frac{1-\mu}{r_1} - \frac{\mu}{r_2}, \tag{12}$$

where $r_1^2 = (x-\mu)^2 + y^2$, $r_2^2 = (x+1-\mu)^2 + y^2$, and $\mu = m_2/(m_1+m_2)$. In terms of the canonical variables

$$q_1 = x, \qquad q_2 = y, \qquad p_1 = \dot{x} - y, \qquad p_2 = \dot{y} + x, \tag{13}$$

the Hamiltonian appears as

$$H = \frac{1}{2}(p_1^2 + p_2^2) + p_1 q_2 - p_2 q_1 - \frac{1-\mu}{r_1} - \frac{\mu}{r_2}. \tag{14}$$

The equations of motion are then

$$\dot{q}_1 = \frac{\partial H}{\partial p_1} = p_1 + q_2, \tag{15a}$$

$$\dot{q}_2 = \frac{\partial H}{\partial p_2} = p_2 - q_1, \tag{15b}$$

$$\dot{p}_1 = -\frac{\partial H}{\partial q_1} = p_2 - \frac{1-\mu}{r_1^3}(q_1 - \mu) - \frac{\mu}{r_2^3}(q_1 + 1 - \mu), \tag{15c}$$

$$\dot{p}_2 = -\frac{\partial H}{\partial q_2} = -p_1 - \frac{1-\mu}{r_1^3} q_2 - \frac{\mu}{r_2^3} q_2, \tag{15d}$$

and the Hamiltonian can be rewritten as

$$H = \frac{1}{2}\left(\dot{q}_1^2 + \dot{q}_2^2\right) - \frac{1}{2}\left(q_1^2 + q_2^2\right) - \frac{1-\mu}{r_1} - \frac{\mu}{r_2}. \tag{16}$$

4.1. Integration

The conventional predictor for this system is

$$\tilde{q}_i = q_i + \dot{q}_i \tau, \qquad \tilde{p}_i = p_i + \dot{p}_i \tau, \tag{17}$$

for $i = 1, 2$. Note that, unless specified otherwise, the variables are functions of t. Let

$$\xi_1 = \frac{1}{2} q_1^2, \tag{18a}$$

$$\xi_2 = \frac{1}{2} q_2^2, \tag{18b}$$

$$\xi_3 = \frac{1}{2}\dot{q}_1^2 - \frac{1-\mu}{r_1} - \frac{\mu}{r_2}, \tag{18c}$$

$$\xi_4 = \frac{1}{2}\dot{q}_2^2. \tag{18d}$$

Here

$$H = -\xi_1 - \xi_2 + \xi_3 + \xi_4 \tag{19}$$

is a linear function of the ξs. Differentiating the ξs with respect to time, we get

$$\dot{\xi}_1 = q_1\dot{q}_1, \tag{20a}$$

$$\dot{\xi}_2 = q_2\dot{q}_2, \tag{20b}$$

$$\dot{\xi}_4 = \dot{q}_2\ddot{q}_2 = \dot{q}_2(\dot{p}_2 - \dot{q}_1), \tag{20c}$$

$$\dot{\xi}_3 = \dot{\xi}_1 + \dot{\xi}_2 - \dot{\xi}_4, \tag{20d}$$

on making use of (19), together with the conservation of H. The corrector is given by

$$\xi_i(t+\tau) = \xi_i + \frac{\tau}{2}(\dot{\xi}_i + \dot{\tilde{\xi}}_i), \tag{21}$$

for $i = 1, \ldots, 4$, where $\tilde{\xi}_i$ is simply (18) evaluated at $\tilde{q}_i$, $\tilde{p}_i$ and $t+\tau$. Inverting, the new values of q_i and p_i can be expressed in terms of ξ_i as

$$q_1 = \mathrm{sgn}(\tilde{q}_1)\sqrt{2\xi_1}, \tag{22a}$$

$$q_2 = \mathrm{sgn}(\tilde{q}_2)\sqrt{2\xi_2}, \tag{22b}$$

and, on using (15a) and (15b),

$$p_1 = -q_2 + \mathrm{sgn}(\tilde{p}_1 + \tilde{q}_2)\sqrt{2\xi_3 + \frac{2(1-\mu)}{r_1} + \frac{2\mu}{r_2}}, \tag{23a}$$

$$p_2 = q_1 + \mathrm{sgn}(\tilde{p}_2 - \tilde{q}_1)\sqrt{2\xi_4}. \tag{23b}$$

This example assumes that the mass of one body is negligible to the other two masses and that the other two masses are travelling in circular orbits. The rest of this paper discusses the general case of three or more bodies: no restrictions are placed on the masses of the bodies, and their orbits do not have to be circular, or even periodic.

5. General Three-Body Problem

The derivation of the equations of motion of the general three-body problem in a plane is described in Refs. [13], [14], and [15].

Given three bodies m_1, m_2, and m_3 with position vectors $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, and $\boldsymbol{r}_3$, where each $\boldsymbol{r}_i$ is at location (x_i, y_i), define $\boldsymbol{r}_{ij} = \boldsymbol{r}_j - \boldsymbol{r}_i$, for $i, j = 1, 2, 3$. The potential is

$$V = -\frac{Gm_1m_2}{r_{12}} - \frac{Gm_2m_3}{r_{23}} - \frac{Gm_1m_3}{r_{13}}, \tag{24}$$

where G is the gravitational constant and $r_{ij} = \sqrt{(x_j - x_i)^2 + (y_j - y_i)^2}$ is the distance between the ith and jth bodies.

The system consists of three second-order differential equations,

$$m_1\ddot{\boldsymbol{r}}_1 = -\frac{\partial V}{\partial \boldsymbol{r}_1} = \frac{Gm_1m_2(\boldsymbol{r}_2-\boldsymbol{r}_1)}{r_{12}^3} + \frac{Gm_1m_3(\boldsymbol{r}_3-\boldsymbol{r}_1)}{r_{13}^3}, \tag{25a}$$

$$m_2\ddot{\boldsymbol{r}}_2 = -\frac{\partial V}{\partial \boldsymbol{r}_2} = \frac{Gm_1m_2(\boldsymbol{r}_1-\boldsymbol{r}_2)}{r_{21}^3} + \frac{Gm_2m_3(\boldsymbol{r}_3-\boldsymbol{r}_2)}{r_{23}^3}, \tag{25b}$$

$$m_3\ddot{\boldsymbol{r}}_3 = -\frac{\partial V}{\partial \boldsymbol{r}_3} = \frac{Gm_1m_3(\boldsymbol{r}_1-\boldsymbol{r}_3)}{r_{31}^3} + \frac{Gm_2m_3(\boldsymbol{r}_2-\boldsymbol{r}_3)}{r_{32}^3}. \tag{25c}$$

These equations conserve the total linear momentum $\sum_{i=1}^3 m_i\dot{\boldsymbol{r}}_i$ (which allows us to fix the center of mass at the origin) and total angular momentum $\sum_{i=1}^3 \boldsymbol{r}_i\times m_i\dot{\boldsymbol{r}}_i$. The Hamiltonian

$$H = \sum_{i=1}^3 m_i\dot{\boldsymbol{r}}_i^2 + V, \tag{26}$$

where V is given by (24), is also conserved. We exploit the constancy of the linear momentum and center of mass position to reduce the number of degrees of freedom in the problem. It is convenient to implement this reduction by converting to Jacobi coordinates (e.g., see Refs. [16], [17], and [18]). The remaining constraints of constant total angular momentum and energy are built into the conservative integrator by transforming to a frame where these invariants are linear.

Letting $\boldsymbol{r} = \boldsymbol{r}_2 - \boldsymbol{r}_1 = (r_x, r_y)$, $M = m_1 + m_2 + m_3$, and $\mu = m_1 + m_2$, the location of the center of mass of m_1 and m_2 is seen to be at $\mu^{-1}(m_1\boldsymbol{r}_1 + m_2\boldsymbol{r}_2)$, or, since $m_1\boldsymbol{r}_1 + m_2\boldsymbol{r}_2 + m_3\boldsymbol{r}_3 = \boldsymbol{0}$, at $-\mu^{-1}m_3\boldsymbol{r}_3$. Let $\boldsymbol{\rho} = (\rho_x, \rho_y)$ be the vector from the center of mass of the first two bodies to the third body. Then $\boldsymbol{\rho} = \boldsymbol{r}_3 + \mu^{-1}m_3\boldsymbol{r}_3 = M\mu^{-1}\boldsymbol{r}_3$ and we find

$$\boldsymbol{r}_2 - \boldsymbol{r}_1 = \boldsymbol{r}, \tag{27a}$$

$$\boldsymbol{r}_3 - \boldsymbol{r}_1 = \boldsymbol{\rho} + m_2\mu^{-1}\boldsymbol{r}, \tag{27b}$$

$$\boldsymbol{r}_3 - \boldsymbol{r}_2 = \boldsymbol{\rho} - m_1\mu^{-1}\boldsymbol{r}. \tag{27c}$$

In these coordinates, following (26), the Hamiltonian can be written as

$$H = \frac{1}{2}g_1(\dot{r}_x^2 + \dot{r}_y^2) + \frac{1}{2}g_2(\dot{\rho}_x^2 + \dot{\rho}_y^2) + V \tag{28}$$

in terms of the reduced masses $g_1 = m_1m_2\mu^{-1}$ and $g_2 = m_3\mu/M$, where V is given by (24).

Define $r_x = r\cos\theta$, $r_y = r\sin\theta$, $\rho_x = \rho\cos\Theta$, and $\rho_y = \rho\sin\Theta$. In these polar coordinates, the Hamiltonian can be rewritten

$$H = \frac{p^2}{2g_1} + \frac{P^2}{2g_2} + \frac{\ell^2}{2g_1r^2} + \frac{L^2}{2g_2\rho^2} + V(r,\rho,\theta,\Theta), \tag{29}$$

where p is the linear momentum of the first reduced mass, ℓ is the angular momentum of the first reduced mass, P is the linear momentum of the second reduced mass, L is the angular momentum of the second reduced mass, and $V = V(r,\rho,\theta,\Theta)$ is the potential

energy of the system. The Hamiltonian H and the total angular momentum $\ell + L$ are conserved, and the center of mass remains at the origin for all time.

The equations of motion in polar coordinates are

$$\dot{r} = \frac{\partial H}{\partial p} = \frac{p}{g_1}, \qquad \dot{\theta} = \frac{\partial H}{\partial \ell} = \frac{\ell}{g_1 r^2}, \tag{30a}$$

$$\dot{p} = -\frac{\partial H}{\partial r} = \frac{\ell^2}{g_1 r^3} - \frac{\partial V}{\partial r}, \qquad \dot{\ell} = -\frac{\partial H}{\partial \theta} = -\frac{\partial V}{\partial \theta}, \tag{30b}$$

$$\dot{\rho} = \frac{\partial H}{\partial P} = \frac{P}{g_2}, \qquad \dot{\Theta} = \frac{\partial H}{\partial L} = \frac{L}{g_2 \rho^2}, \tag{30c}$$

$$\dot{P} = -\frac{\partial H}{\partial \rho} = \frac{L^2}{g_2 \rho^3} - \frac{\partial V}{\partial \rho}, \qquad \dot{L} = -\frac{\partial H}{\partial \Theta} = -\frac{\partial V}{\partial \Theta}. \tag{30d}$$

5.1. Integration

The variables can be transformed as

$$\xi_1 = \frac{p^2}{2g_1} + \frac{\ell^2}{2g_1 r^2}, \qquad \xi_2 = \frac{P^2}{2g_2} + \frac{L^2}{2g_2 \rho^2}, \tag{31a}$$

$$\xi_3 = V, \qquad \xi_4 = \rho, \qquad \xi_5 = \ell, \qquad \xi_6 = L, \qquad \xi_7 = \theta, \qquad \xi_8 = \Theta, \tag{31b}$$

so that the conserved Hamiltonian becomes a linear function of the transformed variables: $H = \xi_1 + \xi_2 + \xi_3$. The time derivatives become

$$\dot{\xi}_1 = \frac{p\dot{p}}{g_1} + \frac{\ell r^2 \dot{\ell} - r\ell^2 \dot{r}}{g_1 r^4}, \tag{32a}$$

$$\dot{\xi}_2 = \frac{P\dot{P}}{g_2} + \frac{L\rho^2 \dot{L} - \rho L^2 \dot{\rho}}{g_2 \rho^4}, \tag{32b}$$

$$\dot{\xi}_3 = \frac{\partial V}{\partial r}\dot{r} + \frac{\partial V}{\partial \theta}\dot{\theta} + \frac{\partial V}{\partial \rho}\dot{\rho} + \frac{\partial V}{\partial \Theta}\dot{\Theta}, \tag{32c}$$

$$\dot{\xi}_4 = \dot{\rho}, \qquad \dot{\xi}_5 = \dot{\ell}, \qquad \dot{\xi}_6 = \dot{L}, \qquad \dot{\xi}_7 = \dot{\theta}, \qquad \dot{\xi}_8 = \dot{\Theta}. \tag{32d}$$

The integration procedure is an extension of the method used for the Kepler problem. We can invert to find the original variables as follows,

$$\rho = \xi_4, \qquad \ell = \xi_5, \qquad L = \xi_6, \qquad \theta = \xi_7, \qquad \Theta = \xi_8, \tag{33a}$$

$$r = g(\xi_3, \rho, \theta, \Theta), \tag{33b}$$

$$p = \mathrm{sgn}(\tilde{p}) \sqrt{2g_1 \left(\xi_1 - \frac{\ell^2}{2g_1 r^2} \right)}, \tag{33c}$$

$$P = \mathrm{sgn}(\tilde{P}) \sqrt{2g_2 \left(\xi_2 - \frac{L^2}{2g_2 \rho^2} \right)}. \tag{33d}$$

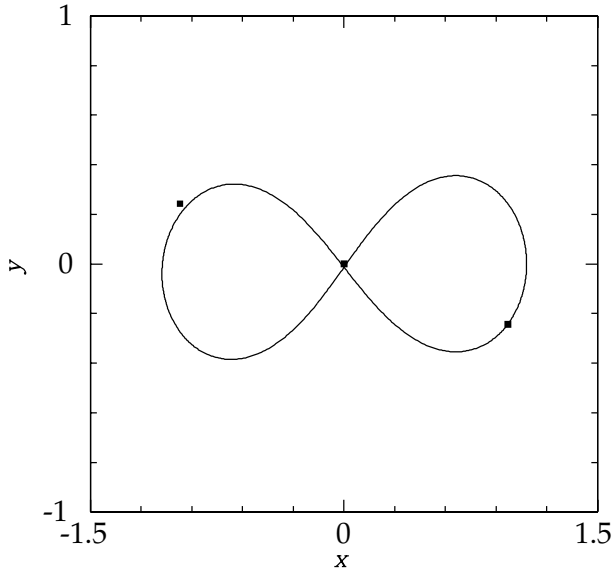

Figure 1. Conservative predictor–corrector solution for a general three-body choreography.

The value of the inverse function g defined by $V(g(\xi_3, \rho, \theta, \Theta), \rho, \theta, \Theta) = \xi_3$ is determined at fixed ρ, θ, Θ by Newton–Raphson iteration, using the predicted value $\tilde{r}$ as an initial guess.

In Fig. 1 we use our conservative predictor–corrector to illustrate the remarkable three-body figure-eight *choreography* discovered by Chenciner and R. Montgomery [19] and located numerically by Simó [20]. The dots indicate the initial positions of the three unit masses. The gravitational constant G is taken to be unity and the initial conditions are those cited in [19]:

$$\begin{aligned}
&\boldsymbol{r}_1 = (0.97000436, -0.24308753), \quad \boldsymbol{r}_2 = (0, 0),\\
&\boldsymbol{r}_3 = (-0.97000436, 0.24308753).\\
&\dot{\boldsymbol{r}}_1 = (0.46620369, 0.43236573), \quad \dot{\boldsymbol{r}}_2 = (-0.93240737, -0.86473146),\\
&\dot{\boldsymbol{r}}_3 = (0.46620369, 0.43236573).
\end{aligned} \tag{34}$$

We used a fixed time step of $\tau = 10^{-4}$ and integrated for a complete choreographic period, during which each mass travels once around the figure eight.

6. General n-Body Problem

The Jacobi coordinates can be extended to $n \geq 2$ bodies in a plane [18, 16]. Let each body of mass m_i have radius vectors $\boldsymbol{r}_i$, where $i = 1, \ldots, n$. Define $\boldsymbol{r}_{ij} = \boldsymbol{r}_j - \boldsymbol{r}_i$ as the vector joining m_i to m_j. Also define $\boldsymbol{C}_i$ to be the center of mass of the first i bodies, where $i = 2, \ldots, n$, and choose the origin of the coordinate system so that $\boldsymbol{C}_n = \boldsymbol{0}$. Let the vectors $\boldsymbol{\rho}_i$ be defined such that

$$\boldsymbol{\rho}_2 = \boldsymbol{r}_{12}, \tag{35a}$$

$$\boldsymbol{\rho}_3 = \boldsymbol{r}_3 - \boldsymbol{C}_2, \tag{35b}$$

$$\ldots \tag{35c}$$

$$\boldsymbol{\rho}_n = \boldsymbol{r}_n - \boldsymbol{C}_{n-1}. \tag{35d}$$

Also,

$$\boldsymbol{r}_{k\ell} = \boldsymbol{\rho}_\ell - \boldsymbol{\rho}_k + \sum_{j=k}^{\ell-1} \frac{m_j \boldsymbol{\rho}_j}{M_j}, \tag{36}$$

where $1 \le k < \ell \le n$, and $M_j = \sum_{k=1}^{j-1} m_k$.§

The reduced masses are

$$g_2 = \frac{m_2 m_1}{M_2}, \tag{37}$$

$$g_3 = \frac{m_3(m_2 + m_1)}{M_3}, \tag{38}$$

$$\ldots \tag{39}$$

$$g_n = \frac{m_n M_{n-1}}{M_n}. \tag{40}$$

The equations of motion in polar coordinates are just an extension of the three-body problem:

$$\dot{\rho}_i = \frac{\partial H}{\partial p_i} = \frac{p_i}{g_i}, \tag{41a}$$

$$\dot{\theta}_i = \frac{\partial H}{\partial \ell_i} = \frac{\ell_i}{g_i \rho_i^2}, \tag{41b}$$

$$\dot{p}_i = -\frac{\partial H}{\partial \rho_i} = \frac{\ell_i^2}{g_i \rho_i^3} - \frac{\partial V}{\partial \rho_i}, \tag{41c}$$

$$\dot{\ell}_i = -\frac{\partial H}{\partial \theta_i} = -\frac{\partial V}{\partial \theta_i}, \tag{41d}$$

where ρ_i, θ_i, p_i and ℓ_i are the radius, angle, linear momentum, and angular momentum, respectively, of the ith reduced mass, for $i = 2, \ldots, n$. The potential is defined to be

$$V = -\sum_{\substack{i,j=1 \\ i<j}}^{n} \frac{G m_i m_j}{r_{ij}} \tag{42}$$

and the total kinetic energy is

$$K = \frac{1}{2} \sum_{i=2}^{n} \left(\frac{p_i^2}{g_i} + \frac{\ell_i^2}{g_i \rho_i^2} \right). \tag{43}$$

It is easy to verify that the Hamiltonian $H = K + V$ is conserved by (41). The total angular momentum $\sum_{i=2}^{n} \ell_i$ is also conserved, and the center of mass remains at the origin for all time.

§ Here $\boldsymbol{\rho}_1$ is a dummy variable that cancels out in the expression for r_{12}.

6.1. Integration

Transform $(\boldsymbol{\rho}, \boldsymbol{\theta}, \boldsymbol{p}, \boldsymbol{\ell})$ to $(\boldsymbol{\zeta}, \boldsymbol{\theta}, \boldsymbol{\eta}, \boldsymbol{\ell})$, where

$$\zeta_2 = V, \tag{44a}$$

$$\zeta_i = \rho_i, \qquad \text{for } \ i = 3, \ldots, n, \tag{44b}$$

$$\eta_i = \frac{p_i^2}{2g_i} + \frac{\ell_i^2}{2g_i\rho_i^2}, \qquad \text{for } \ i = 2, \ldots, n. \tag{44c}$$

Note that H is a linear function of the transformed variables:

$$H = \sum_{i=2}^{n} \eta_i + \zeta_2, \tag{45}$$

as is the total angular momentum $L = \sum_{i=2}^{n} \ell_i$. The time derivatives of $\boldsymbol{\zeta}$ and $\boldsymbol{\eta}$ are given by

$$\dot{\zeta}_2 = \sum_{i=2}^{n} \left(\frac{\partial V}{\partial \rho_i}\dot{\rho}_i + \frac{\partial V}{\partial \theta_i}\dot{\theta}_i \right), \tag{46a}$$

$$\dot{\zeta}_i = \dot{\rho}_i, \qquad \text{for } \ i = 3, \ldots, n, \tag{46b}$$

$$\dot{\eta}_i = \frac{p_i\dot{p}_i}{g_i} + \frac{\ell_i\rho_i^2\dot{\ell}_i - \rho_i\ell_i^2\dot{\rho}_i}{g_i\rho_i^4}, \qquad \text{for } \ i = 2, \ldots, n. \tag{46c}$$

The predictor equations are

$$\tilde{\rho}_i = \rho_i + \dot{\rho}_i\tau, \qquad \tilde{\theta}_i = \theta_i + \dot{\theta}_i\tau, \tag{47a}$$

$$\tilde{p}_i = p_i + \dot{p}_i\tau, \qquad \tilde{\ell}_i = \ell_i + \dot{\ell}_i\tau \tag{47b}$$

and the corrector is given by

$$\zeta_i(t+\tau) = \zeta_i + \frac{\tau}{2}(\dot{\zeta}_i + \dot{\tilde{\zeta}}_i), \qquad \theta_i(t+\tau) = \theta_i + \frac{\tau}{2}(\dot{\theta}_i + \dot{\tilde{\theta}}_i), \tag{48a}$$

$$\eta_i(t+\tau) = \eta_i + \frac{\tau}{2}(\dot{\eta}_i + \dot{\tilde{\eta}}_i), \qquad \ell_i(t+\tau) = \ell_i + \frac{\tau}{2}(\dot{\ell}_i + \dot{\tilde{\ell}}_i), \tag{48b}$$

for $i = 2, \ldots, n$.

One then inverts to get the original variables as functions of the temporary transformed variables:

$$\rho_i = \zeta_i \qquad \text{for } \ i = 3, \ldots, n, \tag{49a}$$

$$\rho_2 = g(\zeta_2, \rho_3, \ldots, \rho_n, \boldsymbol{\theta}), \tag{49b}$$

$$p_i = \operatorname{sgn}(\tilde{p}_i)\sqrt{2g_i\left(\eta_i - \frac{\ell_i^2}{2g_i\rho_i^2}\right)}, \qquad \text{for } \ i = 2, \ldots, n. \tag{49c}$$

The value of the inverse function g defined by

$$V(g(\zeta_2, \rho_3, \ldots, \rho_n, \boldsymbol{\theta}), \rho_3, \ldots, \rho_n, \boldsymbol{\theta}) = \zeta_2 \tag{50}$$

is determined at fixed $\rho_3, \ldots, \rho_n, \boldsymbol{\theta}$ with a Newton–Raphson method, using the predicted value $\tilde{\rho}_2$ as an initial guess.

In Fig. 2, we illustrate Simó's four-body choreography [20]. The motions of one of the four unit masses as determined by the predictor–corrector and conservative predictor–corrector algorithms are compared, using the fixed time step $\tau = 10^{-3}$ to integrate the system from time $t = 0$ to $t = 11.5$. The gravitational constant G is taken to be unity and the initial conditions are given by

$$\begin{aligned}
&\boldsymbol{r}_1 = (1.382857, 0), \quad \boldsymbol{r}_2 = (0, 0.157030),\\
&\boldsymbol{r}_3 = (-1.382857, 0), \quad \boldsymbol{r}_4 = (0, -0.157030),\\
&\dot{\boldsymbol{r}}_1 = (0, 0.584873), \quad \dot{\boldsymbol{r}}_2 = (1.871935, 0),\\
&\dot{\boldsymbol{r}}_3 = (0, -0.584873), \quad \dot{\boldsymbol{r}}_4 = (-1.871935, 0).
\end{aligned} \tag{51}$$

As τ is decreased, the predictor–corrector solution converges to the conservative predictor–corrector solution obtained with a large time step. This emphasizes that the conservative predictor–corrector can be viewed as a finite-time-step generalization of the conventional predictor–corrector, as argued in Ref. [1]. We also compare these solutions to a symplectic map based on the simple second-order kinetic–potential energy splitting

$$\begin{aligned}
\tilde{p}_i &= p_i - \frac{\tau}{2}\frac{\partial}{\partial q_i} V(q_1, q_2, \ldots, q_N),\\
q_i' &= q_i + \tau \frac{\partial}{\partial \tilde{p}_i} K(\tilde{p}_1, \tilde{p}_2, \ldots, \tilde{p}_N),\\
p_i' &= \tilde{p}_i - \frac{\tau}{2}\frac{\partial}{\partial q_i'} V(q_1', q_2', \ldots, q_N'),
\end{aligned} \tag{52}$$

to evolve the canonical variables (q_i, p_i) to (q_i', p_i'), for $i = 1, \ldots, N$. This second-order scheme, which is implemented as the method SKP using Varadi's `NBI` code with $\tau = 10^{-3}$, is similar to the one described by Forest and Ruth [7, 8], with the roles of the coordinates and momenta interchanged.

In Figure 3, we compare the root-mean-square error in the computed trajectory between $t = 0$ and $t = 4\pi$ (twice the period of the choreography), for each of these integration algorithms. The error was computed relative to a fifth-order Runge–Kutta integrator with time step $\tau = 10^{-5}$. Of the three other solutions, we note that the conservative predictor–corrector trajectory is the most accurate. For general n-body integrations, our conservative algorithm was also observed to be more accurate than the second-order symplectic Wisdom–Holman scheme [21, 22, 23], but this is expected since the latter applies only to small perturbations of Keplerian orbits.

7. Conclusion

Conservative integration algorithms can reduce the computational effort required to integrate a system of ordinary differential equations. For example, when the total energy and angular momentum of the n-body problem is conserved, it is possible to obtain accurate trajectories using a larger time step than with conventional integration

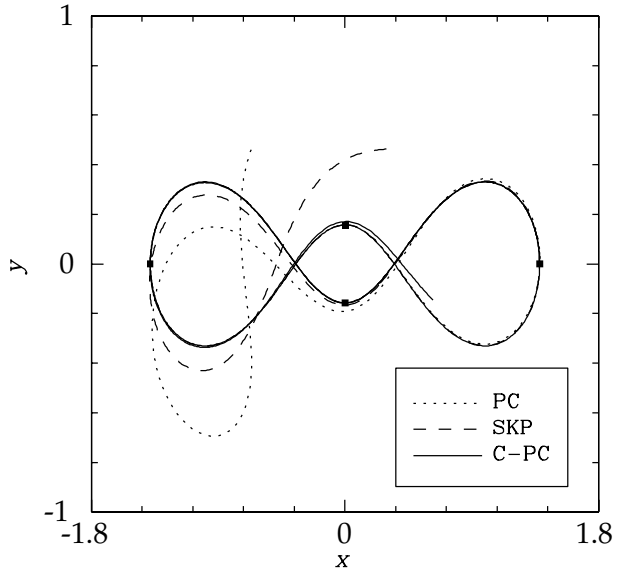

Figure 2. The predictor–corrector (dotted line), symplectic (dashed line) and conservative predictor–corrector (solid line) solutions for a four-body choreography.

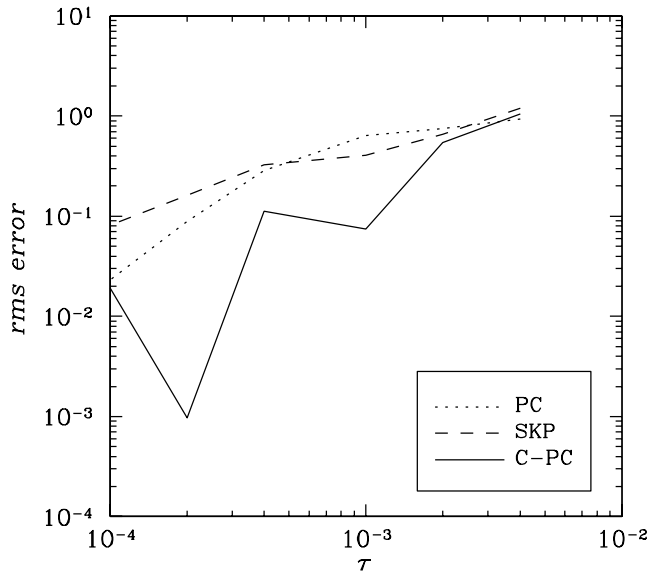

Figure 3. Root-mean-square error of the predictor–corrector (dotted line), symplectic (dashed line) and conservative predictor–corrector (solid line) solutions in Fig. 2.

methods. This is particularly relevant for extremely long-time integrations. In contrast, symplectic methods typically predict a total energy that oscillates about the correct value. In some cases, these oscillations can eventually lead to large excursions from the mean value, similar to random walk diffusion. In addition, there are certain statistical mechanical systems (such as equipartition states of inviscid fluids) where the final mean state is a function of only the initial values of the invariants; for these systems, a conservative integrator is clearly preferable to a symplectic algorithm. However, as

these methods put the integration error into different places, the integration method that is most suitable for a given system ultimately depends on the nature of the physical problem, the integration time scale, and the kinds of questions addressed by the numerical simulation.

In the case of the n-body problem for planar motion, there are six invariants, all of which need to be considered during the integration. Jacobi coordinates were used to reduce the system to an $(n-1)$-body problem in which the linear momentum and center of mass constraints are implicitly built in, leaving fewer conservation laws to be explicitly designed into the algorithm. In Jacobi coordinates, the kinetic energy term of the Hamiltonian remains in diagonal form (a sum of squares); this makes it easy to express the Hamiltonian as a linear function of new variables.

Future work in this area should include extending the numerical code to the full three-dimensional case and regularizing the potential terms to handle collisions and close approaches. One could also build in precession, nutation, and tidal effects into the equations of motion.

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Appendix A. Error Analysis

Here we describe the local error analysis of the second-order conservative predictor–corrector scheme given by (2a) and (3). We assume that both f and T are analytic functions and that the points where T' vanishes are isolated. For notational simplicity, we restrict the analysis to the autonomous one-dimensional ordinary differential equation $dx/dt = f(x)$, for which the exact solution is given by

$$x(t+\tau) = x_0 + \tau f(x_0) + \frac{\tau^2}{2} f'(x_0) f(x_0) + \frac{\tau^3}{6} f(x_0)[f''(x_0) f(x_0) + f'^2(x_0)] + \mathcal{O}(\tau^4). \tag{A.1}$$

The conservative predictor–corrector scheme

$$\tilde{x} = x_0 + \tau f(x_0), \tag{A.2}$$

$$\xi(t+\tau) = \xi_0 + \frac{\tau}{2}\left[T'(x_0) f(x_0) + T'(\tilde{x}) f(\tilde{x})\right] \tag{A.3}$$

yields the solution

$$\begin{aligned}\xi(t+\tau) &= \xi_0 + \frac{\tau}{2}\left[T' f + T' f + \left(T' f\right)' \tau f + \left(T' f\right)'' \frac{\tau^2 f^2}{2} + \mathcal{O}(\tau^3)\right] \\ &= \xi_0 + \tau T' f + \frac{\tau^2}{2}\left(T'' f^2 + T' f' f\right) \\ &\quad + \frac{\tau^3}{4}\left(T''' f^3 + 2T'' f' f^2 + T' f'' f^2\right) + \mathcal{O}(\tau^4),\end{aligned} \tag{A.4}$$

where the expressions on the right-hand side are all evaluated at x_0. The new value of x is then given by

$$\begin{aligned} x(t+\tau) &= T^{-1}\left(\xi(t+\tau)\right) \\ &= T^{-1}(\xi_0) + T^{-1\prime}(\xi_0)\left[\tau T' f + \frac{\tau^2}{2}\left(T'' f^2 + T' f' f\right)\right. \\ &\quad \left. + \frac{\tau^3}{4}\left(T''' f^3 + 2T'' f' f^2 + T' f'' f^2\right) + \mathcal{O}(\tau^4)\right] \\ &\quad + \frac{1}{2} T^{-1\prime\prime}(\xi_0)\left[\tau T' f + \frac{\tau^2}{2}\left(T'' f^2 + T' f' f\right) + \mathcal{O}(\tau^3)\right]^2 \\ &\quad + \frac{1}{6} T^{-1\prime\prime\prime}(\xi_0)\left[\tau T' f + \mathcal{O}(\tau^2)\right]^3 + \mathcal{O}(\tau^4). \end{aligned} \tag{A.5}$$

By implicitly differentiating the identity $T^{-1}(T(x)) = x$, it follows that

$$T^{-1\prime}(\xi_0) = \frac{1}{T'}, \quad T^{-1\prime\prime}(\xi_0) = -\frac{T''}{T'^3}, \quad T^{-1\prime\prime\prime}(\xi_0) = \frac{3T''^2}{T'^5} - \frac{T'''}{T'^4}, \tag{A.6}$$

so that (A.5) simplifies to

$$\begin{aligned} x(t+\tau) &= x_0 + \tau f(x_0) + \frac{\tau^2}{2} f'(x_0) f(x_0) \\ &\quad + \frac{\tau^3}{4}\left[f''(x_0) f^2(x_0) + \frac{T'''(x_0)}{3T'(x_0)} f^3(x_0)\right] + \mathcal{O}(\tau^4). \end{aligned} \tag{A.7}$$

On setting $T(x) = x$, we obtain the usual error estimate for the conventional predictor–corrector. We see that both conservative and conventional schemes are accurate to second order in τ; moreover, for quadratic transformations like $T(x) = x^2$, which in light of Lemma 1 are often useful for enforcing energy conservation, the conservative and conventional schemes agree through third order in τ. The appearance of $T'(x_0)$ in the denominator of the third-order (error) term emphasizes that we must exercise care at singular points of T. Near these points, either a conventional scheme can be used or the time step can be reduced, as previously remarked [2]. Should $T'(x_0) = 0$, the estimate (A.7) should be replaced by

$$x(t+\tau) = T^{-1}\left(T(x_0) + \frac{\tau}{2} T'(\tilde{x}) f(\tilde{x})\right), \tag{A.8}$$

which is guaranteed to have a solution for sufficiently small τ if the points at which T' vanishes are isolated. The transformation is then invertible at $x(t+\tau)$, allowing the integration to be continued beyond the point of singularity.

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