An Exactly Conservative Integrator for the $n$-Body Problem

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Chapter 1

Integrability and the $n$-Body Problem

1.1 Introduction

Much of nature’s behaviour and patterns can be described by differential equations. We can write down the differential equations that describe many physical problems, but we also need to be able to integrate them. This means finding expressions for the functions which satisfy the differential equations and agree with the initial conditions imposed at a particular initial time (Goroff 1993). However, the notion of integrability is very difficult to define precisely. In his essay entitled “Science and Method” (Poincaré 1903), Henri Poincaré attempted to make a clear statement about integrability:

“If we knew exactly the laws of nature and the situation of the universe at the initial moment, we could predict exactly the situation of that same universe at a succeeding moment, but even if it were the case that the natural laws had no longer any secret for us, we could still only know the initial situation approximately. If that enabled us to predict the succeeding situation with the same approximations, that is all we require, and we should say that the phenomenon had been predicted, that it is governed by laws. But it is not always so; it may happen that small differences in the initial conditions produce very great ones in the final phenomena. A small error in the former will produce an enormous error in the latter. Prediction becomes impossible, and we have the fortuitous phenomena.”

The latter cases that Poincaré refers to have some initial conditions where the motion is chaotic. Mathematical research in chaos started in the late 1800s, when Poincaré studied the stability of the solar system. In the special case of iterations of transformations, there are three common characteristics of chaos (Peitgen et al. 1992): sensitive dependence on initial conditions (as described above by Poincaré),
mixing (for any two open sets \(I\) and \(J\) of non-zero measure, one can find initial values in \(I\) that, when integrated, will eventually lead to points in \(J\)), and dense periodic orbits.

To solve such differential equations, one needs to discretize the equations and solve them numerically. However, discretization typically leads to a loss of accuracy; invariants are not necessarily preserved and the phase portrait may be inaccurate. One way of dealing with this problem is to take small time steps. As a result, a computer would require a long time to integrate such a system accurately. An algorithm used to integrate such systems should be as efficient as possible. Is there a way to keep the time step large and still preserve accuracy?

One such integrator, the *conservative predictor-corrector*, was recently developed (Shadwick et al. 1999). This integrator is made efficient by building in the analytical structure of the equations, in particular, by keeping the constants of motion conserved. In this paper, I will be discussing its efficiency and comparing it to the standard predictor-corrector method. The conservative predictor-corrector is believed to be more efficient than the standard predictor-corrector, and I will demonstrate this by applying both integrators to the \(n\)-body problem of classical mechanics, where the “bodies” are the stars/moons/planets of the universe.

### 1.2 Background

Theories of the orbits of the sun and planets have been in place as early as the days before Christ. During this era, the most accepted theories were the *geocentric* scheme of the universe, in which the heavenly bodies rotate around the Earth. The *Almagest*, devised by Claudius Ptolemaeus (Ptolemy), described a geocentric system which lasted for more than 1300 years. He concluded that not all celestial bodies were circling the Earth in perfectly Earth-centered orbits (Williams 1996).

However, in the 15th and 16th centuries, the *heliocentric* system (in which the Earth and other planets revolve around the Sun) was gaining acceptance. Nicholas Copernicus was a major rejuvenator of this system, which had not been popular in earlier times. He suggested a system in which all the known planets had circular orbits around the Sun. Johannes Kepler discarded the assumption of circular orbits in favour of elliptical paths around the sun, with the Sun at one of the foci. His other two laws of planetary motion include: a directed line from the Sun to a planet sweeps out equal areas in equal times, and the square of the period of orbit of each planet is proportional to the cube of its semimajor axis.

In 1687, Isaac Newton published the *Principia*, presenting revolutionary ideas about celestial mechanics, laws of motion, and other ideas. In this book he stated the second law of motion:

\[ F = ma, \]  
(1.1)
where \( \mathbf{a} \) is the acceleration and \( \mathbf{F} \) is the force, and the law of universal gravitation:

\[
\mathbf{F} = \frac{k m_1 m_2}{r^2} \mathbf{r},
\]

which says that there is a universal attraction between all bodies in space. Here, \( \mathbf{F} \) is the attractive gravitational force, \( k \) is a universal gravitational constant, and \( r \) is the distance between the two bodies of mass \( m_1 \) and \( m_2 \).

Since then, much work was done to understand the \( n \)-body problem. Johann Bernoulli proved that the motion of one particle with respect to another is described by a conic section and later won a French Academy Prize for his analytical treatment of the two-body problem (Barrow-Green 1997).

Analyzing the general \( n \)-body problem \( (n \geq 3) \) proved to be a much more difficult task. A vast effort to identify integrals in the three-body problem was launched. In the end, Poincaré was the first to show that there is chaos in the orbital motion of three bodies which mutually exert gravitational forces on each other (Goroﬀ 1993, Peitgen et al. 1992). In the 18th and 19th centuries, both Joseph-Louis Lagrange and Karl Gustav Jacobi were able to minimize the number of free variables by various means, as I will discuss in Chapters 4 and 5 (Barrow-Green 1997, Szebehely 1967, Pollard 1966).

Some special cases of the three-body problem were found by Lagrange and Euler (Diacu & Holmes 1996) and (Pollard 1966). In the 18th century, Euler proved that if three particles of arbitrary finite mass are arranged initially on a line (with suitable initial velocities assigned to the masses), then the particles will move periodically on ellipses, maintaining at all times a collinear configuration. Lagrange showed that a similar thing will happen when the masses are initially on the vertices of an equilateral triangle (i.e., they will move in ellipses, preserving their equilateral configuration).

Another special case is the restricted three-body problem, in which one mass is negligible relative to the other two, to be discussed in Chapter 3.

### 1.3 Motivation for Studying this Problem

A thorough knowledge of the orbits of planets, and a knowledge of how to integrate their equations of motion can allow one to verify the stability of the solar system: will the planets continue moving indefinitely in their present orbits? Or will there eventually be a collision between at least two bodies? Will some bodies leave orbit? Poincaré never found an answer to these questions (Peitgen et al. 1992), despite his discovery of chaos in the general three-body problem.

Another interesting application of the \( n \)-body problem is the idea of historical dating. The underlying idea here is the following: twelve zodiac constellations are placed along the ecliptic (the intersection of the celestial sphere with the plane of the Earth’s orbit). Each of the twelve zodiac constellations is located in a sector approximately 30 degrees long. In everyday language, we think of the sky as a convex
pie and we are dividing the pie into twelve equal pieces. At any given time, each of the planets appears in one of the sectors (that is, appears to be “in” one of the constellations; see Fomenko (1994)). From this a horoscope can be constructed. A horoscope is a chart that shows the positions of the planets with respect to zodiac constellations.

If we know the current position of planets, and we know of an ancient horoscope (which, of course, tells us the position of the planets at that time), we can integrate backwards (using the current positions as initial conditions) and see if, indeed, at that ancient time, the planets were in the location specified by the horoscope. If there is a discrepancy, we can conclude that either the ancient horoscope was dated inaccurately, the constellations in the zodiac have themselves been distorted or shifted, the horoscope was misinterpreted, or that perhaps there are certain years or even centuries that never occurred. The latter has actually been suggested by a group of Russian mathematicians (Fomenko 1994, Taylor 2000).

These controversial but exciting topics inspired me to study the $n$-body problem. For simplicity, I will be looking at the case where all of the planets lie in a plane.
Chapter 2

Conservative Integration and the Kepler Problem

2.1 Description of Conservative Integration

The equations describing the motion of the solar system form a conservative system: the friction which heavenly bodies sustain is so little that no energy is lost. When studying the theory behind the $n$-body problem, one learns that both the total energy and total angular momentum are conserved. It can be argued that any invariants that exist in theory should remain invariant when the system is discretized and integrated on the computer.

One way to preserve these invariants is to transform to a new space where the energy and other conserved quantities are linear functions of the transformed variables, and then transform back to get new values for each variable (Shadwick et al. 1999, Bowman et al. 1997). Often the transformation back involves radicals, and if the argument of the radical is negative, it is still possible to use a finite number of time-step reductions to integrate the system (Bowman et al. 1997). Another way to deal with the negative arguments is to switch to a conventional integrator (predictor-corrector) for that one time step (Kotovych & Bowman 2002).

Given a system of ordinary differential equations
\[ \frac{d\mathbf{x}}{dt} = f(t, \mathbf{x}), \]
where $\mathbf{x} = (x_1, \ldots, x_n)$, the Euler method provides an approximate value $\tilde{\mathbf{x}}$ for the vector $\mathbf{x}$ at the time $t + \tau$, given the value $\mathbf{x}_0$ at the time $t$, by way of the following formula:
\[ \tilde{\mathbf{x}} = \mathbf{x}_0 + \tau f(t, \mathbf{x}_0). \]
(For example, see Press et al. (1992).)

However, it is normally advantageous to use a scheme that is higher order than Euler's method. Consider the second-order predictor-corrector scheme (the first equa-
tion being the predictor and the second being the corrector)

\[
\dot{x} = x_0 + \tau f(t, x_0), \tag{2.1a}
\]

\[
x(t + \tau) = x_0 + \frac{\tau}{2} [f(t, x_0) + f(t + \tau, \dot{x})]. \tag{2.1b}
\]

The basic principle behind conservative predictor–corrector algorithms is the following: let the vector \( x \) be transformed as \( \xi = T(x) \) such that the quantities to be conserved are linear functions of the new variables \( \xi_i, i = 1, \ldots, n \). Then, keeping Eq. (2.1a) as the predictor, apply in the transformed space the corrector:

\[
\dot{\xi}(t + \tau) = \xi_0 + \frac{\tau}{2} [T'(x)f(t, x_0) + T'(|\dot{x}|)f(t + \tau, |\dot{x}|)], \tag{2.2}
\]

where \( \dot{\xi}(t) = T'(\dot{x}) \) and \( T' \) is the derivative of \( T \). The inverse transformation is

\[
x(t + \tau) = T^{-1}(\xi(t + \tau)).
\]

If the transformation involves a square root, then the sign of the root can be taken to be the sign given by the conventional predictor. The examples that I consider in my report will clarify this concept.

According to Iserles (1997), a major drawback of traditional non-conservative integrators is that numbers are often “thrown into the computer.” The mathematical model is discretized according to an algorithm (for example, Runge–Kutta or multigrid) which has nothing to do with the original problem. Instead, we should be developing computational algorithms that reflect known qualitative features of the problem under consideration. The conservative predictor–corrector is an example of such an integrator. In the examples given by Shadwick et al. (1999, 2001), the transformed \( T \) is chosen to work for the system at hand, rather than having one general “formula” that applies to a generic system. With this method, we can get all of the invariants of the \( n \)-body problem conserved exactly, even when using large time steps. This leads to a more accurate picture of the motion of the bodies (Shadwick et al. 1999, figure 9) with a large time step.

According to Ge and Marsden (1988), if an integrator is symplectic (preserves phase space structure) and is conservative (conserves the energy), then it must be exact. Therefore, a drawback with conservative integration is that the phase space structure is not preserved. Likewise, a disadvantage with symplectic integration is that the energy is not conserved.

### 2.2 Kepler Problem

#### 2.2.1 Derivation of the Equations of Motion

The Kepler problem can be described as follows: begin with two bodies \( m_1 \) and \( m_2 \) respectively, located at positions \( r_1 \) and \( r_2 \). The problem can be reduced to an
equivalent one-body problem (a single particle under the influence of a central force of mass $m = m_1 m_2 / (m_1 + m_2)$, at position $r = r_2 - r_1$). The gravitational force given by Eq. (1.2) is derivable from a potential $V = -k/r$, where $r = |r|$, and $k$ is the gravitational constant. This is a conservative system with Hamiltonian

$$H = \frac{1}{2}mv^2 + V,$$

where $v$ is the magnitude of the velocity and $v = dr/dt$.

The equations of motion for the Kepler problem can be derived by letting

$$\mathbf{r} = r\hat{r},$$

where

$$\hat{r} = (\cos \theta, \sin \theta)$$

and

$$\hat{r} = (-\dot{\theta} \sin \theta, \dot{\theta} \cos \theta).$$

If we set

$$\hat{\theta} = (-\sin \theta, \cos \theta),$$

then

$$\dot{\hat{r}} = \dot{\theta} \hat{\theta}.$$

From Eq. (2.4),

$$\dot{\mathbf{r}} = i\hat{r} + r\dot{\theta} \hat{\theta} = \mathbf{v},$$

where $\mathbf{v} = (v_r, v_\theta) = (\dot{r}, r\dot{\theta})$. Differentiating once more, we get

$$\dot{\mathbf{v}} = \ddot{r}\hat{r} + 2r\dot{\theta} \hat{\theta} + r\dot{\theta}^2 \hat{r} - r\dot{\theta}^2 \hat{r}.$$

The acceleration $\mathbf{v}$ per unit mass is, from Eq. (1.1),

$$\dot{\mathbf{v}} = \mathbf{F}/m = -\nabla V/m;$$

that is,

$$\dot{\mathbf{v}} = -\frac{1}{m} \left( \frac{\partial V}{\partial r} \hat{r} + \frac{1}{r} \frac{\partial V}{\partial \theta} \hat{\theta} \right).$$

In particular, since $V$ is independent of $\theta$, only the first term remains. Equating Eq. (2.6) and Eq. (2.7), we find

$$-\frac{1}{m} \left( \frac{\partial V}{\partial r} \right) = \frac{dv_r}{dt} - r\dot{\theta}^2$$

and

$$0 = 2r\dot{\theta} + r\ddot{\theta}. $$

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The last equation can also be written as

\[ 0 = \frac{1}{r} \frac{d}{dt} (r^2 \dot{\theta}), \]

or

\[ \dot{\ell} = 0, \]

where \( \ell = mr^2 \dot{\theta} \) is the conserved angular momentum. (Note that \( m \) is assumed to be constant.) Therefore our equations of motion are

\[ v_r = \frac{dr}{dt}, \]  \hspace{1cm} (2.8a)

\[ \frac{dv_r}{dt} = -\frac{1}{m} \left( \frac{\partial V}{\partial r} \right) + r \ddot{\theta}, \]  \hspace{1cm} (2.8b)

\[ \frac{d\theta}{dt} = \frac{\ell}{mr^2}, \]  \hspace{1cm} (2.8c)

\[ \frac{d\ell}{dt} = 0. \]  \hspace{1cm} (2.8d)

Rewriting the equations in terms of the linear momentum \( p = mv_r \) and the angular momentum \( \ell \) gives

\[ \frac{dr}{dt} = \frac{\partial H}{\partial p} = \frac{p}{m}, \]

\[ \frac{dp}{dt} = -\frac{\partial H}{\partial r} = \frac{\ell^2}{mr^2} - \left( \frac{\partial V}{\partial r} \right), \]

\[ \frac{d\theta}{dt} = \frac{\partial H}{\partial \ell} = \frac{\ell}{mr^2}, \]

\[ \frac{d\ell}{dt} = -\frac{\partial H}{\partial \theta} = 0, \]

where the Hamiltonian is

\[ H = \frac{p^2}{2m} + \frac{\ell^2}{2mr^2} + V(r). \]

Also see Goldstein (1980) for another derivation.

### 2.2.2 Integration

To set the framework for generalizing the two-body problem to the \( n \)-body problem, I slightly modified the presentation in the paper of Shadwick et al. (1999) to make the constant \( \ell \) a variable that is formally being integrated, but which remains constant.
The predictor step of the conservative integrator is given by Eqs. (2.1a), where \( \mathbf{x} = (r, \theta, p, \ell) \). To derive the corrector, we transform the vector \((r, p, \ell)\) to a new space:

\[
\begin{align*}
\xi_1 &= \frac{-k}{r}, \\
\xi_2 &= \frac{p^2}{2m} + \frac{\ell^2}{2mr^2}, \\
\xi_3 &= \ell.
\end{align*}
\]

(Note: unless otherwise specified, each variable is a function of \( t \).) Differentiating these variables and using the fact that \( H = \xi_1 + \xi_2 \) and \( L = \xi_3 \) are both conserved, we find

\[
\begin{align*}
\dot{\xi}_1 &= \frac{kp}{mr^2}, \\
\dot{\xi}_2 &= -\dot{\xi}_1, \\
\dot{\xi}_3 &= 0.
\end{align*}
\]

After applying Eq. (2.2), we use the inverse transformation

\[
\begin{align*}
r &= \frac{-k}{\xi_1}, \\
\ell &= \xi_3, \\
p &= \text{sgn}(\rho)\sqrt{2m\xi_2 - \frac{\ell^2}{r^2}}
\end{align*}
\]

to obtain updated values of the variables. See Shadwick et al. (1999) for details on how the invariance of the Runge–Lenz vector \( \mathbf{A} = \mathbf{v} \times \mathbf{r} + V \mathbf{r} \) is exploited to evolve \( \theta \).

Reworking the Kepler problem gave me a clearer understanding of how to apply conservative integration to the equations of motion of planets. Now that I have looked at the simple case which has an analytic solution, the next step is to integrate the chaotic \( n \)-body problem using methods similar to those used in the Kepler problem. First I will look at a special case of the three-body problem, and then consider the general \( n \)-body case.
Chapter 3

Restricted Three-Body Problem

3.1 Derivation of the Equations of Motion

The following derivation of the equations of motion is taken from Szebehely (1967). Two bodies of masses $m_1$ and $m_2$, called the primaries, revolve around their center of mass in circular orbits. A third body, with a mass $m_3$ that is negligible compared to $m_1$ and $m_2$, moves in a plane defined by the other two revolving bodies but does not influence their motion. The circular restricted three-body problem describes the motion of this third body.

Let $R$ be the distance between the two primaries, $\omega$ be their common angular velocity, $a$ be the distance from the origin (center of mass) to the second primary, $b$ be the distance from the origin to the first primary, and $M = m_1 + m_2$. In the fixed frame, the first mass is located at $(X_1, Y_1)$, the second mass at $(X_2, Y_2)$, and $(X, Y)$ are the coordinates of the massless body (see Fig. 3.1). A balance between the gravitational and centrifugal (see the last term of Eq. (2.6)) forces requires that

\[
\frac{k^2 m_1 m_2}{R^2} = m_2 \omega^2 = m_1 b \omega^2,
\]

where $k$ is the gravitational constant. From this, we see that

\[
\begin{align*}
    k^2 m_1 &= a \omega^2 R^2, \\
    k^2 m_2 &= b \omega^2 R^2, \\
    k^2 M &= \omega^2 R^3.
\end{align*}
\]

As well, $a = m_1 R/M$ and $b = m_2 R/M$. The distances from the massless body to mass $m_1$ and $m_2$ are respectively given by

\[
\begin{align*}
    R_1 &= \sqrt{(X - X_1)^2 + (Y - Y_1)^2}, \\
    R_2 &= \sqrt{(X - X_2)^2 + (Y - Y_2)^2}.
\end{align*}
\]
In terms of these variables, the gravitational potential is given by

\[ V = -\frac{k^2 m_1}{R_1} - \frac{k^2 m_2}{R_2}. \]

Then the equations of motion of \( m_3 \) in the fixed coordinate system are

\[ \ddot{X} = -\frac{dV}{dX}, \]  
(3.1a)

\[ \ddot{Y} = -\frac{dV}{dY}. \]  
(3.1b)

Since the two primaries are traveling in circular orbits, their coordinates can be defined as, denoting time by \( t \),

\[ X_1 = b \cos \omega t, \]
\[ Y_1 = b \sin \omega t, \]
\[ X_2 = -a \cos \omega t, \]
\[ Y_2 = -a \sin \omega t. \]

Therefore, we can write Eqs. (3.1) as

\[ \ddot{X} = -\frac{k^2 m_1 (X - b \cos \omega t)}{R_1^3} - \frac{k^2 m_2 (X + a \cos \omega t)}{R_2^3}, \]  
(3.2a)
\[ Y = -\frac{k^2 m_1(Y - b \sin \omega t)}{R_1^3} - \frac{k^2 m_2(Y + a \sin \omega t)}{R_2^3}. \] (3.2b)

We want to convert this to a coordinate system that will result in a potential with no explicit dependence on time. We transform to a rotating frame. Let \((\mathcal{X}, \mathcal{Y})\) be the coordinates of the massless body in the rotating frame. Then

\[ X = \mathcal{X} \cos \omega \mathcal{t} - \mathcal{Y} \sin \omega \mathcal{t}, \]
\[ Y = \mathcal{X} \sin \omega \mathcal{t} + \mathcal{Y} \cos \omega \mathcal{t}. \]

We transform to the complex variables \(z = \mathcal{X} + i \mathcal{Y}\) and \(Z = X + iY\), where \(i^2 = -1\). Let \(Z = ze^{i\omega t}\), \(Z_1 = be^{i\omega t}\), and \(Z_2 = ae^{i\omega t}\). Then

\[ R_1 = |Z - Z_1|, \]
\[ R_2 = |Z - Z_2|, \]
or
\[ R_1 = |\mathcal{Z} - b| = \sqrt{(\mathcal{X} - b)^2 + \mathcal{Y}^2}, \]
\[ R_2 = |\mathcal{Z} + a| = \sqrt{(\mathcal{X} + a)^2 + \mathcal{Y}^2}. \]

Converting the left-hand sides of Eqs. (3.2) to complex notation and making substitutions in the right-hand sides of these equations gives the following complex form of the equations of motion in the rotating system:

\[ \ddot{z} + 2\omega i \dot{z} - \omega^2 z = -\frac{k^2 m_1(\mathcal{X} - b)}{|\mathcal{X} - b|^3} - \frac{k^2 m_2(\mathcal{X} + a)}{|\mathcal{X} + a|^3}, \]

of which the real and imaginary parts are

\[ \ddot{x} - 2\omega \dot{y} - \omega^2 x = -\frac{k^2 m_1(\mathcal{X} - b)}{R_1^3} - \frac{k^2 m_2(\mathcal{X} + a)}{R_2^3}, \] (3.3a)

\[ \ddot{y} + 2\omega \dot{x} - \omega^2 y = -\frac{k^2 m_1 \mathcal{Y}}{R_1^3} - \frac{k^2 m_2 \mathcal{Y}}{R_2^3}, \] (3.3b)

respectively. Note that the right-hand side has no explicit dependence on time.

We now want to express this in dimensionless coordinates. Let

\[ \mu_1 = \frac{m_1}{M} = \frac{a}{R}, \]
\[ \mu_2 = \frac{m_2}{M} = \frac{b}{R}, \]
\[ t = \omega \mathcal{t}, \]

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\[
x = \frac{\xi}{R},
\]
\[
y = \frac{\eta}{R},
\]
\[
\zeta = \frac{X}{R},
\]
\[
\eta = \frac{Y}{R},
\]
\[
r_1 = \frac{R_1}{R},
\]
\[
r_2 = \frac{R_2}{R}.
\]

Note that \(\mu_1 + \mu_2 = 1\). The nondimensional form of Eqs. (3.3) becomes

\[
x = 2\frac{\xi}{R},
\]
\[
y = 2\frac{\eta}{R},
\]
\[
\zeta = \frac{X}{R},
\]
\[
\eta = \frac{Y}{R},
\]
\[
r_1 = \frac{R_1}{R},
\]
\[
r_2 = \frac{R_2}{R}.
\]

where \(r_1^2 = (x - \mu)^2 + y^2\),
\[
\text{and } \mu = \mu_2. \text{ The Hamiltonian is}
\[
H = \frac{1}{2}(\dot{x}^2 + \dot{y}^2) - \frac{1}{2}(y^2 + x^2) - \frac{1}{r_1} - \frac{\mu}{r_2},
\]

where \(r_1\) and \(r_2\) are defined above.

### 3.2 Integration

Let
\[
q_1 = x,
\]
\[
q_2 = y,
\]
\[
p_1 = \dot{x} - y,
\]
\[
p_2 = \dot{y} + x.
\]

The Hamiltonian then becomes
\[
H = \frac{1}{2}(p_1^2 + p_2^2) + p_1q_2 - p_2q_1 - \frac{1 - \mu}{r_1} - \frac{\mu}{r_2},
\]
where \( r_1 \) and \( r_2 \) are now

\[
\begin{align*}
  r_1^2 &= (q_1 - \mu)^2 + q_2^2, \\
  r_2^2 &= (q_1 + 1 - \mu)^2 + q_2^2.
\end{align*}
\]

The time derivatives of the four variables are

\[
\begin{align*}
  \dot{q}_1 &= \frac{\partial H}{\partial p_1} = p_1 + q_2, \quad (3.6a) \\
  \dot{q}_2 &= \frac{\partial H}{\partial p_2} = p_2 - q_1, \quad (3.6b) \\
  \dot{p}_1 &= -\frac{\partial H}{\partial q_1} = p_2 - \frac{1 - \mu}{r_1^2}(q_1 - \mu) - \frac{\mu}{r_2^2}(q_1 + 1 - \mu), \quad (3.6c) \\
  \dot{p}_2 &= -\frac{\partial H}{\partial q_2} = -p_1 - \frac{1 - \mu}{r_1^2}q_2 - \frac{\mu}{r_2^2}q_2. \quad (3.6d)
\end{align*}
\]

Note that when differentiating the Hamiltonian with respect to one variable, the other variables are kept fixed. The Hamiltonian can now be rewritten as

\[
H = \frac{1}{2}(q_1^2 + q_2^2) - \frac{1}{2}(q_1^2 + q_2^2) - \frac{1 - \mu}{r_1^2} - \frac{\mu}{r_2^2}. \quad (3.7)
\]

The conventional predictor is (refer to Eq. (2.1a)):

\[
\begin{align*}
  \tilde{q}_i &= q_i + \dot{q}_i \tau, \\
  \tilde{p}_i &= p_i + \dot{p}_i \tau,
\end{align*}
\]

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

\[
\begin{align*}
  \xi_1 &= \frac{1}{2} \dot{q}_1^2, \\
  \xi_2 &= \frac{1}{2} \dot{q}_2^2, \\
  \xi_3 &= \frac{1}{2} \dot{q}_1^2 - \frac{1 - \mu}{r_1} - \frac{\mu}{r_2}, \\
  \xi_4 &= \frac{1}{2} \dot{q}_2^2.
\end{align*}
\]

Here

\[
H = -\xi_1 - \xi_2 + \xi_3 + \xi_4 \quad (3.9)
\]

and \( H \) is written as a linear functions of the \( \xi \)s. Differentiating the \( \xi \)s with respect to time, we get

\[
\begin{align*}
  \dot{\xi}_1 &= q_1 \dot{q}_1, \\
  \dot{\xi}_2 &= q_2 \dot{q}_2.
\end{align*}
\]
\[
\begin{align*}
\dot{\xi}_4 &= \dot{q}_2 \ddot{q}_2 = \dot{p}_2 (\dot{p}_2 - \dot{q}_1), \\
\dot{\xi}_3 &= \dot{\xi}_1 + \dot{\xi}_2 - \dot{\xi}_4,
\end{align*}
\]

upon making use of Eq. (3.9) together with the conservation of \(H\). The conservative corrector is given by

\[
\dot{\xi}_i(t + \tau) = \xi_i + \frac{\tau}{2} (\dot{\xi}_i + \ddot{\xi}_i),
\]

for \(i = 1, \ldots, 4\) (refer to Eq. (2.1b)), where \(\ddot{\xi}_i\) is simply Eq. (3.8) evaluated at \(\ddot{q}_i, \ddot{p}_i\) and \(t + \tau\). To invert, we take each variable \(q_i\) and \(p_i\) and write it as a function of \(\xi_i\).

We find

\[
\begin{align*}
q_1 &= \text{sgn}(\ddot{q}_1) \sqrt{2\xi_1}, \\
q_2 &= \text{sgn}(\ddot{q}_2) \sqrt{2\xi_2},
\end{align*}
\]

and, on using Eqs. (3.6a) and (3.6b),

\[
\begin{align*}
p_1 &= -q_2 + \text{sgn}(\ddot{p}_1 + \ddot{q}_2) \sqrt{2\xi_3 + \frac{2(1 - \mu)}{r_1} + \frac{2\mu}{r_2}}, \\
p_2 &= q_1 + \text{sgn}(\ddot{p}_2 - \ddot{q}_1) \sqrt{2\xi_4}.
\end{align*}
\]

The initial conditions are those from Ascher (1998). These initial conditions produce the orbit of the massless body in the rotating frame. I inverted to the fixed frame and plotted all three orbits in Fig. 3.2 and Fig. 3.3. Here, \(\tau = 0.0015\) and the period is \(t = 17.1\) in the rotating frame. Time runs from \(t = 0\) to \(t = 17.1\).

The orbit for the predictor–corrector starts to look like the orbit for the conservative predictor–corrector as the time step is reduced to \(\tau = 0.001\).

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. In the graphs, each color represents one of the bodies.
Figure 3.2: The conservative predictor–corrector solution for the restricted three-body problem.

Figure 3.3: The predictor–corrector solution for the restricted three-body problem.
Chapter 4

General Three-Body Problem

4.1 Derivation of the Equations of Motion

The following derivation of the equations of motion of the general three-body problem in a plane is taken from Barrow-Green (1997), Kovalevsky (1967), and Szebehely (1967).

Assume that there are three bodies $m_1$, $m_2$, and $m_3$ with position vectors $r_1$, $r_2$, and $r_3$, where each $r_i$ is at location $(x_i, y_i)$. Define $r_{ij} = r_j - r_i$, where $i, j = 1, 2, 3$. The distances between the three bodies are

$$r_{ij} = \sqrt{(x_j - x_i)^2 + (y_j - y_i)^2}.$$

The potential is

$$V = -\frac{km_1 m_2}{r_{12}} - \frac{km_2 m_3}{r_{23}} - \frac{km_1 m_3}{r_{13}},$$

where $k$ is the gravitational constant. The equations of motion are

$$m_i \ddot{r}_i = -\frac{\partial V}{\partial r_i},$$

where $i = 1, 2, 3$. The system consists of three second-order differential equations for the vectors $r_i$, written as follows:

$$m_1 \ddot{r}_1 = \frac{km_1 m_2 (r_2 - r_1)}{r_{12}^3} + \frac{km_1 m_3 (r_3 - r_1)}{r_{13}^3},$$

$$m_2 \ddot{r}_2 = \frac{km_1 m_2 (r_1 - r_2)}{r_{21}^3} + \frac{km_2 m_3 (r_3 - r_2)}{r_{23}^3},$$

$$m_3 \ddot{r}_3 = \frac{km_1 m_3 (r_1 - r_3)}{r_{31}^3} + \frac{km_2 m_3 (r_2 - r_3)}{r_{32}^3}.$$
Note that $\sum_{i=1}^{3} m_i \dot{r}_i = 0$, which implies the conservation of linear momentum:

$$\sum_{i=1}^{3} m_i \dot{r}_i = a,$$

and so

$$\sum_{i=1}^{3} m_i r_i = at + b,$$

where $a$ and $b$ are constants of integration. If we set $a = b = 0$, then the center of mass is at the origin. The conservation of angular momentum may be written as

$$\sum_{i=1}^{3} r_i \times m_i \dot{r}_i = c,$$

where $c$ is a constant of integration. Finally, the conserved Hamiltonian can be written as:

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

(4.2)

where $V$ is given by Eq. (4.1). Using these integrals allows us to reduce the number of free variables, making the system easier to integrate.

However, due to inaccuracies that arise when discretizing the above equations, many algorithms written to integrate the above system will not guarantee the conservation of linear momentum, angular momentum, and the energy. Therefore, it was helpful to convert to Jacobi coordinates, where the linear momentum and center of mass constraints are used to reduce the number of degrees of freedom in the equations of motion. The remaining constraints are forced constant by conservative integration. Information on Jacobi coordinates can be found in Khilmi (1961), Pollard (1966), and Roy (1988).

The idea behind Jacobi coordinates is this: begin with the equations of motion above. Let $r = r_2 - r_1$, where $r = (r_x, r_y)$. Set $M = m_1 + m_2 + m_3$ and $\mu = m_1 + m_2$. The location of the center of mass of $m_1$ and $m_2$ is at $\mu^{-1}(m_1 r_1 + m_2 r_2)$, or since $m_1 r_1 + m_2 r_2 + m_3 r_3 = 0$, at $-\mu^{-1} m_3 r_3$. Take $\rho$ to be the vector from the center of mass of the first two bodies to the third body, where $\rho = (\rho_x, \rho_y)$. Then $\rho = r_3 + \mu^{-1} m_3 r_3 = M \mu^{-1} r_3$ (see Fig. 4.1).

Therefore,

$$r_2 - r_1 = r,$$
$$r_3 - r_1 = \rho + m_2 \mu^{-1} r,$$
$$r_3 - r_2 = \rho - m_1 \mu^{-1} r.$$

In these coordinates, following Eq. (4.2), the Hamiltonian can be written as

$$H = \frac{1}{2} g_1 (r_x^2 + r_y^2) + \frac{1}{2} g_2 (\rho_x^2 + \rho_y^2) + V$$
in terms of the reduced masses $g_1 = m_1 m_2 \mu^{-1}$ and $g_2 = m_3 M^{-1} \mu$, and where $V$ is given by Eq. (4.1).

The next step is to convert the above equations to polar coordinates. Define $r_x = r \cos \theta$, $r_y = r \sin \theta$, $r = |\mathbf{r}|$, $\rho_x = \rho \cos \Theta$, $\rho_y = \rho \sin \Theta$, and $\rho = |\rho|$.

In polar coordinates, the Hamiltonian can be rewritten

$$H = \frac{p_x^2}{2g_1} + \frac{p_y^2}{2g_2} + \frac{\ell^2}{2gr^2} + \frac{L^2}{2g\rho^2} + V(r, \rho, \theta, \Theta),$$

(4.3)

where $p$ is the linear momentum of the first reduced mass, $\ell$ 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,

$$V = -\frac{m_1 m_2}{r} - \frac{m_1 m_3}{\sqrt{\rho^2 + m_2 \mu^2 r^2 + 2 \rho m_2 \mu^{-1} r \cos(\Theta - \theta)}} - \frac{m_2 m_3}{\sqrt{\rho^2 + m_1 \mu^2 r^2 - 2 \rho m_1 \mu^{-1} r \cos(\Theta - \theta)}}.$$  

(4.4)

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

The equations of motion in polar coordinates (derived the same way as in the Kepler problem) are

$$\dot{r} = \frac{\partial H}{\partial p} = \frac{p}{g_1},$$

(4.5a)
\[ \dot{\theta} = \frac{\partial H}{\partial \ell} = \frac{\ell}{g_1 r^2}, \]  
\[ \dot{\rho} = -\frac{\partial H}{\partial r} = \frac{\ell^2}{g_1 r^3} - \frac{\partial V}{\partial r}, \]  
\[ \dot{\varphi} = \frac{\partial H}{\partial \theta} = -\frac{\partial V}{\partial \theta}, \]  
\[ \dot{\rho} = \frac{\partial H}{\partial P} = \frac{P}{g_2}, \]  
\[ \dot{\Theta} = \frac{\partial H}{\partial L} = \frac{L}{g_2 \rho^2}, \]  
\[ \dot{\rho} = -\frac{\partial H}{\partial \rho} = \frac{L^2}{g_2 \rho^3} - \frac{\partial V}{\partial \rho}, \]  
\[ \dot{\Theta} = -\frac{\partial H}{\partial \Theta} = -\frac{\partial V}{\partial \Theta}. \]  

### 4.2 Integration

We transform the variables as follows:

\[ \xi_1 = \frac{p^2}{2g_1} + \frac{\ell^2}{2g_1 r^2}, \]  
\[ \xi_2 = \frac{P^2}{2g_2} + \frac{L^2}{2g_2 \rho^2}, \]  
\[ \xi_3 = V, \]  
\[ \xi_4 = \rho, \]  
\[ \xi_5 = \ell, \]  
\[ \xi_6 = L, \]  
\[ \xi_7 = \theta, \]  
\[ \xi_8 = \Theta. \]

All variables are functions of \( t \), unless otherwise specified. Note that our conserved quantity \( H \) becomes a linear function of the transformed variables:

\[ H = \xi_1 + \xi_2 + \xi_3. \]

The time derivatives become

\[ \dot{\xi}_1 = \frac{p \dot{p}}{g_1} + \frac{\ell r^2 \dot{\ell} - r \ell^2 \dot{r}}{g_1 r^4}, \]
\[
\begin{align*}
\dot{\xi}_2 &= \frac{P\dot{P}}{g_2} + \frac{L\rho^2 \dot{L} - \rho L^2 \dot{\rho}}{g_2 \rho^4}, \\
\dot{\xi}_3 &= \frac{\partial V}{\partial \theta}, \\
\dot{\xi}_4 &= \dot{\rho}, \\
\dot{\xi}_5 &= \dot{\ell}, \\
\dot{\xi}_6 &= \dot{L}, \\
\dot{\xi}_7 &= \dot{\theta}, \\
\dot{\xi}_8 &= \dot{\Theta}.
\end{align*}
\]

The procedure for integration that I use is similar to what I had done with the Kepler problem. Upon inverting to find the original variables as functions of the transformed variables, we obtain
\[
\begin{align*}
\ell &= \xi_5, \\
L &= \xi_6, \\
\theta &= \xi_7, \\
\Theta &= \xi_8, \\
\rho &= \xi_4, \\
r &= \rho(\xi_3, \rho, \theta, \Theta), \\
p &= \text{sgn}(\rho) \sqrt{2g_1 \left( \xi_1 - \frac{\ell^2}{2g_1 r^4} \right)}, \\
P &= \text{sgn}(\tilde{P}) \sqrt{2g_2 \left( \xi_2 - \frac{L^2}{2g_2 \rho^2} \right)}.
\end{align*}
\]
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 \( \rho, \theta, \Theta \) with a Newton–Raphson method, using the predicted value \( \tilde{r} \) as an initial guess.

The initial conditions for Fig. 4.2 and Fig. 4.3 are computed by Simó (2000) and cited in Chenciner & Montgomery (2000). Here, \( \tau = 6.5 \times 10^{-5} \) and each mass goes once around the figure eight. The period is 6.33. As \( \tau \) is decreased, the graph of the predictor–corrector begins to look more like that of the conservative predictor–corrector. When \( \tau = 5.1 \times 10^{-5} \), the two graphs are identical in appearance. In these graphs, each color represents one of the bodies.

In the next chapter, I extend the above results to the general \( n \)-body case, where \( n \geq 2 \).
Figure 4.2: The conservative predictor–corrector solution for the general three-body problem.

Figure 4.3: The predictor–corrector solution for the general three-body problem.
Chapter 5

General $n$-Body Problem

5.1 Derivation of the Equations of Motion

The Jacobi coordinates can be extended to $n$ bodies in a plane, as discussed by Roy (1988) and Khilmi (1961), where $n \geq 2$.

Let $n$ masses $m_i$ have radius vectors $r_i$, where $i = 1, \ldots, n$. Define $r_{ij} = r_j - r_i$ as the vector joining $m_i$ to $m_j$. Also define $C_i$ 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 $C_n = 0$. Let the vectors $\rho_i$ be defined such that

\[
\rho_2 = r_{12},
\]

\[
\rho_3 = r_3 - C_2,
\]

\[
\ldots
\]

\[
\rho_n = r_n - C_{n-1}.
\]

(See Fig. 5.1.) Also

\[
r_{k\ell} = \rho_\ell - \rho_k + \sum_{j=k}^{\ell-1} \frac{m_j \rho_j}{M_j},
\]

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

The reduced masses are

\[
g_2 = \frac{m_2 m_1}{M_2},
\]

\[
g_3 = \frac{m_3 (m_2 + m_1)}{M_3},
\]

\[
\ldots
\]

\[
g_n = \frac{m_n M_{n-1}}{M_n}.
\]

$^1$Note that $\rho_1$ is a dummy variable that cancels out in the expression for $r_{12}$.
Figure 5.1: Jacobi coordinates for the general $n$-body problem.

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

\begin{align*}
\dot{\rho}_i &= \frac{\partial H}{\partial \rho_i} = \frac{p_i}{g_i}, \quad (5.1a) \\
\dot{\theta}_i &= \frac{\partial H}{\partial \theta_i} = \frac{\ell_i}{g_i \rho_i^2}, \quad (5.1b) \\
\dot{p}_i &= -\frac{\partial H}{\partial \rho_i} = \frac{\ell_i^2}{g_i \rho_i^3} - \frac{\partial V}{\partial \rho_i}, \quad (5.1c) \\
\dot{\ell}_i &= -\frac{\partial H}{\partial \theta_i} = -\frac{\partial V}{\partial \theta_i}, \quad (5.1d)
\end{align*}

where $\rho_i$, $\theta_i$, $p_i$ and $\ell_i$ are the radius, angle, linear momentum, and angular momentum, respectively, of the $i$th reduced mass, for $i = 2, \ldots, n$. The potential is defined to be

$$V = -\sum_{i,j=1 \atop i \neq j}^n \frac{m_i m_j}{r_{ij}}$$

and the total kinetic energy is

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

It is easy to verify that the Hamiltonian $H = K + V$ is conserved by Eqs. (5.1). Its derivatives are taken with respect to one variable at a time; all the other variables are
held fixed. 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.

### 5.2 Integration

Transform \((\rho, \theta, p, \ell)\) to \((\zeta, \theta, \eta, \ell)\). Set up the variables as follows:

\[
\begin{align*}
\zeta_2 &= V, \\
\zeta_i &= \rho_i, \quad \text{for } i = 3, \ldots, n, \\
\eta_i &= \frac{p_i^2}{2g_i} + \frac{\ell_i^2}{2g_i\rho_i^2}, \quad \text{for } i = 2, \ldots, n.
\end{align*}
\]

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

\[
H = \sum_{i=2}^{n} \eta_i + \zeta_2.
\]

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

\[
\begin{align*}
\dot{\zeta}_2 &= \sum_{i=2}^{n} \left( \frac{\partial V}{\partial \rho_i} \dot{\rho}_i + \frac{\partial V}{\partial \theta_i} \dot{\theta}_i \right), \\
\dot{\zeta}_i &= \dot{\rho}_i, \quad \text{for } i = 3, \ldots, n, \\
\dot{\eta}_i &= \frac{p_i \dot{p}_i}{g_i} + \frac{\ell_i \rho_i^2 \dot{\ell}_i - \rho_i \ell_i^2 \dot{\rho}_i}{g_i \rho_i^4}, \quad \text{for } i = 2, \ldots, n.
\end{align*}
\]

Recall that

\[
\begin{align*}
\tilde{\rho}_i &= \rho_i + \dot{\rho}_i \tau, \\
\tilde{\theta}_i &= \theta_i + \dot{\theta}_i \tau, \\
\tilde{p}_i &= p_i + \dot{p}_i \tau, \\
\tilde{\ell}_i &= \ell_i + \dot{\ell}_i \tau
\end{align*}
\]

is the predictor for each variable \( x_i \) and the corrector is

\[
\begin{align*}
\zeta_i(t + \tau) &= \zeta_i + \frac{\tau}{2}(\dot{\zeta}_i + \ddot{\zeta}_i), \\
\theta_i(t + \tau) &= \theta_i + \frac{\tau}{2}(\dot{\theta}_i + \ddot{\theta}_i), \\
\eta_i(t + \tau) &= \eta_i + \frac{\tau}{2}(\dot{\eta}_i + \ddot{\eta}_i), \\
\ell_i(t + \tau) &= \ell_i + \frac{\tau}{2}(\dot{\ell}_i + \ddot{\ell}_i).
\end{align*}
\]
for $i = 2, \ldots, n$.

We then invert to get our original variables as functions of the temporary transformed variables:

\[
\ell_i(t + \tau) = \ell_i + \frac{\tau}{2}(\dot{\ell}_i + \ddot{\ell}_i),
\]

\[
\theta_i(t + \tau) = \theta_i + \frac{\tau}{2}(\dot{\theta}_i + \ddot{\theta}_i),
\]

\[
\rho_i = \zeta_i \quad \text{for } i = 3, \ldots, n,
\]

\[
\rho_2 = g(\zeta_2, \rho_3, \ldots, \rho_n, \Theta),
\]

\[
p_i = \text{sgn}(\tilde{p}_i) \sqrt{2g_i \left( \eta_i - \frac{f_i^2}{2g_i\rho_i^2} \right)}, \quad \text{for } i = 2, \ldots, n.
\]

The value of the inverse function $g$ defined by

\[
V(g(\zeta_2, \rho_3, \ldots, \rho_n, \Theta), \rho_3, \ldots, \rho_n, \Theta) = \zeta_2
\]

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

The initial conditions for Fig. 5.2 and Fig. 5.3 are computed by Simó (2000) and cited in Chenciner & Montgomery (2000). Here, $\tau = 2 \times 10^{-3}$ and each mass goes once around the curve. The period is 6.33. As $\tau$ is decreased, the graph of the predictor–corrector begins to look more like that of the conservative predictor–corrector. When $\tau = 1 \times 10^{-3}$, the two graphs identical in appearance. In these graphs, each color represents one of the bodies.
Figure 5.2: The conservative predictor–corrector solution for the general four-body problem.

Figure 5.3: The predictor–corrector solution for the general four-body problem.
Chapter 6
Conclusion

In this work, we have seen that conservative integration algorithms can shorten the time it takes a computer to integrate a system of equations accurately.

In the restricted three-body problem, when the Hamiltonian was conserved, I was able to obtain bounded orbits for all three bodies with a much larger time step than when I was not using conservative integration.

The general $n$-body problem was a much more difficult problem to solve. For planar motion, this problem has six invariants, all of which need to be considered when integrating. Making use of Jacobi coordinates for this problem was very useful, since the problem was converted to an $(n - 1)$-body problem through the use of the linear momentum and center of mass constraints. (However, note that there are different ways of using these constraints to reduce the number of degrees of freedom.) The advantage of this is that fewer quantities were left for me to conserve when designing the algorithm. As well, the kinetic energy term of the Hamiltonian remains in diagonal form (a sum of squares) even after converting to Jacobi coordinates. This advantage made it easier for me rewrite the Hamiltonian as a linear function of the transformed variables.

From this project, I have learned a lot about the fundamentals of physics, numerical integration of ordinary differential equations, and classical mechanics. Future work in this area can include modifying the code for the three-dimensional case, and regularizing the equations of motions to handle collisions and close approaches. Further work can include building in precession, nutation, and tidal effects into the equations of motion.
Bibliography


