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Numerical ODE solvers that preserve first integrals

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NUMERICAL ODE SOLVERS THAT PRESERVE FIRST INTEGRALS

By

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CHAPTER 1

GENERAL OVERVIEW

Quantity measurement of the change in energy by a force from any dynamical action has been used for modern dynamical mechanics. Newtonian mechanics need a free body diagram to analyze positions, velocities, accelerations, and forces acting on any dynamical systems. From a free body diagram, vectors are another thing that we have to keep track of cross and dot products, so Newtonian mechanics is required to know the analysis of vectors or vector mechanics. Momentum and forces are essential features in vector mechanics. Unlike Newtonian mechanics, analyzing energy methods requires knowledge of kinetic energy and potential function. Since kinetic energy, potential functions, and work are scalar quantities, we do not have to analyze vector mechanics. By analyzing energy along with variational calculus, Lagrangian Dynamics and Hamiltonian Dynamics have been established. In Chapter 2, we review these two dynamics systems in terms of how they were developed and how they were used in mechanics.

Understanding of constraint would also help in modern dynamical mechanics. In Newtonian mechanics, the constraint forces such as boundary conditions and initial conditions are required to be known in addition to applied forces. Because coordinates used are dependent on the system, we need to take account of all the constraint forces. However, using generalized coordinates that are independent of the system (we will also review in Chapter 2), we can embed constraint equations that will be seen in Lagrange's Equations of Motion (Chapter 2). The number of degrees of freedom in generalized coordinates is the same as the equation of motion. The number of degrees of freedom in space is different than that in configuration space (collection of generalized coordinates). For example, a freely moving particle has three degrees of freedom in space and six degrees of freedom for generalized coordinates, three for position and three for orientation, in configuration space. Having six equations of motion in configuration space rather than three equations of motion and constraints in space, for Newtonian mechanics, this particular example is embedding the constraint equation into the system of equations. Therefore, it is easier to solve for the constraints because constraints in configuration space are adjoined to the problem formulation as side conditions.

Thus we need to discuss briefly the classification of constraints. There are four kinds of constraints: holonomic, nonholonomic, rheonomic, and scleronomic. There are two forms of equations that will consider holonomic constraints; they are either surface constant or time dependent.

$$f(x_1, x_2, x_3) = constant \text{ and } \quad f(x_1, x_2, x_3, t) = constant$$

Nonholonomic constraints are constraints that cannot be expressed in form of holonomic constraints. Some examples of the rate of changes are inequalities and nonintegrable differential expressions.

$$g(x_1, x_2, x_3, t) > 0$$

$$A_1 dx_1 + A_2 dx_2 + A_3 dx_3 + A_0 dt = 0$$

Rheonomic constraints are constraints that time, t, appears explicitly at least in a constraint for a given system of equations (like nonautonomous equations). Scleronomic constraints are constraints that time, t, does not appear explicitly in any constraint for a given system of equations (like autonomous equations). In this paper, we will look into all kinds of constraints that are embedded into systems of equations and solve for them numerically.

Once we get the solution from Lagrange's Equations of Motion (Chapter 2), the result describes a single point in the configuration space. Because analyzing energy methods are based on kinetic energy and potential functions, we should have scalar quantities such as the result was a single point. An infinite number of different solutions may be encountered with different velocities at the same point. For example, a simple spring-weight oscillator can have different velocities at a single position (slower and faster velocities will be encountered at the same point in the middle of a spring while oscillating). Therefore considering position and velocity independently will be much more valuable. The motion of a point in the plane is analyzed by having one axis for the position and the other for the velocity. This is called a phase space, and it is the logical plane for analysis.

In later Chapters we will discuss numerical solutions of a system of equations by Lagrangian, Hamiltonian, and First Integral solutions, like holonomic constraint system (explained in later Chapters). Lagrangian systems are holonomic systems for which the forces are derivable from a generalized potential function $V(\vec{q}, \dot{\vec{q}}, t)$, and so are Hamiltonian systems. Again, since results are scalar quantities, we can take advantage of solving them numerically. When compared with conventional numerical methods that are applied to the equations of motion of classical mechanics, such quantities conserve the total energy and momenta only in the order of the truncation error; round-off errors are eliminated.

CHAPTER 2

BACKGROUND

2.1 INTRODUCTION LAGRANGIAN DYNAMICS

To systematize equations of motion, coordinates used should be independent of the system. Thus, generalized coordinates are introduced. Although a freely moving rigid body, as an example, has three degrees of freedom, it can be determined by six coordinates: three coordinates is for the position of the center of mass of the body and three others for the orientation of the body in space. Therefore, a freely moving rigid body that is like two independent masses moving freely in space, requires a total of six coordinate specifications. The details of units are not important as long as the six values uniquely describe the configuration of the system. The collection of all possible points with the coordinates is called configuration space.

Before we go into Lagrangian Dynamics, we need to discuss about the kinetic energy of a system because both Lagrange and Hamilton analyzed dynamics based on energy. A single particle moving in space has kinetic energy as,

$$T = \tfrac{1}{2} m \sum_{i=1}^{3} \dot{x}_i^2 \qquad (2.1.1)$$

In here, $\dot{x}$ is a total time derivative. If we choose q_1, q_2, and q_3 are generalized coordinates, we must have transformation between the physical and generalized coordinates as,

$$x_i = x_i(q_1, q_2, q_3, t) \qquad (2.1.2)$$

Taking total derivatives to the transformation with respect to time will be,

$$\frac{dx_i}{dt} = \sum_{j=1}^{3}\left[\frac{\partial x_i}{\partial q_j}\cdot \dot{q}_j\right] + \frac{\partial x_i}{\partial t} \tag{2.1.3}$$

Substituting absolute velocity of (2.1.3) into (2.1.1), the kinetic energy of a particle becomes (using tensor analysis),

$$T = \tfrac{1}{2}m\left(\frac{\partial x_i}{\partial q_j}\cdot \dot{q}_j + \frac{\partial \dot{x}_i}{\partial t}\right)\cdot\left(\frac{\partial x_i}{\partial q_k}\cdot \dot{q}_k + \frac{\partial \dot{x}_i}{\partial t}\right) \tag{2.1.4}$$

$$= \tfrac{1}{2}m\left(\frac{\partial x_i}{\partial q_j}\frac{\partial x_i}{\partial q_k}\dot{q}_j\dot{q}_k + \frac{\partial x_i}{\partial q_j}\dot{q}_j\frac{\partial \dot{x}_i}{\partial t} + \frac{\partial x_i}{\partial q_k}\dot{q}_k\frac{\partial \dot{x}_i}{\partial t} + \left(\frac{\partial \dot{x}_i}{\partial t}\right)^2\right)$$

$$= \tfrac{1}{2}m\frac{\partial x_i}{\partial q_j}\frac{\partial x_i}{\partial q_k}\dot{q}_j\dot{q}_k + m\frac{\partial x_i}{\partial q_j}\frac{\partial \dot{x}_i}{\partial t}\dot{q}_j + \tfrac{1}{2}m\left(\frac{\partial \dot{x}_i}{\partial t}\right)^2$$

so that

$$T = \tfrac{1}{2}\sum_{j=1}^{3}\sum_{k=1}^{3}\alpha_{jk}\dot{q}_j\dot{q}_k + \sum_{j=1}^{3}\beta_j\dot{q}_j + \gamma$$

where

$$\alpha_{jk} = m\frac{\partial x_i}{\partial q_j}\frac{\partial x_i}{\partial q_k} \qquad \beta_j = m\frac{\partial x_i}{\partial q_j}\frac{\partial \dot{x}_i}{\partial t} \qquad \text{and} \qquad \gamma = \tfrac{1}{2}m\left(\frac{\partial \dot{x}_i}{\partial t}\right)^2$$

Thus, the kinetic energy is transformed as a scalar function of the generalized coordinates and velocities.

$$T = T(\vec{q}, \dot{\vec{q}}, t) \tag{2.1.5}$$

which has total of three generalized coordinates and three generalized velocities.

Likewise, for an N particle system in three-dimensional space, absolute velocities of the system are

$$\dot{x}_i = \frac{dx_i}{dt} = \sum_{j=1}^{n} \left[\frac{\partial x_i}{\partial q_j} \cdot \dot{q}_j \right] + \frac{\partial x_i}{\partial t} \tag{2.1.6}$$

Also, the total kinetic energy of N-particle system in terms of the generalized coordinates and velocities is,

$$T = \tfrac{1}{2} \sum_{j=1}^{3N} \sum_{k=1}^{3N} \alpha_{jk} \dot{q}_j \dot{q}_k + \sum_{j=1}^{3N} \beta_j \dot{q}_j + \gamma \tag{2.1.7}$$

again,

$$T = T(\vec{q}, \dot{\vec{q}}, t) \tag{2.1.8}$$

which has total of $3N$ generalized coordinates and $3N$ generalized velocities.

Grouping with respect to the powers of the generalized velocities, we can write the total kinetic energy as,

$$T = T_2 + T_1 + T_0 \tag{2.1.9}$$

Also generalized momentum, p_i, is defined as the rate of change of the total kinetic energy with respect to a particular component of generalized velocity $\dot{q}_i$.

$$p_i = \frac{\partial T}{\partial \dot{q}_i} \tag{2.1.10}$$

Both Lagrangian Dynamics and Hamiltonian Dynamics are based on analysis of energy along with variational methods. Therefore, instead of generating the equations of motion from free body diagrams, we will analyze the variation of energy and the minimum number of coordinates to characterize the dynamics of the system. The formulation of the dynamics problems in terms of generalized coordinates is called Lagrangian Dynamics.

The governing equation in vector form for the i-th particle is,

$$\vec{F}_i = m_i \vec{a}_i = \frac{d\vec{p}_i}{dt} \tag{2.1.11}$$

We will now analyze the analytical mechanics. The time rate of change of the generalized momentum corresponding to the k-th-generalized coordinate is,

$$\dot{p}_k = \frac{d}{dt}(p_k) = \frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_k}\right) \tag{2.1.12}$$

Because of the total kinetic energy of the system for N-particles systems in Cartesian coordinates is,

$$T = \tfrac{1}{2}\sum_{i=1}^{N} m_i(\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2) \tag{2.1.13}$$

Thus p_k becomes,

$$p_k = \frac{\partial T}{\partial \dot{q}_k} = \sum_{i=1}^{N} m_i\left[\dot{x}_i \frac{\partial \dot{x}_i}{\partial \dot{q}_k} + \dot{y}_i \frac{\partial \dot{y}_i}{\partial \dot{q}_k} + \dot{z}_i \frac{\partial \dot{z}_i}{\partial \dot{q}_k}\right] \tag{2.1.14}$$

Using the transformation from (2.1.6) and taking partial derivatives with respect to $\dot{q}$ becomes

$$\frac{\partial \dot{x}_i}{\partial \dot{q}_k} = \frac{\partial x_i}{\partial q_k} \tag{2.1.15}$$

Thus, equation (2.1.14) becomes,

$$p_k = \frac{\partial T}{\partial \dot{q}_k} = \sum_{i=1}^{N} m_i\left[\dot{x}_i \frac{\partial x_i}{\partial q_k} + \dot{y}_i \frac{\partial y_i}{\partial q_k} + \dot{z}_i \frac{\partial z_i}{\partial q_k}\right] \tag{2.1.16}$$

Also, taking time derivative becomes,

$$\dot{p}_k = \frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_k}\right) \tag{2.1.17}$$

$$\dot{p}_k = \sum_{i=1}^{N} m_i \left[\ddot{x}_i \frac{\partial x_i}{\partial q_k} + \ddot{y}_i \frac{\partial y_i}{\partial q_k} + \ddot{z}_i \frac{\partial z_i}{\partial q_k} \right]$$
$$+ \sum_{i=1}^{N} m_i \left[\dot{x}_i \frac{d}{dt}\left(\frac{\partial x_i}{\partial q_k} \right) + \dot{y}_i \frac{d}{dt}\left(\frac{\partial y_i}{\partial q_k} \right) + \dot{z}_i \frac{d}{dt}\left(\frac{\partial z_i}{\partial q_k} \right) \right] \tag{2.1.18}$$

According to Newton's Second Law, the first summation of (2.1.18) becomes,

$$F_{ix} = m_i \ddot{x}_i$$

$$F_{iy} = m_i \ddot{y}_i$$

$$F_{iz} = m_i \ddot{z}_i$$

For the second summation of (2.1.18), we will again use equation (2.1.6)

$$\frac{d}{dt}(x_i) = \sum_{j=1}^{3} \frac{\partial}{\partial q_j}(x_i)\dot{q}_j + \frac{\partial}{\partial t}(x_i)$$

and replacing x_i with $\frac{\partial x_i}{\partial q_k}$ in the equation, and its derivative with respect of time will be

$$\frac{d}{dt}\left(\frac{\partial x_i}{\partial q_k} \right) = \sum_{j=1}^{n} \frac{\partial}{\partial q_j}\left(\frac{\partial x_i}{\partial q_k} \right)\dot{q}_j + \frac{\partial}{\partial t}\left(\frac{\partial x_i}{\partial q_k} \right)$$

$$= \sum_{j=1}^{n} \frac{\partial^2 x_i}{\partial q_j \partial q_k}\dot{q}_j + \frac{\partial^2 x_i}{\partial t \partial q_k}$$

$$= \frac{\partial}{\partial q_k}\left[\sum_{j=1}^{n} \frac{\partial x_i}{\partial q_j}\dot{q}_j + \frac{\partial x_i}{\partial t} \right]$$

$$\frac{d}{dt}\left(\frac{\partial x_i}{\partial q_k} \right) = \frac{\partial}{\partial q_k}[\dot{x}_i] = \frac{\partial \dot{x}_i}{\partial q_k}$$

where n is the coordinates, and N is number of particles.

Thus, equation (2.1.18) becomes,

$$\dot{p}_k = \frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_k} \right) = Q_k + \sum_{i=1}^{N} m_i \left[\dot{x}_i \frac{\partial \dot{x}_i}{\partial q_k} + \dot{y}_i \frac{\partial \dot{y}_i}{\partial q_k} + \dot{z}_i \frac{\partial \dot{y}_i}{\partial q_k} \right]$$

$$= Q_k + \frac{\partial}{\partial q_k}\left[\frac{1}{2}\sum_{i=1}^{N} m_i\left(\dot{x}_i^2 + \dot{y}_i^2 + \dot{z}_i^2\right)\right]$$

$$= Q_k + \frac{\partial T}{\partial q_k}$$

Therefore, the Lagrange's Equation of Motion becomes,

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}_k}\right) - \frac{\partial T}{\partial q_k} = Q_k \qquad (2.1.19)$$

We will now briefly discuss three different types of Lagrangian Dynamic's systems. They are Conservative, Non-conservative and Dissipative Lagrangian systems.

Conservative Lagrangian Systems

For a conservative system, $L = T - V$,where V is a generalized potential function usually given as

$$V = V(\vec{q}) \qquad (2.1.20)$$

Therefore,

$$Q_k = -\frac{\partial V}{\partial q_k} \qquad \text{and} \qquad \frac{\partial V}{\partial \dot{q}_k} = 0$$

as we have usually seen.

Thus, the Lagrange's Equation of Motion becomes,

$$\frac{d}{dt}\left(\frac{\partial\left(T(\vec{q},\dot{\vec{q}},t) - V(\vec{q})\right)}{\partial \dot{q}_k}\right) - \frac{\partial T(\vec{q},\dot{\vec{q}},t)}{\partial q_k} = Q_k = -\frac{\partial V(\vec{q})}{\partial q_k}$$

$$\frac{d}{dt}\left(\frac{\partial\left(T(\vec{q},\dot{\vec{q}},t) - V(\vec{q})\right)}{\partial \dot{q}_k}\right) - \frac{\partial\left(T(\vec{q},\dot{\vec{q}},t) - V(\vec{q})\right)}{\partial q_k} =$$

$$\frac{d}{dt}\left(\frac{\partial L(\vec{q},\dot{\vec{q}},t)}{\partial \dot{q}_k}\right) - \frac{\partial L(\vec{q},\dot{\vec{q}},t)}{\partial q_k} = 0 \qquad (2.1.21)$$

Therefore Lagrange's equations of motions are,

$$p_k = \frac{\partial (T - V)}{\partial \dot{q}_k} = \frac{\partial L}{\partial \dot{q}_k} \tag{2.1.22a}$$

$$\dot{p}_k = \frac{d}{dt}\frac{\partial (T - V)}{\partial \dot{q}_k} = \frac{\partial T}{\partial q_k} - \frac{\partial V}{\partial q_k} = \frac{\partial L}{\partial q_k} \tag{2.1.22b}$$

Non-conservative Lagrangian Systems

For a non-conservative system, assuming generalized potential function V exists in a way that is given as,

$$Q_k = \frac{d}{dt}\left[\frac{\partial V(\vec{q},\dot{\vec{q}},t)}{\partial \dot{q}_k}\right] - \frac{\partial V(\vec{q},\dot{\vec{q}},t)}{\partial q_k} \tag{2.1.23}$$

If we substitute the given generalized force into Lagrange's equations (2.1.19), we have

$$\frac{d}{dt}\left[\frac{\partial T(\vec{q},\dot{\vec{q}},t)}{\partial \dot{q}_k}\right] - \frac{\partial T(\vec{q},\dot{\vec{q}},t)}{\partial q_k} = \frac{d}{dt}\left[\frac{\partial V(\vec{q},\dot{\vec{q}},t)}{\partial \dot{q}_k}\right] - \frac{\partial V(\vec{q},\dot{\vec{q}},t)}{\partial q_k} \tag{2.1.24}$$

Since $L(\vec{q},\dot{\vec{q}},t) = T(\vec{q},\dot{\vec{q}},t) - V(\vec{q},\dot{\vec{q}},t)$, we get

$$\frac{d}{dt}\left[\frac{\partial L(\vec{q},\dot{\vec{q}},t)}{\partial \dot{q}_k}\right] - \frac{\partial L(\vec{q},\dot{\vec{q}},t)}{\partial q_k} = 0 \tag{2.1.25}$$

We cannot say the above equation is conservative system although (2.1.25) is similar to (2.1.21) because the generalized potential function does not depend on the generalized coordinates only. Therefore a conservative system is a special case of a Lagrangian system.

For the general non-conservative system, not assuming the generalized potential function as (2.1.23) or not derivable from a generalized potential function, we can split Q_k as

$$Q_k = Q_k^{cons} + Q_k^{nonc} = -\frac{\partial V}{\partial q_k} + Q_k^{nc} \tag{2.1.26}$$

where the conservative component is derivable from a potential function.

Thus, constructing the Lagrangian function $L = T - V$, we formulate the Lagrange's equations of motion as,

$$\frac{d}{dt}\left[\frac{\partial L(\vec{q},\dot{\vec{q}},t)}{\partial \dot{q}_k}\right] - \frac{\partial L(\vec{q},\dot{\vec{q}},t)}{\partial q_k} = Q_k^{nc} \qquad k = 1, 2, \ldots, n \tag{2.1.27}$$

where Q_k^{nc} are generalized forces which is not derivable from a potential function.

Dissipative Lagrangian Systems

If we have dissipative systems as

$$F_{ix} = -c_{x_i}\dot{x}_i$$

$$F_{iy} = -c_{y_i}\dot{y}_i$$

$$F_{iz} = -c_{z_i}\dot{z}_i$$

The virtual work done by these dissipative forces under a set of virtual displacement is,

$$\delta W = \sum_i \vec{F} \cdot \delta\vec{r} = -\sum_{i=1}^{N}\left(c_{x_i}\dot{x}_i\delta x_i + c_{y_i}\dot{y}_i\delta y_i + c_{z_i}\dot{z}_i\delta z_i\right) \tag{2.1.28}$$

where

$$\delta x_i = \sum_{j=1}^{n} \frac{\partial x_i}{\partial q_j} \cdot \delta q_j \qquad \text{and} \qquad \delta t = 0$$

Also, using equation (2.1.15),

$$\frac{\partial \dot{x}_i}{\partial \dot{q}_k} = \frac{\partial x_i}{\partial q_k}$$

the virtual work done (2.1.28) becomes

$$\delta W = -\sum_{k=1}^{n}\left[\tfrac{1}{2}\sum_{k=1}^{N}\frac{\partial}{\partial \dot{q}_k}\left(c_{x_i}\dot{x}_i^2 + c_{y_i}\dot{y}_i^2 + c_{z_i}\dot{z}_i^2\right)\right]\delta q_k \tag{2.1.29}$$

Therefore in general we can split more on Q_k as,

$$Q_k = Q_k^{cons} + Q_k^{nonc} + D = -\frac{\partial V}{\partial q_k} + Q_k^{nc} + D \tag{2.1.30}$$

where

$$D = \tfrac{1}{2}\sum_{k=1}^{N}\left(c_{x_i}\dot{x}_i^2 + c_{y_i}\dot{y}_i^2 + c_{z_i}\dot{z}_i^2\right) \tag{2.1.31}$$

D is known as Rayleigh's Dissipation Function. The Lagrange's equations of motion then is,

$$\frac{d}{dt}\left[\frac{\partial L(\vec{q},\dot{\vec{q}},t)}{\partial \dot{q}_k}\right] - \frac{\partial L(\vec{q},\dot{\vec{q}},t)}{\partial q_k} + \frac{\partial D(\vec{q},\dot{\vec{q}},t)}{\partial \dot{q}_k} = Q_k^* \tag{2.1.32}$$

where Q_k^* is a generalized force which is not derivable from a potential function or a dissipation function.

2.2 INTRODUCTION HAMILTONIAN DYNAMICS

Now we show how to transform Lagrangian Dynamics into Hamiltonian Dynamics. We can review the Legendre Transformation for the connection between Lagrangian and Hamiltonian functions.

If $f(x)$ a twice-differentiable function which is strictly convex,

$$f''(x) > 0 \tag{2.2.1}$$

and let p be a *tangential coordinate* defined as

$$p = f'(x) \tag{2.2.2}$$

The Lagendre Transformation is given as

$$g(p) = xp - f(x) \tag{2.2.3}$$

so that

$$\frac{dg}{dp} = x + p\frac{dx}{dp} - \frac{df}{dx}\frac{dx}{dp} = x$$

and

$$px - g(p) = px - (xp - f(x)) = f(x)$$

Therefore, Lagendre Transformation has a property that p is the tangential coordinate for $g(p)$ and x is the tangential coordinate for $f(x)$. Therefore is completely symmetrical.

As an example, if $\varphi(x) = \log x$, then $p = \frac{\partial\varphi(x)}{\partial x} = (\log e)\frac{1}{x}$ so that $x = \frac{\log e}{p}$ and

$\varphi(x) = \log\left(\frac{\log e}{p}\right)$. Thus finally, the Legendre transformation of $\varphi(x)$ is

$$g(p) = px - \varphi(x) = \log e - \log\left(\frac{\log e}{p}\right)$$

$$= \log\left(\frac{e}{\log e}\right) + \log p = 0.7965 + \log p$$

Now we can apply a Legendre transformation to a function of several variables.

Let $f(x_1, x_2,\ldots, x_n; y_1, y_2,\ldots,y_m)$ be a function of $n + m$ variables where

$$\det\left[\frac{\partial^2 f}{\partial y_i \partial y_j}\right] \neq 0 \qquad (2.2.4)$$

We introduce new coordinates

$$z_i = \frac{\partial f}{\partial y_i} \qquad i = 1, 2, \ldots, m \qquad (2.2.5)$$

Now we can define the Legendre transformation of f, with respect to the variables $y_1, y_2,\ldots,y_m$ as

$$g(x_1, x_2,\ldots, x_n; z_1, z_2,\ldots, z_m) = \sum_{i=1}^{m} y_i z_i - f \qquad (2.2.6)$$

$$\frac{\partial g}{\partial x_k} = -\frac{\partial f}{\partial x_k} \qquad \text{where } k = 1, 2,\ldots, n. \qquad (2.2.7)$$

Also,

$$f(x_1, x_2,\ldots, x_n; z_1, z_2,\ldots, z_m) = \sum_{i=1}^{m} y_i z_i - g \qquad (2.2.8)$$

Again the transformations are completely symmetrical like in one-dimensional case. There is one more property that is the variables $x_1, x_2,\ldots, x_n$ do not *actively* participate in the transformation.

Therefore, the dual function H, the Hamiltonian function transform from Lagrangian function through Legendre Transformation then is

$$H = \sum_{i=1}^{n} p_i \dot{q}_i - L \qquad (2..2.9)$$

Lagrangian function can then be rewritten with the Hamiltonian as

$$L = \sum_{i=1}^{n} p_i \dot{q}_i - H \tag{2.2.10}$$

where

$$\frac{\partial H}{\partial q_i} = -\frac{\partial L}{\partial q_i} \tag{2.2.11}$$

Thus, if we want to write so-called Hamilton's Canonical Equations, similar to Lagrange's equations, we have

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \tag{2.2.12a}$$

but for the $\dot{q}_i$ notice the generalized coordinates q_i are not transformed by (2.2.7), therefore

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \tag{2.2.12b}$$

Thus we have a total of $2n$ first-order differential equations.

An example of Hamilton's Canonical Equation of Motion is given below.

$$H = \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + \frac{p_\phi^2}{2mr^2 \sin^2\theta} + V(r,\theta,\phi)$$

The canonical equations are:

$$\dot{r} = \frac{\partial H}{\partial p_r} = \frac{p_r}{m}, \qquad \dot{\theta} = \frac{\partial H}{\partial p_\theta} = \frac{p_\theta}{mr^2}, \qquad \dot{\phi} = \frac{\partial H}{\partial p_\phi} = \frac{p_\phi}{mr^2 \sin^2\theta}$$

$$\dot{p}_r = -\frac{\partial H}{\partial r} = \frac{p_\theta^2}{mr^3} + \frac{p_\phi^2}{mr^3 \sin^2\theta} - \frac{\partial V}{\partial r}$$

$$\dot{p}_\theta = -\frac{\partial H}{\partial \theta} = \frac{p_\phi^2 \cos\theta}{mr^2 \sin^3\theta} - \frac{\partial V}{\partial \theta}$$

$$\dot{p}_\phi = -\frac{\partial H}{\partial \phi} = -\frac{\partial V}{\partial \phi}$$

For the Hamiltonian, one more property can be observed. Since both Hamiltonian and Lagrangian both were established from kinetic energy expressing in terms of generalized momenta and generalized velocities, we will look very closely on distinguish the two expression. Hamiltonian is also a form of energy with expression in terms of the generalized momenta instead of generalized velocities because generalized coordinates are not transformed for the generalized velocities; we can compare (2.1.22) and (2.2.12). Therefore, T_1 from the (2.1.9) is zero. Therefore

$$H = \sum_{i=1}^{n} p_i \dot{q}_i - L = (T_2 + T_0)_H - (T_2 + T_0 - V)_L$$

$$H = T_2 - T_0 + V \qquad \text{by (2.2.11)}$$

Furthermore, for natural systems, the kinetic energy is purely quadratic in the velocities. That is

$$T = T_2 \qquad \text{and} \qquad T_0 = 0$$

and so the Hamiltonian is

$$H = T + V \tag{2.2.13}$$

which is the total mechanical energy of the system.

The time rate of change of the Hamiltonian is

$$\frac{dH}{dt} = \sum_{i=1}^{n} \left[\frac{\partial H}{\partial q_i} \dot{q}_i + \frac{\partial H}{\partial p_i} \dot{p}_i \right] + \frac{\partial H}{\partial t}$$

The summation represents the implicit dependence on t through the coordinates and momenta. The last term represents the explicit dependence of the Hamiltonian on time t. If we substitute the canonical equations,

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \qquad \text{and} \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}$$

we have

$$\frac{dH}{dt} = \sum_{i=1}^{n} [- \dot{p}_i \dot{q}_i + \dot{q}_i \dot{p}_i] + \frac{\partial H}{\partial t}$$

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} \tag{2.2.14}$$

The total mechanical energy is conserved that is a special case for the Hamiltonian (such as the conservative systems are the special case for the Lagrengian Dynamics). Conservative in here means the autonomous system, time is not explicitly express in the system of equations that is shown in (2.2.14). Therefore the interesting statement is that the Hamiltonian function H is a constant throughout the evolution of the system. That is, the Hamiltonian is an integral of the motion (also called first integral of equation, we will discuss on later sections), representing the conservation of some portion of total energy.

Furthermore, since t is not active in the Legendre transformation, it follows from the property (2.2.7) that

$$\frac{\partial H}{\partial t} = - \frac{\partial L}{\partial t} \tag{2.2.15}$$

which means that the variable t appears in the Hamiltonian if and only if t appears in the Lagrangian function.

If we consider the Hamiltonian as the velocity field of fluid in the Eulerian description such that the vector fields are given as

$$\dot{x}_1 = F_1(x_1, x_2, t)$$

$$\dot{x}_2 = F_2(x_1, x_2, t)$$

The collection of curves that are tangent to the velocity field at any fixed instant of time are called *steamlines* which can shown as $\frac{dx_1}{F_1} = \frac{dx_2}{F_2}$

If fluid is incompressible, there is no change in volume of particles moves along the flow field; the shape may change during the motion. Thus the incompressibility of the fluid is

$$div(\vec{v}) = \frac{\partial F_1}{\partial x_1} + \frac{\partial F_2}{\partial x_2} = 0$$

Therefore, the Hamiltonian in a stream function for the flow of an imaginary fluid in $2n$-dimensional space becomes

$$div(\vec{v}) = \sum_{i=1}^{n} \frac{\partial \dot{q}_i}{\partial q_i} + \sum_{i=1}^{n} \frac{\partial \dot{p}_i}{\partial p_i} = 0 \tag{2.2.16}$$

where

$$F_1 = \dot{q}_i = \frac{\partial H}{\partial p_i} \qquad \text{and} \qquad F_2 = \dot{p}_i = -\frac{\partial H}{\partial q_i}$$

so that

$$div(\vec{v}) = \sum_{i=1}^{n} \frac{\partial^2 H}{\partial p_i \partial q_i} - \sum_{i=1}^{n} \frac{\partial^2 H}{\partial q_i \partial p_i} = 0$$

Therefore using Liouville's Theorem, we can build Hamiltonian (*Example 2.2.2*). There is one thing to be noted that $div(\vec{v}) = 0$ does not necessarily means the conservative system of Hamiltonian; it just means Hamiltonian can be easily built (*Example 2.2.2*). In Chapter 3, We will discuss how to check analytically whether if the given Hamiltonian is conservative or not.

Some examples of transforming from Lagrangian to Hamiltonian or vise visa, verifying Hamiltonian systems using Liouville's Theorem, and finding the Hamiltonian and finding Lagrangian by given canonical equations will be shown below.

Example 2.2.1

If the Lagrangian is given as

$$L = \tfrac{1}{2}\dot{x}^2 - \tfrac{1}{2}\omega^2 x^2 + \varepsilon x \dot{x}^2 - \delta x^3$$

using (2.1.22a)

$$p = \frac{\partial L}{\partial \dot{q}} = x = \frac{\partial L}{\partial \dot{x}} = 2\dot{x} + 2x\dot{x}$$

and (2.2.9)

$$H = \sum_{i=1}^{n} p_i \dot{q}_i - L = p\dot{q} - L = (2\dot{x} + 2x\dot{x})\dot{x} - \tfrac{1}{2}\dot{x}^2 - \tfrac{1}{2}\omega^2 x^2 + \varepsilon x\dot{x}^2 - \delta x^3$$

$$H = \tfrac{1}{2}\dot{x}^2 + \tfrac{1}{2}\omega^2 x^2 + \varepsilon x\dot{x}^2 + \delta x^3$$

Thus the Hamiltonian can be determined.

Analyzing *example 2.2.1*, if we assume we have $T = \tfrac{1}{2}\dot{x}^2 + \varepsilon x\dot{x}^2$ and $V = \tfrac{1}{2}\omega^2 x^2 + \delta x^3$, conservative system with T_2 and $T_1 = T_0 = 0$, then we can clearly define Lagrangian system, $L = T - V$ and Hamiltonian $H = T + V$. See *example 2.2.6*.

Example 2.2.2

$$\dot{x}_1 = x_1 + x_2$$

$$\dot{x}_2 = x_1 - x_2$$

In order to determine if system of equations is Hamiltonian, we use Liouville's Theorem on that system of equations of a particle in two dimension.

$$\sum_{i=1}^{n} \frac{\partial \dot{q}_i}{\partial q_i} + \sum_{i=1}^{n} \frac{\partial \dot{p}_i}{\partial p_i} = \frac{\partial \dot{x}_1}{\partial x_1} + \frac{\partial \dot{x}_2}{\partial x_2} = 1 - 1 = 0$$

Therefore Equations in *example 2.2.2* satisfy Liouville's Theorem and it is a Hamiltonian system. Thus, we can construct a Hamiltonian equation using potential function approach.

$$\dot{x}_1 = \frac{\partial H(x_1, x_2)}{\partial x_2} = x_1 + x_2$$

$$H(x_1, x_2) = x_1 x_2 + \frac{x_2^2}{2} + F(x_1) \qquad \text{and} \qquad \frac{\partial H(x_1, x_2)}{\partial x_1} = x_2 + F'(x_1)$$

Also,

$$-\dot{x}_2 = \frac{\partial H(x_1, x_2)}{\partial x_1} = -x_1 + x_2$$

Therefore,

$$F'(x_1) = -x_1 \qquad \text{and} \qquad F(x_1) = -\frac{x_1^2}{2} + C$$

Finally,

$$H(x_1, x_2) = x_1 x_2 + \frac{x_2^2}{2} - \frac{x_1^2}{2} + C$$

We will use this example in later sections.

Example 2.2.3

$$\dot{x}_1 = x_1 + 2x_2$$

$$\dot{x}_2 = x_1^2 - x_2^2$$

Again using Liouville's Theorem to determine if the system of equations are Hamiltonian,

$$\sum_{i=1}^{n} \frac{\partial \dot{q}_i}{\partial q_i} + \sum_{i=1}^{n} \frac{\partial \dot{p}_i}{\partial p_i} = \frac{\partial \dot{x}_1}{\partial x_1} + \frac{\partial \dot{x}_2}{\partial x_2} = 1 - 2y \neq 0$$

Therefore the given system is not a Hamiltonian system

We can also use Liouville's Theorem for nonautonomous systems to find Hamiltonian such as *Example 2.2.4*.

Example 2.2.4

$$\dot{x}_1 = x_1 t - 2x_2$$

$$\dot{x}_2 = x_1^2 + x_2 t^2$$

Again using Liouville's Theorem to determine if the system of equations are Hamiltonian,

$$\sum_{i=1}^{n} \frac{\partial \dot{q}_i}{\partial q_i} + \sum_{i=1}^{n} \frac{\partial \dot{p}_i}{\partial p_i} = \frac{\partial \dot{x}_1}{\partial x_1} + \frac{\partial \dot{x}_2}{\partial x_2} = t + t^2 \neq 0$$

Therefore the given system is not a Hamiltonian system

Example 2.2.5

$$\dot{x}_1 = x_1 t + 2x_2$$

$$\dot{x}_2 = x_1 t^2 - x_2 t$$

Again using Liouville's Theorem to determine if the system of equations are Hamiltonian,

$$\sum_{i=1}^{n} \frac{\partial \dot{q}_i}{\partial q_i} + \sum_{i=1}^{n} \frac{\partial \dot{p}_i}{\partial p_i} = \frac{\partial \dot{x}_1}{\partial x_1} + \frac{\partial \dot{x}_2}{\partial x_2} = t - t = 0$$

Therefore the given system is a Hamiltonian system

$$\dot{x}_1 = \frac{\partial H(x_1, x_2)}{\partial x_2} = x_1 t + 2x_2$$

$$H(x_1, x_2) = x_1 x_2 t + x_2^2 + F(x_1) \qquad \text{and} \qquad \frac{\partial H(x_1, x_2)}{\partial x_1} = x_2 t + F'(x_1)$$

Also,

$$-\dot{x}_2 = \frac{\partial H(x_1, x_2)}{\partial x_1} = -x_1 t^2 + x_2 t$$

Therefore,

$$F'(x_1) = -x_1 t^2 \quad \text{and} \qquad F(x_1) = -\frac{x_1^2 t^2}{2} + C$$

Finally,

$$H(x_1, x_2) = x_1 x_2 t + x_2^2 - \frac{x_1^2 t^2}{2} + C$$

Example 2.2.6

Consider a mass that only a spring attaches to the wall.

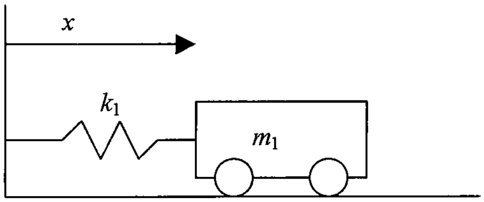

Figure 2.2.1 A mass is attached to the wall only by a spring

Kinetic and potential energy of the system will be

$$T = \tfrac{1}{2} m\dot{x}^2$$
$$V = +\tfrac{1}{2} mx^2$$

and because the system is conservative, the Lagrangian will be

$$L = T - V = \tfrac{1}{2} m\dot{x}^2 - \tfrac{1}{2} mx^2$$

or for our convenience,

$$L = T - V = \tfrac{1}{2} m\dot{q}^2 - \tfrac{1}{2} mq^2$$

so that

$$p=\frac{\partial L}{\partial \dot{q}}=m\dot{q} \quad \text{and} \quad \dot{p}=\frac{\partial L}{\partial q}=-mq$$

$$H=p\dot{q}-L=m\dot{q}^2-(\tfrac{1}{2}m\dot{q}^2-\tfrac{1}{2}mq^2)=\tfrac{1}{2}m\dot{q}^2+\tfrac{1}{2}mq^2$$

Therefore,

$$H=\tfrac{1}{2}m\dot{x}^2+\tfrac{1}{2}mx^2=T+V$$

We can also prove that Hamiltonian is kinetic energy plus potential energy for conservative systems.

Example 2.2.7

If one of the canonical equations for a single degree of freedom Hamiltonian system is given as

$$\dot{p}=p^2-2q+2p$$

then, we can find H because

$$\dot{p}=-\frac{\partial H}{\partial q}=p^2-2q+2p$$

$$H(q,p)=-p^2q+q^2-2pq+F(p)$$

and

$$\dot{q}=\frac{\partial H}{\partial p}=-2pq-2q+F'(p) \tag{2.2.17}$$

Also, we can determine $\dot{q}$ because it's a Hamiltonian system, so Liouville's Theorem has to satisfy such that

$$\sum_{i=1}^{n}\frac{\partial \dot{q}_i}{\partial q_i}+\sum_{i=1}^{n}\frac{\partial \dot{p}_i}{\partial p_i}=\frac{\partial \dot{q}}{\partial q}+\frac{\partial \dot{p}}{\partial p}=\frac{\partial \dot{q}}{\partial q}+2p+2=0$$

$$\frac{\partial \dot{q}}{\partial q} = -2p - 2$$

$$\dot{q} = -2pq - 2q + F(p) \qquad (2.2.18)$$

Comparing (2.2.17) and (2.2.18), we find that

$$F'(p) = F(p)$$

so that $F(p)$ can be either exponential or zero.

If zero is simple, we can choose $F(p)$ to be e^p. Therefore,

$$\dot{q} = -2pq - 2q + e^p$$

and

$$H(q,p) = -p^2 q + q^2 - 2pq + e^p$$

also if we want to convert H to L, we need

$$\dot{q}p = -2p^2 q - 2pq + pe^p$$

Thus,

$$L(q,p) = \dot{q}p - H = -2p^2 q - 2pq + pe^p + p^2 q - q^2 + 2pq - e^p = -p^2 q - q^2 + (p-1)e^p$$

CHAPTER 3

ANALYTICAL PREDICATION OF CONSERVATIVE SYSTEMS FROM THE HAMILTONIAN AND FIRST INTEGRALS

3.1 ENERGY PRESERVING ALGORITHMS

For the application of the Hamiltonian, we need to introduce the energy preserving algorithms. The energy preservation shows some interesting properties of conservation in Hamiltonian. It is given as

$$\vec{M}\vec{a}_{n+1} + \vec{K}(\vec{d}_{n+1}) = \vec{F}_n \tag{3.1.1}$$

$$\vec{d}_{n+1} = \vec{d}_n + \tfrac{1}{2}\Delta t(\vec{v}_n + \vec{v}_{n+1}) \tag{3.1.2}$$

$$\vec{v}_{n+1} = \vec{v}_n + \tfrac{1}{2}\Delta t\lambda(\vec{a}_n + \vec{a}_{n+1}) \tag{3.1.3}$$

$$\lambda = \frac{2[U(\vec{d}_{n+1}) - U(\vec{d}_n)]}{(\vec{d}_{n+1} - d_n)^T\left[\vec{K}(\vec{d}_{n+1}) + \vec{K}(\vec{d}_n)\right]} \tag{3.1.4}$$

$$\vec{d}_0 = \vec{d} \tag{3.1.5}$$

$$\vec{v}_0 = \vec{v} \tag{3.1.6}$$

where $\vec{U}$ is the potential that generates $\vec{K}$, i.e., $DU = \vec{K}$. This algorithm obeys the identity

$$E(\vec{d}_{n+1}, \vec{v}_{n+1}) = E(\vec{d}_n, \vec{v}_n) + \tfrac{1}{2}(\vec{d}_{n+1} - \vec{d}_n)^T(\vec{F}_{n+1} + \vec{F}_n) \tag{3.1.7}$$

The energy-preserving algorithm (3.1.1)-(3.1.6) can be defined for a general Hamiltonian system (finite or infinite-dimensional) as well,

$$\dot{\vec{q}} = \frac{\partial H}{\partial \vec{p}} \qquad \dot{\vec{p}} = -\frac{\partial H}{\partial \vec{q}} \tag{3.1.8}$$

by the following implicit scheme

$$\vec{q}_{n+1} = \vec{q}_n + \Delta t \frac{(H(\vec{q}_{n+1}, \vec{p}_{n+1}) - H(\vec{q}_{n+1}, \vec{p}_n))}{\vec{\lambda}^T (\vec{p}_{n+1} - \vec{p}_n)} \vec{\lambda} \tag{3.1.9}$$

$$\vec{p}_{n+1} = \vec{p}_n - \Delta t \frac{(H(\vec{q}_{n+1}, \vec{p}_n) - H(\vec{q}_n, \vec{p}_n))}{\vec{\mu}^T (\vec{q}_{n+1} - \vec{q}_n)} \vec{\mu} \tag{3.1.10}$$

In which:

$$\vec{\lambda} = \frac{\partial H}{\partial \vec{p}} (\alpha \vec{q}_{n+1} + (1-\alpha)\vec{q}_n, \beta \vec{p}_{n+1} + (1-\beta)\vec{p}_n) \tag{3.1.11}$$

and;

$$\vec{\mu} = \frac{\partial H}{\partial \vec{q}} (\gamma \vec{q}_{n+1} + (1-\gamma)\vec{q}_n, \delta \vec{p}_{n+1} + (1-\delta)\vec{p}_n) \tag{3.1.12}$$

where α, β, γ, δ are arbitrarily chosen in the interval [0,1].

For the proof of conservation of energy,

Equation (3.1.9) becomes,

$$(\vec{q}_{n+1} - \vec{q}_n) \cdot (\vec{p}_{n+1} - \vec{p}_n) = \Delta t \frac{(H(\vec{q}_{n+1}, \vec{p}_{n+1}) - H(\vec{q}_{n+1}, \vec{p}_n))}{\vec{\lambda}^T} \vec{\lambda}$$

Take transpose to both side

$$((\vec{q}_{n+1} - \vec{q}_n) \cdot (\vec{p}_{n+1} - \vec{p}_n))^T = \Delta t \frac{(H(\vec{q}_{n+1}, \vec{p}_{n+1}) - H(\vec{q}_{n+1}, \vec{p}_n))}{\vec{\lambda}^T} \vec{\lambda}^T$$

then,

$$\frac{((\vec{q}_{n+1} - \vec{q}_n) \cdot (\vec{p}_{n+1} - \vec{p}_n))^T}{\Delta t} = H(\vec{q}_{n+1}, \vec{p}_{n+1}) - H(\vec{q}_{n+1}, \vec{p}_n) \tag{3.1.13}$$

Also (3.1.10) becomes

$$\frac{((\vec{p}_{n+1} - \vec{p}_n)(\vec{q}_{n+1} - \vec{q}_n))^T}{\Delta t} = -(H(\vec{q}_{n+1}, \vec{p}_n) - H(\vec{q}_n, \vec{p}_n))$$

$$= -H(\vec{q}_{n+1}, \vec{p}_n) + H(\vec{q}_n, \vec{p}_n) \tag{3.1.14}$$

subtracting (3.1.14) from (3.1.13) becomes

$$\frac{\left((\vec{q}_{n+1}-\vec{q}_n)(\vec{p}_{n+1}-\vec{p}_n)\right)^T-\left((\vec{p}_{n+1}-\vec{p}_n)(\vec{q}_{n+1}-\vec{q}_n)\right)^T}{\Delta t}=0=H(\vec{q}_{n+1},\vec{p}_{n+1})-H(\vec{q}_n,\vec{p}_n)$$

so that

$$H(\vec{q}_{n+1},\vec{p}_{n+1})=H(\vec{q}_n,\vec{p}_n)$$

Example 3.1.1

Example in simple harmonic Oscillator

$$H(q,p)=\frac{\omega^2 q^2}{2}+\frac{p^2}{2}$$

since $n = 1$, one particle,

$$\dot{q}=\frac{\partial H}{\partial p}=p \qquad \text{and} \qquad \dot{p}=-\frac{\partial H}{\partial q}=-\omega^2 q$$

and we want to show the system is conservative using energy preserving algorithms. So,

$$\lambda=\frac{\partial H}{\partial p}(\alpha q_{n+1}+(1-\alpha)q_n,\beta p_{n+1}+(1-\beta)p_n)$$

$$\lambda=\beta p_{n+1}+(1-\beta)p_n \qquad \text{and} \qquad \lambda^T=\lambda$$

and

$$\mu=\frac{\partial H}{\partial q}(\gamma q_{n+1}+(1-\gamma)q_n,\delta p_{n+1}+(1-\delta)p_n)$$

$$\mu=\omega^2(\gamma q_{n+1}+(1-\gamma)q_n) \qquad \text{and} \qquad \mu^T=\mu$$

then,

$$q_{n+1}=q_n+\Delta t\frac{(H(q_{n+1},p_{n+1})-H(q_{n+1},p_n))}{(p_{n+1}-p_n)}$$

$$q_{n+1} = q_n + \Delta t \frac{\left[\left(\frac{\omega^2 q_{n+1}^2}{2} + \frac{p_{n+1}^2}{2}\right) - \left(\frac{\omega^2 q_{n+1}^2}{2} + \frac{p_n^2}{2}\right)\right]}{p_{n+1} - p_n}$$

$$q_{n+1} = q_n + \frac{\Delta t}{2} \frac{(p_{n+1}^2 - p_n^2)}{p_{n+1} - p_n}$$

$$q_{n+1} = q_n + \frac{\Delta t}{2}(p_{n+1} + p_n) \qquad (3.1.15)$$

$$p_{n+1} = p_n - \Delta t \frac{(H(q_{n+1}, p_n) - H(q_n, p_n))}{(q_{n+1} - q_n)}$$

$$p_{n+1} = p_n - \Delta t \frac{\left[\left(\frac{\omega^2 q_{n+1}^2}{2} + \frac{p_n^2}{2}\right) - \left(\frac{\omega^2 q_n^2}{2} + \frac{p_n^2}{2}\right)\right]}{q_{n+1} - q_n}$$

$$p_{n+1} = p_n - \frac{\Delta t}{2} \frac{(\omega^2 (q_{n+1}^2 - q_n^2))}{q_{n+1} - q_n}$$

$$p_{n+1} = p_n - \frac{\omega^2 \cdot \Delta t}{2}(q_{n+1} + q_n) \qquad (3.1.16)$$

Now we have two finite difference equations such (3.1.15) and (3.1.16)

If we can proof $H(q_{n+1},p_{n+1})=H(q_n,p_n)=\frac{\omega^2 q^2}{2}+\frac{p^2}{2}=$*constant*, the system will be conservative, and the phase curve will be elliptical.

Thus,

$$H(q_{n+1},p_{n+1})=\frac{\omega^2 q_{n+1}^2}{2}+\frac{p_{n+1}^2}{2}$$

$$=\frac{\omega^2}{2}\left(q_n+\frac{\Delta t}{2}(p_{n+1}+p_n)\right)^2+\frac{1}{2}\left(p_n-\frac{\omega^2\cdot\Delta t}{2}(q_{n+1}+q_n)\right)^2$$

$$=\frac{\omega^2}{2}\left(q_n+\frac{\Delta t}{2}(p_{n+1}+p_n)\right)^2+\frac{1}{2}\left(p_n-\frac{\omega^2\cdot\Delta t}{2}\{q_n+\frac{\Delta t}{2}(p_{n+1}+p_n)+q_n\}\right)^2$$

$$=\frac{\omega^2}{2}\left(q_n^2+\Delta t q_n(p_{n+1}+p_n)+\frac{(\Delta t)^2}{4}(p_{n+1}+p_n)^2\right)$$

$$+\frac{1}{2}\left(p_n^2-\omega^2\cdot\Delta t\cdot p_n\{2q_n+\frac{\Delta t}{2}(p_{n+1}+p_n)\}+\frac{\omega^4\cdot(\Delta t)^2}{4}\{2q_n+\frac{\Delta t}{2}(p_{n+1}+p_n)\}^2\right)$$

where $(\Delta t)^2 \approx 0$

Thus,

$$=\frac{\omega^2}{2}q_n^2+\frac{\omega^2\Delta t q_n}{2}(p_{n+1}+p_n)+\frac{p_n^2}{2}-\omega^2\cdot\Delta t\cdot p_n q_n-\frac{\omega^2(\Delta t)^2 p_n}{4}(p_{n+1}+p_n)$$

again $(\Delta t)^2 \approx 0$,

Therefore,

$$=\frac{\omega^2}{2}q_n^2+\frac{\omega^2\Delta t q_n}{2}p_{n+1}+\frac{\omega^2\Delta t q_n}{2}p_n+\frac{p_n^2}{2}-\omega^2\cdot\Delta t\cdot p_n q_n$$

$$=\frac{\omega^2}{2}q_n^2+\frac{\omega^2\Delta t q_n}{2}p_{n+1}-\frac{\omega^2\Delta t q_n}{2}p_n+\frac{p_n^2}{2}$$

$$=\frac{\omega^2}{2}q_n^2+\frac{\omega^2\Delta t q_n}{2}(p_{n+1}-p_n)+\frac{p_n^2}{2}$$

and we know from (3.1.16) that

$$p_{n+1}-p_n=-\frac{\omega^2\cdot\Delta t}{2}(q_{n+1}+q_n)$$

Therefore

$$H(q_{n+1},p_{n+1})=\frac{\omega^2}{2}q_n^2+\frac{\omega^2\Delta t q_n}{2}\left(-\frac{\omega^2\cdot\Delta t}{2}(q_{n+1}+q_n)\right)+\frac{p_n^2}{2}$$

$$H(q_{n+1},p_{n+1})=\frac{\omega^2}{2}q_n^2-\frac{\omega^4(\Delta t)^2 q_n}{4}(q_{n+1}+q_n)+\frac{p_n^2}{2}$$

since $(\Delta t)^2 \approx 0$,

$$H(q_{n+1}, p_{n+1}) = \frac{\omega^2}{2} q_n^2 + \frac{p_n^2}{2} = H(q_n, p_n) = constant.$$

Therefore we proved that the given simple Harmonic Oscillator Hamiltonian system is conservative.

We will now find out whether the given Duffing equation is conservative or not using energy preserving algorithms.

<u>*Example 3.1.2*</u>

We know the given Duffing equation does not have damping so that

$$\ddot{x} + x^3 + x = 0$$

So we can write

$$\dot{x} = y$$

$$\dot{y} = -x - x^3$$

By using Liouville's Theorem,

$$\sum_{i=1}^{n} \frac{\partial \dot{q}_i}{\partial q_i} + \sum_{i=1}^{n} \frac{\partial \dot{p}_i}{\partial p_i} = \frac{\partial \dot{x}}{\partial x} + \frac{\partial \dot{y}}{\partial y} = 0 + 0 = 0$$

The system is Hamiltonian. Thus,

$$\dot{x} = \dot{q} = \frac{\partial H}{\partial p} = \frac{\partial H}{\partial y} = p = y \qquad \text{and} \qquad H(x, y) = \frac{y^2}{2} + F(x)$$

$$\frac{\partial H}{\partial x} = F'(x)$$

also

$$-\dot{y} = x + x^3 = -\dot{p} = \frac{\partial H}{\partial q} = \frac{\partial H}{\partial x}$$

Thus,

$$F'(x) = x + x^3 \qquad \text{and} \qquad F(x) = \frac{x^2}{2} + \frac{x^4}{4}$$

Finally,

$$H(x,y) = \frac{y^2}{2} + \frac{x^2}{2} + \frac{x^4}{4}$$

or for our convenience set,

$$H(q,p) = \frac{p^2}{2} + \frac{q^2}{2} + \frac{q^4}{4}$$

where,

$$\dot{q} = \frac{\partial H}{\partial p} = p \qquad \text{and} \qquad -\dot{p} = \frac{\partial H}{\partial q} = q + q^3$$

We now show that the system is conservative using energy preserving algorithms. So,

$$\lambda = \frac{\partial H}{\partial p}(\alpha q_{n+1} + (1-\alpha)q_n, \beta p_{n+1} + (1-\beta)p_n)$$

$$\lambda = \beta p_{n+1} + (1-\beta)p_n \qquad \text{and} \qquad \lambda^T = \lambda$$

and

$$\mu = \frac{\partial H}{\partial q}(\gamma q_{n+1} + (1-\gamma)q_n, \delta p_{n+1} + (1-\delta)p_n)$$

$$\mu = \gamma(q_{n+1} + q_{n+1}^3) + (1-\gamma)(q_n + q_n^3) \qquad \text{and} \qquad \mu^T = \mu$$

then,

$$q_{n+1} = q_n + \Delta t \frac{(H(q_{n+1}, p_{n+1}) - H(q_{n+1}, p_n))}{(p_{n+1} - p_n)}$$

$$q_{n+1} = q_n + \Delta t \frac{\left[\left(\frac{q_{n+1}^2}{2} + \frac{q_{n+1}^4}{4} + \frac{p_{n+1}^2}{2}\right) - \left(\frac{q_{n+1}^2}{2} + \frac{q_{n+1}^4}{4} + \frac{p_n^2}{2}\right)\right]}{p_{n+1} - p_n}$$

$$q_{n+1} = q_n + \frac{\Delta t}{2}\frac{(p_{n+1}^2 - p_n^2)}{p_{n+1} - p_n}$$

$$q_{n+1} = q_n + \frac{\Delta t}{2}(p_{n+1} + p_n) \tag{3.1.17}$$

In here, do not try to solve $\frac{q_{n+1}^2}{2} = \frac{1}{2}\left(q_n + \frac{\Delta t}{2}(p_{n+1} + p_n)\right)^2$ and set $(\Delta t)^2 \approx 0$. q_{n+1} and p_{n+1} are to be solved simultaneously.

$$p_{n+1} = p_n - \Delta t\frac{(H(q_{n+1}, p_n) - H(q_n, p_n))}{(q_{n+1} - q_n)}$$

$$p_{n+1} = p_n - \Delta t\frac{\left[\left(\frac{q_{n+1}^2}{2} + \frac{q_{n+1}^4}{4} + \frac{p_n^2}{2}\right) - \left(\frac{q_n^2}{2} + \frac{q_n^4}{4} + \frac{p_n^2}{2}\right)\right]}{q_{n+1} - q_n}$$

$$p_{n+1} = p_n - \frac{\Delta t}{2}\frac{\left[\left(q_{n+1}^2\right) - \left(q_n^2\right)\right]}{q_{n+1} - q_n} - \frac{\Delta t}{4}\frac{\left[\left(q_{n+1}^4\right) - \left(q_n^4\right)\right]}{q_{n+1} - q_n}$$

$$p_{n+1} = p_n - \frac{\Delta t}{2}(q_{n+1} + q_n) - \frac{\Delta t}{4}(q_{n+1} + q_n)(q_{n+1}^2 + q_n^2) \tag{3.1.18}$$

Now we have two finite difference equations such (3.1.17) and (3.1.18). Using these two equations for the next point in H,

$$H(q_{n+1}, p_{n+1}) = \frac{q_{n+1}^2}{2} + \frac{q_{n+1}^4}{4} + \frac{p_{n+1}^2}{2} \tag{3.1.19}$$

substituting (3.1.17) and (3.1.18) into (3.1.19)

$$= \frac{1}{2}\left(q_n + \frac{\Delta t}{2}(p_{n+1} + p_n)\right)^2 + \frac{1}{4}\left[\left(q_n + \frac{\Delta t}{2}(p_{n+1} + p_n)\right)^2\right]^2$$

$$+ \frac{1}{2}\left[p_n - \frac{\Delta t}{2}\left(q_n + \frac{\Delta t}{2}(p_{n+1} + p_n) + q_n\right) - \frac{\Delta t}{4}\left(q_n + \frac{\Delta t}{2}(p_{n+1} + p_n) + q_n\right)\left\{\left(q_n + \frac{\Delta t}{2}(p_{n+1} + p_n)\right)^2 + q_n^2\right\}\right]^2$$

setting $(\Delta t)^2 \approx 0$

$$=\tfrac{1}{2}\left(q_n^2+\Delta t q_n(p_{n+1}+p_n)\right)+\tfrac{1}{4}\left(q_n^2+\Delta t q_n(p_{n+1}+p_n)\right)^2$$
$$+\tfrac{1}{2}\left[p_n-\frac{\Delta t}{2}(2q_n)-\frac{\Delta t}{4}(2q_n)\left(\{q_n^2+\Delta t q_n(p_{n+1}+p_n)\}+q_n^2\right)\right]^2$$

$$=\tfrac{1}{2}\left(q_n^2+\Delta t q_n(p_{n+1}+p_n)\right)+\tfrac{1}{4}\left(q_n^4+2\Delta t q_n^3(p_{n+1}+p_n)\right)$$
$$+\tfrac{1}{2}\left[p_n-\Delta t q_n-\frac{\Delta t}{2}q_n\left(2q_n^2+\Delta t q_n(p_{n+1}+p_n)\right)\right]^2$$

$$=\tfrac{1}{2}\left(q_n^2+\Delta t q_n(p_{n+1}+p_n)\right)+\tfrac{1}{4}\left(q_n^4+2\Delta t q_n^3(p_{n+1}+p_n)\right)+\tfrac{1}{2}\left(p_n-\Delta t q_n-\Delta t q_n^3\right)^2$$

$$=\tfrac{1}{2}\left(q_n^2+\Delta t q_n(p_{n+1}+p_n)\right)+\tfrac{1}{4}\left(q_n^4+2\Delta t q_n^3(p_{n+1}+p_n)\right)+\tfrac{1}{2}\left(p_n^2-2\Delta t p_n q_n-2\Delta t p_n q_n^3\right)$$

$$=\tfrac{1}{2}q_n^2+\frac{\Delta t}{2}q_n(p_{n+1}+p_n)+\tfrac{1}{4}q_n^4+\frac{\Delta t}{2}q_n^3(p_{n+1}+p_n)+\tfrac{1}{2}p_n^2-\Delta t p_n q_n-\Delta t p_n q_n^3$$

Now, we substitute equation (3.1.18), so we get

$$=\tfrac{1}{2}q_n^2+\frac{\Delta t}{2}q_n\left[p_n-\frac{\Delta t}{2}(q_{n+1}+q_n)-\frac{\Delta t}{4}(q_{n+1}+q_n)(q_{n+1}^2+q_n^2)+p_n\right]+\tfrac{1}{4}q_n^4$$
$$+\frac{\Delta t}{2}q_n^3\left[p_n-\frac{\Delta t}{2}(q_{n+1}+q_n)-\frac{\Delta t}{4}(q_{n+1}+q_n)(q_{n+1}^2+q_n^2)+p_n\right]+\tfrac{1}{2}p_n^2-\Delta t p_n q_n-\Delta t p_n q_n^3$$

again, setting $(\Delta t)^2 \approx 0$

$$=\tfrac{1}{2}q_n^2+\frac{\Delta t}{2}q_n[2p_n]+\tfrac{1}{4}q_n^4+\frac{\Delta t}{2}q_n^3[2p_n]+\tfrac{1}{2}p_n^2-\Delta t p_n q_n-\Delta t p_n q_n^3$$

$$=\tfrac{1}{2}q_n^2+\Delta t p_n q_n+\tfrac{1}{4}q_n^4+\Delta t p_n q_n^3+\tfrac{1}{2}p_n^2-\Delta t p_n q_n-\Delta t p_n q_n^3$$

Therefore,

$$H(q_{n+1},p_{n+1})=\frac{q_{n+1}^2}{2}+\frac{q_{n+1}^4}{4}+\frac{p_{n+1}^2}{2}=\frac{q_n^2}{2}+\frac{q_n^4}{4}+\frac{p_n^2}{2}=H(q_n,p_n)=constant$$

Therefore we proof the given system of Duffing equations is conservative. The phase curves will be closed contours.

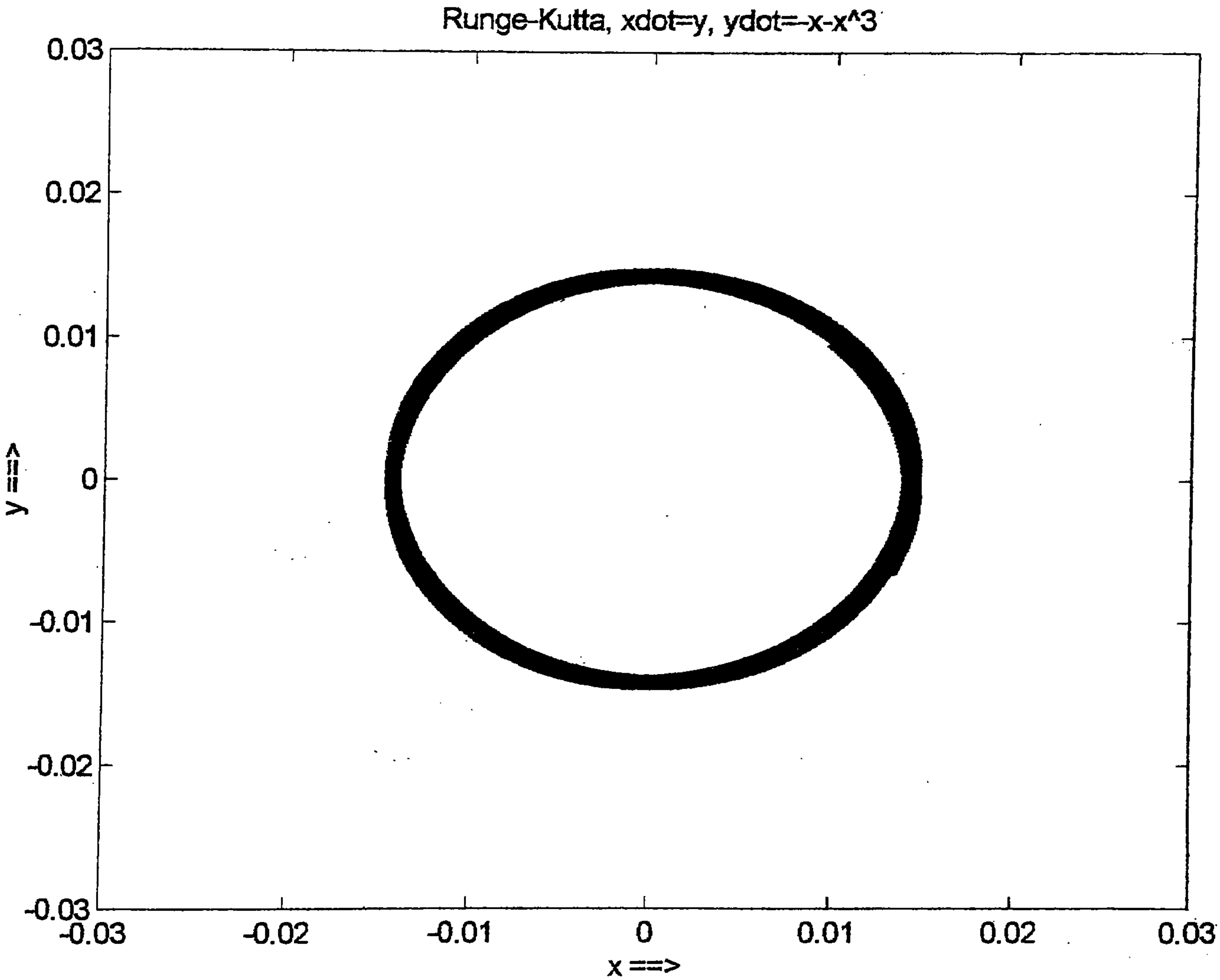

Figure 3.1.1 Runge-Kutta approximation for *example 3.1.2*

Example 3.1.3

From *example 2.2.2*

$$H(x_1,x_2)=x_1x_2+\frac{x_2^2}{2}-\frac{x_1^2}{2}+C$$

For our convince, let $C=0$,

$$H(q,p)=qp+\frac{p^2}{2}-\frac{q^2}{2}$$

To show the above Hamiltonian is conservative or not, we can again use energy preservation algorithms,

$$\dot{q}=\frac{\partial H}{\partial p}=q+p \quad \text{and} \quad -\dot{p}=\frac{\partial H}{\partial q}=-q+p$$

So, it follows that:

$$\lambda=\frac{\partial H}{\partial p}(\alpha q_{n+1}+(1-\alpha)q_n,\beta p_{n+1}+(1-\beta)p_n)$$

$$\lambda=\alpha q_{n+1}+(1-\alpha)q_n+\beta p_{n+1}+(1-\beta)p_n \quad \text{with} \quad \lambda^T=\lambda$$

and,

$$\mu=\frac{\partial H}{\partial q}(\gamma q_{n+1}+(1-\gamma)q_n,\delta p_{n+1}+(1-\delta)p_n)$$

$$\mu=-\gamma q_{n+1}-(1-\gamma)q_n+\delta p_{n+1}+(1-\delta)p_n \quad \text{with} \quad \mu^T=\mu$$

Then,

$$q_{n+1}=q_n+\Delta t\frac{(H(q_{n+1},p_{n+1})-H(q_{n+1},p_n))}{(p_{n+1}-p_n)}$$

$$q_{n+1}=q_n+\Delta t\frac{\left[\left(q_{n+1}\cdot p_{n+1}-\frac{q_{n+1}^2}{2}+\frac{p_{n+1}^2}{2}\right)-\left(q_n\cdot p_n-\frac{q_{n+1}^2}{2}+\frac{p_n^2}{2}\right)\right]}{p_{n+1}-p_n}$$

$$q_{n+1} = q_n + \frac{\Delta t}{2} \frac{(p_{n+1}^2 - p_n^2)}{p_{n+1} - p_n}$$

$$q_{n+1} = q_n + \frac{\Delta t}{2}(p_{n+1} + p_n) \tag{3.1.20}$$

In here, do not try to solve $\frac{q_{n+1}^2}{2} = \frac{1}{2}\left(q_n + \frac{\Delta t}{2}(p_{n+1} + p_n)\right)^2$ and set $(\Delta t)^2 \approx 0$. q_{n+1} and p_{n+1} are to be solved simultaneously. Hence

$$p_{n+1} = p_n - \Delta t \frac{(H(q_{n+1}, p_n) - H(q_n, p_n))}{(q_{n+1} - q_n)}$$

$$p_{n+1} = p_n - \Delta t \frac{\left[\left(q_{n+1} \cdot p_n - \frac{q_{n+1}^2}{2} + \frac{p_n^2}{2}\right) - \left(q_n \cdot p_n - \frac{q_n^2}{2} + \frac{p_n^2}{2}\right)\right]}{q_{n+1} - q_n}$$

$$p_{n+1} = p_n + \frac{\Delta t}{2} \frac{\left[\left(q_{n+1}^2\right) - \left(q_n^2\right)\right]}{q_{n+1} - q_n} - \Delta t \frac{(q_{n+1} - q_n) p_n}{q_{n+1} - q_n}$$

$$p_{n+1} = p_n + \frac{\Delta t}{2}(q_{n+1} + q_n) - \Delta t p_n$$

$$p_{n+1} = p_n + \frac{\Delta t}{2}\left((q_{n+1} + q_n) - 2p_n\right) \tag{3.1.21}$$

Now we have two finite difference equations such (3.1.20) and (3.1.21). Using these two equations for the next point in H.

$$H(q_{n+1}, p_{n+1}) = q_{n+1} \cdot p_{n+1} + \frac{p_{n+1}^2}{2} - \frac{q_{n+1}^2}{2} \tag{3.1.22}$$

substituting (3.1.20) and (3.1.21) into (3.1.22)

$$= \left(q_n + \frac{\Delta t}{2}(p_{n+1} + p_n)\right) \cdot \left(p_n + \frac{\Delta t}{2}\left((q_{n+1} + q_n) - 2p_n\right)\right)$$
$$+ \frac{1}{2}\left(p_n + \frac{\Delta t}{2}\left((q_{n+1} + q_n) - 2p_n\right)\right)^2 - \frac{1}{2}\left(q_n + \frac{\Delta t}{2}(p_{n+1} + p_n)\right)^2$$

setting $(\Delta t)^2 \approx 0$

$$=q_n \cdot p_n + \frac{\Delta t}{2} q_n\left((q_{n+1}+q_n)-2p_n\right)+\frac{\Delta t}{2} p_n(p_{n+1}+p_n)$$
$$+\tfrac{1}{2}\left(p_n^2+\Delta t p_n\left((q_{n+1}+q_n)-2p_n\right)\right)-\tfrac{1}{2}\left(q_n^2+\Delta t q_n(p_{n+1}+p_n)\right)$$

We again substitute (3.3.20),

$$=q_n \cdot p_n + \frac{\Delta t}{2} q_n\left(q_n+\frac{\Delta t}{2}(p_{n+1}+p_n)+q_n-2p_n\right)+\frac{\Delta t}{2} p_n(p_{n+1}+p_n)$$
$$+\tfrac{1}{2}\left(p_n^2+\Delta t p_n\left(q_n+\frac{\Delta t}{2}(p_{n+1}+p_n)+q_n-2p_n\right)\right)-\tfrac{1}{2}\left(q_n^2+\Delta t q_n(p_{n+1}+p_n)\right)$$

$$=q_n \cdot p_n + \frac{\Delta t}{2} q_n\left(2q_n+\frac{\Delta t}{2}(p_{n+1}+p_n)-2p_n\right)+\frac{\Delta t}{2} p_n(p_{n+1}+p_n)$$
$$+\tfrac{1}{2}\left(p_n^2+\Delta t p_n\left(2q_n+\frac{\Delta t}{2}(p_{n+1}+p_n)-2p_n\right)\right)-\tfrac{1}{2}\left(q_n^2+\Delta t q_n(p_{n+1}+p_n)\right)$$

setting $(\Delta t)^2 \approx 0$

$$=q_n \cdot p_n + \Delta t q_n^2 - \Delta t q_n p_n + \frac{\Delta t}{2} p_n(p_{n+1}+p_n)$$
$$+\tfrac{1}{2}\left(p_n^2+2\Delta t q_n p_n-2\Delta t p_n^2\right)-\tfrac{1}{2}\left(q_n^2+\Delta t q_n(p_{n+1}+p_n)\right)$$

$$=q_n \cdot p_n + \Delta t q_n^2 - \Delta t q_n p_n + \frac{\Delta t}{2} p_n(p_{n+1}+p_n)$$
$$+\frac{p_n^2}{2}+\Delta t q_n p_n-\Delta t p_n^2-\frac{q_n^2}{2}-\frac{\Delta t}{2} q_n(p_{n+1}+p_n)$$

$$=q_n \cdot p_n + \Delta t q_n^2 + \frac{\Delta t}{2} p_n(p_{n+1}+p_n)$$
$$+\frac{p_n^2}{2}-\Delta t p_n^2-\frac{q_n^2}{2}-\frac{\Delta t}{2} q_n(p_{n+1}+p_n)$$

$$=q_n \cdot p_n + \Delta t q_n^2 + \frac{\Delta t}{2} p_n(p_{n+1}+p_n)$$
$$+\frac{p_n^2}{2}-\Delta t p_n^2-\frac{q_n^2}{2}-\frac{\Delta t}{2} q_n(p_{n+1}+p_n)$$

We now substitute (3.1.21), so we get

$$=q_n \cdot p_n + \Delta t q_n^2 + \frac{\Delta t}{2} p_n \left(p_n + \frac{\Delta t}{2}((q_{n+1}+q_n)-2p_n) + p_n \right)$$

$$+\frac{p_n^2}{2} - \Delta t p_n^2 - \frac{q_n^2}{2} - \frac{\Delta t}{2} q_n \left(p_n + \frac{\Delta t}{2}((q_{n+1}+q_n)-2p_n) + p_n \right)$$

$$=q_n \cdot p_n + \Delta t q_n^2 + \frac{\Delta t}{2} p_n \left(2p_n + \frac{\Delta t}{2}((q_{n+1}+q_n)-2p_n) \right)$$

$$+\frac{p_n^2}{2} - \Delta t p_n^2 - \frac{q_n^2}{2} - \frac{\Delta t}{2} q_n \left(2p_n + \frac{\Delta t}{2}((q_{n+1}+q_n)-2p_n) \right)$$

again, setting $(\Delta t)^2 \approx 0$

$$=q_n \cdot p_n + \Delta t q_n^2 + \Delta t p_n^2 + \frac{p_n^2}{2} - \Delta t p_n^2 - \frac{q_n^2}{2} - \Delta t q_n p_n$$

$$=q_n \cdot p_n + \frac{p_n^2}{2} - \frac{q_n^2}{2} + \Delta t q_n (q_n - p_n)$$

Therefore

$$H(q_{n+1}, p_{n+1}) = q_{n+1} \cdot p_{n+1} + \frac{p_{n+1}^2}{2} - \frac{q_{n+1}^2}{2} = q_n \cdot p_n + \frac{p_n^2}{2} - \frac{q_n^2}{2} + \Delta t q_n (q_n - p_n) \neq H(q_n, p_n) \neq constant$$

Therefore we proof the given system of equations is not conservative. The phase curve will not have closed contours. In this example, we showed that conservative systems are a special case of Lagrangian or Hamiltonian systems. Not all Hamiltonian systems are conservative.

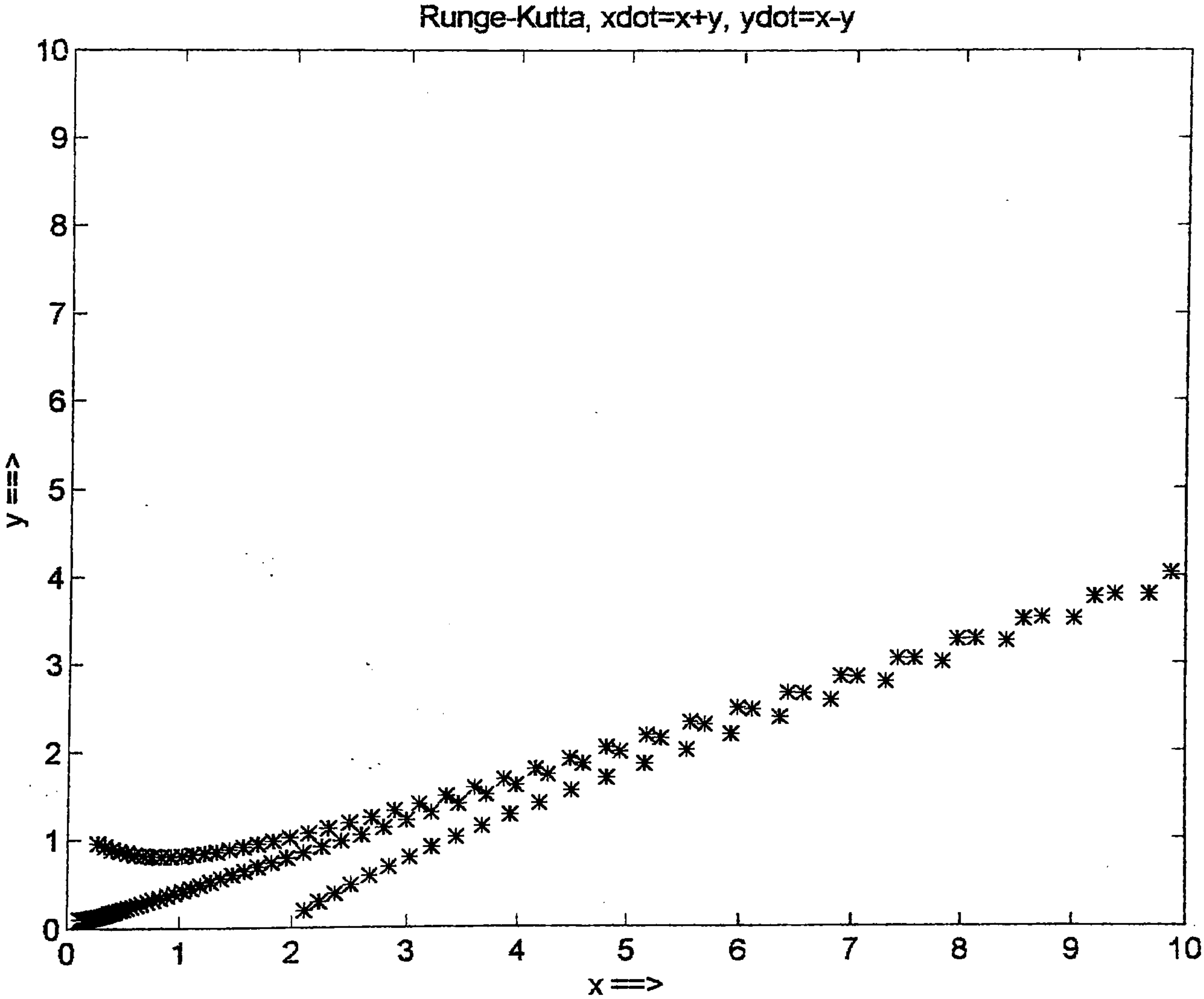

Figure 3.1.2 Runge-Kutta approximation for *example 3.1.3*

3.2 FIRST INTEGRAL FROM EULER-LAGRANGE EQUATION

From Euler-Lagrange equation, we have

$$\frac{\partial F}{\partial y} - \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right) = 0 \tag{3.2.1}$$

where F is a functional, a function of a function, such as

$$F = F(x, y, y')$$

and we have second order equation

$$\frac{\partial F}{\partial y} - \left[\frac{\partial}{\partial x}\left(\frac{\partial F}{\partial y'}\right)dx + \frac{\partial}{\partial y}\left(\frac{\partial F}{\partial y'}\right)dy + \frac{\partial}{\partial y'}\left(\frac{\partial F}{\partial y'}\right)dy'\right] = 0$$

There are two special cases from Euler-Lagrange equations.

Case I

If F is a functional of function x and y',

$$F = F(x, y')$$

then the Euler-Lagrange equation becomes

$$\frac{\partial F(x, y')}{\partial y'} = constant \tag{3.2.2}$$

because

$$\frac{\partial F(x, y')}{\partial y} = 0$$

Case II

If F is a functional of function y and y',

$$F = F(y, y')$$

then the Euler-Lagrange equation becomes

$$F(y, y') - y' \frac{\partial F(x, y')}{\partial y'} = constant \tag{3.2.3}$$

Equation (3.2.2) and (3.2.3) are first-order differential equations. One less equation has to be integrated. Physically, a first integral represents the conservation of a certain quantity. The left-hand sides of equation (3.2.2) and (3.2.3) represent the quantities that are conserved.

CHAPTER 4

NUMERICAL ODE SOLVERS THAT PRESERVE FIRST INTEGRAL

4.1 ORBITAL DERIVATIVES AND FIRST INTEGRAL

As we have discussed on page 2 of Chapter 1, equations in which the independent variable t does not occur explicitly are called autonomous equations. A vector equation of autonomous can be written as

$$\dot{x} = f(x) \qquad (4.1.1)$$

In here, we call equation (4.1.1) an autonomous differential equation because t does not explicitly appear in the equation.

A point in phase space with coordinates x_1 (t), x_2 (t), ... , x_n (t) for certain t, is called a phase point. In general, for increasing t, a phase point shall move through phase-space. In carrying out the projection into phase space, we do not generally know the solution curves of equation (4.1.1), but it is simple to formulate a differential equation describing the behavior of the orbits in phase space.

Equation (4.1.1) can be written out in components as

$$\dot{x}_i = f_i(x) \qquad ; i = 1, \dots, n$$

We now use one of the components of x, such as x_1, as a new independent variable. In order to get x_1 to be such independent variable, $f_1(x) \neq 0$. Therefore

$$\frac{dx_1}{dt} = f_1(x) \qquad \text{and} \qquad \frac{dx_k}{dt} = f_k(x)$$

and dividing dx_1 into dx_k, we have

$$\frac{dx_k}{dx_1} = \frac{df_k(x)}{f_1(x)} \qquad k = 2, \dots, n \qquad (4.1.2)$$

Example 4.1.1

Harmonic oscillator $\ddot{x} + x = 0$

The equivalent vector equation in with $x = x_1, \dot{x} = x_2$

$$\dot{x}_1 = x_2 \qquad \dot{x}_2 = -x_1$$

The orbits of given two dimensional Phase space are described by

$$\frac{dx_2}{dx_1} = -\frac{x_1}{x_2}$$

$$x_2 dx_2 = -x_1 dx_1$$

Integration yields

$$x_1^2 + x_2^2 = constant$$

Or using Liouville's Theorem,

$$\sum_{i=1}^{n} \frac{\partial \dot{q}_i}{\partial q_i} + \sum_{i=1}^{n} \frac{\partial \dot{p}_i}{\partial p_i} = \frac{\partial \dot{x}_1}{\partial x_1} + \frac{\partial \dot{x}_2}{\partial x_2} = 0 - 0 = 0$$

Therefore the system is a Hamiltonian system

$$\dot{x}_1 = \frac{\partial H(x_1, x_2)}{\partial x_2} = x_2$$

$$H(x_1, x_2) = \frac{x_2^2}{2} + F(x_1) \qquad \text{and} \qquad \frac{\partial H(x_1, x_2)}{\partial x_1} = F'(x_1)$$

Also,

$$-\dot{x}_2 = \frac{\partial H(x_1, x_2)}{\partial x_1} = x_1$$

Therefore,

$$F'(x_1) = x_1 \qquad \text{and} \qquad F(x_1) = \frac{x_1^2}{2} + C$$

Finally,

$$H(x_1,x_2)=\frac{x_2^2}{2}+\frac{x_1^2}{2}+C$$

$$H(x,\dot{x})-C=\frac{(\dot{x})^2}{2}+\frac{x^2}{2}$$

Solutions of system (4.1.2) in phase space are called orbits. In equation (4.1.2), time has been eliminated, so it can be integrated in a number of cases, producing a relation between the components of the solution vector. Since simple harmonic oscillator is conservative, $H(x_1, x_2) = C$ is constant, differentiation with respect to t gives,

$$\dot{x}\ddot{x}+x\dot{x}=\dot{x}(\ddot{x}+x)=0$$

Now we will introduce the concept of orbital derivative. Let L_t be the orbital derivative. Consider the differentiable function I: $\boldsymbol{R}^n \rightarrow \boldsymbol{R}$ and the vector function x: $\boldsymbol{R} \rightarrow \boldsymbol{R}^n$. The derivative L_t of the function I along the vector function x, parameterized by t, is

$$L_t I = \frac{\partial I}{\partial x}\dot{x} = \frac{\partial I}{\partial x_1}\dot{x}_1 + \frac{\partial I}{\partial x_2}\dot{x}_2 + \ldots + \frac{\partial I}{\partial x_n}\dot{x}_n$$

If we consider the equation $\dot{x} = f(x)$, $x \in D \subset \boldsymbol{R}^n$; and if

$$L_t I = 0,$$

then $I(x)$ is called first integral of equation. In *example 4.1.1*

$$L_t H = \frac{\partial H}{\partial x_1}\dot{x}_1 + \frac{\partial H}{\partial x_2}\dot{x}_2 = x_1\dot{x}_1 + x_2\dot{x}_2 = x\dot{x} + \dot{x}(-x) = 0$$

Therefore, H in *example 4.1.1* will be a first integral of equation I. If a surface is constant or if the rate of changes are integrable, it means the system of equations involve holonomic constraints.

Example 4.1.2

Let us consider so-called Volterra-Lotka equations

$$\dot{x} = ax - bxy$$

$$\dot{y} = bxy - cy$$

The equation for the orbits in the phase plane is

$$\frac{dy}{dx} = \frac{x}{y}\frac{a - by}{bx - c}$$

Thus the equation is separable and integration yield

$$bx - c\ln x + by - a\ln y = C = I(x, y)$$

We will now check with orbital derivative,

$$L_t I = \frac{\partial I}{\partial x}\dot{x} + \frac{\partial I}{\partial y}\dot{y} = \left(b - \frac{c}{x}\right)(ax - bxy) + \left(b - \frac{a}{y}\right)(bxy - cy)$$

$$= (bx - c)(a - by) + (by - a)(bx - c) = 0$$

Therefore resultant $I(x, y)$ is a first integral of the equation. This may also involve holonomic constraints. However, Volterra-Lotka has some interesting properties that if we now let $p = \ln x \rightarrow x = e^p$ and $q = \ln y \rightarrow y = e^q$ the equations can be observed as Hamiltonian

$$\dot{x} = \frac{\partial x}{\partial p}\frac{\partial p}{\partial t} = e^p \dot{p} = (a - be^q)e^p \rightarrow \dot{p} = (a - be^q)$$

$$\dot{y} = \frac{\partial y}{\partial q}\frac{\partial q}{\partial t} = e^q \dot{q} = (be^p - c)e^q \rightarrow \dot{q} = (be^p - c)$$

$$H(q, p) = be^p - cp + be^q - aq$$

So that Where the resultant H is Hamiltonian and

$$\dot{p} = -\frac{\partial H}{\partial q} \qquad \text{and} \qquad \dot{q} = \frac{\partial H}{\partial p}$$

Another approach of finding a first integral is rather simple for conservative problems. Consider *example 3.1.2* and rewrite two system of equations into

$$\ddot{x} + x + x^3 = 0$$

Where we introduce $f(x) = x + x^3$

So that multiplying by $\dot{x}$ becomes

$$\dot{x}\ddot{x} + \dot{x}(x + x^3) = 0 \qquad \text{or} \qquad \frac{d}{dt}\left(\tfrac{1}{2}\dot{x}^2\right) + \frac{d}{dt}\int\left(x + x^3\right)dx = 0$$

$$\frac{d}{dt}\left(\tfrac{1}{2}\dot{x}^2\right) + \frac{d}{dt}\left(\frac{x^2}{2} + \frac{x^4}{4}\right) = 0$$

Therefore the first integral of the equation is then

$$I = \tfrac{1}{2}\dot{x}^2 + \frac{x^2}{2} + \frac{x^4}{4} = constant$$

That is just the advantage of finding the first integral equation in conservative systems.

<u>*Example 4.1.3*</u>

Let us now look at three-dimensional system of equations

$$A\dot{x} = (B - C)yz \qquad B\dot{y} = (C - A)zx \qquad C\dot{z} = (A - B)xy$$

The equations for the orbits in the phase plane are

$$\frac{dx}{dy} = \frac{y}{x}\left(\frac{B-C}{A}\right)\left(\frac{B}{C-A}\right) \rightarrow ((C-A)A)xdx = (B(B-C))ydy$$

$$((C - A)A)x^2 + (B(C - B))y^2 = I_1(x, y)$$

$$\frac{dy}{dz} = \frac{z}{y}\left(\frac{C-A}{B}\right)\left(\frac{C}{A-B}\right) \rightarrow ((A-B)B)ydy = (C(C-A))zdz$$

$$((B - A)B)y^2 + (C(C - A))z^2 = I_2(y, z)$$

Now we have to construct in a three-dimensional differentiable function $I = I(x, y, z)$, so we have to use the so called Lyapunov function construction.. If we let $y = z = 0$, then x becomes arbitrary such as x_0. Then, I_1 or $I_1(x, y)- I_1(x_0, 0)$ is not sign definite in a neighborhood of $(x_0, 0, 0)$ and I_2 is semidefinite. One of the ways to construct a Lyapunov function is

$$I(x,y,z) = [I_1(x,y) - I_1(x_0,0)]^2 + I_2(y,z)$$

$$= [A(C-A)x^2 + B(C-B)y^2 - A(C-A)x_0^2]^2 + B(B-A)y^2 + C(C-A)z^2$$

$$\begin{aligned} I(x,y,z) = {} & A(C-A)x^4 + 2A(C-A)B(C-B)x^2y^2 - 2A^2(C-A)^2x^2x_0^2 + B^2(C-B)^2y^4 \\ & -2AB(C-A)(C-B)x_0^2y^2 + A^2(C-A)^2x_0^4 + B(B-A)y^2 + C(C-A)z^2 \end{aligned} \tag{4.1.3}$$

We will now check with orbital derivative,

$$L_tI = \frac{\partial I}{\partial x}\dot{x} + \frac{\partial I}{\partial y}\dot{y} + \frac{\partial I}{\partial z}\dot{z}$$

$$\frac{\partial I}{\partial x}\dot{x} = [4A^2(C-A)^2x^3 + 4A(C-A)B(C-B)xy^2 - 4A^2(C-A)^2xx_0^2]\left(\frac{(B-C)}{A}\right)yz$$

$$\frac{\partial I}{\partial y}\dot{y} = [4A(C-A)B(C-B)x^2y - 4B^2(C-B)^2y^3 - 4AB(C-A)(C-B)x_0^2y + 2B(B-A)y]\left(\frac{(C-A)}{B}\right)zx$$

$$\frac{\partial I}{\partial z}\dot{z} = 2C(C-A)z\left(\frac{(A-B)}{C}\right)xy$$

$$\begin{aligned} L_tI = {} & 4A(B-C)(C-A)^2x^3yz + 4B(C-A)(C-B)(B-C)xy^3z - 4A(C-A)^2(B-C)xx_0^2xyz \\ & + 4A(C-B)(C-A)^2x^3yz - 4B(C-A)(C-B)^2xy^3z \qquad - 4A(C-A)^2(C-B)xx_0^2yz \\ & + 2(C-A)(B-A)xyz + 2(C-A)(A-B)xyz \\ = {} & 0 \end{aligned}$$

Indeed, the resultant I in (4.1.3) is a first integral of the equation and give holonomic constraints.

4.2 INTEGRAL-PRESERVING NUMERICAL INTEGRATOR SYSTEMS

In the last section we showed that the first Integral of the equation, $I(x)$ is a constant (4.2.1), and it is typically a holonomic constraint. A system of equations that involves damping can be thought of as embedding of scleronomic constraints, because time t is implicitly involved. Consider:

$$I(\vec{x}) = constant \tag{4.2.1}$$

Taking the time derivative gives

$$\frac{\partial I}{\partial t} = \frac{\partial I}{\partial x_1}\frac{dx_1}{dt} + \frac{\partial I}{\partial x_2}\frac{dx_2}{dt} + \cdots + \frac{\partial I}{\partial x_n}\frac{dx_n}{dt} = 0$$

$$\frac{\partial I}{\partial t} = (\vec{\nabla} I)\cdot\frac{d\vec{x}}{dt} = (\vec{\nabla} I)\cdot F(\vec{x}) = 0 \qquad \because I(\vec{x}) = constant \tag{4.2.2}$$

If we know $I(\vec{x}_n) = constant$, we should be able to construct $I(\vec{x}_{n+1})$ similar to the energy preserving algorithms in Chapter 3. Therefore, as *a first step* we need to find a skew symmetric matrix, S, that has property ($S^T = -S$), i.e.,

$$S^T = -S = \begin{bmatrix} 0 & S_{12} \\ -S_{21} & 0 \end{bmatrix}$$

Now we can convert the system to *skew-gradient form*:

$$[S(\vec{x})]\cdot[\vec{\nabla} I(\vec{x})] = \frac{d\vec{x}}{dt} = F(\vec{x}) \tag{4.2.3}$$

Multiplying with $(\vec{\nabla} I)^T$ to both sides will give

$$(\vec{\nabla} I)^T [S](\vec{\nabla} I) = (\vec{\nabla} I)^T \cdot F(\vec{x}) = (\vec{\nabla} I)\cdot F(\vec{x}) \tag{4.2.4}$$

Taking the transpose of both sides

$$\left((\vec{\nabla} I)^T [S](\vec{\nabla} I)\right)^T = (\vec{\nabla} I)^T [S]^T (\vec{\nabla} I) = (\vec{\nabla} I)\cdot F(\vec{x})$$

where $\left((\vec{\nabla} I)^T\right)^T = (\vec{\nabla} I)$ is obvious. Also because $S^T = -S$,

$$-(\vec{\nabla}I)^T[S](\vec{\nabla}I) = (\vec{\nabla}I)\cdot F(\vec{x})$$

or

$$(\vec{\nabla}I)^T[S](\vec{\nabla}I) = -(\vec{\nabla}I)\cdot F(\vec{x}) \tag{4.2.5}$$

Thus comparing (4.2.4) and (4.2.5), we have

$$\vec{\nabla}I\cdot F(\vec{x}) = -\vec{\nabla}I\cdot F(\vec{x}) \qquad \text{or} \qquad \vec{\nabla}I\cdot F(\vec{x}) = 0 \tag{4.2.6}$$

Equation (4.2.6) is the same as equation (4.2.2). Therefore the skew symmetric matrix does not change the meaning of the first integral of the equation that is I is constant. Therefore, we want to find such S, skew-symmetric as a first step.

The next step is splitting. The n- dimensional vector fields

$$\vec{F} = \sum_{k=1}^{n} F_k \frac{\partial}{\partial x_k}$$

is split, using the skew-symmetry of S, into essentially 2-dimensional vector fields

$$\vec{F}_{ij} = S_{ij}\left[\frac{\partial I}{\partial x_j}\frac{\partial}{\partial x_i} - \frac{\partial I}{\partial x_i}\frac{\partial}{\partial x_j}\right]$$

This is not splitting into $2n$ systems of equations. The components x_i from the I split into n two-dimensional vector fields. Each of the vector fields, $\vec{F}_{ij}$, is equivalent to the system of equations

$$\frac{dx_i}{dt} = S_{ij}\frac{\partial I}{\partial x_j} \tag{4.2.7a}$$

$$\frac{dx_j}{dt} = -S_{ij}\frac{\partial I}{\partial x_i} \tag{4.2.7b}$$

$$\frac{dx_k}{dt} = 0 \qquad \text{where} \qquad k \neq i, j \tag{4.2.7c}$$

It immediately follows that

$$\vec{F}_{ij}[I(\vec{x})] = S_{ij}\left[\frac{\partial I}{\partial x_j}\frac{\partial I}{\partial x_i} - \frac{\partial I}{\partial x_i}\frac{\partial I}{\partial x_j}\right] = 0$$

Therefore, $I(\vec{x})$ is also a first integral for each of the system of *ODEs* (4.2.7) similar to the operator, *skew-gradient form*, to (4.2.3).

The final step is to write down first-order integral-preserving numerical integrators for the system similar to energy preserving algorithms. They are given by

$$x_i^* = x_i + \Delta t S_{ij}\frac{I(x_i^*, x_j^*) - I(x_i^*, x_j)}{x_j^* - x_j}$$

$$x_j^* = x_j - \Delta t S_{ij}\frac{I(x_i^*, x_j) - I(x_i, x_j)}{x_i^* - x_i}$$

$$x_k^* = x_k \qquad\qquad k \neq i, j$$

in which the asterisk (-*) represents the updated values

Note that

$$\vec{\lambda} = (\vec{\lambda})^T = S_{ij}\frac{\partial I}{\partial x_j}(\alpha x_i^* + (1-\alpha)x_i, \beta x_j^* + (1-\beta)x_j)$$
$$= \left[S_{ij}\frac{\partial I}{\partial x_j}(\alpha x_i^* + (1-\alpha)x_i, \beta x_j^* + (1-\beta)x_j)\right]^T$$

$$\vec{\mu} = (\vec{\mu})^T = S_{ij}\frac{\partial I}{\partial x_i}(\gamma x_i^* + (1-\gamma)x_i, \delta x_j^* + (1-\delta)x_j)$$
$$= \left[S_{ij}\frac{\partial I}{\partial x_i}(\gamma x_i^* + (1-\gamma)x_i, \delta x_j^* + (1-\delta)x_j)\right]^T$$

Example 4.2.1

We again take *example 3.1.2*

$$\dot{x}_1 = x_2$$

$$\dot{x}_2 = -x_1 - x_1^3$$

which has the Hamiltonian,

$$H(x_1, x_2) = \frac{x_1^2}{2} + \frac{x_1^4}{4} + \frac{x_2^2}{2} + C$$

is also a first integral of equations I because

$$L_t H = \frac{\partial H}{\partial x_1}\dot{x}_1 + \frac{\partial H}{\partial x_2}\dot{x}_2 = (x_1 + x_1^3)x_2 + x_2(-x_1 - x_1^3) = 0$$

Therefore $H = I$. Now we need to find the skew-symmetric matrix,

$$[S]\cdot[\vec{\nabla} I] = \begin{bmatrix} 0 & S_{12} \\ -S_{21} & 0 \end{bmatrix} \begin{bmatrix} x_1 + x_1^3 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_2 \\ -x_1 - x_1^3 \end{bmatrix}$$

where $S_{12} = 1$. After splitting the vector fields, the system of equations becomes

$$\dot{x}_1 = S_{12}\frac{\partial I}{\partial x_2} = x_2$$

$$\dot{x}_2 = -S_{12}\frac{\partial I}{\partial x_1} = -1(x_1 + x_1^3) = -x_1 - x_1^3$$

Which is the same as the original system of equations in this case. Therefore a first-order integral-preserving numerical integrators for the system are

$$x_1^* = x_1 + \Delta t S_{12}\frac{I(x_1^*, x_2^*) - I(x_1^*, x_2)}{x_2^* - x_2}$$

$$x_1^* = x_1 + \Delta t \frac{\left[\frac{(x_1^*)^2}{2} + \frac{(x_1^*)^4}{4} + \frac{(x_2^*)^2}{2}\right] - \left[\frac{(x_1^*)^2}{2} + \frac{(x_1^*)^4}{4} + \frac{(x_2)^2}{2}\right]}{x_2^* - x_2}$$

$$x_1^* = x_1 + \Delta t \frac{\frac{1}{2}\left((x_2^*)^2 - (x_2)^2\right)}{x_2^* - x_2}$$

$$x_1^* = x_1 + \frac{\Delta t}{2}(x_2^* + x_2) \tag{4.2.8}$$

$$x_2^* = x_2 - \Delta t S_{12} \frac{I(x_1^*, x_2) - I(x_1, x_2)}{x_1^* - x_1}$$

$$x_2^* = x_2 - \Delta t \frac{\left[\frac{(x_1^*)^2}{2} + \frac{(x_1^*)^4}{4} + \frac{(x_2)^2}{2}\right] - \left[\frac{(x_1)^2}{2} + \frac{(x_1)^4}{4} + \frac{(x_2)^2}{2}\right]}{x_1^* - x_1}$$

$$x_2^* = x_2 - \Delta t \frac{\frac{1}{2}\left((x_1^*)^2 - (x_1)^2\right)}{x_1^* - x_1} - \Delta t \frac{\frac{1}{4}\left((x_1^*)^2 - (x_1)^2\right)\cdot\left((x_1^*)^2 + (x_1)^2\right)}{x_1^* - x_1}$$

$$x_2^* = x_2 - \frac{\Delta t}{2}\left(x_1^* + x_1\right) - \frac{\Delta t}{4}\left(x_1^* + x_1\right)\cdot\left((x_1^*)^2 + (x_1)^2\right) \tag{4.2.9}$$

Substituting (4.2.8) into (4.2.9)

$$x_2^* = x_2 - \frac{\Delta t}{2}\left(x_1 + \frac{\Delta t}{2}(x_2^* + x_2) + x_1\right) - \frac{\Delta t}{4}\left(x_1 + \frac{\Delta t}{2}(x_2^* + x_2) + x_1\right)\cdot\left((x_1 + \frac{\Delta t}{2}(x_2^* + x_2))^2 + (x_1)^2\right)$$

setting $(\Delta t)^2 \approx 0$ (Without setting $(\Delta t)^2 \approx 0$, x_2^* is coupled and leads to cubic order terms which are not separable. Thus, we will set $(\Delta t)^2 \approx 0$ only if it is necessary).

$$x_2^* = x_2 - \frac{\Delta t}{2}(2x_1) - \frac{\Delta t}{4}(2x_1)\cdot\left((x_1)^2 + \Delta t x_1(x_2^* + x_2) + (x_1)^2\right)$$

$$x_2^* = x_2 - \Delta t x_1 - \frac{\Delta t}{2}(x_1)\cdot\left(2(x_1)^2\right)$$

$$x_2^* = x_2 - \Delta t x_1 - \Delta t x_1^3 \tag{4.2.10}$$

Substituting (4.210) into (4.2.8)

$$x_1^* = x_1 + \frac{\Delta t}{2}(x_2 - \Delta t x_1 - \Delta t x_1^3 + x_2)$$

$$x_1^* = x_1 + \Delta t x_2 - \frac{(\Delta t)^2}{2}(x_1 + x_1^3) \tag{4.2.11}$$

Finally, the system of equations from example 3.1.2 can not only predict that the phase curves are close contours, conservative, but we can also predict the next value in the phase plane at a given time step using first integral of equation or Hamiltonian in this case. *Figure 4.2.1a* shows Adams-Bashforth approximation of above example. *Figure 4.2.1b* shows Integral-Preserving approximation of above example. *Figure 4.2.1c* shows comparison between Runge-Kutta, Adams-Bashforth, and Integral-Preserving of above example.

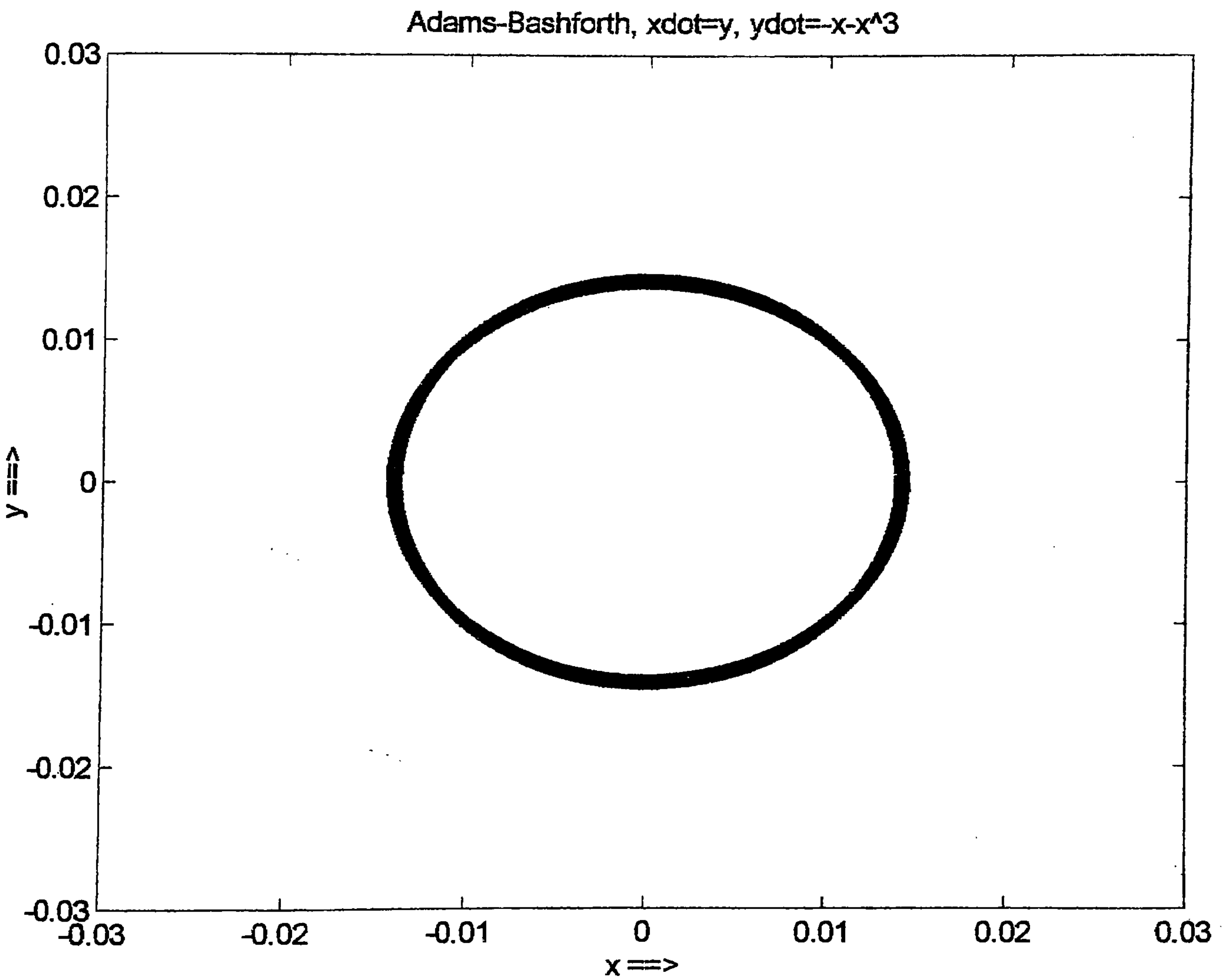

Figure 4.2.1a Adams-Bashforth approximation for *example 4.2.1*

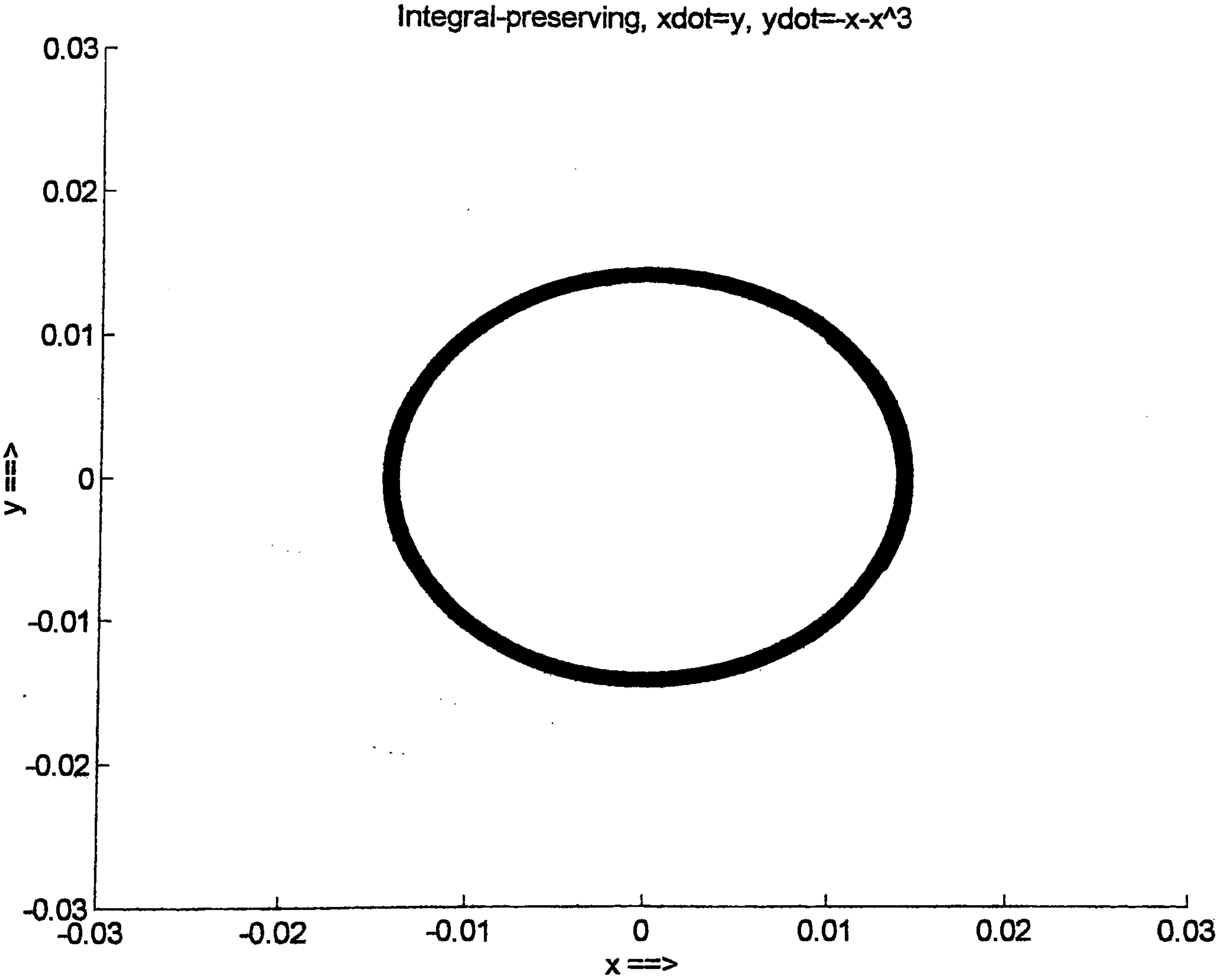

Figure 4.2.1b Integral-Preserving approximation for *example 4.2.1*

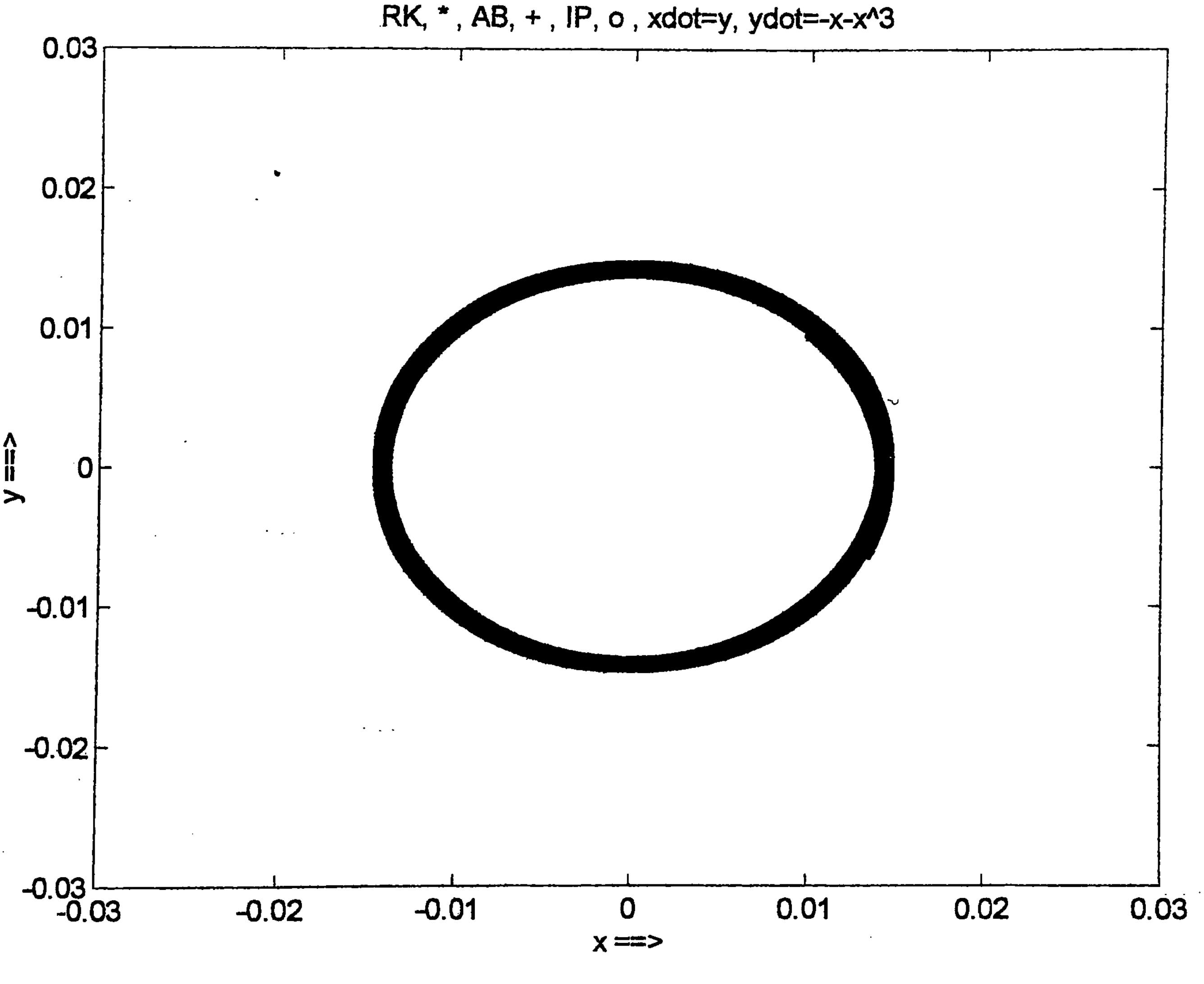

Figure 4.2.1c Comparison between Runge-Kutta, Adams-Bashforth, and Integral-preserving for *example 4.2.1*

Example 4.2.2

We again take *example 3.1.2*

$$\dot{x}_1 = x_1 + x_2$$

$$\dot{x}_2 = x_1 - x_2$$

which has the Hamiltonian,

$$H(x_1, x_2) = x_1 x_2 + \frac{x_2^2}{2} - \frac{x_1^2}{2} + C$$

is also a first integral of equations *I* because

$$L_t H = \frac{\partial H}{\partial x_1}\dot{x}_1 + \frac{\partial H}{\partial x_2}\dot{x}_2 = (x_2 - x_1)(x_1 + x_2) + (x_1 + x_2)(x_1 - x_2) = 0$$

Therefore $H = I$. Now we need to find the skew-symmetric matrix,

$$[S]\cdot[\vec{\nabla} I] = \begin{bmatrix} 0 & S_{12} \\ -S_{21} & 0 \end{bmatrix}\begin{bmatrix} x_2 - x_1 \\ x_1 + x_2 \end{bmatrix} = \begin{bmatrix} x_1 + x_2 \\ x_1 - x_2 \end{bmatrix}$$

where $S_{12} = 1$. After splitting the vector fields, the system of equations becomes

$$\dot{x}_1 = S_{12}\frac{\partial I}{\partial x_2} = x_1 + x_2$$

$$\dot{x}_2 = -S_{12}\frac{\partial I}{\partial x_1} = -1(x_2 - x_1) = x_1 - x_2$$

Which is the same as the original system of equations in this case. Therefore a first-order integral-preserving numerical integrators for the system are

$$x_1^* = x_1 + \Delta t S_{12}\frac{I(x_1^*, x_2^*) - I(x_1^*, x_2)}{x_2^* - x_2}$$

$$x_1^* = x_1 + \Delta t\frac{\left[x_1^* x_2^* + \frac{(x_2^*)^2}{2} - \frac{(x_1^*)^2}{2}\right] - \left[x_1^* x_2 + \frac{(x_2)^2}{2} - \frac{(x_1^*)^2}{2}\right]}{x_2^* - x_2}$$

$$x_1^* = x_1 + \Delta t \frac{x_1^*(x_2^* - x_2) + \frac{1}{2}\left((x_2^*)^2 - (x_2)^2\right)}{x_2^* - x_2}$$

$$x_1^* = x_1 + \Delta t\left(x_1^* + \tfrac{1}{2}\left(x_2^* + x_2\right)\right)$$

$$x_1^*(1-\Delta t) = x_1 + \frac{\Delta t}{2}\left(x_2^* + x_2\right)$$

$$x_1^* = \frac{x_1 + \frac{\Delta t}{2}\left(x_2^* + x_2\right)}{(1-\Delta t)} \tag{4.2.12}$$

$$x_2^* = x_2 - \Delta t S_{12} \frac{I(x_1^*, x_2) - I(x_1, x_2)}{x_1^* - x_1}$$

$$x_2^* = x_2 - \Delta t \frac{\left[x_1^* x_2 + \frac{(x_2)^2}{2} - \frac{(x_1^*)^2}{2}\right] - \left[x_1 x_2 + \frac{(x_2)^2}{2} - \frac{(x_1)^2}{2}\right]}{x_1^* - x_1}$$

$$x_2^* = x_2 - \Delta t \frac{x_2(x_1^* - x_1) - \frac{1}{2}\left((x_1^*)^2 - (x_1)^2\right)}{x_1^* - x_1}$$

$$x_2^* = x_2 - \Delta t\left(x_2 - \tfrac{1}{2}\left(x_1^* + x_1\right)\right)$$

$$x_2^* = x_2(1-\Delta t) + \frac{\Delta t}{2}\left(x_1^* + x_1\right) \tag{4.2.13}$$

substituting (4.2.12) into (4.2.13)

$$x_2^* = x_2(1-\Delta t) + \frac{\Delta t}{2}\left(\frac{x_1 + \frac{\Delta t}{2}\left(x_2^* + x_2\right)}{(1-\Delta t)} + x_1\right)$$

$$x_2^*(1-\Delta t) = x_2(1-\Delta t)^2 + \frac{\Delta t}{2}\left(x_1 + \frac{\Delta t}{2}\left(x_2^* + x_2\right) + x_1(1-\Delta t)\right)$$

$$x_2^*(1-\Delta t) = x_2(1-\Delta t)^2 + \frac{\Delta t}{2}\left(2x_1 + \frac{\Delta t}{2}\left(x_2^* + x_2\right) - x_1 \Delta t\right)$$

$$4x_2^*(1-\Delta t) = 4x_2(1-\Delta t)^2 + 4x_1\Delta t + (\Delta t)^2(x_2^* + x_2) - 2x_1(\Delta t)^2$$

$$4x_2^*(1-\Delta t-(\Delta t)^2)=4x_2(1-2\Delta t+(\Delta t)^2)+(\Delta t)^2x_2+4x_1\Delta t-2x_1(\Delta t)^2$$

$$x_2^*=\frac{4x_2(1-2\Delta t)+5(\Delta t)^2x_2+4x_1\Delta t-2x_1(\Delta t)^2}{4(1-\Delta t-(\Delta t)^2)} \tag{4.2.14}$$

Substituting (4.2.14) into (4.2.12)

$$x_1^*=\frac{x_1+\frac{\Delta t}{2}\left(\frac{4x_2(1-2\Delta t)+5(\Delta t)^2x_2+4x_1\Delta t-2x_1(\Delta t)^2+4(1-\Delta t-(\Delta t)^2)x_2}{4(1-\Delta t-(\Delta t)^2)}\right)}{(1-\Delta t)}$$

$$x_1^*=\frac{x_1+\frac{\Delta t}{2}\left(\frac{8x_2-12\Delta tx_2+(\Delta t)^2x_2+4x_1\Delta t-2x_1(\Delta t)^2}{4(1-\Delta t-(\Delta t)^2)}\right)}{(1-\Delta t)}$$

$$x_1^*=\frac{x_1+\left(\frac{8\Delta tx_2-12(\Delta t)^2x_2+(\Delta t)^3x_2+4x_1(\Delta t)^2-2x_1(\Delta t)^3}{8(1-\Delta t-(\Delta t)^2)}\right)}{(1-\Delta t)}$$

$$x_1^*=\left(\frac{8\Delta tx_2-12(\Delta t)^2x_2+(\Delta t)^3x_2+4x_1(\Delta t)^2-2x_1(\Delta t)^3+8x_1-8\Delta tx_1-8(\Delta t)^2x_1}{(8-8\Delta t)(1-\Delta t-(\Delta t)^2)}\right)$$

$$x_1^*=\left(\frac{8\Delta tx_2-12(\Delta t)^2x_2+(\Delta t)^3x_2+8x_1-8\Delta tx_1-4(\Delta t)^2x_1-2x_1(\Delta t)^3}{(8-8\Delta t)(1-\Delta t-(\Delta t)^2)}\right) \tag{4.2.15}$$

Finally, the given system of equations can predict that the phase curves are open contours by *example 3.1.3*, not conservative. Also, we can predict the next value in the phase plane at a given time step using first integral of equation or Hamiltonian in this case. *Figure 4.2.2a* shows Adams-Bashforth approximation of above example. *Figure 4.2.2b* shows Integral-Preserving approximation of above example. *Figure 4.2.2c* shows comparison between Runge-Kutta, Adams-Bashforth, and Integral-Preserving of above example

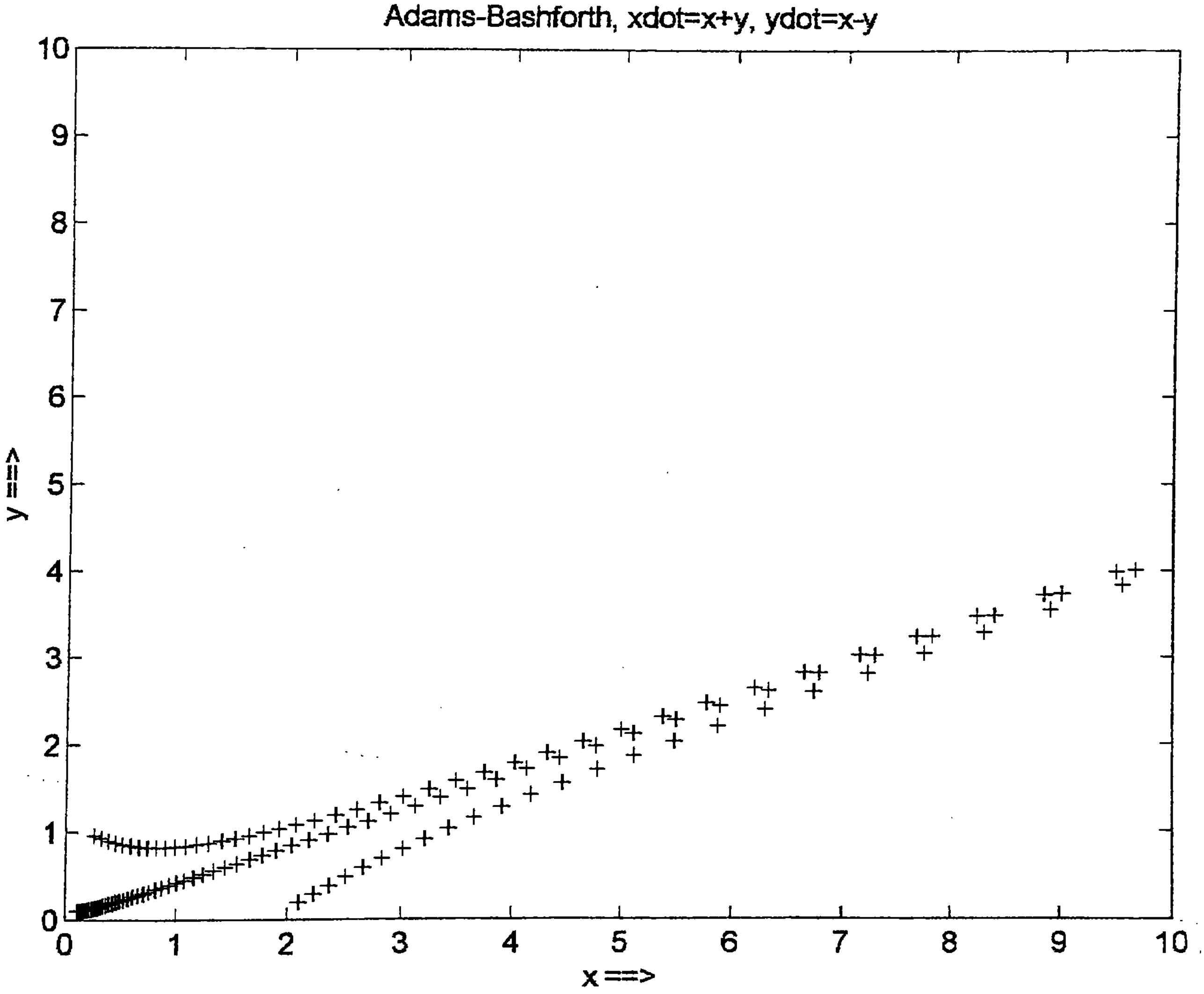

Figure 4.2.2a Adams-Bashforth approximation for *example 4.2.2*

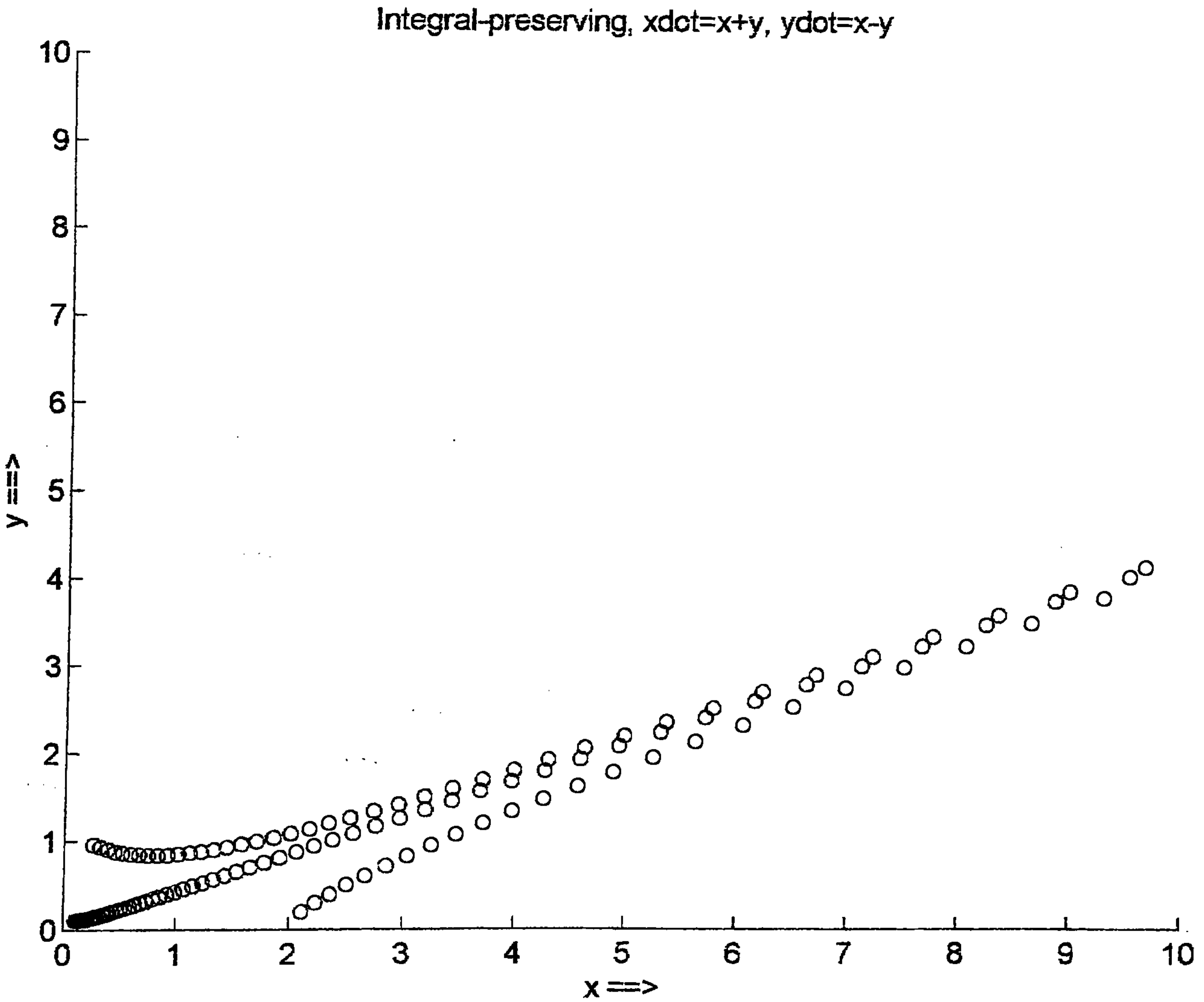

Figure 4.2.2b Integral-Preserving approximation for *example 4.2.2*

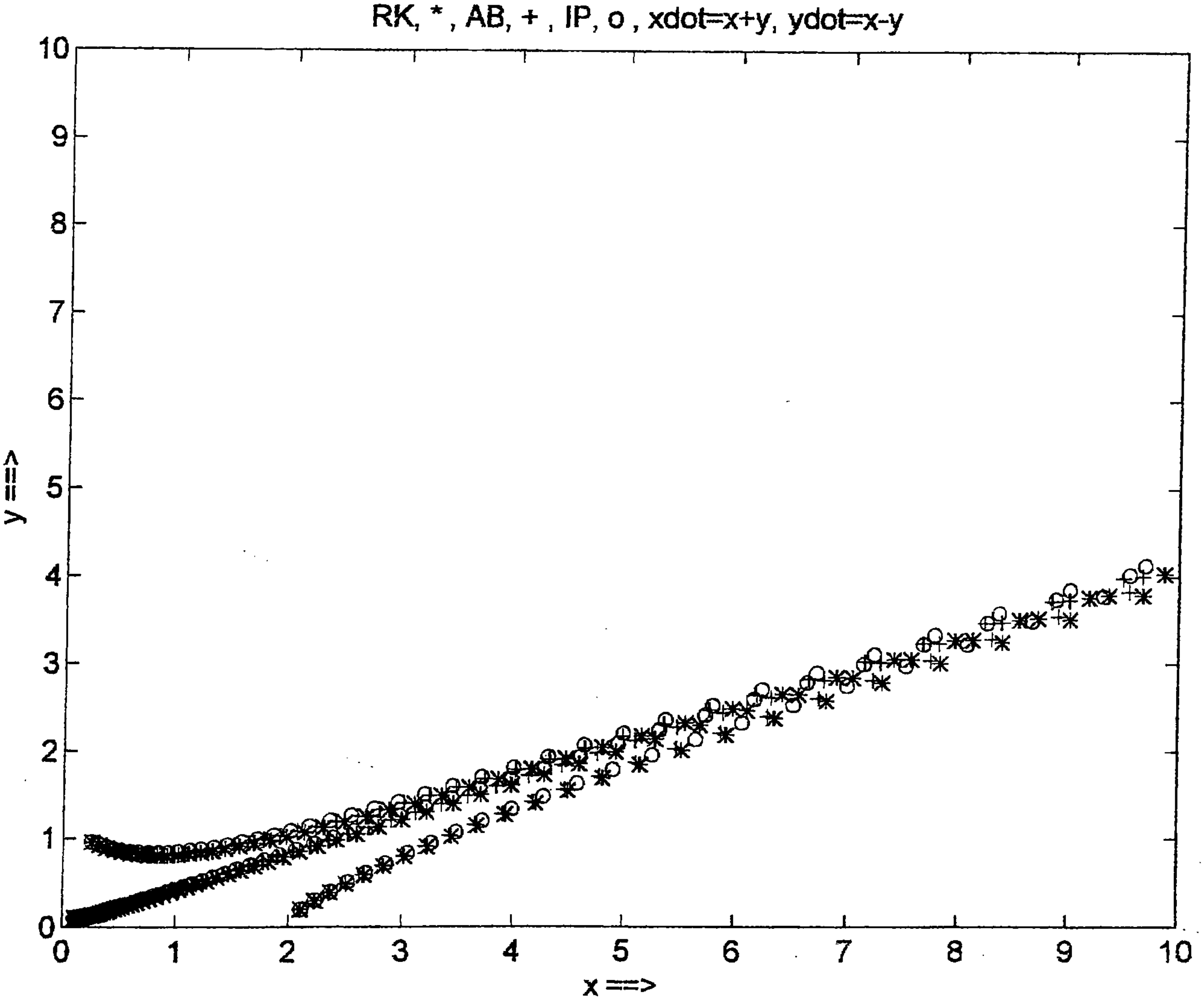

Figure 4.2.2c Comparison between Runge-Kutta, Adams-Bashforth, and Integral-preserving for *example 4.2.2*

Example 4.2.3

In order for us to understand splitting vector fields, we should study a three dimensional problem.

$$\frac{dx_1}{dt} = e^{x_3}$$

$$\frac{dx_2}{dt} = e^{x_1} + e^{x_3}$$

$$\frac{dx_2}{dt} = Be^{x_1} + e^{x_2}$$

Either the orbital derivative, $L_t I = 0$ or $(\vec{\nabla} I) \cdot F(\vec{x}) = 0$ will give us the first integral of the equations. That is,

$$(\vec{\nabla} I) \cdot F(\vec{x}) = \frac{\partial I}{\partial x_1}\dot{x}_1 + \frac{\partial I}{\partial x_2}\dot{x}_2 + \frac{\partial I}{\partial x_3}\dot{x}_3 = 0$$

$$\frac{\partial I}{\partial x_1}e^{x_3} + \frac{\partial I}{\partial x_2}\left(e^{x_1} + e^{x_3}\right) + \frac{\partial I}{\partial x_3}\left(Be^{x_1} + e^{x_2}\right) = 0$$

Let $\frac{\partial I}{\partial x_1} = a$, $\frac{\partial I}{\partial x_2} = b$, and $\frac{\partial I}{\partial x_3} = c$. Thus,

$$ae^{x_3} + b\left(e^{x_1} + e^{x_3}\right) + c\left(Be^{x_1} + e^{x_2}\right) = 0$$

The parameters a, b, and c do not have to be zero.

$$(b + Bc)e^{x_1} + ce^{x_2} + (a + b)e^{x_3} = 0$$

Letting $a + b = 0$, we have

$$(b + Bc)e^{x_1} + ce^{x_2} = 0$$

$$-ae^{x_1} + c(Be^{x_1} + e^{x_2}) = 0$$

$$a = c(B + e^{x_2 - x_1})$$

we can choose $c = 1$ for our convenience so that

$$a = \frac{\partial I}{\partial x_1} = (B + e^{x_2 - x_1}) \tag{4.2.16a}$$

$$b = \frac{\partial I}{\partial x_2} = -B - e^{x_2 - x_1} \tag{4.2.16b}$$

$$c = \frac{\partial I}{\partial x_3} = 1 \tag{4.2.16c}$$

Now we will solve three-dimensional potential form in order to find the first integral of the equations, I. Integrating equation (4.2.16a) with respect to x_1 gives

$$I(x_1, x_2, x_3) = Bx_1 - e^{x_2 - x_1} + I(x_2, x_3) \tag{4.2.17}$$

Take derivative to above equation with respect to x_2 and compare with (4.2.16b)

$$\frac{\partial I(x_1, x_2, x_3)}{\partial x_2} = -e^{x_2 - x_1} + \frac{\partial I(x_2, x_3)}{\partial x_2} = b = -B - e^{x_2 - x_1}$$

$$\frac{\partial I(x_2, x_3)}{\partial x_2} = -B$$

Integrate the equation with respect to x_2.

$$I(x_2, x_3) = -Bx_2 + I(x_3) \tag{4.2.18}$$

Take derivative to above equation with respect to x_3 and compare with (4.2.16c)

$$\frac{\partial I(x_2, x_3)}{\partial x_3} = \frac{\partial I(x_3)}{\partial x_3} = c = 1$$

Integrate the equation with respect to x_3.

$$I(x_3) = x_3 \tag{4.2.19}$$

Combining (4.2.17), (4.2.18), and (4.2.19), we have the first integral of the equations.

$$I(x_1, x_2, x_3) = -e^{x_2 - x_1} + B(x_1 - x_2) + x_3$$

Now we need to find the skew-symmetric matrix, S,

$$[s].\left[\vec{\nabla} I\right]=[F]=\begin{bmatrix}0 & S_{12} & S_{13}\\ -S_{12} & 0 & S_{23}\\ -S_{13} & -S_{23} & 0\end{bmatrix}\begin{bmatrix}e^{x_2-x_1}+B\\ -e^{x_2-x_1}-B\\ 1\end{bmatrix}=\begin{bmatrix}e^{x_3}\\ e^{x_1}+e^{x_3}\\ Be^{x_1}+e^{x_2}\end{bmatrix}$$

solving three equations and three unknowns yield

$$[S]=\begin{bmatrix}0 & 0 & e^{x_3}\\ 0 & 0 & (e^{x_1}+e^{x_3})\\ -e^{x_3} & -(e^{x_1}+e^{x_3}) & 0\end{bmatrix}$$

We will now split three two-dimensional vector fields so that we will have three sets of systems of equations in which each set has two system equations. That is

For x_1 and x_2 plane, $S_{12} = 0$.

$$\frac{dx_1}{dt}=S_{12}\frac{\partial I}{\partial x_2}=0$$

$$\frac{dx_2}{dt}=-S_{12}\frac{\partial I}{\partial x_1}=0$$

For x_1 and x_3 plane, $S_{13} =. e^{x_3}$

$$\frac{dx_1}{dt}=S_{13}\frac{\partial I}{\partial x_3}=e^{x_3}\cdot 1$$

$$\frac{dx_3}{dt}=-S_{13}\frac{\partial I}{\partial x_1}=-e^{x_3}(e^{x_2-x_2}+B)$$

For x_2 and x_3 plane, $S_{23} =. e^{x_1}+e^{x_3}$

$$\frac{dx_2}{dt}=S_{23}\frac{\partial I}{\partial x_3}=(e^{x_1}+e^{x_3})\cdot 1$$

$$\frac{dx_3}{dt}=-S_{23}\frac{\partial I}{\partial x_2}=-(e^{x_1}+e^{x_3})(-e^{x_2-x_2}-B)$$

We will show how to find the new values from the x_1 - x_2 plane in the next example. Let us now choose x_1 - x_3 plane to solve new values of x_1 and x_3. For that, we have to treat x_2 as a constant. Using the first order integral-preserving numerical integrators, we get

$$x_1^* = x_1 + \Delta t \frac{(-e^{x_2 - x_1^*} + B(x_1^* - x_2) + x_3^*) - (-e^{x_2 - x_1^*} + B(x_1^* - x_2) + x_3)}{x_3^* - x_3}$$

$$x_1^* = x_1 + \Delta t \frac{x_3^* - x_3}{x_3^* - x_3}$$

$$x_1^* = x_1 + \Delta t$$

and

$$x_3^* = x_3 - \Delta t \frac{(-e^{x_2 - x_1^*} + B(x_1^* - x_2) + x_3) - (-e^{x_2 - x_1} + B(x_1 - x_2) + x_3)}{x_1^* - x_1}$$

$$x_3^* = x_3 - \Delta t \frac{(-e^{x_2 - x_1^*} + e^{x_2 - x_1}) + B(x_1^* - x_1)}{x_1^* - x_1}$$

substituting $x_1^* = x_1 + \Delta t$ into above equation yields,

$$x_3^* = x_3 - \Delta t \frac{(-e^{x_2 - x_1 - \Delta t} + e^{x_2 - x_1}) + B\Delta t}{\Delta t}$$

$$x_3^* = x_3 + e^{x_2 - x_1}(e^{-\Delta t} - 1) - B\Delta t$$

$$x_3^* = x_3 + e^{x_2 - x_1} \frac{1 - e^{\Delta t}}{e^{\Delta t}} - B\Delta t$$

Now we can show the new value for x_1 and x_3 in x_1 - x_3 plane. The same procedure can be done for x_2 - x_3 plane.

Example 4.2.4

Consider: $\dot{x}_1 = x_1 + x_2$

$\dot{x}_2 = x_1 - x_1 x_2$

which does not satisfy the Liouville's Theorem so that it is not an Hamiltonian system.

$$\sum_{i=1}^{n} \frac{\partial \dot{q}_i}{\partial q_i} + \sum_{i=1}^{n} \frac{\partial \dot{p}_i}{\partial p_i} = \frac{\partial \dot{x}_1}{\partial x_1} + \frac{\partial \dot{x}_2}{\partial x_2} = 1 - x_1 \neq 0$$

To find the first integral, we have to set the orbital derivative of F to be zero.

$$L_t I = \frac{\partial I}{\partial x_1}\dot{x}_1 + \frac{\partial I}{\partial x_2}\dot{x}_2 = \frac{\partial I}{\partial x_1}(x_1 + x_2) + \frac{\partial I}{\partial x_2}(x_1 - x_1 x_2) = 0$$

let $\frac{\partial I}{\partial x_1} = a$ and $\frac{\partial I}{\partial x_2} = b$ so that

$$a(x_1 + x_2) + b(x_1 - x_1 x_2) = 0 \qquad \text{and} \qquad (a + b(1 - x_2))x_1 + a x_2 = 0$$

let $b = -a$

$$(a - a(1 - x_2))x_1 + a x_2 = 0 \qquad \text{and} \qquad (a x_2)x_1 + a x_2 = a x_2(1 + x_1) = 0$$

Therefore $a = b = 0$, and I is just an arbitrary constant. Therefore, the system of equations may have involved a nonintegrable differential expression (nonholonomic constraints may be embedded in the given system) that vanishes in the attempt to find the skew symmetric, S. Then the skew-symmetric matrix can not be defined. Thus, still preserving, the first integral, we cannot predict the next point in the phase space. *Figure 4.2.3* shows Runge-Kutta approximation, and *Figure 4.2.4* shows Adams-Bashforth approximation of above example. One may find above two figures are not similar because both are unstable systems, and the proof is beyond the scope of this thesis since the integral preserving method would not give the prediction.

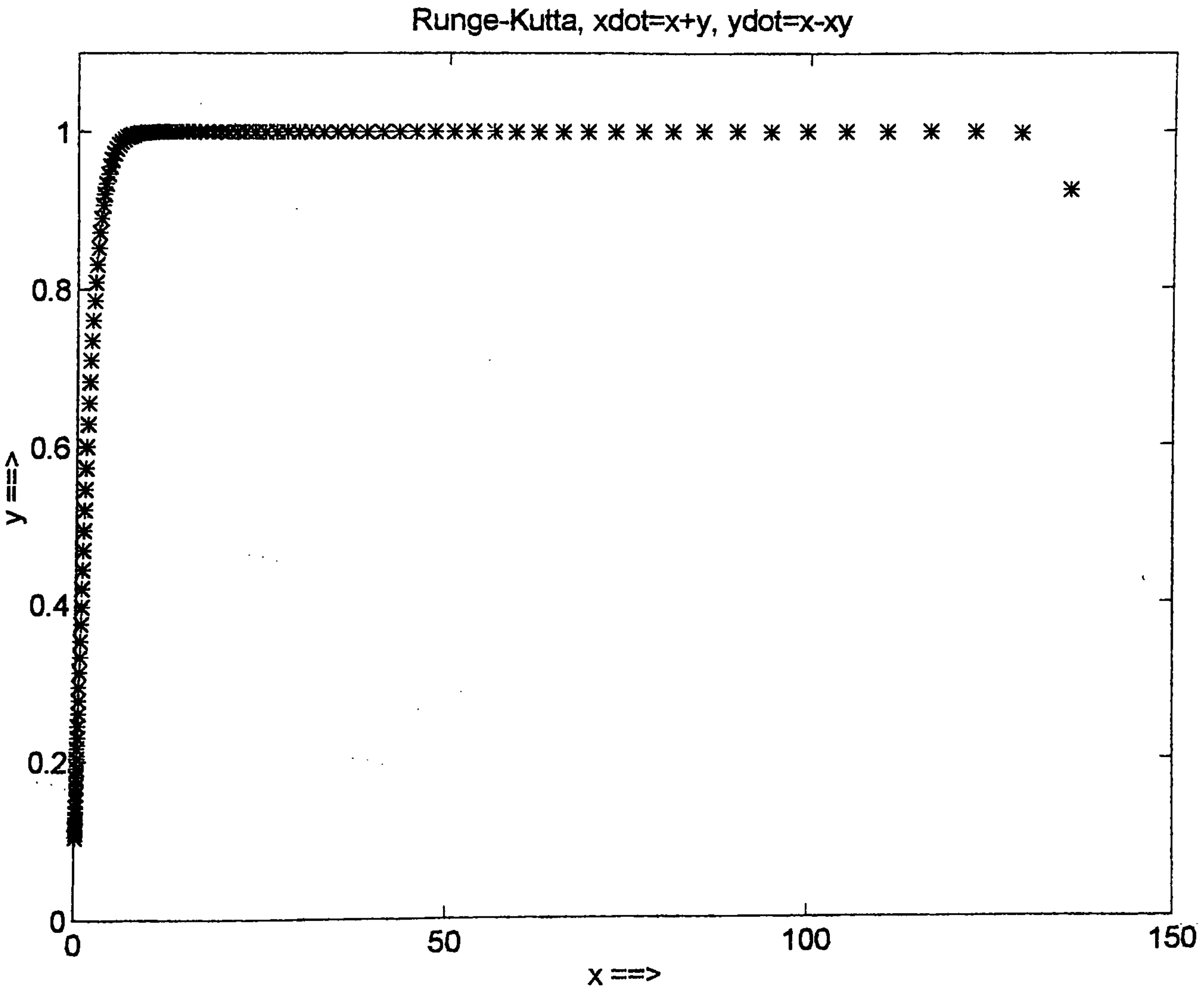

Figure 4.2.3 Runge-Kutta approximation for *example 4.2.4*

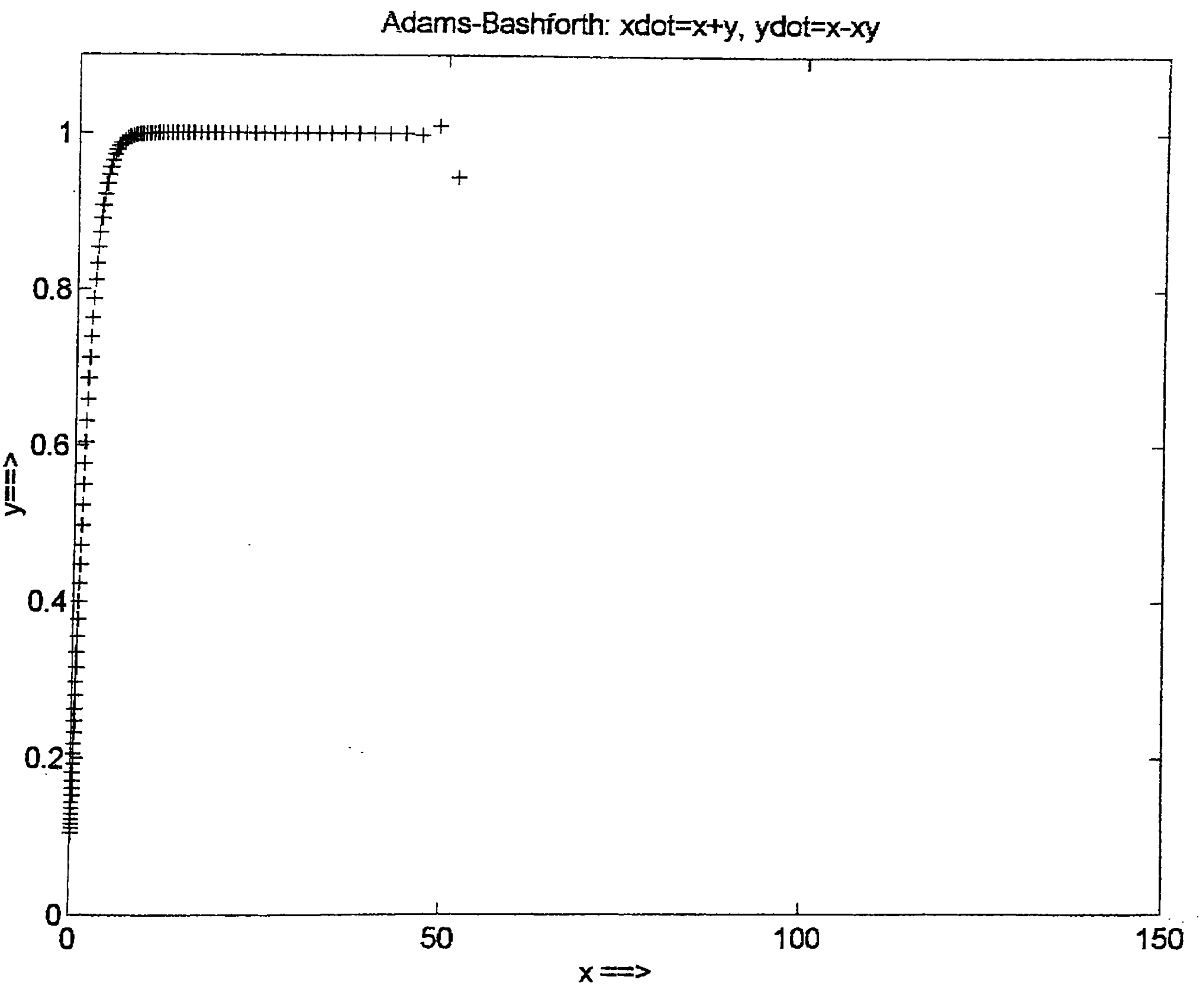

Figure 4.2.4 Adams-Bashforth approximation for *example 4.2.4*

Up until now we have been given problems without damping. If the problem have some damping, a dissipation function, or a generalized force that is not derivable from a potential function or dissipation, we still can find the first integral of the system. First integrals of these systems appear to be embedded scleronomic constraints (time implicitness involves even after writing as system of equations).

Example 4.2.5

Consider

$$\ddot{x}+(1-x^2)\dot{x}=0$$

$$\dot{x}_1=x_2$$

$$\dot{x}_2=-x_2+x_1^2x_2$$

which does not satisfy the Liouville's Theorem so that it is not an Hamiltonian system.

$$\sum_{i=1}^{n}\frac{\partial \dot{q}_i}{\partial q_i}+\sum_{i=1}^{n}\frac{\partial \dot{p}_i}{\partial p_i}=\frac{\partial \dot{x}_1}{\partial x_1}+\frac{\partial \dot{x}_2}{\partial x_2}=0-1+x_1^2\neq 0$$

Taking the orbital derivative and set L_tI to be zero gives

$$L_tI=\frac{\partial I}{\partial x_1}\dot{x}_1+\frac{\partial I}{\partial x_2}\dot{x}_2=\frac{\partial I}{\partial x_1}(x_2)+\frac{\partial I}{\partial x_2}(-x_2+x_1^2x_2)=0$$

let $\frac{\partial I}{\partial x_1}=a$ and $\frac{\partial I}{\partial x_2}=b$ so that

$$a(x_2)+b(-x_2+x_1^2x_2)=0$$

$$a+b(-1+x_1^2)=0$$

$$a=b(1-x_1^2)$$

let $b = 1$ so that

$$a = \frac{\partial I}{\partial x_1} = (1 - x_1^2) \qquad \text{and} \qquad b = \frac{\partial I}{\partial x_2} = 1$$

Integrating a with respect to x_1, we get

$$I = x_1 - \frac{x_1^3}{3} + I(x_2)$$

Take derivative above equation with respect to x_2 and compare with b.

$$\frac{\partial I}{\partial x_2} = I'(x_2) = b = 1$$

Therefore, integrating with respect to x_1 gives

$$I(x_2) = x_2 + C$$

Thus

$$I = x_1 - \frac{x_1^3}{3} + x_2 + C$$

Then the skew-symmetric matrix is then

$$[S]\cdot[\vec{\nabla} I] = \begin{bmatrix} 0 & S_{12} \\ -S_{12} & 0 \end{bmatrix} \begin{bmatrix} 1 - x_1^2 \\ 1 \end{bmatrix} = \begin{bmatrix} x_2 \\ -x_2 + x_1^2 x_2 \end{bmatrix}$$

S_{12} becomes arbitrary and $S_{12} = \dot{x}_1 = x_2$. Also, splitting the vector fields, the system of equations becomes

$$\dot{x}_1 = S_{12}\frac{\partial I}{\partial x_2} = S_{12} = x_2$$

$$\dot{x}_2 = -S_{12}\frac{\partial I}{\partial x_1} = x_2(x_1^2 - 1)$$

A first-order integral-preserving numerical integrators for the system are

$$x_1^* = x_1 + \Delta t S_{12} \frac{I(x_1^*, x_2^*) - I(x_1^*, x_2)}{x_2^* - x_2}$$

$$x_1^* = x_1 + \Delta t x_2 \frac{\left(x_1^* - \frac{(x_1^*)^3}{3} + x_2^*\right) - \left(x_1^* - \frac{(x_1^*)^3}{3} + x_2\right)}{x_2^* - x_2}$$

$$x_1^* = x_1 + \Delta t x_2 \tag{4.2.20}$$

also,

$$x_2^* = x_2 - \Delta t x_2 \frac{I(x_1^*, x_2) - I(x_1, x_2)}{x_1^* - x_1}$$

$$x_2^* = x_2 - \Delta t x_2 \frac{\left(x_1^* - \frac{(x_1^*)^3}{3} + x_2\right) - \left(x_1 - \frac{x_1^3}{3} + x_2\right)}{x_1^* - x_1}$$

$$x_2^* = x_2 - \Delta t x_2 + \frac{\Delta t x_2}{3} \frac{((x_1^*)^3 - x_1^3)}{(x_1^* - x_1)} \tag{4.2.21}$$

substituting (4.2.20) into (4.2.21)

$$x_2^* = x_2 - \Delta t x_2 + \frac{\Delta t x_2}{3} \frac{(x_1^3 + 3\Delta t x_1^2 x_2 + 3(\Delta t)^2 x_1 x_2^2 + x_2^3 (\Delta t)^3 - x_1^3)}{(x_1 + \Delta t x_2 - x_1)}$$

$$x_2^* = x_2 - \Delta t x_2 + \frac{\Delta t x_2}{3} \frac{(3\Delta t x_1^2 x_2 + 3(\Delta t)^2 x_1 x_2^2 + x_2^3 (\Delta t)^3)}{\Delta t x_2}$$

$$x_2^* = x_2 - \Delta t x_2 + \Delta t x_1^2 x_2 + (\Delta t)^2 x_1 x_2^2 + \frac{x_2^3 (\Delta t)^3}{3}$$

Figure 4.2.5a shows Runge-Kutta approximation of above example. *Figure 4.2.5b* shows Adams-Bashforth approximation of above example. *Figure 4.2.5c* shows Integral-Preserving approximation of above example. *Figure 4.2.5d* shows comparison between, Runge-Kutta, Adams-Bashforth, and Integral-Preserving of above example.

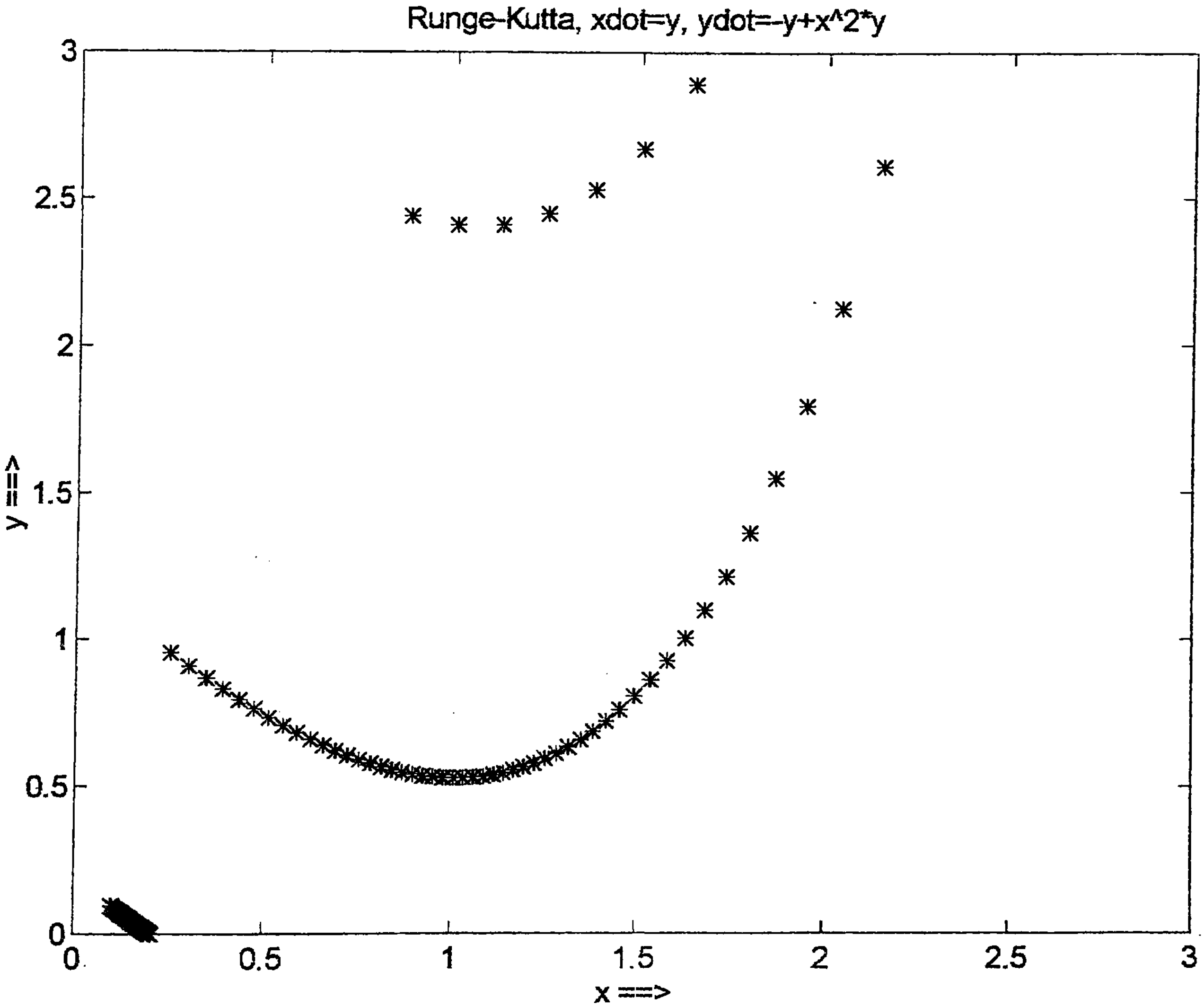

Figure 4.2.5a Runge-Kutta approximation for *example 4.2.5*

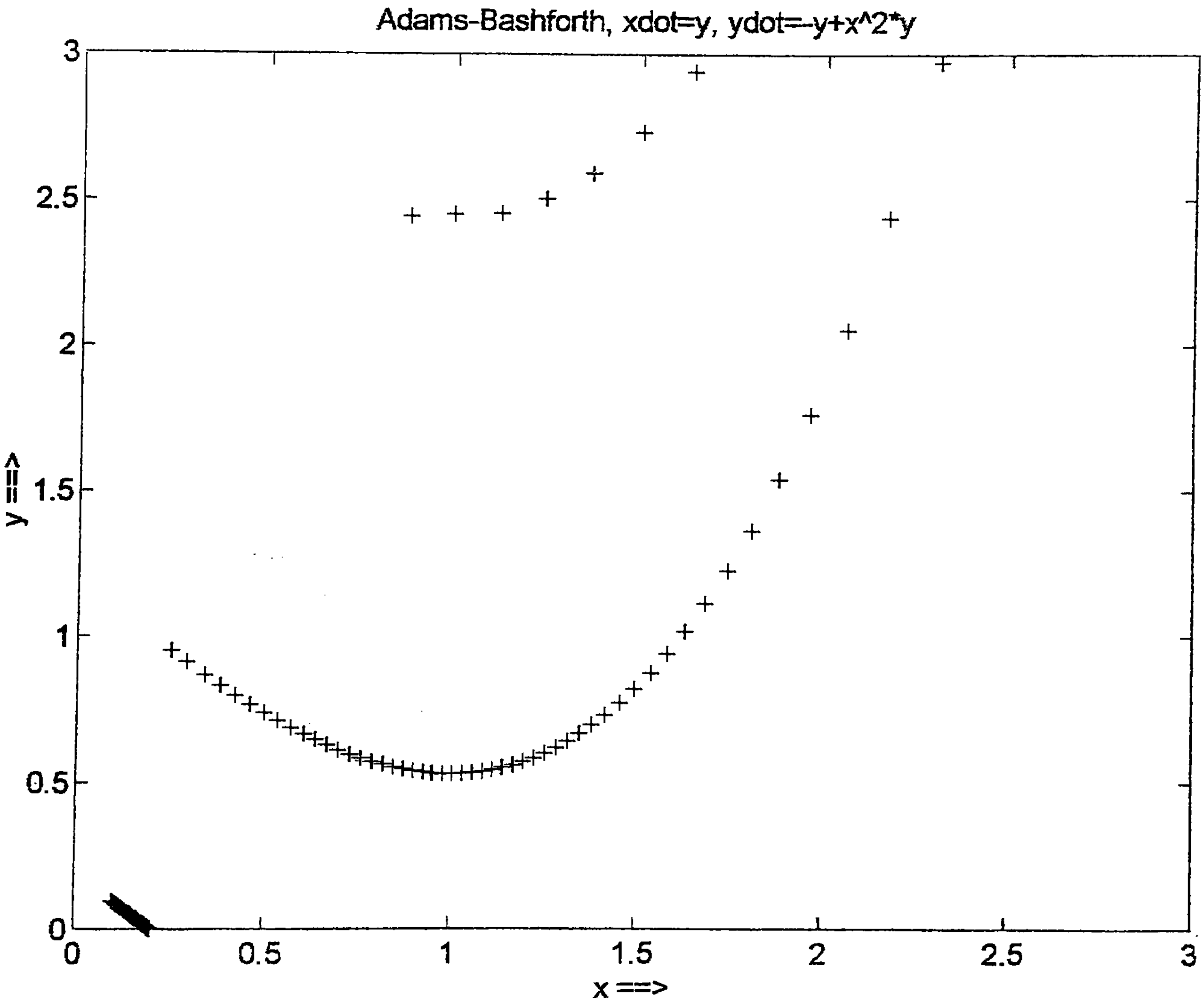

Figure 4.2.5b Adams-Bashforth approximation for *example 4.2.5*

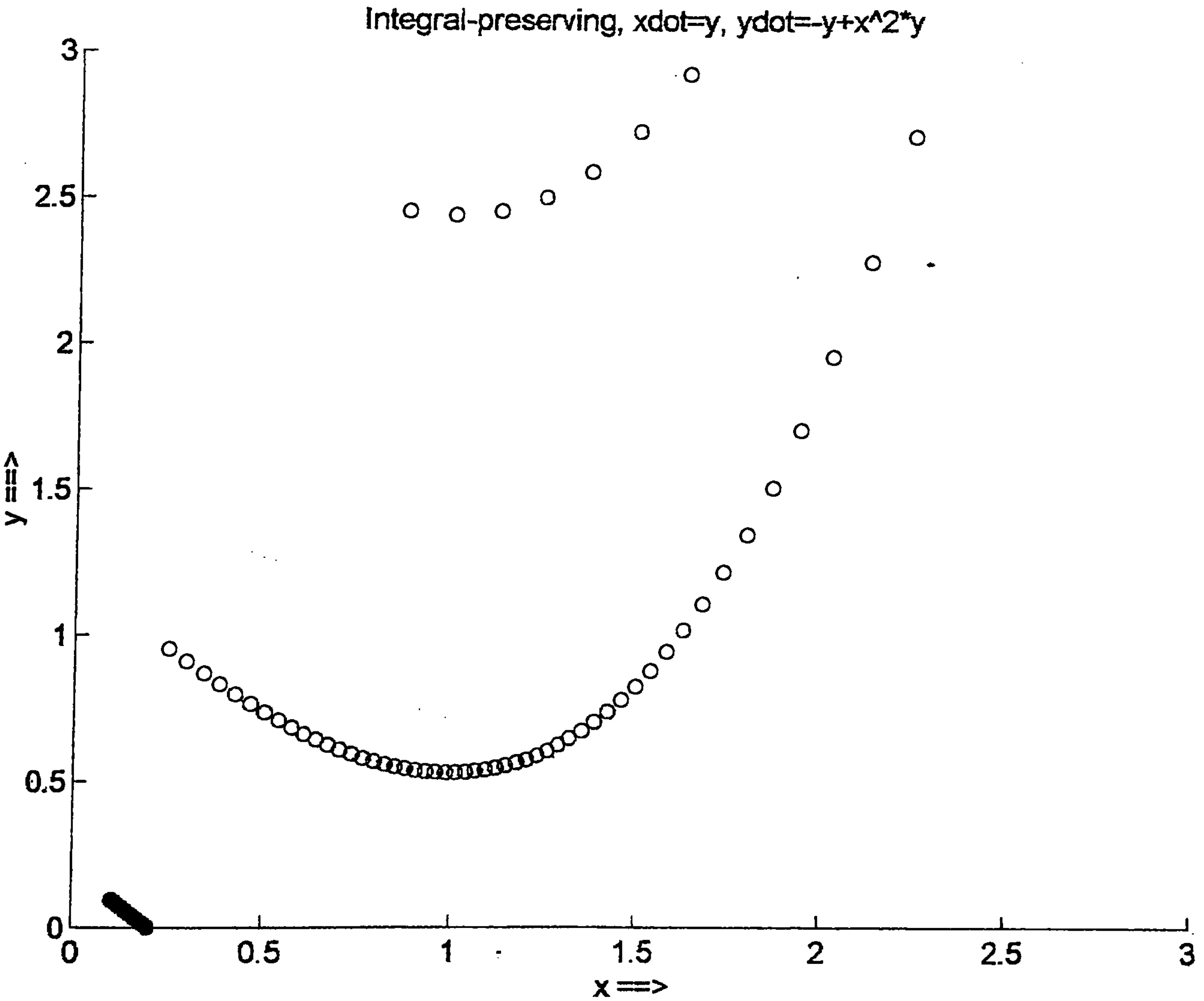

Figure 4.2.5c Integral-preserving approximation for *example 4.2.5*

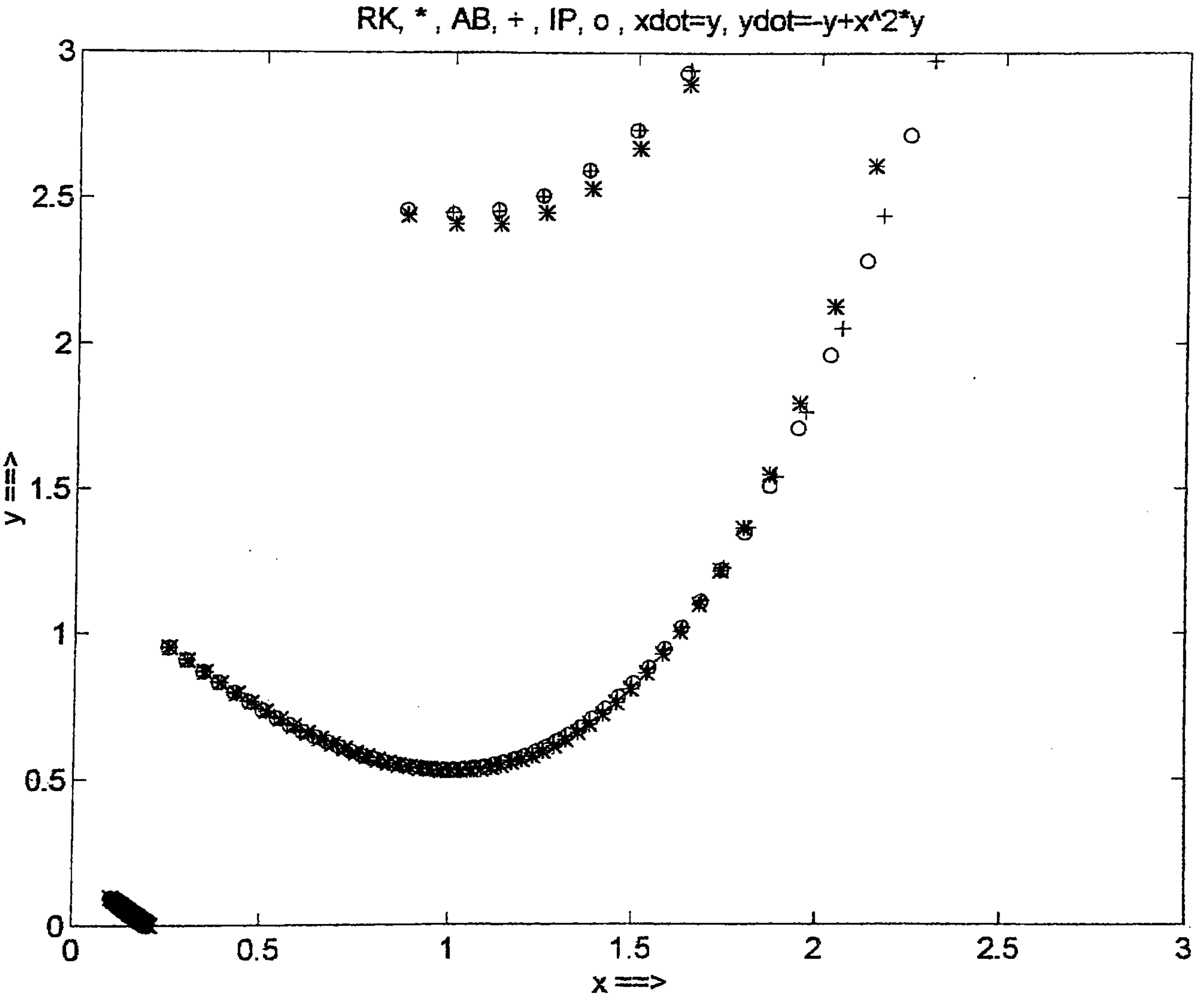

Figure 4.2.5d Comparison between Runge-Kutta, Adams-Bashforth, and Integral-preserving for *example 4.2.5*

Example 4.2.6

Consider the next example of dissipation and a generalized force that is not derivable from a potential function or a dissipation function.

$$\ddot{x}+(1-x^2)\dot{x}^2=0$$

That is,

$$\dot{x}_1=x_2$$

$$\dot{x}_2=-x_2^2+x_1^2x_2^2$$

which does not satisfy the Liouville's Theorem so that it is not a Hamiltonian system.

$$\sum_{i=1}^{n}\frac{\partial \dot{q}_i}{\partial q_i}+\sum_{i=1}^{n}\frac{\partial \dot{p}_i}{\partial p_i}=\frac{\partial \dot{x}_1}{\partial x_1}+\frac{\partial \dot{x}_2}{\partial x_2}=0-2x_2+2x_1^2x_2\neq 0$$

To find the first integral, we have to set the orbital derivative of F to be zero.

$$L_tI=\frac{\partial I}{\partial x_1}\dot{x}_1+\frac{\partial I}{\partial x_2}\dot{x}_2=\frac{\partial I}{\partial x_1}(x_2)+\frac{\partial I}{\partial x_2}(-x_2^2+x_1^2x_2^2)=0$$

let $\frac{\partial I}{\partial x_1}=a$ and $\frac{\partial I}{\partial x_2}=b$ so that

$$a(x_2)+b(-x_2+x_1^2x_2^2)=0$$

$$a+bx_2(-1+x_1^2)=0$$

$$a=bx_2(1-x_1^2)$$

we cannot let b = 1 because, if b = 1

$$a=\frac{\partial I}{\partial x_1}=x_2(1-x_1^2) \quad \text{and} \qquad b=\frac{\partial I}{\partial x_2}=1$$

Integrating a with respect to x_1, we get

$$I=x_1x_2-\frac{x_1^3x_2}{3}+I(x_2)$$

Take derivative above equation with respect to x_2 and compare with b.

$$\frac{\partial I}{\partial x_2} = x_1 - \frac{x_1^3}{3} + I'(x_2) = b = 1$$

The above cannot be true or cannot be equalized. Therefore $a = b$ must be zero. Thus a first integral of the given system is an arbitrary constant similar to *example 4.2.4*.

$$I = constant$$

Then the skew-symmetric matrix can not be defined. The next point in the phase space cannot be established. Also, conventional numerical methods show that the vectors fields are approaching to a constant point like exponential. *Figure 4.2.6a* shows Runge-Kutta approximation of above example. *Figure 4.2.6b* Adams-Bashforth approximation of above example

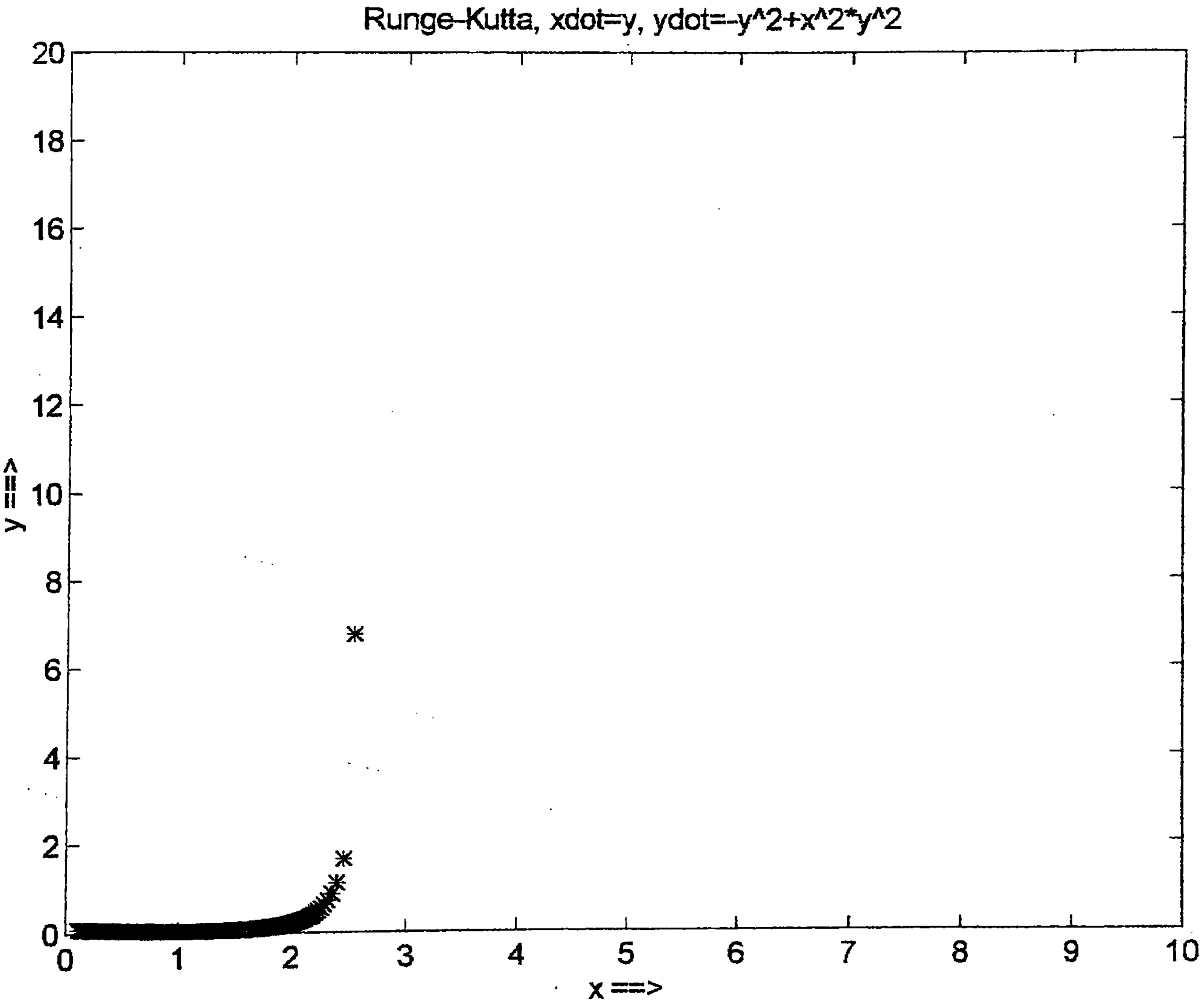

Figure 4.2.6a Runge-Kutta approximation for *example 4.2.6*

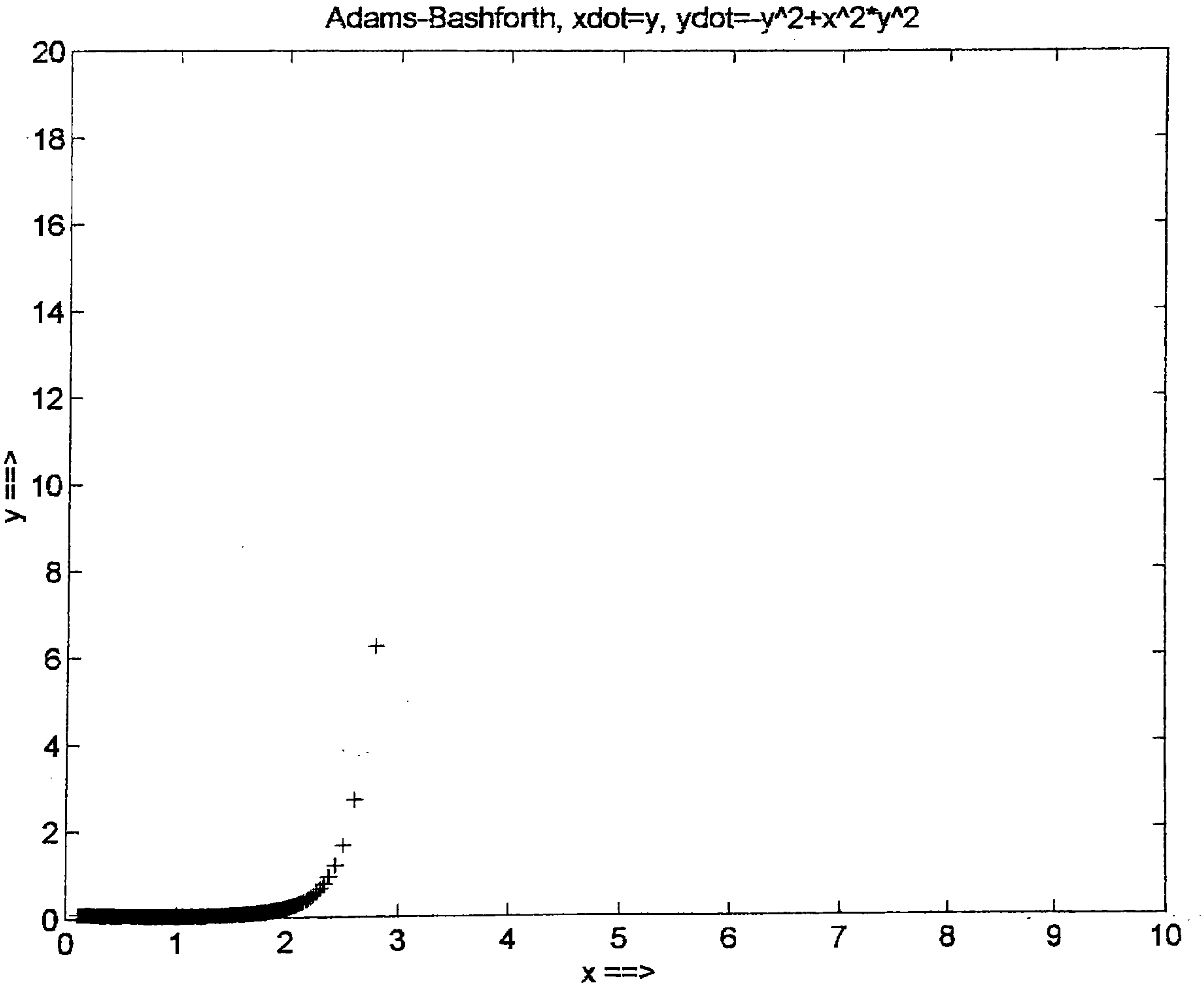

Figure 4.2.6b Adams-Bashforth approximation for *example 4.2.6*

We now need to discuss one last kind of constraint that are embedded in the system of equations. That is, rheonomic constraints such as nonautonomous system of equations. Now we will take *example 2.2.5* for further studies. We will keep in mind that the only difference between *example 2.2.5* and *example 2.2.4* is that one has a Hamiltonian and one does not. We are now trying to find first integral of the equation with time t explicitly shown in the system of equations.

<u>*Example 4.2.7*</u>

$$\dot{x}_1 = x_1 t + 2x_2$$

$$\dot{x}_2 = x_1 t^2 - x_2 t$$

Again using Liouville's Theorem to determine if the system of equations are Hamiltonian,

$$\sum_{i=1}^{n} \frac{\partial \dot{q}_i}{\partial q_i} + \sum_{i=1}^{n} \frac{\partial \dot{p}_i}{\partial p_i} = \frac{\partial \dot{x}_1}{\partial x_1} + \frac{\partial \dot{x}_2}{\partial x_2} = t - t = 0$$

To find the first integral, we have to set the orbital derivative of F to be zero.

$$L_t I = \frac{\partial I}{\partial x_1}\dot{x}_1 + \frac{\partial I}{\partial x_2}\dot{x}_2 = \frac{\partial I}{\partial x_1}(x_1 t + 2x_2) + \frac{\partial I}{\partial x_2}(x_1 t^2 - x_2 t) = 0$$

let $\frac{\partial I}{\partial x_1} = a$ and $\frac{\partial I}{\partial x_2} = b$ so that

$$a(x_1 t + 2x_2) + b(x_1 t^2 - x_2 t) = 0$$

$$(at + bt^2)x_1 + (2a - bt)x_2 = 0$$

If we let $a = b\frac{t}{2}$

$$(a + bt)x_1 = 0$$

which leads to

$$a + bt = \frac{bt}{2} + bt = \frac{3bt}{2} = 0 \Rightarrow b = 0 \Rightarrow a = 0$$

Again the result shows that first integral of equation is an arbitrary constant, and we cannot predict the next point in the phase space. It cannot also be predicted by Runge-Kutta or Adams-Bashforth methods; it may be because the 'time' step and the explicit 'time' shown in the equations may not be separated in the calculations (both h and x will be 'time' in the equations of appendix). One may find the details on classifications of 'time' and may predict the solutions for Runge-Kutta and/or Adams-Bashforth, but again the results from Runge-Kutta and Adams-Bashforth are beyond the scope of this thesis since the Integral Preserving method can not be predicted. Also, embedding rheonomic constraints in the system of equations (time explicitness) behaves like that of nonholonomic constraints. Essentially, there is no numerical solution for rheonomic constraints or nonautonomous systems by Integral Preserving method.

CHAPTER 5

SUMMARY AND CONCLUSIONS

Lagrangian Dynamics and Hamiltonian Dynamics driven by kinetic energies and momenta through generalized coordinates have been reviewed. The classification of constraint forces is also reviewed. Round off errors are eliminated by preserving energies. More accurate numerical solutions are believed to be solved by energy preserving method with only truncation error. By preserving the first integrals, we have interesting results such that for a system of equations whether we can predict numerical solution more accurately or whether we cannot predict numerical solution at all (when the first integral is an arbitrary constant) by energy preserving algorithms.

For a conservative Hamiltonian system (example 4.2.1), the Hamiltonian is the same as the first integral (because it satisfies both Liouville's Theorem and orbital derivatives), and it can have more accurate numerical solution. The solution matched up with conventional numerical methods. Such system can be viewed as a holonomic system because the surface is integrable and is a constant after preserving the first integral. For non-conservative Hamiltonian system (example 4.2.2), the solution still exists, and the Hamiltonian is again the same as the first integral. The solution matched up with conventional numerical methods; we can also assume the system was holonomic system. For the particular example (example 4.2.2), the system is semi-stable. Integral preserving may show better results by observing points (quantities) which are closer packed than the ones from conventional methods.

For some non-Hamiltonian system (example 4.2.4), the first integral was shown to be an arbitrary constant. We can clearly see this kind of system as nonholonomic system;

the potential functions from the set of equations cannot be integrated (non-integratable) to find a first integral. There will not be any numerical solution by integral preserving method for this kind of system.

For damping problems where time is implicitly involved, scleronomic systems, the Hamiltonians are not usually the same as the first integrals (example 4.2.5 and 4.2.6). If we find the first integral is constant, other than arbitrary one, scleronomic system can have more accurate solution (example 4.2.5). If we find a first integral that is an arbitrarily constant (example 4.2.6), scleronomic system can not have integral preserving numerical solution.

For rheonomic system, where a system of equations has time explicitness, the Hamiltonian may or may not be the same as the first integral. Rheonomic systems do not have numerical solution by energy preservation algorithms because the first integrals always give arbitrary constant.

Therefore, we can predict whether we can have integral preserving numerical solutions (more accurate solutions) or not by preserving the first integrals because the solutions exist only if we have non-arbitrary first integrals constants. In addition, we know that sets of equations may be viewed as embedding constraint equations into the problem formulation. In this way the constraint forces do not appear in the equations of motion. By adjoining constraints to the problem formulation, some or all of the constraint forces may be solved for after the generalized coordinates have been obtained. The equations of motion for the configuration coordinates are free of constraint forces. These forces are then expressed in terms of the motion of the system, based on Lagrange's equations for the auxiliary constraint variables. Thus, constraints are not to be kept track as initial conditions or boundary conditions while solving numerical solutions by energy preserving algorithm. Along with embedding constraints into problem formulation, predicting the first integral (to find numerical solutions to be more accurate without keeping track of initial conditions and boundary conditions) gives more appealing method to use as a new and improved numerical method.

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Appendix

All the examples in this thesis have a time step of 0.01s.

Runge Kutta Method for Two First Order Ordinary differential Equations

Given: $dz/dx = z' = f(x, y, z)$ with initial condition $z = z_i$ at $x = x_i$
$dy/dx = y' = g(x, y, z)$ with initial condition $y = y_i$ at $x = x_i$

$K_1 = hf(x_i, y_i, z_i)$
$K_2 = hf(x_i + h/2, y_i + J_1/2, z_i + K_1/2)$
$K_3 = hf(x_i + h/2, y_i + J_2/2, z_i + K_2/2)$
$K_4 = hf(x_i + h, y_i + J_3, z_i + K_3)$

$z_{i+1} = z_i + (K_1 + 2K_2 + 2K_3 + K_4)/6$

$J_1 = hg(x_i, y_i, z_i)$
$J_2 = hg(x_i + h/2, y_i + J_1/2, z_i + K_1/2)$
$J_3 = hg(x_i + h/2, y_i + J_2/2, z_i + K_2/2)$
$J_4 = hg(x_i + h, y_i + J_3, z_i + K_3)$

$y_{i+1} = y_i + (J_1 + 2J_2 + 2J_3 + J_4)/6$

Adams-Bashforth 4th Order Formula for Two First Order Simultaneous Equations

$$\frac{dy}{dx} = f(x,y,z); y(x_i) = y_i$$

$$\frac{dz}{dx} = g(x,y,z); z(x_i) = z_i$$

$$y_{i+1} = y_i + \frac{h}{24}(-9f_{i-3} + 37f_{i-2} - 59f_{i-1} + 55f_i)$$

$$z_{i+1} = z_i + \frac{h}{24}(-9g_{i-3} + 37g_{i-2} - 59g_{i-1} + 55g_i)$$