Numerical Methods Preserving First Integrals of Hamiltonian Systems

by

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Dedicated to My Parents

for their endless love, support and encouragement

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Abstract

The main aim of this thesis is to numerically preserve quadratic first integrals of Hamiltonian systems using symplectic method. We use classical Noether approach to calculate Noether symmetries and corresponding first integrals of Hamiltonian systems. Furthermore, by using complex Lie symmetry method we determine the Noether-like operators and associated first integrals of two dimensional system of Harmonic oscillator. For the numerical preservation of the first integrals of Hamiltonian systems, we integrate these systems with two stages Gauss symplectic Runge-Kutta method of order four. It is observed that only symplectic methods show good long time preservation of the first integrals.

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Chapter 1

Introduction

In real world, physical phenomena can be analyzed and understood by the process of mathematical modeling. These models describe the dynamics of related physical phenomenon. For example, motion of mechanical systems in Physics, chemical reactions in Chemistry, population dynamics in Biology, stock trends in Economics, are all studied through their mathematical models. These models are expressed in the language of ordinary differential equations (ODEs) or partial differential equations (PDEs). In this thesis, we will explore an important class of ODEs known as Hamiltonian system. These systems have some conserved quantities. Our main aim is to calculate these conserved quantities and then numerically integrate Hamiltonian systems such that their solutions also preserve the conserved quantities.

1.1 Hamiltonian Systems

Hamiltonian mechanics was first formulated by Irish mathematician William Rowan Hamilton in 1824 to describe evolution of the dynamical systems [30]. Hamiltonian mechanics is a form of classical mechanics, in which equations of motion depend on generalized coordinates q_i and generalized momenta p_i. The Hamiltonian equations of motion are defined as

$$\begin{aligned} p_i' &= -\frac{\partial H}{\partial q_i}, \\ q_i' &= \frac{\partial H}{\partial p_i}, \end{aligned} \tag{1.1}$$

for $i = 1, 2, \cdots, n$. The terms p'_i and q'_i represent the derivatives of functions p and q with respect to time t, where $p_i = (p_1, p_2, \cdots, p_n)$, $q_i = (q_1, q_2, \cdots, q_n)$ are generalized coordinates and momenta respectively. $H(p, q)$ is called the total energy of Hamiltonian system and it is also known as Hamiltonian which depends upon position and momentum [16].

The number of (p_i, q_i) pairs in Hamilton's equations represent the number of degrees of freedom of a Hamiltonian system. In many physical systems, Hamiltonian is in separable form, and is defined as sum of the kinetic and potential energies of the system i.e.

$$H(p, q) = K(p) + T(q), \tag{1.2}$$

where $K(p)$ represents kinetic energy and $T(q)$ is the potential energy.

In Lagrangian framework, the equations of motion are given as

$$\frac{\partial L}{\partial q_i} = \frac{d}{dt}\left(\frac{\partial L}{\partial q'_i}\right), \tag{1.3}$$

where L is the Lagrangian of the system (1.1) and is defined as the difference of kinetic and potential energy of the system which is written as

$$H(p, q) = K(p) - T(q). \tag{1.4}$$

Moreover, we can also write $y = (p, q)$, then equation (1.1) takes the form

$$\frac{dy}{dt} = J^{-1}\nabla H, \tag{1.5}$$

where $\nabla = (\partial_{p_1}, \cdots, \partial_{p_n}, \partial_{q_1}, \cdots, \partial_{q_n})$ is the gradient operator and J is skew symmetric matrix having I as $n \times n$ identity matrix i.e.

$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}.$$

Example 1.1.1. Harmonic Oscillator

A Harmonic oscillator is a mass spring system having kinetic energy $\frac{p^2}{2m}$ and potential energy $\frac{1}{2}kq^2$, where p is momentum, q is distance of spring from equilibrium position and k is a spring constant. The total energy of a system is given by

$$H(p,q) = \frac{p^2}{2m} + \frac{kq^2}{2}. \tag{1.6}$$

In the case, when $m = k = 1$, differential equations for Harmonic oscillator are

$$\begin{aligned} p' &= -q, \\ q' &= p. \end{aligned} \tag{1.7}$$

Hamiltonian systems possess some remarkable properties due to their special structure, which are described in the following section.

1.1.1 Energy Conservation

In the case of autonomous Hamiltonian systems, the total energy of the system remains conserved. The total energy is first integral and is given as

$$\frac{dH}{dt} = \sum_{i=1}^{n} \frac{\partial H}{\partial p_i} p_i' + \sum_{i=1}^{n} \frac{\partial H}{\partial q_i} q_i'. \tag{1.8}$$

By using equation (1.1), we have

$$\frac{dH}{dt} = \sum_{i=1}^{n} \frac{\partial H}{\partial p_i}\left(-\frac{\partial H}{\partial q_i}\right) + \sum_{i=1}^{n} \frac{\partial H}{\partial q_i}\left(\frac{\partial H}{\partial p_i}\right) \quad = 0. \tag{1.9}$$

This shows that the value of the Hamiltonian remains constant. Thus for a conservative system, trajectories in phase space are confined to a constant energy surface.

1.1.2 Symplectic Structure

Another important qualitative property of Hamiltonian system is that their phase flow is symplectic [15], which means that area is preserved in the phase space. For the Hamiltonian systems the phase space is a $2n$-dimensional space with (p, q) coordinates. There are different ways to check symplecticity. Here, we explain one of them.

Area Preservation through Jacobian:
A linear mapping $\phi : (p, q) \to (p^*, q^*)$ is symplectic if,

$$\phi'^T J \phi' = J.$$

To prove that the transformation ϕ is area preserving, we assume that the Jacobian of transformation has a unit determinant.

$$\phi' = \begin{pmatrix} \frac{\partial p^*}{\partial p} & \frac{\partial p^*}{\partial q}, \\ \frac{\partial q^*}{\partial p} & \frac{\partial q^*}{\partial q} \end{pmatrix},$$

$$= \frac{\partial p^*}{\partial p}\frac{\partial q^*}{\partial q} - \frac{\partial p^*}{\partial q}\frac{\partial q^*}{\partial p} = I.$$

We have,

$$\phi'^T J \phi' = \begin{pmatrix} \frac{\partial p^*}{\partial p} & \frac{\partial q^*}{\partial p} \\ \frac{\partial p^*}{\partial q} & \frac{\partial q^*}{\partial q} \end{pmatrix} \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial p^*}{\partial p} & \frac{\partial p^*}{\partial q} \\ \frac{\partial q^*}{\partial p} & \frac{\partial q^*}{\partial q} \end{pmatrix}.$$

$$= \begin{pmatrix} \frac{\partial p^* \partial q^*}{\partial p \partial p} - \frac{\partial p^* \partial q^*}{\partial p \partial p} & \frac{\partial p^* \partial q^*}{\partial p \partial q} - \frac{\partial p^* \partial q^*}{\partial q \partial p} \\ \frac{\partial p^* \partial q^*}{\partial q \partial p} - \frac{\partial p^* \partial q^*}{\partial p \partial q} & \frac{\partial p^* \partial q^*}{\partial q \partial q} - \frac{\partial p^* \partial q^*}{\partial q \partial q} \end{pmatrix}.$$

Thus

$$\phi'^T J \phi' = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} = J.$$

1.2 Symmetries and Conservation laws

Symmetry is a transformation that leaves a geometrical object invariant. Invariant means that the structural properties of the geometrical object remain unchanged. A more precise definition of symmetry in mathematics is that it is a transformation which leaves the differential equation invariant. Some examples of point symmetry are translation, rotation and reflection and scaling. In case of reflection, any geometrical shape is reflected about the axis. Then the shape, angle and size of that shape remain the same, the only difference is we get the reflected image in the opposite direction. In other words, we can say the orientation of the shape gets changed. Similarly in translation, if an object is displaced in some direction then it will remain invariant.

In the nineteenth century, a Norwegian mathematician, Marius Sophus Lie introduced a remarkable method of solving differential equations using continuous groups of transformations, known as Lie groups [21]. He proposed that under continuous transformations differential equations will remain invariant and these transformations map solution to another solution of the same differential equation. Lie symmetry method is an important tool to find the solution of linear as well as nonlinear DEs. Another application of Lie's work is to find first integrals (conservative laws) of DEs which plays an important role in order reduction and to study physical properties of dynamical systems. For a given system, the existence of a symmetry means that a conserved physical quantity exists.

In this section, we review some basic definitions and concepts of Lie symmetry analysis [4, 18]. We use Lie symmetry methods to calculate the first integrals of our Hamiltonian systems.

1.2.1 Point Transformation

An n^{th} order ODE is given as

$$E(t, y, y', y'', \cdots, y^{(n)}) = 0, \tag{1.10}$$

where t is independent and y is the dependent variables, respectively. While dealing with differential equations, one tries to simplify the equation by an appropriate change of variables, that is the transformation of dependent and independent variables.

$$\tilde{t} = \tilde{t}(t, y), \qquad \tilde{y} = \tilde{y}(t, y). \tag{1.11}$$

Equation (1.11) is known as point transformation as it maps point (t, y) to point $(\tilde{t}, \tilde{y})$. Consider an invertible point transformation which depends on at least one arbitrary parameter ϵ,

$$\tilde{t} = \tilde{t}(t, y; \epsilon), \qquad \tilde{y} = \tilde{y}(t, y; \epsilon), \tag{1.12}$$

having identity at $\epsilon = 0$,

$$\tilde{t}(t, y; 0) = t, \qquad \tilde{y}(t, y; 0) = y,$$

where $\epsilon \in \mathbb{R}$. The transformations (1.12) form a one-parameter group of point transformations [31]. A one-parameter group of point transformations leaves the family of solution curves of ODEs invariant.

1.2.2 Lie Symmetry Generator and its Prolongation

To explain the idea of infinitesimal transformations we consider the point transformations (1.12) and expand its Taylor's series at $\epsilon = 0$,

$$\begin{aligned} \tilde{t} = \tilde{t}(t, y; \epsilon) = \tilde{t}\mid_{\epsilon=0} + \epsilon \frac{\partial \tilde{t}}{\partial \epsilon}\mid_{\epsilon=0} + \ldots, = t + \epsilon \mathbf{X} t + \ldots, \\ \tilde{y} = \tilde{y}(t, y; \epsilon) = \tilde{y}\mid_{\epsilon=0} + \epsilon \frac{\partial \tilde{y}}{\partial \epsilon}\mid_{\epsilon=0} + \ldots, = y + \epsilon \mathbf{X} y + \ldots, \end{aligned} \tag{1.13}$$

where the functions $\xi(t, y)$ and $\eta(t, y)$ are defined as,

$$\xi(t, y) = \frac{\partial \tilde{t}}{\partial \epsilon}\mid_{\epsilon=0}, \qquad \eta(t, y) = \frac{\partial \tilde{y}}{\partial \epsilon}\mid_{\epsilon=0}. \tag{1.14}$$

The operator $\mathbf{X}$

$$\mathbf{X} = \xi(t, y)\frac{\partial}{\partial t} + \eta(t, y)\frac{\partial}{\partial y}, \tag{1.15}$$

is called the infinitesimal generator or infinitesimal operator of the transformations (1.12). The functions ξ and η are the components of tangent vector $\mathbf{X}$.

Example 1.2.1.
The one-parameter group of rotation is given by,

$$\begin{aligned} \tilde{t} &= t \cos \epsilon - y \sin \epsilon, \\ \tilde{y} &= t \sin \epsilon + y \cos \epsilon, \end{aligned} \tag{1.16}$$

where

$$\begin{aligned} \xi(t, y) &= \frac{\partial \tilde{t}}{\partial \epsilon}\mid_{\epsilon=0} = -y, \\ \eta(t, y) &= \frac{\partial \tilde{y}}{\partial \epsilon}\mid_{\epsilon=0} = t. \end{aligned} \tag{1.17}$$

The associated infinitesimal generator of rotation is,

$$\mathbf{X} = -y\frac{\partial}{\partial t} + t\frac{\partial}{\partial y}. \tag{1.18}$$

In order to apply a point transformation (1.12) to an ODE, we have to extend (prolong) the point transformation (1.12) to the derivatives $y^{(n)}$. The prolongation of the infinitesimal generator gives the following expressions

$$\begin{aligned}
\tilde{t} &= t + \epsilon\xi(t, y) + \cdots = t + \epsilon\mathbf{X}t + \cdots, \\
\tilde{y} &= y + \epsilon\eta(t, y) + \cdots = y + \epsilon\mathbf{X}y + \cdots, \\
\tilde{y}' &= y' + \epsilon\eta^{(1)}(t, y, y') + \cdots = y' + \epsilon\mathbf{X}y' + \cdots, \\
&\vdots \\
\tilde{y}^{(n)} &= y^{(n)} + \epsilon\eta^{(n)}(t, y, y', \cdots, y^{(n)}) + \ldots = y^{(n)} + \epsilon\mathbf{X}y^{(n)} + \cdots,
\end{aligned} \tag{1.19}$$

where $\eta^{(1)}, \ldots, \eta^{(n)}$ are the prolongation coefficients of $\eta(t, y)$. For $\eta^{(1)}$ we have

$$\eta^{(1)} = \frac{d\eta}{dt} - y'\frac{d\xi}{dt}. \tag{1.20}$$

Similarly $\eta^{(n)}$ is defined in [26] as,

$$\eta^{(n)} = \frac{d\eta^{(n-1)}}{dt} - y^{(n)}\frac{d\xi}{dt}, \qquad n \geq 2, \tag{1.21}$$

for positive integer n. Here $\frac{d}{dt}$ is the differential operator

$$\frac{d}{dt} = \frac{\partial}{\partial t} + y'\frac{\partial}{\partial y} + y''\frac{\partial}{\partial y'} + \cdots + y^{(n)}\frac{\partial}{\partial y^{(n-1)}}. \tag{1.22}$$

Thus, the prolongation of symmetry generator up to n^{th} order is represented by,

$$\mathbf{X}^{(n)} = \xi\frac{\partial}{\partial t} + \eta\frac{\partial}{\partial y} + \eta^{(1)}\frac{\partial}{\partial y'} + \eta^{(2)}\frac{\partial}{\partial y''} + \ldots + \eta^{(n)}\frac{\partial}{\partial y^{(n)}}. \tag{1.23}$$

The first two prolongation coefficients $\eta^{(1)}$ and $\eta^{(2)}$ are expressed as

$$\begin{aligned}
\eta^{(1)} =& \eta_t + (\eta_y - \xi_t)y' - \xi_y y'^2 \\
\eta^{(2)} =& \eta_{tt} + (2\eta_{ty} - \xi_{tt})y' + (\eta_{yy} - 2\xi_{ty})y'^2 - \xi_{yy}y'^3 \\
&+ (\eta_y - 2\xi_t - 3\xi_y y')y''.
\end{aligned} \tag{1.24}$$

Theorem 1.2.1. An n^{th} order ODE admits a group of symmetries with generator $\mathbf{X}$ if and only if

$$\mathbf{X}^{(n)} E \mid_{E=0} = 0, \tag{1.25}$$

holds, where $\mathbf{X}^{(n)}$ denotes n^{th} order prolongation of the symmetry generator (1.15). The proof is given in [31].

Example 1.2.2.
Consider free particle differential equation

$$y'' = 0. \tag{1.26}$$

By applying second order extension of generator $\mathbf{X}$ on equation (1.26)

$$\mathbf{X}^{(2)} y''|_{y''=0} = 0, \tag{1.27}$$

gives

$$\eta^{(2)} = 0. \tag{1.28}$$

Inserting the value of (1.24) in the above expression, we get

$$\eta_{tt} + (2\eta_{ty} - \xi_{tt})y' + (\eta_{yy} - 2\xi_{ty})y'^2 - \xi_{yy}y'^3 = 0. \tag{1.29}$$

Now comparing coefficients of different power of y', we obtain

$$\begin{aligned} y'^0 \quad &: \eta_{tt} = 0, \\ y'^1 \quad &: 2\eta_{ty} - \xi_{tt} = 0, \\ y'^2 \quad &: \eta_{yy} - 2\xi_{ty} = 0, \\ y'^3 \quad &: \xi_{yy} = 0. \end{aligned} \tag{1.30}$$

Solving the above system, we get

$$\begin{aligned} \xi(t,y) &= (a_1 t + a_2)y + a_3 t^2 + a_7 t + a_8, \\ \eta(t,y) &= a_1 y^2 + (a_3 t + a_4)y + a_5 t + a_6, \end{aligned} \tag{1.31}$$

where $a_1, a_2, \cdots, a_8$ are arbitrary constants. Thus, we obtain eight Lie point symmetry generators.

$$
\begin{aligned}
\mathbf{X}_1 &= ty\frac{\partial}{\partial t} + y^2\frac{\partial}{\partial y},\\
\mathbf{X}_2 &= y\frac{\partial}{\partial t},\\
\mathbf{X}_3 &= t^2\frac{\partial}{\partial t} + ty\frac{\partial}{\partial y},\\
\mathbf{X}_4 &= y\frac{\partial}{\partial y},\\
\mathbf{X}_5 &= t\frac{\partial}{\partial y},\\
\mathbf{X}_6 &= \frac{\partial}{\partial y},\\
\mathbf{X}_7 &= t\frac{\partial}{\partial t},\\
\mathbf{X}_8 &= \frac{\partial}{\partial t}.
\end{aligned}
\tag{1.32}
$$

1.2.3 Conservation Laws

A conservation law is a quantity of an isolated physical system which does not dissipate with time i.e., the quantity remain conserved. It is a function of the dependent variables that is a constant along each trajectory of the system [6]. Examples of conserved quantities are energy, linear momentum and angular momentum, etc. In case of energy conservation, the total energy in an isolated system does not change with time, though it may change its form. Conserved quantities of DEs are also known as the first integrals of these equations. They are also called constants of motion or invariants. Mathematically they are represented as

$$
\frac{dI}{dt} = 0, \tag{1.33}
$$

here I is any function of dependent variables. So for a conservative system the rate of change in I with respect to time is zero. In the case of Hamiltonian system, the Hamiltonian is a first integral.

1.3 Numerical Methods for Hamiltonian Systems

In this section, we give a brief introduction of numerical methods which are used to find approximate solutions of ODEs. The solutions of ODEs give enormous insight in the evolution of underlying physical system. In some cases, these equations can be solved analytically but most of the time it is not possible to find their analytical solutions. Therefore, approximation techniques are used to find their solutions. Different numerical methods are available: such as the one-step methods like the Runge-Kutta methods and multistep methods to find the numerical solution of ODEs [13].

During the past few years, special interest has been developed in studying numerical schemes that preserve some qualitative characteristic of the flow of differential equations [23]. The reason is that many physical systems have some hidden geometrical properties, such as symplectic structure, symmetries, phase-space volume, Lyapunov functions and first integrals. Standard numerical methods completely ignores the preservation of such quantities, therefore we are interested in numerical methods that preserve the geometric properties of ODEs, while also showing good stability and convergence. These methods are termed as structure preserving numerical methods. They are very helpful in stimulation of dynamical systems for long time periods. If traditional numerical methods are used to solve Hamiltonian systems, then they will not preserve Hamiltonian structure. Therefore, we are using structure preserving numerical methods for the solutions of Hamiltonian systems.

In this thesis, we are considering symplectic numerical methods for the preservation of the first integrals of Hamiltonian systems. Pioneering work on symplectic numerical methods was by Ruth [28], de-Vogelaere and Feng [11]. Sanz-Serna, Suris [3,29] and Lasagni, found that by having suitable choice of coeffcients implicit Runge-Kutta methods become symplectic. Only one-step methods can be symplectic [14]. Symplectic numerical methods are helpful in long time stimulation of Hamiltonian systems.

The outline of the thesis as follows: In Chapter 1, we give a brief introduction of Hamiltonian systems and some of its properties togather with a brief introduction of suitable numerical methods. Then, we review some basic definitions and concepts of Lie symmetry analysis. In Chapter 2, we present Noether's theorem and explain how it is used to calculate the first integrals of Hamiltonian systems. We then define complex Lie symmetries and discuss complex Noether approach and Noether-like operators to determine the first integrals for complex system of ODEs.

In Chapter 3, a review of the traditional numerical methods for solving system of ODEs and conservative problems is given. In Chapter 4, we calculate first integrals of Hamiltonian systems. The invariants for complex ODEs are determined by using Noether's theorem for restricted system of complex ODEs. In Chapter 5, numerical experiments are performed to check preservation of the first integrals using symplectic Runge-Kutta method. In last chapter, we discuss numerical results which we have achieved and conclude the results.

Chapter 2

Noether Symmetries and First Integrals

In this chapter, we review some basic definitions and formulas related to Noether symmetries and first integrals of ODEs. Then we briefly explain some results related to complex Noether symmetries, which are used to calculate first integrals for restricted complex ODEs.

The connection between symmetries and conservation laws is one of the most profound relation discovered in the twentieth century. Conservation laws play a significant role in finding the solutions of differential equations [12, 26]. Different methods have been developed over the years to calculate conservation laws or first integrals of system of ODEs. These methods are: the direct method, the characteristic or multiplier method, the celebrated Noether approach and partial Noether approach. Details are given in [17, 20, 22, 25]. A large amount of literature is available regarding symmetries and construction of first integrals for scalar ODEs. In this thesis, we are using Noether approach to calculate the first integral for real ODEs and restricted complex ODEs.

In 1918, Amalie Emmy Noether, a German mathematician, established a classical relation which relates variational symmetries (symmetries of a variational problem) with conservation laws for Euler-Lagrange equations [24]. She proved that there exists a correspondence between each variational symmetries and conservation laws (first integrals) of the associated Euler-Lagrange equations. For example, a system which is invariant under time translation gives conservation of energy, while a system which remains invariant under space translation and rotations is related with conservation of linear momentum and angular momentum. Using the relation between Noether symmetries and first integrals we can reduce and derive the exact solutions of ODEs. Here, to calculate the first integrals of second order ODEs, we restrict our consideration of Lagrangian up to only first order derivative.

A function $L(t, y, y')$ is a Lagrangian for a second order ODE

$$y'' = f(t, y, y'), \tag{2.1}$$

if equation (2.1) is equivalent to the Euler-Lagrange equation

$$\frac{\partial L}{\partial y} - \frac{d}{dt}(\frac{\partial L}{\partial y'}) = 0. \tag{2.2}$$

Definition 2.0.1. The operator

$$\mathbf{X} = \xi(t, y)\frac{\partial}{\partial t} + \eta(t, y)\frac{\partial}{\partial y}, \tag{2.3}$$

is called a Noether point symmetry generator [9] corresponding to the Lagrangian $L(t, y, y')$ of equation (2.1), if there exist a function $B(t, y)$ known as gauge function such that the following condition holds,

$$\mathbf{X}^{(1)}(L) + D(\xi)L = D(B), \tag{2.4}$$

where $\mathbf{X}^{(1)}$ is first order prolongation of symmetry generator and $D = \frac{d}{dt}$ is the total differential operator.

Noether's Theorem 2.0.1.
If $\mathbf{X}$ is a Noether point symmetry generator of a given Lagrangian $L(t, y, y')$, then there exist a function

$$I = \xi L + (\eta - \xi y')\frac{\partial L}{\partial y'} - B, \tag{2.5}$$

known as Noether first integral of the Euler-Lagrange equation (2.2), with respect to symmetry generator $\mathbf{X}$ [27].

Theorem 2.0.2.
The first integral I associated with Noether point symmetry $\mathbf{X}$ satisfies the condition

$$\mathbf{X}^{(1)}I = 0. \tag{2.6}$$

2.1 Noether Symmetries and First Integrals for System of ODEs

In this section, we extend the operator of Noether symmetry generator for two-dimensional system of ODEs.

Consider a generalized system of second order ODEs

$$\begin{aligned} y'' &= f(t, y, z, y', z'), \\ z'' &= g(t, y, z, y', z'), \end{aligned} \tag{2.7}$$

having t as independent variable and y, z as two real dependent variables. The symmetry generator is defined as,

$$\mathbf{X} = \xi(t, y, z)\frac{\partial}{\partial t} + \eta(t, y, z)\frac{\partial}{\partial y} + \zeta(t, y, z)\frac{\partial}{\partial z}, \tag{2.8}$$

where the total derivative is,

$$D = \frac{d}{dt} = \frac{\partial}{\partial t} + y'\frac{\partial}{\partial y} + z'\frac{\partial}{\partial z}. \tag{2.9}$$

The first order extension of symmetry generator $\mathbf{X}$ is given in [20] as,

$$\begin{aligned} \mathbf{X}^{(1)} &= \xi(t, y, z)\frac{\partial}{\partial t} + \eta(t, y, z)\frac{\partial}{\partial y} + \zeta(t, y, z)\frac{\partial}{\partial z} + \eta^{(1)}(t, y, z, y', z')\frac{\partial}{\partial y'} \\ &+ \zeta^{(1)}(t, y, z, y', z')\frac{\partial}{\partial z'}, \end{aligned} \tag{2.10}$$

where $\eta^{(n)}$ and $\zeta^{(n)}$ are defined as,

$$\begin{aligned} \eta^{(n)} &= \frac{d\eta^{(n-1)}}{dt} - y^{(n)}\frac{d\xi}{dt}, \\ \zeta^{(n)} &= \frac{d\zeta^{(n-1)}}{dt} - z^{(n)}\frac{d\xi}{dt}. \end{aligned} \tag{2.11}$$

The values of $\eta^{(1)}$ and $\zeta^{(1)}$ are calculated by using equation (2.11),

$$\begin{aligned} \eta^{(1)} &= \eta_t + (\eta_y - \xi_t)y' + (\eta_z - y'\xi_z)z' - y'^2\xi_y, \\ \zeta^{(1)} &= \zeta_t + (\eta_z - \xi_t)z' + (\zeta_y - z'\xi_y)y' - z'^2\xi_z. \end{aligned} \tag{2.12}$$

Now we present the formula to calculate Noether point symmetries and associated first integrals for two-dimensional system of ODEs.

A system of ODEs of the form (2.7) admits the Lagrangian $L(t, y, z, y', z')$, if it is equivalent to the Euler-Lagrange equations

$$\begin{aligned} \frac{d}{dt}\left(\frac{\partial L}{\partial y'}\right) - \frac{\partial L}{\partial y} = 0, \\ \frac{d}{dt}\left(\frac{\partial L}{\partial z'}\right) - \frac{\partial L}{\partial z} = 0. \end{aligned} \tag{2.13}$$

Theorem 2.1.1.
If $\mathbf{X}$ is a Noether symmetry generator of a given Lagrangian $L(t, y, z, y', z')$, then

$$I = \xi L + (\eta - \xi y')\frac{\partial L}{\partial y'} + (\zeta - \xi z')\frac{\partial L}{\partial z'} - B, \tag{2.14}$$

is called Noether first integral [10] of system of ODEs (2.7), associated with $\mathbf{X}$.

2.2 Restricted Complex ODEs

In complex symmetry analysis, we deal with systems of differential equations involving complex variables. They are called complex differential equations because their dependent variables are complex functions of either real or complex independent variables. Writing the complex variables into real and imaginary parts, yields system of two ODEs if we have real independent variable, and system of two PDEs if we have complex independent variable. Thus a complex ODE can be represented by a system of two second order real ODEs. Examples include system of two coupled Harmonic oscillators and system of free particle equations.

Consider general form of a second order complex ODE

$$y''(t) = \omega(t, y, y'). \tag{2.15}$$

We restrict $y(t)$ to be complex dependent function of a single real independent variable t. Substituting $y(t)$ as,

$$y(t) = f(t) + ig(t), \tag{2.16}$$

and using the assumption,

$$\omega(t, y(t)) = \omega_1(t, f, g) + i\omega_2(t, f, g), \tag{2.17}$$

we get the following system of ODEs

$$\begin{aligned} f'' &= \nu_1(t, f, g, f'g'), \\ g'' &= \nu_2(t, f, g, f', g'), \end{aligned} \tag{2.18}$$

where ω is a complex analytic function and its components ν_1 and ν_2 are arbitrary real functions.

Example 2.2.1. Consider the Harmonic oscillator equation

$$y''(t) = -y(t). \tag{2.19}$$

Using equation (2.16), we get

$$\begin{aligned} f'' &= -f, \\ g'' &= -g. \end{aligned} \tag{2.20}$$

Note that the general solution of equation (2.19) has the form

$$y(t) = a\cos t + b\sin t, \tag{2.21}$$

where $a = a_1 + ia_2$ and $b = b_1 + ib_2$. We can get the general solution of equation (2.20) by putting the value of a and b in (2.21).

$$\begin{aligned} f(t) &= a_1 \cos t + b_1 \sin t, \\ g(t) &= a_2 \cos t + b_2 \sin t. \end{aligned} \tag{2.22}$$

2.3 Symmetry Condition for Complex ODEs

Consider general form of an n^{th} order restricted complex ODE

$$y^{(n)}(t) = \omega(t, y, y', \cdots, y^{(n-1)}). \tag{2.23}$$

The infinitesimal complex Lie point transformations are defined by

$$\tilde{t} = t(t, y; \epsilon), \qquad \tilde{y} = y(t, y; \epsilon), \tag{2.24}$$

where ϵ is a complex parameter. The infinitesimal complex symmetry generator is defined as,

$$\mathbf{Z} = \tau(t,y)\frac{\partial}{\partial t} + \chi(t,y)\frac{\partial}{\partial y}. \tag{2.25}$$

The prolonged symmetry generator for n^{th} order complex ODE is given as

$$\mathbf{Z}^{(n)} = \tau(t,y)\frac{\partial}{\partial t} + \chi\frac{\partial}{\partial y} + \chi^{(1)}\frac{\partial}{\partial y'} + \ldots + \chi^{(n)}\frac{\partial}{\partial y^{(n)}}, \tag{2.26}$$

where

$$\chi^{(n)} = \frac{d\chi^{(n-1)}}{dt} - y^{(n)}\frac{d\tau}{dt}. \tag{2.27}$$

The differential operator is

$$\frac{d}{dt} = \frac{\partial}{\partial t} + y'\frac{\partial}{\partial y} + y''\frac{\partial}{\partial y'} + \cdots + y^{(n)}\frac{\partial}{\partial y^{(n-1)}}. \tag{2.28}$$

2.4 Noether Symmetry Condition and First Integrals for Complex ODEs

In this section we review some basic definitions and concepts related to complex Euler-Lagrange equation, complex Lagrangian, complex Noether symmetries in order to deal with restricted second order complex ODEs [1,2]. For complex case we consider y to be a complex function of real independent variable t. Consider second order complex ODE

$$y''(t) = \omega(t,y,y'), \tag{2.29}$$

$L(t,y,y')$ is a complex Lagrangian of restricted complex ODE (2.29), if it is equivalent to the Euler-Lagrange equation

$$\frac{\partial L}{\partial y} - \frac{d}{dt}\left(\frac{\partial L}{\partial y'}\right) = 0. \tag{2.30}$$

Definition 2.4.1. The operator (2.25) is called complex Noether point symmetry generator of (2.29) corresponding to a complex Lagrangian $L(t,y,y')$, if there exists a complex gauge function $B(t,y)$ such that

$$\mathbf{Z}^{(1)}(L) + D(\tau)L = D(B), \tag{2.31}$$

where $\mathbf{Z}^{(1)}$ is first order prolongation of symmetry generator $\mathbf{Z}$.

Noether's Theorem 2.4.1.
If $\mathbf{Z}$ is a complex Noether point symmetry corresponding to a complex Lagrangian $L(t, y, y')$ of Eq. (2.29), then there exists a function I

$$I = \tau L + (\chi - \tau y')\frac{\partial L}{\partial y'} - B, \tag{2.32}$$

known as complex first integral of (2.29).

Theorem 2.4.2.
The first integral I associated with complex Noether point symmetry $\mathbf{Z}$, satisfies the following condition

$$\mathbf{Z}^{(1)} I = 0. \tag{2.33}$$

2.5 Noether-Like Operators and Associated First Integrals

Noether-like operators [10] play an essential role in writing down the first integrals for Euler Lagrange system of ODEs. Two real Lagrangians for system of two second-order ODEs are obtained by restricting the domain of a complex Lagrangian.

In order to calculate Noether-like operators, suppose that L is a complex Lagrangian of restricted complex ODE

$$L(t, y, y') = L_1 + iL_2. \tag{2.34}$$

Therefore, we have two Lagrangians L_1 and L_2 that satisfy complex Euler-Lagrange equations

$$\begin{aligned} \frac{\partial L_1}{\partial f} + \frac{\partial L_2}{\partial g} - \frac{d}{dt}\left(\frac{\partial L_1}{\partial f'} + \frac{\partial L_2}{\partial g'}\right) = 0, \\ \frac{\partial L_2}{\partial f} - \frac{\partial L_1}{\partial g} - \frac{d}{dt}\left(\frac{\partial L_2}{\partial f'} - \frac{\partial L_1}{\partial g'}\right) = 0. \end{aligned} \tag{2.35}$$

The operators

$$\begin{aligned} \mathbf{X} &= \tau_1 \frac{\partial}{\partial t} + \chi_1 \frac{\partial}{\partial f} + \chi_2 \frac{\partial}{\partial g} \\ \mathbf{Y} &= \tau_2 \frac{\partial}{\partial t} + \chi_2 \frac{\partial}{\partial f} - \chi_1 \frac{\partial}{\partial g} \end{aligned} \tag{2.36}$$

are called Noether-Like operators [2], corresponding to the Lagrangian L_1 and L_2, if there exist $B_1(t, f, g)$ and $B_2(t, f, g)$ gauge functions such that

$$\begin{aligned} &\mathbf{X}^{(1)} L_1 - \mathbf{Y}^{(1)} L_2 + (d_t \tau_1) L_1 - (d_t \tau_2) L_2 = d_t B_1, \\ &\mathbf{X}^{(1)} L_2 + \mathbf{Y}^{(1)} L_1 + (d_t \tau_1) L_2 + (d_t \tau_2) L_1 = d_t B_2, \end{aligned} \tag{2.37}$$

where $\mathbf{Z} = \mathbf{X} + i\mathbf{Y}$, and $\mathbf{X}^{(1)}$ and $\mathbf{Y}^{(1)}$ are the first order prolongation of Noether-Like operators, defined as

$$\begin{aligned} \mathbf{X}^{(1)} &= \tau_1 \partial_t + \chi_1 \partial_f + \chi_2 \partial_g + \chi_1^{(1)} \partial_{f'} + \chi_2^{(1)} \partial_{g'}, \\ \mathbf{Y}^{(1)} &= \tau_2 \partial_t + \chi_2 \partial_f - \chi_1 \partial_g + \chi_2^{(1)} \partial_{f'} - \chi_1^{(1)} \partial_{g'}. \end{aligned} \tag{2.38}$$

The two first integrals [10] corresponding to Noether-like operator $\mathbf{X}$ and $\mathbf{Y}$ of equation (2.18) are

$$\begin{aligned} I_1 &= \tau_1 L_1 - \tau_2 L_2 + \partial f' L_1 (\chi_1 - f' \tau_1 - g' \tau_2) - \partial f' L_2 (\chi_2 - f' \tau_2 - g' \tau_1) - B_1, \\ I_2 &= \tau_1 L_2 + \tau_2 L_1 + \partial f' L_2 (\chi_1 - f' \tau_1 - g' \tau_2) + \partial f' L_1 (\chi_2 + f' \tau_2 - g' \tau_1) - B_2. \end{aligned} \tag{2.39}$$

Chapter 3

Symplectic Runge-Kutta Methods

Numerical methods are used to approximate the exact solution of ODEs. These methods are helpful in understanding the dynamics of physical systems. In this chapter, we review geometric numerical integrators. These are specialized numerical methods which preserve geometric properties of Hamiltonian systems. In particular we are interested in one-step symplectic Runge-Kutta methods. We take Gauss-Legendre Runge-Kutta method of order four for the numerical integration of Hamiltonian systems.

3.1 Conservation of First Integrals

Hamiltonian systems belong to a special class of ODEs where the solutions possess first integrals. In this thesis, we explain two types of first integrals,

- Linear first integral
- Quadratic first integral

3.1.1 Linear First Integral

A non-constant function $I(y)$ is the linear first integral of an initial value problem [14]

$$y' = f(y(t)), \quad y(t_0) = y_0, \tag{3.1}$$

if it satisfies

$$\frac{dI}{dt} = I'(y)f(y) = 0, \qquad \forall y, \tag{3.2}$$

which means that the solution $y(t)$ of (3.1) satisfies

$$I(y(t)) = I(y_0) = constant. \tag{3.3}$$

Example 3.1.1. Consider system of Lotka-Volterra equations

$$\begin{aligned} u' &= u(v-2), \\ v' &= v(1-u). \end{aligned} \tag{3.4}$$

The above system contains $I(u, v) = \ln u - u + 2\ln v - v$ as a first integral [15]. By applying definition of linear first integral we get

$$\frac{dI}{dt} = (\frac{1}{u}.u') - u' + (\frac{2}{v}.v') - v'. \tag{3.5}$$

Substituting the value of u', v' in (3.5), we obtain

$$\begin{aligned} \frac{dI}{dt} &= \frac{1}{u}\{u(v-2)\} - u(v-2) + \frac{2}{v}\{v(1-u)\} - v(1-u) \\ &= (v-2) - u(v-2) + 2(1-u) - v(1-u) \\ &= 0. \end{aligned} \tag{3.6}$$

This shows that I is the first integral of the Lotka-Volterra problem.

3.1.2 Quadratic First Integral

A quadratic function

$$Q(y) = y^t Ay, \tag{3.7}$$

is called first integral of (3.1) if,

$$Q'(y) = y^t Af(y) = 0, \qquad \forall y, \tag{3.8}$$

where A is symmetric square matrix [13].

Example 3.1.2. Consider Harmonic oscillator equations

$$p' = -q, \qquad q' = p, \tag{3.9}$$

Consider the quadratic function

$$Q(y) = (p \quad q)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} p \\ q \end{pmatrix}, \tag{3.10}$$

where

$$y = \begin{pmatrix} p \\ q \end{pmatrix}, \tag{3.11}$$

By using (3.8), we get

$$\frac{dQ}{dt} = (p \quad q)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} -q \\ p \end{pmatrix} = 0. \tag{3.12}$$

Thus $Q(y)$ is a quadratic first integral of (3.9).

3.2 Runge-Kutta Methods

Runge-Kutta methods were discovered by two German mathematicians Carl Runge and Martin Kutta in 1901 [5]. These methods belong to the family of one-step methods to find the numerical solutions of initial value problems.

Consider an autonomous initial value problem

$$y' = f(y(t)), \qquad y(t_0) = y_0, \tag{3.13}$$

where $f : \mathbb{R}^n \longrightarrow \mathbb{R}^n$. An s-stage implicit Runge-Kutta method is defined as

$$\begin{aligned} Y_i &= y_{n-1} + \sum_{j=1}^{s} a_{ij} h f(Y_j), \qquad i = 1, 2, \cdots, s, \\ y_n &= y_{n-1} + \sum_{i=1}^{s=} b_i h f(Y_i), \end{aligned} \tag{3.14}$$

where h is the stepsize. In case of non-autonomous system Runge-Kutta method is given by,

$$\begin{aligned} Y_i &= y_{n-1} + h\sum_{j=1}^{s} a_{ij} f(t_n + c_j h, Y_j), \qquad i = 1, 2, \cdots, s \\ y_n &= y_{n-1} + h\sum_{i=1}^{s} b_i f(t_n + c_i h, Y_i), \end{aligned} \tag{3.15}$$

where Y_i are the stages. The output value y_n represents numerical approximation of the actual solution at time t_n.
The coefficients of Runge-Kutta methods $[a, b, c]$ can be expressed in the form of a tableau, known as the Butcher tableau

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array}.$$

The coefficient b_i are called quadrature weights of the method, the matrix $A = [a_{ij}]$ is the Runge-Kutta matrix and c_i are the abscissas.

Runge-Kutta methods are explicit if the matrix A is strictly lower triangular that is

$$a_{ij} = 0, \quad j \geq i, \quad j = 1, 2, \cdots, s \tag{3.16}$$

The implementation of explicit Runge-Kutta methods is more convenient because they require less computation time in solving ODEs.

Example 3.2.1. The Euler method is the simplest example of Runge-Kutta method having one stage

$$\begin{aligned} Y_1 &= y_n, \\ y_{n+1} &= y_n + hf(Y_1). \end{aligned} \tag{3.17}$$

It can be written in tableau form

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}.$$

Example 3.2.2. The classical explicit Runge-Kutta method of order four having 4 stages is given below

$$\begin{aligned}
Y_1 &= y_n, \\
Y_2 &= y_n + \frac{1}{2}hf(Y_1), \\
Y_3 &= y_n + \frac{1}{2}hf(Y_2), \\
Y_4 &= y_n + hf(Y_3), \\
y_{n+1} &= y_n + \left(\frac{1}{6}hf(Y_1) + \frac{1}{3}hf(Y_2) + \frac{1}{3}hf(Y_3) + \frac{1}{6}hf(Y_4)\right).
\end{aligned} \tag{3.18}$$

The Butcher tableau is given as

$$\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \\
\frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\
1 & 0 & 0 & 1 & 0 \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array}.$$

3.3 Order Conditions of Runge-Kutta Methods

To find the order of a numerical method, we need to compare the Taylor series of the numerical solution with the Taylor series of exact solution. The order condition of the Runge-Kutta method can be found by using explicit as well as implicit method. To calculate the order of Runge-Kutta method, we first understand the concept of elementary differentials

$$\begin{aligned}
y' &= \mathbf{f}, \\
y'' &= \mathbf{f}'\mathbf{f}, \\
y''' &= \mathbf{f}''(\mathbf{f}\ \mathbf{f}) + \mathbf{f}'\mathbf{f}'\mathbf{f}, \\
y^{(4)} &= \mathbf{f}'''(\mathbf{f}\ \mathbf{f}\ \mathbf{f}) + 2\mathbf{f}''(\mathbf{f}\ \mathbf{f}'\ \mathbf{f}) + 2\mathbf{f}'\mathbf{f}''(\mathbf{f}\ \mathbf{f}) + \mathbf{f}'\mathbf{f}'\mathbf{f}'\mathbf{f}, \\
y^{(5)} &= \mathbf{f}^{(4)}(\mathbf{f}\ \mathbf{f}\ \mathbf{f}\ \mathbf{f}) + 4\mathbf{f}'''(\mathbf{f}'\mathbf{f}\ \mathbf{f}\ \mathbf{f}) + 2\mathbf{f}'''(\mathbf{f}\ \mathbf{f}\ \mathbf{f}'\ \mathbf{f}) + 4\mathbf{f}''(\mathbf{f}'\ \mathbf{f}\ \mathbf{f}'\ \mathbf{f}) + 2\mathbf{f}''(\mathbf{f}\ \mathbf{f}''\ \mathbf{f}\ \mathbf{f}) \\
&\quad + 2\mathbf{f}'\mathbf{f}'''(\mathbf{f}\ \mathbf{f}\ \mathbf{f}) + 2\mathbf{f}''\mathbf{f}''(\mathbf{f}\ \mathbf{f}\ \mathbf{f}) + 4\mathbf{f}'\mathbf{f}''(\mathbf{f}'\ \mathbf{f}\ \mathbf{f}) + 3\mathbf{f}''\mathbf{f}'\mathbf{f}'(\mathbf{f}\ \mathbf{f}).
\end{aligned} \tag{3.19}$$

The terms $\mathbf{f}'\mathbf{f}, \mathbf{f}'\mathbf{f}'\mathbf{f}$, etc. are known as elementary differentials. Consider general form of explicit Runge-Kutta method for solving autonomous ODEs

$$
\begin{aligned}
Y_i &= y_{n-1} + \sum_{j=1}^{i-1} a_{ij} h f(Y_j), \qquad i = 1, 2, \cdots, s \\
y_n &= y_{n-1} + \sum_{i=1}^{s} b_i h f(Y_i).
\end{aligned}
\tag{3.20}
$$

For $\mathbf{s} = 3$ stages, we have

$$
\begin{aligned}
Y_1 &= y_{n-1}, \\
Y_2 &= y_{n-1} + ha_{21} f(Y_1), \\
Y_3 &= y_{n-1} + ha_{31} f(Y_1) + ha_{32} f(Y_2),
\end{aligned}
\tag{3.21}
$$

where

$$f(Y_1) = f(y_{n-1}), \tag{3.22}$$

$$f(Y_2) = f(y_{n-1} + ha_{21} f(y_{n-1})). \tag{3.23}$$

Then

$$Y_3 = y_{n-1} + ha_{31} f(y_{n-1}) + ha_{32} f(y_{n-1} + ha_{21} f(y_{n-1})), \tag{3.24}$$

By Taylor series expansion, we get

$$f(y_{n-1} + ha_{21} f(y_{n-1})) = f(y_{n-1}) + ha_{21} f' f(y_{n-1}) + \frac{h^2}{2} a_{21} f'' f f(y_{n-1}) + O(h^3). \tag{3.25}$$

Using equation (3.25) in (3.24)

$$Y_3 = y_{n-1} + ha_{31} f(y_{n-1}) + ha_{32} f(y_{n-1}) + h^2 a_{32} a_{21} f' f(y_{n-1}) + O(h^3), \tag{3.26}$$

where

$$
\begin{aligned}
f(Y_3) =& f(y_{n-1} + h(a_{31} + a_{32}) f(y_{n-1}) + h^2 a_{32} a_{21} f' f(y_{n-1}) + O(h^3)) \\
=& f(y_{n-1}) + hc_3 f' f(y_{n-1}) + \frac{h^2}{2} c_3^2 f'' f^{(2)}(y_{n-1}) \\
&+ h^2 (a_{32} a_{21} f' f(y_{n-1}) f') + O(h^3).
\end{aligned}
\tag{3.27}
$$

Since the output value is

$$y_n = y_{n-1} + h(b_1 f(Y_1) + b_2 f(Y_2) + b_3 f(Y_3)). \tag{3.28}$$

Using the values of (3.32), (3.25) and (3.27) in equation (3.28)

$$\begin{aligned} y_n &= y_{n-1} + h(b_1 + b_2 + b_3) f(y_{n-1}) + h^2 (b_2 c_2 + b_3 c_3) f' f(y_{n-1}) \\ &+ \frac{h^3}{2}(b_2 c_2^2 + b_3 c_3^2) f'' f^{(2)}(y_{n-1}) + h^3 b_3 a_{32} c_2 f' f' f(y_{n-1}) + O(h^4). \end{aligned} \tag{3.29}$$

Now, expanding the Taylor series of exact solution

$$y(t_n) = y(t_{n-1}) + h y'(t_{n-1}) + \frac{h^2}{2!} y''(t_{n-1}) + \frac{h^3}{3!} y^{(3)}(t_{n-1}) + O(h^4). \tag{3.30}$$

Putting values of equation (3.19) in (3.30) and the comparing it with (3.29), we get

$$\begin{aligned} b_1 + b_2 + b_3 &= 1, \\ b_2 c_2 + b_3 c_3 &= \frac{1}{2}. \\ b_2 c_2^2 + b_3 c_3^2 &= \frac{1}{3}, \\ b_3 a_{32} c_2 &= \frac{1}{6}. \end{aligned} \tag{3.31}$$

Thus to achieve an order of 3, Runge-Kutta method must satisfy the following four order conditions

$$\sum_{i=1}^{3} b_i = 1, \tag{3.32}$$

$$\sum_{i=2}^{3} b_i c_i = \tfrac{1}{2}, \tag{3.33}$$

$$\sum_{i=2}^{3} b_i c_i^2 = \tfrac{1}{3}, \tag{3.34}$$

$$\sum_{i=1}^{3} b_i a_{ij} c_j = \tfrac{1}{6}. \tag{3.35}$$

This shows that by increasing the order of Runge-Kutta methods, order conditions also increases.

3.4 Implicit Runge-Kutta Methods

Implicit Runge-Kutta methods were introduced by Kuntzmann and Butcher in 1960 [3]. Runge-Kutta methods are implicit if $a_{ij} \neq 0$ for some $j \geq i$. In order to evaluate its stages, we either need Newton iteration method or fixed point method because at each stage the value of Y_i vector depends on Y_j. Implicit Runge-Kutta methods are very helpful in solving stiff differential equations. Another advantage of these methods is the ability to show good stability.

The Implicit Runge-Kutta methods are obtained from famous Gauss-Legendre polynomial. They are known as Gauss methods. These methods requires s stages and the highest possible order is $2s$. By choosing the $c_i's$ as zeroes of the shifted Gauss-Legendre Polynomial $P(t)$ on $[0, 1]$.

$$P_s(t) = \frac{s!}{2s} \sum_{m=0}^{s} (-1)^{(s-m)} \binom{s}{m} \binom{s+m}{m} x^m. \tag{3.36}$$

For $s = 1$, we get

$$P_1(t) = -\frac{1}{2} + t, \tag{3.37}$$

having root $c_1 = 0$. The 1-stage implicit midpoint rule of order 2 is given by

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}.$$

When we put $s = 2$, we get

$$P_2(t) = t^2 - t + \frac{1}{6}, \tag{3.38}$$

having roots

$$c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6}, \qquad c_2 = \frac{1}{2} + \frac{\sqrt{3}}{6}. \tag{3.39}$$

The coefficient of 2-stages implicit Runge-Kutta method of order four can be represented through Butcher tableau

$$
\begin{array}{c|cc}
\frac{1}{2}-\frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4}-\frac{\sqrt{3}}{6} \\
\frac{1}{2}+\frac{\sqrt{3}}{6} & \frac{1}{4}+\frac{\sqrt{3}}{6} & \frac{1}{4} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}. \tag{3.40}
$$

3.5 Symplectic Runge-Kutta Methods

In this thesis, we consider symplectic Runge-Kutta method for the numerical preservation of the first integrals of Hamiltonian systems. The Runge-Kutta methods of order s are symplectic if numerical solution satisfies

$$
< y_n, y_n > = < y_{n-1}, y_{n-1} >, \tag{3.41}
$$

and if coefficients of Runge-Kutta methods satisfy the following condition

$$
b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \quad \text{for all} \quad i, j = 1, 2, \ldots, s. \tag{3.42}
$$

Equation (3.42) is known as symplectic condition for Runge-Kutta methods. For a conservative system, we have

$$
< Y_i, f(Y_i) > = 0, \tag{3.43}
$$

Inserting value of Y_i in the above expression

$$
< y_{n-1} + \sum_{j=1}^{s} a_{ij} h f(Y_j), f(Y_i) > = 0, \tag{3.44}
$$

we get

$$
< y_{n-1}, f(Y_i) > = -h \sum_{i,j=1}^{s} a_{ij} < f(Y_j), f(Y_i) > . \tag{3.45}
$$

Now to prove equation (3.41), consider

$$
\begin{aligned}
< y_n, y_n > &= < y_{n-1} + \sum_{i=1}^{s} b_i h f(Y_i), y_{n-1} + \sum_{i=1}^{s} b_j h f(Y_i) >, \\
< y_n, y_n > &= < y_{n-1}, y_{n-1} > + h < y_{n-1}, \sum_{i=1}^{s} b_i f(Y_i) > + h < \sum_{i=1}^{s} b_j f(Y_i), y_{n-1} > \\
&\quad + < h^2 \sum_{i=1}^{s} b_i f(Y_i), \sum_{i=1}^{s} b_j f(Y_j) >,
\end{aligned} \tag{3.46}
$$

we have

$$< y_n, y_n > =< y_{n-1}, y_{n-1} > +h\sum_{i=1}^{s} b_i < y_{n-1}, f(Y_i) > +h\sum_{i=1}^{s} b_j < f(Y_i), y_{n-1} >$$
$$+ h^2 \sum_{i,j=1}^{s} b_i b_j < f(Y_i), f(Y_j) >, \tag{3.47}$$

By using value of (3.45) in above expression, we obtain

$$< y_n, y_n > =< y_{n-1}, y_{n-1} > -h^2 \sum_{i,j=1}^{s} b_i a_{ij} < f(Y_j), f(Y_i) > -h^2 \sum_{i,j=1}^{s} b_j a_{ji} < f(Y_j), f(Y_i) >$$
$$+ h^2 \sum_{i,j=1}^{s} b_i b_j < f(Y_j), f(Y_i) >,$$

$$< y_n, y_n > =< y_{n-1}, y_{n-1} > -h^2 \sum_{i,j=1}^{s} (b_i a_{ij} + b_j a_{ji} - b_i b_j) < f(Y_j), f(Y_i) >, \tag{3.48}$$

since

$$< y_n, y_n >=< y_{n-1}, y_{n-1} >,$$

therefore

$$h^2 \sum_{i,j=1}^{s} (b_i(a_{ij} + b_j a_{ji} - b_i b_j) < f(Y_j), f(Y_i) >= 0.$$

As

$$< f(Y_j), f(Y_i) >\neq 0,$$

Therefore

$$h^2 \sum_{i,j=1}^{s} b_i(a_{ij} + b_j a_{ji} - b_i b_j) = 0.$$

A Runge-Kutta method is symplectic if its coefficients satisfy the following condition

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \qquad \forall \;\; i, j = 1, 2, \cdots, n. \tag{3.49}$$

Only implicit Runge-Kutta methods can be symplectic. Therefore, we only consider two stages implicit Gauss Legendre Runge-Kutta method of order four given as

Gauss-2:

$$\begin{array}{c|cc} \frac{1}{2}-\frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4}-\frac{\sqrt{3}}{6} \\ \frac{1}{2}+\frac{\sqrt{3}}{6} & \frac{1}{4}+\frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}. \tag{3.50}$$

Chapter 4

First Integrals of Hamiltonian Systems

In this chapter, we calculate the first integrals of Hamiltonian systems. As discussed in Chapter 2, there are different methods to construct first integrals for ODEs. Here, we use classical Noether approach to calculate Noether symmetries and associated first integrals of Hamiltonian systems. Then by using complex symmetry method we calculate the first integrals for system of restricted complex ODEs.

4.1 Simple Pendulum

A simple pendulum is a two dimensional nonlinear oscillating system having equation of motion

$$y'' = -\sin y, \tag{4.1}$$

which admits Lagrangian

$$L(t, y, y') = \frac{y'^2}{2} + \cos y. \tag{4.2}$$

The Lagrangian (4.2) satisfy the Euler-Lagrange equation (2.2). Using equation (2.4), we get Noether symmetry determining equation

$$-\eta \sin y + y'(\eta_t + \xi_y \cos y) + y'^2(\eta_y - \frac{\xi_t}{2}) - y'^3\frac{\xi_y}{2} + \xi_t \cos y = B_t + y'B_y, \tag{4.3}$$

Separating the coefficients of y' and its powers, we obtain a system of four partial differential equations.

$$\begin{aligned} -\eta\sin y + \cos y\xi_t - B_t &= 0,\\ \eta_t + \cos y\xi_y - B_y &= 0,\\ \eta_y - \frac{\xi_t}{2} &= 0,\\ -\frac{\xi_y}{2} &= 0. \end{aligned} \tag{4.4}$$

Solving the system (4.4) gives

$$\xi(t, y) = \quad a_1, \qquad \eta(t, y) = \quad 0, \tag{4.5}$$

where a_1 is arbitrary constant. One Noether symmetry is obtained

$$\mathbf{X}_1 = \frac{\partial}{\partial t}, \tag{4.6}$$

By utilizing equation (2.5) we obtain

$$I_1 = \frac{y'^2}{2} - \cos y. \tag{4.7}$$

where the first integral I_1 represents total energy of the system.

4.2 Kepler Problem

The equations of motion of the Kepler problem are

$$\begin{aligned} x'' &= -\frac{x}{(x^2+y^2)^{\frac{3}{2}}},\\ y'' &= -\frac{y}{(x^2+y^2)^{\frac{3}{2}}}, \end{aligned} \tag{4.8}$$

where prime represent the differentiation of x and y with respect to t. The above system admits the Lagrangian of the form

$$L(t, x, y, x', y') = \frac{1}{2}(x'^2 + y'^2) + \frac{1}{\sqrt{x^2+y^2}}, \tag{4.9}$$

By utilizing equation (2.4), we get

$$\begin{aligned} B_t + x'B_x - y'B_y = &- \frac{x\eta}{(x^2+y^2)^{\frac{3}{2}}} - \frac{y\zeta}{(x^2+y^2)^{\frac{3}{2}}} + x'\{\eta_t + x'(\eta_x - \xi_t) + y'\eta_y - x'^2\xi_x - x'y'\xi_y\} \\ &+ y'\{\zeta_t + y'(\zeta_y - \xi_t) + x'\zeta_x - y'^2\xi_y - x'y'\xi_x\} + \frac{1}{2}(x'^2 + y'^2)\xi_t + \frac{\xi_t}{\sqrt{x^2+y^2}} \\ &+ \frac{1}{2}(x'^2+y'^2)\xi_x x' + \frac{\xi_x x'}{\sqrt{x^2+y^2}} + \frac{1}{2}(x'^2+y'^2)\xi_y y' + \frac{\xi_y y'}{\sqrt{x^2+y^2}}. \end{aligned} \tag{4.10}$$

On comparing coefficients of x', y' and their powers, we obtain

$$\begin{aligned} -\frac{x\eta}{(x^2+y^2)^{\frac{3}{2}}} - \frac{y\zeta}{(x^2+y^2)^{\frac{3}{2}}} + \frac{\xi_t}{\sqrt{x^2+y^2}} - B_t &= 0, \\ -\eta_t + \frac{\xi_x}{\sqrt{x^2+y^2}} - B_x &= 0, \\ -\zeta_t + \frac{\xi_y}{\sqrt{x^2+y^2}} - B_y &= 0, \\ \eta_x - \frac{\xi_t}{2} &= 0, \\ \zeta_y - \frac{\xi_t}{2} &= 0 \\ \eta_y + \zeta_x &= 0 \\ \xi_x = \xi_y &= 0 \end{aligned} \tag{4.11}$$

Solving the system yields

$$\xi = a_1, \qquad \eta = -a_2 y, \qquad \zeta = a_2 x, \qquad B = a_3, \tag{4.12}$$

Thus, we get two independent symmetry generators.

$$\begin{aligned} \mathbf{X}_1 &= \frac{\partial}{\partial t}, \\ \mathbf{X}_2 &= t\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}. \end{aligned} \tag{4.13}$$

In order to evaluate the two first integrals, we insert the value of equation (4.12) in (2.14), which gives

$$
\begin{aligned}
I_1 =& \frac{1}{2}(x'^2 + y'^2) - \frac{1}{\sqrt{x^2 + y^2}}, \\
I_2 =& xy' - yx'.
\end{aligned}
\tag{4.14}
$$

Here I_1 represents the total energy whereas I_2 is angular momentum of the system.

4.3 Henon-Heiles Problem

The Henon-Heiles model describes the motion of stars around the galactic center. Here, we consider the motion in the xy plane. To determine the Noether symmetries and associated constants of motion, we take equations of motion

$$
\begin{aligned}
x'' &= -x - 2xy, \\
y'' &= -y - x^2 + y^2.
\end{aligned}
\tag{4.15}
$$

The above system admits the Lagrangian

$$
L(t, x, y, x', y') = \frac{1}{2}(x'^2 + y'^2) + V(x, y), \tag{4.16}
$$

where $V(x, y)$ is the generalize form of Henon-Heiles potential

$$
V(x, y) = \frac{1}{2}(x^2 + y^2) + Ax^3 + Bx^2y + Cxy^2 + Dy^3, \tag{4.17}
$$

having A, B, C and D as real parameters. Here we consider a special case of Henon-Heiles potential in which the value of parameters are $A = 0$, $B = 1$, $C = 0$ and $D = -\frac{1}{3}$ respectively.

$$
V(x, y) = \frac{1}{2}(x^2 + y^2) + x^2y - \frac{1}{3}y^3. \tag{4.18}
$$

Then equation (4.16) takes the form

$$
L(t, x, y, x', y') = \frac{1}{2}(x'^2 + y'^2) - \frac{1}{2}(x^2 + y^2) - x^2y - \frac{1}{3}y^3. \tag{4.19}
$$

Using equation (4.19) and (2.10) in (2.4) and then comparing coefficients of x', y' and their powers, we get

$$\begin{aligned}
-x\eta - 2xy\eta - y\zeta - x^2\zeta - y^2\zeta - \frac{1}{2}(x^2+y^2)\xi_t - x^2y\xi_t + \frac{1}{3}y^3\xi_t - B_t =& \; 0,\\
\eta_t - \frac{1}{2}(x^2+y^2)\xi_x - x^2y\xi_x + \frac{1}{3}y^3\xi_x - B_x =& 0,\\
\zeta_t - \frac{1}{2}(x^2+y^2)\xi_y - x^2y\xi_y + \frac{1}{3}y^3\xi_y - B_y =& 0,\\
\eta_x - \xi_t + \frac{1}{2}\ \xi_t =& 0,\\
\zeta_y - \xi_t + \frac{1}{2}\ \xi_t =& 0,\\
\eta_y - \zeta_x =& 0,\\
\frac{1}{2}\ \xi_x =& 0,\\
\frac{1}{2}\ \xi_y =& 0.
\end{aligned} \tag{4.20}$$

The solution of above system of equations give value of ξ, η and ζ.

$$\xi = a_1, \qquad \eta = 0, \qquad \zeta = 0. \tag{4.21}$$

For this particular case, one Noether symmetry is obtained

$$\mathbf{X}_1 = \frac{\partial}{\partial t}, \tag{4.22}$$

where the first integral is calculated by using (2.14),

$$I_1 = \frac{1}{2}(x'^2 + y'^2) + \frac{1}{2}(x^2 + y^2) + x^2y - \frac{1}{3}y^3. \tag{4.23}$$

4.4 Harmonic Oscillator

Consider the second order ordinary differential equation

$$y'' = -k^2 y \tag{4.24}$$

having k as a spring constant and it explains the motion of a Harmonic oscillator. For convenience we choose different values of k^2 to determine the first integrals of corresponding equations. Since Lagrangian of the system is known, so we can compute symmetry group and associated constants of motion by using an explicit formula provided by Noether theorem. Here, we take different values of constant k^2 to obtained first integrals for our real and complex system.

***Case I*: when $k^2 = 1$ and y is real**

In the first case, when $k^2 = 1$ and $y(t)$ is real valued function, then equation (4.24) becomes one-dimensional Harmonic oscillator equation

$$y'' = -y, \tag{4.25}$$

having standard Lagrangian [25]

$$L = \frac{y'^2}{2} - \frac{y^2}{2}. \tag{4.26}$$

Using the Lagrangian in equation (2.4), gives the following determining equation

$$-\eta y + \eta_t y' + (\eta_y - \frac{1}{2}\xi_t)y'^2 - \frac{1}{2}\xi_y y'^3 - \frac{1}{2}\xi_t y^2 - \frac{1}{2}\xi_y y^2 y' - B_t - y' B_y = 0. \tag{4.27}$$

On comparing different powers of y' yields, system of four partial differential equations. Solving this system we get

$$\begin{aligned} \xi(t, y) &= a_1 + a_2 \sin 2t + a_3 \cos 2t, \\ \eta(t, y) &= (a_2 \cos 2t - a_3 \sin 2t)y + a_4 \sin t + a_5 \cos t, \\ B(t, y) &= -(a_2 \sin 2t + a_3 \cos 2t)y^2 + (a_4 \cos t - a_5 \sin t)y. \end{aligned} \tag{4.28}$$

We obtain five Noether symmetries of equation (4.25)

$$\begin{aligned} \mathbf{X}_1 &= \frac{\partial}{\partial t}, \\ \mathbf{X}_2 &= \sin 2t \, \frac{\partial}{\partial t} + y \cos 2t \, \frac{\partial}{\partial y}, \\ \mathbf{X}_3 &= \cos 2t \, \frac{\partial}{\partial t} - y \sin 2t \, \frac{\partial}{\partial y}, \\ \mathbf{X}_4 &= \cos 2t \, \frac{\partial}{\partial y}, \\ \mathbf{X}_5 &= \sin 2t \, \frac{\partial}{\partial y}. \end{aligned} \tag{4.29}$$

Using Lagrangian (4.26) and values of (4.28) in (2.5), we get the following first integrals

$$\begin{aligned} I_1 &= \frac{y'^2}{2} + \frac{y^2}{2}, \\ I_2 &= y' \cos t + y \sin t, \\ I_3 &= y' \sin t - y \cos t, \\ I_4 &= -\frac{1}{2}y'^2 \cos 2t - yy' \sin 2t + \frac{1}{2}y^2 \cos 2t, \\ I_5 &= \frac{1}{2}y'^2 \sin 2t + yy' \cos 2t - \frac{1}{2}y^2 \sin 2t. \end{aligned} \tag{4.30}$$

We observe that amongst five first integrals of Harmonic oscillator, only two are independent. Here I_2 and I_3 as the consider as independent quantities.

$$\begin{aligned} I_1 &= \frac{1}{4}(I_2^2 + I_3^2), \\ I_4 &= -\frac{1}{2}(I_2^2 - I_3^2), \\ I_5 &= \frac{1}{4}(I_2 I_3) \end{aligned} \tag{4.31}$$

Case II: **when $k^2 = 1$ and y is complex**

When we take $k^2 = 1$ and $y(t)$ as a complex dependant function $y = f + ig$ having f and g as real functions, we get a system of Harmonic oscillators. The complex symmetry analysis will help us to calculate first integrals of system of Harmonic oscillator. we have the following equations of motion for Harmonic oscillator

$$\begin{aligned} f'' &= -f, \\ g'' &= -g, \end{aligned} \tag{4.32}$$

which admits the Lagrangians

$$\begin{aligned} L_1 &= \frac{1}{2}(f'^2 - g'^2 - f^2 + g^2), \\ L_2 &= f'g' - fg. \end{aligned} \tag{4.33}$$

Using Lagrangians L_1 and L_2 in Noether like symmetry condition (2.38) gives

$$
\begin{aligned}
&- f\chi_1 + g\chi_2 + f'(\chi_{1t}) + f'^2(\chi_{1f} + \chi_{2g} - \tau_{1t}) - g'^2(\chi_{1f} + \chi_{2g} - \tau_{1t}) \\
&- 2f'g'(\chi_{2f} - \chi_{1g} - \tau_{2t}) + f'^3(\tau_{1f} + \tau_{2g}) + g'^3(\tau_{2f} - \tau_{1g}) - 3f'^2g'(\tau_{2f} - \tau_{1g}) \\
&- 3f'g'^2(\tau_{1f} + \tau_{2g}) + \frac{1}{2}f'^2(\tau_{1t}) - \frac{1}{2}g'^2(\tau_{1t}) - \frac{1}{2}f'^3(\tau_{1f} + \tau_{2g}) + f'g'(\tau_{2t}) \\
&- \frac{1}{2}f'^2g'(\tau_{2f} - \tau_{1g}) - \frac{1}{2}f'g'^2(\tau_{1f} + \tau_{2g}) + \frac{1}{2}g'^3(\tau_{2f} - \tau_{1g}) - \frac{1}{2}f^2(\tau_{1t}) \\
&- f'^2g'(\tau_{2f} - \tau_{1g}) - f'g'^2(\tau_{1f} + \tau_{2g}) - \frac{1}{2}f'f^2(\tau_{1f} + \tau_{2g}) + \frac{1}{2}f^2g'(\tau_{2f} - \tau_{1g}) \\
&+ \frac{1}{2}g^2(\tau_{1t}) + fg(\tau_{2t}) + \frac{1}{2}f'g^2(\tau_{1f} + \tau_{2g}) - \frac{1}{2}g^2g'(\tau_{2f} - \tau_{1g}) + f'(fg)(\tau_{2f} - \tau_{1g}) \\
&+ g'(fg)(\tau_{1f} + \tau_{2g}) - B_{1t} - f'(B_{1f} + B_{2g}) - g'(B_{2f} - B_{1g}) = 0,
\end{aligned}
\tag{4.34}
$$

and

$$
\begin{aligned}
&- g\chi_1 - f\chi_2 + f'(\chi_{2t}) + f'^2(\chi_{2f} - \chi_{1g} - \tau_{2t}) - g'^2(\chi_{2f} - \chi_{1g} - \tau_{2t}) \\
&+ 2f'g'(\chi_{1f} + \chi_{2g} - \tau_{1t}) - f'^3(\tau_{2f} - \tau_{1g}) - g'^3(\tau_{1f} + \tau_{2g}) + 3f'^2g'(\tau_{1f} \\
&+ \tau_{2g}) - 3f'g'^2(\tau_{2f} - \tau_{1g}) + \frac{1}{2}f'^2(\tau_{2t}) + \frac{1}{2}f'^3(\tau_{2f} - \tau_{1g}) + \frac{1}{2}f'^2g'(\tau_{1f} + \tau_{2g}) \\
&- \frac{1}{2}g'^2(\tau_{2t}) - \frac{1}{2}f'g'^2(\tau_{2f} - \tau_{1g}) - \frac{1}{2}g'^3(\tau_{1f} + \tau_{2g}) + f'g'(\tau_{1t}) + f'^2g'(\tau_{1f} + \tau_{2g}) \\
&- f'g'^2(\tau_{2f} - \tau_{1g}) - \frac{1}{2}f^2\tau_{2t} - \frac{1}{2}f'f^2(\tau_{2f} - \tau_{1g}) - \frac{1}{2}f^2g'(\tau_{1f} + \tau_{2g}) + \frac{1}{2}g^2\tau_{2t} \\
&+ \frac{1}{2}f'g^2(\tau_{2f} - \tau_{1g}) - fg\tau_{1t} + \frac{1}{2}g^2g'(\tau_{1f} + \tau_{2g}) - f'fg(\tau_{1f} + \tau_{2g}) + g'fg(\tau_{2f} - \tau_{1g}) \\
&- B_{2t} - f'(B_{2f} - B_{1g}) - g'(B_{1f} + B_{2g}) = 0.
\end{aligned}
\tag{4.35}
$$

On comparing the coefficients of independent variables, yields a system of partial differential equations.

$$\begin{aligned}
&\tau_{1f}+\tau_{2g}=0,\\
&\tau_{2f}-\tau_{1g}=0,\\
&\chi_{1f}+\chi_{2g}-\frac{1}{2}\tau_{1t}=0,\\
&\chi_{2f}-\chi_{1g}-\frac{1}{2}\tau_{2t}=0,\\
&-f\chi_1+g\chi_2-\frac{1}{2}(f^2-g^2)\tau_{1t}+(fg)\tau_{2t}=B_{1t},\\
&-g\chi_1-f\chi_2-\frac{1}{2}(f^2-g^2)\tau_{2t}-(fg)\tau_{1t}=B_{2t},\\
&\chi_{1t}-\frac{1}{2}(f^2-g^2)\tau_{1f}-\frac{1}{2}(f^2-g^2)\tau_{2g}+(fg)(\tau_{2f}-\tau_{1g})-B_{1f}-B_{2g}=0,\\
&-\chi_{2t}-\frac{1}{2}(f^2-g^2)\tau_{2f}+\frac{1}{2}(f^2-g^2)\tau_{1g}+(fg)(\tau_{1f}+\tau_{2g})+B_{2f}-B_{1g}=0,
\end{aligned}\tag{4.36}$$

Solving the system (4.36) gives nine Noether like symmetry generators

$$\begin{aligned}
\mathbf{X}_1&=\frac{\partial}{\partial t},\\
\mathbf{X}_2&=\sin t\frac{\partial}{\partial f},\\
\mathbf{X}_3&=\sin t\frac{\partial}{\partial g},\\
\mathbf{X}_4&=\cos t\frac{\partial}{\partial f},\\
\mathbf{X}_5&=\cos t\frac{\partial}{\partial g},\\
\mathbf{X}_6&=\sin 2t\frac{\partial}{\partial t}+f\ \cos 2t\ \frac{\partial}{\partial f}+g\ \cos 2t\ \frac{\partial}{\partial g},\\
\mathbf{X}_7&=g\ \cos 2t\ \frac{\partial}{\partial f}-f\ \cos 2t\ \frac{\partial}{\partial g},\\
\mathbf{X}_8&=\cos 2t\ \frac{\partial}{\partial t}-f\ \sin 2t\ \frac{\partial}{\partial f}-g\ \sin 2t\ \frac{\partial}{\partial g},\\
\mathbf{X}_9&=-g\ \sin 2t\ \frac{\partial}{\partial f}+f\ \sin 2t\ \frac{\partial}{\partial g}.
\end{aligned}\tag{4.37}$$

By utilizing equation (2.39), we obtain the following first integrals

$$\begin{aligned}
I_{1,1} &= (f'^2 - g'^2 - f^2 + g^2)\sin 2t - 2(ff' - gg')\cos 2t,\\
I_{1,2} &= 2(f'g' - fg)\sin 2t - 2(fg' + f'g)\cos 2t,\\
I_{2,1} &= (f'^2 - g'^2 - f^2 + g^2)\cos 2t + 2(f'f - g'g)\sin 2t,\\
I_{2,2} &= 2(f'g' - fg)\cos 2t + 2(fg' + f'g)\sin 2t,\\
I_{3,1} &= -2f'\cos t - 2f\sin t,\\
I_{3,2} &= -2g'\cos t - 2g\sin t,\\
I_{4,1} &= -2f'\sin t + 2f\cos t,\\
I_{4,2} &= -2g'\sin t + 2g\cos t,\\
I_{5,1} &= f'^2 - g'^2 - f^2 + g^2,\\
I_{5,2} &= 2f'g' + 2fg.
\end{aligned} \tag{4.38}$$

Case III: when k and y are complex

For k and y to be complex functions $k = \alpha + i\beta$ and $y = f + ig$, the following coupled system of harmonic oscillators is obtained

$$\begin{aligned}
f'' &= -(\alpha^2 - \beta^2)f + 2\alpha\beta g,\\
g'' &= -(\alpha^2 - \beta^2)g - 2\alpha\beta f,
\end{aligned} \tag{4.39}$$

having two Lagrangians

$$\begin{aligned}
L_1 &= \frac{1}{2}(f'^2 - g'^2) - \frac{1}{2}(\alpha^2 - \beta^2)(f^2 - g^2) + 2\alpha\beta fg,\\
L_2 &= f'g' - \alpha\beta(f^2 - g^2) - (\alpha^2 - \beta^2)fg.
\end{aligned} \tag{4.40}$$

On comparing the coefficients of independent variables, yields a system of partial differential equations

$$
\begin{aligned}
&\tau_{1f}+\tau_{2g}=0,\\
&\tau_{2f}-\tau_{1g}=0,\\
&\chi_{1f}+\chi_{2g}-\frac{1}{2}\tau_{1t}=0,\\
&\chi_{2f}-\chi_{1g}-\frac{1}{2}\tau_{2t}=0,\\
&-(\alpha^2-\beta^2)f\chi_1+(\alpha^2-\beta^2)g\chi_2+2\alpha\beta(g\chi_1+f\chi_2)=B_{1t},\\
&-(\alpha^2-\beta^2)g\chi_1-(\alpha^2-\beta^2)f\chi_2-2\alpha\beta(f\chi_1+g\chi_2)=B_{2t},\\
&\chi_{1t}-\frac{1}{2}(\alpha^2-\beta^2)(f^2-g^2)(\tau_{1f}+\tau_{2g})+\alpha\beta(f^2-g^2)(\tau_{2f}-\tau_{1g})\\
&+2\alpha\beta fg(\tau_{1f}+\tau_{2g})-B_{1f}-B_{2g}=0,\\
&-\chi_{2t}+\frac{1}{2}(\alpha^2-\beta^2)(f^2-g^2)(\tau_{2f}-\tau_{1g})+\alpha\beta(f^2-g^2)(\tau_{1f}+\tau_{2g})\\
&-2\alpha\beta fg(\tau_{2f}-\tau_{1g})+B_{2f}-B_{1g}=0.
\end{aligned}
\tag{4.41}
$$

The following nine Noether-like operators are obtained by solving the system (4.41)

$$
\begin{aligned}
\mathbf{X}_1&=\frac{\partial}{\partial t},\\
\mathbf{X}_2&=\sin(\alpha t)\cosh(\beta t)\frac{\partial}{\partial f}+\cos(\alpha t)\sinh(\beta t)\frac{\partial}{\partial g},\\
\mathbf{X}_3&=\cos(\alpha t)\sinh(\beta t)\frac{\partial}{\partial f}-\sin(\alpha t)\cosh(\beta t)\frac{\partial}{\partial g},\\
\mathbf{X}_4&=\cos(\alpha t)\cosh(\beta t)\frac{\partial}{\partial f}-\sin(\alpha t)\sinh(\beta t)\frac{\partial}{\partial g},\\
\mathbf{X}_5&=-\sin(\alpha t)\sinh(\beta t)\frac{\partial}{\partial f}-\cos(\alpha t)\cosh(\beta t)\frac{\partial}{\partial g},
\end{aligned}
$$

$$\mathbf{X}_6 = \sin(2\alpha t)\cosh(2\beta t)\frac{\partial}{\partial t} + \{(\alpha f - \beta g)\cos(2\alpha t)\cosh(2\ \beta t) + (\alpha g + \beta f)\sin(2\alpha t)\sinh(2\beta t)\}\frac{\partial}{\partial f}$$
$$+ \{(\alpha g + \beta f)\cos(2\alpha t)\cosh(2\beta t) - (\alpha f - \beta g)\sin(2\alpha t)\sinh(2\beta t)\}\frac{\partial}{\partial g},$$

$$\mathbf{X}_7 = \cos(2\alpha t)\sinh(2\beta t)\frac{\partial}{\partial t} + \{(\alpha g + \beta f)\cos(2\alpha t)\cosh(2\beta t) - (\alpha f - \beta g)\sin(2\alpha t)\sinh(2\beta t)\}\frac{\partial}{\partial f}$$
$$- \{(\alpha f - \beta g)\cos(2\alpha t)\cosh(2\beta t) + (\alpha g + \beta f)\sin(2\alpha t)\sinh(2\beta t)\}\frac{\partial}{\partial g},$$

$$\mathbf{X}_8 = \cos(2\alpha t)\cosh(2\beta t)\frac{\partial}{\partial t} + \{(\alpha f - \alpha\beta g)\sin(2\alpha t)\cosh(2\beta t) - (\alpha g + \beta f)\cos(2\alpha t)\sinh(2\beta t)\}\frac{\partial}{\partial f}$$
$$+ \{(\alpha_1 f - \alpha_2 g)\cos(2\alpha_1 t)\sinh(2\alpha_2 t) + (\alpha_1 g + \alpha_2 f)\sin(2\alpha_1 t)\cosh(2\alpha_2 t)\}\frac{\partial}{\partial g},$$

$$\mathbf{X}_9 = -\sin(2\alpha t)\sinh(2\beta t)\frac{\partial}{\partial t} + \{(\alpha f - \beta g)\cos(2\alpha t)\sinh(2\beta t) + (\alpha g + \beta f)\sin(2\alpha t)\cosh(2\beta t)\}\frac{\partial}{\partial f}$$
$$- \{(\alpha f - \beta g)\sin(2\alpha t)\cosh(2\beta t) - (\alpha g + \beta f)\cos(2\alpha t)\sinh(2\beta t)\}\frac{\partial}{\partial g}. \tag{4.42}$$

Using equation (2.39), we obtained the following first integrals of the system (4.39).

$$I_{1,1} = (\alpha^2 - \beta^2)(f^2 - g^2) - 2\alpha\beta fg + f'^2 - g'^2,$$

$$I_{1,2} = 2(\alpha^2 - \beta^2)fg + 2\alpha\beta(f^2 - g^2) + 2f'g',$$

$$I_{2,1} = f'\sin(\alpha t)\cosh(\beta t) - g'\cos(\alpha t)\sinh(\beta t) - (\alpha f - \beta g)\cos(\alpha t)\cosh(\beta t)$$
$$- (\alpha g + \beta f)\sin(\alpha t)\sinh(\beta t), \tag{4.43}$$

$$I_{2,2} = g'\sin(\alpha t)\cosh(\beta t) + f'\cos(\alpha t)\sinh(\beta t) + (\alpha g + \beta f)\cos(\alpha t)\cos(\beta t)$$
$$- (\alpha f - \beta g)\sin(\alpha t)\sinh(\beta t),$$

$$
\begin{aligned}
I_{3,1} &= f' \cos(\alpha t)\cosh(\beta t) + g' \sin(\alpha t)\sinh(\beta t) + (\alpha f - \beta g)\sin(\alpha t)\cosh(\beta t) \\
&\quad - (\alpha g + \beta f)\cos(\alpha t)\sinh(\beta t),
\end{aligned}
$$

$$
\begin{aligned}
I_{3,2} &= g' \cos(\alpha t)\cosh(\beta t) - f' \sin(\alpha t)\sinh(\beta t) + (\alpha g + \beta f)\sin(\alpha t)\cosh(\beta t) \\
&\quad + (\alpha f - \beta g)\cos(\alpha t)\sinh(\beta t),
\end{aligned}
$$

$$
\begin{aligned}
I_{4,1} &= \frac{1}{2}[\{(\alpha^2 - \beta^2)(f^2 - g^2) - 4\alpha\beta fg - (f'^2 - g'^2)\}\sin(2\alpha t)\cosh(2\beta t) \\
&\quad - \{2\alpha\beta(f^2 - g^2) + 2(\alpha^2 - \beta^2)fg - 2f'g'\}]\cos(2\alpha t)\sinh(2\beta t) \\
&\quad + \{\alpha(ff' - gg') - \beta(fg' + gf')\}\cos(2\alpha t)\cosh(2\beta t) \\
&\quad + \{\alpha(fg' - gf') + \beta(ff' - g'g)\}\sin(2\alpha t)\sinh(2\beta t),
\end{aligned}
$$

$$
\begin{aligned}
I_{4,2} &= \frac{1}{2}[\{(\alpha^2 - \beta^2)(f^2 - g^2) - 4\alpha\beta fg - (f'^2 - g'^2)\}\cos(2\alpha t)\sinh(2\beta t) \\
&\quad + \{2\alpha\beta(f^2 - g^2) + 2fg(\alpha^2 - \beta^2) - 2f'g'\}]\sin(2\alpha t)\cosh(2\beta t) \\
&\quad + [\{\alpha(fg' + f'g) + \beta(ff' - gg')\}\cos(2\alpha t)\cosh(2\beta t)] \\
&\quad - [\{\alpha(ff' - gg') + \beta(fg' + f'g)\}\sin(2\alpha t)\sinh(2\beta t)],
\end{aligned}
$$

$$
\begin{aligned}
I_{5,1} &= \frac{1}{2}[\{(\alpha^2 - \beta^2)(f^2 - g^2) - 4\alpha\beta fg - (f'^2 - g'^2)\}\cos(2\alpha t)\cosh(2\beta t) \\
&\quad + \{2\alpha\beta(f^2 - g^2) + 2(\alpha^2 - \beta^2)fg - 2f'g'\}]\sin(2\alpha t)\sinh(2\beta t) \\
&\quad + \{\alpha(fg' + gf') + \beta(ff' - gg')\}\cos(2\alpha t)\sinh(2\beta t) \\
&\quad - \{\alpha(ff' - gg') + \beta(fg' + gf')\}\sin(2\alpha t)\cosh(2\beta t),
\end{aligned}
$$

$$
\begin{aligned}
I_{5,2} &= \frac{1}{2}[\{-(\alpha^2 - \beta^2)(f^2 - g^2) + 4\alpha\beta fg + (f'^2 - g'^2)\}\sin(2\alpha t)\sinh(2\beta t) \\
&\quad + \{2\alpha\beta(f^2 - g^2) + 2fg(\alpha^2 - \beta^2) - 2f'g'\}]\cos(2\alpha t)\cosh(2\beta t) \\
&\quad - [\{\alpha(fg' + f'g) - \beta(ff' - gg')\}\sin(2\alpha t)\cosh(2\beta t)] \\
&\quad - [\{\alpha(ff' - gg') + \beta(fg' + f'g)\}\cos(2\alpha t)\sinh(2\beta t)].
\end{aligned}
$$

Chapter 5

Numerical Experiments

In this chapter, we numerically integrate Hamiltonian systems using symplectic Runge-Kutta method and look at the preservation of quadratic first integrals of Hamiltonian systems for long time period. For implementation we have used symplectic implicit Runge-Kutta methods for the preservation of all first integrals. We have used fixed stepsize for the implementation of numerical methods. To evaluate implicit stages we have used modified Newton iterations. The numerical results show good preservation of first integrals.

The graphs are plotted by taking time along x-axis and absolute error in first integrals along y-axis. The absolute error in the first integrals is basically the difference between the value of first integral I calculated at initial value $I(y_0)$ with the value of first integral calculated at each point of the approximated solution $I(y_n)$. The error formula is given by,

$$Error = |I(y_n) - I(y_0)|$$

.

5.1 Simple Pendulum

A simple pendulum consists of a particle of mass m attached with a light inextensible rod of unit length. The motion of the rod is along vertical plane. The equations of motion of the simple pendulum are defined as

$$\begin{aligned} y_1' &= -\sin y_2, \\ y_2' &= y_1. \end{aligned} \tag{5.1}$$

The total energy of the system is given in (4.7). We have applied Gauss-2 method on Simple pendulum with initial values $y_1 = 0$, $y_2 = 0.01$. We have taken 100,000 steps and stepsize is $h = 0.01$. Figure 5.1 shows good long time conservation of first integral as the error is bounded by 0.8×10^{-9}.

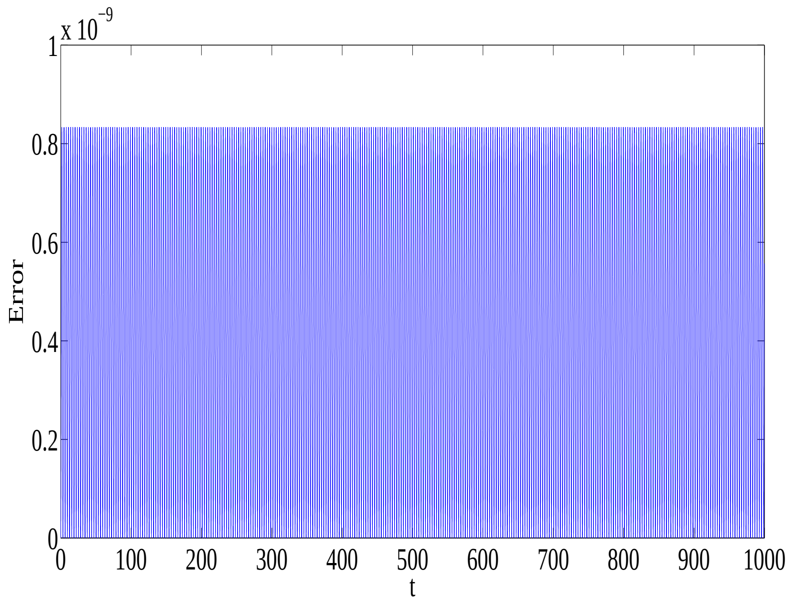

Figure 5.1: Error in integral I_1 of Simple pendulum using Gauss-2 method.

5.2 Kepler Problem

The classical Kepler problem explains the motion of two bodies interacting with each other by a gravitational force. The governing equations of motion are

$$\begin{aligned} y_1' &= y_3, \\ y_2' &= y_4, \\ y_3' &= \frac{-y_1}{(y_1^2+y_2^2)^{\frac{3}{2}}}, \\ y_4' &= \frac{-y_2}{(y_1^2+y_2^2)^{\frac{3}{2}}}. \end{aligned} \tag{5.2}$$

Hamiltonian systems can be written more compactly in the form of canonical coordinates (p_i, q_i). For convenience we have taken (y_3, y_4) as generalized momenta and (y_1, y_2) as generalised position coordinates. To get an elliptic orbits, the eccentricity is taken as $0 < e \leq 1$. The initial conditions are

$$(y_1, y_2, y_3, y_4) = (1-e,\ 0,\ 0,\ \sqrt{\frac{1+e}{1-e}}). \tag{5.3}$$

The conserved quantities is I_1 and I_2 which represents the total energy and angular momentum of the system is given in equation (4.14).

We have used Gauss-2 method on Kepler problem to check preservation of the first integrals. We have taken stepsize $h = 0.01$ for $100,000$ steps. The absolute error in integral I_1, I_2 is plotted in Figure 5.2 and Figure 5.3 respectively. The following results are obtained, when eccentricity is $e = 0.6$. The results shows that absolute error does not grow with time which mean that error will remain bounded for long time period.

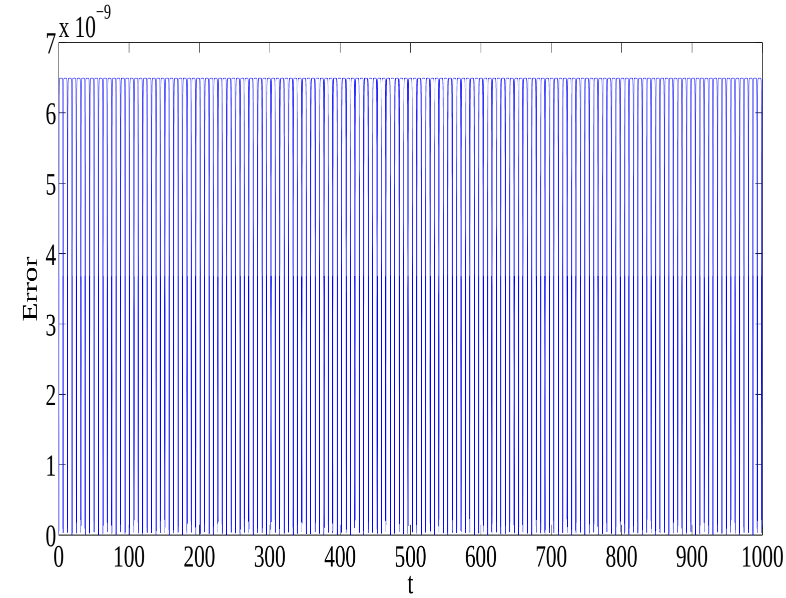

Figure 5.2: Error in integral I_1 of Kepler problem using Gauss-2 method.

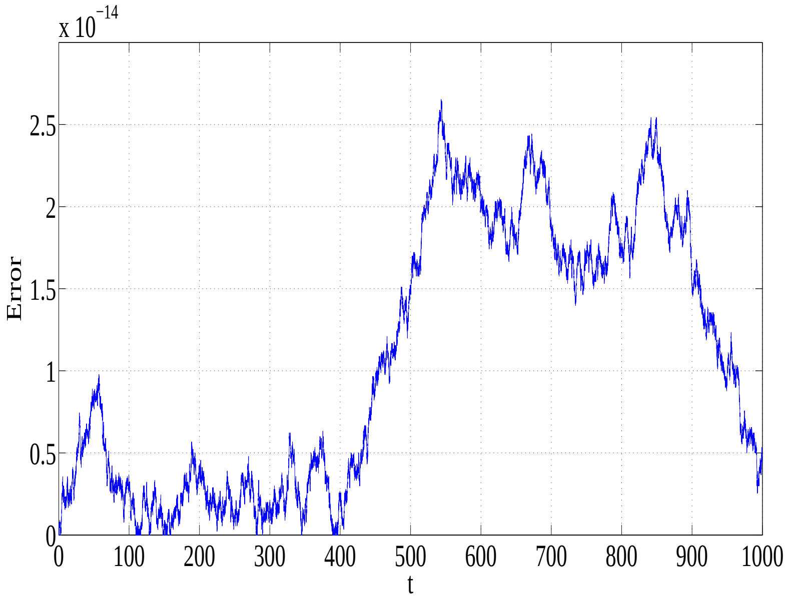

Figure 5.3: Error in integral I_2 of Kepler problem using Gauss-2 method.

5.3 Henon-Heiles Problem

The Henon-Heiles problem explains the motion of stars along the galactic center. The equations of motion are

$$\begin{aligned} y_1' &= y_3, \\ y_2' &= y_4, \\ y_3' &= -y_1 - 2y_1y_2, \\ y_4' &= -y_2 - y_1^2 + y_2^2. \end{aligned} \tag{5.4}$$

having initial value [19],

$$(y_1, y_2, y_3, y_4) = (0, 0, \sqrt{0.3185}, 0), \tag{5.5}$$

where the first integral is given in (4.23). Figure 5.4 shows absolute error in integral I_1. Gauss-2 method is used to check preservation of first integral with stepsize 0.01 and $n = 100,000$ steps.

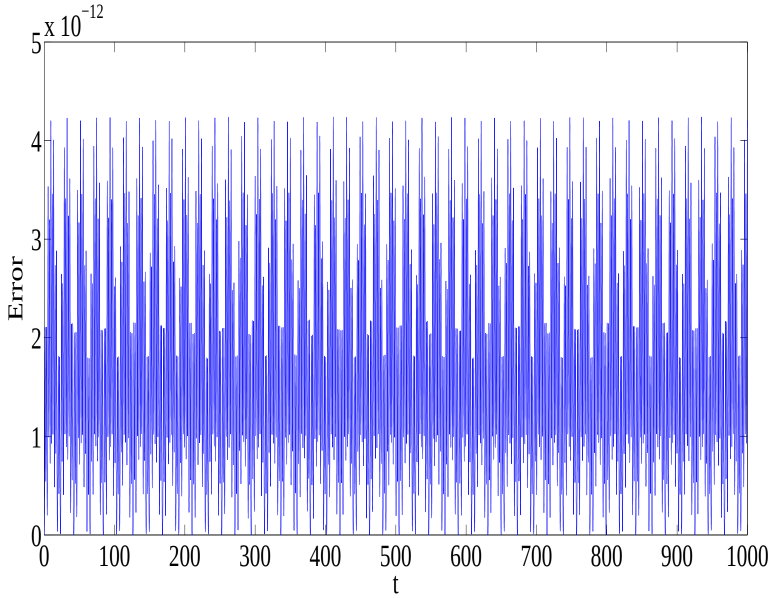

Figure 5.4: Error in integral I_1 of the Henon-Heiles problem using Gauss-2 method.

5.4 Harmonic Oscillator

Case I: **when $k^2 = 1$ and y is real**

Harmonic oscillator explains the motion of a unit mass m attached to a spring of length l. The differential equations of Harmonic oscillator are

$$\begin{aligned} y_1' &= -y_2, \\ y_2' &= \ \ y_1. \end{aligned} \tag{5.6}$$

The first integrals of one-dimensional Harmonic oscillator are calculated in Chapter 4. There are total five first integral of Harmonic oscillator. Amongst these five first integrals only two are independent, here we consider I_2 and I_3 to be the independent quantities.

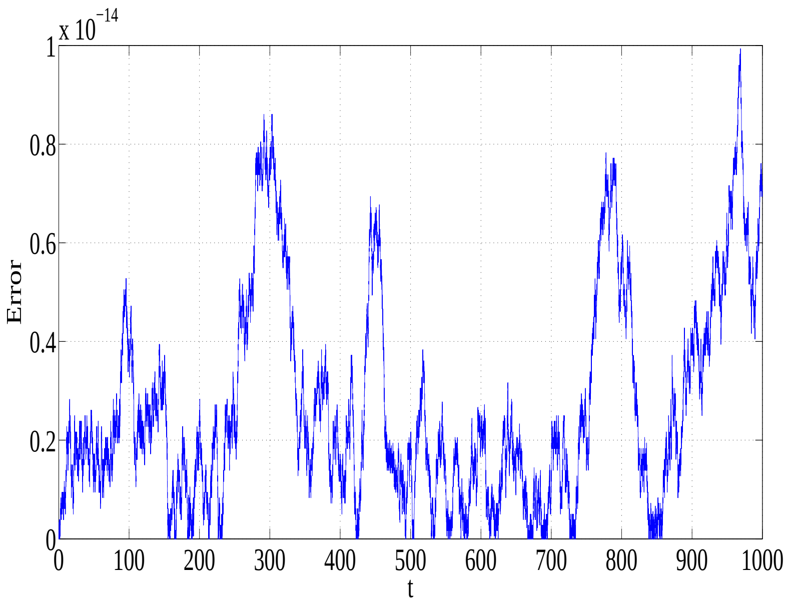

Figure 5.5: Error in integral I_1 of Harmonic oscillator using Gauss-2 method.

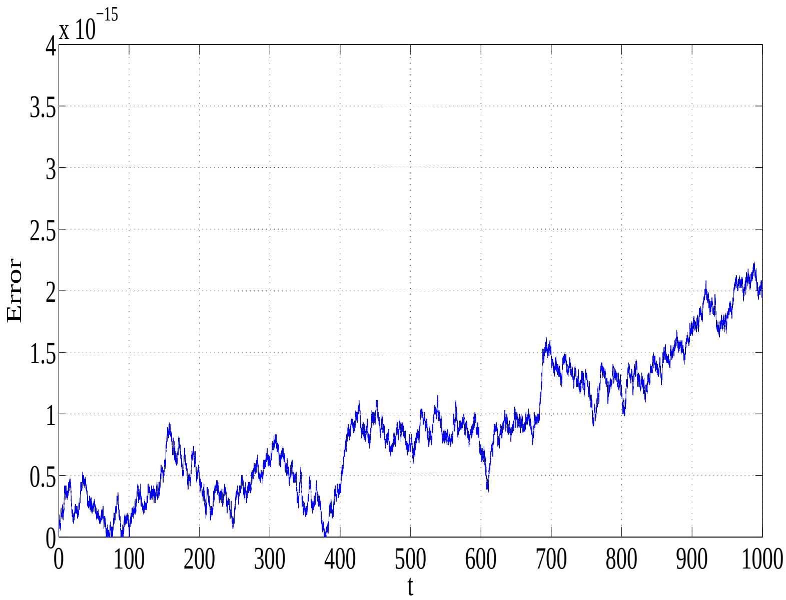

Figure 5.6: Error in integral I_2 of Harmonic oscillator using Gauss-2 method.

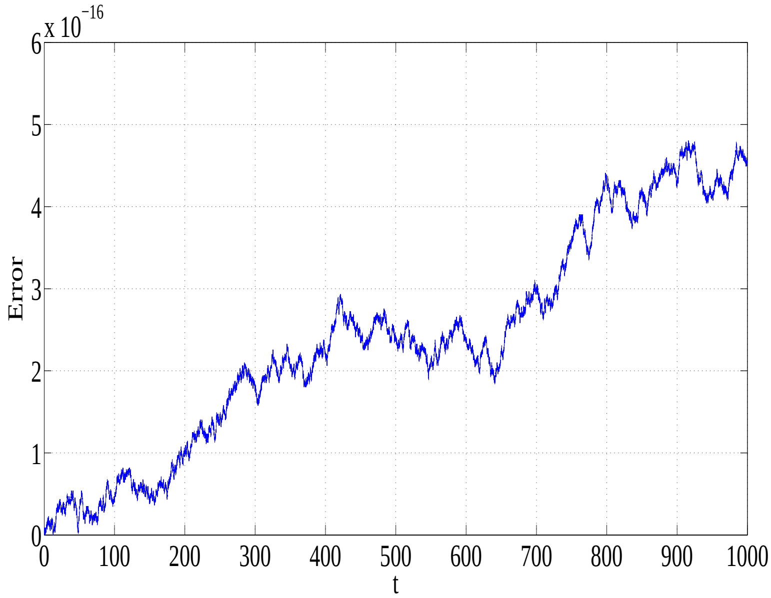

Figure 5.7: Error in integral I_3 of Harmonic oscillator using Gauss-2 method.

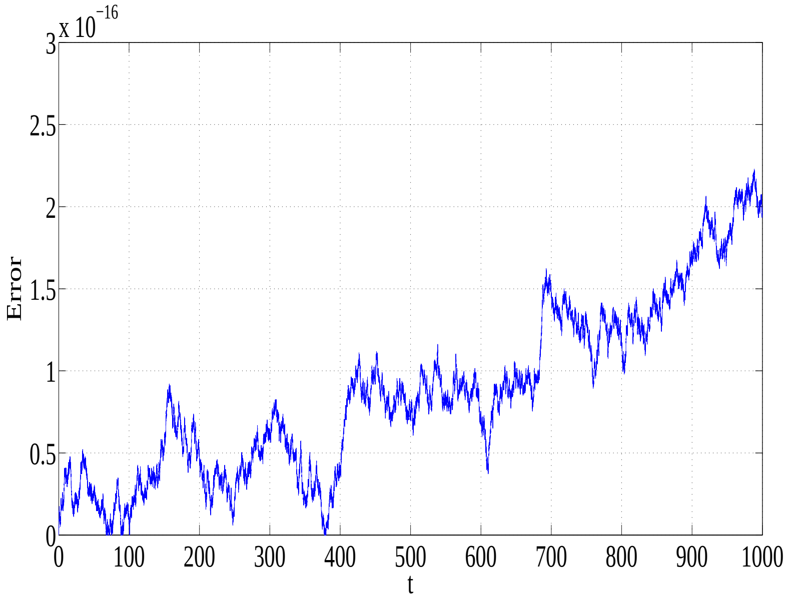

Figure 5.8: Error in integral I_4 of Harmonic oscillator using Gauss-2 method.

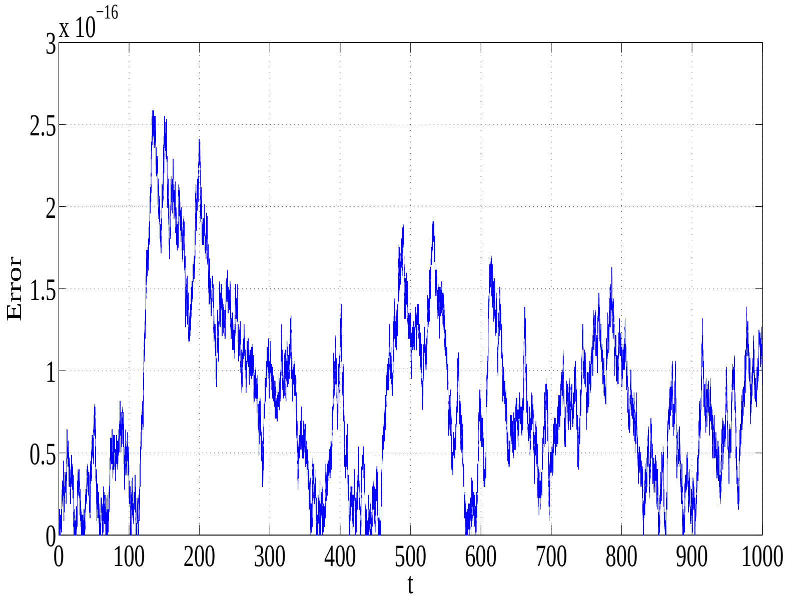

Figure 5.9: Error in integral I_5 of Harmonic oscillator using Gauss-2 method.

We have plotted absolute error in the first integrals by using symplectic Gauss-2 method. We have taken $n = 100,000$ and stepsize $h = 0.01$. The error in first integrals, is plotted in Figure 5.5, Figure 5.6, Figure 5.7, Figure 5.8 and Figure 5.9 respectively. The initial conditions are $[0, 1]$, $[1, 0]$, $[0, 0.1]$, $[0.1, 0]$, $[0.1, 0.1]$. The results have shown the error does not grow out of bound. This shows symplectic Gauss-2 method show good long time preservation of all the first integrals.

***Case II*: when $k^2 = 1$ and y is complex**

Harmonic oscillator consists of two oscillator each of mass m connected by a spring. The differential equations of the system are given as

$$\begin{aligned} y_1' &= y_3, \\ y_2' &= y_4, \\ y_3' &= -y_1, \\ y_4' &= -y_2. \end{aligned} \tag{5.7}$$

We have integrated system of equations (5.7) using symplectic Gauss-2 method. We have taken $h = 0.01$ and $n = 100,000$ steps. The absolute error in the first integrals $I_{1,1}$, $I_{1,2}$, $I_{2,1}$, $I_{2,2}$, $I_{3,1}$, $I_{3,2}$, $I_{4,1}$, $I_{4,2}$, $I_{5,1}$, $I_{5,2}$, are plotted in Figures $5.10, 5.11, \cdots, 5.19$ respectively.

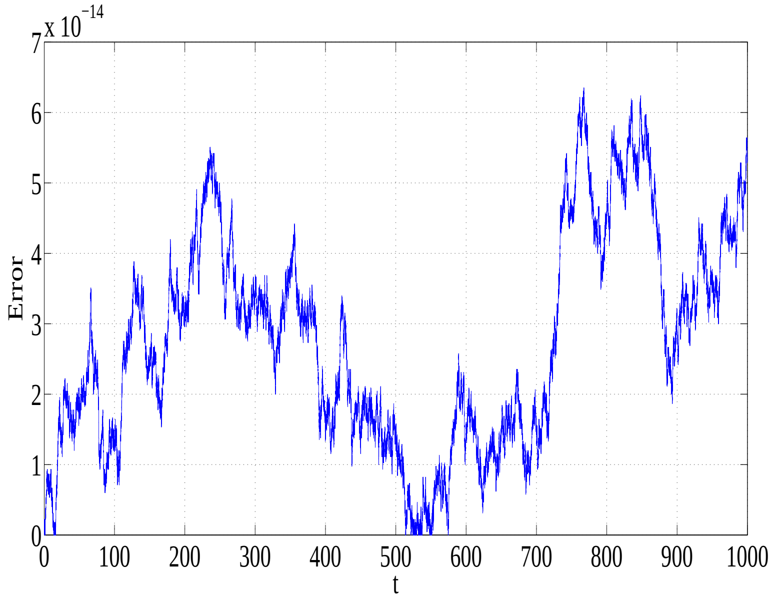

Figure 5.10: Error in integral $I_{1,1}$ of Harmonic oscillator using Gauss-2 method.

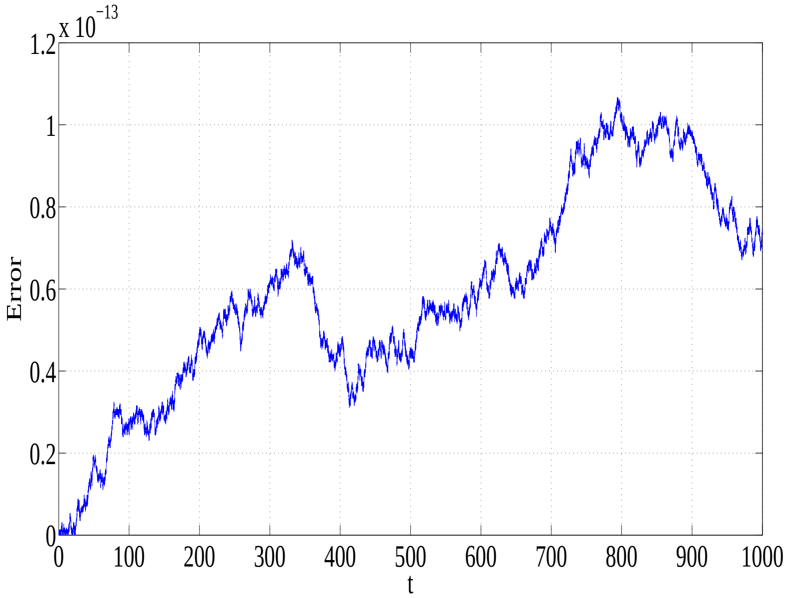

Figure 5.11: Error in integral $I_{1,2}$ of Harmonic oscillator using Gauss-2 method.

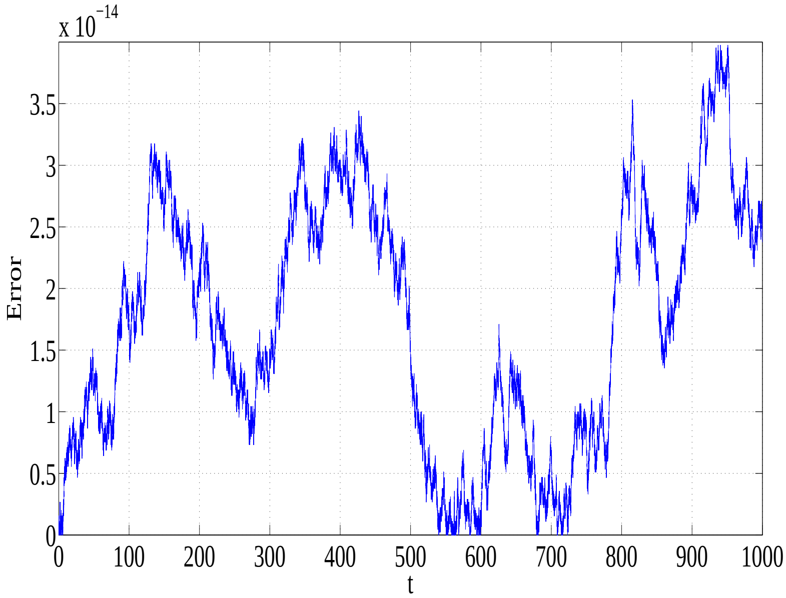

Figure 5.12: Error in integral $I_{2,1}$ of Harmonic oscillator using Gauss-2 method,

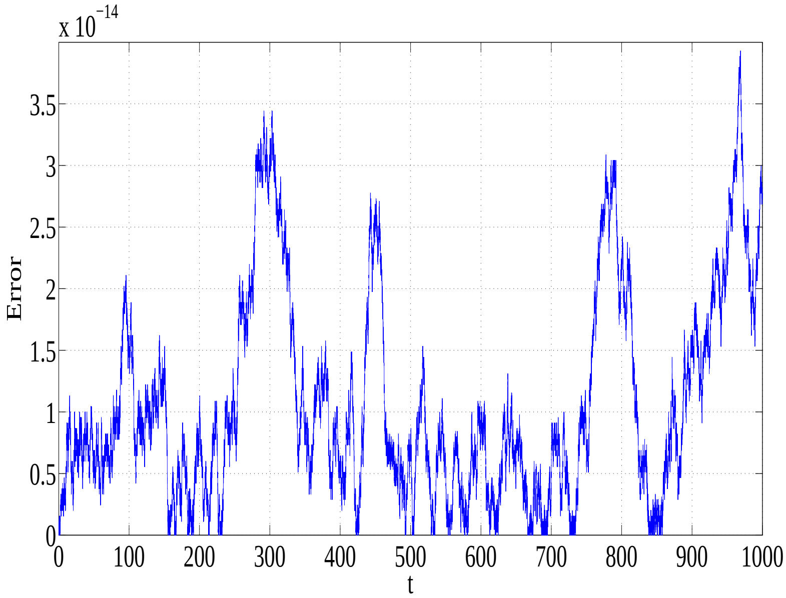

Figure 5.13: Error in integral $I_{2,2}$ of Harmonic oscillator using Gauss-2 method.

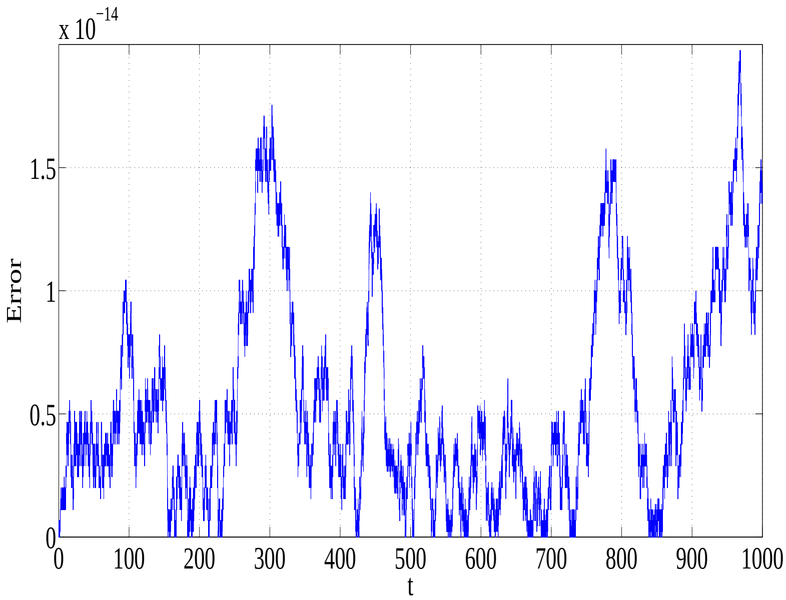

Figure 5.14: Error in integral $I_{3,1}$ of Harmonic oscillator using Gauss-2 method.

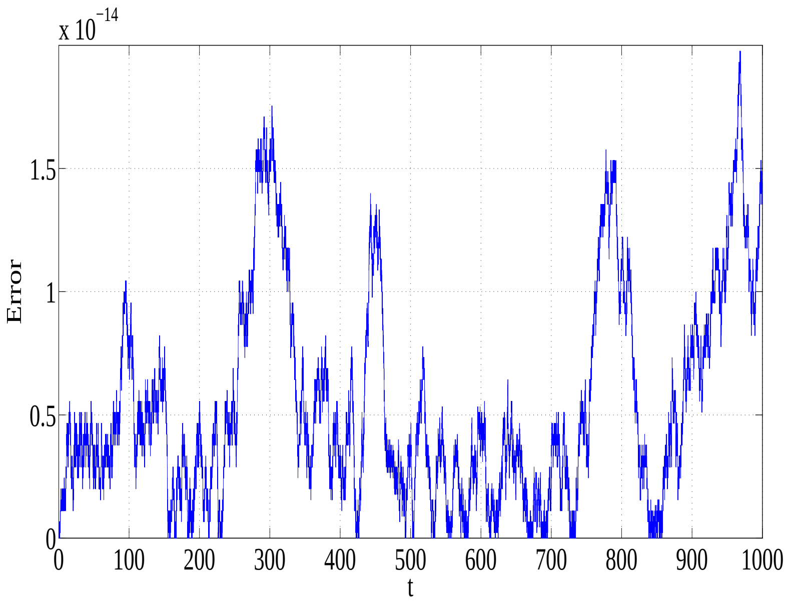

Figure 5.15: Error in integral $I_{3,2}$ of Harmonic oscillator using Gauss-2 method.

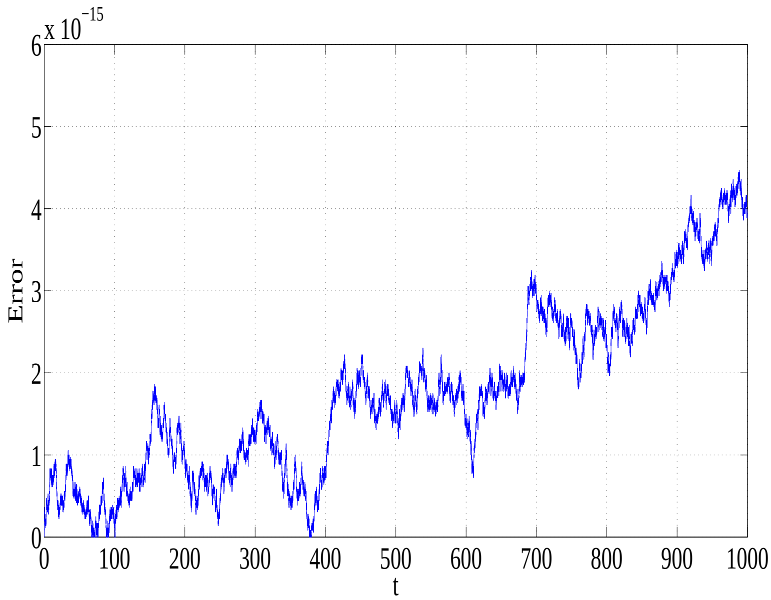

Figure 5.16: Error in integral $I_{4,1}$ of Harmonic oscillator using Gauss-2 method.

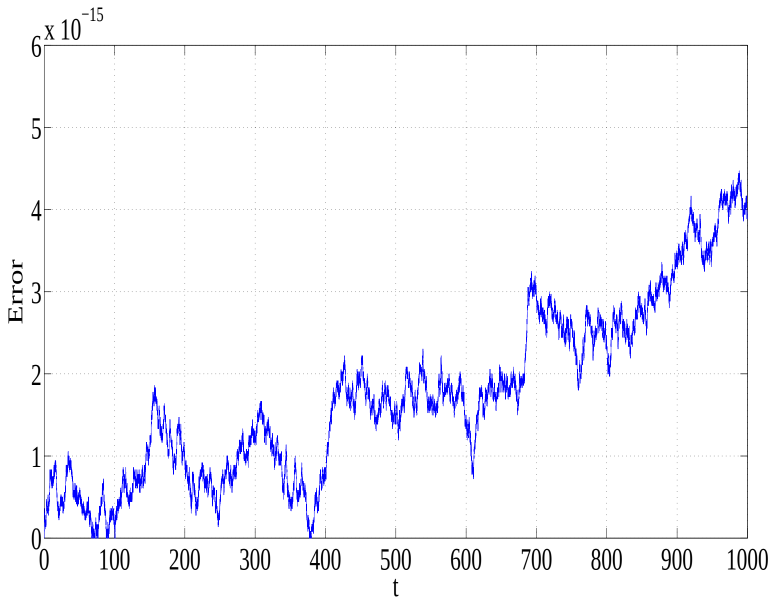

Figure 5.17: Error in integral $I_{4,2}$ of Harmonic oscillator using Gauss-2 method.

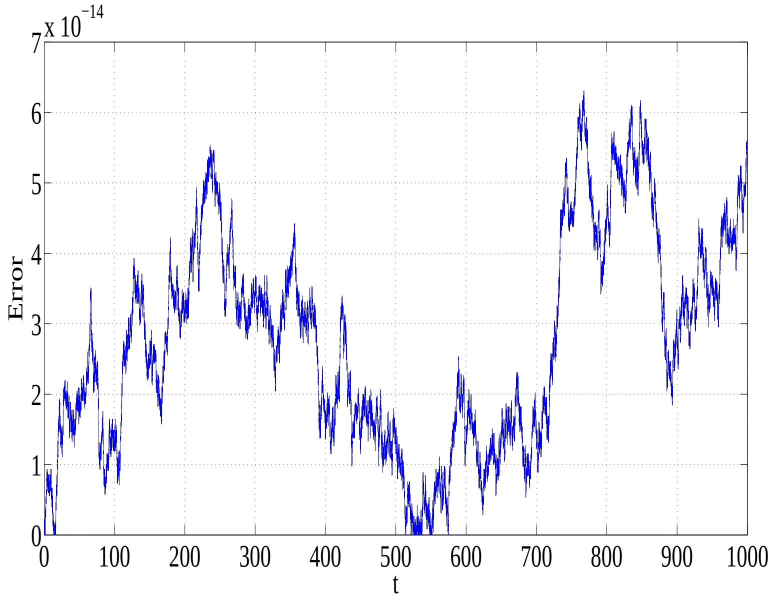

Figure 5.18: Error in integral $I_{5,1}$ of Harmonic oscillator using Gauss-2 method.

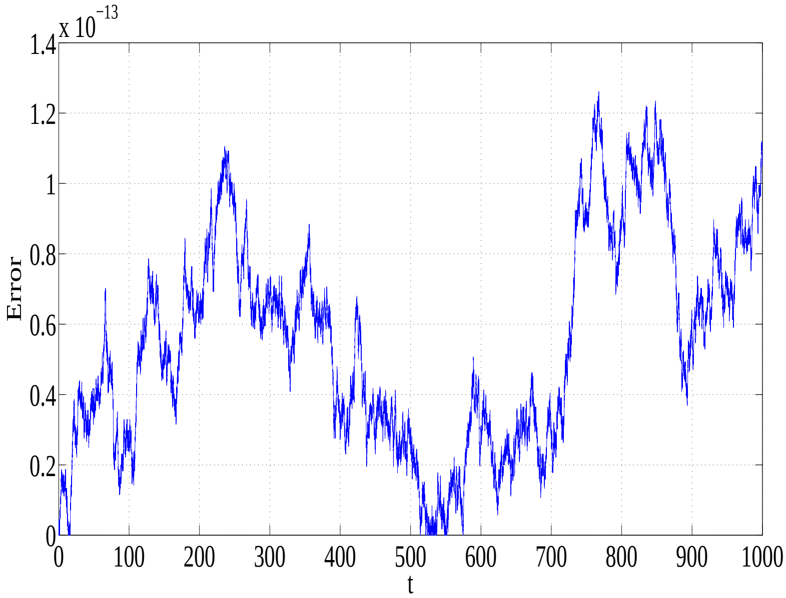

Figure 5.19: Error in integral $I_{5,2}$ of Harmonic oscillator using Gauss-2 method.

Case III: **when k and y are complex**

A coupled time-independent harmonic oscillators consists of two objects of mass m attached with three springs. The equations of motion are

$$\begin{aligned} y_1' &= y_3, \\ y_2' &= y_4, \\ y_3' &= -\alpha y_1 + \beta y_2, \\ y_4' &= -\alpha y_2 - \beta y_1. \end{aligned} \tag{5.8}$$

We have plotted the absolute error in integrals $I_{1,1}$, $I_{1,2}$, $I_{2,1}$, $I_{3,1}$, $I_{3,2}$, $I_{4,1}$, $I_{4,2}$, $I_{5,1}$ and $I_{5,2}$ using stepsize $h = 0.01$ and number of steps $n = 100,000$. The absolute error in the first integrals are plotted in Figures $5.20, 5.21, \cdots, 5.27$ respectively.

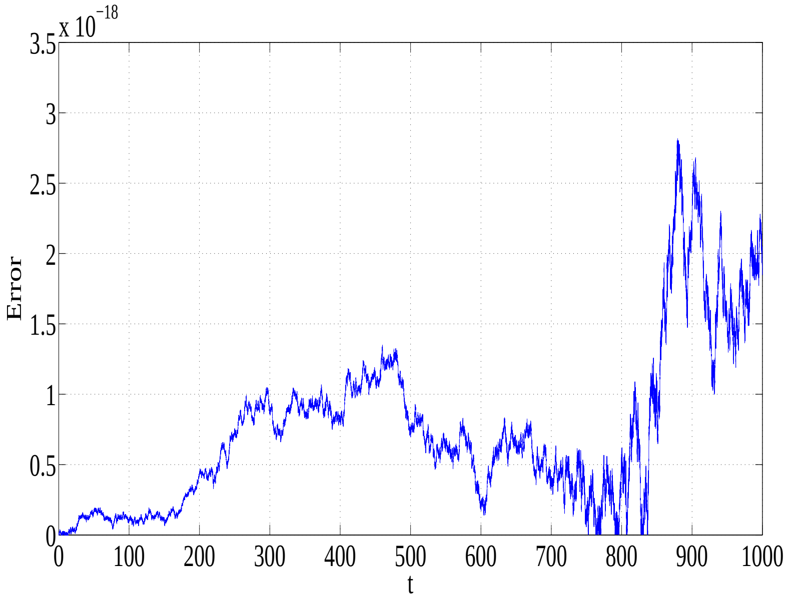

Figure 5.20: Error in integral $I_{1,1}$ of coupled Harmonic oscillator using Gauss-2 method.

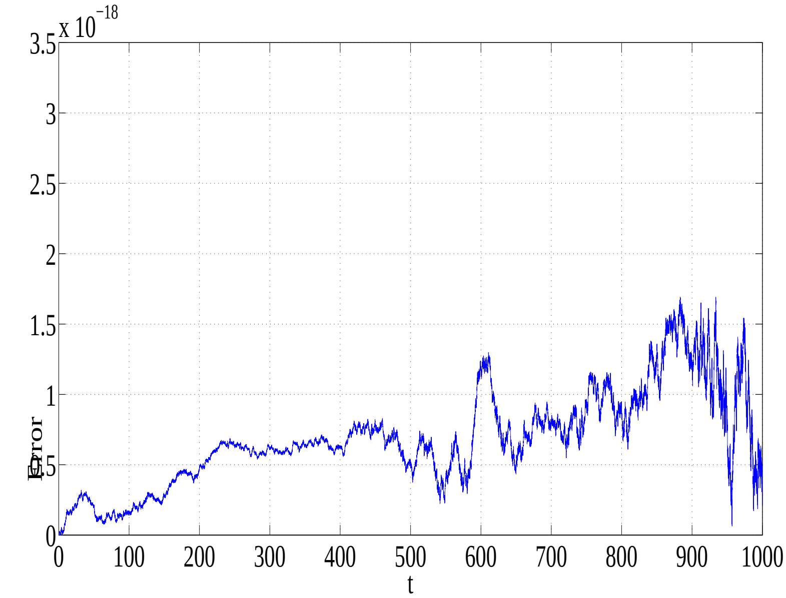

Figure 5.21: Error in integral $I_{1,2}$ of coupled Harmonic oscillator using Gauss-2 method.

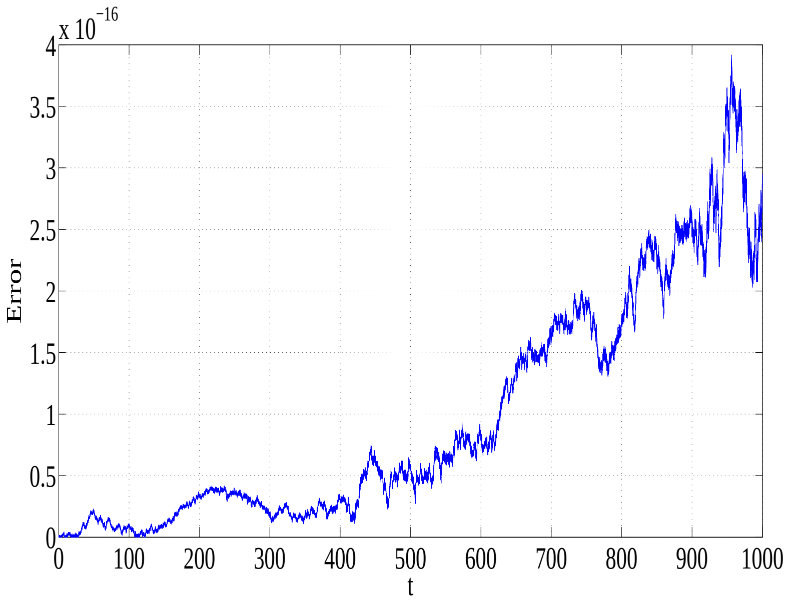

Figure 5.22: Error in integral $I_{2,1}$ of coupled Harmonic oscillator using Gauss-2 method.

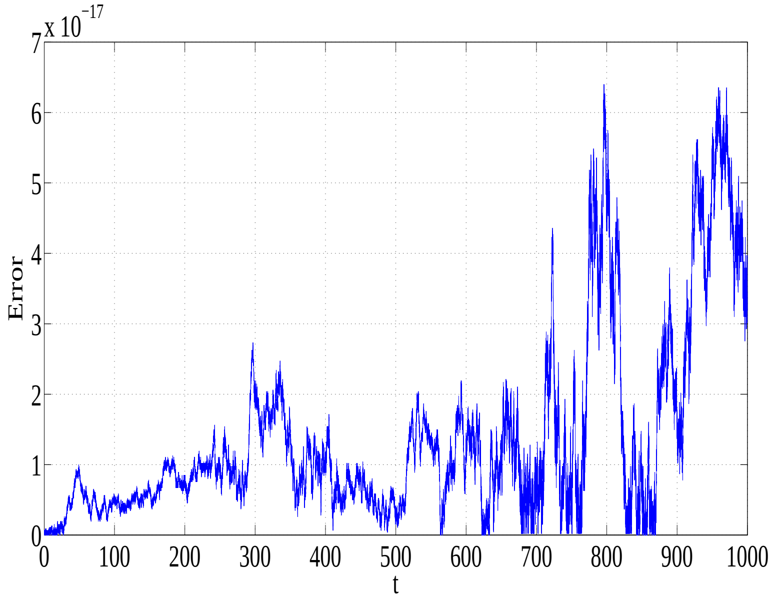

Figure 5.23: Error in integral $I_{2,2}$ of coupled Harmonic oscillator using Gauss-2 method.

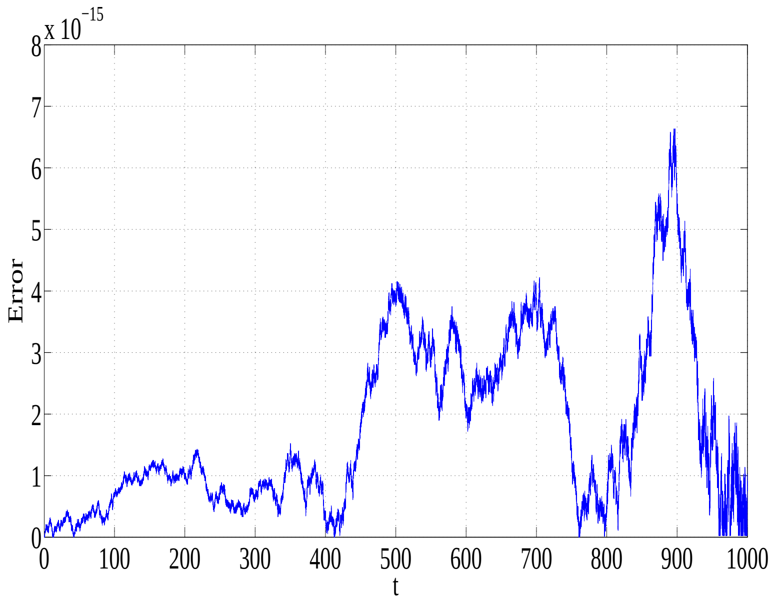

Figure 5.24: Error in integral $I_{3,1}$ of coupled Harmonic oscillator using Gauss-2 method.

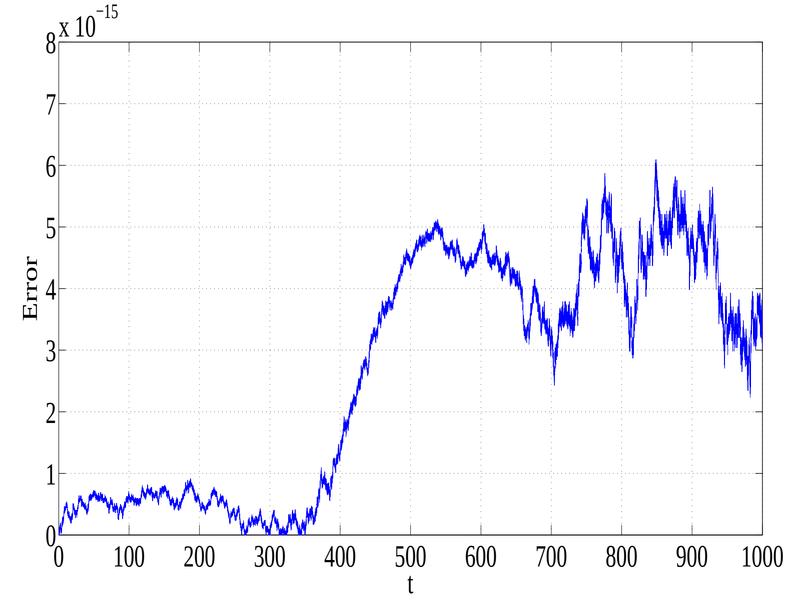

Figure 5.25: Error in integral $I_{3,2}$ of coupled Harmonic oscillator using Gauss-2 method.

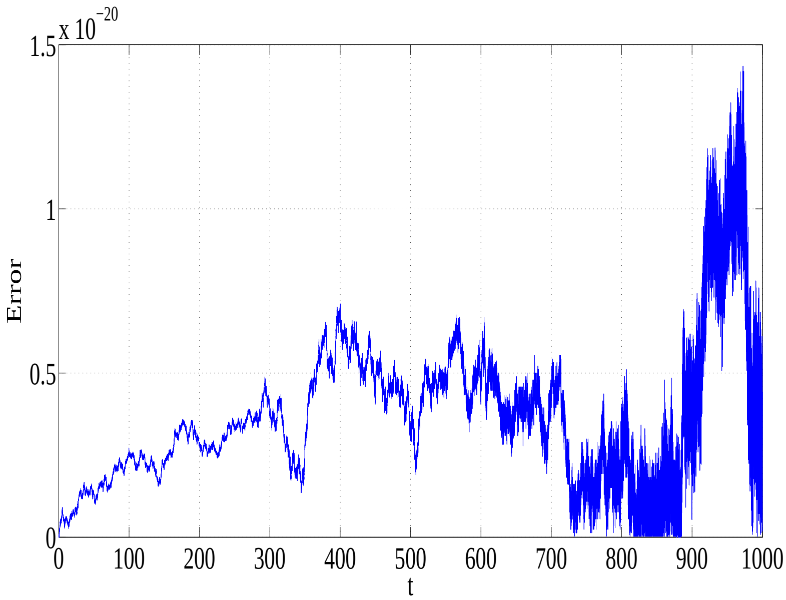

Figure 5.26: Error in integral $I_{4,1}$ of coupled Harmonic oscillator using Gauss-2 method.

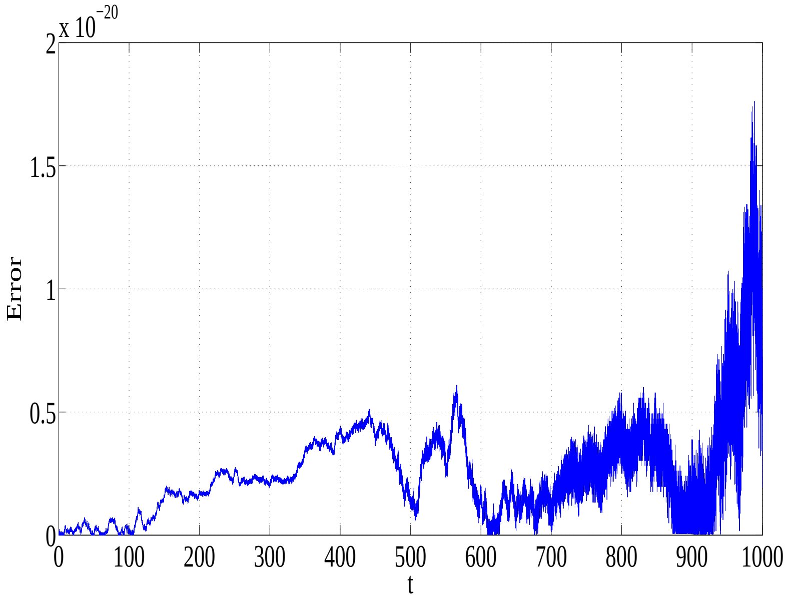

Figure 5.27: Error in integral $I_{4,2}$ of coupled Harmonic oscillator using Gauss-2 method.

Chapter 6

Conclusion

In this thesis, we have studied numerical preservation of first integrals of Hamiltonian systems. We have used classical Noether theorem to calculate Noether symmetries and associated first integrals of Hamiltonian systems. We have evaluated first integrals of Simple pendulum, Kepler problem, Henon-Heiles problem and Harmonic oscillator by using Noether approach. Then we have extended our work by using complex symmetry method to calculate first integrals of system of Harmonic oscillators. Furthermore, it is seen that the two dimensional coupled Harmonic oscillators can be represented by one restricted complex ordinary differential equation. We have determined Noether-like symmetries and associated first integrals corresponding to uncoupled and coupled two dimensional system of Harmonic oscillators.

In these cases, we observe that amongst five first integrals of one dimensional Harmonic oscillator only two first integrals I_2 and I_3 are independent. The other three first integrals which are I_1, I_4 and I_5 can be written as linear combination of these two integrals. Similarly for the complex case, amongst ten first integrals, only four first integrals are independent for each system of equations.

Since we are interested in the numerical conservation of the first integrals of Hamiltonian systems, we have taken order four symplectic Runge-Kutta method for the integration. These first integrals are quadratic in nature, so symplectic Runge-Kutta method has successfully been used. Through this approach, a good long time preservation of the first integrals of single as well as system of Harmonic oscillators is observed.

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