Experimental Behaviour of some Symplectic and G-symplectic Methods for the Numerical Solution of Conservative Systems

By

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Dedicated

To My Parents

Acknowledgements

Praise is to Allah Almighty, the Kind and the Compassionate, who created us and blessed us with intellect so that we can discover and serve his creations. I humbly bow my head before ALMIGHTY ALLAH, Who bestowed on me His blessings and gave me courage to present this piece of work. I invoke peace for Holy Prophet HAZRAT MUHAMMAD (PBUH) who is forever a torch of guidance for humanity as whole.

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Abstract

Hamiltonian equations define a range of physical systems like planetary motion, Harmonic Oscillator and many more. Numerical methods provide an approximate flow of these Hamiltonian equations.

For the solution of Hamiltonian systems, one should use numerical methods that preserve the qualitative features of such systems like energy and symplecticity of the flow. In this thesis, we investigate symplectic and G-symplectic numerical methods for Hamiltonian systems. In addition, we experiment with composition of different G-symplectic methods to avoid parasitic corruption of numerical solution that arises due to the multivalue nature of the general linear methods.

Contents

Chapter 1

Introduction

Ordinary differential equations model the behaviour of a function of one or more variables. In real world, many problems of science and engineering are modeled as systems of ordinary differential equations (ODEs). A first order ordinary differential equation (ODE) with the initial condition is of the form,

$$y' = f(x, y(x)), \qquad y(x_0) = y_0, \tag{1.1}$$

where the y' denotes the derivative of the function with respect to x.
If the time variable x is taken as a component of y, the ODE becomes autonomous,

$$y' = f(y(x)), \qquad y(x_0) = y_0. \tag{1.2}$$

The existence and uniqueness of the solution of an ODE is very important and is given by the Lipschitz condition [2].

Definition : A function g satisfies the Lipschitz condition if for all a,$b \in R^N$, there exist a Lipschitz constant L s.t

$$||g(a) - g(b)|| \leq L||a - b||,$$

where $||.||$ is a norm on R^N.
Most of the time we cannot find the exact solutions of the differential equations, so there is a need of finding approximate solutions using numerical methods. While talking about the solution of ODE by using numerical methods, we divide the methods into one-step methods, multi-step methods and general linear methods. We will

discuss one-step methods in Chapter 2 and general linear methods in Chapter 3 respectively in detail, however a brief introduction is provided here.

Conceptually in numerical methods, we require the value of unknown function at an initial point and this will lead us to find the solution at the next point and so on. One step methods such as Euler method just need value of a function at a particular point and its derivatives to determine the function value at next point [10–12]. In other words, at each step the solution point is treated as an initial value problem.

$$y_{n+1} = y_n + hf(x_n, y_n). \tag{1.3}$$

The Euler method is the simplest example of a one-step method [14]. The Euler method is low order method, that is of order 1. Higher order one step methods include Runge–Kutta methods which will be discussed later in the thesis but a general form is given as

$$Y_s = y_n + h\sum_{j=1}^{i-1} a_{ij} f(Y_j), \qquad i = 1, 2, \ldots, s \tag{1.4}$$

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f(Y_i). \tag{1.5}$$

Here Y_i are the stages calculated at c_i (nodes), b_i are the weights anda_{ij} is the coefficient matrix for the RK method. In these methods before taking the next step, we ignore all the previous information. We have many more methods such as Adams–Bashforth and Adams–Moulton methods, which are multi-step methods. Multi-step methods use all the previous information for their solution [6, 9]. It means that multi-step methods require values of the function and their derivatives at several points. In case of linear multi-step methods, a linear combination of the values of the function and its derivatives at several points are taken in account.

A general linear method is a multivalue and multiderivative method which is of the form

$$Y = hAf(Y^n) + Uy^{[n-1]} \tag{1.6}$$

$$y^{[n]} = hBf(Y^n) + Vy^{[n-1]} \tag{1.7}$$

Here we denote the output approximation by $y_i^{[n]}, i = 1, 2, \ldots, r$, evaluated from step number n, the stage values by $Y_i^{[n]}, i = 1, 2, \ldots, s$ and the stage derivatives by

$f(Y_i^{[n]}), i = 1, 2, \ldots, s$. And A, B, U, V are the matrices representing a general linear method.

1.0.1 Hamiltonian System

The set of differential equations with Hamiltonian H define the Hamiltonian system, i.e.

$$p_i' = -\frac{\partial H}{\partial q_i}, \qquad q_i' = \frac{\partial H}{\partial p_i}, \qquad i = 1, 2, \ldots, n, \tag{1.8}$$

where the p' and q' denotes the derivative of the function p and q with respect to x and q_i are generalized coordinates and p_i are generalized momenta. The Hamiltonian function was firstly introduced by Hamilton in 1824 [17, 19]. Hamiltonian systems posses the remarkable property of the conservation of energy

$$\begin{aligned} \frac{d}{dt}H(p,q) &= \frac{\partial H}{\partial p}p' + \frac{\partial H}{\partial q}q', \\ &= -\frac{\partial H}{\partial p}\frac{\partial H}{\partial q} + \frac{\partial H}{\partial q}\frac{\partial H}{\partial p} = 0. \end{aligned}$$

Thus

$$H(p(x), q(x)) = H(p(0), q(0)) = C.$$

1.0.2 Symlecticity

Hamiltonian systems have a remarkable property that their phase flow is symplectic [12]. This means that the oriented area founded by the vectors (p_i, q_i) of the Hamiltonian systems (1.8) is preserved. Let ψ_H is the solution operator of the Hamiltonian system(1.8) such that,

$$\psi_H : (p(0), q(0)) \mapsto (p(t), q(t)).$$

where

$$f = \begin{bmatrix} -\frac{\partial H}{\partial q} \\ \frac{\partial H}{\partial p} \end{bmatrix}$$

which is true for the Hamiltonian system (1.8). We see that for the Hamiltonian system (1.8),

$$div f = 0.$$

Therefore ψ_H is symplectic. Consider an area A of phase space defined by the vectors (p_i, q_i). If the system evolves over some period of time, then we see that the area of the elements of phase space is conserved along the motion of the system as shown in the Figure 1.1.

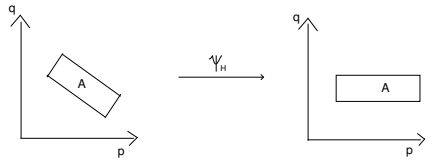

Figure 1.1: Area preservation

In fact, it can be shown that area of phase space elements are conserved for all Hamiltonian systems.

1.0.3 Symplectic Integrators

Symplectic integrators are actually the numerical methods which are especially designed for the solution of the Hamiltonian systems. A numerical method is called symplectic if when applied to Hamiltonian systems, it generates numerical solution which inherits the property of symplecticness [15]. In this thesis, we consider RK methods and General Linear method to be symplectic. These symplectic methods can be applied to general system of differential equations of Hamiltonian systems and achieve symplecticness.

1.0.4 Linear and Quadratic invariants

Hamiltonian systems are among those differential equations where the solution possesses invariants. Consider an initial value problem

$$y' = f(y(x)), \qquad y(x_0) = y_0. \tag{1.9}$$

A non constant function $F(y)$ is called first integral of (1.9) if

$$F'(y)f(y) = 0, \qquad \forall y.$$

This implies every solution $y(x)$ of (1.9) satisfies

$$F(y(x)) = F(y_0) = Constant.$$

Synonymously with "first integral", the terms, linear invariant or conserved quantity or constant of motion are used. Consider a quadratic function,

$$C(y) = y^T S y,$$

where S is a symmetric square matrix. $C(y)$ is a quadratic invariant of (1.9) if

$$y^T S f(y) = 0, \qquad \forall y.$$

1.0.5 Simple Pendulum

A Simple Pendulum consists of a bob (point mass) m suspended from a rigid point. When the bob is moved little aside from the equilibrium and released, it execute Simple Harmonic Motion (SHM) about the equilibrium position. The distance of the bob from the point of suspension is fixed l (length of the massless rod) and the generalized coordinate is the angle q.

Considering the reference level for zero potential energy as a horizontal plane passing through the point of suspension, the set of differential equations with Hamiltonian H defines the Hamiltonian system as

$$p' = -\frac{\partial H}{\partial q} = -\sin(q), \qquad q' = \frac{\partial H}{\partial p} = p, \tag{1.10}$$

where H denotes the total energy conserved in Simple Pendulum and is given as

$$H = \frac{p^2}{2} - \cos(q). \tag{1.11}$$

The symplectic nature of the Simple Pendulum can be seen by applying the symplectic Implicit RK method on eq(1.14). The result is shown in the Figure 1.2. It is a circular region and preserves the area.

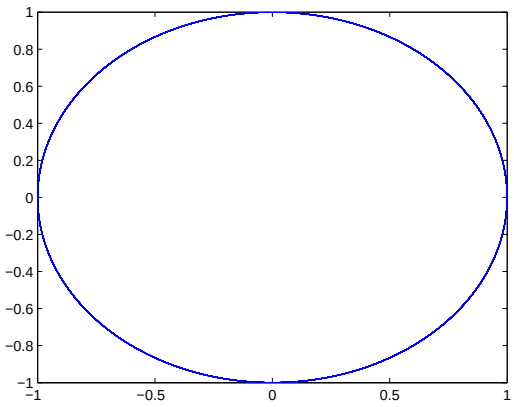

Figure 1.2: Symplecticity of Implicit RK for Simple pendulum

Chapter 2

Runge-Kutta Method

Runge–Kutta methods belong to the family of one step methods. By solving the ODE (1.1), these methods will give us approximations y_{n+1} in terms of y_n only, and thus they produce a one-dimensional map. The RK methods consist of implicit and explicit iterative methods for the numerical solutions of ODEs [1,3,4]. These methods were first introduced by the German mathematicians *C.Runge* and *M.W.Kutta* in 1900. A general form of s-stage explicit RK method is given as

$$Y_i = y_n + h\sum_{j=1}^{i-1} a_{ij} f(x_n + c_j h, Y_j), \qquad i = 1, 2, \ldots, s, \tag{2.1}$$

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f(x_n + c_i h, Y_i). \tag{2.2}$$

where a_{ij} is matrix of non zero coefficients, c_i are the nodal points, b_i are the RK weights. It is convenient to represent a RK method by a tableau of the form given below which is called the Butcher's tableau,

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} = \begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \ldots & a_{1s} \\ c_2 & a_{12} & a_{22} & \ldots & a_{2s} \\ \vdots & \vdots & \vdots & \ldots & \vdots \\ \hline & b_1 & b_2 & \ldots & b_s \end{array}$$

where

a_{ij} : RK cofficients

b_i : RK wights

c_i : RK nodes

$$i, j = 1, 2, \ldots, s$$

stages of RK method.

Since RK methods are classified as explicit and implicit methods, but because of the stability limitations, explicit RK method are less applicable. Also explicit RK method cannot efficiently solve Hamiltonian systems when they are not in separable form.

2.0.6 Implicit Runge–Kutta Methods

The Implicit RK methods are obtained from the famous Guass–Legendre formulae by choosing the c_i's as zeroes of the shifted Guass–Legendre Polynomial $P(x)$ on $[0, 1]$, where

$$P\ (x) = \frac{s!}{2s} \sum_{r=0}^{s} (-1)^{s-r} \begin{pmatrix} s \\ r \end{pmatrix} \begin{pmatrix} s+r \\ r \end{pmatrix} x^r.$$

For $s = 1$, we have

$$P\ (x) = -\frac{1}{2} + x,$$

which has root

$$c = \frac{1}{2}.$$

Thus we get 1 stage Implicit RK method of order 2 as

$$\begin{array}{c|cc} \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Now choose $s = 2$, we have

$$P\ (x) = x^2 - x + \frac{1}{6},$$

which has roots

$$c = \frac{1}{2} - \frac{\sqrt{3}}{6}, \qquad \frac{1}{2} + \frac{\sqrt{3}}{6}.$$

And we have 2 stage Implicit RK method of order 4. Its Butcher's tableau is

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

2.0.7 Order Conditions for Runge–Kutta Methods

To check the order of a Runge–Kutta method, one has to compare the numerical solution with the Taylor series expansion of the exact solution. Here we obtained the order of a Runge–Kutta method by using explicit method and further use it for the Implicit method [8, 18]. To find the order of a Runge–Kutta method we first introduce the concept of Elementary Differentials, that is

$$y' = f, \tag{2.3}$$

$$y'' = f_x + f f_y = f'f, \tag{2.4}$$

$$y''' = f_{xx} + 2f f_{xy} + f^2 f_{yy} + f f_y^2 = f''(f,f) + f'f'f. \tag{2.5}$$

where $f'f$, $f'f'f$, etc are called Elementary differentials.
Now we consider the general form of explicit RK method for solving autonomous system of ODEs.

$$Y_i = y_n + h\sum_{j=1}^{i-1} a_{ij} f(x_n + c_j, hY_j), \qquad i = 1, 2, \ldots, s. \tag{2.6}$$

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f(x_n + c_i h, Y_i). \tag{2.7}$$

For three stages, $s = 3$

$$Y_1 = y_n, \tag{2.8}$$

$$Y_2 = y_n + h a_{21} f(Y_1), \tag{2.9}$$

$$Y_3 = y_n + h a_{31} f(Y_1) + h a_{32} f(Y_2). \tag{2.10}$$

We have to find $f(Y_2)$,

$$f(Y_2) = f(y_n + h a_{21} f(y_n)), \tag{2.11}$$

$$= f(y_n) + h a_{21} f'f(y_n) + \frac{h^2}{2!} a_{21} f''f(y_n) + O(h^3). \tag{2.12}$$

Therefore,

$$Y_3 = y_n + ha_{31}f(y_n) + ha_{32}f(y_n) + h^2a_{32}a_{21}f'f(y_n) + \tfrac{h^3}{2}a_{32}a_{21}f''f(y_n) + O(h^3), \tag{2.13}$$

The output value is

$$y_{n+1} = y_n + hb_1f(Y_1) + hb_2f(Y_2) + hb_3f(Y_3), \tag{2.14}$$

using the values of $f(Y_1), f(Y_2)$ and $f(Y_3)$ and on simplifying them we get

$$y_{n+1} = y_n + h(b_1 + b_2 + b_3)f(y_n) + h^2(b_2c_2 + b_3c_3)f'f(y_n) + h^3(\tfrac{1}{2}(b_2c_2^2 + b_3c_3^2)f^{(2)}ff(y_n) + b_3a_{32}c_2f'ff') + O(h^4). \tag{2.15}$$

Now we compare (2.15) with the Taylor series of exact solution given as,

$$y_{n+1} = y(x_n + h) = y(x_n) + hy'(x_n) + \frac{h^2}{2!}y^{(2)}(x_n) + \frac{h^3}{3!}y^{(3)}(x_n) + O(h^4).$$

and get

$$b_1 + b_2 + b_3 = 1, \tag{2.16}$$

which is condition of 1^{st} order.

Further,

$$b_2c_2 + b_3c_3 = \frac{1}{2}, \tag{2.17}$$

is conditions for $2nd$ order.

And

$$b_2c_2^2 + b_3c_3^2 = \frac{1}{3}, \tag{2.18}$$

$$b_3a_{32}c_2 = \frac{1}{6}. \tag{2.19}$$

are conditions for $3rd$ order. In general for an RK method to achieve order 3, it must satisfies

$$\sum_{i=1}^{3} bi = 1, \tag{2.20}$$

$$\sum_{i=1}^{3} b_ic_i = \frac{1}{2}, \tag{2.21}$$

$$\sum_{i=1}^{3} b_ic_i^2 = \frac{1}{3}, \tag{2.22}$$

$$\sum_{i=1}^{3} b_ia_{ij}c_j = \frac{1}{6}. \tag{2.23}$$

2.0.8 Order Conditions in Terms of Trees

Trees play an important role in the numerical methods for solving ODEs. Introducing the concept of tress along the formulation of order conditions of the differential equations. There is a difficulty in obtaining order conditions for higher orders by usual method, so for avoiding this problem there is a tree-based approach for investigating the order of various methods.

Tree:A tree is a connected graph with no cycles. If we fix one vertex as a root we get a rooted tree. Number of vertices of a tree is called the order of a tree. It is denoted by $r(t)$. Examples of trees are given in Figures 2.1, 2.2, 2.3, 2.4.

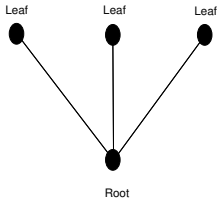

Figure 2.1: A Tree of order 4

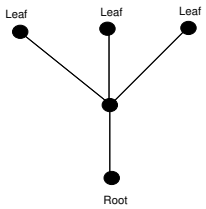

Figure 2.2: A Tree of order 5

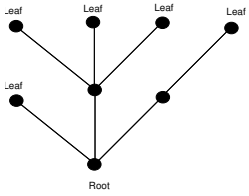

Figure 2.3: A Tree of order 8

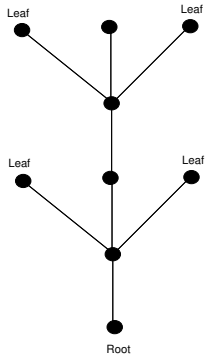

Figure 2.4: A Tree of order 9

Density: It is the product of the order of tree and the order of subtrees when the root is chopped off. It is denoted by γ. Consider the tree in Figure 2.5. Its density is $\gamma(t) = 4.3.1.1 = 12$.

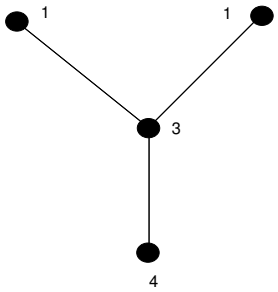

Figure 2.5: Tree

Elementary weights: Elementary weights are algebraic expressions involving the coefficients of an RK method. Elementary weights has an important relation with the order of the RK method, by which one can easily find an order of any tree.

Theorem: If $y(x)$ is k-times differentiable then

$$\frac{d^k y}{dx^k} = y^k(x) = \sum \alpha(t) F(t)(y(x)). \tag{2.24}$$

If we put $k = 1$ in the above relation, then we have

$$y'(x) \quad = \quad \sum \alpha(t) F(t)(y(x)). \tag{2.25}$$

If we consider the Taylor series of RK method

$$y(x_{n+1}) = y(x_n) + hy'(x_n) + h^2/2!y^{(2)}(x_n) + \ldots + O(h^{p+1}), \quad (2.26)$$

$$= y(x_n) + \sum h^k/k!y^k(x_n) + O(h^{p+1}), \quad (2.27)$$

using (2.24) in (2.26), we have

$$= y(x_n) + \sum h^k/k! \sum \alpha(t)F(t)(y(x_n)) + O(h^{p+1}), \quad (2.28)$$

$$= y(x_n) + \sum h^{r(t)}1/(\sigma(t)\gamma(t))F(t)(y(x_n)) + O(h^{p+1}), \quad (2.29)$$

which is the Taylor series of the exact solution in terms of elementary differentials. The RK method written in terms of elementary weights is given by the formula

$$y_{n+1} = y_n + \sum \varphi(t)/\sigma(t)h^{r(t)}F(t)(y_n) + O(h^{p+1}). \quad (2.30)$$

Compare equations (2.28), (2.29)

$$\varphi(t) = \frac{1}{\gamma(t)}.$$

This is the order condition for the RK method.

Consider a tree in Figure 2.6. The elementary weight is

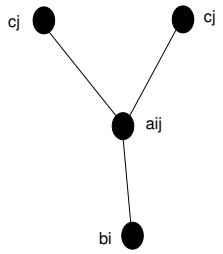

Figure 2.6: Tree of Order 4

$$\varphi(t) = b_i a_{ij} c_j^2.$$

And the density is

$$\gamma(t) = \frac{1}{12}.$$

So the order condition for the tree in Figure 2.6 is

$$b_i a_{ij} c_j^2 = 12.$$

2.0.9 Symplectic Runge–Kutta Method

Hamiltonian systems posses the property of energy conservation and symplecticity. Standard numerical methods fall short preserving these properties when numerically solving hamiltonian system. Therefore, we need symplectic RK methods. Consider an initial value problem

$$y' = f(y(x)), \qquad y(x_0) = y_0.$$

To check whether the RK method is preserving symplecticity or in other words it is quadratic invariant or not, we proceed as follows.
For a conservative system,

$$< Y_i, f(Y_i) > \;=\; 0, \tag{2.31}$$

$$< y_0 + h\sum_{i=1}^{s} a_{ij} f(Y_j), f(Y_i) > \;=\; 0, \tag{2.32}$$

$$< y_0, f(Y_i) > \;=\; -h\sum_{i,j=1}^{s} a_{ij} < f(Y_j), f(Y_i) > . \tag{2.33}$$

For the output value

$$y_i \;=\; y_0 + h\sum_{i=1}^{s} b_i f(Y_i). \tag{2.34}$$

For the numerical solution of RK methods to be symplectic, Consider

$$< y_1, y_1 > \;=\; < y_0 + h\sum_{i=1}^{s} b_i f(Y_i), y_0 + h\sum_{j=1}^{s} b_j f(Y_j) >, \tag{2.35}$$

or

$$\begin{aligned} < y_1, y_1 > =& < y_0, y_0 > + h\textstyle\sum_{i=1}^{s} b_i < y_0, f(Y_i) > + h\sum_{j=1}^{s} b_j < f(Y_j), y_0 > \\ &+ h^2 \textstyle\sum_{i,j=1}^{s} b_i b_j < f(Y_i), f(Y_j) >. \end{aligned} \tag{2.36}$$

Using (2.32) in (2.35) we have,

$$\begin{aligned} < y_1, y_1 > =& < y_0, y_0 > + h\textstyle\sum_{i=1}^{s} b_i(-h)\sum_{i,j=1}^{s} a_{ij} < f(Y_j, f(Y_i) > \\ &+ h\textstyle\sum_{j=1}^{s} b_j(-h)\sum_{i,j=1}^{s} a_{ij} < f(Y_i), Y_j) > \\ &+ h^2 \textstyle\sum_{j=1}^{s} b_i b_j < f(Y_i), f(Y_j) >, \end{aligned} \tag{2.37}$$

or

$$< y_1, y_1 > \;=\; < y_0, y_0 > -h^2 \sum_{i,j=1}^{s} [b_i a_{ij} + b_j a_{ji} - b_i b_j] < f(y_i), f(y_j) > . \tag{2.38}$$

For the symplecticity, we must have

$$b_i a_{ij} + b_j a_{ji} - b_i b_j \quad = \quad 0. \tag{2.39}$$

The RK method with above property is called symplectic RK method.

2.0.10 Order Conditions for symplectic Runge–Kutta Method

To obtain the order conditions for symplectic Runge–Kutta method, consider two special types of trees as

- Superfluous trees
- Non-Superfluous trees

A tree is called superfluous if it generates identical rooted tree when any two adjacent nodes of trees are taken as a root. Otherwise it is said to be non-superfluous tree. In example of a tree of order 4, given in Figure 2.7. If we consider nodes b and c as a root, both approaches will generate same rooted trees and that is why the underlying tree is called superfluous tree.

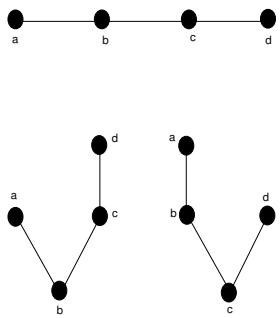

Figure 2.7: Tree

Let us consider a tree of order 4, as shown in Figure 2.8. By considering the nodes a and b as roots, it will generate different rooted trees as shown in the figure, so the underlying tree is non-superfluous tree.

For symplectic RK method, the order conditions related to the superfluous trees are not required at all, while of all those related to non-superfluous trees, we need

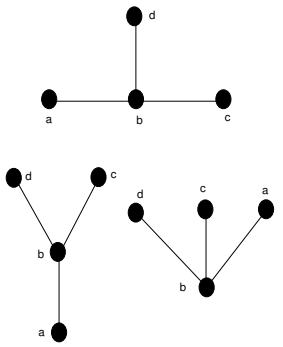

Figure 2.8: Tree

only one.

Let's discuss that how number of order conditions reduces in symplectic RK method. Suppose the method is of order at least 1, then it must satisfy

$$\sum_{i=1}^{s} b_i \quad = \quad 1. \tag{2.40}$$

Consider the symplectic condition and take summation

$$\sum_{i,j=1}^{s} b_i a_{ij} + \sum_{i,j=1}^{s} b_j a_{ji} - \sum_{i,j=1}^{s} b_i b_j \quad = \quad 0. \tag{2.41}$$

Then we have

$$\sum_{i,j=1}^{s} b_i a_{ij} \quad = \quad \frac{1}{2}. \tag{2.42}$$

The above equation is nothing but the $2nd$ order condition. Therefore for symplectic RK method the second order condition is automatically satisfied and hence not required.

Suppose the method is of order at least 2, then we have

$$\sum_{i=1}^{s} b_i c_i \quad = \quad \frac{1}{2}. \tag{2.43}$$

Consider the symplectic condition,

$$b_i a_{ij} + b_j a_{ji} - b_i b_j \quad = \quad 0, \tag{2.44}$$

Multiply with c_j and take summation,

$$\sum_{i.j=1}^{s} b_i a_{ij} c_j + \sum_{i,j=1}^{s} b_j c_j a_{ji} - \sum_{i,j=1}^{s} b_i b_j c_j \quad = \quad 0, \tag{2.45}$$

Take $s = 1, 2$, the above equation becomes of the form

$$\begin{aligned} & b_1a_{11}c_1 + b_1a_{12}c_2 + b_2a_{21}c_1 + b_2a_{22}c_2 \\ & + b_1c_1a_{11} + b_1c_1a_{12} + b_2c_2a_{21} + b_2c_2a_{22} \\ & - b_1b_1c_1 - b_1b_2c_2 - b_2b_1c_1 - b_2b_2c_2 = 0. \end{aligned} \tag{2.46}$$

Now again consider the symplectic condition

$$b_ia_{ij} + b_ja_{ji} - b_ib_j \;\; = \;\; 0, \tag{2.47}$$

For two stages, the matrix form of symplectic condition is

$$G = \begin{bmatrix} b_1a_{11} + b_1a_{11} - b_1b_1 & b_1a_{12} + b_2a_{21} - b_1b_2 \\ b_2a_{21} + b_1a_{12} - b_2b_1 & b_2a_{22} + b_2a_{22} - b_2b_2 \end{bmatrix}$$

multiply with c_j, where $j = 1, 2$,

$$G = \begin{bmatrix} b_1a_{11} + b_1a_{11} - b_1b_1 & b_1a_{12} - b_2a_{21} + b_1b_2 \\ b_2a_{21} + b_1a_{12} - b_2b_1 & b_2a_{22} - b_2a_{22} + b_2b_2 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

or

$$G = \begin{bmatrix} 2b_1a_{11}c_1 - b_1^2c_1 & b_1a_{12}c_2 + b_2a_{21}c_2 - b_1b_2c_2 \\ b_2a_{21}c_1 + b_1a_{12}c_1 - b_2b_1c_1 & 2b_2a_{22} - b_2^2c_2 \end{bmatrix}$$

Taking sum of rows and columns, we get the equation of the form

$$2b_1a_{11}c_1 - b_1^2c_1 + b_1a_{12}c_2 + b_2a_{21}c_2 - b_1b_2c_2 + b_2a_{21}c_1 + b_1a_{12}c_1 - b_2b_1c_1 + 2b_2a_{22} - b_2^2c_2 \;\; = \;\; 0,$$

The above equation is as same of equation (2.46). For the $3rd$ order conditions, consider the symplectic condition, multiply with c_j, take summation and use (2.39) and (2.41), we have

$$\sum_{i,j=1}^{s} b_ia_{ij}c_j + \sum_{i,j=1}^{s} b_jc_ja_{ji} - \sum_{i,j=1}^{s} b_ib_jc_j \;\; = \;\; 0, \tag{2.48}$$

$$\sum_{i,j=1}^{s} b_ia_{ij}c_j + \sum_{j=1}^{s} b_jc_jc_j - \frac{1}{2} \;\; = \;\; 0, \tag{2.49}$$

$$\sum_{i,j=1}^{s} b_ia_{ij}c_j + \sum_{j=1}^{s} b_jc_{j^2} - (\frac{1}{6} + \frac{1}{3}) \;\; = \;\; 0, \tag{2.50}$$

$$(\sum_{i,j=1}^{s} b_ia_{ij}c_j - \frac{1}{6}) + (\sum_{j=1}^{s} b_jc_{j^2} - \frac{1}{3}) \;\; = \;\; 0. \tag{2.51}$$

If

$$\Sigma b_i a_{ij} c_j - \frac{1}{6} = 0, \tag{2.52}$$

is satisfied, the other condition

$$\Sigma b_i c_{j^2} - \frac{1}{3} = 0, \tag{2.53}$$

is automatically satisfied.
The equations (2.52) and (2.53) represents the order conditions for order 3, so for order 3 we need only one condition out of the two conditions.

Notice that the number of order conditions for symplectic RK method is less than the number of order conditions for a general RK method, as shown in Table.

That is the symplectic RK method requires less number of conditions, as order progresses, as compared to the non-symplectic RK method.

Order	General RK method	Symplectic RK method
1	1	1
2	2	1
3	4	2
4	8	3
5	17	6

Order conditions for general and symplectic RK method up to order 5.

Chapter 3

General Linear Methods

A general linear method (GLM) is a multistep multivalue method for the numerical solution of initial value problem and is a generalization of linear multistep and Runge–Kutta methods. It was introduced by *Gragg* and *Stetter* in 1964 [5,6,9].The main characteristic of General linear method (GLM) is that stage derivatives are evaluated along the stages within the steps. These are methods where a collection of vectors forms the input at the beginning of step and a similar collection is passed on as output from the current step. Let us denote the output approximation by $y_i^{[n]}, i = 1, 2, \ldots, r$, evaluated from step number n, the stage values by $Y_i^{[n]}, i = 1, 2, \ldots, s$ and the stage derivatives by $f(Y_i^{[n]}), i = 1, 2, \ldots, s$.

At the starting, the quantities denoted by $y_i^{[n-1]}, i = 1, 2, \ldots, r$, are available from approximations computed in step $n - 1$.

Let h be the stepsize, then for the convenience we have

$$y^{[n-1]} = \begin{bmatrix} y_1^{[n-1]} \\ y_2^{[n-1]} \\ \vdots \\ y_r^{[n-1]} \end{bmatrix}, y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix}, hf(Y) = \begin{bmatrix} hf(Y_1^{[n]}) \\ hf(Y_2^{[n]}) \\ \vdots \\ hf(Y_r^{[n]}) \end{bmatrix},$$

The general form of GLM is given as

$$Y = hAf(Y^n) + Uy^{[n-1]}$$
$$y^{[n]} = hBf(Y^n) + Vy^{[n-1]},$$

where $\begin{bmatrix} A & B & U & V \end{bmatrix}$ completely defines a GLM.

3.0.11 Runge–Kutta Method as General Linear Method

RK methods can easily be written as GLM. The matrix A is same as that of matrix of RK methods. The matrix B is b^T, where b is the vector of RK method [21]. We assume that the input vector is an approximation to $y(x_{n-1})$. As an example we consider a general 2nd order RK method as

$$Y_1 = ha_{11}f(Y_1) + ha_{12}f(y_2) + y_0, \tag{3.1}$$

$$Y_2 = ha_{21}f(Y_1) + ha_{22}f(y_2) + y_0, \tag{3.2}$$

$$y_1 = hb_1f(Y_1) + h_2f(y_2) + y_0. \tag{3.3}$$

Since RK methods have single input, by taking U=1 and V=1, it takes the form of a GLM as

$$\left[\begin{array}{cc|c} a_{11} & a_{12} & 1 \\ a_{21} & a_{22} & 1 \\ \hline b_1 & b_2 & 1 \end{array}\right]$$

In general we have the form, which as

$$\left[\begin{array}{cccc|c} a_{11} & a_{12} & \dots & a_{1s} & 1 \\ a_{21} & a_{22} & \dots & a_{2s} & 1 \\ \vdots & \vdots & \dots & \vdots & \vdots \\ a_{s1} & a_{s2} & \dots & a_{ss} & 1 \\ \hline b_1 & b_2 & \dots & b_s & 1 \end{array}\right]$$

3.0.12 Concept of G-symplecticity

Symplecticity is a property of Hamiltonian system which is maintained by one step methods so as with RK methods. Multistep multiderivative methods cannot posses the symplectic property, until they can acquire just one value of the current step from the previous one, means the GLM is reduced to RK method [20].

By the symplectic behaviour, we mean that the inner product of the values at the initial point is same as the inner product of the values at the later point. In GLM we have multiple inputs with multiple outputs. To accommodate them, we introduce a G-matrix and define a G-norm as

$$||y||_G^2 =< y, y >_G= \sum_{i,j=1}^{r} g_{i,j} < y_i, y_j >, \tag{3.4}$$

where g_{ij} is the ij^{th} entry of matrix G. Also we have a diagonal sxs matrix $D = d_i$ such that

$$< y^{[n]}, y^{[n]} >_G \;\; = \;\; < y^{[n-1]}, y^{[n-1]} >_G + 2h \sum d_i < Y_i, F_i > . \tag{3.5}$$

For the conservation, we must have

$$< y^{[n]}, y^{[n]} >_G \;\; = \;\; < y^{[n-1]}, y^{[n-1]} >_G, \tag{3.6}$$

means that

$$2h \sum d_i < Y_i, F_i >= 0.$$

Theorem 1: A GLM is said to be G-symplectic if we have a symmetric matrix G and a diagonal matrix D s.t

$$G = V^T G V$$
$$DU = B^T G V$$
$$DA + A^T D = B^T G B$$

It should be noted that GLM cannot posses true quadratic invariants and hence cannot be symplectic. However, GLM can preserve quadratic behaviour of invariants in a G-norm and such a GLM is called a G-symplectic GLM [13].

Example: Consider an example of G-symplectic general linear method,

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{cc|cc} \frac{3-\sqrt{3}}{6} & 0 & 1 & -\frac{3-2\sqrt{3}}{3} \\ \frac{\sqrt{3}}{3} & \frac{3-\sqrt{3}}{6} & 1 & \frac{3-2\sqrt{3}}{3} \\ \hline \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & -1 \end{array}\right].$$

This method is G-symplectic with

$$G = \begin{bmatrix} 1 & 0 \\ 0 & \frac{3-2\sqrt{3}}{3} \end{bmatrix}$$

and

$$D = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}$$

We have

$$< y_1^{[n]}, y_1^{[n]} >_G \;=\; < y_1^{[n-1]}, y_1^{[n-1]} >_G . \tag{3.7}$$

$$\sum_{i,j=1}^{2} g_{i,j} < y_i^{[n]}, y_j^{[n]} >_G \;=\; \sum_{i,j=1}^{2} g_{i,j} < y_i^{[n-1]}, y_j^{[n-1]} >_G . \tag{3.8}$$

$$\begin{aligned} g_{11} < y_1^{[n]}, y_1^{[n]} > + g_{22} < y_2^{[n]}, y_2^{[n]} > = g_{11} < y_1^{[n-1]}, y_1^{[n-1]} > \\ + g_{22} < y_2^{[n-1]}, y_2^{[n-1]} >, \end{aligned} \tag{3.9}$$

where $g_{11} = 1$ and $g_{22} = \frac{3-2\sqrt{3}}{3}$, Therefore, instead of preserving true quadratic behaviour

$$< y_1^{[n]}, y_1^{[n]} > \;=\; < y_1^{[n-1]}, y_1^{[n-1]} > . \tag{3.10}$$

The linear combination

$$\begin{aligned} < y_1^{[n]}, y_1^{[n]} > + \tfrac{3-2\sqrt{3}}{3} < y_2^{[n]}, y_2^{[n]} > = < y_1^{[n-1]}, y_1^{[n-1]} > \\ + \tfrac{3-2\sqrt{3}}{3} < y_2^{[n-1]}, y_2^{[n-1]} > \end{aligned} \tag{3.11}$$

is preserved.

3.0.13 Methods

As it is mentioned earlier that a GLM consists of multiple vectors as inputs and outputs. Generally in ODE's, we always have an initial condition from where we get an initial value. In dealing with GLM, one value is obtained from the initial condition and the remaining values are obtained by applying a starting method. Here we consider two methods naming P method and N method along with their starting methods,

P Method:

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{cc|cc} \frac{3+\sqrt{3}}{6} & 0 & 1 & -\frac{3+2\sqrt{3}}{3} \\ -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 & \frac{3+2\sqrt{3}}{3} \\ \hline \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & -1 \end{array}\right].$$

The starting method is

$$\left[\begin{array}{cc|c} \frac{3+\sqrt{3}}{6} & 0 & 1 \\ -\frac{3+\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 \\ \hline 0 & 0 & 1 \\ \frac{\sqrt{3}-1}{8} & -\frac{\sqrt{3}-1}{8} & 0 \end{array}\right].$$

N Method:

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{cc|cc} \frac{3-\sqrt{3}}{6} & 0 & 1 & -\frac{3-2\sqrt{3}}{3} \\ \frac{\sqrt{3}}{3} & \frac{3-\sqrt{3}}{6} & 1 & \frac{3-2\sqrt{3}}{3} \\ \hline \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & -1 \end{array}\right].$$

The starting method is

$$\left[\begin{array}{cc|c} \frac{3-\sqrt{3}}{6} & 0 & 1 \\ -\frac{3-\sqrt{3}}{3} & \frac{3-\sqrt{3}}{6} & 1 \\ \hline 0 & 0 & 1 \\ -\frac{\sqrt{3}+1}{8} & -\frac{\sqrt{3}+1}{8} & 0 \end{array}\right].$$

It should be noted that the methods we considered above are G-symplectic methods. Consider P method

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{cc|cc} \frac{3+\sqrt{3}}{6} & 0 & 1 & -\frac{3+2\sqrt{3}}{3} \\ -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} & 1 & \frac{3+2\sqrt{3}}{3} \\ \hline \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & -1 \end{array}\right],$$

with

$$G = \begin{bmatrix} 1 & 0 \\ 0 & \frac{3+2\sqrt{3}}{3} \end{bmatrix},$$

and

$$D = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}.$$

For the method to be G-symplectic it should satisfied all the axioms of the Theorem 1 given above that is, $G = V^T GV, DU = B^T GV, DA + A^T D = B^T GB$.

Since

$$A = \begin{bmatrix} \frac{3+\sqrt{3}}{6} & 0 \\ -\frac{\sqrt{3}}{3} & \frac{3+\sqrt{3}}{6} \end{bmatrix},$$

$$B = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{bmatrix},$$

$$U = \begin{bmatrix} 1 & -\frac{3+2\sqrt{3}}{3} \\ 1 & \frac{3+2\sqrt{3}}{3} \end{bmatrix},$$

$$V = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

$$V^T GV = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}^T \begin{bmatrix} 1 & 0 \\ 0 & \frac{3+2\sqrt{3}}{3} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -\frac{3+2\sqrt{3}}{3} \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 \\ 0 & \frac{3+2\sqrt{3}}{3} \end{bmatrix} = G$$

So first condition is satisfied.

Now consider,

$$DU = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix} \begin{bmatrix} 1 & -\frac{3+2\sqrt{3}}{3} \\ 1 & \frac{3+2\sqrt{3}}{3} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1}{2} & -\frac{3+2\sqrt{3}}{6} \\ \frac{1}{2} & \frac{3+2\sqrt{3}}{6} \end{bmatrix}.$$

Now consider,

$$B^T GV = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{bmatrix}^T \begin{bmatrix} 1 & 0 \\ 0 & \frac{3+2\sqrt{3}}{3} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1}{2} & -\frac{3+2\sqrt{3}}{6} \\ \frac{1}{2} & \frac{3+2\sqrt{3}}{6} \end{bmatrix} = DU.$$

Second condition $DU = B^T GV$ is also satisfied.

Now consider,

$$DA + A^T D = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix} \begin{bmatrix} \frac{3+\sqrt{3}}{6} & 0 \\ -\frac{\sqrt{3}}{3} & -\frac{3-\sqrt{3}}{6} \end{bmatrix} + \begin{bmatrix} \frac{3+\sqrt{3}}{6} & 0 \\ -\frac{\sqrt{3}}{3} & -\frac{3-\sqrt{3}}{6} \end{bmatrix}^T \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix},$$

$$= \begin{bmatrix} \frac{3+\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} \\ -\frac{\sqrt{3}}{6} & \frac{3+\sqrt{3}}{6} \end{bmatrix}.$$

Now consider,

$$B^T G B = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{bmatrix}^T \begin{bmatrix} 1 & 0 \\ 0 & \frac{3+2\sqrt{3}}{3} \end{bmatrix} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} \end{bmatrix},$$

$$= \begin{bmatrix} \frac{3+\sqrt{3}}{6} & -\frac{\sqrt{3}}{6} \\ -\frac{\sqrt{3}}{6} & \frac{3+\sqrt{3}}{6} \end{bmatrix} = DA + A^T D.$$

This satisfies the third condition of the G-symplectic theorem.

Also N method is G-symplectic with

$$G = \begin{bmatrix} 1 & 0 \\ 0 & \frac{3-2\sqrt{3}}{3} \end{bmatrix},$$

and

$$D = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}.$$

3.0.14 Parasitic Solution

Consider the example of Simple Pendulum discussed in Chapter 1 to which we apply the P method with initial condition $p = 0, q = 1.5$ by taking stepsize 0.01 for 10^6 number of steps, we plot the graph between error and time. Along x-axis, we have time and at y-axis, we have error in energy. The result of energy conservation given in Figure 3.2 shows that error in energy is bounded by 10^{-4}, means that the behaviour of energy conservation is reasonable. On increasing the amplitude of the Simple Pendulum that is by changing the value of q from 1.5 to 2.4 the Figure 3.2 shows that the error has increased, so the energy is not conserved now.

Both the results are different from each other, it is clear that when we replace the value by $q = 2.3$, the error increases. By which we can say that, as the amplitude is increased, there is a complete change in results. And this change is because of parasitic effect. The parasitic effect is caused when the actual solution value is dominated by related parasitic value.

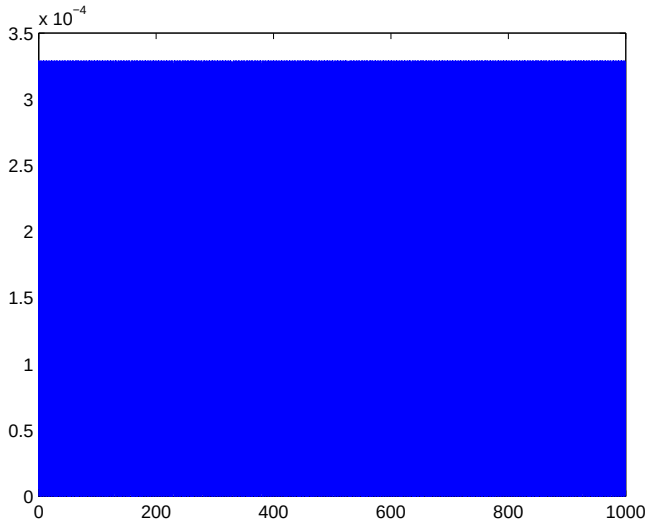

Figure 3.1: Error in Energy conservation of the Simple Pendulum for P method using q=1.5

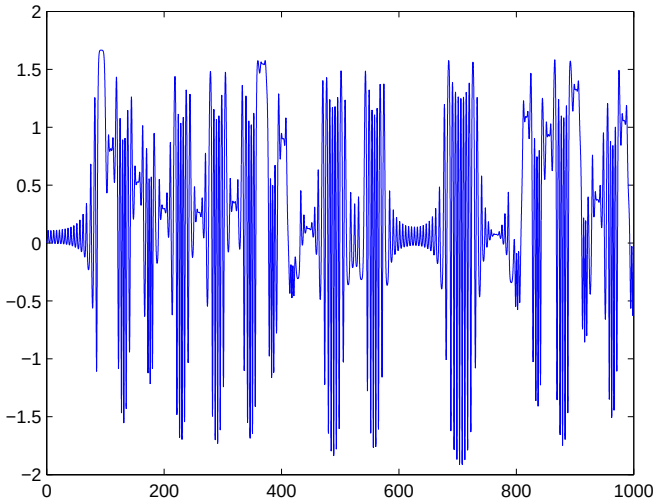

Figure 3.2: Error in Energy conservation of the Simple Pendulum for P method using q=2.3

We consider a typical step of the general linear method to study the effect of parasitism.

$$\left[\begin{array}{c} Y_1 \\ Y_2 \\ \hline y_1^{[1]} \\ y_2^{[1]} \end{array}\right] = \left[\begin{array}{cc|cc} a_{11} & a_{12} & u_{11} & u_{12} \\ a_{21} & a_{22} & u_{21} & u_{22} \\ \hline b_{11} & b_{12} & 1 & 0 \\ b_{21} & b_{22} & 0 & -1 \end{array}\right] \left[\begin{array}{c} hf(Y_1) \\ hf(Y_2) \\ \hline y_1^{[0]} \\ y_2^{[0]} \end{array}\right]$$

$$\begin{aligned} Y_1 &= ha_{11}F_1 + ha_{12}F_2 + u_{11}y_1^{[n-1]} + u_{12}y_2^{[n-1]}, \\ Y_2 &= ha_{21}F_1 + ha_{22}F_2 + u_{11}y_1^{[n-1]} + u_{12}y_2^{[n-1]}, \\ y_1^{[n]} &= hb_{11}F_1 + hb_{12}F_2 + y_1^{[n-1]}, \\ y_2^{[n]} &= hb_{11}F_1 + hb_{12}F_2 + y_2^{[n-1]}, \end{aligned}$$

where,

$$F_i = f(Yi).$$

Here $y_1^{[1]}$ approximates the exact solution, the second component $y_2^{[1]}$ approximates the second derivative [13]. To see how the $y_2^{[1]}$ can propagate a parasitic corruption, we introduce a change at the start of step,

$$y_2^{[n-1]} \to y_2^{[n-1]} + (-1)^{n-1}x_{n-1}. \tag{3.12}$$

This will also effects the stage values Y_i

$$Y_i + \delta Y_i = ha_{11}F_1 + ha_{12}F_2 + u_{11}y_1^{[n-1]} + u_{12}(y_2^{[n-1]} + (-1)^{n-1}x_{n-1}), \tag{3.13}$$

which means that

$$\delta Y_i \approx u_{12}(-1)^{n-1}x_{n-1}. \tag{3.14}$$

The change in the values of stage derivatives is

$$F_i \to F_i + \delta F_i = f(Y_i + \delta Y_i \frac{\partial f}{\partial y}), \tag{3.15}$$

which means that

$$\delta F_i \frac{\partial f}{\partial y} \approx u_{12}(-1)^{n-1}x_{n-1}, \tag{3.16}$$

Now the change at step n should be

$$y_2^{[n]} \to y_2^{[n]} + (-1)^n x_n, \tag{3.17}$$

$$y_2^{[n]} + (-1)^n x_n \approx hb_{21}F_1 + hb_{22}F_2 + hb_{21}\delta F_1 y_2^{[n-1]} + hb_{22}\delta F_2 y_2^{[n-1]} - (y_2^{[n-1]} + (-1)^{n-1}x_{n-1}), \tag{3.18}$$

$$y_2^{[n]}+(-1)^n x_n \approx hb_{21}F_1+hb_{22}F_2+hb_{21}\delta F_1 u_{21}^{[n-1]}+hb_{22}\delta F_2 u_{22}^{[n-1]}-y_2^{[n-1]}-(-1)^{n-1}x_{n-1}, \tag{3.19}$$

$$= (-1)^{n-1}x_{n-1} + (-1)^{n-1}h(b_{21}+b_{22})\frac{\partial f}{\partial y}x_{n-1}, \tag{3.20}$$

$$x_n = 1 - h(b_{21}+b_{22})\frac{\partial f}{\partial y}x_{n-1}. \tag{3.21}$$

where

$$\upsilon = -b_{21}u_{12} + b_{22}u_{22},$$

is the growth rate for the parasitic component x_n. In matrix form we have,

$$BU = \begin{bmatrix} 1 & 0 \\ 0 & -\upsilon \end{bmatrix}.$$

We have to cancel the effect of parasitism which is possible only when $\upsilon = 0$. The parasitic component of method P is

$$\upsilon_P = \frac{1+2\sqrt{3}}{3}.$$

and the parasitic component of method N is

$$\upsilon_N = \frac{1-2\sqrt{3}}{3}.$$

3.0.15 Composition of method P and N to annihilate parasitism

We have observed the numerical solution by general linear method using P method and N method. Both methods suffer from the parasitic solution. We want to control the parasitic behaviour and we calculate these parasitic coefficients given as

$$\upsilon_P = \frac{1+2\sqrt{3}}{3}, \qquad \upsilon_N = \frac{1-2\sqrt{3}}{3}.$$

These will be referred to as P (denoting a positive value of υ) and N (indicating negative υ). It will be noted that these numbers are similar to each other but having opposite sign of $\sqrt{3}$. We note that we can apply P and N methods side by side in a composition to avoid the parasitic growth. One such composition is given in [7] which is,

$$N^7PN^{14}PN^{14}PN^{14}PN^{14}PN^{14}PN^{14}PN^{13}P\ldots$$

This means that we first apply N methods seven times and then apply method P. Then we apply method N 14 times and then apply method P. This process continues until we reach at step 113 where we apply method N 13 times instead of 14 times.

Chapter 4

Numerical Experiments

We are interested in those numerical methods that preserve the qualitative behaviour of the problems for long time. The methods chosen for implementation include the famous one step fourth order Gauss symplectic Runge-Kutta method, denoted as IRK, the G-symplectic general linear method denoted as method P and method N and composition of method P and method N as discussed in Chapter 3 and is denoted as method COM. It should be noted that we have used a fixed stepsize in all numerical methods. We have applied these methods for solving Hamiltonian systems. Each problem is accompanied by the numerical results and a discussion.

4.0.16 Simple Pendulum

Consider the equation of Simple Pendulum

$$p' = -\frac{\partial H}{\partial q} \qquad q' = \frac{\partial H}{\partial p} \tag{4.1}$$

$$= -\sin(q), \qquad = p. \tag{4.2}$$

Let H denotes the total energy conserved in Simple Pendulum and is given as

$$H = \frac{p^2}{2} - \cos(q). \tag{4.3}$$

We apply IRK method by taking $p = 0$, $q = 1.2$ with stepsize 0.01 for 10^6 steps and the result of energy conservation is given in Figure 4.1 shows that the energy is well conserved.

We again apply the IRK method by taking $q = 2.3$ with same stepsize of 0.01 and number of steps and check for the conservation of energy. The result is shown

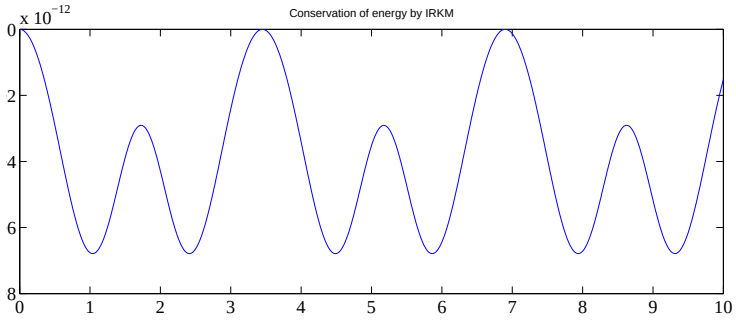

Figure 4.1: Error in Energy conservation of the Simple Pendulum for IRK using q=1.2, p=0.

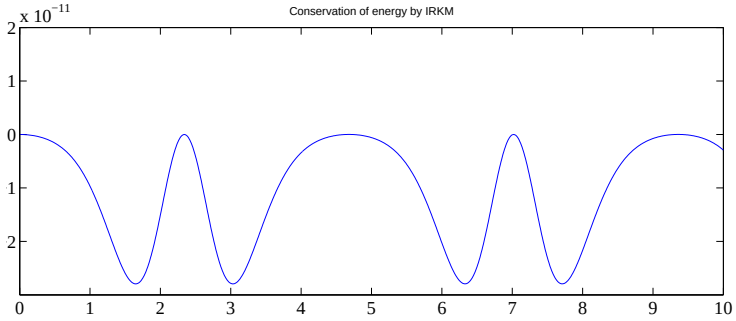

Figure 4.2: Error in Energy conservation of the Simple Pendulum for IRK using q=2.3.

in Figure 4.2. The energy is again well conserved.

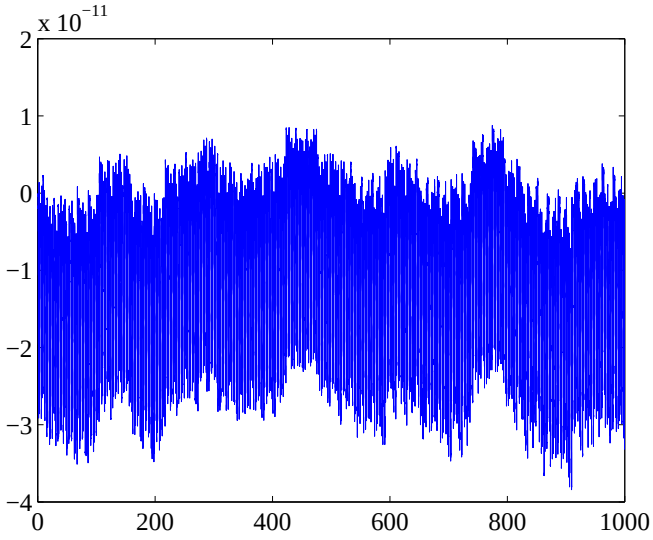

Figure 4.3: Error in Energy conservation of the Simple Pendulum for COM, using q=2.3.

Then we implemented Composition method (COM) using the same stepsize of 0.01 mentioned above for 10^5 steps. The energy is totaly conserved as shown in Figure 4.3.

4.0.17 Harmonic Oscillator

The equation of Harmonic Oscillator is given as

$$\begin{aligned} p' &= -\frac{\partial H}{\partial q} & q' &= \frac{\partial H}{\partial p} \\ &= -q, & &= p. \end{aligned}$$

The energy H is given as

$$H = \frac{p^2}{2} + \frac{q^2}{2}.$$

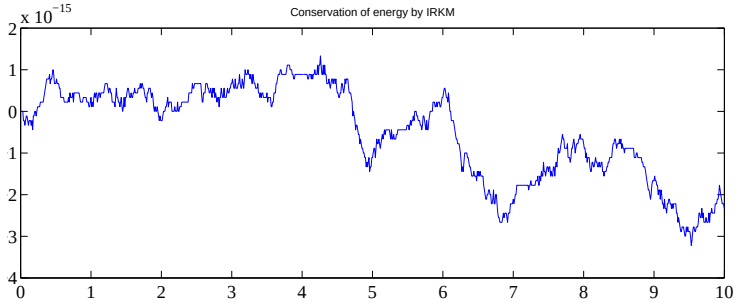

Figure 4.4: Error in Energy conservation of the Harmonic Oscillator for IRK, q=1.2.

We apply IRK method by taking $p = 0$, $q = 1.2$ with stepsize 0.01 for $1,000,000$ steps and the result is shown in the Figure 4.4. We then changed the value of q by 2.3 and the result is given in the Figure 4.5. Both results show that the energy is conserved.

The Figure 4.6 shows behaviour of the general linear method P method by choosing $q = 1.5$ for 1,000,000 steps with same stepsize of 0.01 and we get good conservation of energy.

Similar results for the conservation of energy are obtained using general linear method N with $q = 2.3$ as shown in Figure 4.7.

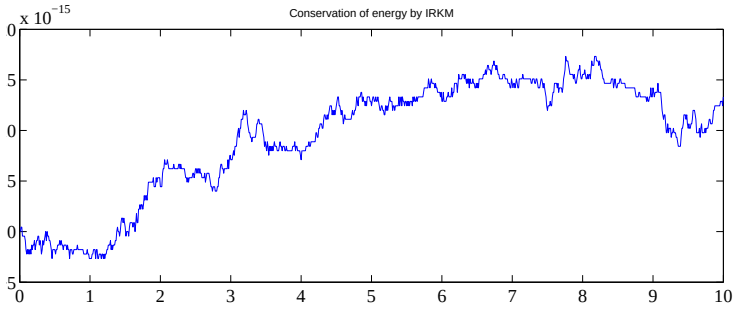

Figure 4.5: Error in Energy conservation of the Harmonic Oscillator for IRK, q=2.3.

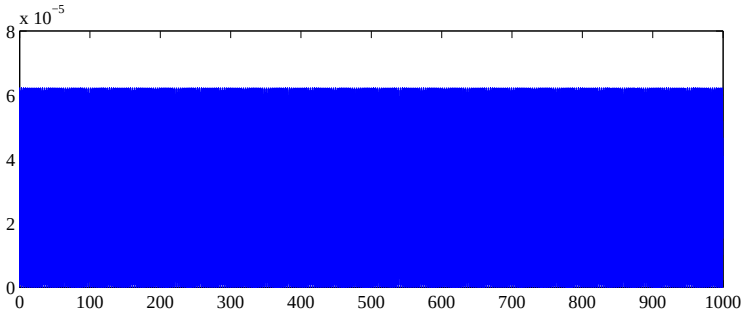

Figure 4.6: Error in Energy conservation of the Harmonic Oscillator for P method, q=1.5.

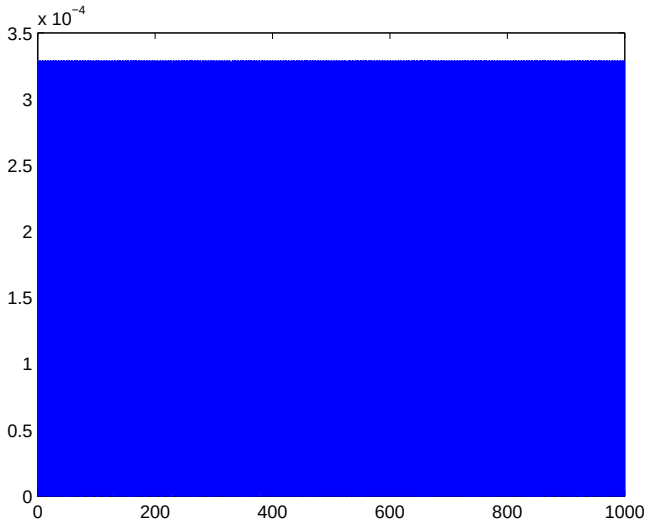

Figure 4.7: Error in Energy conservation of the Harmonic Oscillator for N method, q=2.3.

Then we implemented COM method for the numerical solution of the Harmonic Oscillator with 0.01 stepsize and 100,000 number of steps. The results shown in Figure 4.8 that the energy is again conserved in this case.

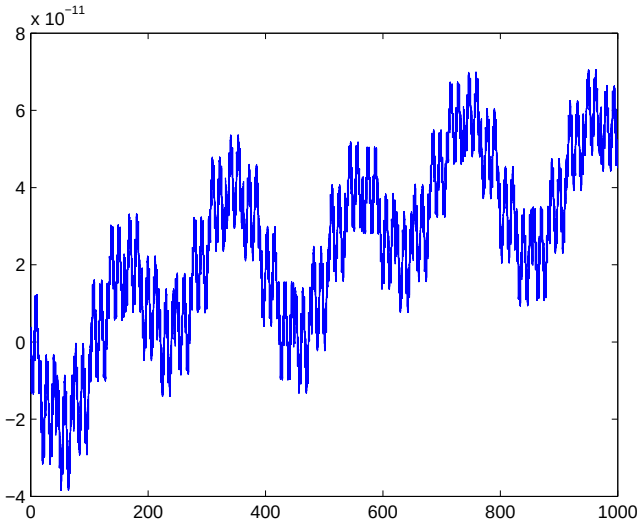

Figure 4.8: Error in Energy conservation of the Harmonic Oscillator for COM, q=2.3.

4.0.18 Kepler Problem

A common problem is Kepler's two body problem. Usually this problem is related with planetary orbital motion. It defines the motion of one body orbiting another. The mathematical equation governing the motion are

$$\begin{aligned} q_1' &= p_1, \\ q_2' &= p_2, \\ p_1' &= \frac{q_1}{(q_1^2+q_2^2)^{3/2}}, \\ p_2' &= \frac{q_2}{(q_1^2+q_2^2)^{3/2}}. \end{aligned}$$

The energy H is given as

$$H = \frac{p_1^2+p_2^2}{2} - \frac{1}{\sqrt{q_1^2+q_2^2}}.$$

In this section, we study the conservation of energy of the Kepler problem with $e = 0, e = 0.1, e = 0.5$ and stepsize 0.01 for one million steps using IRK method. Good energy conservation is observed in all cases as shown in Figures 4.9, 4.10 and 4.11 respectively.

We apply the general linear method N and method P by choosing $e = 0.1$ for 1,000,000 steps with same stepsize 0f 0.01 and the results in Figures 4.12 and 4.13

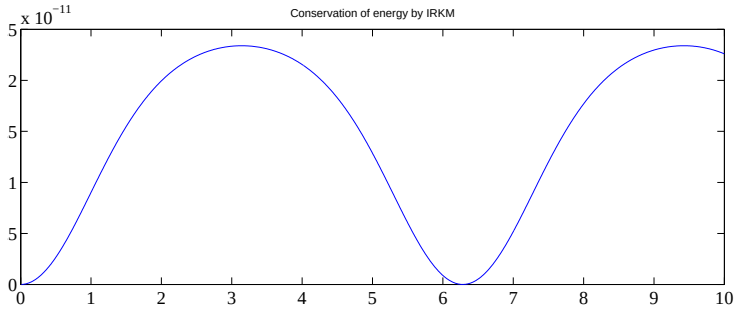

Figure 4.9: Error in Energy conservation of the Kepler two body problem for IRK, e=0.

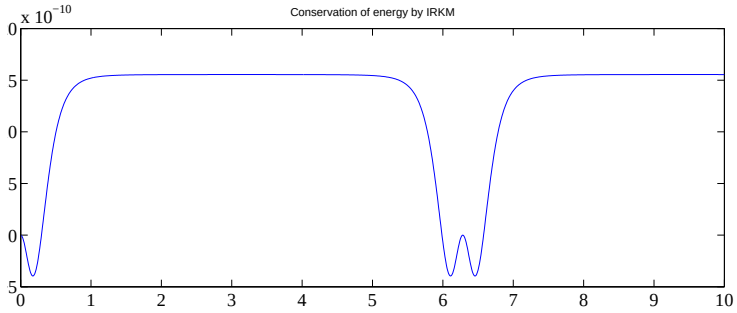

Figure 4.10: Error in Energy conservation of the Kepler two body problem for IRK, e=0.1.

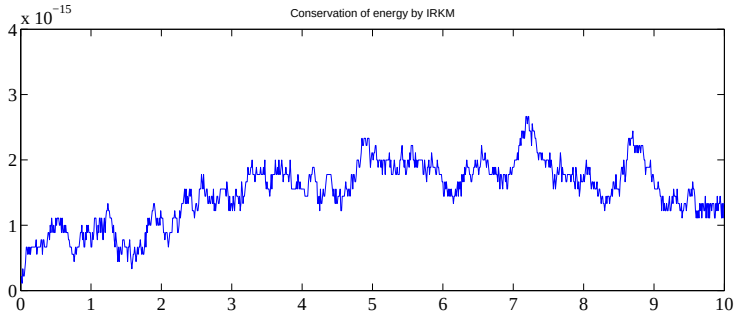

Figure 4.11: Error in Energy conservation of the Kepler two body problem for IRK, e=0.5.

shows that they are comparable to the behaviour of the energy conservation by IRK method.

Then we implemented COM method using 0.01 stepsize and $100,000$ steps and the results are shown in Figure 4.14. The energy is conserved in this case as well.

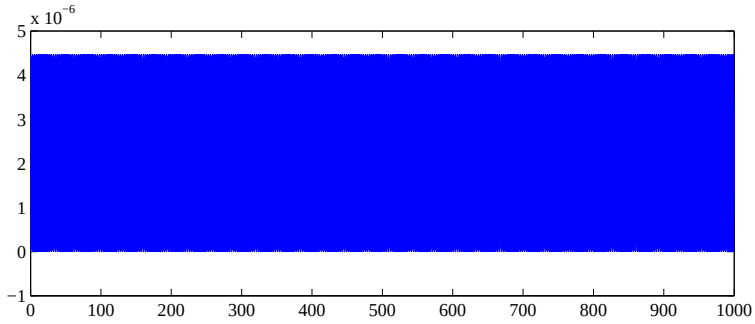

Figure 4.12: Error in Energy conservation of the Kepler two body problem for N method, e=0.1.

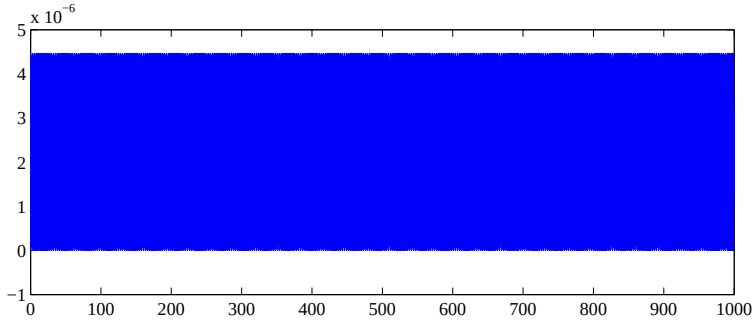

Figure 4.13: Error in Energy conservation of the Kepler two body problem for P method, e=0.1.

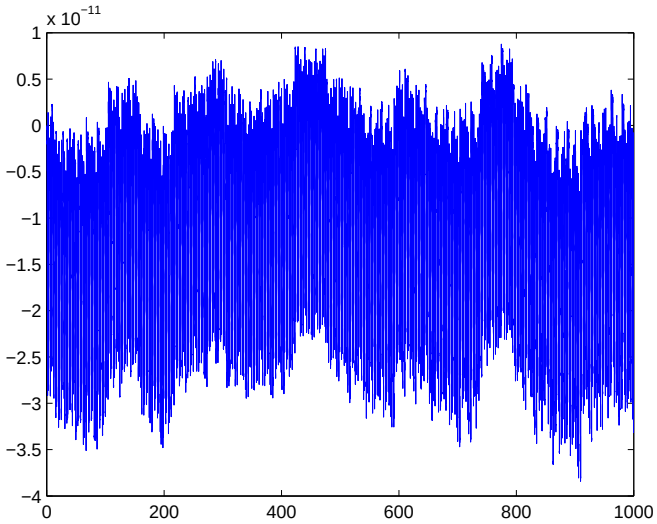

Figure 4.14: Error in Energy conservation of the Kepler two body problem for COM, e=0.1.

4.0.19 Jovian Problem

Jovian problem represents the orbital motion of the Sun and the four planets Jupiter, Saturn, Uranus and Neptune, considering their bodies as point masses [16]. The

equation of motion is written as

$$r_i'' = \sum_{j=1, j\neq i}^{5} \frac{u_j(r_j(x) - r_i(x))}{||r_j(x) - r_i(x)||_2^3}.$$

where the $||.||_2$ denotes the L_2 norm, $u_j = Gm_j$, where G is the gravitational constant and m_j is the mass of j^{th} body.

H is given as

$$H = \frac{1}{2}\sum_{i=1}^{5} m_i r_i'.r_i' - G \sum_{j=1, j\neq i}^{5} \frac{m_i m_j}{||r_j(x) - r_i(x)||_2}.$$

The values of u_j are given in the Appendix A.

The Figure 4.15 shows the behaviour of the energy conservation by IRK method, with stepsize of 0.01 and 10^6 number of steps. The energy is well conserved.

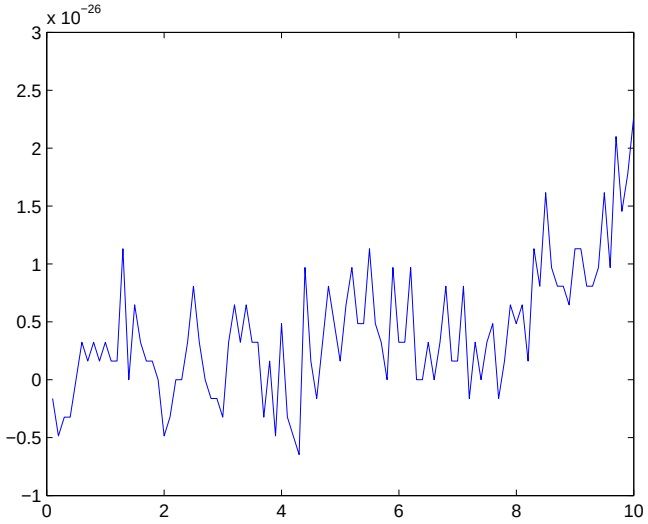

Figure 4.15: Error in Energy conservation of the Jovian problem for IRK.

The Figure 4.20 shows the behaviour of the general linear method P for 10^6 number of steps with 0.01 stepsize. We get conservation of energy.

Similar result for energy conservation is obtained using the general linear method N as shown in the Figure 4.21.

Figure 4.18 shows the conservation of energy by COM with 0.01 stepsize and 10^5 steps. The energy is conserved in this case as well.

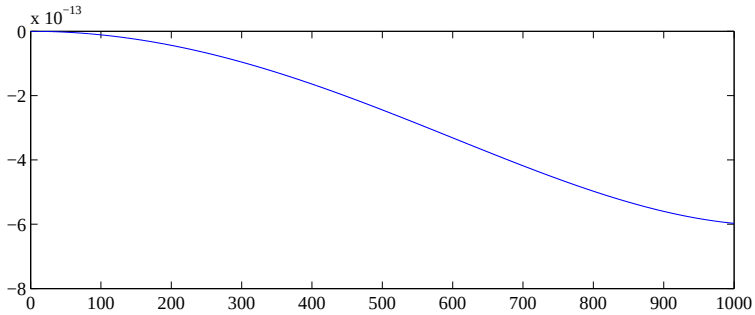

Figure 4.16: Error in Energy conservation of the Jovian problem for P method.

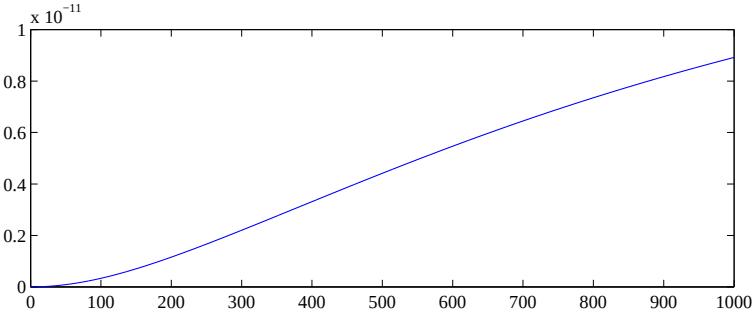

Figure 4.17: Error in Energy conservation of the Jovian problem for N method.

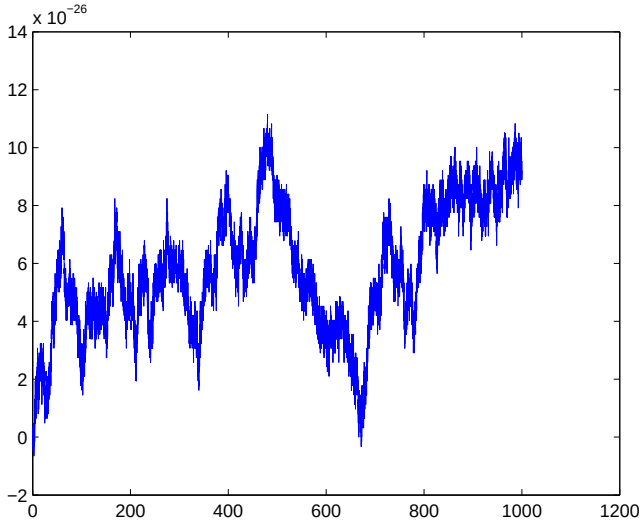

Figure 4.18: Error in Energy conservation of the Jovian problem for COM.

4.0.20 Helin-Roman-Crockett (HRC) Problem

The Helin-Roman-Crockett (HRC) problem models a comet having multiple close approaches with Jupiter [16]. The equations of motion are the same as those for the Jovian Problem with the addition of the following equations for the position r_6 of

the comet

$$r_6'' = \sum_{j=1, j\neq i}^{5} \frac{u_j(r_j(x) - r_6(x))}{||r_j(x) - r_6(x)||_2^3}.$$

The results are same as in the case of the Jovian problem, because the mass of the comet is negligible.

4.0.21 9-Planets Problem

This 9-planet problem is similar to the Jovian problem with additional five planets.i.e Mercury, Venus, Earth, Mars and Pluto [16]. The equation of motion is same as in Jovian Problem but the number of bodies is now ten.

The conservation of energy of the 9 body problem with 0.01 stepsize and $1,000,000$ number of steps using IRK. Good energy conservation is observed as shown in the Figure 4.19.

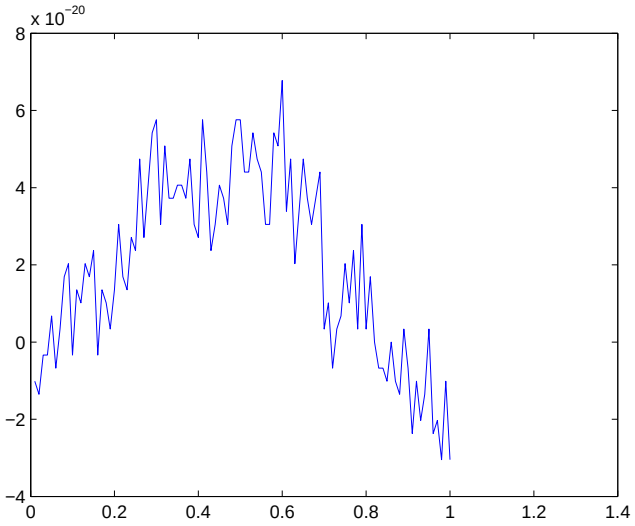

Figure 4.19: Error in Energy conservation of the 9 body problem for IRK.

The Figure 4.20 shows the behaviour of the general linear method P for $1,000,000$ number of steps with step size of 0.01. We get conservation of energy.
Similar result for energy conservation is obtained using the general linear method N as shown in the Figure 4.21.

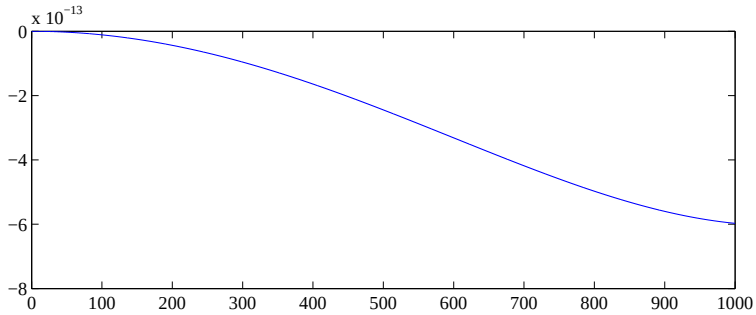

Figure 4.20: Error in Energy conservation of the 9 body problem for P method.

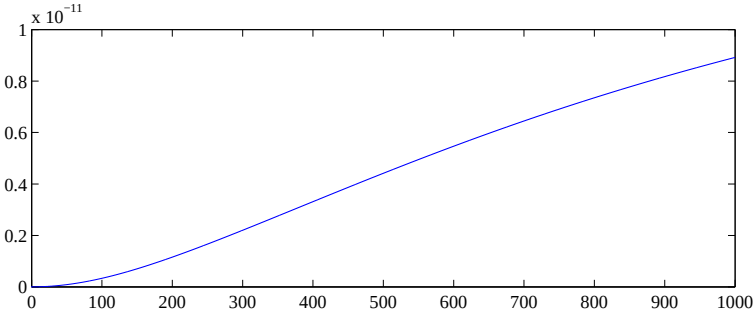

Figure 4.21: Error in Energy conservation of the 9 body problem for N method.

The Figure 4.22 represents the behaviour of the energy conservation by COM with 0.01 stepsize and $100,000$ steps. The energy is conserved in this case as well.

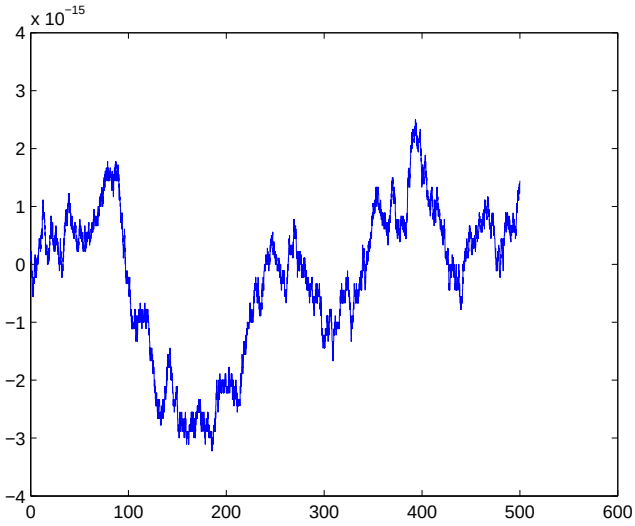

Figure 4.22: Error in Energy conservation of the 9 body problem for COM.

Chapter 5

Conclusion

The goal of this thesis was to study efficient numerical methods for the energy conservation of Hamiltonian systems. We considered two methods, Implicit Runge–Kutta methods and G-symplectic General Linear methods. In all experiments we used fixed stepsize. We used various problems such as Harmonic Oscillator, Simple Pendulum, Kepler, Jovian, Nine body, Helin-Roman-Crockett (HRC) problem in this thesis.

In Chapter 1, we gave an introduction of Hamiltonian systems and symplectic Integrators. We also discussed the numerical methods for the solution of ODEs. Chapter 2 deals with Runge–Kutta methods and their symplecticity. In Chapter 3, we discussed general linear methods and introduced the concept of their G-symplecticity. The growth of parasitic solution of the G-symplectic general linear methods was also investigated. In Chapter 4, we implemented symplectic implicit Runge–Kutta method, G-symplectic general linear method and the composition of two G-symplectic methods of fourth order in a sequence for the control of parasitic component. General symplectic linear method provide an alternative approach to numerically solve Conservative systems like Hamiltonian systems such that qualitative feature is preserved. We studied the energy conservation of Hmailtonian systems in all cases.

5.1 Appendix

5.1.1 Jovian Problem

The Gm for five bodies ordered from SUN, Jupiter, Saturn, Uranus and Neptune are

$$m_1 = 0.295912208285591095E-03$$

$$m_2 = 0.295912208285591095E-03$$

$$m_3 = 0.282534590952422643E-06$$

$$m_4 = 0.845971518568065874E-07$$

$$m_4 = 0.129202491678196939E-07$$

$$m_5 = 0.152435890078427628E-07$$

and the initial conditions

	x	y	z
Sun	4.5041709931760E-03	7.629617246855896E-04	2.642173714857008E-04
Jupiter	-5.37970523578697608E+00	-8.30484073974418041E-01	-2.24831631285812891E-01
Saturn	7.89439586897901350E+00	4.59647081929466859E+00	1.55869642252380332E+00
Uranus	-1.82653939237009090E+01	-1.16195110729092122E+00	-2.50107720935801844E-01
Neptune	-1.60550335112138710E+01	-2.39421866167270672E+01	-9.40016532150945853E+00
Sun	-2.686979799291859E-07	5.225296222968518E-06	2.248930945915554E-06
Jupiter	1.09209442155944167E-03	-6.51806804633966371E-03	-2.82076550685720154E-03
Saturn	-3.21747131481691839E-03	4.33585784900737449E-03	1.92866675819078661E-03
Uranus	2.21271749628262749E-04	-3.76242860345373065E-03	-1.65099556049815467E-03
Neptune	2.64285432917179465E-03	-1.49826690091408224E-03	-6.79022140848015384E-04

Table A.1: Rows 1 to 5 list the initial position and rows 6 to 10 the initial velocity.

5.1.2 Nine Planets Problem

The Gm for ten bodies ordered from Sun to Neptune are

$$m_1 = (0.017202098952)/2$$

$$m_2 = m_1/6023600$$

$$m_3 = m_1/408523.5$$

$$m_4 = m_1/328900.53$$

$$m_5 = m_1/3098710$$

$$m_6 = m_1/1047.355$$

$$m_7 = m_1/3498.5$$

$$m_8 = m_1/22869.0$$

$$m_9 = m_1/19314.0$$

$$m_{10} = m_1/3000000.0$$

and the initial conditions

	x	y	z
Sun	0.9301259103994515E-03	0.2292733100662641E-02	0.9059057664779422E-03
Mercury	0.3448565760800415E+00	0.4790821305397614E-01	-0.1001813144545456E-01
Venus	0.1438953102536455E+00	0.6492977991345496E+00	0.2833883064268579E+00
Earth	-0.1354345700443955E+00	0.8956906559576626E+00	0.3883642504058149E+00
Mars	-0.1368903850273021E+01	0.8454279811185666E+00	0.4247388123779079E+00
Jupiter	0.3350294349606409E+01	-0.3471468715911917E+01	-0.1571243780627322E+01
Saturn	-0.8971574942371711E+01	0.2281974741233523E+01	0.1331244515477938E+01
Uranus	-0.1002073869416921E+01	0.1732580120637246E+02	0.7605730952182388E+01
Neptune	-0.2919365061270080E+02	-0.7716992458897807E+01	-0.2426339472522292E+01
Pluto	-0.2623272065610510E+02	0.2056426815315656E+02	0.1444546303354718E+02
Sun	-0.4559774360194479E-05	-0.3150250493626429E-05	-0.1274328432609927E-05
Mercury	-0.8471091819370054E-02	0.2561145505678817E-01	0.1458557100780699E-01
Venus	-0.1989837205370269E-01	0.3109969215624964E-02	0.2658171477313190E-02
Earth	-0.1732455862288979E-01	-0.2247454982261186E-02	-0.9746354441906539E-03
Mars	-0.7389123605631364E-02	-0.9480508889767826E-02	-0.4152929465094740E-02
Jupiter	0.5581083375222116E-02	0.4959110886728884E-02	0.1991002598306760E-02
Saturn	-0.1862811731356904E-02	-0.4987008831911066E-02	-0.1981531741239860E-02
Uranus	-0.3959813937377914E-02	-0.3790640356065674E-03	-0.1101243197204039E-03
Neptune	0.8161882834578905E-03	-0.2775248510073856E-02	-0.1157390358868530E-02
Pluto	-0.1320448472641354E-02	-0.2623278455987146E-02	-0.4283576834589079E-03

Table A.2: Rows 1 to 10 list the initial position and rows 11 to 20 the initial velocity.

5.1.3 HRC Problem

The Gm for five bodies ordered from Sun, Jupiter, Saturn, Uranus and Neptune are

$$m_1 = 2.959122082855911025 82E-4$$

$$m_2 = 2.825342103445926254 72E-7$$

$$m_3 = 8.459468504830659292 85E-8$$

$$m_4 = 1.288816238138034888 51E-8$$

$$m_5 = 1.532112481284276189 18E - 8$$

and the initial conditions are

	x	y	z
Sun	0.6669198564440767E-02	-0.7235114664408392E-03	-0.1130654423787794E-03
Jupiter	-0.4929481880506559E+01	-0.2310910532399841E+01	0.1197889941614212E+00
Saturn	-0.5559462159881659E+01	0.7217090743352659E+01	0.1008764843911512E+00
Uranus	-0.1051479684851656E+02	-0.1555904864202644E+02	0.7740390484943622E-01
Neptune	0.1636130229890141E+01	0.2982856616501356E+02	-0.6473579962266688E+00
Asteroid	-0.3965267044277659E+01	0.3060320798461592E+00	0.2949122108880113E+00
Sun	-0.1597551822288177E-05	0.7254098157790906E-05	-0.3038348598973975E-07
Jupiter	0.3109433296611612E-02	-0.6477134819096109E-02	-0.4357172559451174E-04
Saturn	-0.4717678753258388E-02	-0.3413503592855709E-02	0.2469252827795303E-03
Uranus	0.3227888778570112E-02	-0.2386568620156909E-02	-0.5061978789868374E-04
Neptune	-0.3152327294479188E-02	0.1931132154044109E-03	0.6952342277721326E-04
Asteroid	-0.1800219023380088E-02	-0.8521337694196810E-02	0.1052106206437703E-03

Table A.3: Rows 1 to 6 list the initial position and rRows 7 to 12 the initial velocity.

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