On the Construction of Symplectic Integrators via Vandermonde Transformation

by

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Dedicated to My Husband

For his endless love, support and encouragement

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Samina Ashrsf

Abstract

The physical problems like the planetary motion, simple pendulum and many others are governed by Hamiltonian equations. We provide approximate solution of Hamiltonian equations by using structure preserving numerical methods.
The numerical methods which preserve the qualitative features of Hamiltonian system like energy conservation and symplecticity are used for the long term integration of Hamiltonian system. In this thesis we construct symplectic numerical methods like symplectic Runge-Kutta and symplectic partitioned Runge-Kutta methods. Particularly we deal with the symplectic implicit Runge-Kutta and symplectic implicit partitioned Runge-Kutta methods, like Gauss, Radau-I, Radau-II and Lobatto-III for Hamiltonian systems. We have implemented all these methods and draw a comparison between the results.

Contents

Chapter 1

Introduction

Differential Equations (DEs) play an important role in different fields of sciences. For example, in Engineering, DEs describe the flow of electrical currents through the series circuits, in Chemistry, DEs describe the rates of chemical reactions and in Physics, DEs model Newton's law. Usually these DEs are ordinary differential equations (ODEs), because they are most suitable mathematical form which can be used to understand above mention phenomena. In this thesis, we are concerned with the solutions for the system of ODEs.

Generally, the system of ODEs with initial conditions are known as the initial value problem (IVP) and is given as

$$y'(t) = f(t, y(t)), \quad y(t_0) = y_0, \tag{1.0.1}$$

where $y'(t) = \frac{dy}{dt}$ denotes the derivative of function with respect to time t, y is the flow of ODE which represents the solution of (1.0.1). In autonomous IVPs, t is taken as the argument of the vector y that is

$$y'(t) = f(y(t)), \quad y(t_0) = y_0.$$

The system of first order ODEs with initial conditions has the form,

$$\begin{aligned}
y_1' &= f_1(t, y_1, y_2, y_3, ...y_n) \qquad y_1(t_0) = y_1,\\
y_2' &= f_2(t, y_1, y_2, y_3, ...y_n) \qquad y_2(t_0) = y_2,\\
\vdots &= \vdots\\
y_n' &= f_n(t, y_1, y_2, y_3, ...y_n) \qquad y_n(t_0) = y_n.
\end{aligned}$$

Example 1.0.1. Let $T(t)$ denotes the temperature of body at any time t, and constant temperature of the surrounding medium is T_m. If the rate in which a body cools is represented by $\frac{dT}{dt}$, then by Newton's law of cooling is

$$\frac{dT}{dt} \propto T - T_m,$$

or

$$\frac{dT}{dt} = k(T - T_m)$$

where k is a proportionality constant. The body is in a state of cooling, when $k < 0$ and we have $T > T_m$ [9].

If $f(y)$ satisfies a Lipschitz condition [8], then the solution of (1.0.1) must exist and is unique.

Definition 1.0.2. A function $f(t, y)$ satisfies a Lipschitz condition in the variable y on a set $E \subset \mathbb{R}^2$ if a constant $L > 0$ exist with

$$|f(t, y_1) - f(t, y_2)| \leq \mathbf{L}|y_1 - y_2|,$$

whenever (t, y_1) and (t, y_2) are in E. The constant L is called a Lipschitz constant for f.

Example 1.0.3. Let $y' = f(t, y) = t|y|$ and
consider a set

$$E = \{(t, y)| \ \ 1 \leq t \leq 2 \ \text{ and } \ -3 \leq y \leq 4\}.$$

Now

$$|f(t, y_1) - f(t, y_2)| = |t|y_1| - t|y_2|| = |t|||y_1| - |y_2|| \leq 2|y_1 - y_2|.$$

Thus f satisfies a Lipschitz condition on E in the variable y with Lipschitz constant $L = 2$. It means that the solution of this DE must exist and unique.

1.1 Hamiltonian systems

Classical mechanics is a branch of physics in which we study the motion of bodies. Hamiltonian mechanics was first formulated by William Rowan Hamilton. Hamiltonian mechanics is an improved form of classical mechanics. Hamiltonian theory works in three different disciplines (equations of motion, partial differential equations and variational principles) but here we shall use his theory about equations of motion. In Hamiltonian mechanics, the equations of motion depend on the generalized co-ordinates q_i and generalized momenta p_i. These equations are known as Hamiltonian system [7, 10], with Hamiltonian H such that

$$\begin{aligned} p_i' &= -\frac{\partial H}{\partial q_i} \\ q_i' &= \frac{\partial H}{\partial p_i}, \end{aligned} \tag{1.1.1}$$

where $'$ denotes the derivative of function with respect to time t

$$p_i = (p_1, p_2, p_3 .....p_n),$$

$$q_i = (q_1, q_2, q_3.....q_n),$$

having $2n$ degree of freedom. In other words, Hamiltonian systems are mathematical function that can be used to develop the equations of motion of a dynamical system. Normally H represents the total energy of the underlying mechanical system. Usually Hamiltonian can be written as a linear combination of kinetic energy and potential energy,

$$H(p, q) = T(p) + V(q),$$

where T is kinetic energy and V is potential energy. Hamiltonian of this form is said to be separable.

Example 1.1.1. Harmonic oscillator. The equations of motion of the Harmonic oscillator define a Hamiltonian system with generalized momenta p and generalized coordinates q and are given as

$$q' = p, \quad p' = -q.$$

The total energy H is given as

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

Some remarkable properties of Hamiltonian systems [10] are given below.

1.2 Energy conservation

Energy is one of the physical quantities that is conserved in our universe. If the Hamiltonian function H is autonomous then the energy is conserved such that

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

Thus H conserves energy

$$H(p(t), q(t)) = H(p(0), q(0)) = \text{constant}.$$

1.3 Symplecticity

Symplecticity is a qualitative feature of Hamiltonian systems. There are many ways to explain the notion of symplecticity. One of them is discussed here.

- symplecticity in terms of jacobian.

Consider a linear transformation $\Psi : (p, q) \mapsto (p^\star, q^\star)$. Ψ is symplectic if,

$$\Psi'^t J \Psi' = J.$$

Here

$$J = \begin{pmatrix} 0 & \text{I} \\ \text{-I} & 0 \end{pmatrix},$$

is a $2n \times 2n$ matrix, I is $n \times n$ identity matrix.
To prove this, suppose that the jacobian of transformation has a unit determinant.

$$\Psi' = \begin{pmatrix} \frac{\partial p}{\partial p^\star} & \frac{\partial p}{\partial q^\star} \\ \frac{\partial q}{\partial p^\star} & \frac{\partial q}{\partial q^\star} \end{pmatrix}.$$

Now

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

Thus

$$\Psi'^t J \Psi' = \begin{pmatrix} \frac{\partial p \partial q}{\partial p^\star \partial p^\star} - \frac{\partial p \partial q}{\partial p^\star \partial p^\star} & \frac{\partial p}{\partial p^\star}\frac{\partial q}{\partial q^\star} - \frac{\partial p}{\partial q^\star}\frac{\partial q}{\partial p^\star} \\ -\frac{\partial p}{\partial p^\star}\frac{\partial q}{\partial q^\star} + \frac{\partial p}{\partial q^\star}\frac{\partial q}{\partial p^\star} & \frac{\partial p \partial q}{\partial q^\star \partial q^\star} - \frac{\partial p \partial q}{\partial q^\star \partial q^\star} \end{pmatrix},$$

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

Hence Ψ is symplectic.

1.4 Symplectic integrators

Energy conservation and symplecticity are the properties of Hamiltonian systems. We want those numerical methods that preserve symplecticity. However, all Runge-Kutta methods do not preserve this property when we solve Hamiltonian system numerically. Therefore we need symplectic Runge-Kutta methods.
Solving the Hamiltonian system, we can verify that Runge-Kutta methods are symplectic if the approximate solution will satisfy the following relation.

$$< p_{n+1}, q_{n+1} >=< p_n, q_n >,$$

where p_{n+1}, q_{n+1} and p_n, q_n are the approximate solutions of Hamiltonian systems at t_{n+1} and t_n respectively. In this thesis, we have considered Runge-Kutta methods and partitioned Runge-Kutta methods to be symplectic.

1.5 Linear and quadratic invariants

Hamiltonian systems are those DEs whose solution possess invariants. There are two types of invariants, we have studied, in this thesis: one is called linear invariant and other is called quadratic invariant [4, 5].

Linear invariant: Suppose that an initial value problem is

$$z' = f(z(t)), \qquad z(t_0) = z_0. \tag{1.5.1}$$

A non constant function $L(z)$ is known as linear invariant (first integral) of (1.5.1) if

$$L'(z)f(z) = 0, \qquad \forall\, z.$$

This means the solution $z(t)$ of (1.5.1) satisfies

$$L(z(t)) = L(z_0) = \text{constant}.$$

For example, in a conservative system the Hamiltonian function H is a Linear invariant of (1.1.1) by applying the definition of linear invariant on H then

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

$$H' = \begin{bmatrix} \frac{\partial H}{\partial p} & \frac{\partial H}{\partial q} \end{bmatrix},$$

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

Quadratic invariants: Consider a quadratic function

$$Q(z) = z^t C z,$$

where C is a square symmetric matrix. It is an invariant of (1.5.1)
if

$$z^t C f(z) =< z^t, f(z) >= 0, \quad \forall z.$$

This condition holds for conservative systems. We consider an example of quadratic invariant

Harmonic oscillator: Consider the quadratic function

$$Q(z) = z^t C(z),$$

$$Q(z) = \begin{pmatrix} p & q \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} p \\ q \end{pmatrix}, \tag{1.5.2}$$

where

$$z = \begin{pmatrix} p \\ q \end{pmatrix}.$$

(1.5.2) is an invariant of the equation of motion of of Harmonic oscillator (4.3) because

$$z^t C f(z) = \begin{pmatrix} p & q \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} -q \\ p \end{pmatrix} = 0.$$

Chapter 2

Runge-Kutta methods and partitioned Runge-Kutta methods

2.1 Runge-Kutta methods

Two German scientists Carl Runge (1856 − 1927) and Martin Kutta (1867 − 1944) developed the Runge-Kutta methods [2, 3] in 1901 for the numerical solution of ODEs. Carl Runge developed numerical methods for solving the ODEs that appeared in his study of atomic spectra. These numerical methods are still used today. He used so much mathematics in his research that physicists thought he was a mathematician and he did so much physics that mathematicians thought he was a physicist.

Runge-Kutta methods belong to the family of one step methods to calculate numerical solutions of initial value problems

$$y' = f(y(t)), \quad y(t_0) = y_0. \tag{2.1.1}$$

Rung-Kutta methods give an approximate solution of (2.1.1) at time $t_n = nh$ where $n = 0, 1, 2 \dots$ and h is the stepsize. The general form of Runge-Kutta methods in case of autonomous is,

$$\begin{aligned} Y_i &= y_{n-1} + \sum_{j=1}^{s} a_{ij} h f(Y_j), \qquad i = 1, 2 \dots s, \\ y_n &= y_{n-1} + \sum_{i=1}^{s} b_i h f(Y_i), \end{aligned} \tag{2.1.2}$$

and in case of non-autonomous,

$$Y_i = y_{n-1} + \sum_{j=1}^{s} a_{ij} h f(t_n + c_j h, Y_j), \qquad i = 1, 2 \ldots s,$$
$$y_n = y_{n-1} + \sum_{i=1}^{s} b_i h f(t_n + c_i h, Y_i),$$

where Y_i are s stage calculated during the integration from time t_{n-1} to t_n, y_n is an approximate solution. A Runge-Kutta method can also be represented by Butcher tableau as [2],

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

where b_i are called the quadrature weights of the method. The

$$c_i = \sum_{j=1}^{s} a_{ij}, \qquad \text{for} \quad i = 1, 2....s, \tag{2.1.3}$$

are the quadrature nodes of the method at which the stages Y_i are calculated. Runge-Kutta methods are explicit if $a_{ij} = 0$ for $i \leq j$ which means that the stages can be calculated sequentially. This requires less computation time for solving ODEs. Runge-Kutta methods are implicit if $a_{ij} \neq 0$ for some $i \leq j$. The stages then become implicit and we need either fixed point iteration or Newton Raphson method to evaluate them.

Example 2.1.1. Fourth-stage explicit Runge-Kutta method of order 4:

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

$$\begin{aligned} Y_1 &= y_0, \\ Y_2 &= y_0 + \frac{h}{2} f(Y_1), \\ Y_3 &= y_0 + \frac{h}{2} f(Y_2), \\ Y_4 &= y_0 + \frac{h}{1} f(Y_3), \\ y_1 &= y_0 + \frac{h}{6} f(Y_1) + \frac{2h}{6} f(Y_2) + \frac{2h}{6} f(Y_3) + \frac{h}{6} f(Y_4). \end{aligned}$$

Example 2.1.2. Two-stages implicit Runge-Kutta method of order 4:

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

$$\begin{aligned} Y_1 &= y_0 + \frac{h}{4} f(Y_1) + h(\frac{1}{4} - \frac{\sqrt{3}}{6}) f(Y_2), \\ Y_2 &= y_0 + h(\frac{1}{4} + \frac{\sqrt{3}}{6}) f(Y_1) + \frac{h}{4} f(Y_2), \\ y_1 &= y_0 + \frac{h}{2} f(Y_1) + \frac{h}{2} f(Y_2). \end{aligned}$$

2.2 Order conditions for Runge-Kutta methods

The order conditions [1] for a Runge-Kutta method (2.1.2) represent a relation between the coefficients of a Runge-Kutta method such that if these conditions are satisfied, then the method have a particular order. To find the order conditions of Runge-Kutta method we have to compare the numerical solution with the Taylor expansion of exact solution. We accessed the order conditions of Runge-Kutta method by using an explicit method as well as an implicit method. To find the order of the Runge-Kutta method we first explain the concept of elementary differentials which is as follows.

$$\begin{aligned} y' &= f, \\ y'' &= f'f, \\ y''' &= f''(f,f) + f'f'f, \\ y^{iv} &= f'''(f,f,f) + 2f''(f,f',f) + 2f'f''(f,f) + f'f'f'f, \\ y^{v} &= f^{iv}(f,f,f,f) + 4f'''(f',f,f,f) + 2f'''(f,f,f',f) + 4f''(f',f,f',f) + 2f''(f,f'',f,f) \\ &\quad + 2f'f'''(f,f,f) + 2f''f''(f,f,f) + 4f'f''(f',f,f) + 3f''f'f'(f,f), \end{aligned} \tag{2.2.1}$$

where f, $f'f$ etc are called elementary differentials. The general form of explicit Runge-Kutta method is

$$\begin{aligned} Y_i &= y_{n-1} + \sum_{j=1}^{i-1} a_{ij} h f(Y_j), \qquad i = 1, 2, \ldots s, \\ y_n &= y_{n-1} + \sum_{i=1}^{s} b_i h f(Y_i), \end{aligned} \tag{2.2.2}$$

and

$$c_i = \sum_{j=1}^{s} a_{ij} = 0, \qquad i = 1, 2, ...s, \tag{2.2.3}$$

is the consistency condition.

For $s = 3$,

$$Y_1 = y_{n-1}. \tag{2.2.4}$$

$$Y_2 = y_{n-1} + ha_{21}f(Y_1), \tag{2.2.5}$$

by using equation (2.2.4) in equation (2.2.5)

$$Y_2 = y_{n-1} + hc_2 f(y_{n-1}), \tag{2.2.6}$$

$$Y_3 = y_{n-1} + ha_{31}f(y_{n-1}) + ha_{32}f(Y_2), \tag{2.2.7}$$

by using equation (2.2.6) in equation (2.2.7),

$$Y_3 = y_{n-1} + ha_{31}f(y_{n-1}) + ha_{32}f(y_{n-1} + hc_2 f(y_{n-1})). \tag{2.2.8}$$

Using Taylor series,

$$f(y_{n-1} + hc_2 f(y_{n-1})) = f(y_{n-1}) + hc_2 f'f(y_{n-1}) + \frac{h^2}{2}c_2^2 f''ff(y_{n-1}) + O(h^3), \tag{2.2.9}$$

by using equation (2.2.9) in equation (2.2.8)

$$\begin{aligned} Y_3 &= y_{n-1} + h(a_{31} + a_{32})f(y_{n-1}) + h^2 a_{32}c_2 f'f(y_{n-1}) + O(h^3) \\ f(Y_3) &= f(y_{n-1} + hc_3 f(y_{n-1}) + h^2 a_{32}c_2 f'f(y_{n-1}) + O(h^3)), \end{aligned}$$

and

$$f(Y_3) = f(y_{n-1}) + hc_3 f'f(y_{n-1})) + h^2(\frac{1}{2}c_3^2 f''f^2(y_{n-1}) + a_{32}c_2 f'f'f(y_{n-1})) + O(h^3). \tag{2.2.10}$$

$$y_n = y_{n-1} + hb_1 f(Y_1) + hb_2 f(Y_2) + hb_3 f(Y_3) + O(h^4), \tag{2.2.11}$$

by using equations (2.2.4), (2.2.9) and (2.2.10) in equation (2.2.11)

$$\begin{aligned} y_n = y_{n-1} &+ hb_1 f(y_{n-1}) + hb_2(f(y_{n-1}) + hc_2 f'f(y_{n-1}) + \frac{h^2}{2}c_2^2 f''f(y_{n-1})) \\ &+ hb_3(f(y_{n-1}) + hc_3 f'f(y_{n-1}) + h^2(\frac{1}{2}c_3^2 f''f^2(y_{n-1}) + a_{32}c_2 f'f'f(y_{n-1})) + O(h^4), \end{aligned}$$

$$\begin{aligned} y_n = y_{n-1} &+ h(b_1 + b_2 + b_3)f(y_{n-1}) + h^2(b_2c_2 + b_3c_3)f'f(y_{n-1}) \\ &+ h^3(\frac{1}{2}(b_2c_2^2 + b_3c_3^2)f''ff(y_{n-1}) + b_3a_{32}c_2 f'f'f(y_{n-1})) + O(h^4)). \end{aligned} \tag{2.2.12}$$

Now the Taylor series of exact solution is

$$y(t_n) = y(t_{n-1}) + hy'(t_{n-1}) + \frac{h^2}{2!}y''(t_{n-1}) + \frac{h^3}{3!}y'''(t_{n-1}) + O(h^4). \tag{2.2.13}$$

By using equation (2.2.1) in equation (2.2.13), comparing it with equation (2.2.12) we have

$$\sum_{i=1}^{3} b_i = 1, \tag{2.2.14}$$

which is the condition of Runge-Kutta methods of order 1.

$$\sum_{i=2}^{3} b_i c_i = \frac{1}{2}, \tag{2.2.15}$$

which is the condition of Runge-Kutta methods of order 2.

$$\begin{aligned} \sum_{i=2}^{3} b_i c_i^2 &= \frac{1}{3}, \\ b_3 a_{32} c_2 &= \frac{1}{6}, \end{aligned} \tag{2.2.16}$$

which are the conditions of Runge-Kutta methods of order 3.

2.3 Symplectic Runge-Kutta methods

As discussed in chapter 1, we need the Runge-Kutta methods which when applied to Hamiltonian system or conservative system can preserve their inherent qualitative features, such Runge-Kutta methods are called symplectic Runge-Kutta methods [4,11]. The Runge-Kutta methods (2.1.2) are symplectic if the numerical solution y_n of (2.1.1) satisfies

$$< y_n, y_n >=< y_{n-1}, y_{n-1} > . \tag{2.3.1}$$

This is only possible if the coefficient of Runge-Kutta methods (2.1.2) satisfies

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0 \quad \forall \ i, j = 1, 2, \cdots s. \tag{2.3.2}$$

Equation (2.3.2) is called the symplectic condition for Runge-Kutta methods.
Proof:

Since for a conservative system, as given in quadratic invariant in section (1.5)

$$z^t C f(z) =< z^t, f(z) >= 0, \forall \ z, \tag{2.3.3}$$

where C is identity matrix. For the Runge-Kutta method (2.1.2), we apply (2.3.3) on the stages of the Runge-Kutta method. Therefore

$$< Y_i, f(Y_i) >= 0,$$

using (2.1.2) in above equation we have

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

$$< y_{n-1}, f(Y_i) >= -h\sum_{j=1}^{s} a_{ij} < f(Y_j), f(Y_i) > . \quad (2.3.4)$$

To prove equation (2.3.1), take the left hand side of it and using (2.1.2) we get

$$< y_n, y_n > =< y_{n-1} + h\sum_{i=1}^{s} b_i f(Y_i), y_{n-1} + h\sum_{i=1}^{s} b_i f(Y_i) >, \quad (2.3.5)$$

$$=< y_{n-1}, y_{n-1} > +h\sum_{i=1}^{s} b_i < y_{n-1}, f(Y_i) > +h\sum_{i=1}^{s} b_i < f(Y_i), y_{n-1} >$$

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

Using equation (2.3.4) in above equation, we have

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

$$+ h^2\sum_{ij=1}^{s} b_i b_j < f(Y_j), f(Y_i) >,$$

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

Now

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

If and only if

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

Since

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

therefore

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

hence

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \qquad \forall\ i, j = 1, 2...s.$$

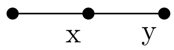
2.4 Trees and its use in Runge-Kutta methods

Trees [2] play an important role in the development of Runge-Kutta methods. We have the following definitions.

Trees and rooted trees.

Tree is simply a connected graph with no cycles. It is the combination of vertices and edges. Tree becomes a rooted tree if we fixed one vertex of it as root. We indicate the root by placing it at the bottom of a tree diagram. [1, 7]

As an example we can take a tree $\hat{t}$

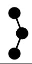
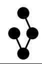
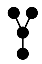


$\hat{t}$

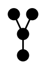
and its rooted trees are

$\hat{t}_x$ $\hat{t}_y$

Let **T** denotes the set of all rooted trees including the empty tree which has zero vertices and edges. A single tree with only one vertex is represented by τ and is denoted by •. A tree with two vertices is represented by $[\tau]$ and is denoted by . The following table represents some rooted trees and their notations.

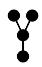
Rooted trees						
Notations	$[\tau^2]$	$[[\tau]]$	$[\tau^3]$	$[\tau[\tau]]$	$[[\tau^2]]$	$[[[\tau]]]$

Order: The number of vertices of a tree is called the order of the tree and is denoted by $r(\hat{t})$.
For example

$\hat{t} =$  $\qquad r(\hat{t}) = 4$

Density: It is a product of the order of the trees and the order of subtrees when the tree is chopped off. It is denoted by $\gamma(\hat{t})$.

For example

$\hat{t} =$  $\qquad \gamma(\hat{t}) = 12$

Elementary Differentials: To find out the order of a Runge-Kutta method, the numerical solution is compared with the Taylor series expansion of the exact solution. For the comparison, $f(y(t))$ needs to be differentiated several times as follows

$$
\begin{aligned}
y' &= f, \\
y'' &= f'f, \\
y''' &= f''(f,f) + f'f'f, \\
y^{iv} &= f'''(f,f,f) + 2f''(f,f',f) + 2f'f''(f,f) + f'f'f'f, \\
y^{v} &= f^{iv}(f,f,f,f) + 4f'''(f',f,f,f) + 2f'''(f,f,f',f) + 4f''(f',f,f',f) + 2f''(f,f'',f,f) \\
&\quad + 2f'f'''(f,f,f) + 2f''f''(f,f,f) + 4f'f''(f',f,f) + 3f''f'f'(f,f).
\end{aligned}
$$

A set of elementary differentials is denoted by $F(t)$.

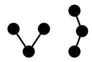
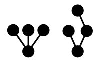
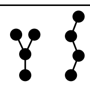
Rooted trees	Elementary differentials
	f
	$f'f$
	$f''(f,f), \quad f'f'f$
	$f'''(f,f,f),\ f''(f,f',f)$
	$f'f''(f,f),\ f'f'f'f$

Table 2.1: Elementary differentials and their rooted trees.

Elementary Weight: For each tree $\hat{t}$, a corresponding polynomial can be obtained in the coefficients of the Runge-Kutta methods known as elementary weight. It is represented by $\Phi(\hat{t})$. In other words, it is a linear combination of b_i, a_{ij} and c_j. Thus single vertex is represented by quadrature weights that is, $b_1,\ b_2, \dots b_s$. The end vertex of each edge is represented by quadrature nodes of the method at which the stages Y_i calculated that is, $c_1,\ c_2, \dots c_s$. The edge which has edges on both sides is represented by $a_{ij},\ \forall\ i,j = 1,2,\dots s$.

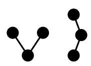
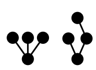
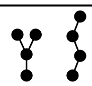
Rooted trees	Elementary weight
	$\sum_{i=1}^{s} b_i$
	$\sum_{i=1}^{s} b_i c_i$
	$\sum_{i=1}^{s} b_i c_i^2, \quad \sum_{i,j=1}^{s} b_i a_{ij}$
	$\sum_{i=1}^{s} b_i c_i^3, \quad \sum_{i,j=1}^{s} b_i c_i a_{ij} c_j$
	$\sum_{i,j=1}^{s} b_i a_{ij} c_j^2, \quad \sum_{i,j,k=1}^{s} b_i a_{ij} a_{jk} c_k$

Table 2.2: Elementary weights and their rooted trees.

Taylor series of exact solution in terms of trees [4] is given as

$$y(t_{n+1}) = y(t_n) + \sum h^{r(\hat{t})} 1/(\sigma(\hat{t})\gamma(\hat{t}))F(t)(y(t_n)) + O(h^{p+1}). \tag{2.4.1}$$

The numerical solution of Runge-Kutta method written in terms of trees [7] is given as

$$y_{n+1} = y_n + \sum \frac{h^{r(\hat{t})}\Phi(\hat{t})}{\sigma(\hat{t})} F(t)y(t_n) + O(h^{p+1}). \tag{2.4.2}$$

Comparing equations (2.4.1) and (2.4.2), we have

$$\Phi(\hat{t}) = \frac{1}{\gamma(\hat{t})}, \tag{2.4.3}$$

where $\hat{t}$, $r(\hat{t})$ and $\Phi(\hat{t})$ are rooted tree, order and elementary weight of that rooted tree respectively. So the equation (2.4.3) is the order condition for the Runge-Kutta method.

Example 2.4.1. Consider a tree $\hat{t} =$ .
The elementary weight is

$$\Phi(\hat{t}) = \sum_{i,j=1}^{s} b_i a_{ij} c_j^2.$$

And the density is

$$\gamma(\hat{t}) = 12.$$

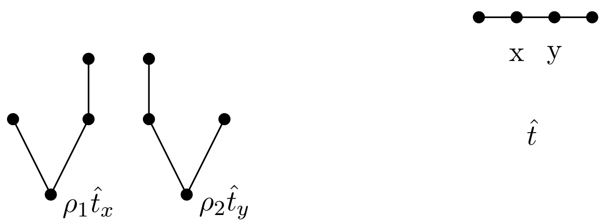
The order condition for this tree is

$$\Phi(\hat{t}) = \frac{1}{\gamma(\hat{t})}$$

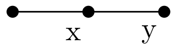
$$\Phi(\hat{t}) = \sum_{i,j=1}^{s} b_i a_{ij} c_j^2 = \frac{1}{12}$$

2.5 Superfluous trees and non-superfluous trees

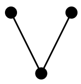
A tree is called superfluous [7], if it generates identical rooted trees when any two adjacent nodes of the tree are taken as a root. Consider a tree $\hat{t}$ which have vertices x and y. Let x is taken as root and $\rho_1\hat{t}_x$ is rooted tree. If we take y as root and $\rho_2\hat{t}_y$ is rooted tree.



As we can see that $\rho_1\hat{t}_x$ and $\rho_2\hat{t}_y$ represents two identical rooted trees so underlying tree is superfluous tree. The important thing is we can choose any two adjacent vertices as roots. A superfluous tree has even number of vertices.
We consider another tree $\hat{t}_1$ which have vertices x and y. Let x is taken as root and $\rho_3\hat{t}_{1x}$ is a rooted tree. If we take y as root and $\rho_3\hat{t}_{1y}$ is rooted tree.



$\hat{t}_1$



$\rho_3\hat{t}_{1x}$

$\rho_4\hat{t}_{1y}$

We can see that $\rho_3\hat{t}_{1x}$ and $\rho_4\hat{t}_{1y}$ are two different rooted trees. So we did not get two identical rooted trees for any of the two adjacent vertices being taken as root. Thus tree $\hat{t}_1$ is a non-superfluous tree. A non-superfluous tree has odd number of vertices.

2.6 Order conditions for symplectic Runge-Kutta methods in terms of rooted trees

The symplectic Runge-Kutta methods have a particular order if the order conditions are satisfied which is a relation between the coefficients of these methods. The order conditions for symplectic Runge-Kutta methods [2, 12] are less then the order conditions for general Runge-Kutta methods. This is due to the fact the superfluous trees do not contribute in the order conditions while non-superfluous trees contribute half number of order conditions. The following table shows the possible rooted trees of order 1 to 4 for Runge-Kutta methods.

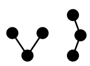
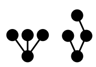
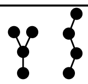
Order	rooted trees	order conditions
1		$\sum_{i=1}^{s} b_i = 1$
2		$\sum_{i=1}^{s} b_i c_i = \frac{1}{2}$
3		$\sum_{i=1}^{s} b_i c_i^2 = \frac{1}{3}, \quad \sum_{i,j=1}^{s} b_i a_{ij} c_j = \frac{1}{6}$
4		$\sum_{i=1}^{s} b_i c_i^3 = \frac{1}{4}, \quad \sum_{i,j=1}^{s} b_i c_i a_{ij} c_j = \frac{1}{8}$
4		$\sum_{i,j=1}^{s} b_i a_{ij} c_j^2 = \frac{1}{12}, \quad \sum_{i,j,k=1}^{s} b_i a_{ij} a_{jk} c_k = \frac{1}{24}$

Table 2.3: Order conditions and their rooted trees.

Now lets discuss the symplectic condition (2.3.2) of Runge-Kutta methods which is not effected by the following procedure:

1. First multiply symplectic condition by c_i then take summation.

2. First apply summation over symplectic condition then multiply it by c_i

In both cases we have same expression.
Proof:
Consider the symplectic condition (2.3.2) of Runge-Kutta methods.

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0. \quad \forall i, j = 1, 2, \ldots s. \tag{2.6.1}$$

Multiply equation (2.6.1) with c_j

$$b_i a_{ij} c_j + b_j c_j a_{ji} - b_i b_j c_j = 0. \quad \forall i, j = 1, 2, \ldots s. \tag{2.6.2}$$

Apply summation over equation (2.6.2) when $s = 2$, and after simplification, equation (2.6.2) becomes,

$$2b_1a_{11}c_1 + b_1a_{12}c_2 + b_2a_{21}c_1 + 2b_2a_{22}c_2 + b_1c_1a_{12} + b_2c_2a_{21} - b_1b_1c_1 - b_1b_2c_2 - b_2b_1c_1 - b_2b_2c_2 = 0. \tag{2.6.3}$$

Now first apply summation over equation (2.6.2) when $s = 2$,

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

multiply by c_j,

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

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

$$2b_1a_{11}c_1 - b_1^2c_1 + b_1a_{12}c_2 + b_2a_{21}c_2 - b_1b_2c_2 + b_2a_{21}c_1 + b_1a_{12}c_1 - b_2b_1c_1 + 2b_2a_{22}c_2 - b_2^2c_2 = 0. \tag{2.6.4}$$

We can see that equations (2.6.3) and (2.6.4) are same which shows that symplectic condition of Runge-Kutta methods is not being effected by the procedure.

Lets discuss that how number of order conditions reduces in symplectic Runge-Kutta methods.

For order 1.

We have only one possible tree •, which gives us only one order condition that is

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

•

There is only one order condition for one order symplectic Runge-Kutta methods.

For order 2.

We have one superfluous tree

which does not contribute in order conditions. For example consider the symplectic condition of Runge-Kutta methods from equation (2.3.2) then apply the summation over i and j from 1 to s, then we have

$$\sum_{i,j} b_i a_{ij} + \sum_{i,j} b_j a_{ji} - \sum_{i,j} b_i b_j = 0, \tag{2.6.5}$$

$$\Rightarrow 2 \sum_{i,j} b_i a_{ij} - 1 = 0,$$

$$\Rightarrow \sum_{i,j} b_i a_{ij} = \frac{1}{2}.$$

The order condition for $2nd$ order symplectic Runge-Kutta methods will automatically satisfy. The total number of order conditions for order two are one.

For order 3.

For order three, we have only one tree that is non-superfluous, that generates two rooted trees. This non-superfluous tree gives only one order condition. For example, consider the symplectic condition of Runge-Kutta methods from equation (2.3.2) multiply by c_j then apply the summation over i and j from 1 to s, then we have

$$\sum_{i,j} b_i a_{ij} c_j + \sum_{i,j} b_j c_j a_{ji} - \sum_{i,j} b_i b_j c_j = 0,$$

$$\sum_{i,j} b_i a_{ij} c_j + \sum_{i,j} b_j c_j a_{ji} - \frac{1}{2} = 0,$$

$$\sum_{i,j} b_i a_{ij} c_j + \sum_{i,j} b_j c_j a_{ji} - (\frac{1}{3} + \frac{1}{6}) = 0,$$

$$(\sum_{i,j} b_i a_{ij} c_j - \frac{1}{6}) + (\sum_{i,j} b_j c_j^2 - \frac{1}{3}) = 0.$$

From this we shall also take only one condition because second one will be automatically satisfied. The total number of order conditions for order three are two.

For order 4.

For order four, we have two trees: one is superfluous tree and second one is non-superfluous tree.

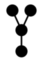
Superfluous tree does not give any order condition. A non-superfluous tree generates two rooted trees. This tree will give only one order condition. Now we want to see that how this tree is contributing in order conditions. Multiply symplectic condition of Runge-Kutta methods from equation (2.3.2) by c_j^2 then take the summation over i and j from 1 to s, then we have

$$\sum_{i,j} b_i a_{ij} c_j^2 + \sum_{i,j} b_j c_j^2 a_{ji} - \sum_{i,j} b_i b_j c_j^2 = 0,$$

$$\sum_{i,j} b_i a_{ij} c_j^2 + \sum_{i,j} b_j c_j^2 a_{ji} - \frac{1}{3} = 0,$$

$$\sum_{i,j} b_i a_{ij} c_j^2 + \sum_{i,j} b_j c_j^2 a_{ji} - (\frac{1}{4} + \frac{1}{12}) = 0,$$

$$(\sum_{i,j} b_i a_{ij} c_j^2 - \frac{1}{12}) + (\sum_{i,j} b_j c_j^2 a_{ji} - \frac{1}{4}) = 0.$$

From this we shall pick only one condition and second one will be automatically satisfied.
The total number of order conditions for order four are three.
Number of order conditions of Runge-Kutta methods and symplectic Runge-Kutta methods are given below in the following table.

Order	Number of order conditions for Runge-Kutta methods	Number of order conditions for symplectic Runge-Kutta methods
1	1	1
2	2	1
3	4	2
4	8	3
5	17	6

Table 2.4: Number of order conditions.

2.7 Partitioned Runge-Kutta methods

Sometime we deal with partitioned system of ODEs as follows

$$\begin{aligned} u' &= a(u, v), \\ v' &= b(u, v). \end{aligned} \tag{2.7.1}$$

To numerically solve equation (2.7.1) we can apply Partitioned Euler method which is given below

$$\begin{aligned} u_{n+1} &= u_n + ha(u_n, v_{n+1}), \\ v_{n+1} &= v_n + hb(u_n, v_{n+1}). \end{aligned} \tag{2.7.2}$$

where u_n is treated by implicit Euler method and v_n by explicit Euler method. Vogelaere introduced an important property of this method in 1956, which is symplecticity, that's why we call it symplectic Euler method.

Consider a system of ODEs as follows,

$$\begin{aligned} p' &= f(q), \qquad p(t_0) = p_0, \\ q' &= g(p), \qquad q(t_0) = q_0, \end{aligned} \tag{2.7.3}$$

because we are working on separable Hamiltonian systems. It is sometimes possible to solve the above mentioned ODEs using one Runge-Kutta method (a_{ij}, b_i) for one ODE and second one with different Runge-Kutta method $(\hat{a_{ij}}, \hat{b_i})$.

Suppose that b_i, a_{ij} and $\hat{b_i}$, $\hat{a_{ij}}$ be the coefficients of two Runge-Kutta methods. A partitioned Runge-Kutta method [1] for the solution of (2.7.3) is given by

$$\begin{aligned} P_i &= p_{n-1} + h\sum_{j=1}^{s} a_{ij} f(Q_j), \qquad 1 \le i \le s, \\ Q_i &= q_{n-1} + h\sum_{j=1}^{s} \hat{a}_{ij} g(P_j), \qquad 1 \le i \le s, \\ p_n &= p_{n-1} + h\sum_{i=1}^{s} b_i f(Q_i), \\ q_n &= q_{n-1} + h\sum_{i=1}^{s} \hat{b}_i g(P_i), \end{aligned} \tag{2.7.4}$$

where P_i and Q_i are the stages, p_n and q_n are the approximated solutions and s is the number of stages. A partitioned Runge-Kutta method [5,11] is represented by Butcher tableau

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \dots & a_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array} \qquad \begin{array}{c|cccc} \hat{c}_1 & \hat{a}_{11} & \hat{a}_{12} & \cdots & \hat{a}_{1s} \\ \hat{c}_2 & \hat{a}_{21} & \hat{a}_{22} & \dots & \hat{a}_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \hat{c}_s & \hat{a}_{s1} & \hat{a}_{s2} & \cdots & \hat{a}_{ss} \\ \hline & \hat{b}_1 & \hat{b}_2 & \cdots & \hat{b}_s \end{array}$$

where b_i and $\hat{b}_i$ are called the quadrature weights of the method. And

$$c_i = \sum_{j=1}^{s} a_{ij}, \quad \text{for} \;\; i = 1, 2...s, \qquad\qquad \hat{c}_i = \sum_{j=1}^{s} \hat{a}_{ij}, \quad \text{for} \;\; i = 1, 2...s,$$

are the quadrature nodes of the method at which the stages P_i and Q_i are calculated.

Example 2.7.1. The symplectic Euler method (2.7.2) is an example of partitioned Runge-Kutta method where the implicit Euler method $b_1 = 1$, $a_{11} = 1$ is combined with the explicit Euler method $b_1 = 1$, $a_{11} = 0$.

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

$$\begin{aligned} P_1 &= p_0 + hf(Q_1), \\ Q_1 &= q_0, \\ p_1 &= p_0 + hf(Q_1), \\ q_1 &= q_0 + hg(P_1). \end{aligned}$$

Example 2.7.2. An other example of partitioned Runge-Kutta method is,

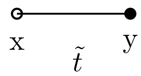
$$\begin{array}{c|cc} 0 & \frac{1}{8} & -\frac{1}{8} \\ \frac{2}{3} & \frac{5}{8} & \frac{1}{24} \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array} \qquad\qquad \begin{array}{c|cc} \frac{1}{3} & \frac{5}{24} & \frac{1}{8} \\ 1 & \frac{3}{8} & \frac{5}{8} \\ \hline & \frac{1}{4} & \frac{3}{4} \end{array}$$

$$\begin{aligned} P_1 &= p_0 + \frac{h}{8}f(Q_1) - \frac{h}{8}f(Q_2), \\ P_2 &= p_0 + \frac{5h}{8}f(Q_1) + \frac{h}{24}f(Q_2), \\ Q_1 &= q_0 + \frac{5h}{24}g(P_1) + \frac{h}{8}g(P_2), \\ Q_2 &= q_0 + \frac{3h}{8}g(P_1) + \frac{5h}{8}g(P_2), \\ p_1 &= p_0 + \frac{3h}{4}f(Q_1) + \frac{h}{4}f(Q_2), \\ q_1 &= q_0 + \frac{h}{4}g(P_1) + \frac{3h}{4}g(P_2). \end{aligned}$$

2.8 Bicolour trees and its use in partitioned Runge-Kutta methods

Trees play an important role in the development of partitioned Runge-Kutta methods. We have the following definitions.

Bicolour trees and bicolour rooted trees: Bicolour tree [1, 7] is simply a connected graph with no cycles. It is the combination of vertices and edges, its vertices have two colors one is black and other is white. It becomes a bicolour rooted tree if we fixed one vertex of it as root. We indicate the root by placing it at the bottom of a tree diagram. As an example we can take a bicolour tree



$\tilde{t}$

and its bicolour rooted trees are

The terms order, elementary weight and elementary differential are same as described in section 2.4.

Use of bicolour rooted trees in partitioned Runge-Kutta methods: Consider a system of ODEs as follows,

$$\begin{aligned} p' &= f(q), \quad p(t_0) = p_0, \\ q' &= g(p), \quad q(t_0) = q_0. \end{aligned} \tag{2.8.1}$$

The elementary differentials are

$$\begin{aligned} p' &= f(q), \\ p'' &= \frac{\partial f}{\partial q} g, \\ p''' &= \frac{\partial^2 f}{\partial q^2}(g, g) + \frac{\partial f \partial g}{\partial q \partial p} f. \end{aligned} \tag{2.8.2}$$

or

$$\begin{aligned} p' &= f, \\ p'' &= f_q g, \\ p''' &= f_{qq}(g, g) + f_q g_q g. \end{aligned} \tag{2.8.3}$$

where f, $f_q g$ etc. are elementary differentials. Similarly we can find the elementary differentials for $q' = g(p)$.

Bicolour rooted trees	Order	Elementary differentials	Elementary weights
	1	f	$\sum_{i=1}^{s} b_i$
	2	$f_q g$	$\sum_{ij=1}^{s} b_i \hat{a}_{ij}$
	3	$f_{qq}(g,g)$	$\sum_{i=1}^{s} b_i \hat{c}_i^2$
	3	$f_q g_p f$	$\sum_{ijk=1}^{s} b_i \hat{a}_{ij} c_j$

Table 2.5: Some bicolour rooted trees and their various functions.

Note: Here two same colour vertices do not connect with same edge.

2.9 Order conditions for partitioned Runge-Kutta methods

The order conditions [1] for a partitioned Runge-Kutta methods can be found by the same pattern as followed in Runge-Kutta methods. To find the order conditions of partitioned Runge-Kutta methods we have to compare the numerical solution with the Taylor series of exact solution. We calculate the order conditions of partitioned Runge-Kutta method by using explicit method as well as implicit method. To find the order of partitioned Runge-Kutta method we first explain the concept of elementary differentials that is

$$\begin{aligned} p' &= f(q), \\ p'' &= \frac{\partial f}{\partial q} g, \\ p''' &= \frac{\partial^2 f}{\partial q^2}(g,g) + \frac{\partial f \partial g}{\partial q \partial p} f \\ q' &= g(p), \\ q'' &= \frac{\partial g}{\partial p} f, \\ q''' &= \frac{\partial^2 g}{\partial p^2}(f,f) + \frac{\partial g \partial f}{\partial p \partial q} g. \end{aligned} \tag{2.9.1}$$

The general form of explicit partitioned Runge-Kutta method is

$$\begin{aligned}
P_i &= p_{n-1} + h\sum_{j=1}^{i-1} a_{ij} f(Q_j), \qquad 1 \le i \le s,\\
Q_i &= q_{n-1} + h\sum_{j=1}^{i-1} \hat{a}_{ij} g(P_j), \qquad 1 \le i \le s,\\
p_n &= p_{n-1} + h\sum_{i=1}^{s} b_i f(Q_i),\\
q_n &= q_{n-1} + h\sum_{i=1}^{s} \hat{b}_i g(P_i),
\end{aligned} \tag{2.9.2}$$

The following two relations are called the consistency conditions of methods.

$$\begin{aligned}
c_i &= \sum_{j=1}^{s} a_{ij} = 0, \qquad i = 1, 2, ...s,\\
\hat{c}_i &= \sum_{j=1}^{s} \hat{a}_{ij} = 0, \qquad i = 1, 2, ...s.
\end{aligned}$$

For $s = 2$,

$$\begin{aligned}
P_1 &= p_{n-1},\\
Q_1 &= p_{n-1}.
\end{aligned} \tag{2.9.3}$$

$$\begin{aligned}
P_2 &= p_{n-1} + ha_{21} f(q_{n-1}),\\
Q_2 &= p_{n-1} + h\hat{a}_{21} g(p_{n-1}).
\end{aligned} \tag{2.9.4}$$

By using equation (2.9.4) the approximate solution becomes

$$\begin{aligned}
p_n &= p_{n-1} + hb_1 f(q_{n-1}) + hb_2 f(q_{n-1} + h\hat{a}_{21} g(p_{n-1})),\\
q_n &= p_{n-1} + h\hat{b}_1 g(p_{n-1}) + h\hat{b}_1 g(p_{n-1} + ha_{21} f(q_{n-1})),
\end{aligned} \tag{2.9.5}$$

$$\begin{aligned}
p_n &= p_{n-1} + hb_1 f(q_{n-1}) + hb_2 f(q_{n-1}) + h^2 b_2 \hat{a}_{21} \frac{\partial f}{\partial q_{n-1}} g(p_{n-1})) + O(h^3),\\
q_n &= p_{n-1} + h\hat{b}_1 g(p_{n-1}) + h\hat{b}_1 g(p_{n-1}) + h^2 \hat{b}_2 a_{21} \frac{\partial g}{\partial p_{n-1}} f(q_{n-1})) + O(h^3).
\end{aligned} \tag{2.9.6}$$

Now the Taylor series of the exact solution is

$$\begin{aligned}
p(t_n) &= p(t_{n-1}) + hp'(t_{n-1}) + \frac{h^2}{2!} p''(t_{n-1}) + O(h^3),\\
q(t_n) &= q(t_{n-1}) + hq'(t_{n-1}) + \frac{h^2}{2!} q''(t_{n-1}) + O(h^3).
\end{aligned} \tag{2.9.7}$$

Now using (2.9.1) in equation (2.9.7) then comparing it with equation (2.9.6), we have the following order conditions.
For first order partitioned Runge-Kutta methods,

$$\begin{aligned} \sum_{i=1}^{2} b_i &= 1, \\ \sum_{i=1}^{2} \hat{b}_i &= 1. \end{aligned} \tag{2.9.8}$$

For second order partitioned Runge-Kutta methods,

$$\begin{aligned} \hat{b}_2 a_{21} &= \frac{1}{2}, \\ b_2 \hat{a}_{21} &= \frac{1}{2}. \end{aligned} \tag{2.9.9}$$

In general,
For first order partitioned Runge-Kutta methods,

$$\begin{aligned} \sum_{i=1}^{s} b_i &= 1, \\ \sum_{i=1}^{s} \hat{b}_i &= 1. \end{aligned} \tag{2.9.10}$$

For second order partitioned Runge-Kutta methods,

$$\begin{aligned} \sum_{ij=1}^{s} \hat{b}_i a_{ij} &= \frac{1}{2}, \\ \sum_{ij=1}^{s} b_i \hat{a}_{ij} &= \frac{1}{2}. \end{aligned} \tag{2.9.11}$$

For third order partitioned Runge-Kutta methods,

$$\begin{aligned} \sum_{i,j=1}^{s} \hat{b}_i c_i a_{ij} &= \frac{1}{3}, \\ \sum_{i,j=1}^{s} b_i \hat{c}_i \hat{a}_{ij} &= \frac{1}{3}, \\ \sum_{i,j=1}^{s} b_i \hat{a}_{ij} c_j &= \frac{1}{6}, \\ \sum_{i,j=1}^{s} \hat{b}_i a_{ij} \hat{c}_j &= \frac{1}{6}. \end{aligned} \tag{2.9.12}$$

2.10 Symplectic partitioned Runge-Kutta methods

Symplecticity of Runge-Kutta methods were discussed in chapter 1. In the same way symplecticity of partitioned Runge-Kutta methods [4, 11] also discussed here. Consider an IVP which is given in equation (2.7.3) and partitioned Runge-Kutta method (2.7.4). Partitioned Runge-Kutta method is symplectic, if numerical solution vectors p_n and q_n of partitioned Runge-Kutta methods (2.7.4) satisfy

$$< p_{n+1}, q_{n+1} >=< p_n, q_n > . \tag{2.10.1}$$

This is only possible if the coefficients of partitioned Runge-Kutta 2.7.4 methods satisfy

$$b_i \hat{a}_{ij} + \hat{b}_j a_{ji} - b_i \hat{b}_j = 0, \qquad i, j = 1, 2, \dots s. \tag{2.10.2}$$

Equation (2.10.2) is said to be symplectic condition.
Proof:
For a conservative system, as given in quadratic invariant in section (1.5)

$$z^t C f(z) =< z^t, f(z) >= 0, \forall \qquad z, \tag{2.10.3}$$

where C is identity matrix, now for partitioned Runge-Kutta methods (2.7.4), we apply (2.10.3) on the stages of partitioned Runge-Kutta methods. Therefore,

$$< P_i, g(P_i, Q_i) >= 0,$$

using (2.7.4)

$$< p_n + h \sum_{j=1}^{s} a_{ij} f(P_j, Q_j), g(P_i, Q_i) >= 0,$$

$$< p_n, g(P_i, Q_i) >= -h \sum_{j=1}^{s} a_{ij} < f(P_j, Q_j), g(P_i, Q_i) > . \tag{2.10.4}$$

Again consider

$$< Q_i, f(P_i, Q_i) >= 0,$$

using (2.7.4)

$$< q_n + h \sum_{j=1}^{s} \hat{a}_{ij} f(P_j, Q_j), f(P_i, Q_i) >= 0,$$

$$< q_n, f(P_i, Q_i) >= -h \sum_{j=1}^{s} \hat{a}_{ij} < g(P_j, Q_j), f(P_i, Q_i) > . \tag{2.10.5}$$

Take the left hand side of equation (2.10.1) using equation (2.7.4) we have

$$< p_{n+1}, q_{n+1} > =< p_n + h\sum_{i=1}^{s} b_i f(P_i, Q_i), q_n + h\sum_{i=1}^{s} \hat{b}_i g(P_i, Q_i) >,$$

$$< p_{n+1}, q_{n+1} > =< p_n, q_n > +h\sum_{i=1}^{s} \hat{b}_i < p_n, g(P_i, Q_i) > +h\sum_{i=1}^{s} b_i < f(P_i, Q_i), q_n, >$$

$$+ h^2 \sum_{ij=1}^{s} b_i\hat{b}_i < f(P_i.Q_i), g(P_i, Q_i) > .$$

Now using equations (2.10.4) and (2.10.5) in above equation

$$< p_{n+1}, q_{n+1} > =< p_n, q_n > -h^2 \sum_{ij=1}^{s} \hat{b}_j a_{ji} < f(P_i, Q_i), g(P_j, Q_j) >$$

$$- h^2 \sum_{ij=1}^{s} b_i \hat{a}_{ij} < f(P_j, Q_j), g(P_i, Q_i) > +h^2 \sum_{ij=1}^{s} b_i\hat{b}_j < f(P_j, Q_j), g(P_i, Q_i) >,$$

$$< p_{n+1}, q_{n+1} > =< p_n, q_n > +h^2 \sum_{ij=1}^{s} (-b_i\hat{a}_{ij} - \hat{b}_j a_{ji} + b_i\hat{b_j}) < f(P_j, Q_j), g(P_i, Q_i) > .$$

Now we have our required equation

$$< p_{n+1}, q_{n+1} >=< p_n, q_n > .$$

If and only if

$$h^2 \sum_{ij=1}^{s} (-b_i\hat{a}_{ij} - \hat{b}_j a_{ji} + b_i\hat{b_j}) < f(P_j, Q_j), g(P_i, Q_i) >= 0.$$

Since

$$< f(P_j, Q_j), g(P_i, Q_i) >\neq 0,$$

therefore

$$h^2 \sum_{ij=1}^{s} (-b_i\hat{a}_{ij} - \hat{b}_j a_{ji} + b_i\hat{b_j}) = 0,$$

hence

$$b_i\hat{a}_{ij} + \hat{b}_j a_{ji} - b_i\hat{b_j} = 0. \qquad i, j = 1, 2...s.$$

2.11 Order conditions for symplectic partitioned Runge-Kutta methods using rooted trees

To define order conditions for symplectic partitioned Runge-Kutta methods we use the bicolour trees which have been already discussed. Superfluous bicolour trees and non-superfluous bicolour trees are playing main role in construction of order conditions for

symplectic partitioned Runge-Kutta methods. The difference between these trees is that a non-superfluous bicolour tree gives two order conditions while a superfluous bicolour tree generates only one order condition.
The vertices of trees for that Runge-Kutta methods by which one can solve $p' = f(q)$ are represented by filled circle. The vertices of trees for that Runge-Kutta methods which can be use to solve $q' = g(p)$ are represented by empty circle. The following table shows the possible trees of order 1 to 4.

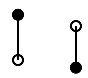
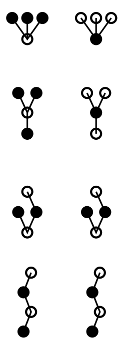
Order	rooted trees	order conditions
1		$\sum_{i=1}^{s} b_i = 1 \quad \sum_{i=1}^{s} \hat{b}_i = 1$
2		$\sum_{i=1}^{s} \hat{b}_i c_i = \frac{1}{2} \quad \sum_{i=1}^{s} b_i \hat{c}_i = \frac{1}{2}$
3		$\sum_{i=1}^{s} \hat{b}_i c_i^2 = \frac{1}{3} \quad \sum_{i=1}^{s} b_i \hat{c}_i^2 = \frac{1}{3}$
3		$\sum_{i,j=1}^{s} b_i \hat{a}_{ij} c_j = \frac{1}{6} \quad \sum_{i,j=1}^{s} \hat{b}_i a_{ij} \hat{c}_j = \frac{1}{6}$
4		$\sum_{i=1}^{s} \hat{b}_i c_i^3 = \frac{1}{4} \quad \sum_{i=1}^{s} b_i \hat{c}_i^3 = \frac{1}{4}$
		$\sum_{i,j=1}^{s} b_i \hat{a}_{ij} c_j^2 = \frac{1}{12} \quad \sum_{i,j=1}^{s} \hat{b}_i a_{ij} \hat{c}_j^2 = \frac{1}{12}$
		$\sum_{i,j=1}^{s} \hat{b}_i c_i a_{ij} \hat{c}_j = \frac{1}{8} \quad \sum_{i,j=1}^{s} b_i \hat{c}_i \hat{a}_{ij} c_j = \frac{1}{8}$
		$\sum_{i,j,k=1}^{s} \hat{b}_i a_{ij} \hat{a}_{jk} c_k = \frac{1}{24} \quad \sum_{i,j,k=1}^{s} b_i \hat{a}_{ij} a_{jk} \hat{c}_k = \frac{1}{24}$

Table 2.6: Bicolour rooted trees and their order conditions up to order 4.

Here the location of root of bicolour rooted tree does not effect the order conditions at all.
For order 1
We have two possible superfluous bicolour trees ● and ○ which give us two order conditions such that,

$$\sum_{i=1}^{s} b_i = 1, \quad \sum_{i=1}^{s} \hat{b}_i = 1.$$

The total number of order conditions for order one are two.

For order 2

We have one superfluous bicolour tree

which generates only one order condition. For example consider the symplectic condition (2.10.2) of partitioned Runge-Kutta methods then apply the summation over i and j from 1 to s, then we have

$$\sum_{ij=1}^{s} \hat{b}_i a_{ij} + \sum_{ji=1}^{s} b_j \hat{a}_{ji} - \sum_{ij=1}^{s} b_i \hat{b}_j = 0,$$

$\Rightarrow$

$$(\sum_{ij=1}^{s} \hat{b}_i a_{ij} - \frac{1}{2}) + (\sum_{ji=1}^{s} b_j \hat{a}_{ji} - \frac{1}{2}) = 0.$$


From this we shall take only one condition because second is automatically be satisfied. Thus the total number of order conditions for order two are three.

For order 3

For order three, these two non-superfluous bicolour trees

generate four bicolour rooted trees such that two pairs are identical. Thus these non-superfluous bicolour trees give only two order conditions. For example, consider the symplectic condition (2.10.2) of partitioned Runge-Kutta methods, multiply it by c_j, and apply the summation over i and j from 1 to s, then we have

$$\sum_{ij=1}^{s} b_i \hat{a}_{ij} c_j + \sum_{ji=1}^{s} \hat{b}_j c_j a_{ji} - \sum_{ij=1}^{s} b_i \hat{b}_j c_j = 0, \tag{2.11.1}$$

$\Rightarrow$

$$\sum_{ij=1}^{s} b_i \hat{a}_{ij} c_j + \sum_{ji=1}^{s} \hat{b}_j c_j a_{ji} - \frac{1}{2} = 0,$$

$\Rightarrow$

$$\sum_{ij=1}^{s} b_i \hat{a}_{ij} c_j + \sum_{ji=1}^{s} \hat{b}_j c_j a_{ji} - (\frac{1}{3} + \frac{1}{6}) = 0.$$

$\Rightarrow$

$$(\sum_{ij=1}^{s} b_i \hat{a}_{ij} c_j - \frac{1}{6}) + (\sum_{ji=1}^{s} \hat{b}_j c_j a_{ji} - \frac{1}{3}) = 0.$$


From this we shall also take only one condition because second one will be automatically satisfied. Now for second order condition again multiply symplectic condition (2.10.2) of partitioned Runge-Kutta method by $\hat{c}_i$ then take the summation over i and j from 1 to s, then we have

$$\sum_{ij=1}^{s} b_i\hat{c}_i\hat{a}_{ij} + \sum_{ji=1}^{s} \hat{b}_j a_{ji}\hat{c}_i - \sum_{ij=1}^{s} b_i\hat{c}_j\hat{b}_j = 0,$$

$\Rightarrow$

$$\sum_{ij=1}^{s} b_i\hat{c}_j^2 + \sum_{ji=1}^{s} \hat{b}_j a_{ji}\hat{c}_i - \frac{1}{2} = 0,$$

$\Rightarrow$

$$\sum_{ij=1}^{s} b_i\hat{c}_j^2 + \sum_{ji=1}^{s} \hat{b}_j a_{ji}\hat{c}_i - (\frac{1}{6} + \frac{1}{2}) = 0,$$

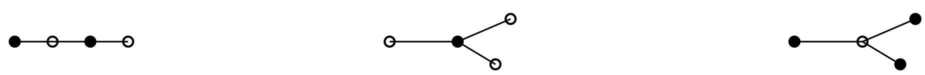
$\Rightarrow$

$$(\sum_{ij=1}^{s} b_i\hat{c}_j^2 - \frac{1}{3}) + (\sum_{ji=1}^{s} \hat{b}_j a_{ji}\hat{c}_i - \frac{1}{6}) = 0.$$

From this we shall also pick only one condition because second one will be automatically satisfied. Thus total number of order conditions for order three are five.

For order 4

For order four, we have one superfluous bicolour tree and two non-superfluous bicolour trees.



Superfluous bicolour tree gives one order condition. Two non-superfluous bicolour trees generate four bicolour rooted trees such that two pairs are identical. These trees give only two order conditions. Now we want to see that how these trees are contributing in order conditions. Multiply symplectic condition (2.10.2) of partitioned Runge-Kutta methods by c_j^2 then take the summation over i and j from 1 to s, then we have

$$\sum_{ij=1}^{s} b_i\hat{a}_{ij}c_j^2 + \sum_{ji=1}^{s} \hat{b}_j c_j^2 a_{ji} - \sum_{ij=1}^{s} \hat{b}_j c_j^2 b_i = 0,$$

$\Rightarrow$

$$\sum_{ij=1}^{s} b_i\hat{a}_{ij}c_j^2 + \sum_{ji=1}^{s} \hat{b}_j c_j^2 a_{ji} - \frac{1}{3} = 0,$$

⇒

$$(\sum_{ij=1}^{s} b_i \hat{a}_{ij} c_j^2 - \frac{1}{12}) + (\sum_{ji=1}^{s} \hat{b}_j c_j^2 a_{ji} - \frac{1}{4}) = 0.$$

From this we shall take only one condition because second one is automatically be satisfied. Again multiply symplectic condition (2.10.2) of partitioned Runge-Kutta methods by $\hat{c}_i^2$ then take the summation over i and j from 1 to s, then we have

$$\sum_{ij=1}^{s} b_i \hat{c}_i^2 \hat{a}_{ij} + \sum_{ji=1}^{s} \hat{b}_j a_{ji} \hat{c}_i^2 - \sum_{ij=1}^{s} b_i \hat{c}_i^2 \hat{b}_j = 0,$$

⇒

$$\sum_{ij=1}^{s} b_i \hat{c}_i^2 \hat{a}_{ij} + \sum_{ji=1}^{s} \hat{b}_j a_{ji} \hat{c}_i^2 - \frac{1}{3} = 0,$$

⇒

$$\sum_{ij=1}^{s} b_i \hat{c}_i^2 \hat{a}_{ij} + \sum_{ji=1}^{s} \hat{b}_j a_{ji} \hat{c}_i^2 - (\frac{1}{12} + \frac{1}{4}) = 0,$$

⇒

$$(\sum_{ij=1}^{s} b_i \hat{c}_i^2 \hat{a}_{ij} - \frac{1}{4}) + (\sum_{ji=1}^{s} \hat{b}_j a_{ji} \hat{c}_i^2 - \frac{1}{2}) = 0.$$

Now for third order condition, again multiply symplectic condition (2.10.2) of partitioned Runge-Kutta method by $a_{jk}\hat{c}_k$, we have

$$\sum_{ij=1}^{s} b_i \hat{a}_{ij} a_{jk} \hat{c}_k + \sum_{ji=1}^{s} \hat{b}_j a_{ji} a_{jk} \hat{c}_k - \sum_{ij=1}^{s} b_i \hat{b}_j a_{jk} \hat{c}_k = 0,$$

⇒

$$\sum_{ij=1}^{s} b_i \hat{a}_{ij} a_{jk} \hat{c}_k + \sum_{ji=1}^{s} \hat{b}_j a_{ji} a_{jk} \hat{c}_k - \frac{1}{6} = 0,$$

⇒

$$\sum_{ij=1}^{s} b_i \hat{a}_{ij} a_{jk} \hat{c}_k + \sum_{ji=1}^{s} \hat{b}_j a_{ji} a_{jk} \hat{c}_k - (\frac{1}{24} + \frac{1}{8}) = 0,$$

⇒

$$(\sum_{ij=1}^{s} b_i \hat{a}_{ij} a_{jk} \hat{c}_k - \frac{1}{24}) + (\sum_{ji=1}^{s} \hat{b}_j a_{ji} a_{jk} \hat{c}_k - \frac{1}{8}) = 0.$$

Therefore total number of order conditions for symplectic partitioned Runge-Kutta methods of order four are eight. Number of order conditions for partitioned Runge-Kutta method and symplectic partitioned Runge-Kutta method are given below in Table

Order	Number of order conditions for partioned Runge-Kutta methods	Number of order conditions for symplectic partitioned Runge-Kutta methods
1	1	2
2	4	3
3	8	5
4	16	8
5	34	14

Table 2.7: Number of order conditions.

Chapter 3

Construction of symplectic Runge-Kutta methods and partitioned Runge-Kutta methods with V-transformation

3.1 Construction of symplectic Runge-Kutta methods

In this chapter we are going to construct symplectic Runge-Kutta methods and symplectic partitioned Runge-Kutta methods with the help of Vandermonde transformation. For a Runge-Kutta method (2.1.2) we need to find the values of a's, b's and c's. Our strategy is to write the values of a's and b's in terms of c's. We then choose the values of c's [2,6] from shifted Legendre polynomial on the interval $[0,1]$. The shifted Legendre polynomial of degree s on the interval $[0,1]$ is,

$$P_s^* = \frac{d^s}{dt^s}(t^s(t-1)^s) \tag{3.1.1}$$

Gauss:
The values of c_i's are the zeros of shifted Legendre polynomial.
Radau-I:
$c_1 = 0$, the remaining c_i are chosen as the zeros of $P_s^*(x)$+$P_{s-1}^*(x)$.
Radau-II:
$c_s = 1$, the remaining c_i are chosen as the zeros of $P_s^*(x)$-$P_{s-1}^*(x)$.
Lobatto-III:
$c_1 = 0$ and $c_s = 1$,
the remaining c_i are chosen as the zeros of $P_s^*(x)$-$P_{s-2}^*(x)$.

Note: If we have s-stage Gauss, Radau-I, Radau-II and Lobatto-III Runge-Kutta methods then the order of these methods is $2s$, $2s-1$, $2s-1$ and $2s-2$ respectively.

Using Vandermonde transformation [6, 7], we can construct the symplectic Runge-Kutta methods. For this we use the pre and post multiplication of Vandermonde matrix with symplectic condition of Runge-Kutta method (2.1.2).
Consider a Runge-Kutta method $[\mathbf{A}, b^T, c]$ and consider the Vandermonde matrix V given as,

$$V = c_i^{j-1} = \begin{bmatrix} 1 & c_1 & c_1^2 & \dots & c_1^{s-1} \\ 1 & c_2 & c_2^2 & \dots & c_2^{s-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & c_s & c_s^2 & \dots & c_s^{s-1} \end{bmatrix}$$

Multiply symplectic condition (2.3.2) of Runge-Kutta methods with matrix V as follows

$$c_i^{k-1}(b_i a_{ij} + b_j a_{ji} - b_i b_j) c_j^{l-1} = 0, \;\; \forall\, i, j, k, l = 1, 2...s. \tag{3.1.2}$$

For order two, put $l, k = 1, 2$, and then take summation over i and j from 1 to s.
For $l = 1$, $k = 1$,

$$\sum_{i,j} b_i a_{ij} + \sum_{i,j} b_j a_{ji} - \sum_{i,j} b_i b_j = 0. \tag{3.1.3}$$

For $l = 1$, $k = 2$,

$$\sum_{i,j} b_i c_i a_{ij} + \sum_{i,j} b_j a_{ji} c_i - \sum_{i,j} b_i c_i b_j = 0. \tag{3.1.4}$$

For $l = 2$, $k = 1$,

$$\sum_{i,j} b_i a_{ij} c_j + \sum_{i,j} b_j c_j a_{ji} - \sum_{i,j} b_i b_j c_j = 0. \tag{3.1.5}$$

For $l = 2$, $k = 2$,

$$\sum_{i,j} b_i c_i a_{ij} c_j + \sum_{i,j} b_j c_j a_{ji} c_i - \sum_{i,j} b_i c_i b_j c_j = 0. \tag{3.1.6}$$

We are constructing method of order two, then following order conditions (2.2.14) and (2.2.15) must satisfy

$$\sum_{i}^{s} b_i = 1, \qquad \sum_{i=1}^{s} b_i c_i = \frac{1}{2}. \tag{3.1.7}$$

Using equations (3.1.7) in equations (3.1.3)-(3.1.6) we have

$$\sum_{i,j} b_i a_{ij} = \frac{1}{2}, \quad \text{or} \quad \sum_{i} b_i c_i = \frac{1}{2}. \tag{3.1.8}$$

$$\sum_{i,j} b_i c_i a_{ij} + \sum_{i,j} b_j a_{ji} c_i = \frac{1}{2}. \tag{3.1.9}$$

$$\sum_{i,j} b_i a_{ij} c_j + \sum_{i,j} b_j c_j a_{ji} = \frac{1}{2}. \tag{3.1.10}$$

$$\sum_{i,j} b_i c_i a_{ij} c_j = \frac{1}{8}. \tag{3.1.11}$$

Now for the values of b_2 we consider the relation

$$b_i(c_i - c_1) = b_i c_i - b_i c_1. \tag{3.1.12}$$

Take summation over i from 1 to s and use the equations (3.1.7) we have

$$\sum_i b_i(c_i - c_1) = \sum_i b_i c_i - \sum_i b_i c_1,$$

$$b_2(c_2 - c_1) = \frac{1}{2} - c_1,$$

$$b_2 = \frac{(\frac{1}{2} - c_1)}{c_2 - c_1}.$$

Similarly we can get

$$b_1 = \frac{(\frac{1}{2} - c_2)}{c_1 - c_2}.$$

Now to calculate a_{11} we consider the following relation,

$$b_i(c_i - c_2)a_{ij}(c_j - c_2) = b_i c_i a_{ij} c_j - b_i c_i a_{ij} c_2 - b_i a_{ij} c_j c_2 + b_i a_{ij} c_2 c_2,$$

take the summation over i and j, and use equations (3.1.7)-(3.1.11) we have

$$a_{11} = \frac{\frac{1}{8} - \frac{c_2}{3} - \frac{c_2}{6} + \frac{c_2 c_2}{2}}{b_1(c_1 - c_2)(c_1 - c_2)}.$$

Similarly we have

$$a_{12} = \frac{\frac{1}{8} - \frac{c_1}{3} - \frac{c_2}{6} + \frac{c_2 c_1}{2}}{b_1(c_1 - c_2)(c_2 - c_1)},$$

$$a_{21} = \frac{\frac{1}{8} - \frac{c_2}{3} - \frac{c_1}{6} + \frac{c_1 c_2}{2}}{b_2(c_2 - c_1)(c_1 - c_2)},$$

$$a_{22} = \frac{\frac{1}{8} - \frac{c_1}{3} - \frac{c_1}{6} + \frac{c_1 c_1}{2}}{b_2(c_2 - c_1)(c_2 - c_1)}.$$

A class of two stages symplectic Runge-Kutta methods can be found by choosing c_1 and c_2. We can choose c_1 and c_2 as the zeros of shifted Legendre polynomial.

Gauss: $s = 2$

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

Radau-I: $s = 2$

$$\begin{array}{c|cc} 0 & \frac{1}{8} & \frac{-1}{8} \\ \frac{2}{3} & \frac{7}{24} & \frac{3}{8} \\ \hline & \frac{1}{4} & \frac{3}{4} \end{array}$$

Radau-II: $s = 2$

$$\begin{array}{c|cc} \frac{1}{3} & \frac{3}{8} & \frac{-1}{24} \\ 1 & \frac{7}{8} & \frac{1}{8} \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array}$$

For order three

Put $l, k = 1, 2, 3,$ in equation (3.1.4) and then take summation over i and j from 1 to s.

For $l = 1$, $k = 1$,

$$\sum_{i,j} b_i a_{ij} + \sum_{i,j} b_j a_{ji} - \sum_{i,j} b_i b_j = 0. \tag{3.1.13}$$

For $l = 1$, $k = 2$,

$$\sum_{i,j} b_i c_i a_{ij} + \sum_{i,j} b_j a_{ji} c_i - \sum_{i,j} b_i c_i b_j = 0. \tag{3.1.14}$$

For $l = 1$, $k = 3$,

$$\sum_{i,j} b_i c_i^2 a_{ij} + \sum_{i,j} b_j a_{ji} c_i^2 - \sum_{i,j} b_i c_i^2 b_j = 0. \tag{3.1.15}$$

For $l = 2$, $k = 1$,

$$\sum_{i,j} b_i a_{ij} c_j + \sum_{i,j} b_j c_j a_{ji} - \sum_{i,j} b_i b_j c_j = 0. \tag{3.1.16}$$

For $l = 3$, $k = 1$,

$$\sum_{i,j} b_i a_{ij} c_j^2 + \sum_{i,j} b_j c_j^2 a_{ji} - \sum_{i,j} b_i b_j c_j^2 = 0. \tag{3.1.17}$$

For $l = 2$, $k = 2$,

$$\sum_{i,j} b_i c_i a_{ij} c_j + \sum_{i,j} b_j c_j a_{ji} c_i - \sum_{i,j} b_i c_i b_j c_j = 0. \tag{3.1.18}$$

For $l = 3$, $k = 3$,

$$\sum_{i,j} b_i c_i^2 a_{ij} c_j^2 + \sum_{i,j} b_j c_j^2 a_{ji} c_i^2 - \sum_{i,j} b_i c_i^2 b_j c_j^2 = 0. \tag{3.1.19}$$

In order to construct method of order three, the following order conditions (2.2.14), (2.2.15) and (2.2.16) must satisfy.

$$\sum_{i=1}^{s} b_i = 1, \qquad \sum_{i=1}^{s} b_i c_i = \frac{1}{2}, \qquad \sum_{i=1}^{s} b_i c_i^2 = \frac{1}{3}, \qquad \sum_{i,j=1}^{s} b_i a_{ij} c_j = \frac{1}{6}. \tag{3.1.20}$$

Using equations (3.1.20) in equations (3.1.13)-(3.1.19) we have

$$\sum_{i,j} b_i a_{ij} = \frac{1}{2} \quad \text{or} \quad \sum_{i} b_i c_i = \frac{1}{2}. \tag{3.1.21}$$

$$\sum_{i,j} b_i c_i a_{ij} + \sum_{i,j} b_j a_{ji} c_i = \frac{1}{2}. \tag{3.1.22}$$

$$\sum_{i,j} b_i c_i^2 a_{ij} + \sum_{i,j} b_j a_{ji} c_i^2 = \frac{1}{3}. \tag{3.1.23}$$

$$\sum_{i,j} b_i a_{ij} c_j + \sum_{i,j} b_j c_j a_{ji} = \frac{1}{2}. \tag{3.1.24}$$

$$\sum_{i,j} b_i a_{ij} c_j^2 + \sum_{i,j} b_j c_j^2 a_{ji} = \frac{1}{3}. \tag{3.1.25}$$

$$\sum_{i,j} b_i c_i a_{ij} c_j = \frac{1}{8}. \tag{3.1.26}$$

$$\sum_{i,j} b_i c_i^2 a_{ij} c_j^2 = \frac{1}{18}. \tag{3.1.27}$$

Now for the values of b_1, b_2 and b_3 we consider the following relations respectively.

$$b_i(c_i - c_2)(c_i - c_3) = b_i c_i^2 - b_i c_i c_3 - b_i c_i c_2 + b_i c_2 c_3, \tag{3.1.28}$$

$$b_i(c_i - c_1)(c_i - c_3) = b_i c_i^2 - b_i c_i c_3 - b_i c_i c_1 + b_i c_1 c_3,$$

$$b_i(c_i - c_1)(c_i - c_2) = b_i c_i^2 - b_i c_i c_2 - b_i c_i c_1 + b_i c_1 c_2,$$

In equation (3.1.28) take summation over i from 1 to s, using equations (3.1.20) and (3.1.21), we have

$$b_i(c_i - c_2)(c_i - c_3) = b_i c_i^2 - b_i c_i c_3 - b_i c_i c_2 + b_i c_2 c_3,$$

$$b_1(c_1 - c_2)(c_1 - c_3) = \frac{1}{3} - \frac{c_3}{2} - \frac{c_2}{2} + c_2 c_3,$$

$$b_1 = \frac{(2 - 3(c_3 + c_2 - 2c_2 c_3))}{(6(c_1 - c_2)(c_1 - c_3))}.$$

Similarly we have

$$b_2 = \frac{(2 - 3(c_3 + c_1 - 2c_1 c_3))}{(6(c_2 - c_1)(c_2 - c_3))}.$$

$$b_3 = \frac{(2 - 3(c_1 + c_2 - 2c_2 c_1))}{(6(c_3 - c_2)(c_3 - c_1))}.$$

Now for the value of a_{11} consider the following relation

$$b_i(c_i-c_2)(c_i-c_3)a_{ij}(c_j-c_2)(c_j-c_3) = b_ic_i^2a_{ij}c_j^2 - b_ic_i^2a_{ij}c_jc_3 - b_ic_i^2a_{ij}c_jc_2 + b_ic_i^2a_{ij}c_2c_3$$
$$- b_ic_ia_{ij}c_j^2c_3 + b_ic_ia_{ij}c_jc_3c_3 + b_ic_ia_{ij}c_jc_3c_2 - b_ic_ia_{ij}c_2c_3c_3 - b_ic_ia_{ij}c_j^2c_2 + b_ic_ia_{ij}c_jc_2c_3$$
$$+ b_ic_ia_{ij}c_jc_2c_2 - b_ic_ia_{ij}c_2c_3c_2 + b_ia_{ij}c_j^2c_3c_2 - b_ia_{ij}c_jc_3c_3c_2c_3 - b_ia_{ij}c_jc_3c_2c_2 + b_ia_{ij}c_2c_2c_3c_3.$$

Take summation over i and j from 1 to s, then using equations (3.1.20) and (3.1.21)-(3.1.27) we have

$$b_1(c_1-c_2)(c_1-c_3)a_{11}(c_1-c_2)(c_1-c_3) = \frac{1}{18} - \frac{(c_2+c_3)}{10} + \frac{c_2c_3}{4} - \frac{c_2+c_3}{15} + \frac{(c_2+c_3)(c_2+c_3)}{8} - \frac{c_2c_3(c_2+c_3)}{6} + \frac{c_2c_3}{12} - \frac{c_2c_3(c_2+c_3)}{3} + \frac{c_2c_2c_3c_3}{2},$$

$$a_{11} = \frac{\frac{1}{18} - \frac{(c_2+c_3)}{10} + \frac{c_2c_3}{4} - \frac{c_2+c_3}{15} + \frac{(c_2+c_3)(c_2+c_3)}{8} - \frac{c_2c_3(c_2+c_3)}{6} + \frac{c_2c_3}{12} - \frac{c_2c_3(c_2+c_3)}{3} + \frac{c_2c_2c_3c_3}{2}}{b_1(c_1-c_2)(c_1-c_3)(c_2-c_1)(c_2-c_3)}.$$

Similarly we have

$$a_{12} = \frac{\frac{1}{18} - \frac{(c_1+c_3)}{10} + \frac{c_1c_3}{4} - \frac{c_2+c_3}{15} + \frac{(c_1+c_3)(c_2+c_3)}{8} - \frac{c_2c_3(c_1+c_3)}{6} + \frac{c_2c_3}{12} - \frac{c_1c_3(c_2+c_3)}{3} + \frac{c_2c_3c_1c_3}{2}}{b_1(c_1-c_2)(c_1-c_3)(c_3-c_2)(c_3-c_1)}.$$

$$a_{13} = \frac{\frac{1}{18} - \frac{(c_1+c_2)}{10} + \frac{c_1c_2}{4} - \frac{c_2+c_3}{15} + \frac{(c_1+c_2)(c_2+c_3)}{8} - \frac{c_2c_3(c_1+c_2)}{6} + \frac{c_2c_3}{12} - \frac{c_2c_1(c_2+c_3)}{3} + \frac{c_2c_3c_2c_1}{2}}{b_1(c_1-c_2)(c_1-c_3)(c_1-c_2)(c_1-c_3)}.$$

$$a_{21} = \frac{\frac{1}{18} - \frac{(c_3+c_2)}{10} + \frac{c_3c_2}{4} - \frac{c_1+c_3}{15} + \frac{(c_1+c_3)(c_2+c_3)}{8} - \frac{c_1c_3(c_3+c_2)}{6} + \frac{c_1c_3}{12} - \frac{c_2c_3(c_1+c_3)}{3} + \frac{c_1c_3c_2c_3}{2}}{b_2(c_2-c_1)(c_2-c_3)(c_1-c_2)(c_1-c_3)}.$$

$$a_{22} = \frac{\frac{1}{18} - \frac{(c_3+c_1)}{10} + \frac{c_3c_1}{4} - \frac{c_1+c_3}{15} + \frac{(c_1+c_3)(c_1+c_3)}{8} - \frac{c_1c_3(c_3+c_1)}{6} + \frac{c_1c_3}{12} - \frac{c_1c_3(c_1+c_3)}{3} + \frac{c_1c_3c_3c_1}{2}}{b_2(c_2-c_1)(c_2-c_3)(c_2-c_1)(c_2-c_3)}.$$

$$a_{23} = \frac{\frac{1}{18} - \frac{(c_2+c_1)}{10} + \frac{c_2c_1}{4} - \frac{c_1+c_3}{15} + \frac{(c_1+c_3)(c_1+c_2)}{8} - \frac{c_1c_3(c_2+c_1)}{6} + \frac{c_1c_3}{12} - \frac{c_1c_2(c_1+c_3)}{3} + \frac{c_1c_2c_1c_3}{2}}{b_2(c_2-c_1)(c_2-c_3)(c_3-c_1)(c_3-c_2)}.$$

$$a_{31} = \frac{\frac{1}{18} - \frac{(c_2+c_3)}{10} + \frac{c_2c_3}{4} - \frac{c_1+c_2}{15} + \frac{(c_2+c_3)(c_1+c_2)}{8} - \frac{c_1c_2(c_2+c_3)}{6} + \frac{c_1c_2}{12} - \frac{c_3c_2(c_1+c_2)}{3} + \frac{c_2c_1c_2c_3}{2}}{b_3(c_3-c_1)(c_3-c_2)(c_1-c_2)(c_1-c_3)}.$$

$$a_{32} = \frac{\frac{1}{18} - \frac{(c_1+c_3)}{10} + \frac{c_1c_3}{4} - \frac{c_1+c_2}{15} + \frac{(c_1+c_3)(c_1+c_2)}{8} - \frac{c_1c_2(c_1+c_3)}{6} + \frac{c_1c_2}{12} - \frac{c_3c_1(c_1+c_2)}{3} + \frac{c_1c_2c_1c_3}{2}}{b_3(c_3-c_1)(c_3-c_2)(c_2-c_1)(c_2-c_3)}.$$

$$a_{33} = \frac{\frac{1}{18} - \frac{(c_1+c_2)}{10} + \frac{c_1c_2}{4} - \frac{c_1+c_2}{15} + \frac{(c_1+c_2)(c_1+c_2)}{8} - \frac{c_1c_2(c_1+c_2)}{6} + \frac{c_1c_2}{12} - \frac{c_2c_1(c_1+c_2)}{3} + \frac{c_1c_2c_1c_2}{2}}{b_3(c_3-c_1)(c_3-c_2)(c_3-c_1)(c_3-c_2)}.$$

In this way we get a class of three stages symplectic Runge-Kutta methods by choosing c_1, c_2 and c_3. We can choose c_1, c_2 and c_3 as the zeros of shifted Legender polynomial.

Gauss: $s = 3$

$$
\begin{array}{c|ccc}
\frac{1}{2}-\frac{\sqrt{15}}{10} & \frac{5}{36} & \frac{2}{9}-\frac{\sqrt{15}}{15} & \frac{5}{36}-\frac{\sqrt{15}}{30} \\
\frac{1}{2} & \frac{5}{36}+\frac{\sqrt{15}}{24} & \frac{2}{9} & \frac{5}{36}-\frac{\sqrt{15}}{24} \\
\frac{1}{2}+\frac{\sqrt{15}}{10} & \frac{5}{36}+\frac{\sqrt{15}}{30} & \frac{2}{9}+\frac{\sqrt{15}}{15} & \frac{5}{36} \\
\hline
 & \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array}
$$

Radau-I: $s = 3$

$$
\begin{array}{c|ccc}
0 & \frac{1}{18} & \frac{5}{35}\frac{\sqrt{6}}{-6+\sqrt{6}} & \frac{5}{35}\frac{\sqrt{6}}{6+\sqrt{6}} \\
\frac{6-\sqrt{6}}{10} & \frac{1}{9}\left(\frac{-1+3\sqrt{6}}{-2+3\sqrt{6}}\right) & \frac{-5}{72}\left(\frac{-2+3\sqrt{6}}{-6+\sqrt{6}}\right)\sqrt{6} & \frac{-5}{36}\left(\frac{-25+12\sqrt{6}}{(-2+3\sqrt{6})(6+\sqrt{6})}\right)\sqrt{6} \\
\frac{6+\sqrt{6}}{10} & \frac{1}{9}\left(\frac{1+3\sqrt{6}}{2+3\sqrt{6}}\right) & \frac{-5}{36}\left(\frac{25+12\sqrt{6}}{(2+3\sqrt{6})(-6+\sqrt{6})}\right)\sqrt{6} & \frac{5}{72}\left(\frac{2+3\sqrt{6}}{6+\sqrt{6}}\right)\sqrt{6} \\
\hline
 & \frac{1}{9} & \frac{-5}{36}\sqrt{6}\left(\frac{-2+3\sqrt{6}}{-6+\sqrt{6}}\right) & \frac{5}{36}\sqrt{6}\left(\frac{2+3\sqrt{6}}{6+\sqrt{6}}\right)
\end{array}
$$

Radau-II: $s = 3$

$$\begin{array}{c|ccc}
\frac{4-\sqrt{6}}{10} & \frac{5}{72}(\frac{2+3\sqrt{6}}{6+\sqrt{6}})\sqrt{6} & \frac{5}{36}(\frac{-25+12\sqrt{6}}{(2+3\sqrt{6})(-6+\sqrt{6})})\sqrt{6} & \frac{1}{9(2+3\sqrt{6})} \\
\frac{4+\sqrt{6}}{10} & \frac{5}{36}(\frac{25+12\sqrt{6}}{(-2+3\sqrt{6})(6+\sqrt{6})})\sqrt{6} & \frac{-5}{72}(\frac{-2+3\sqrt{6}}{-6+\sqrt{6}})\sqrt{6} & \frac{-1}{9(-2+3\sqrt{6})} \\
1 & \frac{5}{36}(\frac{1+3\sqrt{6}}{6+\sqrt{6}})\sqrt{6} & \frac{-5}{36}(\frac{-1+3\sqrt{6}}{-6+\sqrt{6}})\sqrt{6} & \frac{1}{18} \\
\hline
 & \frac{5}{36}\sqrt{6}(\frac{2+3\sqrt{6}}{6+\sqrt{6}}) & \frac{-5}{36}\sqrt{6}(\frac{-2+3\sqrt{6}}{-6+\sqrt{6}}) & \frac{1}{9}
\end{array}$$

Lobatto-III: $s = 3$

$$\begin{array}{c|ccc}
0 & \frac{1}{12} & \frac{-1}{15} & \frac{-1}{60} \\
\frac{1}{2} & \frac{11}{60} & \frac{1}{3} & \frac{-1}{60} \\
1 & \frac{11}{60} & \frac{11}{15} & \frac{1}{12} \\
\hline
 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{array}$$

Lobatto-III: $s = 4$

$$\begin{array}{c|cccc}
0 & \frac{1}{24} & \frac{-1}{480}(4\sqrt{5}+15)\sqrt{5} & \frac{-1}{480}(4\sqrt{5}-15)\sqrt{5} & \frac{1}{168} \\
\frac{1}{2}-\frac{\sqrt{5}}{10} & \frac{1}{4200}(74\sqrt{5}+15)\sqrt{5} & \frac{5}{24} & \frac{1}{168}(7\sqrt{5}-18)\sqrt{5} & \frac{-1}{4200}(4\sqrt{5}-15)\sqrt{5} \\
\frac{1}{2}-\frac{\sqrt{5}}{10} & \frac{1}{4200}(74\sqrt{5}-15)\sqrt{5} & \frac{1}{168}(7\sqrt{5}+18)\sqrt{5} & \frac{5}{24} & \frac{-1}{4200}(1054\sqrt{5}-3135)\sqrt{5} \\
1 & \frac{13}{168} & \frac{1}{480}(74\sqrt{5}-15)\sqrt{5} & \frac{1}{480}(1124\sqrt{5}-3135)\sqrt{5} & \frac{1}{24} \\
\hline
 & \frac{1}{12} & \frac{5}{12} & \frac{5}{12} & \frac{1}{12}
\end{array}$$

3.2 Construction of symplectic partitioned Runge-Kutta methods

Symplectic partitioned Runge-Kutta methods [7, 11] can be constructed in the same way as we have constructed symplectic Runge-Kutta methods. By using Vandermonde transformation, we can construct the symplectic partitioned Runge-Kutta methods. For this we use the pre and post multiplication of Vandermonde matrix with the symplectic condition for partitioned Runge-Kutta method (2.7.4).

Consider the symplectic condition (2.10.2) of partitioned Runge-Kutta method which is given as,

$$b_i\hat{a}_{ij} + \hat{b}_j a_{ji} - b_i\hat{b}_j = 0, \quad \forall\, i, j = 1, 2 \ldots s. \tag{3.2.1}$$

Consider the Vandermonde matrix V,

$$V = c_i^{j-1} = \begin{bmatrix} 1 & c_1 & c_1^2 & \ldots & c_1^{s-1} \\ 1 & c_2 & c_2^2 & \ldots & c_2^{s-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & c_s & c_s^2 & \ldots & c_s^{s-1} \end{bmatrix}$$

Multiply the symplectic conditions of prtitioned Runge-Kutta method (2.7.4) from (3.2.1) with matrix V as follows,

$$\hat{c}_i^{k-1}(b_i\hat{a}_{ij} + \hat{b}_j a_{ji} - b_i\hat{b}_j = 0)c_j^{l-1} = 0, \;\; \forall i, j, k, l = 1, 2...s. \tag{3.2.2}$$

where c's are used for that Runge-Kutta methods by which one can solve $p' = f(q)$ as well. $\hat{c}$'s are used for that Runge-Kutta methods which can be used to solve $q' = g(p)$.

For order two, put $l, k = 1, 2$ and take summation over i and j from 1 to s.

For $l, k = 1$

$$\sum_{i,j} b_i\hat{a}_{ij} + \hat{b}_j a_{ji} - b_i\hat{b}_j = 0. \tag{3.2.3}$$

For $l = 1, k = 2$

$$\sum_{i,j} b_i\hat{c}_i a_{ij} + \sum_{i,j} \hat{b}_j a_{ji}\hat{c}_i - \sum_{i,j} b_i\hat{c}_i\hat{b}_j = 0. \tag{3.2.4}$$

For $l = 2, k = 1$

$$\sum_{i,j} b_i\hat{a}_{ij}c_j + \sum_{i,j} \hat{b}_j c_j a_{ji} - \sum_{i,j} b_i\hat{b}_j c_j = 0. \tag{3.2.5}$$

For $l, k = 2$

$$\sum_{i,j} b_i\hat{c}_i\hat{a}_{ij}c_j + \sum_{i,j} \hat{b}_j c_j\hat{a}_{ji}\hat{c}_i - \sum_{i,j} \hat{b}_j c_j b_i\hat{c}_i = 0. \tag{3.2.6}$$

In order to construct method of order two, then following order conditions, (2.9.10) and (2.9.11) must satisfy

$$\sum_{i=1}^{s} b_i = 1, \qquad \sum_{i=1}^{s} \hat{b}_i = 1, \qquad \sum_{i=1}^{s} \hat{b}_i c_i = \frac{1}{2}, \qquad \sum_{i=1}^{s} b_i\hat{c}_i = \frac{1}{2}. \tag{3.2.7}$$

Using equations (3.2.7) in equations (3.2.3)-(3.2.6) we have

$$\sum_{i,j} b_i\hat{a}_{ij} = \frac{1}{2} \quad \text{or} \quad \sum_{i} \hat{b}_j a_{ji} = \frac{1}{2}. \tag{3.2.8}$$

$$\sum_{i,j} b_i\hat{c}_i a_{ij} + \sum_{i,j} \hat{b}_j a_{ji}\hat{c}_i = \frac{1}{2}. \tag{3.2.9}$$

$$\sum_{i,j} b_i\hat{a}_{ij}c_j + \sum_{i,j} \hat{b}_j c_j\hat{a}_{ji} = \frac{1}{2}. \tag{3.2.10}$$

$$\sum_{i,j} b_i\hat{c}_i\hat{a}_{ij}c_j = \frac{1}{8}. \tag{3.2.11}$$

Now for the values of b_2 we consider the relation

$$b_i(\hat{c}_i - \hat{c}_1) = b_i\hat{c}_i - b_i\hat{c}_1, \tag{3.2.12}$$

take summation over i from 1 to s and use the equations (3.2.7) we get

$$\sum_i b_i(\hat{c}_i - \hat{c}_1) = \sum_i b_i\hat{c}_i - \sum_i b_i\hat{c}_1,$$

$$b_2(\hat{c_2} - \hat{c_1}) = \frac{\hat{c_1}}{2} - \hat{c}_1,$$

$$b_2 = \frac{(\frac{1}{2} - \hat{c}_1)}{\hat{c}_2 - \hat{c}_1}.$$

Similarly we have

$$b_1 = \frac{(\frac{1}{2} - \hat{c}_2)}{\hat{c}_1 - \hat{c}_2}.$$

Now for $\hat{b}_2$ we consider the following relation

$$\hat{b}_i(c_i - c_1) = \hat{b}_i c_i - \hat{b}_i c_1,$$

take summation over i from 1 to s and use the equations (3.2.7) we get

$$\sum_i \hat{b}_i(c_i - c_1) = \sum_i \hat{b}_i c_i - \sum_i \hat{b}_i c_1,$$

$$\hat{b}_2(c_2 - c_1) = \frac{1}{2} - c_1,$$

$$\hat{b}_2 = \frac{(\frac{1}{2} - c_1)}{c_2 - c_1}.$$

Similarly we can get

$$\hat{b}_1 = \frac{(\frac{1}{2} - c_2)}{c_1 - c_2}.$$

Now to calculate a_{11} we consider the following relation,

$$\hat{b}_i(c_i - c_2)a_{ij}(\hat{c}_j - c_2) = \hat{b}_i c_i a_{ij}\hat{c}_j - \hat{b}_i c_i a_{ij}\hat{c}_2 - \hat{b}_i a_{ij}\hat{c}_j c_2 + \hat{b}_i a_{ij} c_2\hat{c}_2,$$

take the summation over i and j from 1 to s, and use equations (3.2.7), (3.2.8) and (3.2.11) we have

$$a_{11} = \frac{\frac{1}{8} - \frac{\hat{c}_2}{3} - \frac{c_2}{6} + \frac{c_2\hat{c}_2}{2}}{\hat{b}_1(c_1 - c_2)(\hat{c}_1 - \hat{c}_2)}.$$

Similarly we have

$$a_{12} = \frac{\frac{1}{8} - \frac{\hat{c}_1}{3} - \frac{c_2}{6} + \frac{c_2\hat{c}_1}{2}}{\hat{b}_1(c_1 - c_2)(\hat{c}_1 - \hat{c}_2)}.$$

$$a_{21} = \frac{\frac{1}{8} - \frac{\hat{c}_2}{3} - \frac{c_1}{6} + \frac{c_1\hat{c}_2}{2}}{\hat{b}_2(c_2 - c_1)(\hat{c}_1 - \hat{c}_2)}.$$

$$a_{22} = \frac{\frac{1}{8} - \frac{\hat{c}_1}{3} - \frac{c_1}{6} + \frac{c_1\hat{c}_1}{2}}{\hat{b}_2(c_2 - c_1)(\hat{c}_2 - \hat{c}_1)}.$$

Now consider the relation for the value of $\hat{a}_{11}$

$$b_i(\hat{c}_i - \hat{c}_2)\hat{a}_{ij}(c_j - c_2) = b_i\hat{c}_i\hat{a}_{ij}c_j - b_i\hat{c}_i\hat{a}_{ij}c_2 - b_i\hat{a}_{ij}c_j\hat{c}_2 + b_i\hat{a}_{ij}c_2\hat{c}_2,$$

take the summation over i and j, and use equations (3.2.7)and (3.2.21) we have

$$\hat{a}_{11} = \frac{\frac{1}{8} - \frac{c_2}{3} - \frac{\hat{c}_2}{6} + \frac{c_2\hat{c}_2}{2}}{b_1(\hat{c}_1 - \hat{c}_2)(c_1 - c_2)}.$$

Similarly we have

$$\hat{a}_{12} = \frac{\frac{1}{8} - \frac{c_1}{3} - \frac{\hat{c}_2}{6} + \frac{c_1\hat{c}_2}{2}}{b_1(\hat{c}_1 - \hat{c}_2)(c_2 - c_1)}.$$

$$\hat{a}_{21} = \frac{\frac{1}{8} - \frac{c_2}{3} - \frac{\hat{c}_1}{6} + \frac{\hat{c}_1 c_2}{2}}{b_2(\hat{c}_2 - \hat{c}_1)(c_1 - c_2)}.$$

$$\hat{a}_{22} = \frac{\frac{1}{8} - \frac{c_1}{3} - \frac{\hat{c}_1}{6} + \frac{c_1\hat{c}_1}{2}}{b_2(\hat{c}_2 - \hat{c}_1)(c_2 - c_1)}.$$

In this we get a class of two stages symplectic partitioned Runge-Kutta methods by choosing c_1, c_2, $\hat{c}_1$ and $\hat{c}_2$. We can choose c_1, c_2, $\hat{c}_1$ and $\hat{c}_2$ as the zeros of shifted Legendre polynomial.

Gauss and Radau-I : $s = 2$

$$\begin{array}{c|cc}
\frac{1}{2}-\frac{\sqrt{3}}{6} & \frac{1}{24}(-1+2\sqrt{3})\sqrt{3} & \frac{1}{24}(-3+2\sqrt{3})\sqrt{3} \\
\frac{1}{2}+\frac{\sqrt{3}}{6} & \frac{1}{24}(1+2\sqrt{3})\sqrt{3} & \frac{1}{24}(-3+2\sqrt{3})\sqrt{3} \\
\hline
 & \frac{1}{4} & \frac{3}{4}
\end{array}$$

$$\begin{array}{c|cc}
0 & \frac{1}{12}\sqrt{3} & -\frac{1}{12}\sqrt{3} \\
\frac{2}{3} & \frac{1}{36}(3+4\sqrt{3})\sqrt{3} & \frac{1}{36}(-3+4\sqrt{3})\sqrt{3} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}$$

Gauss and Radua-II : $s = 2$

$$\begin{array}{c|cc}
\frac{1}{2}-\frac{\sqrt{3}}{6} & \frac{1}{24}(-3+4\sqrt{3})\sqrt{3} & -\frac{1}{24}\sqrt{3} \\
\frac{1}{2}+\frac{\sqrt{3}}{6} & \frac{1}{24}(3+4\sqrt{3})\sqrt{3} & \frac{1}{24}\sqrt{3} \\
\hline
 & \frac{3}{4} & \frac{1}{4}
\end{array}$$

$$\begin{array}{c|cc}
\frac{1}{3} & \frac{1}{36}(3+4\sqrt{3})\sqrt{3} & \frac{1}{36}(-3+4\sqrt{3})\sqrt{3} \\
1 & \frac{1}{12}(1+2\sqrt{3})\sqrt{3} & -\frac{1}{12}(-1+2\sqrt{3})\sqrt{3} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}$$

Radau-I and Radau-II: $s = 2$

$$\begin{array}{c|cc} 0 & \frac{1}{8} & -\frac{1}{8} \\ \frac{2}{3} & \frac{5}{8} & \frac{1}{24} \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array} \qquad \begin{array}{c|cc} \frac{1}{3} & \frac{5}{24} & \frac{1}{8} \\ 1 & \frac{3}{8} & \frac{5}{8} \\ \hline & \frac{1}{4} & \frac{3}{4} \end{array}$$

For order three

Put $l, k = 1, 2, 3.$ in equation (3.2.2) and take summation over i and j from 1 to s

For $l, k = 1$

$$\sum_{i,j} b_i \hat{a}_{ij} + \sum_{i,j} \hat{b}_j a_{ji} - \sum_{i,j} b_i \hat{b}_j = 0. \tag{3.2.13}$$

For $l = 1, k = 2$

$$\sum_{i,j} b_i \hat{c}_i \hat{a}_{ij} + \sum_{i,j} \hat{b}_j a_{ji} \hat{c}_i - \sum_{i,j} b_i \hat{c}_i \hat{b}_j = 0. \tag{3.2.14}$$

For $l = 1, k = 3$

$$\sum_{i,j} b_i \hat{c}_i^2 \hat{a}_{ij} + \sum_{i,j} \hat{b}_j a_{ji} \hat{c}_i^2 - \sum_{i,j} b_i \hat{c}_i^2 \hat{b}_j = 0. \tag{3.2.15}$$

For $l = 2, k = 1$

$$\sum_{i,j} b_i \hat{a}_{ij} c_j + \sum_{i,j} \hat{b}_j c_j a_{ji} - \sum_{i,j} b_i \hat{b_j} c_j = 0. \tag{3.2.16}$$

For $l = 3, k = 1$

$$\sum_{i,j} b_i \hat{a}_{ij} c_j^2 + \sum_{i,j} \hat{b}_j c_j^2 a_{ji} - \sum_{i,j} b_i \hat{b_j} c_j^2 = 0. \tag{3.2.17}$$

For $l, k = 2$

$$\sum_{i,j} b_i \hat{c}_i \hat{a}_{ij} c_j + \sum_{i,j} \hat{b}_j c_j a_{ji} \hat{c}_i - \sum_{i,j} b_i \hat{c}_i \hat{b_j} c_j = 0. \tag{3.2.18}$$

For $l, k = 3$

$$\sum_{i,j} b_i \hat{c}_i^2 \hat{a}_{ij} c_j^2 + \sum_{i,j} \hat{b}_j c_j^2 a_{ji} \hat{c}_i^2 - \sum_{i,j} b_i \hat{c}_i^2 \hat{b_j} c_j^2 = 0. \tag{3.2.19}$$

We are constructing method of order three, the following order conditions (2.9.10), (2.9.11) and (2.9.12) must satisfy,

$$\sum_{i}^{s} b_i = 1, \quad \sum_{i}^{s} \hat{b_i} = 1, \quad \sum_{i=1}^{s} b_i \hat{c}_i = \frac{1}{2}, \quad \sum_{i=1}^{s} \hat{b_i} c_i = \frac{1}{2}, \quad \sum_{i=1}^{s} b_i \hat{c}_i^2 = \frac{1}{3}, \quad \sum_{i=1}^{s} \hat{b_i} c_i^2 = \frac{1}{3},$$
$$\sum_{i,j=1}^{s} b_i \hat{a_{ij}} c_j = \frac{1}{6}, \quad \sum_{i,j=1}^{s} \hat{b_i} a_{ij} \hat{c_j} = \frac{1}{6}. \tag{3.2.20}$$

Using equations (3.2.20) in equations (3.2.13)- (3.2.19) we have

$$\sum_{i,j} \hat{b}_j a_{ji} = \frac{1}{2} \text{ or } \sum_{i} b_i \hat{a}_{ij} = \frac{1}{2}. \tag{3.2.21}$$

$$\sum_{i,j} b_i \hat{c}_i \hat{a}_{ij} + \sum_{i,j} \hat{b}_j a_{ji} \hat{c}_i = \frac{1}{2}. \tag{3.2.22}$$

$$\sum_{i,j} b_i \hat{c}_i^2 \hat{a}_{ij} + \sum_{i,j} \hat{b}_j a_{ji} \hat{c}_i^2 = \frac{1}{3}. \tag{3.2.23}$$

$$\sum_{i,j} b_i \hat{a}_{ij} c_j + \sum_{i,j} \hat{b}_j c_j a_{ji} = \frac{1}{2}. \tag{3.2.24}$$

$$\sum_{i,j} b_i \hat{a}_{ij} c_j^2 + \sum_{i,j} \hat{b}_j c_j^2 a_{ji} = \frac{1}{3}. \tag{3.2.25}$$

$$\sum_{i,j} \hat{b}_j c_j a_{ji} \hat{c}_i = \frac{1}{8}. \tag{3.2.26}$$

$$\sum_{i,j} b_i \hat{c}_i^2 \hat{a}_{ij} c_j^2 = \frac{1}{18}. \tag{3.2.27}$$

Now for the values of b_1, b_2 and b_3, we consider the following relations respectively.

$$b_i(\hat{c}_i - \hat{c}_2)(\hat{c}_i - \hat{c}_3) = b_i\hat{c}_i^2 - b_i\hat{c}_i\hat{c}_3 - b_i\hat{c}_i\hat{c}_2 + b_i\hat{c}_2\hat{c}_3, \tag{3.2.28}$$

$$b_i(\hat{c}_i - \hat{c}_1)(\hat{c}_i - \hat{c}_3) = b_i\hat{c}_i^2 - b_i\hat{c}_i\hat{c}_3 - b_i\hat{c}_i\hat{c}_1 + b_i\hat{c}_1\hat{c}_3,$$

$$b_i(\hat{c}_i - \hat{c}_1)(\hat{c}_i - \hat{c}_2) = b_i\hat{c}_i^2 - b_i\hat{c}_i\hat{c}_2 - b_i\hat{c}_i\hat{c}_1 + b_i\hat{c}_1\hat{c}_2,$$

for the value of b_1 apply summation on equation (3.2.28) over i from 1 to s and using equations (3.2.20), we have

$$b_i(\hat{c}_i - \hat{c}_2)(\hat{c}_i - \hat{c}_3) = b_i\hat{c_i^2} - b_i\hat{c}_i\hat{c}_3 - b_i\hat{c}_i\hat{c}_2 + b_i\hat{c}_2\hat{c}_3,$$

$$b_1(\hat{c}_1 - \hat{c}_2)(\hat{c}_1 - \hat{c}_3) = \frac{1}{3} - \frac{\hat{c}_3}{2} - \frac{\hat{c}_2}{2} + \hat{c}_2\hat{c}_3,$$

$$b_1 = \frac{(2 - 3(\hat{c}_3 + \hat{c}_2 - 2\hat{c}_2\hat{c}_3)}{(6(\hat{c}_1 - \hat{c}_2)(\hat{c}_1 - \hat{c}_3))}.$$

Similarly we have

$$b_2 = \frac{(2 - 3(\hat{c}_3 + \hat{c}_1 - 2\hat{c}_1\hat{c}_3))}{(6(\hat{c}_2 - \hat{c}_1)(\hat{c}_2 - \hat{c}_3))}.$$

$$b_3 = \frac{(2 - 3(\hat{c}_1 + \hat{c}_2 - 2\hat{c}_2\hat{c}_1))}{(6(\hat{c}_3 - \hat{c}_2)(\hat{c}_3 - \hat{c}_1))}.$$

To find out the values of $\hat{b_1}$, $\hat{b_2}$ and $\hat{b_3}$ we consider the following relations respectively.

$$\hat{b}_i(c_i - c_2)(c_i - c_3) = \hat{b}_i c_i^2 - \hat{b}_i c_i c_3 - \hat{b}_i c_i c_2 + \hat{b}_i c_2 c_3, \tag{3.2.29}$$

$$\hat{b}_i(c_i - c_1)(c_i - c_3) = \hat{b}_i c_i^2 - \hat{b}_i c_i c_3 - \hat{b}_i c_i c_1 + \hat{b}_i c_1 c_3,$$

$$\hat{b}_i(c_i - c_1)(c_i - c_2) = \hat{b}_i c_i^2 - \hat{b}_i c_i c_2 - \hat{b}_i c_i c_1 + \hat{b}_i c_1 c_2,$$

for the value of $\hat{b_1}$ apply the summation on equation (3.2.29) over i from 1 to s and using equations (3.2.20) and we have,

$$\hat{b}_i(c_i - c_2)(c_i - c_3) = \hat{b}_i c_i^2 - \hat{b}_i c_i c_3 - \hat{b}_i c_i c_2 + \hat{b}_i c_2 c_3,$$

$$\hat{b}_1(c_1-c_2)(c_1-c_3)=\frac{1}{3}-\frac{c_3}{2}-\frac{c_2}{2}+c_2c_3,$$
$$\hat{b}_1=\frac{(2-3(c_3+c_2-2c_2c_3))}{(6(c_1-c_2)(c_1-c_3))}.$$

Similarly we have

$$\hat{b}_2=\frac{(2-3(c_3+c_1-2c_1c_3))}{(6(c_2-c_1)(c_2-c_3))}.$$
$$\hat{b}_3=\frac{(2-3(c_1+c_2-2c_2c_1))}{(6(c_3-c_2)(c_3-c_1))}.$$

Now to calculate the value of a_{11} we consider the following relation,

$$\begin{aligned}\hat{b_i}(c_i-c_2)(c_i-c_3)a_{ij}(\hat{c_j}-\hat{c_2})(\hat{c_j}-\hat{c_3}) &= \hat{b_i}c_i^2a_{ij}\hat{c_j^2}-\hat{b_i}c_i^2a_{ij}\hat{c_j}\hat{c_3}-\hat{b_i}c_i^2a_{ij}\hat{c_j}\hat{c_2}+\hat{b_i}c_i^2a_{ij}\hat{c_2}\hat{c_3}\\ &-\hat{b_i}c_ia_{ij}\hat{c_j^2}c_3+\hat{b_i}c_ia_{ij}\hat{c_j}c_3\hat{c_3}+\hat{b_i}c_ia_{ij}\hat{c_j}c_3\hat{c_2}-\hat{b_i}c_ia_{ij}\hat{c_2}\hat{c_3}c_3-\hat{b_i}c_ia_{ij}\hat{c_j^2}c_2+\hat{b_i}c_ia_{ij}\hat{c_j}c_2\hat{c_3}\\ &+\hat{b_i}c_ia_{ij}\hat{c_j}c_2\hat{c_2}-\hat{b_i}c_ia_{ij}\hat{c_2}\hat{c_3}c_2+\hat{b_i}a_{ij}\hat{c_j^2}c_3c_2-\hat{b_i}a_{ij}\hat{c_j}c_3\hat{c_3}c_2-\hat{b_i}a_{ij}\hat{c_j}c_3\hat{c_2}c_2+\hat{b_i}a_{ij}c_2\hat{c_2}c_3\hat{c_3}.\end{aligned}$$

Take summation over i and j from 1 to s, then using equations (3.2.20) and (3.2.21)-(3.2.27) we have

$$\begin{aligned}\hat{b_1}(c_1-c_2)(c_1-c_3)a_{11}(\hat{c_1}-\hat{c_2})(\hat{c_1}-\hat{c_3}) &= \frac{1}{18}-\frac{(\hat{c_2}+\hat{c_3})}{10}+\frac{\hat{c_2}\hat{c_3}}{4}-\frac{c_2+c_3}{15}+\frac{(c_2+c_3)(\hat{c_2}+\hat{c_3})}{8}\\ &-\frac{\hat{c_2}\hat{c_3}(c_2+c_3)}{3}+\frac{c_2c_3}{12}-\frac{c_2c_3(\hat{c_2}+\hat{c_3})}{6}+\frac{c_2\hat{c_2}c_3\hat{c_3}}{2},\end{aligned}$$

$$a_{11}=\frac{\frac{1}{18}-\frac{(\hat{c_2}+\hat{c_3})}{10}+\frac{\hat{c_2}\hat{c_3}}{4}-\frac{c_2+c_3}{15}+\frac{(c_2+c_3)(\hat{c_2}+\hat{c_3})}{8}-\frac{\hat{c_2}\hat{c_3}(c_2+c_3)}{3}+\frac{c_2c_3}{12}-\frac{c_2c_3(\hat{c_2}+\hat{c_3})}{6}+\frac{c_2\hat{c_2}c_3\hat{c_3}}{2}}{\hat{b_1}(c_1-c_2)(c_1-c_3)(\hat{c_1}-\hat{c_2})(\hat{c_1}-\hat{c_3})}.$$

Similarly we have,

$$a_{12}=\frac{\frac{1}{18}-\frac{(\hat{c_1}+\hat{c_3})}{10}+\frac{\hat{c_1}\hat{c_3}}{4}-\frac{c_2+c_3}{15}+\frac{(\hat{c_1}+\hat{c_3})(c_2+c_3)}{8}-\frac{\hat{c_1}\hat{c_3}(c_2+c_3)}{3}+\frac{c_2c_3}{12}-\frac{c_2c_3(\hat{c_1}+\hat{c_3})}{6}+\frac{c_2\hat{c_3}c_3\hat{c_1}}{2}}{\hat{b_1}(c_1-c_2)(c_1-c_3)(\hat{c_1}-\hat{c_2})(\hat{c_1}-\hat{c_3})}.$$

$$a_{13}=\frac{\frac{1}{18}-\frac{(\hat{c_1}+\hat{c_2})}{10}+\frac{\hat{c_1}\hat{c_2}}{4}-\frac{c_2+c_3}{15}+\frac{(\hat{c_1}+\hat{c_2})(c_2+c_3)}{8}-\frac{c_2c_3(\hat{c_1}+\hat{c_2})}{6}+\frac{c_2c_3}{12}-\frac{\hat{c_1}\hat{c_2}(c_2+c_3)}{3}+\frac{c_2\hat{c_1}c_3\hat{c_2}}{2}}{\hat{b_1}(c_1-c_2)(c_1-c_3)(\hat{c_1}-\hat{c_2})(\hat{c_1}-\hat{c_3})}.$$

$$a_{21}=\frac{\frac{1}{18}-\frac{(\hat{c_3}+\hat{c_2})}{10}+\frac{\hat{c_3}\hat{c_2}}{4}-\frac{c_1+c_3}{15}+\frac{(c_1+c_3)(\hat{c_2}+\hat{c_3})}{8}-\frac{c_1c_3(\hat{c_3}+\hat{c_2})}{6}+\frac{c_1c_3}{12}-\frac{\hat{c_2}\hat{c_3}(c_1+c_3)}{3}+\frac{c_3\hat{c_1}c_2\hat{c_3}}{2}}{\hat{b_2}(c_2-c_1)(c_2-c_3)(\hat{c_1}-\hat{c_2})(\hat{c_1}-\hat{c_3})}.$$

$$a_{22}=\frac{\frac{1}{18}-\frac{(\hat{c_3}+\hat{c_1})}{10}+\frac{\hat{c_3}\hat{c_1}}{4}-\frac{c_1+c_3}{15}+\frac{(c_1+c_3)(\hat{c_1}+\hat{c_3})}{8}-\frac{c_1c_3(\hat{c_3}+\hat{c_1})}{6}+\frac{c_1c_3}{12}-\frac{\hat{c_1}\hat{c_3}(c_1+c_3)}{3}+\frac{c_1\hat{c_3}c_3\hat{c_1}}{2}}{\hat{b_2}(c_2-c_1)(c_2-c_3)(\hat{c_2}-\hat{c_1})(\hat{c_2}-\hat{c_3})}.$$

$$a_{23}=\frac{\frac{1}{18}-\frac{(\hat{c_2}+\hat{c_1})}{10}+\frac{\hat{c_2}\hat{c_1}}{4}-\frac{c_1+c_3}{15}+\frac{(c_1+c_3)(\hat{c_1}+\hat{c_2})}{8}-\frac{c_1c_3(\hat{c_2}+\hat{c_1})}{6}+\frac{c_1c_3}{12}-\frac{\hat{c_1}\hat{c_2}(c_1+c_3)}{3}+\frac{c_1\hat{c_2}c_3\hat{c_1}}{2}}{\hat{b_2}(c_2-c_1)(c_2-c_3)(\hat{c_3}-\hat{c_1})(\hat{c_3}-\hat{c_2})}.$$

$$a_{31} = \frac{\frac{1}{18} - \frac{(\hat{c_2}+\hat{c_3})}{10} + \frac{\hat{c_2}\hat{c_3}}{4} - \frac{c_1+c_2}{15} + \frac{(\hat{c_2}+\hat{c_3})(c_1+c_2)}{8} - \frac{c_1c_2(\hat{c_2}+\hat{c_3})}{6} + \frac{c_1c_2}{12} - \frac{\hat{c_3}\hat{c_2}(c_1+c_2)}{3} + \frac{c_1\hat{c_2}c_2\hat{c_3}}{2}}{\hat{b_3}(c_3-c_1)(c_3-c_2)(\hat{c_1}-\hat{c_2})(\hat{c_1}-\hat{c_3})}.$$

$$a_{32} = \frac{\frac{1}{18} - \frac{(\hat{c_1}+\hat{c_3})}{10} + \frac{\hat{c_1}\hat{c_3}}{4} - \frac{c_1+c_2}{15} + \frac{(\hat{c_1}+\hat{c_3})(c_1+c_2)}{8} - \frac{c_1c_2(\hat{c_1}+\hat{c_3})}{6} + \frac{c_1c_2}{12} - \frac{\hat{c_3}\hat{c_1}(c_1+c_2)}{3} + \frac{c_2\hat{c_1}c_1\hat{c_3}}{2}}{\hat{b_3}(c_3-c_1)(c_3-c_2)(\hat{c_2}-\hat{c_1})(\hat{c_2}-\hat{c_3})}.$$

$$a_{33} = \frac{\frac{1}{18} - \frac{(\hat{c_1}+\hat{c_2})}{10} + \frac{\hat{c_1}\hat{c_2}}{4} - \frac{c_1+c_2}{15} + \frac{(c_1+c_2)(\hat{c_1}+\hat{c_2})}{8} - \frac{c_1c_2(\hat{c_1}+\hat{c_2})}{6} + \frac{c_1c_2}{12} - \frac{\hat{c_2}\hat{c_1}(c_1+c_2)}{3} + \frac{c_1\hat{c_2}c_2\hat{c_1}}{2}}{\hat{b_3}(c_3-c_1)(c_3-c_2)(\hat{c_3}-\hat{c_1})(\hat{c_3}-\hat{c_2})}.$$

Now for the value of $\hat{a}_{11}$ we consider the following relation

$$\begin{aligned}
&b_i(\hat{c_i}-\hat{c_2})(\hat{c_i}-\hat{c_3})\hat{a_{ij}}(c_j-c_2)(c_j-c_3) = b_i\hat{c_i^2}\hat{a_{ij}}c_j^2 - b_i\hat{c^2}_i a_{ij}c_jc_3 - b_i\hat{c_i^2}\hat{a_{ij}}c_jc_2 + b_i\hat{c_i^2}\hat{a_{ij}}c_2c_3 \\
&- b_i\hat{c}_i\hat{a_{ij}}c_j^2\hat{c}_3 + b_i\hat{c}_i\hat{a_{ij}}c_j\hat{c}_3c_3 + b_i\hat{c}_i\hat{a_{ij}}c_j\hat{c}_3c_2 - b_i\hat{c}_i\hat{a_{ij}}c_2\hat{c}_3c_3 - b_i\hat{c}_i\hat{a_{ij}}c_j^2\hat{c}_2 + b_i\hat{c}_i\hat{a_{ij}}c_j\hat{c}_2c_3 \\
&+ b_i\hat{c}_i\hat{a_{ij}}c_jc_2\hat{c}_2 - b_i\hat{c}_i\hat{a_{ij}}c_2c_3\hat{c}_2 + b_i\hat{a_{ij}}c_j^2\hat{c}_3\hat{c}_2 - b_i\hat{a_{ij}}c_j\hat{c}_3c_3\hat{c}_2c_3 - b_i\hat{a_{ij}}c_j\hat{c}_3\hat{c}_2c_2 + b_i\hat{a_{ij}}c_2\hat{c}_2\hat{c}_3c_3.
\end{aligned}$$

Take summation over i and j from 1 to s, then using (3.2.20) and (3.2.21)-(3.2.27) we have,

$$\begin{aligned}
b_1(\hat{c_1}-\hat{c_2})(\hat{c_1}-\hat{c_3})\hat{a_{11}}(c_1-c_2)(c_1-c_3) = {}& \frac{1}{18} - \frac{(c_2+c_3)}{10} + \frac{c_2c_3}{4} - \frac{\hat{c}_2+\hat{c}_3}{15} + \frac{(c_2+c_3)(\hat{c}_2+\hat{c}_3)}{8} \\
& - \frac{\hat{c}_2\hat{c}_3(c_2+c_3)}{6} + \frac{\hat{c}_2\hat{c}_3}{12} - \frac{c_2c_3(\hat{c}_2+\hat{c}_3)}{3} + \frac{\hat{c}_2c_2\hat{c}_3c_3}{2},
\end{aligned}$$

$$\hat{a}_{11} = \frac{\frac{1}{18} - \frac{(c_2+c_3)}{10} + \frac{c_2c_3}{4} - \frac{\hat{c_2}+\hat{c_3}}{15} + \frac{(c_2+c_3)(\hat{c_2}+\hat{c_3})}{8} - \frac{\hat{c_2}\hat{c_3}(c_2+c_3)}{6} + \frac{\hat{c_2}\hat{c_3}}{12} - \frac{c_2c_3(\hat{c_2}+\hat{c_3})}{3} + \frac{\hat{c_2}c_3\hat{c_3}c_2}{2}}{b_1(\hat{c_1}-\hat{c_2})(\hat{c_1}-\hat{c_3})(c_1-c_2)(c_1-c_3)}.$$

Similarly we have

$$\hat{a}_{12} = \frac{\frac{1}{18} - \frac{(c_1+c_3)}{10} + \frac{c_1c_3}{4} - \frac{\hat{c_2}+\hat{c_3}}{15} + \frac{(c_1+c_3)(\hat{c_2}+\hat{c_3})}{8} - \frac{\hat{c_2}\hat{c_3}(c_1+c_3)}{6} + \frac{\hat{c_2}\hat{c_3}}{12} - \frac{c_1c_3(\hat{c_2}+\hat{c_3})}{3} + \frac{\hat{c_2}c_3\hat{c_3}c_1}{2}}{b_1(\hat{c_1}-\hat{c_2})(\hat{c_1}-\hat{c_3})(c_1-c_2)(c_1-c_3)}.$$

$$\hat{a}_{13} = \frac{\frac{1}{18} - \frac{(c_1+c_2)}{10} + \frac{c_1c_2}{4} - \frac{\hat{c_2}+\hat{c_3}}{15} + \frac{(c_1+c_2)(\hat{c_2}+\hat{c_3})}{8} - \frac{\hat{c_2}\hat{c_3}(c_1+c_2)}{6} + \frac{\hat{c_2}\hat{c_3}}{12} - \frac{c_1c_3(\hat{c_2}+\hat{c_3})}{3} + \frac{\hat{c_2}c_1\hat{c_3}c_2}{2}}{b_1(\hat{c_1}-\hat{c_2})(\hat{c_1}-\hat{c_3})(c_1-c_2)(c_1-c_3)}.$$

$$\hat{a}_{21} = \frac{\frac{1}{18} - \frac{(c_3+c_2)}{10} + \frac{c_3c_2}{4} - \frac{\hat{c_1}+\hat{c_3}}{15} + \frac{(\hat{c_1}+\hat{c_3})(c_2+c_3)}{8} - \frac{\hat{c_1}\hat{c_3}(c_3+c_2)}{6} + \frac{\hat{c_1}\hat{c_3}}{12} - \frac{c_2c_3(\hat{c_1}+\hat{c_3})}{3} + \frac{\hat{c_1}c_3\hat{c_3}c_2}{2}}{b_2(\hat{c_2}-\hat{c_1})(\hat{c_2}-\hat{c_3})(c_1-c_2)(c_1-c_3)}.$$

$$\hat{a}_{22} = \frac{\frac{1}{18} - \frac{(c_3+c_1)}{10} + \frac{c_3c_1}{4} - \frac{\hat{c_1}+\hat{c_3}}{15} + \frac{(c_1+c_3)(\hat{c_1}+\hat{c_3})}{8} - \frac{\hat{c_1}\hat{c_3}(c_3+c_1)}{6} + \frac{\hat{c_1}\hat{c_3}}{12} - \frac{c_1c_3(hatc_1+\hat{c_3})}{3} + \frac{\hat{c_1}c_3\hat{c_3}c_1}{2}}{b_2(\hat{c_2}-\hat{c_1})(\hat{c_2}-\hat{c_3})(c_2-c_1)(c_2-c_3)}.$$

$$\hat{a}_{23} = \frac{\frac{1}{18} - \frac{(c_2+c_1)}{10} + \frac{c_2c_1}{4} - \frac{\hat{c_1}+\hat{c_3}}{15} + \frac{(\hat{c_1}+\hat{c_3})(c_1+c_2)}{8} - \frac{\hat{c_1}\hat{c_3}(c_2+c_1)}{6} + \frac{\hat{c_1}\hat{c_3}}{12} - \frac{c_1c_2(\hat{c_1}+\hat{c_3})}{3} + \frac{\hat{c_1}c_2\hat{c_3}c_1}{2}}{b_2(\hat{c_2}-\hat{c_1})(\hat{c_2}-\hat{c_3})(c_3-c_1)(c_3-c_2)}.$$

$$\hat{a}_{31} = \frac{\frac{1}{18} - \frac{(c_2+c_3)}{10} + \frac{c_2c_3}{4} - \frac{\hat{c_1}+\hat{c_2}}{15} + \frac{(c_2+c_3)(\hat{c_1}+\hat{c_2})}{8} - \frac{\hat{c_1}\hat{c_2}(c_2+c_3)}{6} + \frac{\hat{c_1}\hat{c_2}}{12} - \frac{c_3c_2(\hat{c_1}+\hat{c_2})}{3} + \frac{\hat{c_1}c_2\hat{c_2}c_3}{2}}{b_3(\hat{c_3}-\hat{c_1})(\hat{c_3}-\hat{c_2})(c_1-c_2)(c_1-c_3)}.$$

$$\hat{a}_{32} = \frac{\frac{1}{18} - \frac{(c_1+c_3)}{10} + \frac{c_1c_3}{4} - \frac{\hat{c_1}+\hat{c_2}}{15} + \frac{(c_1+c_3)(\hat{c_1}+\hat{c_2})}{8} - \frac{\hat{c_1}\hat{c_2}(c_1+c_3)}{6} + \frac{\hat{c_1}\hat{c_2}}{12} - \frac{c_3c_1(\hat{c_1}+\hat{c_2})}{3} + \frac{\hat{c_2}c_1\hat{c_3}c_1}{2}}{b_3(\hat{c_3}-\hat{c_1})(\hat{c_3}-\hat{c_2})(c_2-c_1)(c_2-c_3)}.$$

$$\hat{a}_{33} = \frac{\frac{1}{18} - \frac{(c_1+c_2)}{10} + \frac{c_1c_2}{4} - \frac{\hat{c_1}+\hat{c_2}}{15} + \frac{(c_1+c_2)(\hat{c_1}+\hat{c_2})}{8} - \frac{\hat{c_1}\hat{c_2}(c_1+c_2)}{6} + \frac{\hat{c_1}\hat{c_2}}{12} - \frac{c_2c_1(\hat{c_1}+\hat{c_2})}{3} + \frac{\hat{c_1}c_2\hat{c_2}c_1}{2}}{b_3(\hat{c_3}-\hat{c_1})(\hat{c_3}-\hat{c_2})(c_3-c_1)(c_3-c_2)}.$$

In this way we get a class of three stages symplectic partitioned Runge-Kutta methods by choosing c_1, c_2 and c_3, $\hat{c_1}$, $\hat{c_2}$ and $\hat{c_3}$. We can choose c_1, c_2 and c_3, $\hat{c_1}$, $\hat{c_2}$ and $\hat{c_3}$ as the zeros of shifted Legendre polynomial.

Gauss and Lobatto-III : $s = 3$

$$\begin{array}{c|ccc}
\frac{1}{2}-\frac{\sqrt{15}}{10} & \frac{2}{15}-\frac{\sqrt{(15)}}{100} & \frac{1}{3}-\frac{2}{25}\sqrt{15} & \frac{1}{30}-\frac{\sqrt{15}}{100} \\
\frac{1}{2} & \frac{5}{24} & \frac{1}{3} & -\frac{1}{24} \\
\frac{1}{2}+\frac{\sqrt{15}}{10} & \frac{2}{15}+\frac{\sqrt{(15)}}{100} & \frac{1}{3}+\frac{2}{25}\sqrt{15} & \frac{1}{30}-\frac{\sqrt{15}}{100} \\
\hline
 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{array}$$

$$\begin{array}{c|ccc}
0 & \frac{1}{18}+\frac{\sqrt{15}}{60} & -\frac{1}{9} & \frac{1}{18}-\frac{\sqrt{15}}{60} \\
\frac{1}{2} & \frac{5}{36}+\frac{\sqrt{15}}{30} & \frac{2}{9} & \frac{5}{36}-\frac{\sqrt{15}}{30} \\
1 & \frac{2}{9}+\frac{\sqrt{15}}{60} & \frac{5}{9} & \frac{2}{9}-\frac{\sqrt{15}}{60} \\
\hline
 & \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array}$$

Chapter 4

Experiments

4.1 Numerical experiments

This chapter includes the results of those numerical methods which preserve the qualitative behaviour of the conservative problems for long time. The methods include symplectic implicit Runge-Kutta and symplectic implicit partitioned Runge-Kutta methods constructed in section 3.1 and 3.2 respectively. Among the symplectic implicit Runge-Kutta methods we have taken Gauss, Radau-I, Radau-II and Lobatto-III. Among the symplectic implicit partitioned Runge-Kutta methods we have taken the pairs Gauss and Lobatto-III, Gauss and Radau-I, Gauss and Radau-II, and Radau-I and Radau-II.

The main purpose of these numerical experiments is to observe the ability of these methods to provide qualitatively correct numerical results over long time. It should be noted that we have used a fixed stepsize in all numerical methods. The numerical methods used here have implicit stages to evaluate. We have used modified Newton iterations.

The absolute value of the difference between total energy of Hamiltonian system at initial point and at each point of approximated solution is calculated afterwards, that is called absolute error in the energy conservation of Hamiltonian system and the results are shown in Figures. In each graph, time is taken along x-axis and absolute error is taken along y-axis.

4.2 Simple pendulum

Consider a Simple pendulum which has unit mass of bob attached with a rod. The length of rod is one unit. The equations of motion of the Simple pendulum define a Hamiltonian system with generalized momenta p and generalized coordinates q and are given as

$$p' = -\sin(q), \qquad q' = p. \tag{4.2.1}$$

The total energy H is given as

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

We have applied symplectic implicit Runge-Kutta methods on Simple pendulum by using the initial values $p = 0$, $q = 1$. We have taken $100,000$ steps and stepsize $h = 0.01$. The absolute error in energy is plotted in Figures 4.1, 4.2, 4.3, 4.4, 4.5, 4.6, 4.7 and 4.8.

For $s = 2$.

Figures 4.1, 4.2 and 4.3 show the energy conservation using two stages Gauss, Radau-I and Radau-II symplectic implicit Runge-Kutta methods. Gauss symplectic implicit Runge-Kutta method produces most accurate result as compared to Radau-I and Radau-II symplectic implicite Runge-Kutta Methods. Now Figures, 4.9, 4.10 and 4.11 represent the energy conservation using Gauss and Radau-I, Gauss and Radau-II and Radau-I and Radau-II symplectic implicit partitioned Runge-Kutta methods. These methods produce approximately same results.

For $s = 3$**.**

Figures 4.4, 4.5, 4.6 and 4.7 show the energy conservation using three stages Gauss, Radau-I, Radau-II and Lobatto-III symplectic Implicite Runge-Kutta methods. Gauss, Radau-I and Radau-II symplectic implicit Runge-Kutta methods give the approximately same and much better results as compared to results obtained by the Lobatto-III. Figure, 4.12 represents the energy conservation using Gauss and Lobatto-III symplectic implicit partitioned Runge-Kutta methods.

For $s = 4$**.**

Figure 4.8 shows the energy conservation using four stages Labatto-III symplectic implicit Runge-Kutta method.

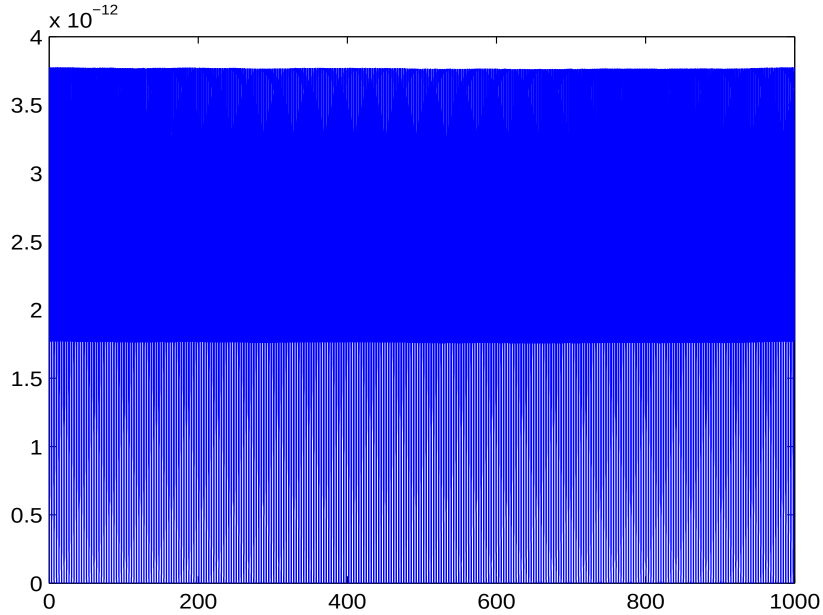


Figure 4.1: Absolute error in energy conservation of Simple pendulum with Gauss when $s = 2$.

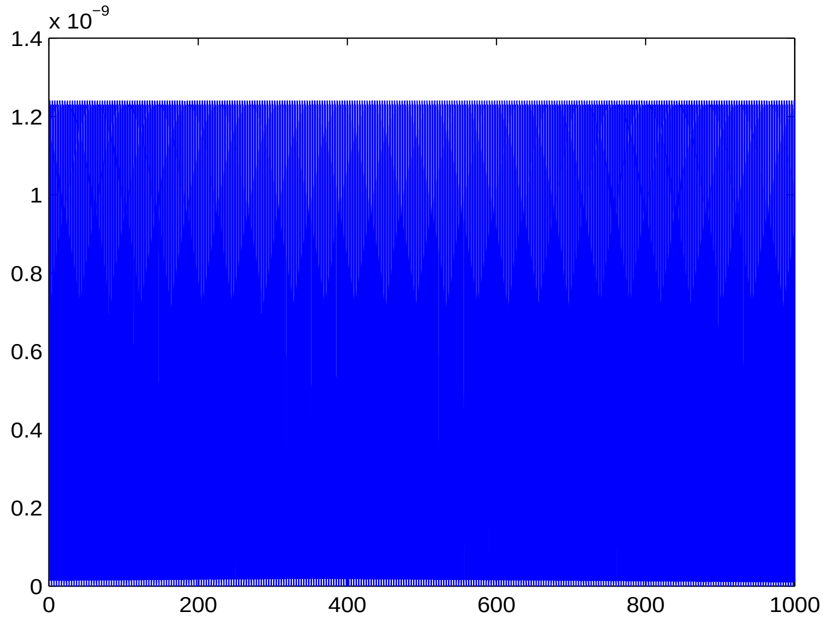


Figure 4.2: Absolute error in energy conservation of Simple pendulum with Radau-I when $s = 2$.

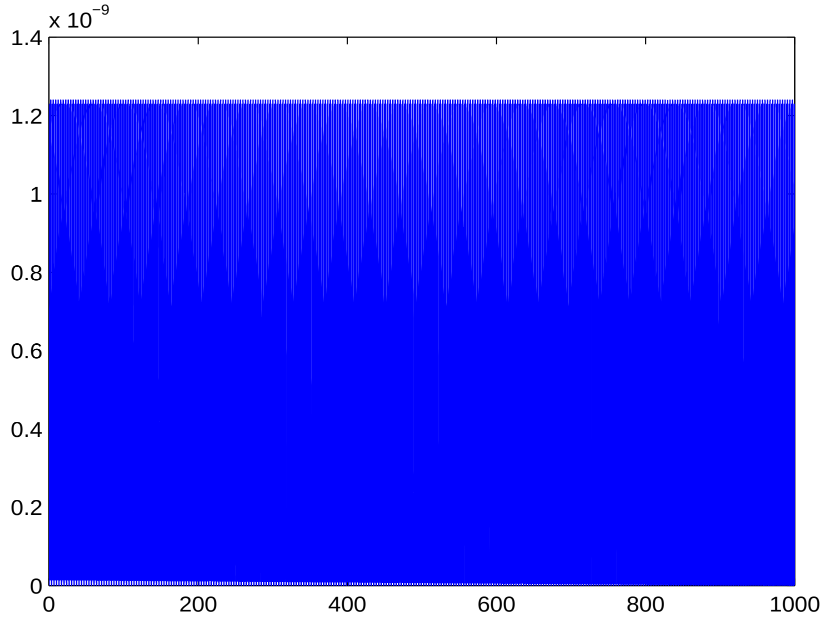


Figure 4.3: Absolute error in energy conservation of Simple pendulum with Radau-II when $s = 2$.

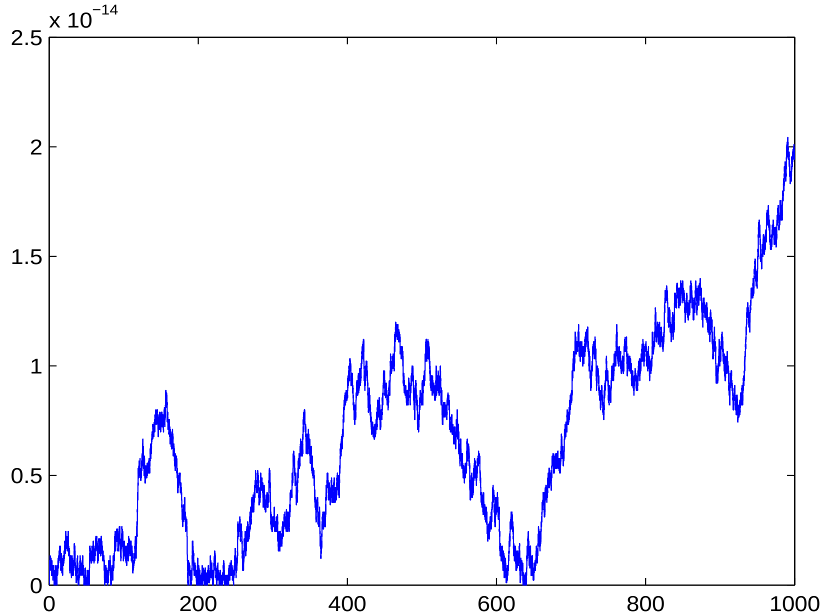


Figure 4.4: Absolute error in energy conservation of Simple pendulum with Gauss when $s = 3$.

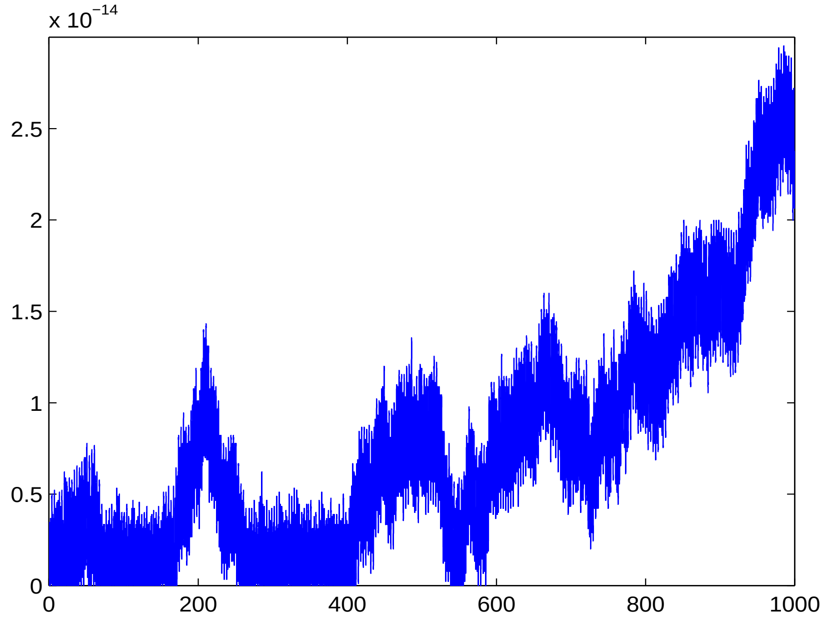


Figure 4.5: Absolute error in energy conservation of Simple pendulum with Radau-I when $s = 3$.

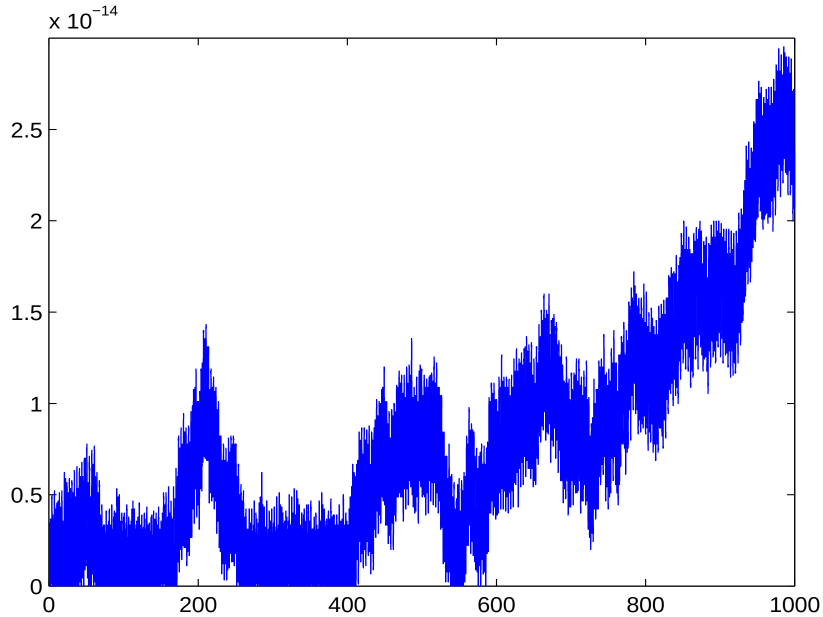


Figure 4.6: Absolute error in energy conservation of Simple pendulum with Radau-II when $s = 3$.

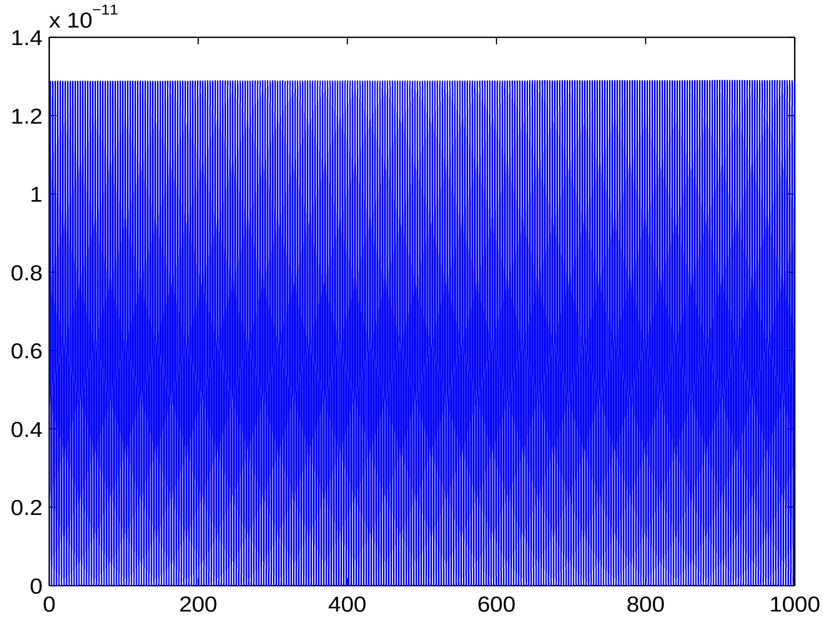


Figure 4.7: Absolute error in energy conservation of Simple pendulum with Lobatto-III when $s = 3$.

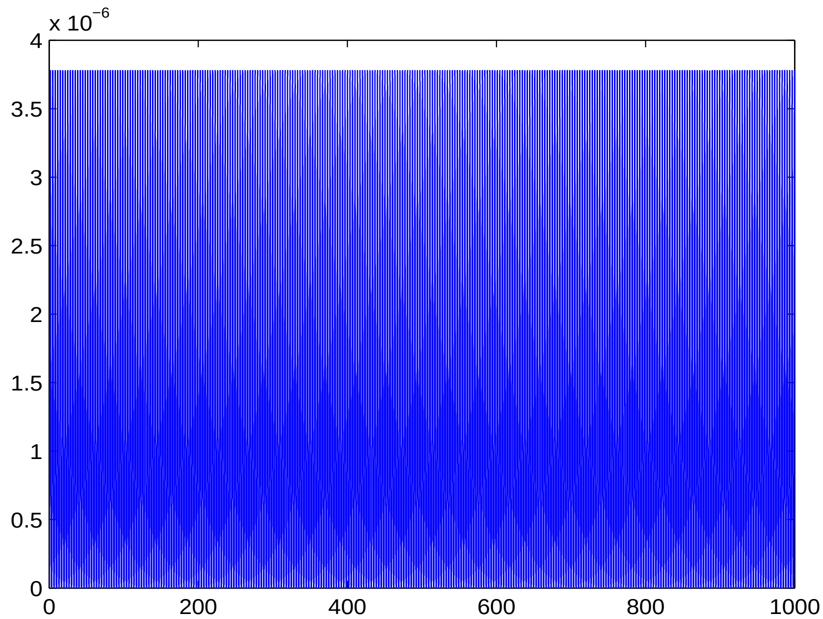


Figure 4.8: Absolute error in energy conservation of Simple pendulum with Lobatto-III when $s = 4$.

Now we have applied symplectic implicit partitioned Runge-Kutta methods on Simple pendulum by using $p = 0$, $q = 1$. We have taken $100,000$ steps and stepsize $h = 0.01$. The absolute error in energy is plotted in Figures 4.9, 4.10, 4.11 and 4.12.

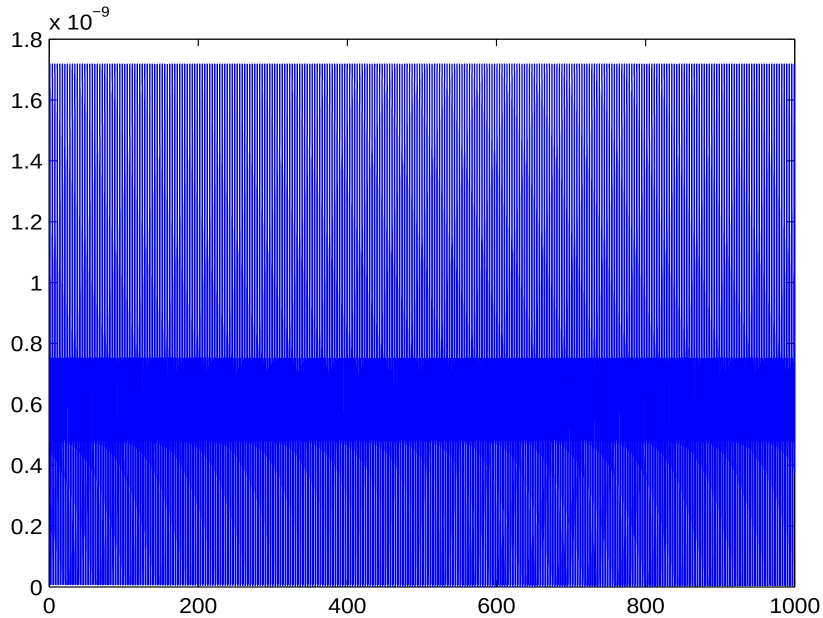


Figure 4.9: Absolute error in energy conservation of Simple pendulum with Gauss and Radau-I when $s = 2$.

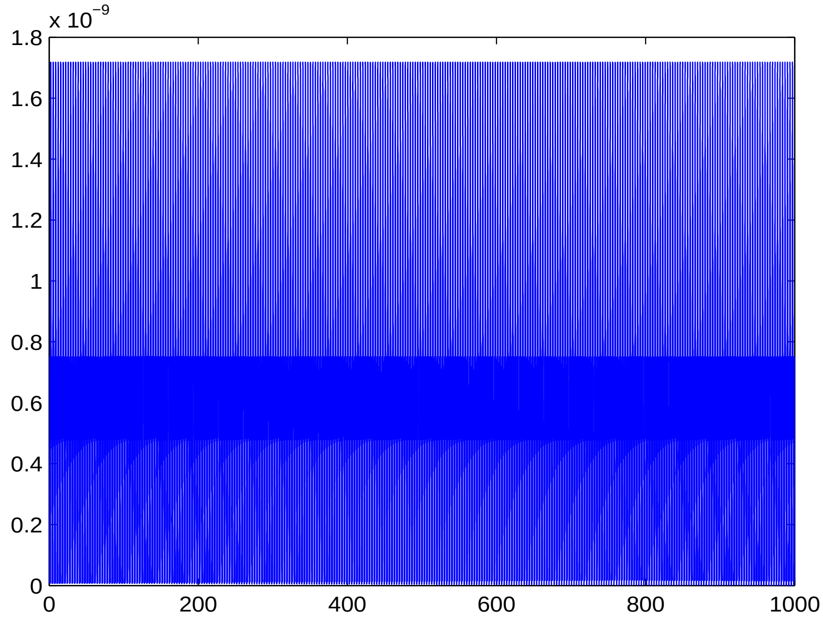


Figure 4.10: Absolute error in energy conservation of Simple pendulum with Gauss and Radau-II when $s = 2$.

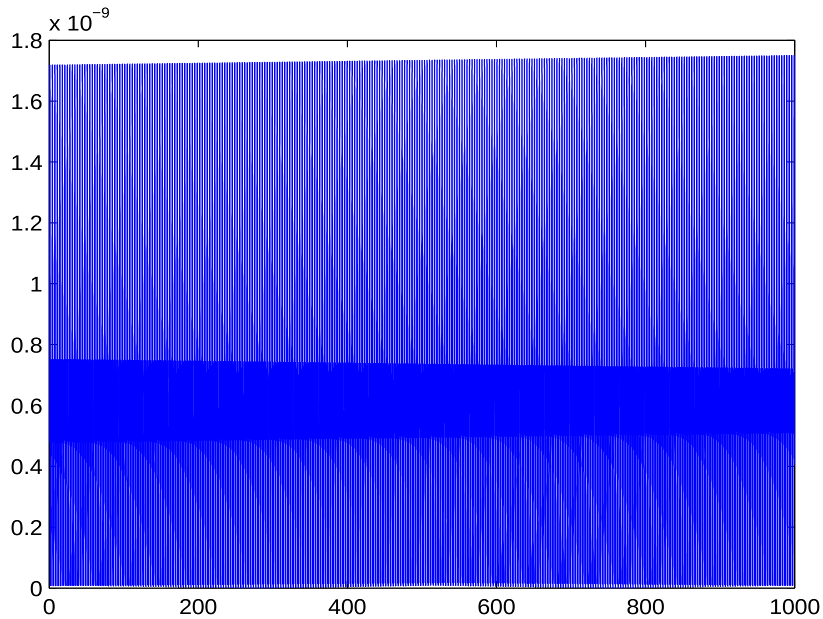


Figure 4.11: Absolute error in energy conservation of Simple pendulum with Radau-I and Radau-II when $s = 2$.

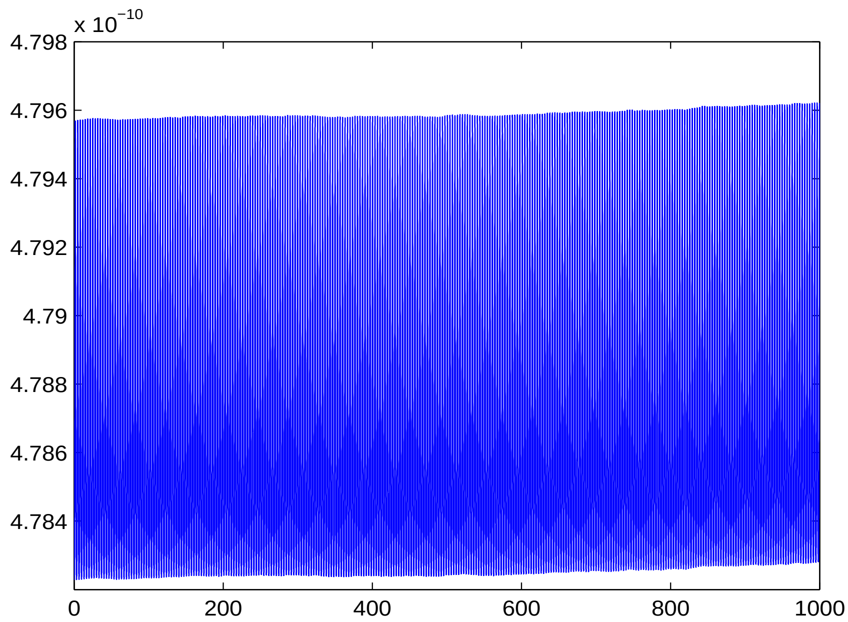


Figure 4.12: Absolute error in energy conservation of Simple pendulum with Gauss and Lobatto-III when $s = 3$.

4.3 Harmonic oscillator

The equations of motion of the Harmonic oscillator defines a Hamiltonian system with generalized momenta p and generalized coordinates q and are given as

$$q' = p, \quad p' = -q.$$

The total energy H is given as

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

We have applied symplectic implicit Runge-Kutta methods on Harmonic oscillator by using $p = 0$, $q = 1$. We have taken $100,000$ steps and stepsize $h = 0.01$. The absolute error in energy is plotted in Figures 4.13, 4.14, 4.15, 4.16, 4.17, 4.18, 4.19 and 4.20.

For $s = 2$.

Figures 4.13, 4.14 and 4.15 show the energy conservation using two stages Gauss, Radau-I and Radau-II symplectic implicit Runge-Kutta methods. These methods produce an approximately same and much better results as compared to symplectic implicit partitioned Runge-Kutta methods.

For $s = 3$.

Figures 4.16, 4.17, 4.18 and 4.19 represent the energy conservation using three stages Gauss, Radau-I, Radau-II and Lobatto-III symplectic implicit Runge-Kutta methods.

These methods produce an approximately same and much better results as compared to symplectic implicit partitioned Runge-Kutta methods.

For $s = 4$.

Figure 4.20 also represent the energy conservation using four stages Lobatto-III symplectic implicit Runge-Kutta method. This method produce much better result.

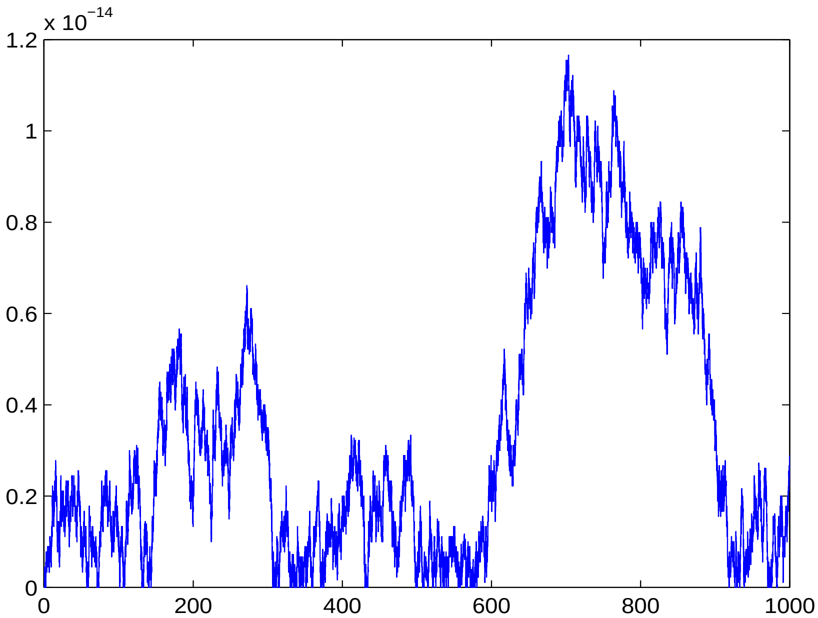


Figure 4.13: Absolute error in energy conservation of Harmonic oscillator with Gauss when $s = 2$.

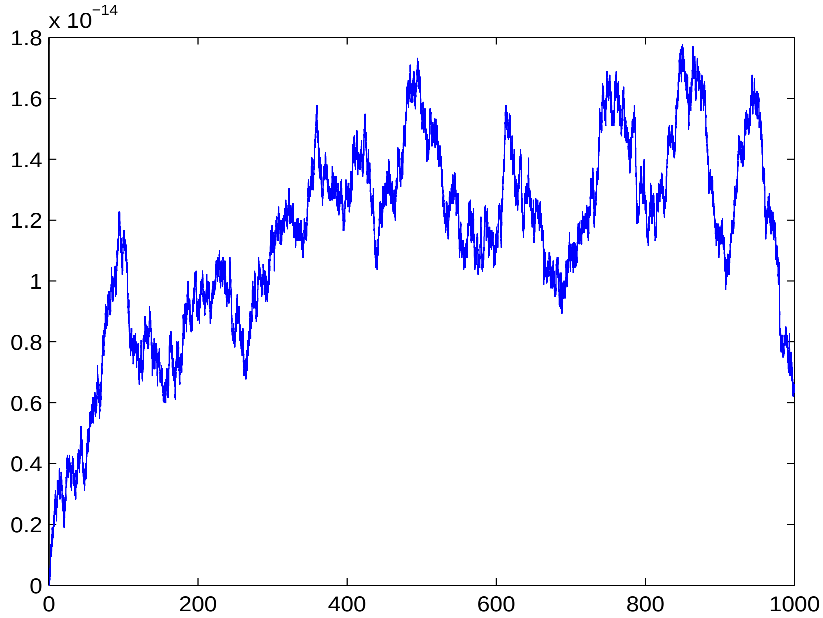


Figure 4.14: Absolute error in energy conservation of Harmonic oscillator with Radau-I when $s = 2$.

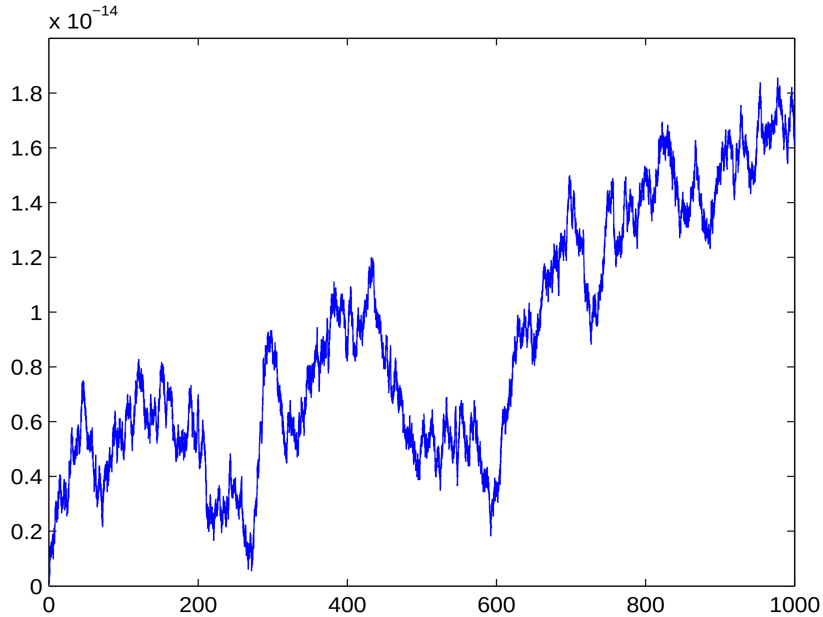


Figure 4.15: Absolute error in energy conservation of Harmonic oscillator with Radau-II when $s = 2$.

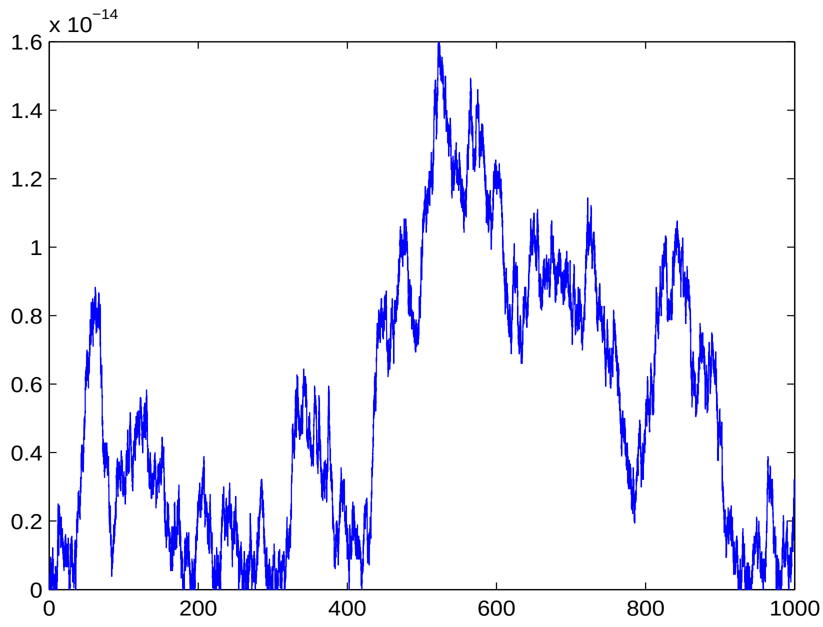


Figure 4.16: Absolute error in energy conservation of Harmonic oscillator with Gauss when $s = 3$.

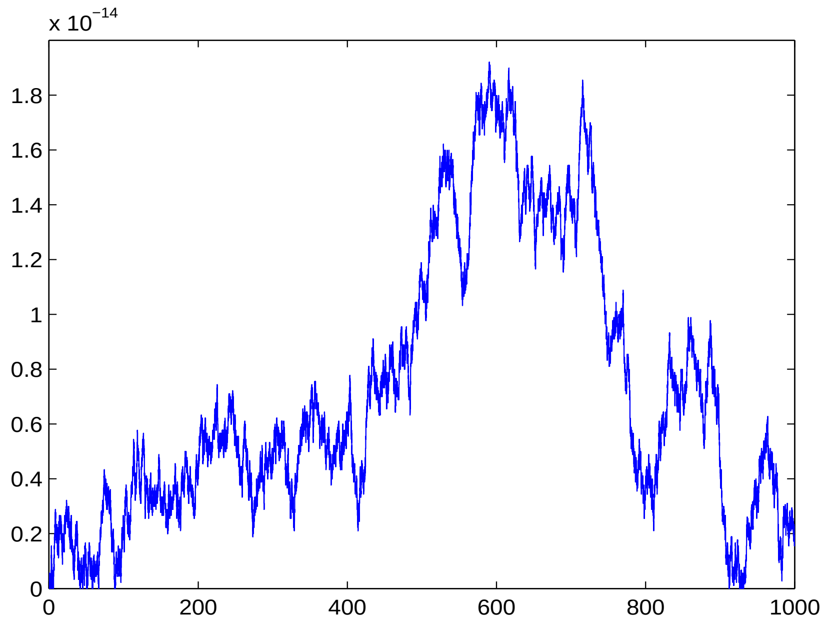


Figure 4.17: Absolute error in energy conservation of Harmonic oscillator with Radau-I when $s = 3$.

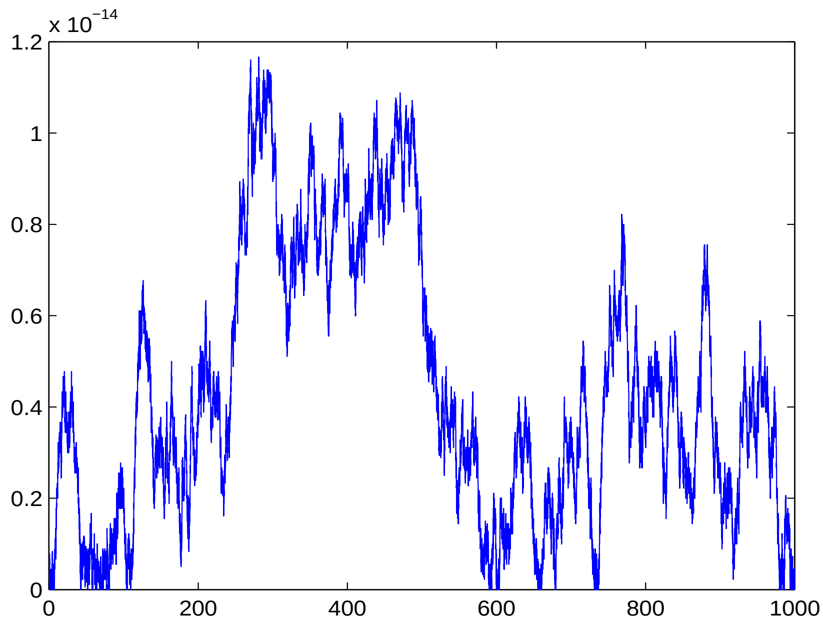


Figure 4.18: Absolute error in energy conservation of Harmonic oscillator with Radau-II when $s = 3$.

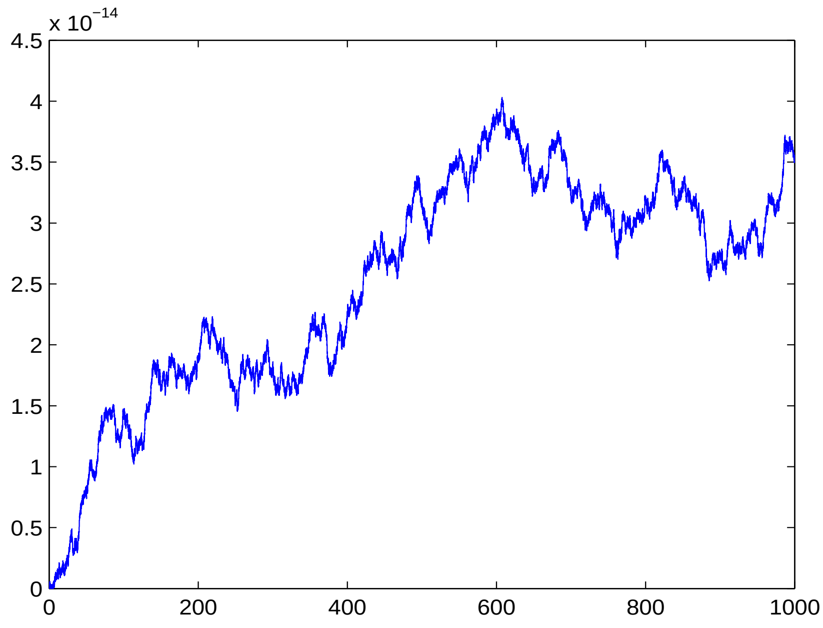


Figure 4.19: Absolute error in energy conservation of Harmonic oscillator with Lobatto-III when $s = 3$.

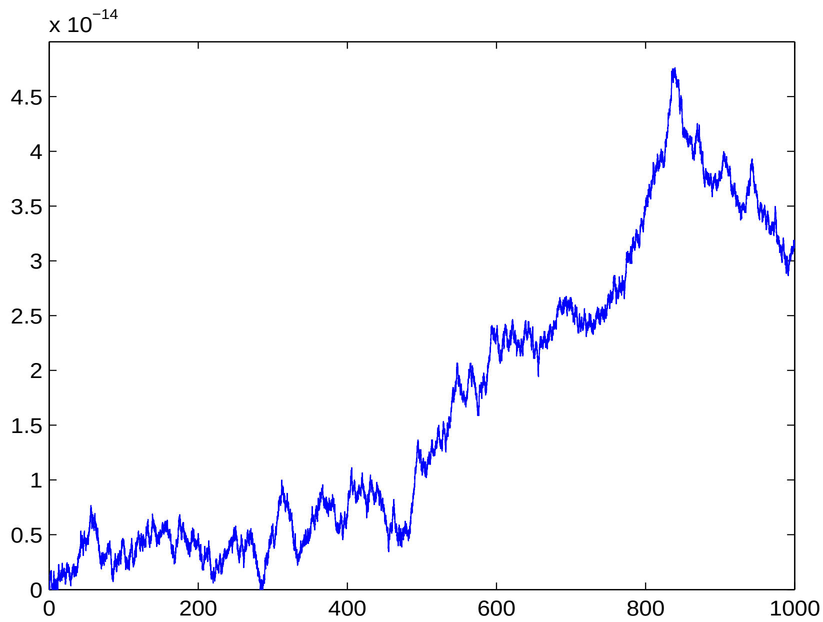


Figure 4.20: Absolute error in energy conservation of Harmonic oscillator with Lobatto-III when $s = 4$.

Now we have applied symplectic implicit partitioned Runge-Kutta methods on Harmonic oscillator by using $p = 0$, $q = 1$, for $100,000$ steps using stepsize $h = 0.01$. The absolute error in energy is plotted in Figures 4.21, 4.22, 4.23 and 4.24. Absolute error is very small that means the energy is conserved.

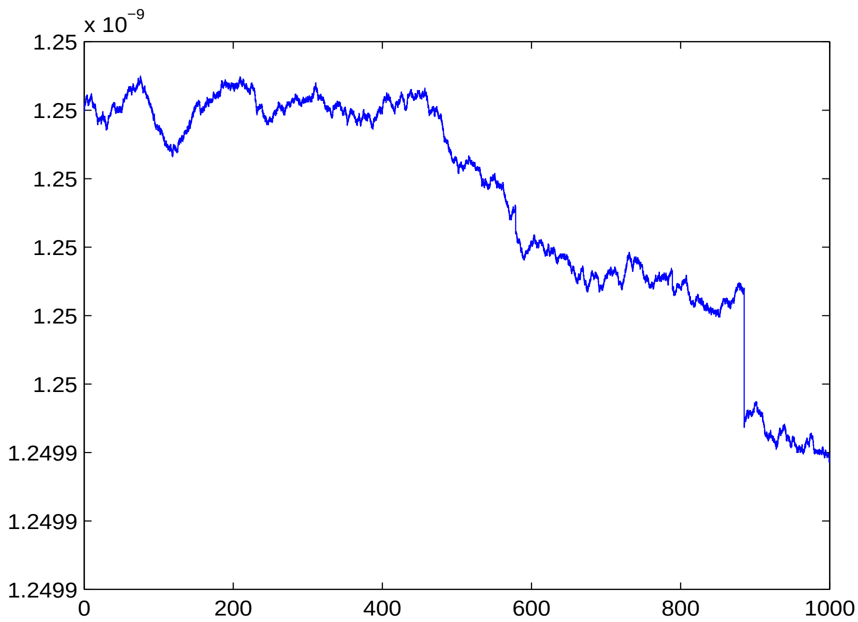


Figure 4.21: Absolute error in energy conservation of Harmonic oscillator with Gauss and Radau-I when $s = 2$.

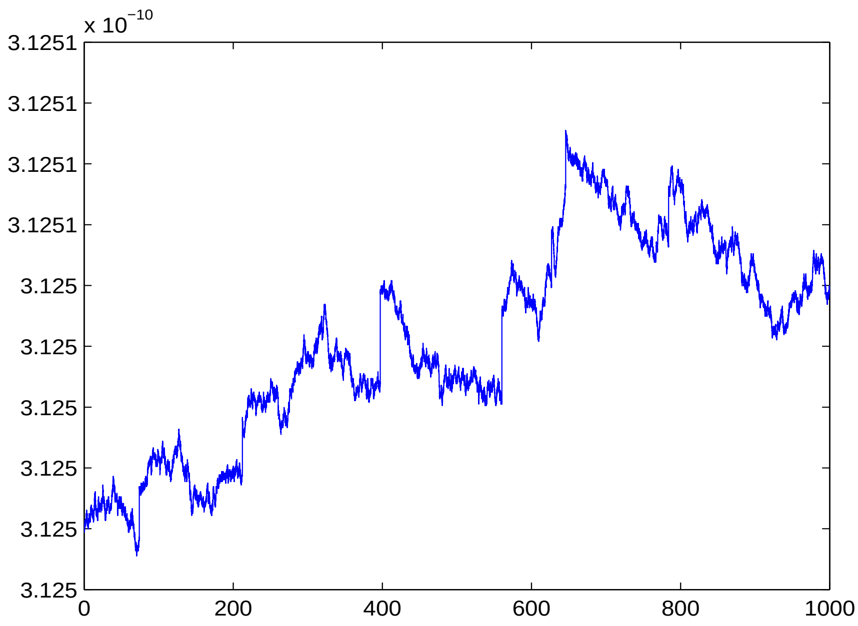


Figure 4.22: Absolute error in energy conservation of Harmonic oscillator with Gauss and Radau-II when $s = 2$.

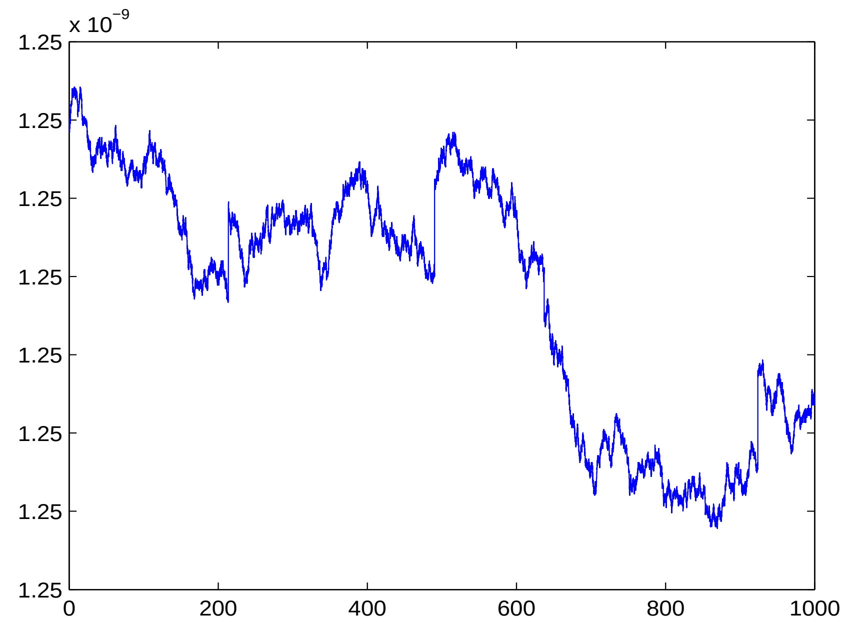


Figure 4.23: Absolute error in energy conservation of Harmonic oscillator with Radau-I and Radau-II when $s = 2$.

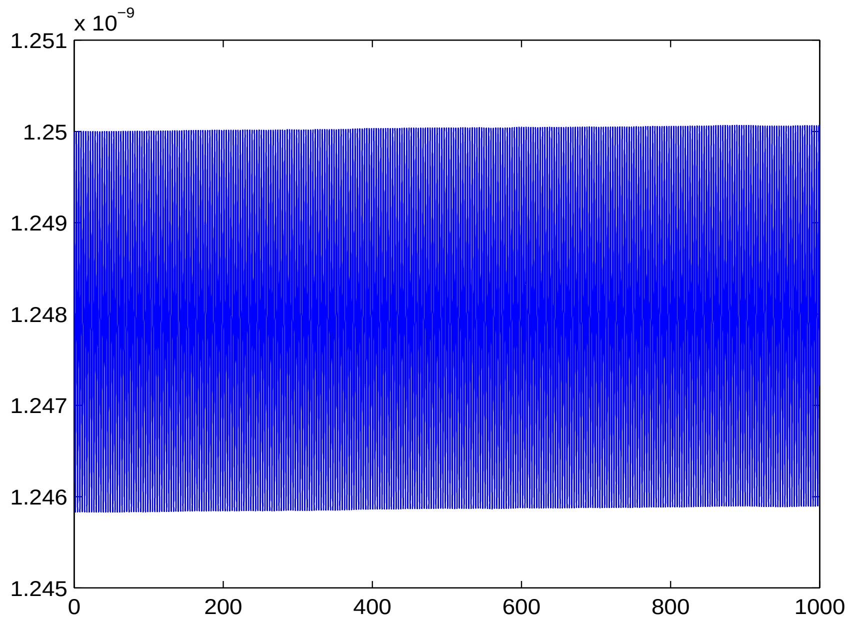


Figure 4.24: Absolute error in energy conservation of Harmonic oscillator with Gauss and Lobatto-III when $s = 3$.

4.4 Kepler problem

The problem in which the motion of a planet revolving around the sun which is considered to be fixed at origin is called the Kepler problem. The equations of motion are,

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

where (q_1, q_2) are the generalized coordinates and (p_1, p_2) are the generalized momenta. The total energy of the system is

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

The initial conditions are

$$(q_1, q_2, p_1, p_2) = (1-e, 0, 0, \sqrt{\frac{1+e}{1-e}}),$$

where $0 \le e < 1$ is the eccentricity of the elliptic orbits which are formed by the motion of one body around the other.

We have applied symplectic implicit Runge-Kutta methods on Kepler problem with $e = 0$ and $e = 0.5$. We have taken 100,000 steps and stepsize $h = \frac{2\pi}{1000}$. The absolute error in energy is plotted in Figures 4.25, 4.26, 4.27, 4.33, 4.34, 4.35, 4.28, 4.29, 4.30, 4.31 4.32, 4.36, 4.37, 4.38 and 4.39.

When eccentricity $e = 0$.

For $s = 2$.

Figures 4.25, 4.26 and 4.27 show the energy conservation using two stages Gauss, Radau-I and Radau-II symplectic implicit Runge-Kutta methods. These methods give the good results. Now the Figures, 4.41, 4.42 and 4.43 also represent the energy conservation using two stages Gauss and Radau-I, Gauss and Radau-II and Radau-I and Radau-II symplectic implicit partitioned Runge-Kutta methods.

For $s = 3$**.**

Figures 4.28, 4.29, 4.30, 4.31 also show the energy conservation using three stages Gauss, Radau-I, Radau-II and Lobatto-III symplectic implicit Runge-Kutta methods. All of these methods produce an approximately same and much better results. Now Figure 4.44 represents the energy conservation using two stages Gauss and Lobatto-III symplectic implicit partitioned Runge-Kutta method.

For $s = 4$**.**

Figure 4.32 shows the energy conservation using four stages Lobatto-III symplectic implicit Runge-Kutta method.

When eccentricity $e = 0.5$.

For $s = 2$**.**

Figures 4.33, 4.34 and 4.35 represent the energy conservation using two stages Gauss, Radau-I, Radau-II and Lobatto-III symplectic implicit Runge-Kutta methods. Gauss symplectic implicit Runge-Kutta method produce the most better result as compared to results obtained by Radau-I and Radau-II symplectic implicit Runge-Kutta methods. Now the Figures 4.45, 4.46 and 4.47 also show the energy conservation using two stages Gauss and Radau-I, Gauss and Radau-II and Radau-I and Radau-II symplectic implicit partitioned Runge-Kutta methods.

For $s = 3$**.**

Figures 4.36, 4.37, 4.38 and 4.39 show the energy conservation using three stages Gauss, Radau-I, Radau-II and Lobatto-III symplectic implicit Runge-Kutta methods. Here Gauss symplectic implicit Runge-Kutta method give the good result as compared to results obtained by Radau-I and Radau-II symplectic implicit Runge-Kutta methods. Figure 4.48 represents the energy conservation using three stages Gauss and Lobatto-III symplectic implicit partitioned Runge-Kutta method.

For $s = 4$**.**

Figure 4.40 represents the energy conservation using four stages Lobatto-III symplectic implicit Runge-Kutta method.

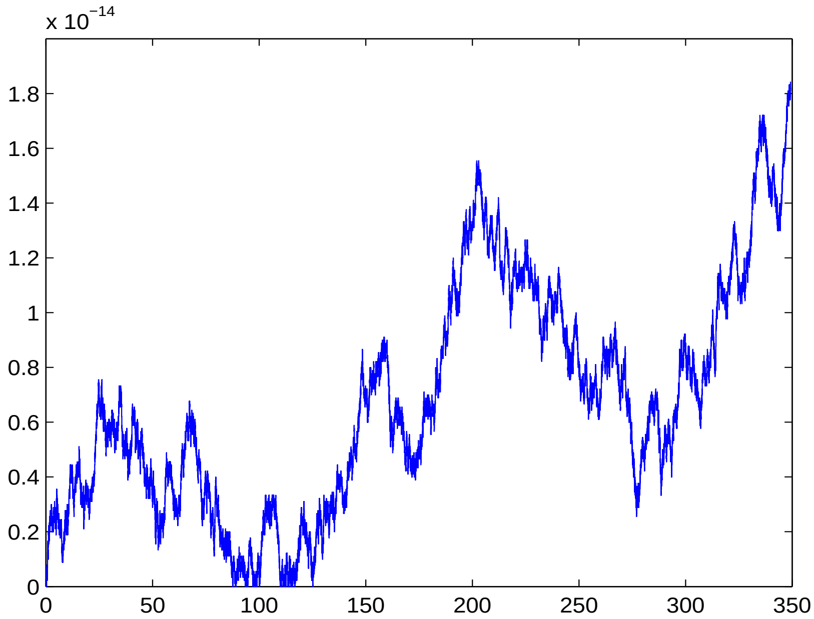


Figure 4.25: Absolute error in energy conservation of Kepler problem ($e = 0$) with Gauss when $s = 2$.

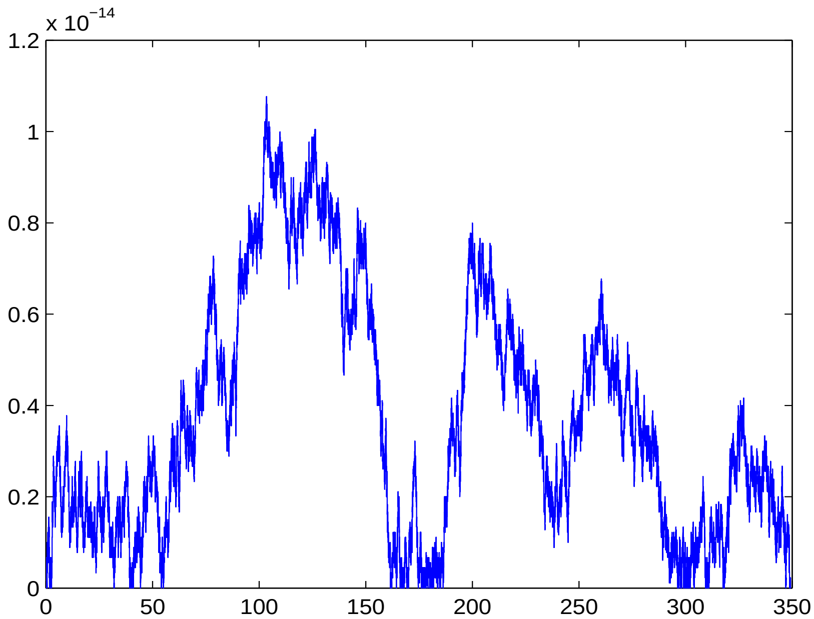


Figure 4.26: Absolute error in energy conservation of Kepler problem ($e = 0$) with Radau-I when $s = 2$.

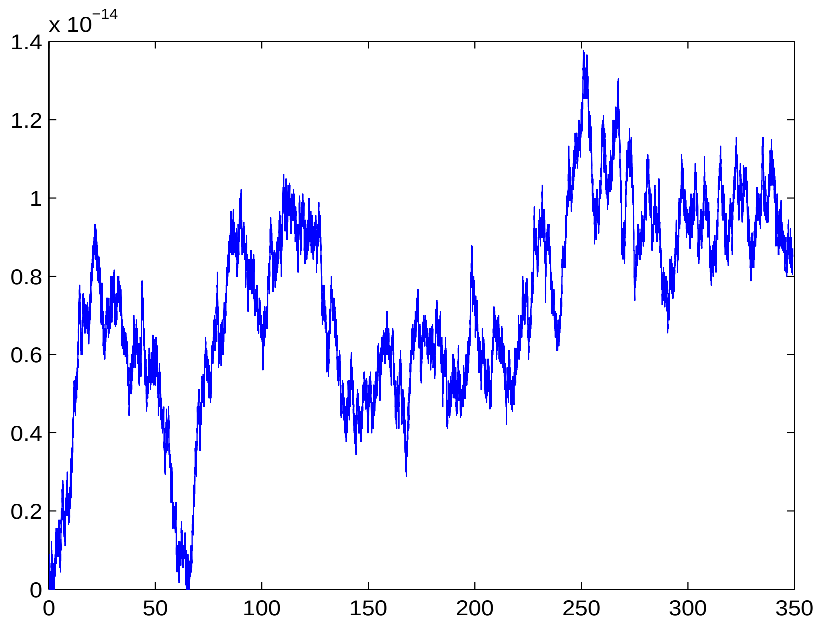


Figure 4.27: Absolute error in energy conservation of Kepler problem ($e = 0$) with Radau-II when $s = 2$.

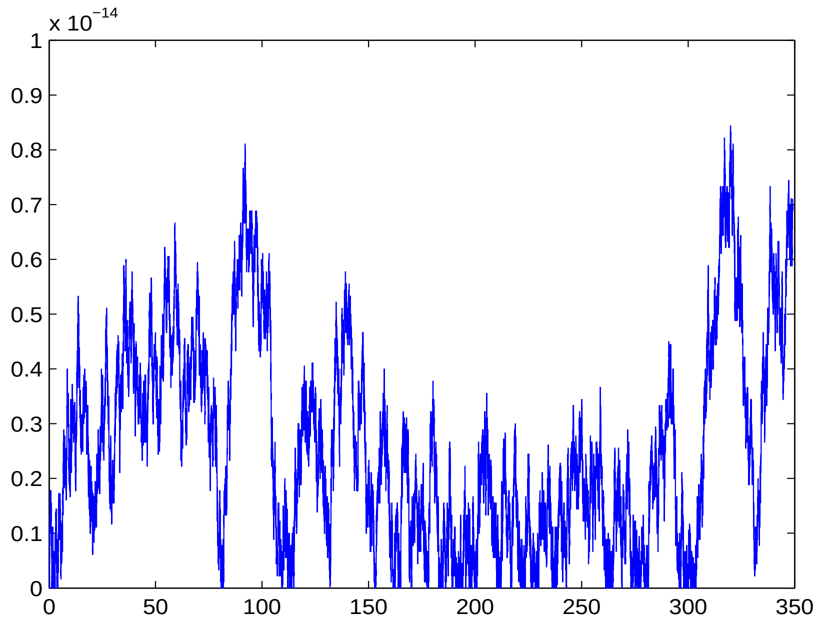


Figure 4.28: Absolute error in energy conservation of Kepler problem ($e = 0$) with Gauss when $s = 3$.

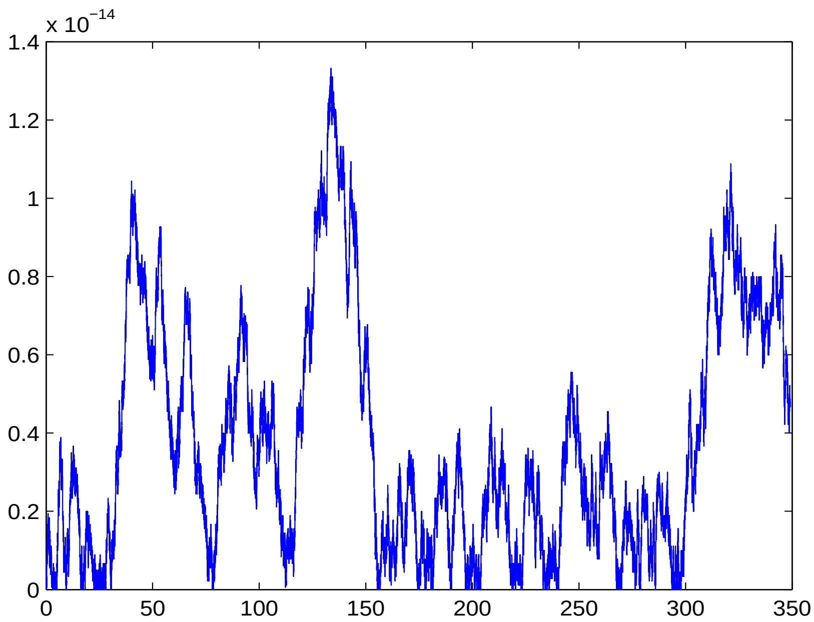


Figure 4.29: Absolute error in energy conservation of Kepler problem ($e = 0$) with Radau-I when $s = 3$.

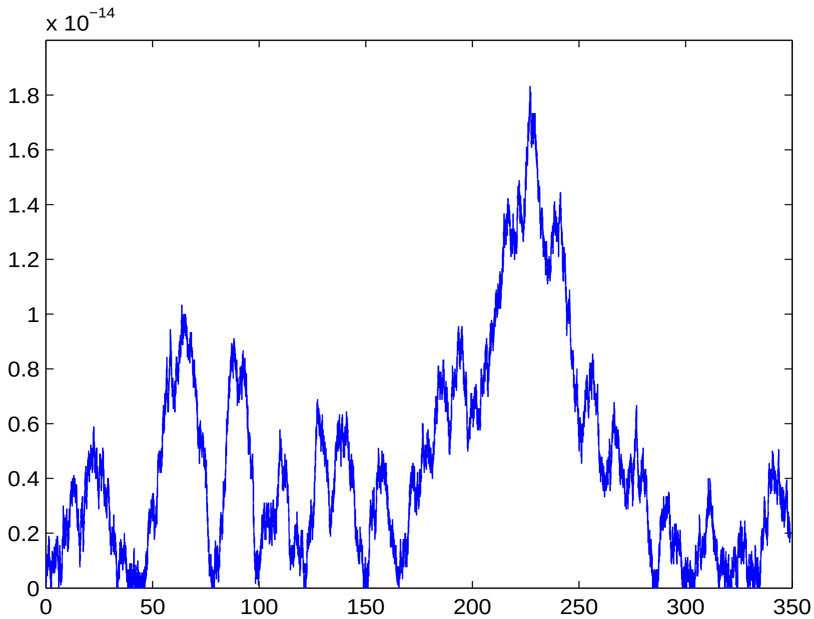


Figure 4.30: Absolute error in energy conservation of Kepler problem ($e = 0$) with Radau-II when $s = 3$.

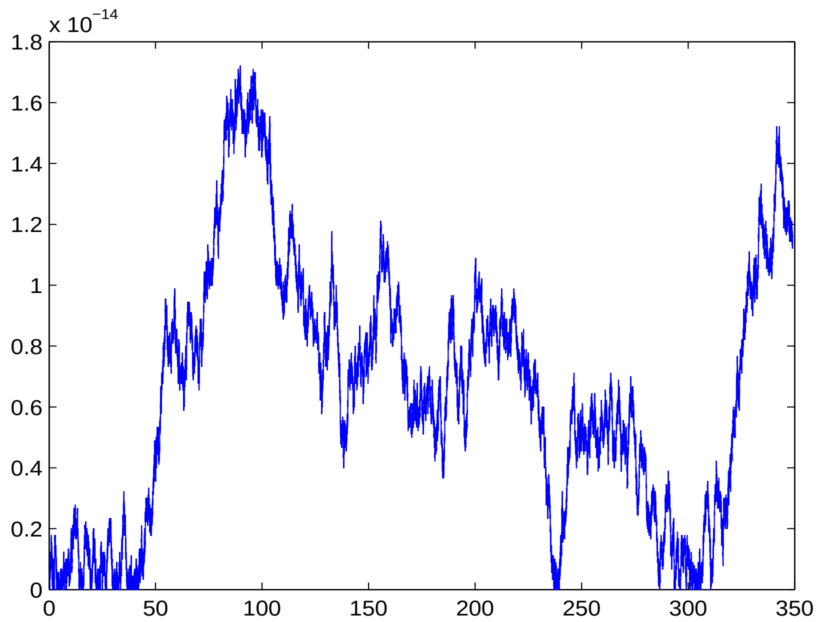


Figure 4.31: Absolute error in energy conservation of Kepler problem ($e = 0$) with Lobatto-III when $s = 3$.

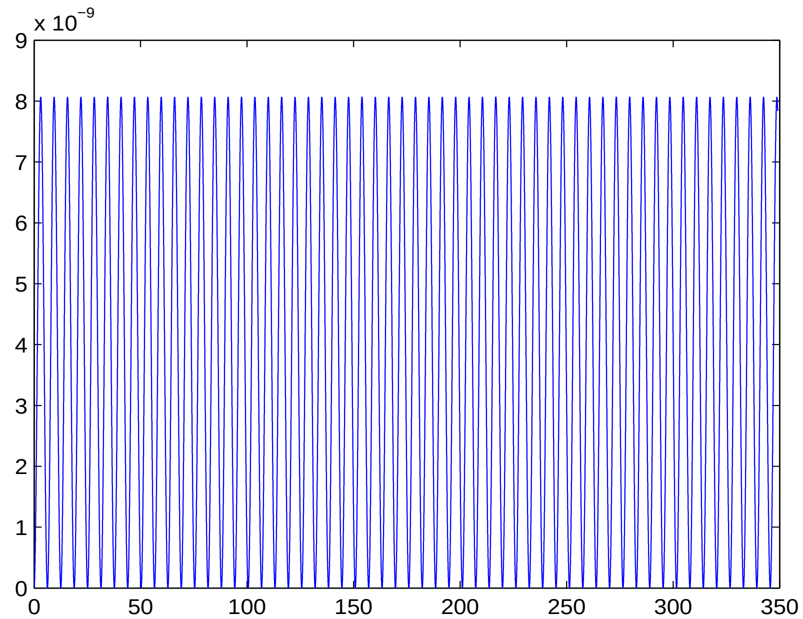


Figure 4.32: Absolute error in energy conservation of Kepler problem ($e = 0$) with Lobatto-III when $s = 4$.

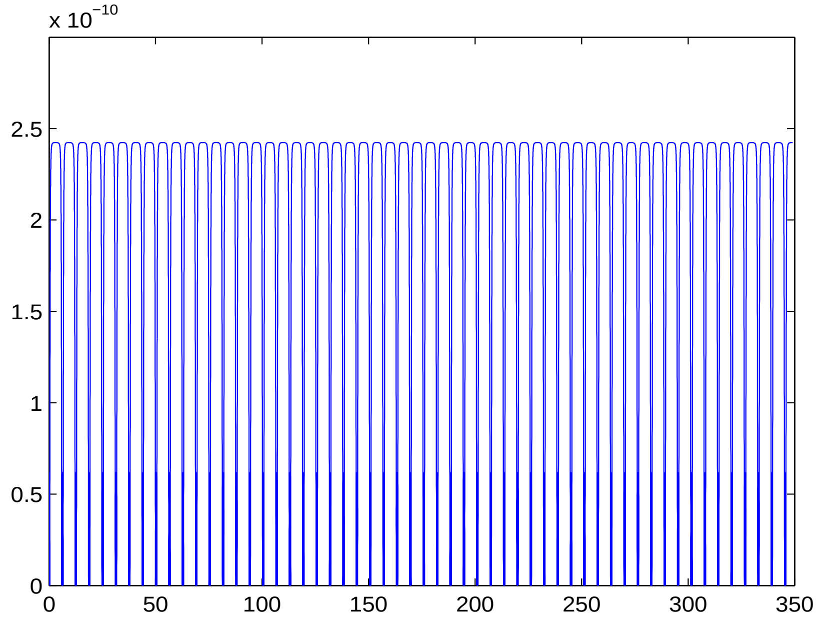


Figure 4.33: Absolute error in energy conservation of Kepler problem ($e = 0.5$) with Gauss when $s = 2$.

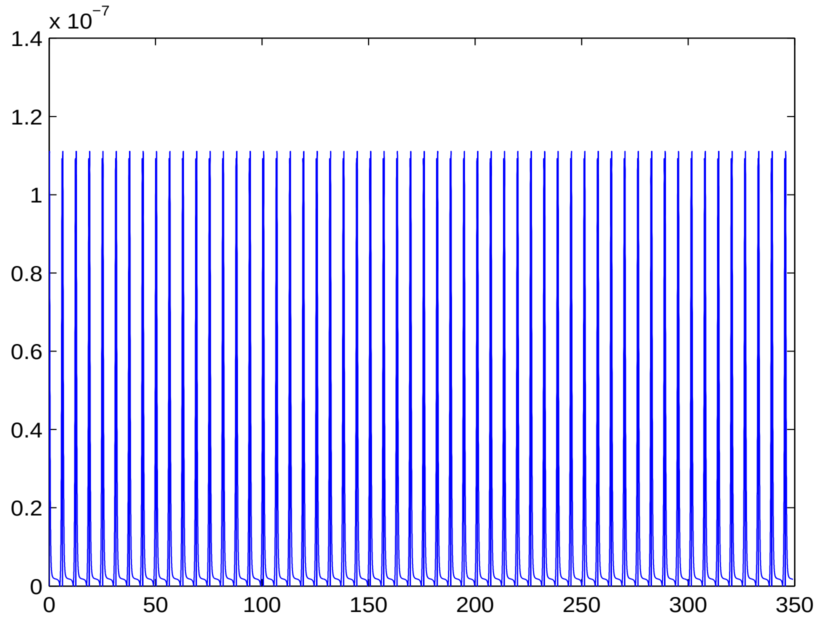


Figure 4.34: Absolute error in energy conservation of Kepler problem ($e = 0.5$) with Radau-I when $s = 2$.

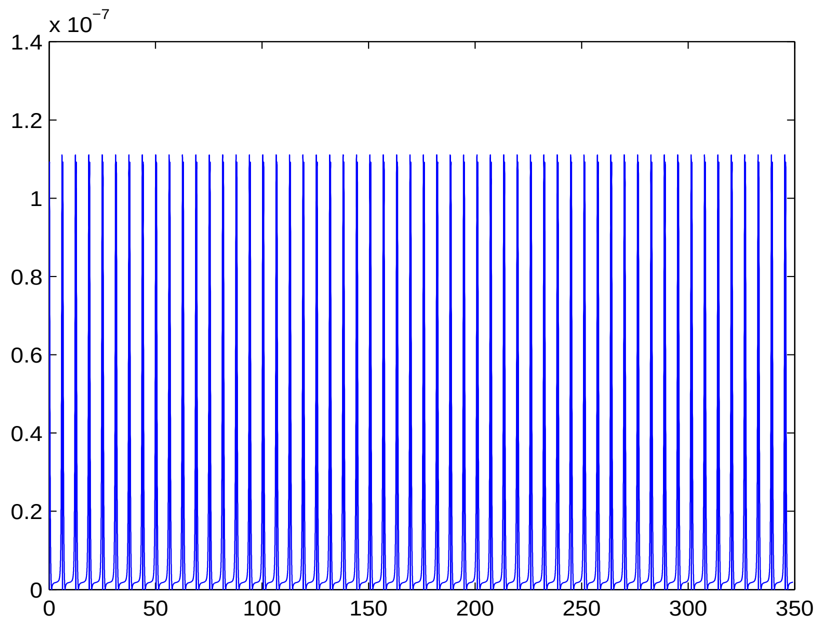


Figure 4.35: Absolute error in energy conservation of Kepler problem ($e = 0.5$) with Radau-II when $s = 2$.

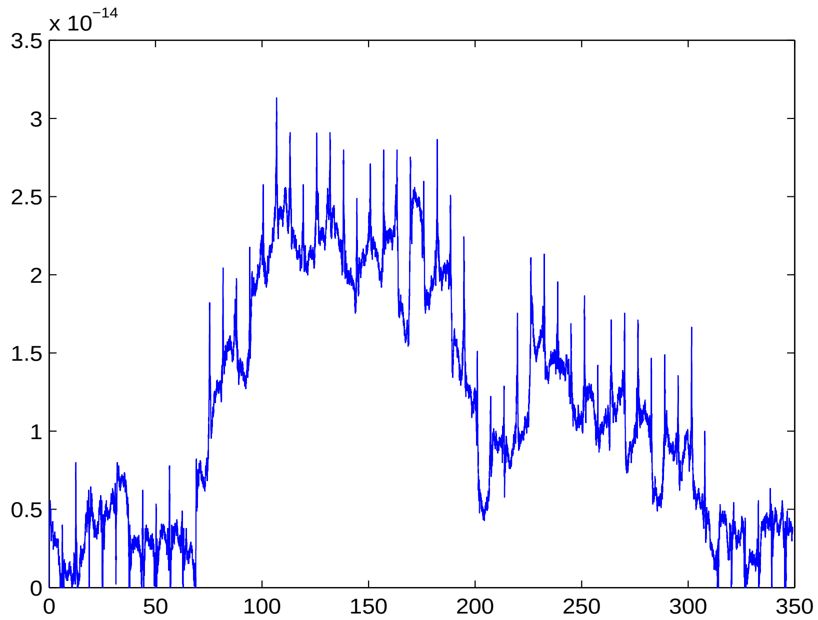


Figure 4.36: Absolute error in energy conservation of Kepler problem ($e = 0.5$) with Gauss when $s = 3$.

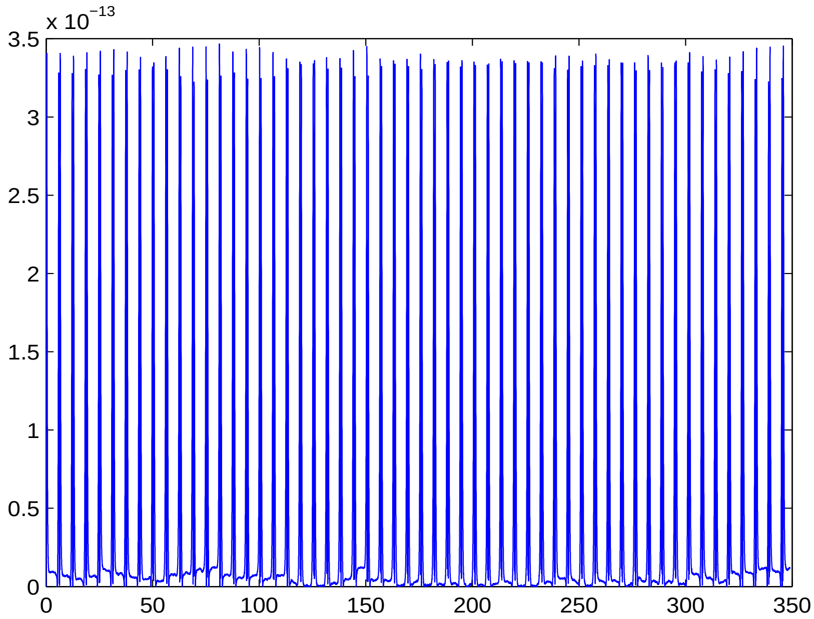


Figure 4.37: Absolute error in energy conservation of Kepler problem ($e = 0.5$) with Radau-I when $s = 3$.

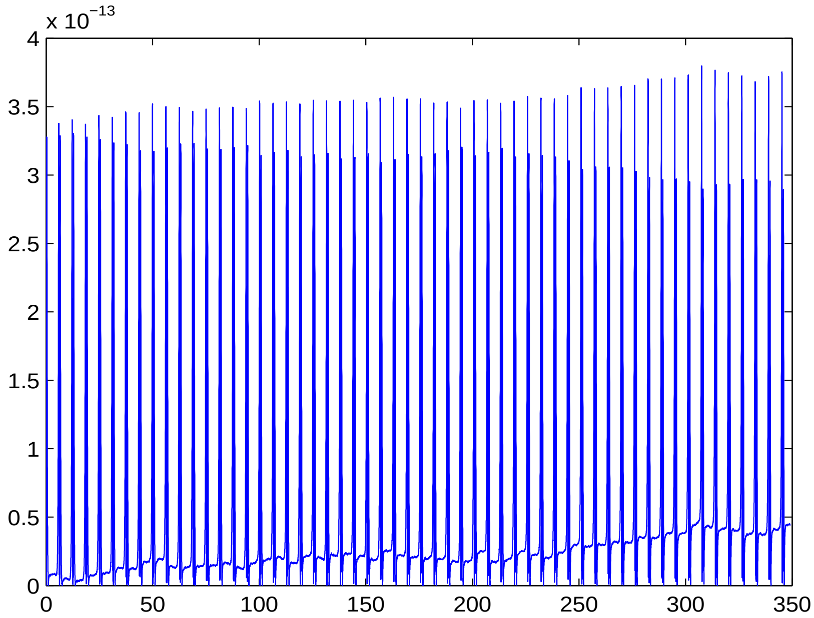


Figure 4.38: Absolute error in energy conservation of Kepler problem ($e = 0.5$) with Radau-II when $s = 3$.

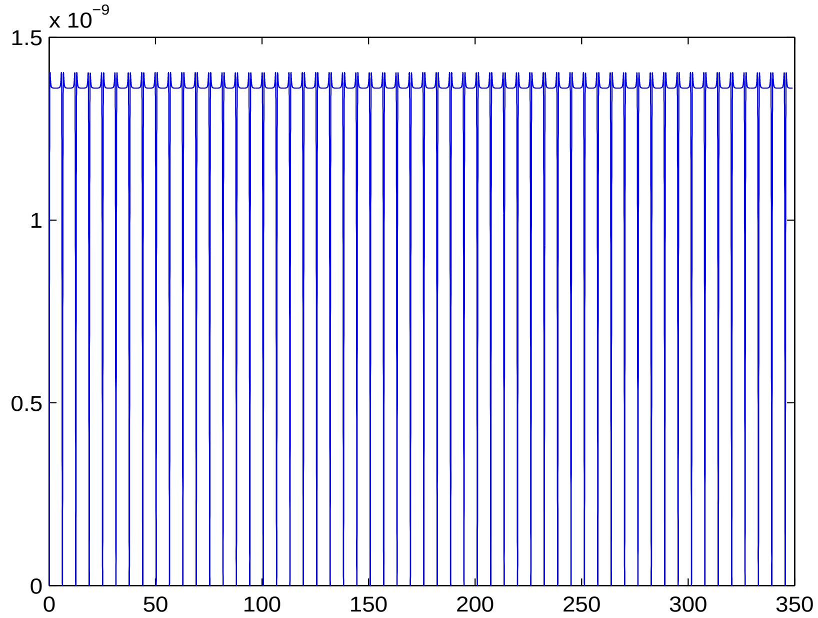


Figure 4.39: Absolute error in energy conservation of Kepler problem ($e = 0.5$) with Lobatto-III when $s = 3$.

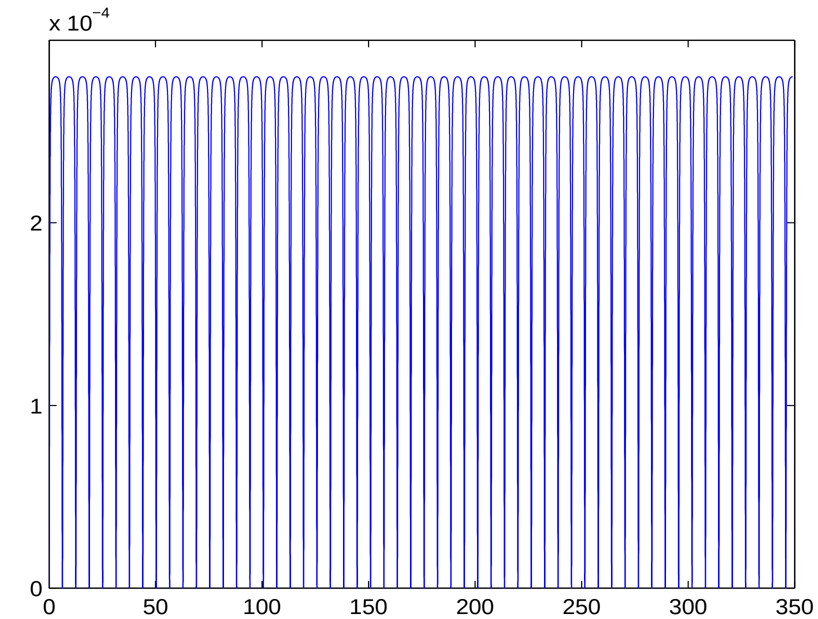


Figure 4.40: Absolute error in energy conservation of Kepler problem ($e = 0.5$) with Lobatto-III when $s = 4$.

Now we have applied symplectic implicit partitioned Runge-Kutta methods on Kepler Problem using $e = 0$ and $e = 0.5$. We have taken $100,000$ steps and stepsize $h = \frac{2\pi}{1000}$. The absolute error in energy is plotted in Figures 4.41, 4.42, 4.43, 4.44, 4.45, 4.46, 4.47 and 4.48. The absolute error is very small that means the energy is conserved.

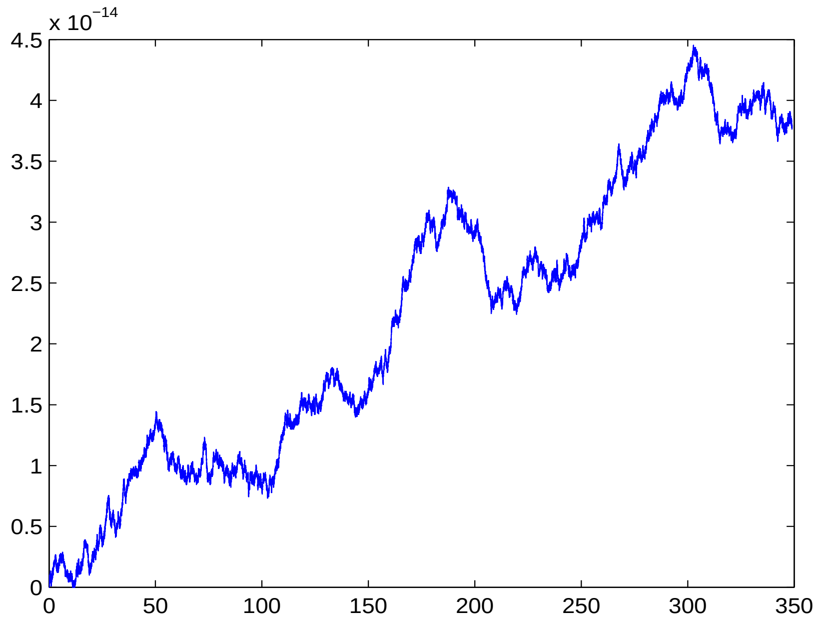


Figure 4.41: Absolute error in energy conservation of Kepler problem ($e = 0$) with Gauss and Radau-I when $s = 2$.

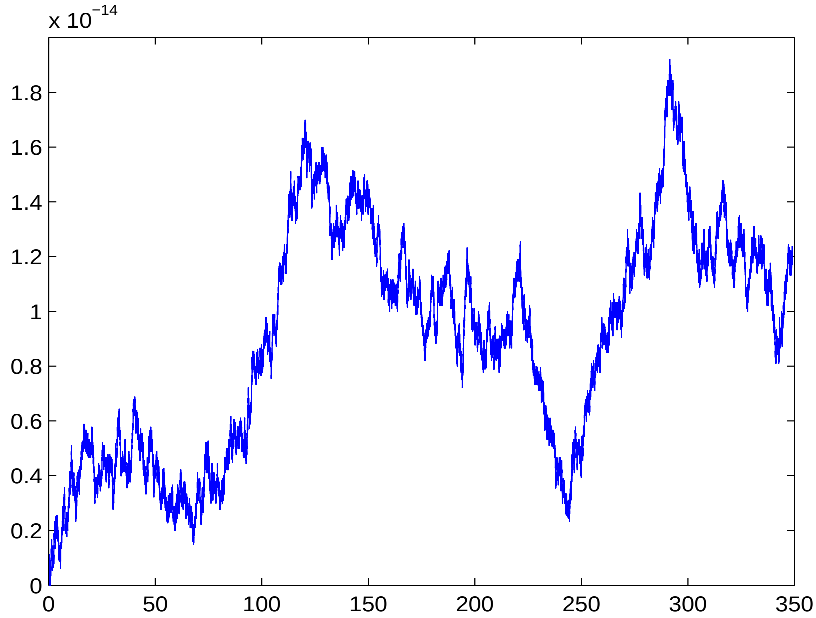


Figure 4.42: Absolute error in energy conservation of Kepler problem ($e = 0$) with Gauss and Radau-II when $s = 2$.

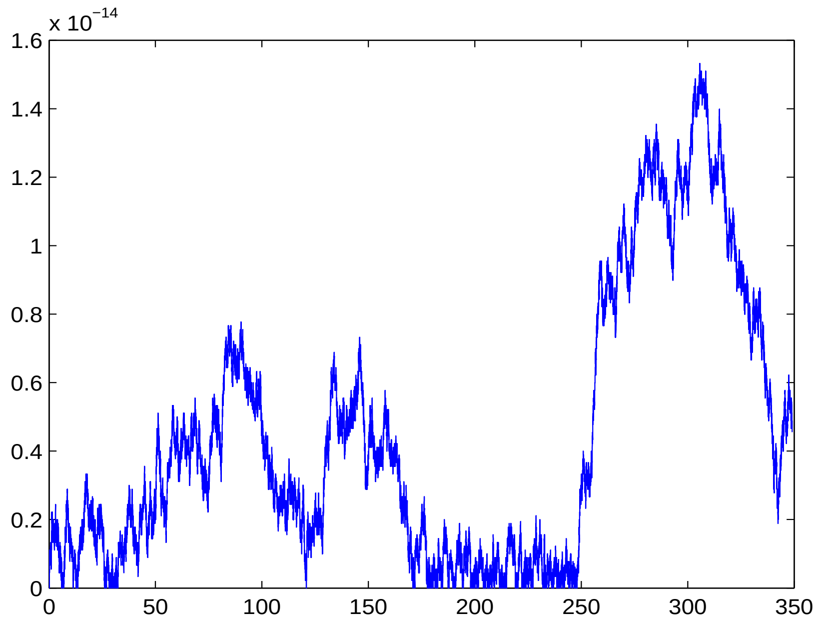


Figure 4.43: Absolute error in energy conservation of Kepler problem ($e = 0$) with Radau-I and Radau-II when $s = 2$.

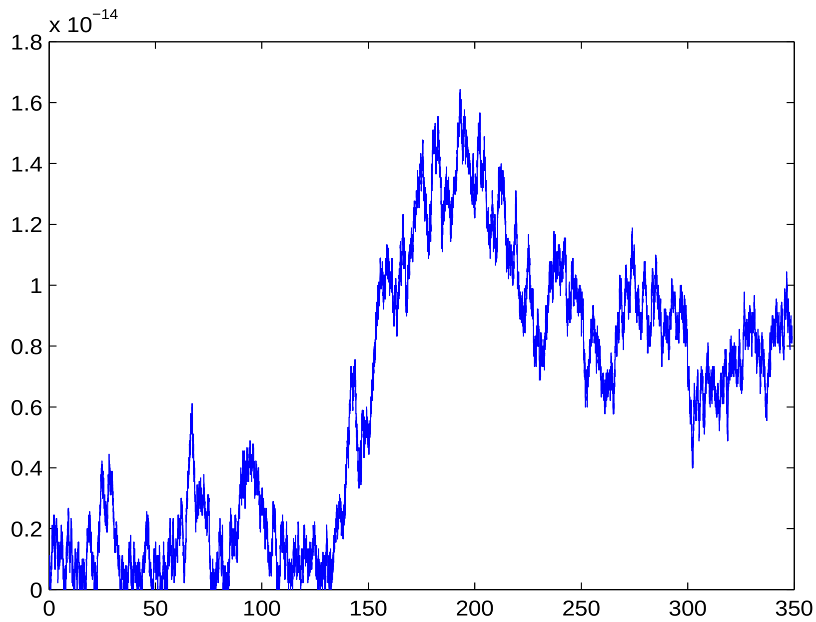


Figure 4.44: Absolute error in energy conservation of Kepler problem ($e = 0$) with Gauss and Lobatto-III when $s = 3$.

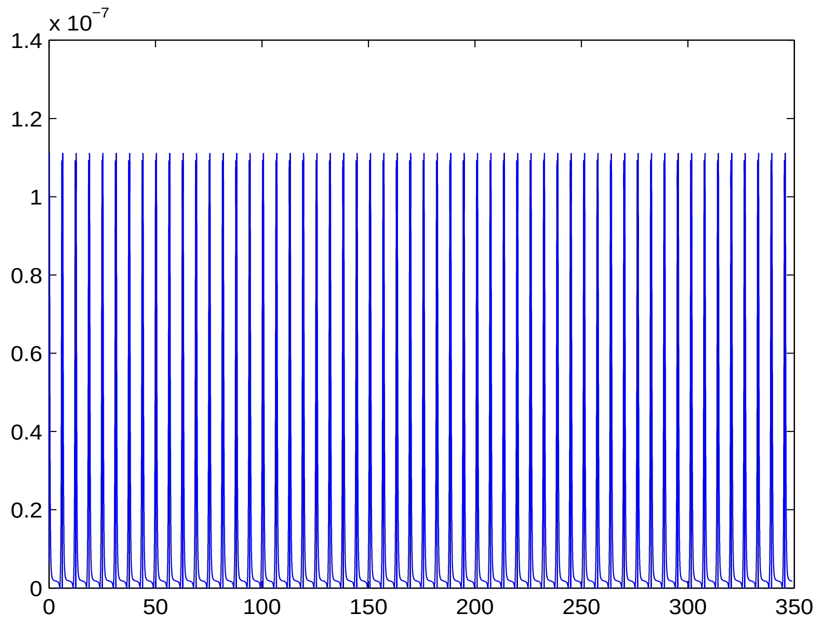


Figure 4.45: Absolute error in energy conservation of Kepler problem ($e = 0.5$) with Gauss and Radau-I when $s = 2$.

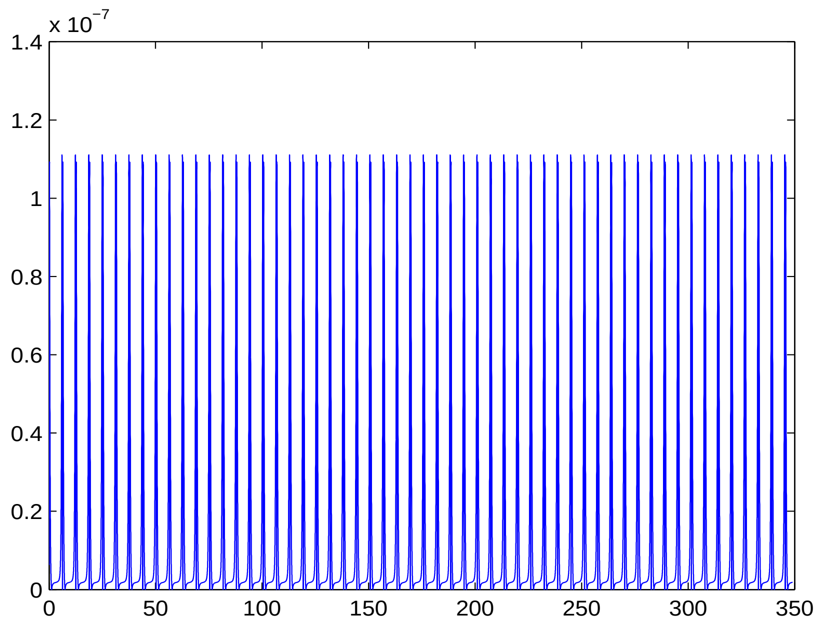


Figure 4.46: Absolute error in energy conservation of Kepler problem ($e = 0.5$) with Gauss and Radau-II when $s = 2$.

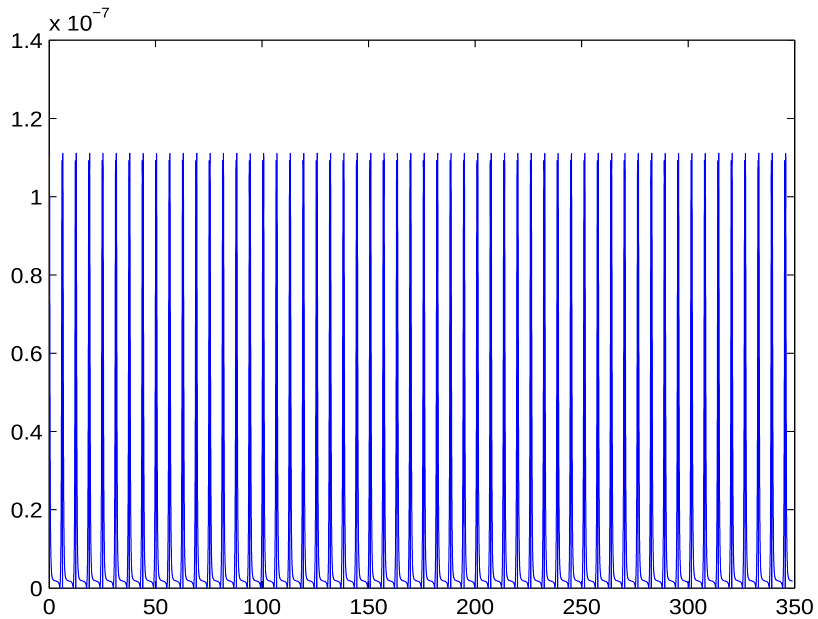


Figure 4.47: Absolute error in energy conservation of Kepler problem ($e = 0.5$) with Radau-I and Radau-II when $s = 2$.

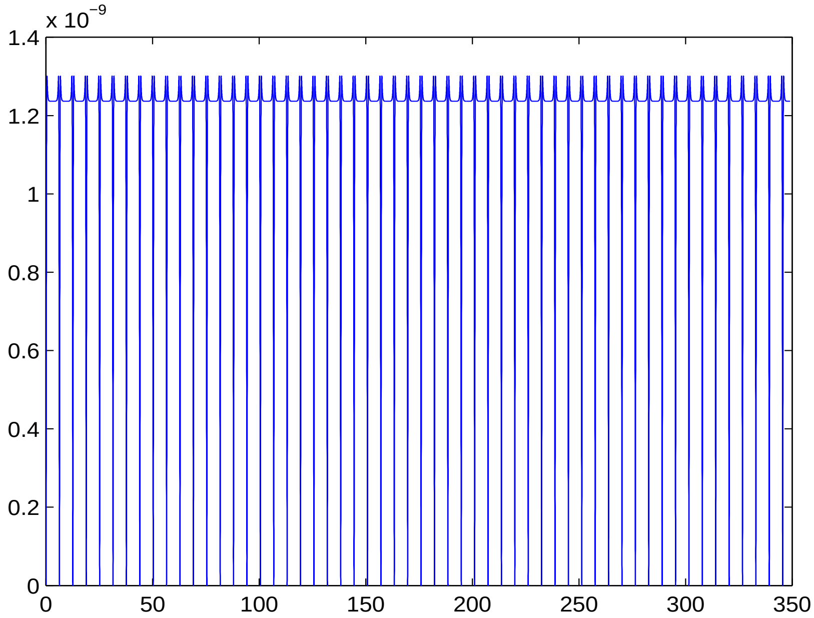


Figure 4.48: Absolute error in energy conservation of Kepler problem ($e = 0.5$) with Gauss and Lobatto-III when $s = 3$.

4.5 Rigid body problem

Rigid bodies are solid objects such that the distance between any two points remain constant. The mathematical equations governing the motion of a rigid body were derived by Euler, named as Euler equations. The equations representing the motion of a rigid body, whose center of mass is at the origin are

$$y_1' = \frac{\omega_{yy} - \omega_{zz}}{\omega_{xx}} y_2 y_3,$$
$$y_2' = \frac{\omega_{zz} - \omega_{xx}}{\omega_{yy}} y_3 y_2,$$
$$y_3' = \frac{\omega_{xx} - \omega_{yy}}{\omega zz} y_1 y_2,$$

where $y = (y_1, y_2, y_3)^T$ are the components of angular velocity around the principal axis and ω_{xx}, ω_{yy}, ω_{zz} are principal moment of inertia. The initial conditions [4] are

$$y_0 = (\cos(1.1), 0, \sin(1.1)).$$
$$H(y_1, y_2, y_3) = \frac{1}{2}\left(\frac{y_1^2}{\omega_1} + \frac{y_2^2}{\omega_2} + \frac{y_3^2}{\omega_3}\right), \tag{4.5.1}$$

which represents the total energy. We have applied symplectic implicit Runge-Kutta methods on Rigid body problem with $100,000$ steps using stepsize $h = 0.01$. The absolute error in energy is plotted in Figures 4.49, 4.50, 4.51, 4.52, 4.53, 4.54, 4.55, and 4.56.

For $s = 2$.

Figures, 4.49, 4.50 and 4.51 show the energy conservation using two stages Gauss, Radau-I and Radau-II symplectic implicit Runge-Kutta methods. All of these methods produce an approximately same and much better results.

For $s = 3$.

Figures 4.52, 4.53, 4.54 and 4.55 also represent energy conservation using three stages Gauss, Radau-I, Radau-II and Lobatto-III symplectic implicit Runge-Kutta Methods. Here Gauss, Radau-I, Radau-II and Lobatto-III symplectic implicit Runge-Kutta methods produce an approximately same and much better results.

For $s = 4$.

Figure 4.56 shows the energy conservation using four stages Lobatto-III symplectic implicit Runge-Kutta method.

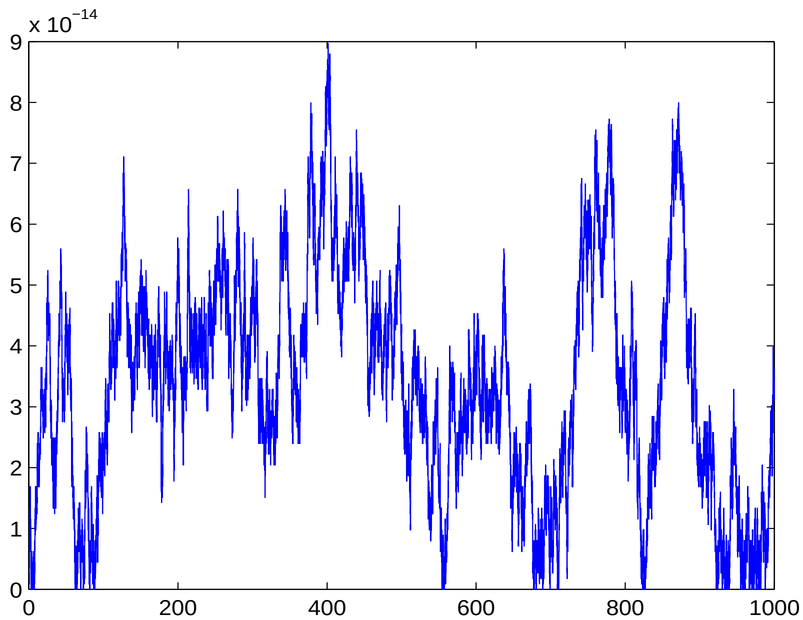


Figure 4.49: Absolute error in energy conservation of Rigid body motion with Gauss when $s = 2$.

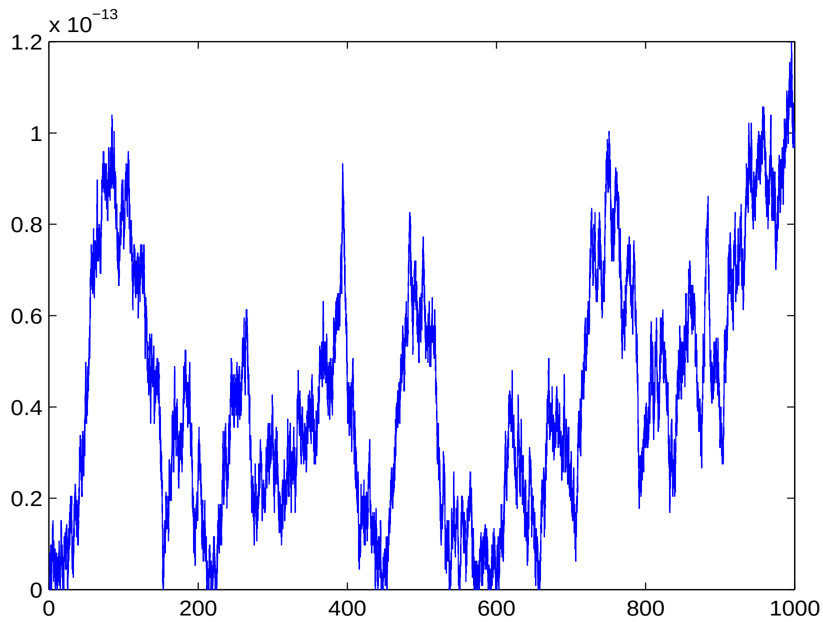


Figure 4.50: Absolute error in energy conservation of Rigid body motion with Radau-I when $s = 2$.

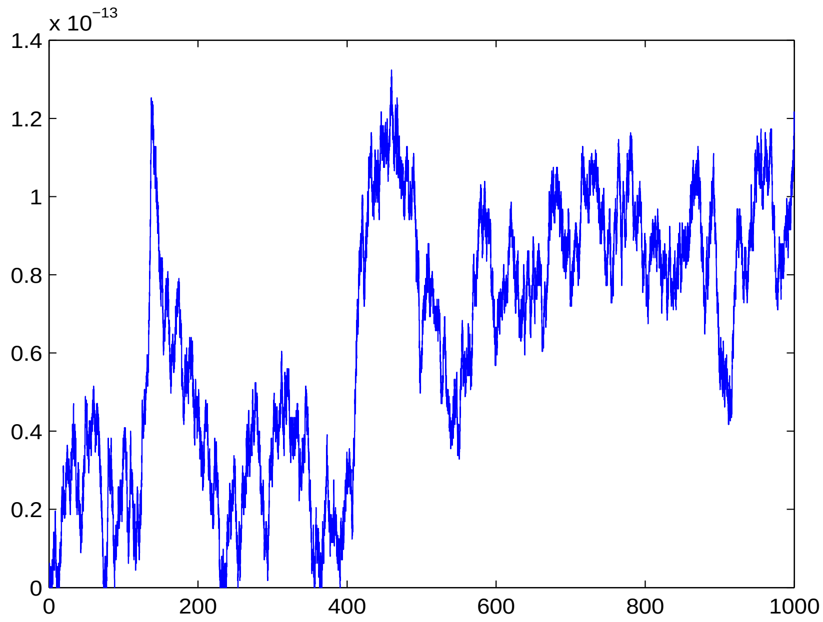


Figure 4.51: Absolute error in energy conservation of Rigid body motion with Radau-II when $s = 2$.

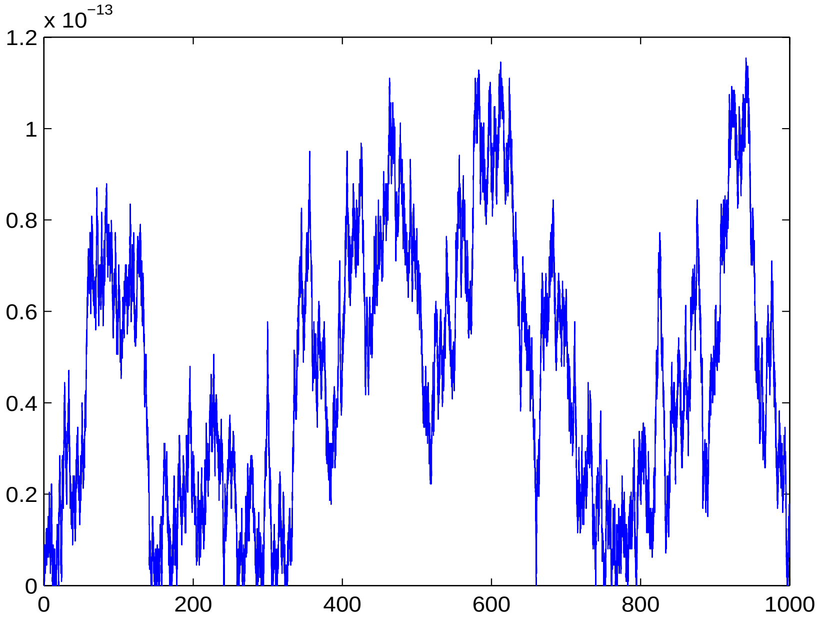


Figure 4.52: Absolute error in energy conservation of Rigid body motion with Gauss when $s = 3$.

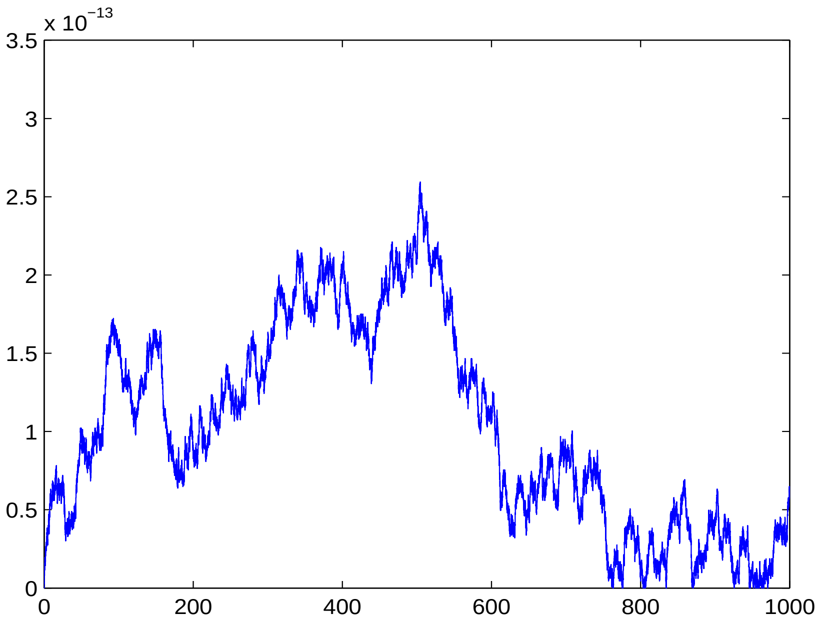


Figure 4.53: Absolute error in energy conservation of Rigid body motion with Radau-I when $s = 3$.

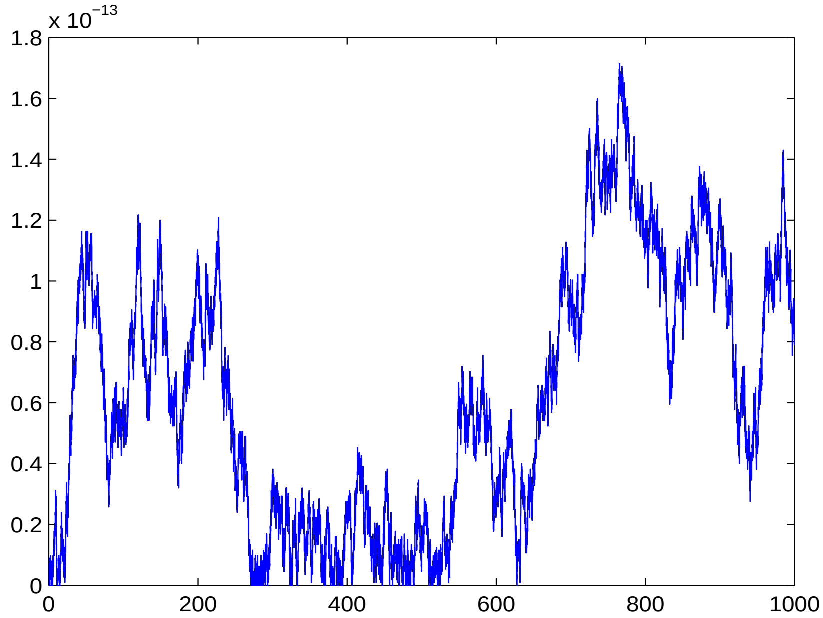


Figure 4.54: Absolute error in energy conservation of Rigid body motion with Radau-II when $s = 3$.

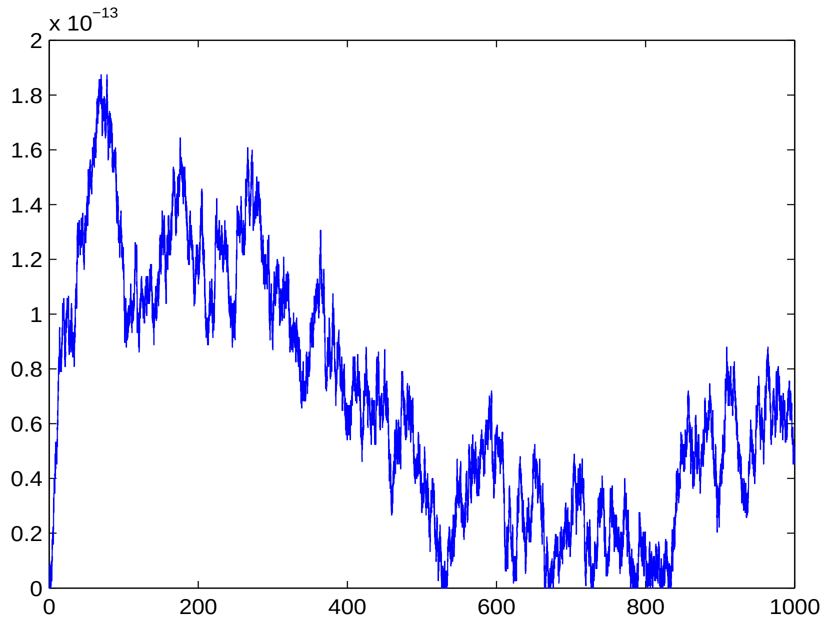


Figure 4.55: Absolute error in energy conservation of Rigid body motion with Lobatto-III when $s = 3$.

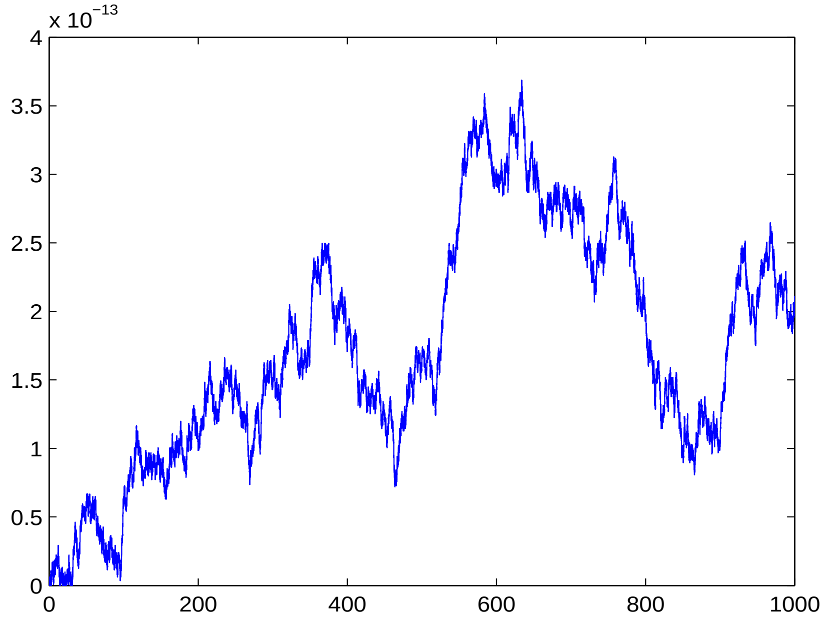


Figure 4.56: Absolute error in energy conservation of Rigid body motion with Lobatto-III when $s = 4$.

Chapter 5

Conclusions and future work

In this thesis we deal with the numerical integration of system of ODEs having quadratic invariants with an emphasis on symplectic implicit Runge-Kutta methods and symplectic implicit partitioned Runge-Kutta methods. We have constructed symplectic implicit Runge-Kutta methods and symplectic implicit partitioned Runge-Kutta methods using Vandermonde transformation. Among the symplectic implicit Runge-Kutta methods we have taken Gauss, Radau-I, Radau-II and Lobatto-III. Among the symplectic implicit partitioned Runge-Kutta methods we have taken the pairs Gauss and Lobatto-III, Gauss and Radau-I, Gauss and Radau-II, and Radau-I and Radau-II.

We have applied these methods on the Hamiltonian systems such as Harmonic oscillator, Simple pendulum, Kepler problem and Rigid body problem. In all experiments we have used fixed stepsize because we have worked on symplectic methods which must satisfy the following condition

$$< p_{n+1}, q_{n+1} >=< p_n, q_n >,$$

where p_{n+1}, q_{n+1} and p_n, q_n are the approximate solutions of Hamiltonian system at t_{n+1} and t_n respectively. These methods give good energy conservation results.

In future we can construct symplectic Nystrom Runge-Kutta methods. For this we can use V-transformation and W-transformation.

Chapter 6

Appendix

6.1 Symplectic implicit Runge-Kutta methods

Gauss: $s = 2$

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

Radau-I: $s = 2$

$$\begin{array}{c|cc} 0 & \frac{1}{8} & \frac{-1}{8} \\ \frac{2}{3} & \frac{7}{24} & \frac{3}{8} \\ \hline & \frac{1}{4} & \frac{3}{4} \end{array}$$

Radau-II: $s = 2$

$$\begin{array}{c|cc} \frac{1}{3} & \frac{3}{8} & \frac{-1}{24} \\ 1 & \frac{7}{8} & \frac{1}{8} \\ \hline & \frac{3}{4} & \frac{1}{4} \end{array}$$

Gauss: $s = 3$

$$
\begin{array}{c|ccc}
\frac{1}{2} - \frac{\sqrt{15}}{10} & \frac{5}{36} & \frac{2}{9} - \frac{\sqrt{15}}{15} & \frac{5}{36} - \frac{\sqrt{15}}{30} \\
\frac{1}{2} & \frac{5}{36} + \frac{\sqrt{15}}{24} & \frac{2}{9} & \frac{5}{36} - \frac{\sqrt{15}}{24} \\
\frac{1}{2} + \frac{\sqrt{15}}{10} & \frac{5}{36} + \frac{\sqrt{15}}{30} & \frac{2}{9} + \frac{\sqrt{15}}{15} & \frac{5}{36} \\
\hline
 & \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array}
$$

Radau-I: $s = 3$

$$
\begin{array}{c|ccc}
0 & \frac{1}{18} & \frac{5}{35}\frac{\sqrt{6}}{-6+\sqrt{6}} & \frac{5}{35}\frac{\sqrt{6}}{6+\sqrt{6}} \\
\frac{6-\sqrt{6}}{10} & \frac{1}{9}(\frac{-1+3\sqrt{6}}{-2+3\sqrt{6}}) & \frac{-5}{72}(\frac{-2+3\sqrt{6}}{-6+\sqrt{6}})\sqrt{6} & \frac{-5}{36}(\frac{-25+12\sqrt{6}}{(-2+3\sqrt{6})(6+\sqrt{6})})\sqrt{6} \\
\frac{6+\sqrt{6}}{10} & \frac{1}{9}(\frac{1+3\sqrt{6}}{2+3\sqrt{6}}) & \frac{-5}{36}(\frac{25+12\sqrt{6}}{(2+3\sqrt{6})(-6+\sqrt{6})})\sqrt{6} & \frac{5}{72}(\frac{2+3\sqrt{6}}{6+\sqrt{6}})\sqrt{6} \\
\hline
 & \frac{1}{9} & \frac{-5}{36}\sqrt{6}(\frac{-2+3\sqrt{6}}{-6+\sqrt{6}}) & \frac{5}{36}\sqrt{6}(\frac{2+3\sqrt{6}}{6+\sqrt{6}})
\end{array}
$$

Radau-II: $s = 3$

$$
\begin{array}{c|ccc}
\frac{4-\sqrt{6}}{10} & \frac{5}{72}(\frac{2+3\sqrt{6}}{6+\sqrt{6}})\sqrt{6} & \frac{5}{36}(\frac{-25+12\sqrt{6}}{(2+3\sqrt{6})(-6+\sqrt{6})})\sqrt{6} & \frac{1}{9(2+3\sqrt{6})} \\
\frac{4+\sqrt{6}}{10} & \frac{5}{36}(\frac{25+12\sqrt{6}}{(-2+3\sqrt{6})(6+\sqrt{6})})\sqrt{6} & \frac{-5}{72}(\frac{-2+3\sqrt{6}}{-6+\sqrt{6}})\sqrt{6} & \frac{-1}{9(-2+3\sqrt{6})} \\
1 & \frac{5}{36}(\frac{1+3\sqrt{6}}{6+\sqrt{6}})\sqrt{6} & \frac{-5}{36}(\frac{-1+3\sqrt{6}}{-6+\sqrt{6}})\sqrt{6} & \frac{1}{18} \\
\hline
 & \frac{5}{36}\sqrt{6}(\frac{2+3\sqrt{6}}{6+\sqrt{6}}) & \frac{-5}{36}\sqrt{6}(\frac{-2+3\sqrt{6}}{-6+\sqrt{6}}) & \frac{1}{9}
\end{array}
$$

Lobatto-III: $s = 3$

$$\begin{array}{c|ccc}
0 & \frac{1}{12} & \frac{-1}{15} & \frac{-1}{60} \\
\frac{1}{2} & \frac{11}{60} & \frac{1}{3} & \frac{-1}{60} \\
1 & \frac{11}{60} & \frac{11}{15} & \frac{1}{12} \\
\hline
 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{array}$$

Lobatto-III: $s = 4$

$$\begin{array}{c|cccc}
0 & \frac{1}{24} & \frac{-1}{480}(4\sqrt{5}+15)\sqrt{5} & \frac{-1}{480}(4\sqrt{5}-15)\sqrt{5} & \frac{1}{168} \\
\frac{1}{2}-\frac{\sqrt{5}}{10} & \frac{1}{4200}(74\sqrt{5}+15)\sqrt{5} & \frac{5}{24} & \frac{1}{168}(7\sqrt{5}-18)\sqrt{5} & \frac{-1}{4200}(4\sqrt{5}-15)\sqrt{5} \\
\frac{1}{2}-\frac{\sqrt{5}}{10} & \frac{1}{4200}(74\sqrt{5}-15)\sqrt{5} & \frac{1}{168}(7\sqrt{5}+18)\sqrt{5} & \frac{5}{24} & \frac{-1}{4200}(1054\sqrt{5}-3135)\sqrt{5} \\
1 & \frac{13}{168} & \frac{1}{480}(74\sqrt{5}-15)\sqrt{5} & \frac{1}{480}(1124\sqrt{5}-3135)\sqrt{5} & \frac{1}{24} \\
\hline
 & \frac{1}{12} & \frac{5}{12} & \frac{5}{12} & \frac{1}{12}
\end{array}$$

6.2 Symplectic implicit partitioned Runge-Kutta methods

Gauss and Radau-I : $s = 2,$

$$
\begin{array}{c|cc}
\frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{24}(-1 + 2\sqrt{3})\sqrt{3} & \frac{1}{24}(-3 + 2\sqrt{3})\sqrt{3} \\
\frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{24}(1 + 2\sqrt{3})\sqrt{3} & \frac{1}{24}(-3 + 2\sqrt{3})\sqrt{3} \\
\hline
 & \frac{1}{4} & \frac{3}{4}
\end{array}
$$

$$
\begin{array}{c|cc}
0 & \frac{1}{12}\sqrt{3} & -\frac{1}{12}\sqrt{3} \\
\frac{2}{3} & \frac{1}{36}(3 + 4\sqrt{3})\sqrt{3} & \frac{1}{36}(-3 + 4\sqrt{3})\sqrt{3} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
$$

Gauss and Radua-II : $s = 2,$

$$
\begin{array}{c|cc}
\frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{24}(-3 + 4\sqrt{3})\sqrt{3} & -\frac{1}{24}\sqrt{3} \\
\frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{24}(3 + 4\sqrt{3})\sqrt{3} & \frac{1}{24}\sqrt{3} \\
\hline
 & \frac{3}{4} & \frac{1}{4}
\end{array}
$$

$$
\begin{array}{c|cc}
\frac{1}{3} & \frac{1}{36}(3 + 4\sqrt{3})\sqrt{3} & \frac{1}{36}(-3 + 4\sqrt{3})\sqrt{3} \\
1 & \frac{1}{12}(1 + 2\sqrt{3})\sqrt{3} & -\frac{1}{12}(-1 + 2\sqrt{3})\sqrt{3} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
$$

Radau-I and Radau-II: $s = 2$,

$$
\begin{array}{c|cc}
0 & \frac{1}{8} & -\frac{1}{8} \\
\frac{2}{3} & \frac{5}{8} & \frac{1}{24} \\
\hline
 & \frac{3}{4} & \frac{1}{4}
\end{array}
\qquad
\begin{array}{c|cc}
\frac{1}{3} & \frac{5}{24} & \frac{1}{8} \\
1 & \frac{3}{8} & \frac{5}{8} \\
\hline
 & \frac{1}{4} & \frac{3}{4}
\end{array}
$$

Gauss and Lobatto-III : $s = 3$,

$$
\begin{array}{c|ccc}
\frac{1}{2} - \frac{\sqrt{15}}{10} & \frac{2}{15} - \frac{\sqrt{(15)}}{100} & \frac{1}{3} - \frac{2}{25}\sqrt{15} & \frac{1}{30} - \frac{\sqrt{15}}{100} \\
\frac{1}{2} & \frac{5}{24} & \frac{1}{3} & -\frac{1}{24} \\
\frac{1}{2} + \frac{\sqrt{15}}{10} & \frac{2}{15} + \frac{\sqrt{(15)}}{100} & \frac{1}{3} + \frac{2}{25}\sqrt{15} & \frac{1}{30} - \frac{\sqrt{15}}{100} \\
\hline
 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{array}
$$

$$
\begin{array}{c|ccc}
0 & \frac{1}{18} + \frac{\sqrt{15}}{60} & -\frac{1}{9} & \frac{1}{18} - \frac{\sqrt{15}}{60} \\
\frac{1}{2} & \frac{5}{36} + \frac{\sqrt{15}}{30} & \frac{2}{9} & \frac{5}{36} - \frac{\sqrt{15}}{30} \\
1 & \frac{2}{9} + \frac{\sqrt{15}}{60} & \frac{5}{9} & \frac{2}{9} - \frac{\sqrt{15}}{60} \\
\hline
 & \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array}
$$

6.3 Implementation of implicit Runge-Kutta methods

The general form of an implicit Runge-Kutta method is

$$
\begin{aligned}
Y_i &= y_{n-1} + \sum_{j=1}^{s} a_{ij} h f(Y_j), \qquad i = 1, 2 \ldots s, \\
y_n &= y_{n-1} + \sum_{i=1}^{s} b_i h f(Y_i),
\end{aligned}
\tag{6.3.1}
$$

We shall use implicit Runge-Kutta method (6.3.1) to solve the system of ODEs. We shall use modified Newton iterations as follows,

$$Y_i = y_{n-1} + a_{i1}hf(Y_1) + a_{i2}hf(Y_2) + a_{i3}hf(Y_3) + \ldots + a_{is}hf(Y_s), \qquad i = 1, 2 \ldots s,$$
$$y_n = y_{n-1} + b_1hf(Y_1) + b_2hf(Y_2) + b_3hf(Y_3) + \ldots + b_shf(Y_s).$$

When $s = 2$,

$$Y_1 = y_{n-1} + a_{11}hf(Y_1) + a_{12}hf(Y_2), \tag{6.3.2}$$

$$Y_2 = y_{n-1} + a_{21}hf(Y_1) + a_{22}hf(Y_2), \tag{6.3.3}$$

$$y_n = y_{n-1} + b_1hf(Y_1) + b_2hf(Y_2). \tag{6.3.4}$$

Let, $Y_1 = Y_1 + \delta Y_1$ using in equation (6.3.2) we have

$$Y_1 + \delta Y_1 = y_{n-1} + a_{11}hf(Y_1 + \delta Y_1) + a_{12}hf(Y_2). \tag{6.3.5}$$

Using taylor series in equation (6.3.5) becomes,

$$Y_1 + \delta Y_1 = y_{n-1} + a_{11}hf(Y_1 + ha_{11}\delta f'Y_1) + a_{12}hf(Y_2), \tag{6.3.6}$$

$\Rightarrow$

$$\delta Y_1 = \frac{y_{n-1} + a_{11}hf(Y_1) + a_{12}hf(Y_2)}{I - ha_{11}f'(Y_1)}. \tag{6.3.7}$$

updated $Y_1 = Y_1^{up}$

$$Y_1^{up} = Y_1 + \delta Y_1. \tag{6.3.8}$$

Similarly we have

$$\delta Y_2 = \frac{y_{n-1} + a_{21}hf(Y_1) + a_{22}hf(Y_2)}{I - ha_{22}f'Y_2}. \tag{6.3.9}$$

updated $Y_2 = Y_2^{up}$

$$Y_2^{up} = Y_2 + \delta Y_2. \tag{6.3.10}$$

Stoping criteria

$$|(Y_1^{up} - Y_1)\&\ (Y_2^{up} - Y_2)| < \frac{1}{2^{50}}. \tag{6.3.11}$$

Here $\frac{1}{2^{50}}$ is machine accuracy.
Then

$$Y_1 = Y_1^{up} \tag{6.3.12}$$

$$Y_2 = Y_2^{up} \tag{6.3.13}$$

After this we use Y_1 and Y_2 from equations (6.3.12) and (6.3.13) in equation (6.3.4) for the approximate numerical solution.

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