Runge-Kutta Methods: Analysis and Implementation

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Author's Declaration

I **Junaid Ahmad** hereby state that my PhD thesis titled:

Runge – Kutta Methods: Analysis and Implementation

is my own work and has not been submitted previously by me for taking any degree from this University

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or anywhere else in the country/world.

At any time if my statement is found to be incorrect even after my Graduate the university has the right to withdraw my PhD degree.

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بِسْمِ اللهِ الرَّحْمٰنِ الرَّحِيْمِ

In the name of Allah

The Most Beneficent and Merciful

O, my Sustainer!
Open my heart and make my task easy for me and loosen the knot from my tongue so that they might understand my speech.

Al-Quran

Dedication

This study is

dedicated to

the people of Pakistan.

Abstract

In this thesis, we have developed new numerical methods in Runge-Kutta family for numerical solution of ordinary differential equations. We have extended the idea of effective order to Runge-Kutta Nyström methods for numerical approximation of second order ordinary differential equations. The composition of Runge-Kutta Nyström methods, the pruning of associated Nyström trees, and conditions for effective order Runge-Kutta Nyström methods up to order five are presented. Also, partitioned Runge-Kutta methods of effective order 4 with 3 stages are constructed. The most obvious feature of these methods is efficiency in terms of implementation cost.

The numerical results verify that the asymptotic error behavior of the effective order 4 partitioned Runge- Kutta methods with 3 stages is similar to that of classical order 4 method which necessarily require 4 stages. Moreover, it is evident from the numerical results that effective order methods are more efficient than their classical order counterpart.

Lastly, a family of explicit symplectic partitioned Runge-Kutta methods are derived with effective order 3 for the numerical integration of separable Hamiltonian systems. The proposed explicit methods are more efficient than existing symplectic implicit Runge-Kutta methods. A selection of numerical experiments on separable Hamiltonian system confirming the efficiency of the approach is also provided with good energy conservation.

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In the end, I would like to acknowledge all my friends and fellows of university life who supported me in this long journey of truth. Needless to say, however, any errors and mistakes remain the scholar's responsibility.

Junaid Ahmad

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Chapter 1

Introduction

Mathematical models are frequently used to describe various physical phenomena, for instance, the blood circulation in veins, the electrical circuit's behaviour in machines, the motion of planetary bodies in outer Solar System or the rate of change of shares in stock exchanges. Generally, these models include ordinary differential equations (ODEs) based on physical systems in which time acts independently while variables associated to physical systems are taken as dependent quantities. Usually, an initial condition is accompanied by the said ODEs, hence, an initial value problem (IVP) is constituted as

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

Such kind of IVP consists of a solution y, a mapping $\mathbb{R} \to \mathbb{R}^n$, time denoted by x and $f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$, where n represents the dimension. Mostly, we consider initial value problems (IVPs) of autonomous nature which carries x as a component of $y(x)$, and is represented as

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

Generally, the higher order differential equations are used to model some physical systems. The system of nth order differential equations of autonomous type is as

$$y^{(n)}(x) = f(y, y', y'', ..., y^{(n-1)}).$$

This kind of system can be solved by using initial values for $y, y', y'', ..., y^{(n-1)}$. The existence and uniqueness of a solution depends on the satisfaction of the Lipschitz condition for the function f [12].

Definition 1. A function $f : \mathbb{R}^m \to \mathbb{R}^m$ satisfies a Lipschitz condition, if for any $X, Y \in \mathbb{R}^m$, there exists a Lipschitz constant M, such that,

$$\|f(X) - f(Y)\| \leq M \|X - Y\|.$$

On the whole, problems involving ODEs can be categorized as stiff and non-stiff types. The first type carries differential equations with vastly fluctuating time components with large Lipschitz constants. While, all the other problems fall in second type.
The system consisting of differential equations of first order show the behavior of the original physical occurrence through its solution. Usually, the analytic process of finding this solution becomes harder often, so we use numerical schemes as an approximation to solution obtained analytically. The numerical schemes uses initial values and the slope provided by the differential equation will direct the movement of the solution. Numerical methods are classified into three major areas, firstly one-step methods , then multistep methods and lastly general linear methods. We have discussed and contributed in one-step methods in this dissertation.

1.1 One-step methods

These methods are used to estimate the value of $y(x)$ at time x_n by using the previous step x_{n-1} information. In this manner, the solution values at different points in $[x_{n-1}, x_n]$ may be calculated by using such methods. Euler's method is the first and simple method which is considered as one-step method. The numerical solutions are obtained by using following Euler's formula

$$y_n = y_{n-1} + hf(y_{n-1}).$$

This formula uses the solution obtained at previous time step t_{n-1} and information of slope at that time to update the solution y_n. Here, $f(y_{n-1})$ represents the slope of tangent line along which the numerical solution propagates. This one-

step method completes this one step with one stage, so it is one stage one-step method. Due to its single stage property, this method needs small time steps to get certain accuracy. We need some one step methods with multistage structure to improve the accuracy and efficiency of numerical schemes which will be our main focus of the study.
In Chapter 2, we will discuss the theory of Runge Kutta (RK) methods for multistage structure. RK methods are divided into explicit and implicit methods. Explicit methods are low cost methods but they are not suitable for stiff differential equations like implicit methods. The general scheme of RK methods of s-stage is

$$
\begin{aligned}
Y_i &= y_0 + h\sum_{j=1}^{s} a_{ij} f(Y_j), \qquad\qquad i = 1, 2, ..., s, \\
y_1 &= y_0 + h\sum_{j=1}^{s} b_j f(Y_j).
\end{aligned}
$$

where b_i, a_{ij}, and Y_i are quadrature weights, coefficient matrix and stage values, respectively. The consistency of these methods is maintained by the condition

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

Here, c_i are known as abscissas of method. These methods are basically constructed through Taylor's series expansion up till certain order of accuracy. By the expansion of this series up to the $O(h^p)$ will decide the order of method. The order of method decides the order conditions of the method, which are the combinations of coefficients b_i, a_{ij} and c_i. As the order of method gets higher the complexity of order conditions also grow. For this, a new approach to RK methods were presented by Butcher in [11] and is known as rooted tree theory. The components of this theory will also be discussed in Chapter 2. This theory is basically a graphical theory which consists of rooted trees. Each tree is a non cyclic representation consisting of edges and vertices and the line join the two roots is linked with differentials. With the help of this modern approach, a new era of RK methods started in which it becomes easier to construct any RK method upto any higher order.
Butcher in [9] presented an idea of effective order to handle the number of stages

for higher order RK methods. For example, for RK methods up to order 4, the number of stages are equal to order of method but for fifth order method, we need at least six stages. Butcher tried to reduce at least one stage for RK 5. The idea of effective order for RK methods is also explained in Chapter 2 along with construction of effective order conditions and derivation of a 2 stages effective order Rk method of order 3.
Lastly, in this chapter, we shall also discuss the application of RK method on Hamiltonian system and this will lead us to symplectic RK methods. Here, we present main concepts regarding Hamiltonian systems and symplecticity.

1.1.1 Hamiltonian systems

Hamiltonian systems belong to Hamiltonian mechanics, in which we study the motion of bodies in the context of their momentum and positions. The momentum coordinates are generally taken as $p_i = (p_1, p_2, ..., p_n)$ while the position coordinates are termed as $q_i = (q_1, q_2, ..., q_n)$. These coordinates constitute a differential equation with the help of a function H (Hamiltonian function) and this system of differential equations is known as Hamiltonian system. Mathematically we write it as

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}, \qquad \dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad i = 1, 2, \cdots, n. \tag{1.1}$$

Let we take $z = (p, q)$, then we write equation (1.1) in the following format as

$$z^{'} = J^{-1} \nabla H. \tag{1.2}$$

Here, ∇ is the operator used to compute the gradient and Jacobian J is a skew symmetric matrix having zeros in principal diagonal and an $n \times n$ identity matrix I in minor diagonal. Mathematically J is given by

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

The Hamiltonian function H forms a separable system called Hamiltonian system [19] as

$$H(p, q) = T(p) + V(q), \tag{1.3}$$

where H is known as the total energy of the system and q and p are generalized coordinates and generalized momenta, respectively. The autonomous Hamiltonian systems have two important properties; one is that the total energy remains constant

$$\frac{dH}{dt} = \frac{\partial H}{\partial p} \cdot \frac{\partial p}{\partial t} + \frac{\partial H}{\partial q} \cdot \frac{\partial q}{\partial t} = 0.$$

1.1.2 Symplecticity

The second important property of Hamiltonian systems is that the phase flow is symplectic which imply that the motion along the phase curve retains the area of a bounded sub-domain in the phase space. Mathematically, we can express it by taking a linear transformation Ψ as

$$\Psi : (p, q) \longrightarrow (p^*, q^*).$$

This linear transformation Ψ is symplectic, if the following equation holds

$$(\Psi')^T J \Psi' = J, \tag{1.4}$$

where Jacobian J is already discussed. To prove this, we take the supposition of unit determinant of the Jacobian matrix obtained by applying it on the transformation. So we have

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

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

So,

$$(\Psi')^T J \Psi' = \begin{bmatrix} -\frac{\partial q^*}{\partial p}\frac{\partial p^*}{\partial p} + \frac{\partial p^*}{\partial p}\frac{\partial q^*}{\partial p} & -\frac{\partial q^*}{\partial p}\frac{\partial p^*}{\partial q} + \frac{\partial p^*}{\partial p}\frac{\partial q^*}{\partial q} \\ -\frac{\partial q^*}{\partial q}\frac{\partial p^*}{\partial p} + \frac{\partial p^*}{\partial q}\frac{\partial q^*}{\partial p} & \frac{\partial q^*}{\partial q}\frac{\partial p^*}{\partial q} + \frac{\partial p^*}{\partial q}\frac{\partial q^*}{\partial q} \end{bmatrix},$$

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

This gives us the proof that Ψ is symplectic. We shall explain this symplectic property of RK methods with its combination to effective order techniques in the last part of Chapter 2.

We know that RK methods are only applicable to first order differential equations. They can be applied to second order ordinary differential equations by converting it to system of first order differential equations. There were need of such methods which can solve second order ODEs directly. One of such direct method was designed by Nystrӧm [8] in 1925 and are known as Runge-Kutta Nystrӧm (RKN) methods. In Chapter 3, we shall discuss its existing literature in the context of rooted tree theory. We shall explain the structure of trees and use of this structure in developing the order conditions of RKN methods. A new approach of effective order for RKN methods will also be the part of this chapter. This chapter will include a comprehensive classification of effective order condition of RKN up to order 5.

In Chapter 4, we shall present our second major contribution in partitioned Runge–Kutta (PRK) methods. PRK methods are basically applicable to separable equations of first order. In the earlier part of this chapter, we shall explain the rooted theory for PRK methods and the use of bi-color rooted trees for these methods and also, discuss their relation with elementary differentials. In the middle part of the chapter, we shall present a complete mechanism for the construction of conditions for effective order of PRK methods along with a comprehensive list of effective order conditions for PRK up to order 5 by maintaining classical order up to 4. In the later part of this chapter, we shall derive a new

PRK method with effective order 4 with 3 stages. This newly built method will give one stage lesser than its counterpart standard PRK method of order 4. In the last part of this chapter, we shall perform some numerical experiments to show the order verification and efficiency in terms of function evaluation of our newly built method.

In Chapter 5, we shall present our third contribution which is related to PRK methods for Hamiltonian type problems. In first part of this chapter, we shall discuss the existing literature on symplectic PRK methods and in the later part of the chapter, we apply effective order technique to these symplectic PRK methods. We shall show the effects of symplectic condition of PRK methods on the effective order conditions of PRK methods and this will be helpful in the derivation of two types of PRK methods for Hamiltonian systems; one is effective order of symplectic PRK methods and second is effective order of mutually adjoint symplectic PRK methods with order 3. In the last part of this final chapter, we shall perform numerical experimentation to implement our numerical scheme for some Hamiltonian systems, like, Kepler's problem and Harmonic oscillator to show the energy behaviour and order verification.

Chapter 2

RK methods with modern approach

The solutions of ordinary differential equations can be obtained by approximating them with numerical methods. These methods are used widely to understand the behaviour of physical systems. There are three sub classes of these methods known as one-step methods, multi-step methods, and general linear methods. In this chapter, we are going to present a brief analysis of RK methods along with their construction mechanism in the context of modern theory of rooted trees.

2.1 Taylor series methods

The idea of one step methods was based on Taylor's series expansion of exact solution. The concept was to approximate the solution of initial value problem

$$\dot{y} = g(t, y), \qquad y(t_0) = y_0, \qquad y \in \mathbb{R}^n, \tag{2.1}$$

at t_{n+1} by qth-degree Taylor polynomial $y(t)$, which is evaluated at any time t_n [29]. For the moment, we take variable time step for the process of integration in such a way that $t_{n+1} = t_n + h_n$ and its approximation becomes

$$\begin{aligned} y_{n+1} &= y_n + \frac{dy}{dt}(t_n, y_n)h_n + \cdots + \frac{1}{r!}\frac{d^q y}{dt^q}(t_n, y_n)h_n^q, \\ &= y_n + g(t_n, y_n)h_n + \cdots + \frac{1}{r!}\frac{d^{q-1}g(t_n, y_n)}{dt^{q-1}}h_n^q. \end{aligned} \tag{2.2}$$

The Equation (2.2) gives the explicit Euler scheme if we place $q = 1$ in it. Generally, the truncation error in these methods is of order $O(h^q)$ and as h grows higher, the accuracy of method also increases but the problem for these methods is mainly due to non-differentiability of functions, which may occur at some of the time steps. On the other side, this simple idea can help efficiently to evaluate the total derivatives $g^k(t_n, y_n) \equiv \frac{d^k g}{dt^k}(t_n, y_n)$ as in (2.2) for numerical integration procedure. The clear approach is to differentiate any function g repeatedly but this procedure becomes more complex as order of "h" grows higher. Thus for differential equation (2.1) second and third derivatives are given as

$$\begin{aligned}
\frac{d^2y}{dt^2} &= \frac{dg}{dt}(t, y), \\
&= g_t(t, y) + g_y(t, y)\dot{y}, \\
&= g_t(t, y) + g_y(t, y)g(t, y) \equiv g_t + g_y g, \\
\frac{d^3y}{dt^3} &= g_{tt} + g_{ty}g + (g_{ty} + g_{yy}g)g + g_y(g_t + g_y g), \\
\vdots &= \vdots \quad \vdots \quad \vdots \quad \vdots \quad \ddots
\end{aligned}$$

The main reason for the failure of Taylor's method was the complications of expressions obtained after repeated differentiation as order of method goes higher. But emergence of automatic differential techniques efficiently make it possible to develop a recurrence formulations for the coefficients of Taylor method. The idea of these techniques was to divide the function into sequence of arithmetic operations and use of binary functions with chain rule [2].

These methods are very suitable to attain an approximated solution with high accuracy for the low dimension ODE systems. Particularly these are suitable for the calculations of orbital periods in the dynamical systems to get an accuracy up to hundreds digits. This is because that these methods permit the automatic selection of step-size and order for gaining desired accuracy. We can conclude that all geometrical aspects of an ODE are well-maintained by these methods up to the order of truncation error.

Ex 2.1.1. Consider the following pendulum problem

$$\dot{q} = p,$$
$$\dot{p} = -sin(q).$$

We apply Taylor method for step $(q_n, p_n) \mapsto ((q_{n+1}, p_{n+1}))$ as follows.
Let take $x = (q, p)^T$, $g = (p, -sin(q))$, $g_t = (0, 0)^T$, Then the derivatives are computed as

$$g_x g = \begin{pmatrix} -sin(q) \\ -pcos(q) \end{pmatrix}, \qquad g_{xx} gg = \begin{pmatrix} 0 \\ p^2 sin(q) \end{pmatrix}, \qquad g_x g_x g = \begin{pmatrix} -pcos(q) \\ -\frac{1}{2} sin(2q) \end{pmatrix}.$$

Then Taylor method expansion up to truncation error of h^4 is

$$\begin{pmatrix} q_{n+1} \\ p_{n+1} \end{pmatrix} = \begin{pmatrix} q_n \\ p_n \end{pmatrix} \text{-h} \begin{pmatrix} -p_n \\ sin(q_n) \end{pmatrix} \text{-} \frac{h^2}{2} \begin{pmatrix} sin(q_n) \\ p_n cos(q_n) \end{pmatrix} + \cdots$$
$$\frac{h^3}{6} \begin{pmatrix} -p_n cos(q_n) \\ (p_n^2 + cos(q_n) + sin(q_n) \end{pmatrix}.$$

2.2 Runge-Kutta methods

The RK methods evaluate the first derivative of $f(x, y)$ many times in one step. Runge [32] in 1895, used Taylor's series expansion to propose this idea first time which was basically an extension to the Euler's method. Later on, Heun [25] and Kutta [28] also contributed in this early development.
The advantages of Runge-Kutta (RK) methods are their stability and managing of variable step-size and order. The disadvantage is regarding high accuracy achievement at high computational cost. These are one step methods and are mostly applicable to initial value problems

$$y' = f(y(x)), \qquad y(x_0) = y_0, \qquad y \in \mathbb{R}^n.$$

The RK methods give an approximation to exact solution $y(x)$ at any time $x_n = nh$ for $n = 0, 1, 2, \cdots$ and step-size h. The general formulation of an s-stage RK method is

$$Y_i = y_{n-1} + h\sum_{j=1}^{s} a_{ij} f(x_{n-1} + hc_j, Y_j), \qquad i = 1, 2, ..., s, \tag{2.3}$$

$$y_n = y_{n-1} + h\sum_{j=1}^{s} b_j f(x_{n-1} + hc_j, Y_j). \tag{2.4}$$

The general form of Butcher's table for RK methods is

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

Table 2.1: General form of Butcher table for RK methods.

where Y_i represent the stages and are computed during integration process for time interval x_{n-1} to x_n.The above formulation also contains three constant coefficients a_{ij}, c_j, b_j, which are used to get good approximation of numerical solution y_n for the actual solution $y(x_n)$. The coefficients a_{ij} are used to calculate internal stages by using the linear combinations of stage derivatives, while b is a weighted vector, which tells the dependence of approximated solution on the derivatives of internal stages. The position of approximations in each step is represented by abscissa vector c. Also the relationships of these constants provide the consistency of RK methods. The suitable consistency is necessary for the solution of problems. A consistent method means difference between numerical integration and exact solution at $x_{n-1} + h$ should approach to zero as h goes nearer to zero. The following consistency conditions must hold for a valid RK method

$$\sum_{j=1}^{s} b_j = 1, \tag{2.5}$$

$$\sum_{j=1}^{s} a_{ij} = c_i, \qquad i = 1, 2, ..., s. \tag{2.6}$$

The configuration of coefficient matrix a_{ij} effects the computational cost of the methods. Due to this, RK methods are further classified into two types as, explicit and implicit methods.

2.2.1 Explicit RK methods

In explicit RK methods, the components $a_{ij} = 0$ for all $i \leq j$. This means that we can compute stages successively. Due to arrival of zeros in upper triangle, the computational time becomes lesser and that is why these methods are very suitable for numerical solutions of ordinary differential equations. There are also some limitations of these methods, like, their stability for solving differential equations of stiff nature and their inability to solve the non separable Hamiltonian systems. The Butcher table for explicit methods is given by

$$\begin{array}{c|cccc} 0 & 0 & 0 & \dots & 0 \\ c_2 & a_{21} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & a_{s2} & \dots & 0 \\ \hline & b_1 & b_2 & \dots & b_s \end{array}$$

Example: Explicit RK method of order 3
Consider the following Butcher table which was presented by Heun's third-order method

$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{3} & \frac{1}{3} & & \\ \frac{2}{3} & 0 & \frac{2}{3} & \\ \hline & \frac{1}{4} & 0 & \frac{3}{4} \end{array}$$

The blank spaces in the upper triangular components of matrix A denote the zero values of a_{ij}. The stage values at n^{th} step of RK scheme can be calculated as follows:

$$
\begin{aligned}
Y_1 &= y_{n-1},\\
Y_2 &= y_{n-1} + h(\frac{1}{3})F_1,\\
Y_3 &= y_{n-1} + h(\frac{2}{3})F_2.
\end{aligned}
$$

The derivative of each stage are:

$$
\begin{aligned}
F_1 &= f(x_{n-1} + h(0), Y_1),\\
F_2 &= f(x_{n-1} + h(\frac{1}{3}), Y_2),\\
F_3 &= f(x_{n-1} + h(1), Y_3).
\end{aligned}
$$

The approximated solution at n^{th} step is

$$y_n = y_{n-1} + h(\frac{1}{4}F_1 + 0F_2 + \frac{1}{6}F_3).$$

For the higher order explicit RK methods required stages are also higher. In fact for $s \leq 4$, the number of stages required are equal to the order of method. As in classic RK method of order 4, we require 4 stages described as

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

2.2.2 Implicit RK methods

Implicit RK method can be represented by the following Butcher table with condition $a_{ij} \neq 0$ for some $i \leq j$.

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

To construct an s-stage RK method of implicit nature for the solution of m-dimensional system of ODE's, we need to solve sm non-linear equations representing the stages. This can be obtained by newton's iterative schemes, which have obviously high computational costs. Due to this, general implicit RK methods are computationally expensive than explicit methods but still these methods are better than explicit methods in terms of less number of stages are required to obtain same order explicit method. Another advantage of these methods is that these can help in solving stiff differential equations along with having a capability of handling Hamiltonian nature differential equations. The Guass-Legendre implicit RK methods are the popular as s-stages are required to get a method of order $2s$. Gauss-Legendre polynomial are used to construct such methods by taking c's of implicit RK methods equal to zero. The legendre polynomial Q_s on the interval $[0, 1]$ is given as

$$Q_s(x) = \frac{s!}{2s} \sum_{n=0}^{s} (-1)^{s-n} \left(\begin{array}{c} s \\ n \end{array} \right) \left(\begin{array}{c} s+n \\ n \end{array} \right) x_n.$$

By placing $s = 1$, the following Gauss-Legendre polynomial is obtained

$$Q_1(x) = -\frac{1}{2} + x.$$

Now by $Q_1(x) = 0$, we get $x = c_1 = \frac{1}{2}$, which represents the node for 1-stage implicit RK method represented in the following table.
For $s = 2$, we will obtain Gauss-Legendre polynomial as follows

$$Q_2(x) = 3x^2 - 3x + \frac{1}{2}.$$

$\frac{1}{2}$	$\frac{1}{2}$
	1

If we take $Q_2(x) = 0$, we shall obtain $c_1 = \dfrac{1}{2} - \dfrac{\sqrt{3}}{6}$ and $c_2 = \dfrac{1}{2} + \dfrac{\sqrt{3}}{6}$ which are the nodes for order 4 with 2-stage implicit RK method [11]. To attain $2s$ order of the method, the values of coefficients b_i and a_{ij} can be calculated by abscissa c_i. The Butcher table for this method is .

$\frac{1}{2}-\frac{\sqrt{3}}{6}$	$\frac{1}{4}$	$\frac{1}{4}-\frac{\sqrt{3}}{6}$
$\frac{1}{2}+\frac{\sqrt{3}}{6}$	$\frac{1}{4}+\frac{\sqrt{3}}{6}$	$\frac{1}{4}$
	$\frac{1}{2}$	$\frac{1}{2}$

2.3 Taylor's series expansion for RK methods construction

The origination of RK methods is based on expansion of Taylor's series. The order of any RK method is basically Taylor's series expansion up till any order of h^m. Let we want to construct explicit RK3 from Taylor's expansion. For this we expand equations (2.3) and (2.4) for $i, j = 1, 2, 3$ and $a_{ij} = 0$ for $i \leq j$, we obtain the following formulation of RK3 with 3 stages:

$$Y_1 = y_0, \tag{2.7}$$

$$Y_2 = y_0 + ha_{21}f(Y_1),$$

$$Y_2 = y_0 + ha_{21}f(y_0), \tag{2.8}$$

$$Y_3 = y_0 + ha_{31}f(Y_1) + ha_{32}f(Y_2),$$

$$Y_3 = y_0 + ha_{31}f(y_0) + ha_{32}f(y_0 + ha_{21}f(y_0)), \tag{2.9}$$

$$y_1 = y_0 + hb_1f(Y_1) + hb_2f(Y_2) + hb_3f(Y_3). \tag{2.10}$$

Using the values of Y_1, Y_2, Y_3 from equations (2.7), (2.8), (2.9) and place it in equation (2.10), we get

$$\begin{aligned} y_1 = y_0 + hb_1 f(y_0) + hb_2 f(y_0 + ha_{21} f(y_0)), \\ + hb_3 f(y_0 + ha_{31} f(y_0) + ha_{32} f(y_0 + ha_{21} f(y_0)). \end{aligned} \tag{2.11}$$

Now we expand the series for $f(y_0 + ha_{21}f(y_0))$ upto h^3 as

$$\begin{aligned} f(y_0 + ha_{21} f(y_0)) = f(y_0) + ha_{21}(f'f) + \frac{h^2 a_{21}}{2!}(f''(f,f) + f'f'f) + \frac{h^3 a_{21}}{3!} \\ \times (f'''(f,f,f) + 4f''f'(f,f) + f'f'f). \end{aligned}$$

The above expression is placed in equation (2.11) gives us the following result

$$\begin{aligned} &y_1 = y_0 + hb_1 f(y_0) + hb_2 f(y_0) + h^2 b_2 a_{21} f'f + \frac{h^3}{2} b_2 a_{21}^2 (f''f + f'f'f) + \mathcal{O}(h^4) \\ &+ hb_3 f(y_0 + ha_{31} f(y_0) + ha_{32} \times (f(y_0) + ha_{21} h(f'f) \\ &+ \frac{h^2 a_{21}}{2!} \times (f''(f,f) + f'f'f) + \frac{h^3 a_{21}}{3!}(f'''(f,f,f) + 4f''f'(f,f) + f'f'f))). \end{aligned} \tag{2.12}$$

The approximated solution for explicit RK method of order3 is obtained after simplification of equation (2.12) as

$$\begin{aligned} &y_1 = y_0 + h(b_1 + b_2 + b_3)f + h^2(b_2 a_{21} + b_3(a_{31} + a_{32}))f'f + h^3 b_3 a_{32} a_{21} \\ &\times (f''(f,f) + f'f'f) + \frac{h^3}{2}(b_2 a_{21}^2 + b_3(a_{31} + a_{32})^2 (f''(f,f) + f'f'f) + \mathcal{O}(h^4). \end{aligned} \tag{2.13}$$

As we know that

$$y_0' = f(y_0) = f. \tag{2.14}$$

The higher order derivatives of equation (2.14) are obtained by differentiating it recursively as

$$\begin{aligned} y_0'' &= f'(y_0) y_0' = f'(y_0) f(y_0) = f'f, \\ y_0''' &= f''(y_0)(y_0') f(y_0) + f'(y_0) f'(y_0)(y_0') = f''ff + f'f'f. \end{aligned}$$

These higher order derivatives are also known as elementary differentials and placed in Equation (2.13) to get

$$\begin{aligned} y_1 &= y_0 + h(b_1 + b_2 + b_3)y_0' + h^2(b_2a_{21} + b_3(a_{31} + a_{32}))y'' \\ &+ h^3 b_3 a_{32} a_{21} y''' + \frac{h^3}{2}(b_2 a_{21}^2 + b_3(a_{31} + a_{32})^2)y''' + \mathcal{O}(h^4). \end{aligned} \tag{2.15}$$

Now we expand Taylor's series to get the exact solution as under

$$y(x_0 + h) = y_0 + hy_0' + \frac{h^2}{2!}y_0'' + \frac{h^3}{3!}y_0''' + \mathcal{O}(h^4). \tag{2.16}$$

The approximated solution obtained in equation (2.15) is compared with exact solution in equation (2.16) will give the following order conditions for explicit RK method of order 3:

$$\begin{aligned} b_1 + b_2 + b_3 &= 1, \\ b_2 a_{21} + b_3(a_{31} + a_{32}) &= \frac{1}{2}, \\ b_2 a_{21}^2 + b_3(a_{31} + a_{32})^2 &= \frac{1}{3}, \\ b_3 a_{32} a_{21} &= \frac{1}{6}. \end{aligned}$$

The consistency conditions $\sum a_{ij} = c_j$ will be utilized to reduce above conditions. The reduced form of these conditions is as follows:

$$\begin{aligned} b_1 + b_2 + b_3 &= 1, \\ b_2 c_2 + b_3 c_3 &= \frac{1}{2}, \\ b_2 c_2^2 + b_3 c_3^2 &= \frac{1}{3}, \\ b_3 a_{32} c_2 &= \frac{1}{6}. \end{aligned} \tag{2.17}$$

The solution of order conditions provided in equation set (2.17) will lead to construction of an explicit Rk3 method. As we have 5 equations and 6 unknowns, we can choose value of any abscissa to get the required result. For the moment, by selecting $c_3 = 1$ following solution is obtained as described in Butcher Table 2.2

0	0	0	0
$\frac{1}{2}$	$\frac{1}{2}$	0	0
1	-1	2	0
	$\frac{1}{6}$	$\frac{2}{3}$	$\frac{1}{6}$

Table 2.2: Butcher table for RK method of order 3.

With the help of the above Table 2.2, we can compute stage values and output values as:

$$
\begin{aligned}
Y_1 &= y_0, \\
Y_2 &= y_0 + \frac{h}{2} f(y_0), \\
Y_3 &= y_0 - hf(y_0) + 2hf(y_0 + \frac{h}{2} f(y_0)), \\
y_1 &= y_0 + \frac{h}{6} f(y_0) + \frac{2h}{3} f(y_0 + \frac{h}{2} f(y_0)) + \frac{h}{6} f(y_0 - hf(y_0) + 2hf(y_0 + \frac{h}{2} f(y_0))).
\end{aligned}
$$

2.4 Rooted trees theory for RK methods construction

The main problem in the construction of RK methods through Taylor's series is that for higher order methods, the complexity of order conditions becomes more difficult. So there was a requirement of a new approach that can handle this problem. For this, Butcher introduced a new way of finding order conditions of RK methods known as rooted trees theory. This theory provided an ease to develop order conditions of any order method. In this section, we shall provide a complete understanding of this theory but before that it is necessary to understand some basic concepts which can help to build an understanding of this theory.

2.4.1 Rooted trees and elementary differentials

A tree is a graphical representation consisting of vertices and edges. A non-cyclic connected graph having one vertex acts as root is called a rooted tree. The rooted trees for RK methods have a connection with elementary differentials given in equation (2.14). As described earlier, elementary differentials are the higher order derivatives for $y_0' = f(y_0)$ and are represented by $F(t)$. A complete classification of elementary differentials up to order 4 is the following:

$$y_0' = f(y_0) = f, \tag{2.18}$$

$$y_0'' = f'(y_0)y_0' = f'(y_0)f(y_0) = f'f, \tag{2.19}$$

$$y_0''' = f''ff + f'f'f, \tag{2.20}$$

$$y_0'''' = f'''fff + f''f'ff + f''ff'f + f''ff'f + f'f''ff + f'f'f'f. \tag{2.21}$$

The elementary differentials are represented by trees as for differential f is denoted by single vertex •. Moreover, the representation of $f'f$ by tree will be . In this representation, vertex with edge denotes the derivative and then end vertex is for function f. A complete classification of all rooted trees and their connection with elementary differentials up to order 4 is provided in the following Table 2.3 .

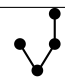
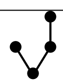
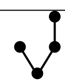
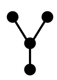
Sr. No.	Elementary differential	Rooted tree	Sr. No.	Elementary differential	Rooted tree
1	f	•	2	$f'f$	
3	$f''ff$		4	$f'f'f$	
5	$f'''fff$		6	$f''f'ff$	
7	$f''ff'f$		8	$f''ff'f$	
9	$f'f''ff$		10	$f'f'f'f$	

Table 2.3: Rooted trees and elementary differentials up to order 4.

Order

The total number of vertices of a tree is termed as order of a rooted tree and is represented by $r(t)$. As an example, we have

$r(t_1) = r(\bullet) = 1$ and $r(t_4) = r($  $) = 3.$

Density

The repetitive product of order of a tree with its chopped sub trees is termed as density and is expressed as $\gamma(t)$. The mathematical representation is

$$\gamma(t) = r(t)\gamma(t_1)\cdots\gamma(t_n),$$

$\gamma(\phi) = 0, \quad \gamma(\bullet) = 1, \quad \gamma($  $) = 2 \times 1 = 2, \quad \gamma($  $) = 3 \times 2 \times 1 = 6.$

Symmetry

The symmetry of the tree is the order of a automorphism group and denoted by $\sigma(t)$ and calculated as

$$\sigma(t) = (\sigma(t_1)^{n_1}\sigma(t_2)^{n_2}...\sigma(t_m)^{n_m})(n_1!\cdots n_{m-1}!n_m!).$$

Moreover, we have relationships among order, densities and symmetries to calculate number of ways of labelling any tree. The labelling of any tree with an order set is denoted by $\alpha(t)$ while labelling with an un-order set is represented by $\beta(t)$. Such relations are provided by Butcher in [11] as

$$\alpha(t) = \frac{r(t)!}{\sigma(t)\gamma(t)},$$
$$\beta(t) = \frac{r(t)!}{\sigma(t)}.$$

2.4.2 Elementary weights

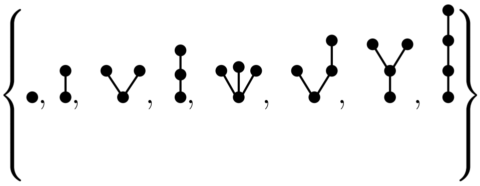
Butcher in [11] showed that coefficients of an RK methods of any stage s are linked to trees through elementary weights Φ as,

$$\Phi(t) = \begin{cases} \sum_{i=1}^{s} b_i, & \text{if } \ t = \tau, \\ \sum_{i=1}^{s} b_i\Phi_i(t_1)\Phi_i(t_2)...\Phi_i(t_m), & \text{if } \ t = [t_1t_2...t_m]. \end{cases}$$

Where $\Phi_i(t)$ is the elementary. The elementary weight related to i^{th}-stage is represented by $\Phi_i(t)$ and is determined as

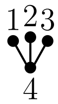
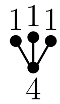
$$\Phi_i(t) = \begin{cases} \sum_{i=j}^{s} a_{ij} = c_i, & \text{if } \; t = \tau, \\ \sum_{i=j}^{s} a_{ij} \Phi_j(t_1)\Phi_j(t_2)...\Phi_i(t_m), & \text{if } \; t = [t_1 t_2 ... t_m]. \end{cases}$$

Let T represents the set consisting of trees up to order 4, then we have

$T =$ .

where $r(t)$ = order and $\gamma(t)$ = density of t.

For tree $t_5 =$ , the values of order, density, $\alpha(t)$, $\beta(t)$, elementary differential and elementary weights are given as:

$r(t_5) = 4$  , $\gamma(t_5) = 4 \times 1 \times 1 \times 1 = 4,$ 

$$\alpha(t_5) = \frac{r(t)!}{\sigma(t)\gamma(t)} = \frac{4!}{6 \times 4} = 1 \;, \qquad \beta(t_5) = \frac{r(t)!}{\sigma(t)} = \frac{4!}{6} = 4$$

$$F(t_5) = f'''(f, f, f), \qquad \Phi(t_5) = \sum_{i=1}^{s} b_i c_i^3.$$

A complete list of all components described above for trees up to order 4 are summarized in the Table 2.4.

2.4.3 Order conditions

Order conditions are basically a relationship between elementary weight function and density. This relationship provides us number of linear and non linear algebraic equations containing the coefficients of RK methods and the solution of these equations will give us the specific RK method. To find this relationship we

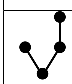
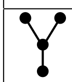
t	$r(t)$	$\gamma(t)$	$\sigma(t)$	$\alpha(t)$	$\beta(t)$	$F(t)$	$\Phi(t)$
•	1	1	1	1	1	f	Σb_i
	2	2	1	1	1	$f'f$	$\Sigma b_i c_i$
	3	3	2	1	3	$f''ff$	$\Sigma b_i c_i^2$
	3	6	1	1	6	$f'f'f$	$\Sigma b_i a_{ij} c_j$
	4	4	6	1	4	$f'''fff$	$\Sigma b_i c_i^3$
	4	8	1	3	24	$f''f'f$	$\Sigma c_i b_i a_{ij} c_j$
	4	12	2	1	12	$f'f''ff$	$\Sigma b_i a_{ij} c_j^2$
	4	24	1	1	24	$f'f'f'f$	$\Sigma b_i a_{ij} a_{jk} c_k$

Table 2.4: Tree notations and different functions up to order 4.

use Taylor's series for exact solution that can be written as

$$y(x_0 + h) = y_0 + \sum_{t \in T} \frac{\alpha(t) h^{r(t)}}{r(t)!} F(t)(y_0).$$

Using the value of $\alpha(t)$ in this equation will give

$$y(x_n + h) = y_n + \sum_{t \in T} \frac{h^{r(t)}}{\sigma(t)\gamma(t)} F(t)(y_n). \tag{2.22}$$

The numerical approximation to Taylor's series is as under

$$y_{n+1} = y_n + \sum_{t \in T} \frac{\beta(t) h^{r(t)}}{r(t)!} \Phi(t) F(t)(y_n).$$

By using the value of $\beta(t)$ in approximated solution will lead to

$$y_1 = y_0 + \sum_{t \in T} \frac{h^{r(t)}}{\sigma(t)} \Phi(t) F(t)(y_0). \tag{2.23}$$

The comparison of approximated and exact solutions provided in equations (2.22) and (2.23) gives us the relationship between elementary weight function and density for the development of order conditions of any RK method of any order with any number of stages.

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

Table 2.5 provides us a complete list of order conditions for RK method up-till order 4.

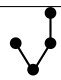
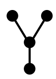
t	$r(t)$	$\gamma(t)$	$\Phi(t) = \frac{1}{\gamma(t)}$	t	$r(t)$	$\gamma(t)$	$\Phi(t) = \frac{1}{\gamma(t)}$
	1	1	$\Sigma b_i = 1$		2	2	$\Sigma b_i c_i = \frac{1}{2}$
	3	3	$\Sigma b_i c_i^2 = \frac{1}{3}$		3	6	$\Sigma b_i a_{ij} c_j = \frac{1}{6}$
	4	4	$\Sigma b_i c_i^3 = \frac{1}{4}$		4	8	$\Sigma c_i b_i a_{ij} c_j = \frac{1}{8}$
	4	12	$\Sigma b_i a_{ij} c_j^2 = \frac{1}{12}$		4	24	$\Sigma b_i a_{ij} a_{jk} c_k = \frac{1}{24}$

Table 2.5: Order conditions of 4-stage RK method.

To construct RK method of order 4 with 4 stages, so we need to expand $\Phi(t)$ for $i, j = 1, 2, 3, 4$. This results in the form of the following algebraic equations:

$$b_1 + b_2 + b_3 + b_4 = 1, \tag{2.24}$$

$$b_2c_2 + b_3c_3 + b_4c_4 = \frac{1}{2}, \tag{2.25}$$

$$b_2c_2^2 + b_3c_3^2 + b_4c_4^2 = \frac{1}{3}, \tag{2.26}$$

$$b_3a_{32}c_2 + b_4a_{42}c_2 + b_4a_{43}c_3 = \frac{1}{6}, \tag{2.27}$$

$$b_2c_2^3 + b_3c_3^3 + b_4c_4^3 = \frac{1}{4}, \tag{2.28}$$

$$b_3c_3a_{32}c_2 + b_4c_4a_{42}c_2 + b_4c_4a_{43}c_3 = \frac{1}{8}, \tag{2.29}$$

$$b_3a_{32}c_2^2 + b_4a_{42}c_2^2 + b_4a_{43}c_3^2 = \frac{1}{12}, \tag{2.30}$$

$$b_4a_{43}a_{32}c_2 = \frac{1}{24}. \tag{2.31}$$

In addition to above eight equations we have three more equations which are necessary to satisfy consistency conditions of a RK method. These are:

$$c_2 = a_{21}, \tag{2.32}$$

$$c_3 = a_{31} + a_{32}, \tag{2.33}$$

$$c_4 = a_{41} + a_{42} + a_{43}. \tag{2.34}$$

Now we have 11 equations to solve for 13 parameters, which means that we have freedom of choosing 2 parameters (two degree of freedom). We choose $c_3 = \frac{1}{4}$ and $c_4 = 1$ and proceed as given in [11]

1. Calculate the values of b_1, b_2, b_3 and b_4 in terms of c_2, c_3, c_4 using equations (2.24), (2.25), (2.26) and (2.28).

2. Equations (2.27), (2.29) and (2.30) are used to get values of coefficients a_{32}, a_{42}, a_{43}.

3. Placing the values of a_{32}, a_{43}, and b_4 in equation (2.31) to get $c_2 = \frac{1}{4}$.

4. The values of a_{21}, a_{31}, a_{41} are calculated by using consistency conditions given in equations (2.32) to (2.34).

The values obtained through step 1 to step 4 are summarized in the following Butcher table for 4 stage explicit RK method of order 4.

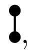
$$\begin{array}{c|cccc} 0 & & & & \\ \frac{1}{4} & \frac{1}{4} & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & \\ 1 & 1 & -2 & 2 & \\ \hline & \frac{1}{6} & 0 & \frac{2}{3} & \frac{1}{6} \end{array}$$

Table 2.6: Butcher table for RK method of order 4.

2.4.4 Simplifying assumptions

With the increase in the order of method, the number of algebraic conditions are also increased and it becomes more difficult to solve these conditions. For this purpose, it is needed to study the connections between the conditions equivalent to different trees. We also see that some set order conditions have some kind of vital role. Due to different variations in difficulty levels of these conditions, we categorized them into the following four parts [11]:

$$\begin{aligned} B(p) &: \sum_{i=1}^{s} b_i c_i^{k-1} = \frac{1}{k}, && && k = 1, 2, \ldots, p, \\ C(\eta) &: \sum_{j=1}^{s} a_{ij} c_j^{k-1} = \frac{c_i^k}{k}, && i = 1, 2, \ldots, s, && k = 1, 2, \ldots, \eta, \\ D(\zeta) &: \sum_{i=1}^{s} b_i c_i^{k-1} a_{ij} = \frac{b_j c_j^k}{k}, && j = 1, 2, \ldots, s, && k = 1, 2, \ldots, \zeta, \\ E(\eta, \zeta) &: \sum_{j=1}^{s} \sum_{i=1}^{s} b_i c_i^{k-1} a_{ij} c_j^{l-1} = \frac{1}{l(k+l)}, && l = 1, 2, \ldots \zeta, && k = 1, 2, \ldots, \eta. \end{aligned}$$

- The condition $B(p)$ shows that method has order p quadrature. Moreover, it satisfies the order conditions of $\bullet$, , ,  $\cdots$ up to order p.

- The $C(\eta)$ condition is associated with the stage order of a method and guarantees that the paired trees, like,  and  produce same order conditions for$k \leq \eta$. This condition shows that elementary weight functions of any two trees are equal which contain factors c_i and $\sum a_{ij}c_j^{k-1}$, while the remaining vertices of both are same.

- $D(\zeta)$ condition provides the relationship among three trees, say, t_1, t_2, and t_3 with elementary weights $b_i c_i^{k-1} a_{ij}$, b_j, and $b_j c_j^k$, respectively. The explicit methods with order 4 having 4 stages must hold $D(1)$.

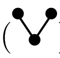
- The $E(\eta, \zeta)$ shows the fact that order condition $\phi(t) = 1/\gamma(t)$ is true for tree $[\tau^{k-1}[\tau^{l-1}]]$ having minimum order $\eta + \zeta$.

2.4.5 B-series and rules for composition

The numerical solution provided in equation (2.23) can be expressed in formal series as

$$B(\lambda(t), y(x)) = \sum_{t \in T} \frac{\lambda(t)}{\sigma(t)} h^{r(t)} F(t)(y(x)),$$

$$= y + h\lambda(\bullet)\mathbf{f}(y) + h^2\lambda(\text{[tree]})\mathbf{f}'\mathbf{f}(y) + h^2\lambda(\text{[tree]})\mathbf{f}''(\mathbf{f},\mathbf{f})(y)\cdots.$$

where $\lambda(t) : T \longrightarrow \mathbb{R}^n$ denotes the elementary weight functions as discussed earlier. Hairer and Warner [24] named this series as Butcher series to present the honour to John Butcher. This series is alternative form of theory presented by Butcher.
The elementary weight function $\mathbf{1}(t)$ is referred as identity mapping and $\lambda^{-1}(t)$ is taken as inverse of elementary weight functions and both are represented as

- $B(\mathbf{1}, y_{n-1}) = y_{n-1}$.

- $y_n = B(\lambda(t), y_{n-1}), \iff y_{n-1} = B(\lambda^{-1}, y_n)$.

Now, let we have two B series $B(\lambda(t), y)$ and $B(\nu(t), y)$ and these can be added and composed as:

- $B(\lambda(t), y) + B(\nu(t), y) = B((\lambda + \nu)(t), y)$.
- $B(\lambda(t), B(\nu(t), y) = B(\lambda\nu(t), y)$.

We can get the product of both functions (λ and ν) with $\lambda(\phi) = 1$ as

$$(\lambda\nu)(t) = \nu(\phi)\lambda(t) + \nu(t) + \sum_{u \prec t} \nu(u)\lambda(t \setminus u). \tag{2.35}$$

In the above equation u and $(t \setminus u)$ are sub-tree and remaining trees, respectively. The term remaining tree is used for the trees which comes after the removal of tree u.
Now for performing composition, we take two RK methods with general form as $[a, b^T, c]$ and $[A, B^T, C]$ having $\lambda(t)$ and $\nu(t)$ as elementary weights, respectively. For better understanding of the composition process, we take two RK methods with 2 stages as

$$\begin{array}{c|cc} c_1 & a_{11} & a_{12} \\ c_2 & a_{21} & a_{22} \\ \hline & b_1 & b_2 \end{array} \qquad \begin{array}{c|cc} C_1 & A_{11} & A_{12} \\ C_2 & A_{21} & A_{22} \\ \hline & B_1 & B_2 \end{array}$$

The equations on the bases of above general Butcher tables are as under:

$$\begin{aligned} Y_1 &= y_0 + a_{11}hf(Y_1) + a_{12}hf(Y_2), & \widetilde{Y}_1 &= y_1 + A_{11}hf(\widetilde{Y}_1) + A_{12}hf(\widetilde{Y}_2), \\ Y_2 &= y_0 + a_{21}hf(Y_1) + a_{22}hf(Y_2), & \widetilde{Y}_2 &= y_1 + A_{21}hf(\widetilde{Y}_1) + A_{22}hf(\widetilde{Y}_2), \\ y_1 &= y_0 + b_1hf(Y_1) + b_2hf(Y_2), & y_2 &= y_1 + B_1hf(\widetilde{Y}_1) + B_2hf(\widetilde{Y}_2), \end{aligned}$$

The composed form of both methods can be obtained by updating $\widetilde{Y}_1$, $\widetilde{Y}_2$ and y_2

by using the value of y_1 as

$$
\begin{aligned}
Y_1 &= y_0 + a_{11}hf(Y_1) + a_{12}hf(Y_2),\\
Y_2 &= y_0 + a_{21}hf(Y_1) + a_{22}hf(Y_2),\\
\widetilde{Y}_1 &= y_0 + b_1hf(Y_1) + b_2hf(Y_2), + A_{11}hf(\widetilde{Y}_1) + A_{12}hf(\widetilde{Y}_2),\\
\widetilde{Y}_2 &= y_0 + b_1hf(Y_1) + b_2hf(Y_2) + A_{21}hf(\widetilde{Y}_1) + A_{22}hf(\widetilde{Y}_2),\\
y_2 &= y_0 + b_1hf(Y_1) + b_2hf(Y_2) + B_1hf(\widetilde{Y}_1) + B_2hf(\widetilde{Y}_2).
\end{aligned}
$$

The butcher table obtained by the composition of two RK methods is as under

$$
\begin{array}{c|cccc}
c_1 & a_{11} & a_{12} & 0 & 0\\
c_2 & a_{21} & a_{22} & 0 & 0\\
C_1+1 & b_1 & b_2 & A_{11} & A_{12}\\
C_2+1 & b_1 & b_2 & A_{21} & A_{22}\\
\hline
 & b_1 & b_2 & B_1 & B_2
\end{array}
\tag{2.36}
$$

This composed table gives different combinations of trees. As an example first order condition which belongs to $t = \bullet$ can be expressed through this composed method as

$$
\begin{aligned}
(\lambda\nu)(t) &= b_1 + b_2 + B_1 + B_2,\\
&= \sum b_i + \sum B_i,\\
&= \lambda(\bullet) + \nu(\bullet).
\end{aligned}
$$

This composition becomes more complex as order of trees grows. A complete list of these compositions in terms of product of elementary weight functions up to order 4 is listed in Table 2.7 below

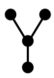
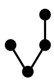
t		$\lambda\nu(t)$
ϕ	t_0	$\nu(t_0)$
	t_1	$\lambda(t_1)\nu(t_0) + \nu(t_1)$
	t_2	$\lambda(t_2)\nu(t_0) + \lambda(t_1)\nu(t_1) + \nu(t_2)$
	t_3	$\lambda(t_3)\nu(t_0) + \lambda(t_2)\nu(t_1) + \lambda(t_1)\nu(t_2) + \nu(t_3)$
	t_4	$\lambda(t_4)\nu(t_0) + \lambda(t_1)^2\nu(t_1) + 2\lambda(t_1)\nu(t_2) + \nu(t_4)$
	t_5	$\lambda(t_5)\nu(t_0) + \lambda(t_3)\nu(t_1) + \lambda(t_2)\nu(t_2) + \lambda(t_1)\nu(t_3) + \nu(t_5)$
	t_6	$\lambda(t_6)\nu(t_0) + \lambda(t_4)\nu(t_1) + \lambda(t_1)^2\nu(t_2) + 2\lambda(t_1)\nu(t_3) + \nu(t_6)$
	t_7	$\lambda(t_7)\nu(t_0) + \lambda(t_1)\lambda(t_2)\nu(t_1) + (\lambda(t_1)^2 + \lambda(t_2))\nu(t_2) + \lambda(t_1)(\nu(t_3) + \nu(t_4)) + \nu(t_7)$
	t_8	$\lambda(t_8)\nu(t_0) + (\lambda(t_1)^3\nu(t_1) + 3(\lambda(t_1)^2\nu(t_2) + 3\lambda(t_1)\nu(t_4) + \nu(t_8)$

Table 2.7: Elementary weight functions product up to order 4.

2.5 Effective order of RK methods

Butcher presented the idea of effective order in [6] and then for the purpose of enhancing the accuracy of RK methods it was revised in [9]. Butcher and Chartier in [12] attained this accuracy for singly implicit RK methods. Butcher and Chan [13] extended this idea to diagonally extended singly implicit RK methods. Sanz-Serna et al., [30] used this idea to increase the efficiency of symplectic integrator for Hamiltonian systems.

In the next part of this section, we are going to present the construction of RK methods with effective order for the following first order differential equations

$$y' = f(y(x)), \qquad y(x_0) = y_0. \tag{2.37}$$

The above system based on initial value can be solved by using conventional RK method described in equations (2.3) and (2.4), we call this method α-method. This method has ability to give solution in one step from $y(x_0)$ to $y(x_0 + h) + \mathcal{O}(h^{p+1})$ by attaining order p with step size h. For method having effective order p, α-method is composed with another method β in such a way that the composition $\beta\alpha\beta^{-1}$ maintains the order p. The β - method is termed as starting method as it is used once at the start to perturb the initial solution while e β^{-1} is used in the end to balance the starting perturbation. In the light of Butcher's definition of effective order, this could be achieved by comparing the composition $\beta\alpha$ with composition $E\beta$ by taking E as exact solution and its value is obtained by the $E = \dfrac{1}{\gamma(t)}$ [21]. The $\beta\alpha$ composition is same as described in Table 2.7 and its general form is

$$(\beta\alpha)(t) = \alpha(\phi)\beta(t) + \alpha(t) + \sum \beta(t \setminus u)\alpha(u). \tag{2.38}$$

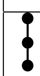
t	u	$t \setminus u$	term
			β_4
			$\beta_2\alpha_1$
			$\beta_1\alpha_2$
			α_4

Table 2.8: The composition of $(\beta\alpha)(t_4)$.

This composition can also be obtained by the process of pruning of trees. In this

procedure we can obtain any sub-tree u by cutting it from main tree t. Thus we get two types of trees u and $(t \setminus u)$. Tree u is termed as α_i while tree $(t \setminus u)$ is referred as β_i. This composition is explained in Table 2.8.
So, we can write

$$\beta\alpha(t_4) = \beta_4 + \beta_2\alpha_1 + \beta_1\alpha_2 + \alpha_4.$$

2.5.1 Effective order RK 3 with 2 stages

The classic RK method of order 3 requires three stages but the effectiver order RK 3 requires only two stages. The procedure starts with finding α- method first by equating last two columns of Table 2.9 with value of $\beta_1 = 0$. Thus we get the following set of equations:

$$\alpha_1 = 1, \tag{2.39}$$

$$\alpha_2 = \frac{1}{2}, \tag{2.40}$$

$$\alpha_3 = \frac{1}{3} + 2\beta_2, \tag{2.41}$$

$$\alpha_4 = \frac{1}{6}. \tag{2.42}$$

t_i	$(\beta\alpha)(t_i)$	$(E\beta)(t_i)$
	$\beta_1 + \alpha_1$	$1 + \beta_1$
	$\beta_2 + \beta_1\alpha_1 + \alpha_2$	$\frac{1}{2} + \beta_1 + \beta_2$
	$\beta_3 + \beta_1^2\alpha_1 + 2\beta_1\alpha_2 + \alpha_3$	$\frac{1}{3} + \beta_1 + 2\beta_2 + \beta_3$
	$\beta_4 + \beta_2\alpha_1 + \beta_1\alpha_2 + \alpha_4$	$\frac{1}{6}+\frac{1}{2}\beta_1 + \beta_2 + \beta_4$

Table 2.9: $\beta\alpha$ and $E\beta$ for the trees up to order 3.

The equations (2.39) to (2.42) can be expressed in terms of elementary weights as

$$\begin{aligned}\sum_{i=1}^{2} b_i &= 1,\\ \sum_{i=1}^{2} b_i c_i &= \frac{1}{2},\\ \sum_{i=1}^{2} b_i c_i^2 &= \frac{1}{3} + 2\sum_{i=1}^{2} B_i C_i,\\ \sum_{i,j=1}^{2} b_i a_{ij} c_j &= \frac{1}{6}.\end{aligned} \tag{2.43}$$

The equations set (2.43) expanded up to 2 stages for the following Butcher table

$$\begin{array}{c|cc} c_1 & a_{11} & 0 \\ c_2 & a_{21} & a_{22} \\ \hline & b_1 & b_2 \end{array}$$

The expanded form of above set of equations is:

$$b_1 + b_2 = 1, \tag{2.44}$$

$$b_1 c_1 + b_2 c_2 = \frac{1}{2}, \tag{2.45}$$

$$b_1 c_1^2 + b_2 c_2^2 = \frac{1}{3} + 2\beta_2, \tag{2.46}$$

$$b_1 a_{11} c_1 + b_2 a_{21} c_1 + b_2 a_{22} c_2 = \frac{1}{6}. \tag{2.47}$$

We use the consistency conditions $a_{11} = c_1$, $a_{21} + a_{22} = c_2$ of RK method to solve equations (2.44), (2.45), (2.47) and obtain the values of b_1, b_2, a_{11}, a_{21}, and a_{22} by taking c_1 and c_2 as parameters given as under:

$$\begin{aligned} b_1 &= -\frac{2c_2 - 1}{2(c_1 - c_2)},\\ b_2 &= \frac{2c_1 - 1}{2(c_1 - c_2)},\\ a_{11} &= c_1,\\ a_{21} &= \frac{-3c_1 + 1 + 6c_1 c_2 - 3c_2}{3(2c_1 - 1)},\\ a_{22} &= \frac{3c_1 - 1}{3(2c_1 - 1)}.\end{aligned} \tag{2.48}$$

As we have two degree of freedom, so we can choose any value of c_1, c_2, like, $c_1 = \frac{1}{3}, c_2 = \frac{2}{3}$ for equations (2.48) to get the following Butcher table for 2 stages α-method.

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

The starting β-method for perturbation is computed by taking $\beta_1 = 0$ and to calculate β_2 from equation (2.45), we calculate the value of α_3 as

$$\begin{aligned} \alpha_3 &= \sum b_i c_i^2 = b_1 c_1^2 + b_2 c_2^2, \\ &= \frac{1}{2}(\frac{1}{9} + \frac{4}{9}), \\ &= \frac{5}{18}. \end{aligned}$$

Using α_3 in Equation (2.45), we get β_2 as

$$\beta_2 = -\frac{1}{36}. \tag{2.49}$$

To maintain the classical order 2, we use

$$\beta_1 = 0. \tag{2.50}$$

The elementary weight form of equations (2.50) and (2.49) is

$$\begin{aligned} \sum B_i &= 0, \\ \sum B_i C_i &= -\frac{1}{36}. \end{aligned} \tag{2.51}$$

The coefficients of Butcher table for explicit starting method of 2 stage for equation set (2.51) are given by

$$
\begin{array}{c|cc}
0 & 0 & 0 \\
C_2 & A_{21} & 0 \\
\hline
 & B_1 & B_2
\end{array}
$$

By expanding equations (2.51), we get:

$$
\begin{aligned}
B_1 + B_2 &= 0, \\
B_2 C_2 &= -\frac{1}{36}.
\end{aligned}
$$

We choose $C_2 = \frac{1}{2}$, and get the following starting method.

$$
\begin{array}{c|cc}
0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & 0 \\
\hline
 & \frac{1}{18} & -\frac{1}{18}
\end{array}
$$

In the end, we calculate β^{-1} method as given in [11] to cancel the effects of starting method.

$$
\begin{array}{c|cc}
0 & -\frac{1}{18} & \frac{1}{18} \\
\frac{1}{2} & \frac{4}{9} & \frac{1}{18} \\
\hline
 & -\frac{1}{18} & \frac{1}{18}
\end{array}
$$

2.6 Symplectic Runge-Kutta methods

Symplecticity is the property of preserving area of any system and when it is combined with RK methods [19] to study the behaviour of Hamiltonian systems, we get a new class of geometric integrators known as symplectic RK methods. The relationship among the coefficients of RK method to be symplectic is

$$
b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \qquad i, j = 1, \cdots, s. \tag{2.52}
$$

Proof : We take the quadratic invariant definition for a function $f(z)$ as

$$z^T M f(z) =< z, f(z) >= 0, \quad \forall z. \tag{2.53}$$

Here M is a symmetric matrix of square dimension. The above definition is applied to RK method as

$$< X_i, f(X_i) >= 0.$$

The equations (2.3) and (2.4) become

$$\begin{aligned} < y_n + \sum_{j=1}^{s} a_{ij} h f(X_j), f(X_i) >= 0, \\ < y_n, f(X_i) >= -h \sum_{j=1}^{s} a_{ij} < f(X_j), f(X_i) > . \end{aligned} \tag{2.54}$$

In addition to this, the inner product of solution y_{n+1} is

$$\begin{aligned} < y_{n+1}, y_{n+1} > &=< y_n + \sum_{i=1}^{s} b_i h f(K_i), y_n + \sum_{i=1}^{s} b_i h f(K_i) >, \\ &=< y_n, y_n > +h \sum_{i=1}^{s} b_i < y_n, f(X_i) > +h \sum_{i=1}^{s} b_i \\ &\quad < f(X_i), y_n > +h^2 \sum_{i,j=1}^{s} b_i b_j < f(X_i), f(X_j) > . \end{aligned} \tag{2.55}$$

Using equations (2.54) and (2.55), we have

$$\begin{aligned} < y_{n+1}, y_{n+1} > &=< y_n, y_n > -h^2 \sum_{i,j=1}^{s} b_i a_{ij} < f(X_j), f(X_i) > -h^2 \sum_{i,j=1}^{s} b_j a_{ji} \\ &\quad < f(X_j), f(X_i) > +h^2 \sum_{i,j=1}^{s} b_i b_j < f(X_j), f(X_i) >, \\ &=< y_n, y_n > -h^2 \sum_{i,j=1}^{s} (b_i a_{ij} + b_j a_{ji} - b_i b_j) < f(X_j), f(X_i) > . \end{aligned}$$

So, for

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

we get

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

As we know that

$$< f(X_j), f(X_i) > \neq 0.$$

So,

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

This proves that

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

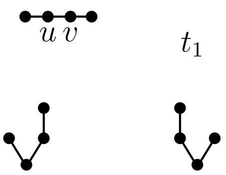
2.7 Order conditions for symplectic RK methods

The trees of RK methods are catogorized into superfluous and non-superfluous trees. These trees are used in reducing the number of order conditions for symplectic RK methods. The structure of these trees is explained as follows.

Superfluous trees:

These are the trees that produce same rooted trees when we make any of neighboring nodes to root of the tree [19].

As an example, let take a tree t_1



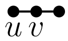
$u(t_1)$ $v(t_1)$

The nodes u and v are next to each other. If we take any of root u or v as a root, the resultant trees $u(t)$ and$v(t)$ become same. So, t_1 tree will be a superfluous tree.

Non-superfluous trees:

A tree in which two adjacent nodes can not generate an identical tree is named as non-superfluous tree [19].

As an example, consider the following tree t_2



t_2

Then $u(t_2)$ becomes a rooted tree when node u is assigned as root while, when node v is taken as root we get different tree $v(t_2)$ as compared to $u(t)$ as shown below.

$u(t_2)$ $v(t_2)$

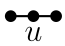
In symplectic RK method case, superfluous trees do not take part in the order condition while we select only one condition out of any set of non-superfluous trees. That is the reason for having less number of conditions in symplectic RK method than standard RK method. This reduction is caused by the use of symplectic condition and the procedure of this reduction is explained as under.

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0. \tag{2.56}$$

Consider a superfluous tree belongs to order 2 condition. By taking summation over the symplectic condition provided in equation (2.56) along with $b_i = 1$ as

$$\begin{aligned} \sum_{i,j} b_i a_{ij} + \sum_{i,j} b_j a_{ji} - \sum_{i} b_i \sum_{j} b_j &= 0, \\ 2\sum_{i,j} b_i a_{ij} - 1 &= 0, \\ \sum_{i,j} b_i a_{ij} &= \frac{1}{2}. \end{aligned}$$

So, this superfluous tree does not act as an order condition in symplectic RK method.

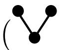
Similarly, 

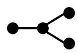
is a non-superfluous tree. We multiply equation (2.56) by c_j by placing summation over i and j, so that, we have

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

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

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

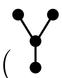
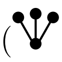
( $-\frac{1}{6}$) + ( $-\frac{1}{3}$) $= 0.$

We see from the above equations, if one of the above is satisfied, other will also be satisfied. So, we take one of these non superfluous trees and remaining trees will be thrown away.
When we look at order 4 trees, we see that tree  is non-superfluous and is superfluous. To develop the relationship between pair of non-superfluous trees, we multiply equation (2.56) with c_j^2 by taking summation over i, j index as

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

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

$$(\sum_{i,j} b_i a_{ij} c_j^2 - \frac{1}{12}) + (\sum_{i,j} b_j c_j^3 - \frac{1}{4}) = 0,$$

( $-\frac{1}{2}$) + ( $-\frac{1}{4}$) $= 0.$

Again we find that the satisfaction of one condition gives the satisfaction of other. So we can take only one out of both.
Similarly, we multiply equation (2.56) with c_j and c_i for superfluous tree, we get

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

$$2 \sum_{i,j} b_i c_i a_{ij} c_j - \frac{1}{4} = 0,$$

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

For symplective RK method, the conditions based on superfluous trees will not be considered as an order conditions, so we leave both of above trees. The number of order conditions of both standard RK and symplectic RK methods are summarized in the following Table (2.10).

order	RK methods	Symplectic RK method
1	1	1
2	2	1
3	4	2
4	8	3
5	17	6

Table 2.10: Number of order conditions for standard and symplectic RK methods up to order 5.

2.8 Derivation of order 3 symplectic RK method

Sanz-serna in [34] gave the general format of diagonally impilcit symplectic RK method. By using this format for order 3, we can calculate the method by solving only two conditions. The general format for order 3 is as under:

$$
\begin{array}{c|ccc}
\frac{b_1}{2} & \frac{b_1}{2} & & \\
b_1 + \frac{b_2}{2} & b_1 & \frac{b_2}{2} & \\
b_1 + b_2 + \frac{b_3}{2} & b_1 & b_2 & \frac{b_3}{2} \\
\hline
 & b_1 & b_2 & b_3
\end{array}
$$

Table 2.11: General format of diagonally implicit symplectic RK method of order 3.

Due to symplectic condition, only two order conditions will participate in the construction of symplectic RK method. Expanded form of these two conditions are as follows:

$$b_1 + b_2 + b_3 = 1, \tag{2.57}$$

$$b_1c_1^2 + b_2c_2^2 + b_3c_3^2 = \frac{1}{3}. \tag{2.58}$$

By replacing the values of $c_1,\ c_2,\ c_3$ using the general form of symlectic RK method in Table (2.11), equation (2.58) gets the following form

$$b_1(\frac{b_1}{2})^2 + b_2(b_1 + \frac{b_2}{2})^2 + b_3(b_1 + b_2 + \frac{b_3}{2})^2 = \frac{1}{3}. \tag{2.59}$$

Sanz-serna used $b_1 = b_3$ in equations (2.57) and (2.59) and solved them to get the values of $b_1 = b_3 = \frac{1}{3}(2 + 2^{\frac{1}{3}} + 2^{-\frac{1}{3}})$ and $b_2 = -\frac{1}{3}(1 + 2^{\frac{4}{3}} + 2^{\frac{2}{3}})$. These values confirm the symplectic condition provided in equation (2.52) and all 4 order conditions of standard RK3 method.

2.9 Symplectic effective order RK methods

The effective order of symplectic RK methods was first developed by Butcher and Gulshad in [16, 26]. Here, we present the derivation of symplectic RK method with two stages. We can move towards this construction by utilizing effective order conditions Table (2.9) for RK method and applying the symplectic conditions on equations set (2.39) to (2.42). In these equations, α_2 links to superfluous tree, so this order condition is satisfied automatically. Moreover, in equation linked to non-superfluous trees ($\alpha_3 + \alpha_4 = \frac{1}{2}$), we can skip any tree out of α_3 and α_4 and hence we choose the condition ($\alpha_3 = \frac{1}{3}$). Now we have to equations for the construction of effective order method as

$$\alpha_1 = 1, \tag{2.60}$$

$$\alpha_3 = \frac{1}{3}. \tag{2.61}$$

We know that, any effective order technique involves starting method, main method, and finishing method. First we present the Butcher table for main method as under

$$
\begin{array}{c|cc}
c_1 & a_{11} & a_{12} \\
c_2 & a_{21} & a_{22} \\
\hline
 & b_1 & b_2
\end{array}
$$

By expanding equations (2.60) and (2.61) in component form as:

$$\sum_{i=1}^{2} b_i = b_1 + b_2 = 1, \tag{2.62}$$

$$\sum_{i=1}^{2} b_i c_i^2 = b_1 c_1^2 + b_2 c_2^2 = \frac{1}{3}. \tag{2.63}$$

Solving equations (2.62) and (2.63) along with consistency and symplectic condition, we get the following set of Butcher's coefficients with c_1 as free parameter:

$$
\begin{aligned}
b_1 &= \frac{1}{4(3c_1^2 - 3c_1 + 1)}, \\
b_2 &= \frac{3(1 + 4c_1^2 - 4c_1)}{4(3c_1^2 - 3c_1 + 1)}, \\
a_{11} &= \frac{1}{8(3c_1^2 - 3c_1 + 1)}, \\
a_{22} &= \frac{3(1 + 4c_1^2 - 4c_1)}{8(3c_1^2 - 3c_1 + 1)}, \\
a_{12} &= \frac{24c_1^3 - 24c_1^2 + 8c_1 - 1}{8(3c_1^2 - 3c_1 + 1)}, \\
a_{21} &= -\frac{12c_1^2 - 18c_1 + 7}{24(2c_1 - 1)(3c_1^2 - 3c_1 + 1)}, \\
c_2 &= \frac{3c_1 - 2}{3(2c_1 - 1)}.
\end{aligned}
$$

For main method (α)-method, we take $c_1 = \dfrac{1}{4}$ and the Butcher table will become

$$
\begin{array}{c|cc}
\frac{1}{4} & \frac{2}{7} & -\frac{1}{28} \\
\frac{5}{6} & \frac{13}{21} & \frac{3}{14} \\
\hline
 & \frac{4}{7} & \frac{3}{7}
\end{array}
$$

Lastly, starting and finishing methods of symplectic nature are developed. As discussed earlier that for all symplectic RK method for $s \leq 3$, we use diagonally implicit configuration of Butcher table as under

$$\begin{array}{c|cc} B_1 & B_1 & 0 \\ B_2 & 2B_1 & B_2 - 2B_1 \\ \hline & 2B_1 & 2B_2 - 4B_1 \end{array}$$

We take $B_1 = \dfrac{1}{6}$ to find the starting method as

$$\begin{array}{c|cc} \frac{1}{6} & \frac{1}{6} & 0 \\ \frac{1}{6} & \frac{1}{3} & -\frac{1}{6} \\ \hline & \frac{1}{3} & -\frac{1}{3} \end{array}$$

The coefficients of β^{-1} table are calculated by using inverse table provided in [11]

$$\begin{array}{c|cc} \frac{1}{6} & -\frac{1}{6} & \frac{1}{3} \\ \frac{1}{6} & 0 & \frac{1}{6} \\ \hline & -\frac{1}{3} & \frac{1}{3} \end{array}$$

A complete compose table of composition $\beta\alpha\beta^{-1}$ takes the form

$$\begin{array}{c|cccccc} \frac{1}{6} & \frac{1}{6} & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{6} & \frac{1}{3} & -\frac{1}{6} & 0 & 0 & 0 & 0 \\ \frac{1}{4} & \frac{1}{3} & -\frac{1}{3} & \frac{2}{7} & -\frac{1}{28} & 0 & 0 \\ \frac{5}{6} & \frac{1}{3} & -\frac{1}{3} & \frac{13}{21} & \frac{3}{14} & 0 & 0 \\ \frac{7}{6} & \frac{1}{3} & -\frac{1}{3} & \frac{4}{7} & \frac{3}{7} & -\frac{1}{6} & \frac{1}{3} \\ \frac{7}{6} & \frac{1}{3} & -\frac{1}{3} & \frac{4}{7} & \frac{3}{7} & 0 & \frac{1}{6} \\ \hline & \frac{1}{3} & -\frac{1}{3} & \frac{4}{7} & \frac{3}{7} & -\frac{1}{3} & \frac{1}{3} \end{array}$$

The coefficients of above table satisfy both conditions, i.e., symplectic and order conditions of standard RK method of order 3.

2.10 Conclusion

In this chapter, we discussed the detailed work already done in the field of RK methods. We started from the Runge work of extending the Euler's scheme to approximate the solution of ordinary differential equations. His approach was to use Taylor's series upto higher derivatives to get more accurate method. We gave Taylor's method approach to solve any system of differential equation. Later on, we presented the process of finding out the order conditions required for the construction of a RK method. As this procedure becomes complex as order of method goes higher, we are required a new way to calculate these order conditions easily. We explored the modern theory of rooted trees presented by J. C. Butcher to develop order conditions of RK methods.

In the next part of the chapter, we explained all aspects of this rooted tree theory by giving details regarding rooted trees, elementary weights, elementary differentials, density, etc. With the help of this theory, we explained and calculated the order conditions of RK4 and by solving these order conditions, we calculated classic explicit RK 4 method using simplifying assumptions. In the last part of the chapter, we moved towards the most recent development in RK methods under the name of effective order of RK methods. We presented all those details that are essential in the construction of an effective order. Use of B-series and composition of two RK methods is explained both in algebraic and graphical way. In the end, we constructed an effective order RK method with order three using 2 stages. Symplectic RK methods are also discussed in detail along with the order conditions and role of super and non-superfluous trees for Hamiltonian systems. Lastly, we discussed a very latest development in symplectic RK methods and that is the construction of effective order for symplectic RK methods. With the help of this technique, we saw that order 3 method with 2 stages can be constructed. This gives us 1 stage benefit than standard symplectic RK method.

In the next chapters, we shall use this effective order technique to RKN methods and PRK methods to present new ideas in this field.

Chapter 3

The effective order of RKN methods

In many practical situations, we deal with system of differential equations containing second order derivatives. The general expression of these type of equations is given by

$$y^{''} = f(x, y, y^{'}). \tag{3.1}$$

A very simple representation of such system in Newton's second law of motion in which force is directly connected with acceleration. As acceleration is the second derivative of displacement, so when we link this force with any physical phenomenon, this will result in second order differential equation. As in the case of Hook's law, the force is directly proportional to displacement x and can be expressed mathematically as follows:

$$\begin{aligned} F &= -kx, \\ ma &= -kx, \\ \frac{d^2x}{dt^2} &= -\frac{k}{m}x. \end{aligned} \tag{3.2}$$

Although any differential equation or system of differential equations containing second order can be solved by classic RK schemes by converting that equation or systems in to first order but in 1925, Nystr$\ddot{o}$m presented the method which can solve such type of differential equations directly with out converting them into the first order. Such direct methods are known as Runge–Kutta Nystr$\ddot{o}$m (RKN) methods [23].

In this chapter, we have presented the techniques to develop a new class of RKN methods which is termed as effective order of RKN methods. We have presented some effective order conditions of RKN up to order 5 along with various combinations of starting and main methods. These combinations can be very useful for researchers to develop effective order RKN methods up to order 5. The following sections will lead us towards such type of conditions.

- Algebraic structure of solution scheme.
- Derivatives of exact solution and their connection with trees.
- Order conditions of RKN up to order 5.
- Pruning of special Nystr*ö*m trees.
- Composition of two RKN methods.
- Inverse of RKN method.
- Effective order conditions of RKN methods.

3.1 Algebraic structure of solution scheme

We have considered the following autonomous system of second order ordinary differential equations (ODEs).

$$y^{''} = f(y), \qquad y(x_0) = y_0, \qquad y^{'}(x_0) = y_0^{'}, \tag{3.3}$$

where y$\in \mathbb{R}^N$ and $f : \mathbb{R}^N \longrightarrow \mathbb{R}^N$. Such system of ODEs can be solved either with standard RK methods by converting them into the corresponding first order system of ODEs or by RKN methods that solve such systems directly. The solution of (3.3) with an s-stage RKN method $[A \ \ \bar{b} \ \ b \ \ c]$ is

$$\begin{aligned} K_i &= y_0 + c_i h y_0^{'} + h^2 \sum_{j=1}^{s} a_{ij} f(k_j), \\ y_1 &= y_0 + h y_0^{'} + h^2 \sum_{i=1}^{s} \bar{b}_i f(k_i), \\ y_1^{'} &= y_0^{'} + h \sum_{i=1}^{s} b_i f(k_i). \end{aligned} \tag{3.4}$$

Where, K_i are internal stages, b_i and $\bar{b}_i$ are quadrature weights, c_i are quadrature nodes and $A = (a_{ij})_{s\times s}$ denotes the matrix of s-stage RKN method. The Butcher table for RKN methods is

$$\begin{array}{c|c} c & A \\ \hline & \bar{b}^T \\ \hline & b^T \end{array}$$

3.2 Derivatives of exact solution and their connection with trees

As in the case with all numerical methods, the order of a RKN method is obtained by comparing the numerical solution with Taylor's series of exact solution. The exact solution contains the higher derivations of given system. The order of derivatives involved in any scheme depicts the order of method. The procedure of taking derivatives obeys chain rule and it becomes more and more complicated as order of the method increases.
Consider the following second order differential equation.

$$y^{''} = f(y, y^{'}), \qquad y(x_0) = y_0, \qquad y^{'}(x_0) = y_0^{'}. \tag{3.5}$$

The repetitive procedure of taking derivatives of equation (3.5) is as follows:

$$\begin{aligned} y^{'} &= y^{'}, \\ y^{''} &= f, \\ y^{'''} &= \frac{\partial f}{\partial y} \cdot y^{'} + \frac{\partial f}{\partial y^{'}} \cdot f, \\ y^{iv} &= \frac{\partial^2 f}{\partial y^2} \cdot (y^{'}, y^{'}) + \frac{\partial f}{\partial y^{'} \partial y} \cdot (f, y^{'}) + \frac{\partial f}{\partial y} \cdot f + \frac{\partial^2 f}{\partial y \partial y^{'}} \cdot (y^{'}, f) + \cdots \\ &\frac{\partial^2 f}{\partial y^{'2}} \cdot (f, f) + \frac{\partial f}{\partial y^{'}} \cdot \frac{\partial f}{\partial y} \cdot y^{'} + \frac{\partial f}{\partial y^{'}} \cdot \frac{\partial f}{\partial y^{'}} \cdot f. \end{aligned} \tag{3.6}$$

We can see that from above set of equations (3.6) as order of derivation increases, complexity of terms also increases. This problem was overcome by rooted tree concept presented by Butcher [11], in which he had linked the vertices of trees with derivative terms of RK methods. On the same pattern, Hairer presented rooted tree for RKN methods. In case of these methods, we have Nyström trees whose vertices are either fat (t=$\circ$) or meager (t= $\bullet$). The terms having derivatives with respect to y are represented by meager vertex while terms containing derivatives with respect to y' are represented by fat vertex . For the system (3.3), we use Special Nyström (SN) trees where we take only fat vertices as root of each rooted tree [23]. Moreover, the trees connected with derivatives of equation set (3.6) are presented in Table 3.1.

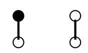
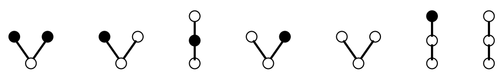
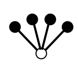
Derivative terms	Trees
y''	
y'''	
y^{iv}	

Table 3.1: Derivative terms and corresponding rooted trees up to order 4.

3.3 Order conditions of RKN up to order 5

The order of RKN method is obtained by comparing Taylor's series of y_1, y_1' with true solutions $y(x_0+h)$ and $y'(x_0+h)$. Based on the algebraic theory of group of RK methods due to Butcher [7], the elements of RKN group are functions from Nyström trees to elementary weights associated to order conditions. Thus for any $\alpha \in G$ acts on a Nyström tree as $\alpha(t_i) = \alpha_i$, such that, we have, for example,

$$\alpha_8 = \alpha(t_8) = \alpha\Bigg(\quad\Bigg) = \sum b_i {c_i}^4.$$



These conditions can be formed by relating elementary weight function $\Phi(t_i)$ with density value $\gamma(t_i)$. The governing equation that creates the conditions is

$$b_i \cdot \Phi(t_i) = \frac{1}{\gamma(t_i)}.$$

For RKN methods, we use thirteen order conditions as illustrated in [23]. A complete detail of all these conditions along with their relevant order is presented in Table 3.2.

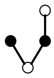
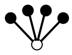
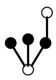
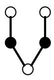
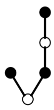
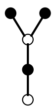
t_i	Trees	order	$\gamma(t_i)$	$\Phi(t_i) = \dfrac{1}{\gamma(t_i)}$
t_1		1	1	$\sum b_i = 1$
t_2		2	2	$\sum b_i c_i = \frac{1}{2}$
t_3		3	3	$\sum b_i c_i^2 = \frac{1}{3}$
t_4		3	6	$\sum b_i a_{ij} = \frac{1}{6}$
t_5		4	4	$\sum b_i c_i^3 = \frac{1}{4}$
t_6		4	8	$\sum b_i c_i a_{ij} = \frac{1}{8}$
t_7		4	24	$\sum b_i a_{ij} c_j = \frac{1}{24}$
t_8		5	5	$\sum b_i c_i^4 = \frac{1}{5}$
t_9		5	10	$\sum b_i c_i^2 a_{ij} = \frac{1}{10}$
t_{10}		5	20	$\sum b_i a_{ij} a_{ik} = \frac{1}{20}$
t_{11}		5	30	$\sum b_i c_i a_{ij} c_j = \frac{1}{30}$
t_{12}		5	60	$\sum b_i a_{ij} c_j^2 = \frac{1}{60}$
t_{13}		5	120	$\sum b_i a_{ij} a_{jk} = \frac{1}{120}$

Table 3.2: Rooted trees and Order conditions up to order 5.

Equations involving coefficients of Butcher's tableau can be derived by expanding order conditions provided in the last column of Table 3.2. These coefficient are used in solution scheme provided in equation set (3.4). For example, the component form of order conditions up to order 4 for an explicit RKN method is presented in the following set of equations:

$$\begin{aligned}
b_1 + b_2 + b_3 + b_4 &= 1, \\
b_2c_2 + b_3c_3 + b_4c_4 &= \frac{1}{2}, \\
b_2c_2^2 + b_3c_3^2 + b_4c_4^2 &= \frac{1}{3}, \\
b_2a_{21} + b_3(a_{31} + a_{32}) + b_4(a_{41} + a_{42} + a_{43}) &= \frac{1}{6}, \\
b_2c_2^3 + b_3c_3^3 + b_4c_4^3 &= \frac{1}{4}, \\
b_2c_2a_{21} + b_3c_3(a_{31} + a_{32}) + b_4c_4(a_{41} + a_{42} + a_{43}) &= \frac{1}{8}, \\
b_3a_{32}c_2 + b_4(a_{42}c_2 + a_{43}c_3) &= \frac{1}{24}.
\end{aligned} \tag{3.7}$$

We are only dealing with Explicit RKN methods, therefore the coefficient $c_1 = a_{11} = a_{22} = a_{33} = a_{44} = 0$ in equations set (3.7). By solving these equations along with consistency condition $\sum a_{ij} = \frac{c_i^2}{2}$, we can form RKN method of order four with three or four stages.

For effective order RKN, we need to develop effective order conditions for RKN so that we are able to develop order 4 method with two stages or order 5 with 3 stages. In [23], RKN method of order four and five with three stages and four stages, respectively, is already constructed from classical order conditions presented in Table 3.2. For effective order conditions we need to make composition of two methods. This composition can be obtained by pruning of trees and algebraically. Both compositions must give the same result. We can assign two elements $\alpha, \beta \in G$ to RKN methods M and S, respectively, for pruning of trees and for their algebraic composition.

3.4 Pruning of special Nystrӧm trees.

For the two RKN methods M and S, their composition for the tree t_7 is given as

$\beta\alpha\Bigg($  $\Bigg) = \beta_7 + \alpha_4 + \beta_2\alpha_2 - \beta_3\alpha_1 + \beta_2\alpha_1 + \alpha_7.$ (3.8)

The terms on right hand side of the equation (3.8) are obtained from Table 3.3. The pruning of a SN tree t yields sub-trees u and $t \setminus u$, such that $t \setminus u$ is the remaining set of trees when u is chopped off t. Columns of Table 3.3 show the procedure of different cuts and their resultant trees as follows:

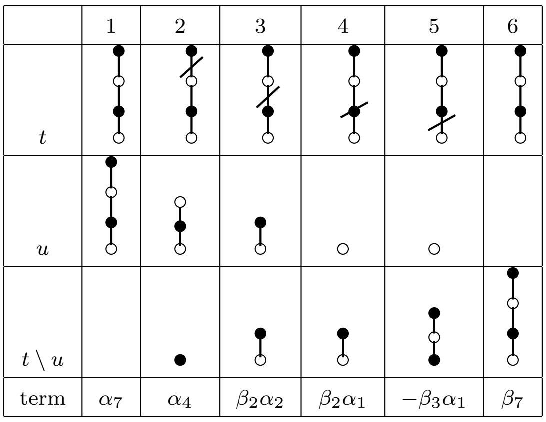


Table 3.3: Calculation for the term $\beta\alpha(t_7)$.

- In column 1, we cut nothing from tree t so $t \setminus u$ is empty and u contains the whole tree t_7.
- In column 2, we cut the edge joining the meager and fat vertex. So, u contains t_4 while $t \setminus u$ contains a single meager vertex. As we are considering only SN trees, where meager vertex cannot be a root of a tree. So, by ignoring the meager vertex tree and considering the order condition of t_4 only, we get the term α_4.
- In column 3, we cut the edge joining fat and meager vertex. The result consists of tree t_2 in both u and $t \setminus u$ and the term we get is $\beta_2\alpha_2$.

- In column 4, when a meager vertex appears between two fat vertices, we cut this meager vertex itself. We get t_1 in u and t_2 in $t \setminus u$, thus giving us the term $\beta_2\alpha_1$.

- In column 5, we cut the edge between the meager and fat vertex. Thus u becomes a fat vertex only and $t \setminus u$ has a tree whose root is a meager vertex. However, we do not take a meager vertex as a root. So we assign the root to the nearest fat vertex and the tree  becomes . Moreover, we change the sign from +ve to -ve of the associated functions $\alpha(t_i)$ and $\beta(t_i)$. Thus we get the term $-\beta_3\alpha_1$.

- In column 6, a complete tree is removed, so u is an empty tree and $t \setminus u$ is the tree itself and the term we get is β_7.

3.5 Composition of two RKN methods

The two RKN methods are composed in such a way that first method enhances solution from y_0 to y_1, while second method took the solution from y_1 to y_2. Thus in the end we get a combined composed form of two methods which will help us in the construction of different sub trees . Consider the following 3-stage RKN methods M and S having Butcher tableau's:

$$
M\text{-method:}\quad
\begin{array}{c|ccc}
c_1 & a_{11} & a_{12} & a_{13} \\
c_2 & a_{21} & a_{22} & a_{23} \\
c_3 & a_{31} & a_{32} & a_{33} \\
\hline
 & \bar{b}_1 & \bar{b}_2 & \bar{b}_3 \\
\hline
 & b_1 & b_2 & b_3
\end{array}\,,
\qquad
S\text{-method:}\quad
\begin{array}{c|ccc}
C_1 & A_{11} & A_{12} & A_{13} \\
C_2 & A_{21} & A_{22} & A_{23} \\
C_3 & A_{31} & A_{32} & A_{33} \\
\hline
 & \bar{B}_1 & \bar{B}_2 & \bar{B}_3 \\
\hline
 & B_1 & B_2 & B_3
\end{array}\,.
$$

Now, we first apply M-method using solution scheme (3.4) to up lift solution from y_0 to y_1 and $y_0^{'}$ to $y_1^{'}$ as:

$$\begin{aligned}
K_1 &= y_0 + hc_1y_0^{'} + h^2[a_{11}f(K_1) + a_{12}f(K_2) + a_{13}f(K_3)],\\
K_2 &= y_0 + hc_2y_0^{'} + h^2[a_{21}f(K_1) + a_{22}f(K_2) + a_{23}f(K_3)],\\
K_3 &= y_0 + hc_3y_0^{'} + h^2[a_{31}f(K_1) + a_{32}f(K_2) + a_{33}f(K_3)],\\
y_1 &= y_0 + hy_0^{'} + h^2[\bar{b}_1f(K_1) + \bar{b}_2f(K_2) + \bar{b}_3f(K_3)],\\
y_1^{'} &= y_0^{'} + h[b_1f(K_1) + b_2f(K_2) + b_3f(K_3)].
\end{aligned} \tag{3.9}$$

S-method is applied on y_1 & $y_1^{'}$ to get y_2 & $y_2^{'}$ by using solution Scheme (3.4) again as:

$$\begin{aligned}
L_1 &= y_1 + hC_1y_1^{'} + h^2[A_{11}f(L_1) + A_{12}f(L_2) + A_{13}f(L_3)],\\
L_2 &= y_1 + hC_2y_1^{'} + h^2[A_{21}f(L_1) + A_{22}f(L_2) + A_{23}f(L_3)],\\
L_3 &= y_1 + hC_3y_1^{'} + h^2[A_{31}f(L_1) + A_{32}f(L_2) + A_{33}f(L_3)],\\
y_2 &= y_1 + hy_1^{'} + h^2[\overline{B}_1f(L_1) + \overline{B}_2f(L_2) + \overline{B}_3f(L_3)],\\
y_2^{'} &= y_1^{'} + h[B_1f(L_1) + B_2f(L_2) + B_3f(L_3)].
\end{aligned} \tag{3.10}$$

Now we place the values of y_1 and $y_1^{'}$ from equation (3.9) into L_1, L_2, L_3, y_2, and $y_2^{'}$ of equation (3.10) to get a composed table of two methods which will uplift the solution from y_0 to y_2. The simplified form of such composition is expressed in the following system:

$$\begin{aligned}
L_1 &= y_0 + h(1 + C_1)y_0^{'} + h^2[(\bar{b}_1 + b_1C_1)f(K_1) + (\bar{b}_2 + b_2C_1)f(K_2) + \cdots\\
&\quad (\bar{b}_3 + b_3C_1)f(K_3) + A_{11}f(L_1) + A_{12}f(L_2) + A_{13}f(L_3)],\\
L_2 &= y_0 + h(1 + C_2)y_0^{'} + h^2[(\bar{b}_1 + b_1C_2)f(K_1) + (\bar{b}_2 + b_2C_2)f(K_2) + \cdots\\
&\quad (\bar{b}_3 + b_3C_2)f(K_3) + A_{21}f(L_1) + A_{22}f(L_2) + A_{23}f(L_3)],\\
L_3 &= y_0 + h(1 + C_3)y_0^{'} + h^2[(\bar{b}_1 + b_1C_3)f(K_1) + (\bar{b}_2 + b_2C_3)f(K_2) + \cdots\\
&\quad (\bar{b}_3 + b_3C_3)f(K_3) + A_{31}f(L_1) + A_{32}f(_2) + A_{33}f(L_3)],\\
y_2 &= y_0 + 2hy_0^{'} + h^2[(\bar{b}_1 + b_1)f(K_1) + (\bar{b}_2 + b_2)f(K_2) + (\bar{b}_3 + b_3)f(K_3) + \cdots\\
&\quad \overline{B}_1f(L_1) + \overline{B}_2f(L_2) + \overline{B}_3f(L_3)],\\
y_2^{'} &= y_0^{'} + h[b_1f(K_1) + b_2f(K_2) + b_3f(K_3) + B_1f(L_1) + B_2f(L_2) + B_3f(L_3)].
\end{aligned} \tag{3.11}$$

The combined table of above composed scheme (3.11) is

c_1	a_{11}	a_{12}	a_{13}	0	0	0
c_2	a_{21}	a_{22}	a_{23}	0	0	0
c_3	a_{31}	a_{32}	a_{33}	0	0	0
$1+C_1$	$\bar{b}_1 + b_1 C_1$	$\bar{b}_2 + b_2 C_1$	$\bar{b}_3 + b_3 C_1$	A_{11}	A_{12}	A_{13}
$1+C_2$	$\bar{b}_1 + b_1 C_2$	$\bar{b}_2 + b_2 C_2$	$\bar{b}_3 + b_3 C_2$	A_{21}	A_{22}	A_{23}
$1+C_3$	$\bar{b}_1 + b_1 C_3$	$\bar{b}_2 + b_2 C_3$	$\bar{b}_3 + b_3 C_3$	A_{31}	A_{32}	A_{33}
	$\bar{b}_1 + b_1$	$\bar{b}_2 + b_2$	$\bar{b}_3 + b_3$	$\overline{B}_1$	$\overline{B}_2$	$\overline{B}_3$
	b_1	b_2	b_3	B_1	B_2	B_3

Table 3.4: Combined composed table of MS scheme.

where $\bar{b}_i = b_i(1-c_i)$ [23] is a simplifying assumption of RKN methods. The algebraic verification of the order condition related to the tree  by using the compact form of composition Table (3.4) is as follows

$$\begin{aligned}
\sum b_i a_{ij} c_j &= \begin{pmatrix} b_i & B_i \end{pmatrix} \begin{pmatrix} a_{ij} & 0 \\ \bar{b}_i + b_i C_i & A_{ij} \end{pmatrix} \begin{pmatrix} c_i \\ 1 + C_i \end{pmatrix}, \\
&= \begin{pmatrix} b_i a_{ij} + B_i(\bar{b}_i + b_i C_i) & B_i A_{ij} \end{pmatrix} \begin{pmatrix} c_i \\ 1 + C_i \end{pmatrix}, \\
&= b_i a_{ij} c_j + B_i c_i (b_i - b_i c_i + b_i C_i) + B_i A_{ij} + B_i A_{ij} C_j, \\
&= b_i a_{ij} c_j + B_i A_{ij} + b_i c_i B_i C_i - b_i c_i^2 B_i + b_i c_i B_i + B_i A_{ij} C_j, \\
&= \beta_7 + \alpha_4 + \beta_2 \alpha_2 - \beta_3 \alpha_1 + \beta_2 \alpha_1 + \alpha_7,
\end{aligned}$$

$$= \beta\alpha\left(\quad\right). \qquad (3.12)$$

In above verification of different sub-trees of t_7, it should be noted that small letter coefficients are the part of M-method and these sub trees are represented by β_i while coefficient represented by capital letters belong to S-method and there sub-trees are represented by α_i. We shall use same method of pruning of all SN trees up to order 5 for construction of effective order conditions of RKN-method.

3.6 Inverse of RKN method

In the previous section, we have constructed the composition of two RKN methods, which is basically forms a multiplicative operation of RKN group. In this section we are going to present identity element and inverse for an equivalence class of RKN. Here, we consider method M_0 as an identity element that maps an initial value to an equal value provided by a given continuous function keeping h is very small in such a way that for any RKN method M, the composition or multiplicative operations of $[M_0 \cdot M] = [M \cdot M_0] = [M]$. For our convenience, we take this identity class as 1. To prove the existence of identity class, we need to construct an inverse of RKN method M such that the composition of this method with its inverse will lead us to identify an equivalence identity class. For the construction of inverse RKN (M^{-1}), we start from method M and its one step movement as described in equation (3.9). This will lead our initial solution from y_0 to y_1. From this scheme, we shall develop a Butcher's table, which enables to move back from y_1 to initial solution y_0. The procedure starts as follows:

$$M\text{-method:}\quad \begin{array}{c|ccc} c_1 & a_{11} & a_{12} & a_{13} \\ c_2 & a_{21} & a_{22} & a_{23} \\ c_3 & a_{31} & a_{32} & a_{33} \\ \hline & \bar{b}_1 & \bar{b}_2 & \bar{b}_3 \\ \hline & b_1 & b_2 & b_3 \end{array}$$

Now, we first apply M-method using solution scheme (3.4) to update solution from y_0 to y_1 as:

$$K_1 = y_0 + hc_1y_0' + h^2[a_{11}f(K_1) + a_{12}f(K_2) + a_{13}f(K_3)], \tag{3.13}$$

$$K_2 = y_0 + hc_2y_0' + h^2[a_{21}f(K_1) + a_{22}f(K_2) + a_{23}f(K_3)], \tag{3.14}$$

$$K_3 = y_0 + hc_3y_0' + h^2[a_{31}f(K_1) + a_{32}f(K_2) + a_{33}f(K_3)], \tag{3.15}$$

$$y_1 = y_0 + hy_0' + h^2[\bar{b}_1f(K_1) + \bar{b}_2f(K_2) + \bar{b}_3f(K_3)], \tag{3.16}$$

$$y_1' = y_0' + h[b_1f(K_1) + b_2f(K_2) + b_3f(K_3)]. \tag{3.17}$$

From equation (3.17), we get $y_0^{'}$ as

$$y_0^{'} = y_1^{'} - h[b_1 f(K_1) + b_2 f(K_2) + b_3 f(K_3)]. \tag{3.18}$$

From equation (3.16), we take the value of y_0 and place $y_0^{'}$ in it from equation (3.18) as under

$$y_0 = y_1 - hy_0^{'} - h^2[\bar{b}_1 f(K_1) + \bar{b}_2 f(K_2) + \bar{b}_3 f(K_3)],$$
$$y_0 = y_1 - h[y_1^{'} - h[b_1 f(K_1) + b_2 f(K_2) + b_3 f(K_3)]] - h^2[\bar{b}_1 f(K_1) + \bar{b}_2 f(K_2) + \bar{b}_3 f(K_3)],$$
$$y_0 = y_1 - hy_1^{'} - h^2[(b_1 - \bar{b}_1) f(K_1) + (b_2 - \bar{b}_2) f(K_2) + (b_3 - \bar{b}_3) f(K_3)]. \tag{3.19}$$

Now using equations (3.18) and (3.19) in equations (3.13), (3.14) and (3.15), we get

$$K_1^{-1} = y_1 + h(c_1 - 1)y_1^{'} + h^2[(b_1(1 - c_1) - \bar{b}_1 + a_{11}) f(K_1) + \cdots$$
$$(b_2(1 - c_1) - \bar{b}_2 + a_{12}) f(K_2)] + (b_3(1 - c_1) - \bar{b}_3 + a_{13}) f(K_3)], \tag{3.20}$$
$$K_2^{-1} = y_1 + h(c_2 - 1)y_1^{'} + h^2[(b_1(1 - c_2) - \bar{b}_1 + a_{21}) f(K_1) + \cdots$$
$$(b_2(1 - c_2) - \bar{b}_2 + a_{22}) f(K_2)] + (b_3(1 - c_2) - \bar{b}_{23} + a_{23}) f(K_3)], \tag{3.21}$$
$$K_3^{-1} = y_1 + h(c_3 - 1)y_1^{'} + h^2[(b_1(1 - c_3) - \bar{b}_1 + a_{31}) f(K_1) + \cdots$$
$$(b_2(1 - c_3) - \bar{b}_2 + a_{32}) f(K_2)] + (b_3(1 - c_3) - \bar{b}_{33} + a_{33}) f(K_3)]. \tag{3.22}$$

The equations (3.18) to (3.22) forms M^{-1} method and whose Butcher's table is as follows:

$c_1 - 1$	$b_1(1 - c_1) - \bar{b}_1 + a_{11}$	$b_2(1 - c_1) - \bar{b}_2 + a_{12}$	$b_3(1 - c_1) - \bar{b}_3 + a_{13}$
$c_2 - 1$	$b_1(1 - c_2) - \bar{b}_1 + a_{21}$	$b_2(1 - c_2) - \bar{b}_2 + a_{22}$	$b_3(1 - c_2) - \bar{b}_3 + a_{23}$
$c_3 - 1$	$b_1(1 - c_3) - \bar{b}_1 + a_{31}$	$b_2(1 - c_3) - \bar{b}_2 + a_{32}$	$b_3(1 - c_3) - \bar{b}_3 + a_{33}$
	$b_1 - \bar{b}_1$	$b_2 - \bar{b}_2$	$b_3 - \bar{b}_3$
	$-b_1$	$-b_2$	$-b_3$

Table 3.5: Inverse of RKN of order 3.

The general form of inverse of RKN method for s-stages is represented by following Butcher's table:

c_1-1	$b_1(1-c_1)-\overline{b}_1+a_{11}$	$b_2(1-c_1)-\overline{b}_2+a_{12}$	$\cdots$	$b_s(1-c_1)-\overline{b}_s+a_{1s}$
c_2-1	$b_1(1-c_2)-\overline{b}_1+a_{21}$	$b_2(1-c_2)-\overline{b}_2+a_{22}$	$\cdots$	$b_s(1-c_2)-\overline{b}_s+a_{2s}$
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
c_s-1	$b_1(1-c_s)-\overline{b}_1+a_{s1}$	$b_2(1-c_s)-\overline{b}_2+a_{s2}$	$\cdots$	$b_3(1-c_s)-\overline{b}_s+a_{ss}$
	$b_1-\overline{b}_1$	$b_2-\overline{b}_2$	$\cdots$	$b_s-\overline{b}_s$
	$-b_1$	$-b_2$	$\cdots$	$-b_s$

Table 3.6: General form of s-stage inverse RKN.

The table above holds the consistency conditions $\sum \frac{c_i^2}{2} = \sum a_{ij}$ by using RKN conditions $\sum \overline{b_i} = \frac{1}{2}$ and $\sum b_i = 1$. This method reverse the action of method M, so it is denoted by M^{-1} and composition of this inverse method with M-method will result as identity equivalence class. The following theorem will prove this result.

Theorem 1. *Let M denotes an RKN-method, then* $[M \cdot M^{-1}] = [M^{-1} \cdot M] = 1$

Proof. First, we present the composition of MM^{-1} by placing the values of y_1 and $y_1^{'}$ from equations (3.16) and (3.17) of M-method in equations (3.20) to (3.22) for stages along with in equations (3.18) and (3.19) for b^T and $\overline{b}^T$ of M^{-1} method, respectively. This will give us composition of MM^{-1} for three stages and is complied in the following butcher's table.

c_1	a_{11}	a_{12}	a_{13}	0	0	0
c_2	a_{21}	a_{22}	a_{23}	0	0	0
c_3	a_{31}	a_{32}	a_{33}	0	0	0
c_1	$\overline{b}_1+b_1(c_1-1)$	$\overline{b}_2+b_2(c_1-1)$	$\overline{b}_3+b_3(c_1-1)$	$b_1(1-c_1)-\overline{b}_1+a_{11}$	$b_2(1-c_1)-\overline{b}_2+a_{12}$	$b_3(1-c_1)-\overline{b}_3+a_{13}$
c_2	$\overline{b}_1+b_1(c_2-1)$	$\overline{b}_2+b_2(c_2-1)$	$\overline{b}_3+b_3(c_2-1)$	$b_1(1-c_2)-\overline{b}_1+a_{21}$	$b_2(1-c_2)-\overline{b}_2+a_{22}$	$b_3(1-c_2)-\overline{b}_3+a_{23}$
c_3	$\overline{b}_1+b_1(c_3-1)$	$\overline{b}_2+b_2(c_3-1)$	$\overline{b}_3+b_3(c_3-1)$	$b_1(1-c_3)-\overline{b}_1+a_{31}$	$b_2(1-c_3)-\overline{b}_2+a_{32}$	$b_3(1-c_3)-\overline{b}_3+a_{33}$
	$\overline{b}_1+b_1$	$\overline{b}_2+b_2$	$\overline{b}_3+b_3$	$b_1-\overline{b}_1$	$b_2-\overline{b}_2$	$b_3-\overline{b}_3$
	b_1	b_2	b_3	$-b_1$	$-b_2$	$-b_3$

Table 3.7: Composition table of MM^{-1}.

Now, for the composition of $M^{-1}M$, we start from equations (3.18) and (3.19) by taking the values of y_0' and y_0 from M^{-1} method and placing it in equations (3.13) to (3.17) to get composed form of $M^{-1}M$ and is represented in the following Butcher's table.

c_1-1	$b_1(1-c_1)-\bar{b}_1+a_{11}$	$b_2(1-c_1)-\bar{b}_2+a_{12}$	$b_3(1-c_1)-\bar{b}_3+a_{13}$	0	0	0
c_2-1	$b_1(1-c_2)-\bar{b}_1+a_{21}$	$b_2(1-c_2)-\bar{b}_2+a_{22}$	$b_3(1-c_2)-\bar{b}_3+a_{23}$	0	0	0
c_3-1	$b_1(1-c_3)-\bar{b}_1+a_{31}$	$b_2(1-c_3)-\bar{b}_2+a_{32}$	$b_3(1-c_3)-\bar{b}_3+a_{33}$	0	0	0
c_1-1	$b_1(c_1-1)-\bar{b}_1$	$b_2(c_1-1)-\bar{b}_2$	$b_3(c_1-1)-\bar{b}_3$	a_{11}	a_{12}	a_{13}
c_2-1	$b_1(c_2-1)-\bar{b}_1$	$b_2(c_2-1)-\bar{b}_2$	$b_3(c_2-1)-\bar{b}_3$	a_{21}	a_{22}	a_{23}
c_3-1	$b_1(c_3-1)-\bar{b}_1$	$b_2(c_3-1)-\bar{b}_2$	$b_3(c_3-1)-\bar{b}_3$	a_{31}	a_{32}	a_{33}
	$-\bar{b}_1$	$-\bar{b}_2$	$-\bar{b}_3$	b_1	b_2	b_3
	$-b_1$	$-b_2$	$-b_3$	b_1	b_2	b_3

Table 3.8: Composition table of $M^{-1}M$.

Each of above composition is P-reducible to M and M^{-1}, respectively, as $(\sum a_{ij})_M = (\sum a_{ij})_{M^{-1}}$ and $(\sum b_i)_M = (\sum b_i)_{M^{-1}}$ for each composition. Thus each method lies in equivalence class 1. $\square$

3.7 Effective order conditions of RKN methods

For the construction of effective order RKN methods up to certain accuracy, we need starting and finishing RKN methods, both of which are applied only once. A RKN method M of classical order q needs starting method S and a finishing method S^{-1} so that SMS^{-1} has the required effective order q. This in turn implies the following relationship must be established for all trees up to order q as shown in Table 3.9.

$$\beta\alpha(t) = E\beta(t),$$

where E represents the exact flow and is given as

$$E(t) = \frac{1}{\gamma(t)},$$

where $\gamma(t)$ is the density of tree t.

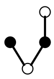
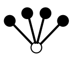
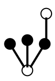
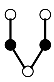
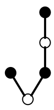
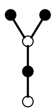
t_i	tree	$(\beta\alpha)(t_i)$	$(E\beta)(t_i)$
t_1		$\beta_1 + \alpha_1$	$1 + \beta_1$
t_2		$\beta_2 + \alpha_1 + \alpha_2$	$\frac{1}{2} + \beta_1 + \beta_2$
t_3		$\beta_3 + 2\alpha_2 + \alpha_1 + \alpha_3$	$\frac{1}{3} + \beta_1 + 2\beta_2 + \beta_3$
t_4		$\beta_4 + \alpha_2\beta_1 + \alpha_1\beta_1 - \alpha_1\beta_2 + \alpha_4$	$\frac{1}{6} + \frac{1}{2}\beta_1 + \beta_2 + \beta_4$
t_5		$\beta_5 + 3\alpha_3 + 3\alpha_2 + \alpha_1 + \alpha_5$	$\frac{1}{4} + \beta_1 + 3\beta_2 + 3\beta_3 + \beta_5$
t_6		$\beta_6 + \beta_1\alpha_3 + 2\beta_1\alpha_2 + \beta_2\alpha_2 + \alpha_4 + \beta_1\alpha_1 - \beta_2\alpha_1 + \alpha_6$	$\frac{1}{8} + \frac{1}{2}\beta_1 + \frac{3}{2}\beta_2 + \beta_3 + \beta_4 + \beta_6$
t_7		$\beta_7 + \alpha_4 + \beta_2\alpha_2 - \beta_3\alpha_1 + \beta_2\alpha_1 + \alpha_7$	$\frac{1}{24} + \frac{1}{6}\beta_1 + \frac{1}{2}\beta_2 + \beta_4 + \beta_8$
t_8		$\beta_8 + 4\alpha_5 + 6\alpha_3 + 4\alpha_2 + \alpha_1 + \alpha_8$	$\frac{1}{5} + \beta_1 + 4\beta_2 + 6\beta3 + 4\beta_5 + \beta_8$
t_9		$\beta_9 + \beta_1\alpha_5 + 3\beta_1\alpha_3 - \beta_2\alpha_3 + 2\alpha_6 + \alpha_4 + 3\beta_1\alpha_2 - 2\beta_2\alpha_2 \cdots$ $+\beta_1\alpha_1 - \beta_2\alpha_1 + \alpha_9$	$\frac{1}{10} + \frac{1}{2}\beta_1 + 2\beta_2 + \frac{5}{2}\beta3 + \beta_4 + \beta_5 + 2\beta_6 + \beta_9$
t_{10}		$\beta_{10} + 2\beta_1\alpha_6 + 2\beta_1\alpha_4 - 2\beta_2\alpha_4 + \beta_1^2\alpha_3 + 2\beta_1^2\alpha_2 \cdots$ $-2\beta_1\beta_2\alpha_2 + \beta_1^2\alpha_1 - 2\beta_1\beta_2\alpha_1 + \beta_2^2\alpha_1 + \alpha_{10}$	$\frac{1}{20} - \frac{1}{4}\beta_1 + \beta_2 + \beta3 + \beta_4 + 2\beta_6 + \beta_{10}$
t_{11}		$\beta_{11} + \alpha_7 + \alpha_6 + \alpha_4 + \beta_2\alpha_3 + 2\beta_2\alpha_2 - \beta_3\alpha_2 + \beta_2\alpha_1 - \beta_3\alpha_1 + \alpha_{11}$	$\frac{1}{30} + \frac{1}{6}\beta_1 + \frac{2}{3}\beta_2 + \frac{1}{2}\beta3 + \beta_4 + \beta_6 + \beta_7 + \beta_{11}$
t_{12}		$\beta_{12} + 2\alpha_7 + \alpha_4 + \beta_3\alpha_2 + \beta_3\alpha_1 - \beta_5\alpha_1 + \alpha_{12}$	$\frac{1}{60} + \frac{1}{12}\beta_1 + \frac{1}{3}\beta_2 + \beta_4 + 2\beta_7 + \beta_{12}$
t_{13}		$\beta_{13} + \beta_1\alpha_7 + \beta_1\alpha_4 - \beta_2\alpha_4 + \beta_4\alpha_2 + \beta_4\alpha_1 - \beta_7\alpha_1 + \alpha_{13}$	$\frac{1}{120} + \frac{1}{8}\beta_1 + \frac{1}{6}\beta_2 + \frac{1}{2}\beta_4 + \beta_7 + \beta_{13}$

Table 3.9: $\beta\alpha$ and $E\beta$ for trees up to order 5.

Comparison of the last two columns of Table 3.9 results in effective order conditions containing $\alpha's$ in terms of $\beta's$ and with the help of these conditions we can calculate starting and main methods of different order. A complete list of effective order conditions for all trees of order up to 5 is provided in Table 3.10.

q	Effective order conditions
1	$\alpha_1 = 1$
2	$\alpha_2 = \beta_1 - \frac{1}{2}$
3	$\alpha_3 = \frac{1}{3} + 2\beta_2 - \beta_1$
	$\alpha_4 = \frac{1}{6} + 2\beta_2 - \beta_1^2$
4	$\alpha_5 = -\frac{1}{4} + 3\beta_3 - 3\beta_2 + \beta_1$
	$\alpha_6 = -\frac{1}{24} + \beta_4 + \beta_3 + \frac{1}{6}\beta_1 - \beta_1\beta_2$
	$\alpha_7 = -\frac{3}{24} + \beta_4 + \beta_3 - 2\beta_2 + \frac{1}{6}\beta_1 + \beta_1^2 - \beta 1\beta_2$
5	$\alpha_8 = \frac{1}{5} + 4\beta_5 - 6\beta 3 + 4\beta_2 - \beta_1$
	$\alpha_9 = \frac{1}{60} + 2\beta_6 + \beta_5 - \beta_4 + \frac{1}{2}\beta 3 + \frac{1}{3}\beta_2 - \frac{1}{12}\beta_1 + 2\beta_2^2 - 3\beta_1\beta_3$
	$\alpha_{10} = \frac{1}{20} - 3\beta_2\beta_1 + 2\beta_6 + 3\beta_2^2 - 2\beta_1\beta_3 + \beta_1^3 - \frac{2}{3}\beta_1^2 + \beta_4 + \beta_3 - 2\beta_1\beta_4 + \frac{4}{3}\beta_2$
	$\alpha_{11} = \frac{1}{30} + \beta_7 + \beta_6 - \beta_4 - \beta_3 + \frac{1}{3}\beta 2 - \frac{1}{6}\beta 1 + \beta_2\beta_1 + \beta_1\beta_3 - 2\beta_2^2$
	$\alpha_{12} = \frac{1}{10} + 2\beta_7 - \beta_4 + \frac{7}{3}\beta 2 - \frac{1}{4}\beta_1 - \frac{5}{2}\beta_3 + \beta_5 - \beta_1\beta_3 - \beta_1^2 + 2\beta_2\beta_1$
	$\alpha_{13} = \frac{1}{120} + 2\beta_7 + \frac{1}{3}\beta_2 + \frac{1}{12}\beta_1 - 2\beta_1\beta_4 + 2\beta_2^2 - \frac{1}{6}\beta_1^2 - \beta_1\beta_3$

Table 3.10: Effective order conditions up to order 5 on α in terms of β .

We can obtain RKN methods M, S and S^{-1} by carefully selecting different values of β to ensure classical order p for the main method M and effective order q for the composition SMS^{-1} as given in Table 3.11.

q	p	Order conditions for main method	Order conditions for starting method
3	2	$\alpha_1 = 1, \alpha_2 = \frac{1}{2}, 6(\alpha_3 - \alpha_4) = 1$	$\beta_1 = 1, \quad \beta_2 = \frac{1}{2}\alpha_3 + \frac{1}{3}$
4	2	$\alpha_1 = 1, \alpha_2 = \frac{1}{2}, 6\alpha_3 - 6\alpha_4 = 1,$ $4\alpha_7 - 4\alpha_6 + 4\alpha_3 = 1,$	$\beta_1 = 1, \beta_2 = \frac{1}{3} + \frac{1}{2}\alpha_3,$ $\beta_3 = \frac{1}{12} + \frac{1}{2}\alpha_3 + \frac{1}{3}\alpha_5,$ $\beta_4 = \frac{1}{8} - \frac{1}{3}\alpha_5 + \alpha_6,$
4	3	$\alpha_1 = 1, \alpha_2 = \frac{1}{2}, \alpha_3 = \frac{1}{3}, \alpha_4 = \frac{1}{6}$ $12\alpha_6 - 12\alpha_7 = 1,$	$\beta_1 = 1, \beta_2 = \frac{1}{2}, \beta_3 = \frac{1}{4} + \frac{1}{3}\alpha_5$ $\beta_3 = \frac{1}{4} + \frac{1}{3}\alpha_5$ $\beta_4 = \frac{1}{8} - \frac{1}{3}\alpha_5 + \alpha_6$
5	2	$\alpha_1 = 1, \alpha_2 = \frac{1}{2}$ $36\alpha_{10} - 36\alpha_9 + 9\alpha_8 + 6\alpha_3 - 9\alpha_3^2 = 1$ $30\alpha_{12} - 60\alpha_{11} + 30\alpha_9 - 15\alpha_8 \cdots$ $+30\alpha_5 - 15\alpha_3 - 45\alpha_3^2 = -4$ $180\alpha_{13} - 360\alpha_{11} + 180\alpha_9 - 45\alpha_8 \cdots$ $+180\alpha_6 + 60\alpha_5 - 30\alpha_3 360\alpha_3^2 = -14$	$\beta_1 = 1, \beta_2 = \frac{1}{3} + \frac{1}{2}\alpha_3$ $\beta_3 = \frac{1}{12} + \frac{1}{2}\alpha_3 + \frac{1}{3}\alpha_5$ $\beta 4 = \frac{1}{8} - \frac{1}{3}\alpha_5 + \alpha_6$ $\beta_5 = -\frac{1}{120}\frac{1}{4}\alpha_8 + \frac{1}{4}\alpha_3 + \frac{1}{2}\alpha_5$ $\beta_6 = \frac{3}{80} + \frac{1}{2}\alpha_6 - \frac{1}{8}\alpha_8 + \frac{1}{12}\alpha_3 - \frac{1}{4}\alpha_3^2 + \frac{1}{2}\alpha_9$ $\beta_7 = -\frac{1}{720} - \frac{1}{12}\alpha_3 + \frac{1}{2}\alpha_6 + \frac{1}{8}\alpha_8 \cdots$ $+\frac{3}{4}\alpha_3^2 - \frac{1}{2}\alpha_9 - \frac{1}{3}\alpha 5 + \alpha_{11}$
5	3	$\alpha_1 = 1, \alpha_2 = \frac{1}{2}, \alpha_3 = \frac{1}{3}, \alpha_4 = \frac{1}{6}$ $12\alpha_7 - 12\alpha_6 = -1; 4\alpha_{10} - 4\alpha_9 + \alpha_8 = 0;$ $10\alpha_{12} - 20\alpha_{11} + 10\alpha_9 - 5\alpha_8 + 10\alpha_5 = 2$ $60\alpha_{13} - 120\alpha_{11} + 60\alpha_9 - 15\alpha_8 + 60\alpha_6 + 20\alpha_5 = 12$	$\beta_1 = 1, \beta_2 = \frac{1}{2}, \beta_3 = \frac{1}{4} + \frac{1}{3}\alpha_5, \beta_4 = \frac{1}{8} - \frac{1}{3}\alpha_5 + \alpha_6,$ $\beta_5 = \frac{3}{40} + \frac{1}{2}\alpha 5 + \frac{1}{4}\alpha_8$ $\beta_6 = \frac{1}{2}\alpha_9 + \frac{3}{80} - \frac{1}{8}\alpha_8 + \frac{1}{2}\alpha_6$ $\beta_7 = \frac{13}{240} + \frac{1}{2}\alpha_6 - \frac{1}{2}\alpha_9 + \frac{1}{8}\alpha 8 - \frac{1}{3}\alpha_5 + \alpha_{11}$
5	4	$\alpha_1 = 1, \alpha_2 = \frac{1}{2}, \alpha_3 = \frac{1}{3}, \alpha_4 = \frac{1}{6},$ $\alpha_5 = \frac{1}{4}, \alpha_6 = \frac{1}{8}, \alpha_7 = \frac{1}{24}$ $4\alpha_{10} - 4\alpha_9 + \alpha_8 = 0$ $20\alpha_{12} - 40\alpha_{11} + 20\alpha_9 - 10\alpha_8 = -1,$ $120\alpha_{13} - 240\alpha_{11} + 120\alpha_9 - 30\alpha_8 = -1$	$\beta_1 = 1, \beta_2 = \frac{1}{2}, \beta_3 = \frac{1}{3}; \beta_4 = \frac{1}{6}$ $\beta_5 = \frac{1}{5} + \frac{1}{4}\alpha_8,$ $\beta_6 = \frac{1}{10} - \frac{1}{8}\alpha_8 + \frac{1}{2}\alpha_9$ $\beta_7 = \frac{1}{30} + \alpha_{11} + \frac{1}{8}\alpha 8 - \frac{1}{2}\alpha_9$

Table 3.11: Effective order q, classical order p conditions for main and starting methods.

3.8 Conclusions

In this chapter, we extended the idea of effective order to RKN methods and provided a classification of effective order conditions up to order 5. Explanation regarding the group structure of RKN methods is discussed by using composition and inverse of RKN method. Existence of identity class is also proved through composition of RKN method with its inverse.

Chapter 4

The effective order methods for PRK method

In Chapter 2, we discussed the effective order techniques for RK methods. In this chapter, we shall apply those techniques to construct effective order of Partitioned Runge-Kutta (PRK) methods, symplectic and mutually adjoint PRK methods for Hamiltonian type systems of differential equations. Thus for the effective order PRK methods, we construct two main methods together with two starting and two finishing methods. The conditions for effective order up to 5 are derived in this chapter. With these conditions we can construct methods with effective order $2 \leq q \leq 5$ such that the main method has classical order $2 \leq p \leq 4$. Moreover, we have constructed an effective order 4 method with 3 stages. This results in obvious reduction of the implementation cost because, order 4 RK methods require 4 stages and it is a well known fact that if a PRK method is of order 4, both RK methods that comprise the PRK method will be of order 4 and hence requires 4 stages [21, 34]. Also, a family of explicit symplectic and mutually adjoint symplectic PRK methods are derived with effective order 3 for the numerical integration of the separable Hamiltonian systems. The numerical experiments on these systems through explicit symplectic and mutually adjoint symplectic PRK methods confirm good energy conservation, which confirms the efficiency of these methods.

4.1 Algebraic structure of PRK methods

Consider a separable system of initial value problem

$$\begin{pmatrix} y \\ z \end{pmatrix}' = \begin{pmatrix} f(z) \\ g(y) \end{pmatrix}, \qquad y(x_0) = y_0, \quad z(x_0) = z_0. \tag{4.1}$$

Such systems arise frequently in Hamiltonian Mechanics. In order to solve such systems, it is natural to use PRK methods for the numerical approximation. Thus, we take two s-stages RK methods $M = [A \;\; b \;\; c]$ and $\tilde{M} = [\tilde{A} \;\; \tilde{b} \;\; \tilde{c}]$ and solve system (4.1) such that the y-components are numerically integrated by M and the z-components with $\widetilde{M}$ as follows

$$\begin{aligned} Y_i &= y_n + h\sum_{j=1}^{s-1} a_{ij} f(Z_j), \qquad Z_i = z_n + h\sum_{j=1}^{s} \widetilde{a}_{ij} g(Y_j) \quad i = 1, 2, ..., s, \\ y_{n+1} &= y_n + h\sum_{j=1}^{s} b_j f(Z_j), \quad z_{n+1} = z_n + h\sum_{j=1}^{s} \widetilde{b}_j g(Y_j), \end{aligned} \tag{4.2}$$

where, Y_i and Z_i are the stages for the y and z variables, b_i and $\widetilde{b}_i$ are quadrature weights, c_i and $\widetilde{c}_i$ are quadrature nodes, $a = (a_{ij})_{s\times s}$ and $\widetilde{a} = (\widetilde{a}_{ij})_{s\times s}$ are matrices of s-stage PRK methods. The Butcher tableaux for: PRK methods are

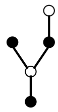
$$\begin{array}{c|c} \text{c} & \text{a} \\ \hline & b^T \end{array}, \qquad \begin{array}{c|c} \widetilde{c} & \widetilde{a} \\ \hline & \widetilde{b}^T \end{array}.$$

4.2 Order conditions and bi-color rooted trees

A rooted tree is a non-cyclic graph containing vertices and edges with one vertex acting as a root. A bi-color rooted tree is a rooted tree such that vertices can either be black or white in color. Bi-color rooted trees with black vertex as root is represented by t whereas $\tilde{t}$ represents bi-color rooted trees with white vertex as root.

Order: The total number of vertices in a bi-color tree is the order of the tree and is represented by $r(t)$.

Density: The density$\gamma(t)$ is a recursive relation computed as a product of the order of a bi-color rooted tree and the densities of the sub trees after pruning the root.

Example: Consider the bi-color tree  with $r(t) = 5$, $\gamma(t) = 5 \times 4 \times 2 = 40$.
Order conditions: By comparing the numerical solutions in equation (4.2) with Taylor's series of the exact solution, we obtain order conditions that must be satisfied to derive practical numerical methods. In order to understand this, we investigate the connection between the derivatives of the exact solution and the bi-color rooted trees. The derivatives of the exact solution are:

$$\begin{aligned} y^{(1)} &= f(z), & z^{(1)} &= g(y), \\ y^{(2)} &= \frac{\partial f}{\partial z} g, & z^{(2)} &= \frac{\partial g}{\partial y} f, \\ y^{(3)} &= \frac{\partial^2 f}{\partial z\, \partial z}(g, g) + \frac{\partial f}{\partial z}\frac{\partial g}{\partial y} f, & z^{(3)} &= \frac{\partial^2 g}{\partial y\, \partial y}(f, f) + \frac{\partial g}{\partial y}\frac{\partial f}{\partial z} g, \\ &\vdots & &\vdots \end{aligned} \tag{4.3}$$

We can represent these formulas graphically using bi-color rooted trees. Thus f is represented by a black vertex and g is represented by a white vertex. The differentiation is represented by an edge. Since we are only considering differential equations of the type equation (4.1), where f depends only on z and g depends only on y. Therefore, we only consider trees in which a black vertex has a white child and vice versa. Such trees are given in Table 4.3 and Table 4.4. The quantities on the right hand side of equation (4.3) are termed as elementary differentials and can be represented by bi-color rooted trees as shown in Table 4.1.

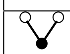
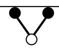
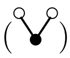
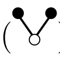
t	Elementary differentials	$\Phi(t)$	$\tilde{t}$	Elementary differentials	$\Phi(\tilde{t})$
●	f	b_i	○	g	$\tilde{b}_i$
	$\frac{\partial f}{\partial z} g$	$b_i \tilde{c}_i$		$\frac{\partial g}{\partial y} f$	$\tilde{b}_i c_i$
	$\frac{\partial^2 f}{\partial z\, \partial z}(g, g),$	$b_i \tilde{c}_i^2,$		$\frac{\partial^2 g}{\partial y\, \partial y}(f, f)$	$\tilde{b}_i c_i^2$
	$\frac{\partial f}{\partial z}\frac{\partial g}{\partial y} f$	$b_i \tilde{a}_{ij} c_j$		$\frac{\partial g}{\partial y}\frac{\partial f}{\partial z} g$	$\tilde{b}_i a_{ij} \tilde{c}_j$

Table 4.1: Elementary differentials and elementary weights of bi-color rooted trees.

The elementary weights $\Phi(t)$ and $\Phi(\tilde{t})$ are nonlinear expressions of the coefficients of PRK methods and can be related to bi-color rooted trees as shown in Table 4.1 [11, 21]. A PRK method is of order p iff

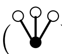
$$\Phi(t) = \frac{1}{\gamma(t)}, \qquad \text{and} \qquad \Phi(\tilde{t}) = \frac{1}{\gamma(\tilde{t})}.$$

for all bi-color rooted trees t and $\tilde{t}$ of order $\leq$p.
Basically, RK methods belong to an algebraic group G whose elements are functions acting on rooted trees. Corresponding to the methods M and $\widetilde{M}$, we define functions $\alpha, \widetilde{\alpha} \in G$ which maps trees to algebraic expressions in the coefficients of the PRK methods, known as elementary weights. The function α acts on trees t and the function $\widetilde{\alpha}$ acts on trees $\widetilde{t}$. For particular t_i & $\widetilde{t}_i$, $\alpha(t_i) = \alpha_i$ and $\widetilde{\alpha}(\widetilde{t}_i) = \widetilde{\alpha}_i$, such that,

$\alpha($  $) = \sum b_i \bar{c}_i{}^2, \qquad \widetilde{\alpha}($  $) = \sum \widetilde{b}_i c_i{}^2.$

4.2.1 Composition of PRK methods

We can define composition of two PRK methods in terms of their functions from group G. Let $\alpha, \widetilde{\alpha}, \beta, \widetilde{\beta} \in G$ corresponding to methods $M, \widetilde{M}, S, \widetilde{S}$, respectively. Multiplicative group operations $\beta\alpha$ and $\widetilde{\beta}\widetilde{\alpha}$ can be defined and we have

$\beta\alpha($  $) = \beta_5 + 3\widetilde{\beta}_1\alpha_3 + 3\widetilde{\beta}_1^2\alpha_2 + \widetilde{\beta}_1^3\alpha_1 + \alpha_5.$ (4.4)

The terms on the right hand side of equation (4.4) are obtained from Table 4.2. Here we have trees t, u, and $t \setminus u$. The tree u is a sub tree of tree t, and $t \setminus u$ is the remaining set of trees when u is chopped off t. We can look at the composition

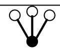
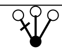
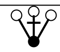
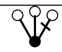
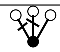
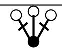
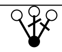
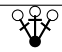
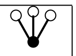
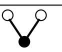
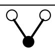
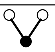
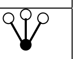
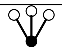
t									
u									
$t \setminus u$		$\circ$	$\circ$	$\circ$	$\circ\circ$	$\circ\circ$	$\circ\circ$	$\circ\circ\circ$	
term	β_5	$\widetilde{\beta}_1\alpha_3$	$\widetilde{\beta}_1\alpha_3$	$\widetilde{\beta}_1\alpha_3$	$\widetilde{\beta}_1^2\alpha_2$	$\widetilde{\beta}_1^2\alpha_2$	$\widetilde{\beta}_1^2\alpha_2$	$\widetilde{\beta}_1^3\alpha_1$	α_5

Table 4.2: Calculation for the term $\beta\alpha(t_5)$.

of PRK methods by considering their Butcher tableaux as follows: Let M, $\widetilde{M}$, S and, $\widetilde{S}$ have Butcher tableaux:

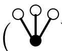
$$
\begin{array}{c|c} \mathrm{c} & \mathrm{a} \\ \hline & b^T \end{array}, \quad
\begin{array}{c|c} \widetilde{c} & \widetilde{a} \\ \hline & \widetilde{b}^T \end{array}, \quad
\begin{array}{c|c} C & A \\ \hline & B^T \end{array}, \quad \text{and} \quad
\begin{array}{c|c} \widetilde{C} & \widetilde{A} \\ \hline & \widetilde{B}^T \end{array}.
$$

The Butcher tableaux for the composition of MS and $\widetilde{M}\widetilde{S}$ are:

$$
\begin{array}{c|cc} c & \mathrm{a} & 0 \\ C + \sum_{i=1}^{s} b_i & b & A \\ \hline & b^T & B^T \end{array}, \quad
\begin{array}{c|cc} \widetilde{c} & \widetilde{a} & 0 \\ \widetilde{C} + \sum_{i=1}^{s} \widetilde{b}_i & \widetilde{b} & \widetilde{A} \\ \hline & \widetilde{b}^T & \widetilde{B}^T \end{array}.
$$

For the composed PRK method, the order condition related to tree  is

$$
\begin{aligned}
b_i\widetilde{c}_i^3 + B_i(\widetilde{C}_i + \widetilde{b}_i)^3 &= b_i\widetilde{c}^3 + 3B_i\widetilde{C}^2\widetilde{b}_i + 3B_i\widetilde{C}_i\widetilde{b}_i^2 + B_i\widetilde{b}_i^3 + B_i\widetilde{C}_i^3, \\
&= \beta_5 + 3\widetilde{\beta}_1\alpha_3 + 3\widetilde{\beta}_1^2\alpha_2 + \widetilde{\beta}_1^3\alpha_1 + \alpha_5, \\
&= \beta\alpha(\text{tree}).
\end{aligned}
$$



4.3 Effective order of PRK methods

A Runge-Kutta method M has an effective order p if there exists a starting method S and a finishing method S^{-1} such that SMS^{-1} has the required order p [9]. For PRK methods, we want to construct two methods M and $\widetilde{M}$ together with two starting methods S and $\widetilde{S}$ and two finishing methods S^{-1} and $\widetilde{S}^{-1}$ in such a way that SMS^{-1} and $\widetilde{S}\widetilde{M}\widetilde{S}^{-1}$ have the required effective order. The starting methods S and $\widetilde{S}$ do not advance the solution but only act as perturbations and are applied only once. The main methods M and $\widetilde{M}$ are then applied for n number of iterations followed by finishing methods S^{-1} and $\widetilde{S}^{-1}$ applied at the end only once to undo the effects of starting methods. The existence of inverse methods S^{-1} and $\widetilde{S}^{-1}$ is guaranteed because RK methods form a group [11].
In order to calculate effective order conditions, we compute $\beta\alpha(t)$, $E\beta(t)$, $\widetilde{\beta}\widetilde{\alpha}(\widetilde{t})$, $E\widetilde{\beta}(\widetilde{t})$ in Table 4.3 and Table 4.4, where E is the exact flow given as

$$
E(t) = \frac{1}{\gamma(t)},
$$

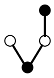
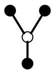
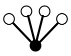
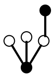
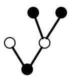
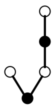
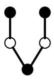
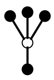
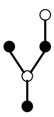
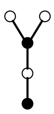
t_i	tree	$(\beta\alpha)(t_i)$	$(E\beta)(t_i)$
t_1		$\beta_1 + \alpha_1$	$1 + \beta_1$
t_2		$\beta_2 + \widetilde{\beta}_1\alpha_1 + \alpha_2$	$\frac{1}{2} + \beta_1 + \beta_2$
t_3		$\beta_3 + \widetilde{\beta}_1^2\alpha_1 + 2\widetilde{\beta}_1\alpha_2 + \alpha_3$	$\frac{1}{3} + \beta_1 + 2\beta_2 + \beta_3$
t_4		$\beta_4 + \beta_1\alpha_2 + \widetilde{\beta}_2\alpha_1 + \alpha_4$	$\frac{1}{6} + \frac{1}{2}\beta_1 + \beta_2 + \beta_4$
t_5		$\beta_5 + 3\widetilde{\beta}_1\alpha_3 + 3\widetilde{\beta}_1^2\alpha_2 + \widetilde{\beta}_1^3\alpha_1 + \alpha_5$	$\frac{1}{4} + \beta_1 + 3\beta_2 + 3\beta_3 + \beta_5$
t_6		$\beta_6 + \widetilde{\beta}_1\alpha_4 + \widetilde{\beta}_2\alpha_2 + \beta_1\alpha_3 + \widetilde{\beta}_1\widetilde{\beta}_2\alpha_1 + \widetilde{\beta}_1\beta_1\alpha_2 + \alpha_6$	$\frac{1}{8} + \frac{1}{2}\beta_1 + \frac{3}{2}\beta_2 + \beta_3 + \beta_4 + \beta_6$
t_7		$\beta_7 + \widetilde{\beta}_3\alpha_1 + 2\beta_1\alpha_4 + \beta_1^2\alpha_2 + \alpha_7$	$\frac{1}{12} + \frac{1}{3}\beta_1 + \beta_2 + 2\beta_4 + \beta_7$
t_8		$\beta_8 + \widetilde{\beta}_4\alpha_1 + \beta_2\alpha_2 + \widetilde{\beta}_1\alpha_4 + \alpha_8$	$\frac{1}{24} + \frac{1}{6}\beta_1 + \frac{1}{2}\beta_2 + \beta_4 + \beta_8$
t_9		$\beta_9 + 4\widetilde{\beta}_1\alpha_5 + 6\widetilde{\beta}_1^2\alpha_3 + 4\widetilde{\beta}_1^3\alpha_2 + \widetilde{\beta}_1^4\alpha_1 + \alpha_9$	$\frac{1}{5} + 4\beta_5 + 6\beta_3 + 4\beta_2 + \beta_1 + \beta_9$
t_{10}		$\beta_{10} + \widetilde{\beta}_2\alpha_3 + 2\widetilde{\beta}_1\alpha_6 + \widetilde{\beta}_1\alpha_5 + \widetilde{\beta}_1^2\alpha_4 + 2\widetilde{\beta}_1\widetilde{\beta}_2\alpha_2$ $+2\widetilde{\beta}_1\beta_1\alpha_3 + \widetilde{\beta}_1^2\widetilde{\beta}_2\alpha_1 + \widetilde{\beta}_1^2\beta_2\alpha_2 + \alpha_{10}$	$\frac{1}{10} + \frac{5}{2}\beta_3 + 2\beta_6 + \beta_5$ $+\beta_4 + 2\beta_2 + \frac{1}{2}\beta_1 + \beta_{10}$
t_{11}		$\beta_{11} + \widetilde{\beta}_1\alpha_7 + \widetilde{\beta}_3\alpha_2 + 2\beta_1\alpha_6 + 2\widetilde{\beta}_1\beta 1\alpha_4$ $+\widetilde{\beta}_1\widetilde{\beta}_3\alpha_1 + \beta_1^2\alpha_3 + \widetilde{\beta}_1\beta_1^2\alpha_2 + \alpha_{11}$	$\frac{1}{15} + \beta_7 + \frac{4}{3}\beta_2 + 2\beta_6 + 2\beta_4$ $+\frac{1}{3}\beta_1 + \beta_3 + \beta_{11}$
t_{12}		$\beta_{12} + \widetilde{\beta}_1\alpha_8 + \widetilde{\beta}_4\alpha_2 + \beta_2\alpha_3 + \widetilde{\beta}_2\alpha_6 + \widetilde{\beta}_1\widetilde{\beta}_4\alpha_1$ $+\widetilde{\beta}_1\beta_1^2\alpha_2 + \widetilde{\beta}_1^2\alpha_4 + \alpha_{12}$	$\frac{1}{30} + \beta_8 + \frac{2}{3}\beta_2 + \frac{1}{2}\beta_3 + \beta_6$ $+\frac{1}{6}\beta_1 1 + \beta_4 + \beta_{12}$
t_{13}		$\beta_{13} + 2\beta_1\alpha_6 + 2\widetilde{\beta}_2\alpha_4 + 2\beta_1\widetilde{\beta}_2\alpha_2 + \beta_1^2\alpha_3 + \widetilde{\beta}_2^2\alpha_1 + \alpha_{13}$	$\frac{1}{20} + 2\beta_6 + \beta_4 + \beta_2 + \beta_3 + \frac{1}{4}\beta_1 + \beta_{13}$
t_{14}		$\beta_{14} + \widetilde{\beta}_5\alpha_1 + 3\beta_1\alpha_7 + 3\beta_1^2\alpha_4 + \beta_1^3\alpha_2 + \alpha_{14}$	$\frac{1}{20} + \frac{1}{4}\beta_1 + 3\beta_7 + 3\beta_4 + \beta_2 + \beta_{14}$
t_{15}		$\beta_{15} + \widetilde{\beta}_6\alpha_1 + \beta_2\alpha_4 + \beta_1\alpha_8 + \widetilde{\beta}_1\alpha_7 + \beta_1\widetilde{\beta}_1\alpha_4 + \beta_1\beta_2\alpha_2 + \alpha_{15}$	$\frac{1}{40} + \frac{1}{8}\beta_1 + \frac{3}{2}\beta_4 + \beta_8 + \beta_7 + \frac{1}{2}\beta_2 + \beta_{15}$
t_{16}		$\beta_{16} + \widetilde{\beta}_7\alpha_1 + \beta_3\alpha_2 + 2\widetilde{\beta}_1\alpha_8 + \widetilde{\beta}_1^2\alpha_4 + \alpha_{16}$	$\frac{1}{40} + \frac{1}{8}\beta_1 + \frac{3}{2}\beta_4 + \beta_8 + \beta_7 + \frac{1}{2}\beta_2 + \beta_{15}$
t_{17}		$\beta_{17} + \widetilde{\beta}_8\alpha_1 + \beta_4\alpha_2 + \widetilde{\beta}_2\alpha_4 + \beta_1\alpha_8 + \alpha_{17}$	$\frac{1}{120} + \frac{1}{24}\beta_1 + \frac{1}{6}\beta_2 + \frac{1}{2}\beta_4 + \beta_8 + \beta_{17}$

Table 4.3: $\beta\alpha$ and $E\beta$ for trees up to order 5.

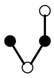
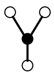
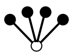
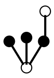
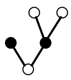
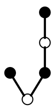
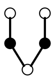
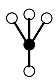
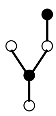
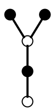
t_i	tree	$(\tilde{\beta}\tilde{\alpha})(t_i)$	$(E\tilde{\beta})(t_i)$
$\tilde{t}_1$		$\tilde{\beta}_1 + \tilde{\alpha}_1$	$1 + \tilde{\beta}_1$
$\tilde{t}_2$		$\tilde{\beta}_2 + \beta_1\tilde{\alpha}_1 + \tilde{\alpha}_2$	$\frac{1}{2} + \tilde{\beta}_1 + \tilde{\beta}_2$
$\tilde{t}_3$		$\tilde{\beta}_3 + \beta_1^2\tilde{\alpha}_1 + 2\beta_1\tilde{\alpha}_2 + \tilde{\alpha}_3$	$\frac{1}{3} + \tilde{\beta}_1 + 2\tilde{\beta}_2 + \tilde{\beta}_3$
$\tilde{t}_4$		$\tilde{\beta}_4 + \tilde{\beta}_1\tilde{\alpha}_2 + \beta_2\tilde{\alpha}_1 + \tilde{\alpha}_4$	$\frac{1}{6} + \frac{1}{2}\tilde{\beta}_1 + \tilde{\beta}_2 + \tilde{\beta}_4$
$\tilde{t}_5$		$\tilde{\beta}_5 + 3\beta_1\tilde{\alpha}_3 + 3\beta_1^2\tilde{\alpha}_2 + \beta_1^3\tilde{\alpha}_1 + \tilde{\alpha}_5$	$\frac{1}{4} + \tilde{\beta}_1 + 3\tilde{\beta}_2 + 3\tilde{\beta}_3 + \tilde{\beta}_5$
$\tilde{t}_6$		$\tilde{\beta}_6 + \beta_1\tilde{\alpha}_4 + \beta_2\tilde{\alpha}_2 + \tilde{\beta}_1\tilde{\alpha}_3 + \beta_1\beta_2\tilde{\alpha}_1 + \beta_1\tilde{\beta}_1\tilde{\alpha}_2 + \tilde{\alpha}_6$	$\frac{1}{8} + \frac{1}{2}\tilde{\beta}_1 + \frac{3}{2}\tilde{\beta}_2 + \tilde{\beta}_3 + \tilde{\beta}_4 + \tilde{\beta}_6$
$\tilde{t}_7$		$\tilde{\beta}_7 + \beta_3\tilde{\alpha}_1 + 2\tilde{\beta}_1\tilde{\alpha}_4 + \tilde{\beta}_1^2\tilde{\alpha}_2 + \tilde{\alpha}_7$	$\frac{1}{12} + \frac{1}{3}\tilde{\beta}_1 + \tilde{\beta}_2 + 2\tilde{\beta}_4 + \tilde{\beta}_7$
$\tilde{t}_8$		$\tilde{\beta}_8 + \beta_4\tilde{\alpha}_1 + \tilde{\beta}_2\tilde{\alpha}_2 + \beta_1\tilde{\alpha}_4 + \tilde{\alpha}_8$	$\frac{1}{24} + \frac{1}{6}\tilde{\beta}_1 + \frac{1}{2}\tilde{\beta}_2 + \tilde{\beta}_4 + \tilde{\beta}_8$
$\tilde{t}_9$		$\tilde{\beta}_9 + 4\beta_1\tilde{\alpha}_5 + 6\beta_1^2\tilde{\alpha}_3 + 4\beta_1^3\tilde{\alpha}_2 + \beta_1^4\tilde{\alpha}_1 + \tilde{\alpha}_9$	$\frac{1}{5} + 4\tilde{\beta}_5 + 6\tilde{\beta}_3 + 4\tilde{\beta}_2 + \tilde{\beta}_1 + \tilde{\beta}_9$
$\tilde{t}_{10}$		$\tilde{\beta}_{10} + \beta_2\tilde{\alpha}_3 + 2\beta_1\tilde{\alpha}_6 + \beta_1\tilde{\alpha}_5 + \beta_1^2\tilde{\alpha}_4 + 2\beta_1\beta_2\tilde{\alpha}_2$ $+2\beta_1\tilde{\beta}_1\tilde{\alpha}_3 + \beta_1^2\beta_2\tilde{\alpha}_1 + \beta_1^2\tilde{\beta}_2\tilde{\alpha}_2 + \tilde{\alpha}_{10}$	$\frac{1}{10} + \frac{5}{2}\tilde{\beta}_3 + 2\tilde{\beta}_6 + \tilde{\beta}_5$ $+\tilde{\beta}_4 + 2\tilde{\beta}_2 + \frac{1}{2}\tilde{\beta}_1 + \tilde{\beta}_{10}$
$\tilde{t}_{11}$		$\tilde{\beta}_{11} + \beta_1\tilde{\alpha}_7 + \beta_3\tilde{\alpha}_2 + 2\tilde{\beta}_1\tilde{\alpha}_6 + 2\beta_1\tilde{\beta}_1\tilde{\alpha}_4$ $+\beta_1\beta_3\tilde{\alpha}_1 + \tilde{\beta}_1^2\tilde{\alpha}_3 + \beta_1\tilde{\beta}_1^2\tilde{\alpha}_2 + \tilde{\alpha}_{11}$	$\frac{1}{15} + \tilde{\beta}_7 + \frac{4}{3}\tilde{\beta}_2 + 2\tilde{\beta}_6 + 2\tilde{\beta}_4$ $+\frac{1}{3}\tilde{\beta}_1 + \tilde{\beta}_3 + \tilde{\beta}_{11}$
$\tilde{t}_{12}$		$\tilde{\beta}_{12} + \beta_1\tilde{\alpha}_8 + \beta_4\tilde{\alpha}_2 + \tilde{\beta}_2\tilde{\alpha}_3 + \beta_2\tilde{\alpha}_6 + \beta_1\beta_4\tilde{\alpha}_1$ $+\beta_1\tilde{\beta}_1^2\tilde{\alpha}_2 + \beta_1^2\tilde{\alpha}_4 + \tilde{\alpha}_{12}$	$\frac{1}{30} + \tilde{\beta}_8 + \frac{2}{3}\tilde{\beta}_2 + \frac{1}{2}\tilde{\beta}_3 + \tilde{\beta}_6$ $+\frac{1}{6}\tilde{\beta}_1 + \tilde{\beta}_4 + \tilde{\beta}_{12}$
$\tilde{t}_{13}$		$\tilde{\beta}_{13} + 2\tilde{\beta}_1\tilde{\alpha}_6 + 2\beta_2\tilde{\alpha}_4 + 2\tilde{\beta}_1\beta_2\tilde{\alpha}_2 + \tilde{\beta}_1^2\tilde{\alpha}_3 + \beta_2^2\tilde{\alpha}_1 + \tilde{\alpha}_{13}$	$\frac{1}{20} + 2\tilde{\beta}_6 + \tilde{\beta}_4 + \tilde{\beta}_2 + \tilde{\beta}_3 + \frac{1}{4}\tilde{\beta}_1 + \tilde{\beta}_{13}$
$\tilde{t}_{14}$		$\tilde{\beta}_{14} + \beta_5\tilde{\alpha}_1 + 3\tilde{\beta}_1\tilde{\alpha}_7 + 3\tilde{\beta}_1^2\tilde{\alpha}_4 + \tilde{\beta}_1^3\tilde{\alpha}_2 + \tilde{\alpha}_{14}$	$\frac{1}{20} + \frac{1}{4}\tilde{\beta}_1 + 3\tilde{\beta}_7 + 3\tilde{\beta}_4 + \tilde{\beta}_2 + \tilde{\beta}_{14}$
$\tilde{t}_{15}$		$\tilde{\beta}_{15} + \beta_6\tilde{\alpha}_1 + \tilde{\beta}_2\tilde{\alpha}_4 + \tilde{\beta}_1\tilde{\alpha}_8 + \beta_1\tilde{\alpha}_7 + \tilde{\beta}_1\beta_1\tilde{\alpha}_4 + \tilde{\beta}_1\tilde{\beta}_2\tilde{\alpha}_2 + \tilde{\alpha}_{15}$	$\frac{1}{40} + \frac{1}{8}\tilde{\beta}_1 + \frac{3}{2}\tilde{\beta}_4 + \tilde{\beta}_8 + \tilde{\beta}_7 + \frac{1}{2}\tilde{\beta}_2 + \tilde{\beta}_{15}$
$\tilde{t}_{16}$		$\tilde{\beta}_{16} + \beta_7\tilde{\alpha}_1 + \tilde{\beta}_3\tilde{\alpha}_2 + 2\beta_1\tilde{\alpha}_8 + \beta_1^2\tilde{\alpha}_4 + \tilde{\alpha}_{16}$	$\frac{1}{40} + \frac{1}{8}\tilde{\beta}_1 + \frac{3}{2}\tilde{\beta}_4 + \tilde{\beta}_8 + \tilde{\beta}_7 + \frac{1}{2}\tilde{\beta}_2 + \tilde{\beta}_{16}$
$\tilde{t}_{17}$		$\tilde{\beta}_{17} + \beta_8\tilde{\alpha}_1 + \tilde{\beta}_4\tilde{\alpha}_2 + \beta_2\tilde{\alpha}_4 + \tilde{\beta}_1\tilde{\alpha}_8 + \tilde{\alpha}_{17}$	$\frac{1}{120} + \frac{1}{24}\tilde{\beta}_1 + \frac{1}{6}\tilde{\beta}_2 + \frac{1}{2}\tilde{\beta}_4 + \tilde{\beta}_8 + \tilde{\beta}_{17}$

Table 4.4: $\tilde{\beta}\tilde{\alpha}$ and $E\tilde{\beta}$ 76 for trees up to order 5.

and $\gamma(t)$ is the density of tree t. For main methods M and $\widetilde{M}$ to have effective order p, we must have $\beta\alpha\beta^{-1}(t) = E(t)$ and $\widetilde{\beta}\widetilde{\alpha}\widetilde{\beta}^{-1}(\widetilde{t}) = E(\widetilde{t})$ for all trees up to order p [11]. This is equivalent to having $\beta\alpha(t) = E\beta(t)$ and $\widetilde{\beta}\widetilde{\alpha}(\widetilde{t}) = E\widetilde{\beta}(\widetilde{t})$, which provide us algebraic conditions that must be satisfied for all trees of order up to p. Table 4.5 illustrates effective order conditions for all trees of order up to 5.

q	Effective order conditions
1	$\alpha_1 = 1, \qquad \widetilde{\alpha}_1 = 1$
2	$\alpha_2 = \frac{1}{2}, \qquad \widetilde{\alpha}_2 = \frac{1}{2}$
3	$\alpha_3 = \frac{1}{3} + 2\beta_2, \qquad \widetilde{\alpha}_3 = \frac{1}{3} + 2\widetilde{\beta}_2$ $\alpha_4 = \frac{1}{6} + \beta_2 - \widetilde{\beta}_2, \qquad \widetilde{\alpha}_4 = \frac{1}{6} + \widetilde{\beta}_2 - \beta_2$
4	$\alpha_5 = \frac{1}{4} + 3\beta_2 + 3\beta_3, \qquad \widetilde{\alpha}_5 = \frac{1}{4} + 3\widetilde{\beta}_2 + 3\widetilde{\beta}_3$ $\alpha_6 = \frac{1}{8} + \frac{3}{2}\beta_2 - \frac{1}{2}\widetilde{\beta}_2 + \beta_3 + \beta_4, \qquad \widetilde{\alpha}_6 = \frac{1}{8} + \frac{3}{2}\widetilde{\beta}_2 - \frac{1}{2}\beta_2 + \widetilde{\beta}_3 + \widetilde{\beta}_4$ $\alpha_7 = \frac{1}{12} + \beta_2 - \widetilde{\beta}_3 + 2\beta_4, \qquad \widetilde{\alpha}_7 = \frac{1}{12} + \widetilde{\beta}_2 - \beta_3 + 2\widetilde{\beta}_4$ $\alpha_8 = \frac{1}{24} + \beta_4 - \widetilde{\beta}_4, \qquad \widetilde{\alpha}_8 = \frac{1}{24} + \widetilde{\beta}_4 - \beta_4$
5	$\alpha_9 = \frac{1}{5} + 4\beta_2 + 6\beta_3 + 4\beta_5, \qquad \widetilde{\alpha}_9 = \frac{1}{5} + 4\widetilde{\beta}_2 + 6\widetilde{\beta}_3 + \widetilde{\beta}_5$ $\alpha_{10} = \frac{1}{10} + 2\beta_2 - \frac{1}{3}\widetilde{\beta}_2 - 2\widetilde{\beta}\beta_2 + \frac{5}{2}\beta_3, \qquad \widetilde{\alpha}_{10} = \frac{1}{10} + 2\widetilde{\beta}_2 - \frac{1}{3}\beta_2 - 2\beta_2\widetilde{\beta}_2 + \frac{5}{2}\widetilde{\beta}_3$ $+\beta_4 + \beta_5 + 2\beta_6 \qquad + \widetilde{\beta_4} + \widetilde{\beta}_5 + 2\widetilde{\beta}_6$ $\alpha_{11} = \frac{1}{15} + \frac{4}{3}\beta_2 + \beta_3 - \frac{1}{2}\widetilde{\beta}_3 + 2\beta_4 + 2\beta_6 + \beta_7, \qquad \widetilde{\alpha}_{11} = \frac{1}{15} + \frac{4}{3}\widetilde{\beta}_2 + \widetilde{\beta}_3 - \frac{1}{2}\beta_3 + 2\widetilde{\beta}_4 + 2\widetilde{\beta}_6 + \widetilde{\beta}_7$ $\alpha_{12} = \frac{1}{30} + \frac{1}{3}\beta_2 - 2\beta_2^2 + \frac{1}{2}\beta_3 + \frac{1}{2}\beta_4 + \beta_6 + \beta_8, \qquad \widetilde{\alpha}_{12} = \frac{1}{30} + \frac{1}{3}\widetilde{\beta}_2 - 2\widetilde{\beta}_2^2 + \frac{1}{2}\widetilde{\beta}_3 + \frac{1}{2}\widetilde{\beta}_4 + \widetilde{\beta}_6 + \widetilde{\beta}_8$ $\alpha_{13} = \frac{1}{20} + \beta_2 - \frac{1}{3}\widetilde{\beta}_2 + \widetilde{\beta}_2^2 - 2\widetilde{\beta}_2\beta_2 \qquad \widetilde{\alpha}_{13} = \frac{1}{20} + \widetilde{\beta}_2 - \frac{1}{3}\beta_2 + \beta_2^2 - 2\beta_2\widetilde{\beta}_2$ $+\beta_3 + \beta_4 + 2\beta_6, \qquad + \widetilde{\beta}_3 + \widetilde{\beta}_4 + 2\widetilde{\beta}_6$ $\alpha_{14} = \frac{1}{20} + \beta_2 + 3\beta_4 - \widetilde{\beta}_5 + 3\beta_7, \qquad \widetilde{\alpha}_{14} = \frac{1}{20} + \widetilde{\beta}_2 + 3\widetilde{\beta}_4 - \beta_5 + 3\widetilde{\beta}_7$ $\alpha_{15} = \frac{1}{40} + \frac{1}{3}\beta_2 - \beta_2^2 + \widetilde{\beta}_2\beta 2 + \frac{3}{2}\beta_4 \qquad \widetilde{\alpha}_{15} = \frac{1}{40} + \frac{1}{3}\widetilde{\beta}_2 - \widetilde{\beta}_2^2 + \beta_2\beta 2 + \frac{3}{2}\widetilde{\beta}_4$ $-\widetilde{\beta}_6 + \beta_7 + \beta_8, \qquad - \beta_6 + \widetilde{\beta}_7 + \widetilde{\beta}_8$ $\alpha_{16} = \frac{1}{60} + \frac{1}{3}\beta_2 - \frac{1}{2}\beta_3 + \beta_4 - \widetilde{\beta}_7 + 2\beta_8, \qquad \widetilde{\alpha}_{16} = \frac{1}{60} + \frac{1}{3}\widetilde{\beta}_2 - \frac{1}{2}\widetilde{\beta}_3 + \widetilde{\beta}_4 - \beta_7 + 2\widetilde{\beta}_8$ $\alpha_{17} = \frac{1}{120} + \frac{1}{6}\beta_2 - \frac{1}{6}\widetilde{\beta}_2 - \widetilde{\beta}_2\beta_2 + \widetilde{\beta}_2^2 + \beta_8 - \widetilde{\beta}_8 \qquad \widetilde{\alpha}_{17} = \frac{1}{120} + \frac{1}{6}\widetilde{\beta}_2 - \frac{1}{6}\beta_2 - \beta_2\widetilde{\beta}_2 + \beta_2^2 + \widetilde{\beta}_8 - \beta_8$

Table 4.5: Effective order 5 conditions on α and $\widetilde{\alpha}$ in terms of β and $\widetilde{\beta}$.

q	p	Order conditions for main methods	Order conditions for starting methods
3	2	$\alpha_1 = \widetilde{\alpha}_1 = 1, \alpha_2 = \widetilde{\alpha}_2 = \frac{1}{2}, \alpha_4 = \frac{1}{6} + \frac{1}{2}\alpha_3 - \frac{1}{2}\widetilde{\alpha}_3, \widetilde{\alpha}_4 = \frac{1}{6} + \frac{1}{2}\widetilde{\alpha}_3 - \frac{1}{2}\alpha_3$	$\beta_1 = \widetilde{\beta}_1 = 0, \beta_2 = \frac{1}{2}\alpha_3 - \frac{1}{6}, \widetilde{\beta}_2 = \frac{1}{2}\widetilde{\alpha}_3 - \frac{1}{6}$
4	2	$\alpha_1 = \widetilde{\alpha}_1 = 1, \alpha_2 = \widetilde{\alpha}_2 = \frac{1}{2}, \alpha_4 = \frac{1}{6} + \frac{1}{2}\alpha_3 - \frac{1}{2}\widetilde{\alpha}_3, \widetilde{\alpha}_4 = \frac{1}{6} + \frac{1}{2}\widetilde{\alpha}_3 - \frac{1}{2}\alpha_3$ $\frac{1}{4} - \widetilde{\alpha}_3 + \frac{2}{3}\alpha_5 + \frac{1}{3}\widetilde{\alpha}_5 - 2\alpha_6 + \alpha_7 = 0,$ $\frac{1}{4} - \alpha_3 + \frac{2}{3}\widetilde{\alpha}_5 + \frac{1}{3}\alpha_5 - 2\widetilde{\alpha}_6 + \widetilde{\alpha}_7 = 0$ $\widetilde{\alpha}_8 = \frac{1}{24} + \frac{1}{2}(\alpha_3 - \widetilde{\alpha}_3) + \frac{1}{3}(\alpha_5 - \widetilde{\alpha}_5) + (\widetilde{\alpha}_6 - \alpha_6)$ $\alpha_8 = \frac{1}{24} + \frac{1}{2}(\widetilde{\alpha}_3 - \alpha_3) + \frac{1}{3}(\widetilde{\alpha}_5 - \alpha_5) + (\alpha_6 - \widetilde{\alpha}_6)$	$\beta_1 = \widetilde{\beta}_1 = 0, \beta_2 = \frac{1}{2}\alpha_3 - \frac{1}{6}, \widetilde{\beta}_2 = \frac{1}{2}\widetilde{\alpha}_3 - \frac{1}{6},$ $\beta_3 = \frac{1}{12} - \frac{1}{2}\alpha_3 + \frac{1}{3}\alpha_5,$ $\widetilde{\beta}_3 = \frac{1}{12} - \frac{1}{2}\widetilde{\alpha}_3 + \frac{1}{3}\widetilde{\alpha}_5,$ $\beta_4 = -\frac{1}{24} - \frac{1}{4}\alpha_3 + \frac{1}{4}\widetilde{\alpha}_3 - \frac{1}{3}\alpha_5 + \alpha_6,$ $\widetilde{\beta}_4 = -\frac{1}{24} - \frac{1}{4}\widetilde{\alpha}_3 + \frac{1}{4}\alpha_3 - \frac{1}{3}\widetilde{\alpha}_5 + \widetilde{\alpha}_6$
4	3	$\alpha_1 = \widetilde{\alpha}_1 = 1, \quad \alpha_2 = \widetilde{\alpha}_2 = \frac{1}{2}, \alpha_3 = \widetilde{\alpha}_3 = \frac{1}{3}, \quad \alpha_4 = \widetilde{\alpha}_4 = \frac{1}{6}$ $\frac{1}{12} - \frac{2}{3}\alpha_5 - \frac{1}{3}\widetilde{\alpha}_5 + 2\alpha_6 - \alpha_7 = 0, \frac{1}{12} - \frac{2}{3}\widetilde{\alpha}_5 - \frac{1}{3}\alpha_5 + 2\widetilde{\alpha}_6 - \widetilde{\alpha}_7 = 0$ $\alpha_8 = \frac{1}{24} + \frac{1}{3}(\widetilde{\alpha}_5 - \alpha_5) + (\alpha_6 - \widetilde{\alpha}_6), \widetilde{\alpha}_8 = \frac{1}{24} + \frac{1}{3}(\alpha_5 - \widetilde{\alpha}_5) + (\widetilde{\alpha}_6 - \alpha_6)$	$\beta_1 = \widetilde{\beta}_1 = \beta_2 = \widetilde{\beta}_2 = 0, \beta_3 = \frac{1}{12} - \frac{1}{2}\alpha_3 + \frac{1}{3}\alpha_5$ $\widetilde{\beta}_3 = \frac{1}{12} - \frac{1}{2}\widetilde{\alpha}_3 + \frac{1}{3}\widetilde{\alpha}_5$
5	2	$\alpha_1 = \widetilde{\alpha}_1 = 1, \quad \alpha_2 = \widetilde{\alpha}_2 = \frac{1}{2},$ $\alpha_4 = \frac{1}{6} + \frac{1}{2}(\alpha_3 - \widetilde{\alpha}_3), \widetilde{\alpha}_4 = \frac{1}{6} + \frac{1}{2}(\widetilde{\alpha}_3 - \alpha_3)$ $\frac{1}{4} - \widetilde{\alpha}_3 + \frac{2}{3}\alpha_5 + \frac{1}{3}\widetilde{\alpha}_5 - 2\alpha_6 + \alpha_7 = 0,$ $\frac{1}{4} - \alpha_3 + \frac{2}{3}\widetilde{\alpha}_5 + \frac{1}{3}\alpha_5 - 2\widetilde{\alpha}_6 + \widetilde{\alpha}_7 = 0$ $\alpha_8 = \frac{1}{24} + \frac{1}{2}(\widetilde{\alpha}_3 - \alpha_3) - \frac{1}{3}(\alpha_5 - \widetilde{\alpha}_5) + (\alpha_6 - \widetilde{\alpha}_6),$ $\widetilde{\alpha}_8 = \frac{1}{24} + \frac{1}{2}(\alpha_3 - \widetilde{\alpha}_3) - \frac{1}{3}(\widetilde{\alpha}_5 - \alpha_5) + (\widetilde{\alpha}_6 - \alpha_6)$ $\alpha_{13} = \frac{1}{36} - \frac{1}{6}\widetilde{\alpha}_3 + \frac{1}{4}\widetilde{\alpha}_3^2 - \frac{1}{4}\alpha_9 + \alpha_{10},$ $\widetilde{\alpha}_{13} = \frac{1}{36} - \frac{1}{6}\alpha_3 + \frac{1}{4}\alpha_3^2 - \frac{1}{4}\widetilde{\alpha}_9 + \widetilde{\alpha}_{10}$ $\alpha_{14} = \frac{2}{15} + \frac{1}{2}\alpha_3 - \widetilde{\alpha}_3 - \frac{3}{2}\widetilde{\alpha}_3\alpha_3 + \alpha_5 + \frac{3}{4}\alpha_9\frac{1}{4}\widetilde{\alpha}_9 - 3\alpha_{10} + 3\alpha_{11},$ $\widetilde{\alpha}_{14} = \frac{2}{15} + \frac{1}{2}\widetilde{\alpha}_3 - \alpha_3 - \frac{3}{2}\alpha_3\widetilde{\alpha}_3 + \widetilde{\alpha}_5 + \frac{3}{4}\widetilde{\alpha}_9\frac{1}{4}\alpha_9 - 3\widetilde{\alpha}_{10} + 3\widetilde{\alpha}_{11}$ $\alpha_{15} = \frac{1}{90} + \frac{1}{12}\alpha_3 - \frac{1}{4}\widetilde{\alpha}_3 - \frac{3}{4}\widetilde{\alpha}_3\alpha_3 + \frac{1}{4}\alpha_3^2 + \frac{1}{6}\widetilde{\alpha}_5 - \frac{1}{6}\alpha_5 + \frac{1}{2}\widetilde{\alpha}_6 + \frac{1}{2}\alpha_6 \cdots$ $+\frac{1}{8}\widetilde{\alpha}_9 + \frac{3}{8}\alpha_9 - \frac{1}{2}\widetilde{\alpha}_{10} - \frac{3}{2}\alpha_{10} + \alpha_{11} + \alpha_{12}$ $\widetilde{\alpha}_{15} = \frac{1}{90} + \frac{1}{12}\widetilde{\alpha}_3 - \frac{1}{4}\alpha_3 - \frac{3}{4}\alpha_3\widetilde{\alpha}_3 + \frac{1}{4}\widetilde{\alpha}_3^2 + \frac{1}{6}\widetilde{\alpha}_5 - \frac{1}{6}\alpha_5 + \frac{1}{2}\widetilde{\alpha}_6 + \frac{1}{2}\alpha_6 \cdots$ $+\frac{3}{8}\widetilde{\alpha}_9 + \frac{1}{8}\alpha_9 - \frac{1}{2}\widetilde{\alpha}_{10} - \frac{3}{2}\alpha_{10} + \alpha_{11} + \alpha_{12}$ $\alpha_{16} = -\frac{37}{180} + \frac{1}{3}\alpha_3 + \alpha_3^2 - \frac{1}{3}\widetilde{\alpha}_5 - \frac{2}{3}\alpha_5\widetilde{\alpha}_6 + \alpha_6 + \frac{1}{4}\alpha_9 - \frac{1}{4}\widetilde{\alpha}_9 \cdots$ $+\widetilde{\alpha}_{10} - \alpha_{10} - \widetilde{\alpha}_{11} + 2\alpha_{12}$ $\widetilde{\alpha}_{16} = -\frac{37}{180} + \frac{1}{3}\widetilde{\alpha}_3 + \widetilde{\alpha}_3^2 - \frac{1}{3}\alpha_5 - \frac{2}{3}\widetilde{\alpha}_5\alpha_6 + \widetilde{\alpha}_6 + \frac{1}{4}\widetilde{\alpha}_9 - \frac{1}{4}\alpha_9 \cdots$ $+\alpha_{10} - \widetilde{\alpha}_{10} - \alpha_{11} + 2\widetilde{\alpha}_{12}$ $\alpha_{17} = \frac{1}{120} + \frac{1}{2}\alpha_3^2 - \frac{1}{4}\widetilde{\alpha}_3\alpha_3 - \frac{1}{4}\widetilde{\alpha}_3^2 + \frac{1}{8}(\alpha_9 - \widetilde{\alpha}_9) \cdots$ $+\frac{1}{2}(\widetilde{\alpha}_{10} - \alpha_{10}) + (\alpha_{12} - \widetilde{\alpha}_{12})$ $\widetilde{\alpha}_{17} = \frac{1}{120} + \frac{1}{2}\widetilde{\alpha}_3^2 - \frac{1}{4}\alpha_3\widetilde{\alpha}_3 - \frac{1}{4}\widetilde{\alpha}_3^2 + \frac{1}{8}(\widetilde{\alpha}_9 - \alpha_9) \cdots$ $+\frac{1}{2}(\widetilde{\alpha}_{10} - \alpha_{10}) + (\widetilde{\alpha}_{12} - \alpha_{12})$	$\beta_1 = \widetilde{\beta}_1 = \beta_2 = \widetilde{\beta}_2 = 0,$ $\beta_3 = \frac{1}{12} - \frac{1}{2}\alpha_3 + \frac{1}{3}\alpha_5, \widetilde{\beta}_3 = \frac{1}{12} - \frac{1}{2}\widetilde{\alpha}_3 + \frac{1}{3}\widetilde{\alpha}_5$ $\beta_4 = -\frac{1}{24} + \frac{1}{4}\widetilde{\alpha}_3 - \frac{1}{4}\alpha_3 - \frac{1}{3}\alpha_5 + \alpha_6,$ $\widetilde{\beta}_4 = -\frac{1}{24} + \frac{1}{4}\alpha_3 - \frac{1}{4}\widetilde{\alpha}_3 - \frac{1}{3}\widetilde{\alpha}_5 + \widetilde{\alpha}_6$ $\beta_5 = -\frac{1}{120} + \frac{1}{4}\alpha_3 - \frac{1}{2}\alpha_5 + \frac{1}{4}\alpha_9,$ $\widetilde{\beta}_5 = -\frac{1}{120} + \frac{1}{4}\widetilde{\alpha}_3 - \frac{1}{2}\widetilde{\alpha}_5 + \frac{1}{4}\widetilde{\alpha}_9$ $\beta_6 = \frac{3}{8} + \frac{1}{24}\alpha_3 - \frac{1}{8}\widetilde{\alpha}_3 + \frac{1}{4}\widetilde{\alpha}_3\alpha_3 \cdots$ $-\frac{1}{2}\alpha_6 - \frac{1}{8}\alpha_9 + \frac{1}{2}\alpha_{10}$ $\widetilde{\beta}_6 = \frac{3}{8} + \frac{1}{24}\widetilde{\alpha}_3 - \frac{1}{8}\alpha_3 + \frac{1}{4}\alpha_3\widetilde{\alpha}_3 - \frac{1}{2}\widetilde{\alpha}_6 - \frac{1}{8}\widetilde{\alpha}_9 + \frac{1}{2}\widetilde{\alpha}_{10}$ $\beta_7 = \frac{11}{90} + \frac{1}{4}\alpha_3 - \frac{1}{2}\widetilde{\alpha}_3 - \frac{1}{2}\widetilde{\alpha}_3\alpha_3 + \frac{1}{6}\widetilde{\alpha}_5 + \frac{1}{3}\alpha_5 \cdots$ $-\alpha_6 + \frac{1}{4}\alpha_9 + \alpha_{11}$ $\widetilde{\beta}_7 = \frac{11}{90} + \frac{1}{4}\widetilde{\alpha}_3 - \frac{1}{2}\alpha_3 - \frac{1}{2}\alpha_3\widetilde{\alpha}_3 + \frac{1}{6}\alpha_5 + \frac{1}{3}\widetilde{\alpha}_5 \cdots$ $-\widetilde{\alpha}_6 + \frac{1}{4}\widetilde{\alpha}_9 + \widetilde{\alpha}_{11}$ $\beta_8 = \frac{7}{360} - \frac{1}{6}\alpha_3 - \frac{1}{4}\widetilde{\alpha}_3\alpha_3 + \frac{1}{2}\alpha_3^2 + \frac{1}{8}\alpha_9 - \frac{1}{2}\alpha_{10} + \alpha_{12}$ $\widetilde{\beta}_8 = \frac{7}{360} - \frac{1}{6}\widetilde{\alpha}_3 - \frac{1}{4}\alpha_3\widetilde{\alpha}_3 + \frac{1}{2}\widetilde{\alpha}_3^2 + \frac{1}{8}\widetilde{\alpha}_9 - \frac{1}{2}\widetilde{\alpha}_{10} + \widetilde{\alpha}_{12}$

q	p	Order conditions for main methods	Order conditions for starting methods
5	3	$\alpha_1=\widetilde{\alpha}_1=1, \alpha_2=\widetilde{\alpha}_2=\frac{1}{2},$ $\alpha_3=\widetilde{\alpha}_3=\frac{1}{3}, \alpha_4=\widetilde{\alpha}_4=\frac{1}{6}$ $\frac{1}{12}-\frac{2}{3}\alpha_5-\frac{1}{3}\widetilde{\alpha}_5+2\alpha_6-\alpha_7=0,$ $\frac{1}{12}-\frac{2}{3}\widetilde{\alpha}_5-\frac{1}{3}\alpha_5+2\widetilde{\alpha}_6-\widetilde{\alpha}_7=0$ $\alpha_8=\frac{1}{24}+\frac{1}{2}(\widetilde{\alpha}_3-\alpha_3)-\frac{1}{3}(\alpha_5-\widetilde{\alpha}_5)+(\alpha_6-\widetilde{\alpha}_6)$ $\widetilde{\alpha}_8=\frac{1}{24}+\frac{1}{2}(\alpha_3-\widetilde{\alpha}_3)-\frac{1}{3}(\widetilde{\alpha}_5-\alpha_5)+(\widetilde{\alpha}_6-\alpha_6)$ $\frac{1}{4}\alpha_9-\alpha_{10}+\alpha_{13}=0,$ $\frac{1}{4}\widetilde{\alpha}_9-\widetilde{\alpha}_{10}+\widetilde{\alpha}_{13}=0$ $\frac{1}{5}-\widetilde{\alpha}_5-\frac{3}{4}\alpha_9+\frac{1}{4}\widetilde{\alpha}_9+3\alpha_{10}-3\alpha_{11}+\alpha_{14}=0$ $\frac{1}{5}-\alpha_5-\frac{3}{4}\widetilde{\alpha}_9+\frac{1}{4}\alpha_9+3\widetilde{\alpha}_{10}-3\widetilde{\alpha}_{11}+\widetilde{\alpha}_{14}=0$ $\frac{1}{10}+\frac{1}{6}\alpha_5-\frac{1}{6}\widetilde{\alpha}_5-\frac{1}{2}\alpha_6-\frac{1}{2}\widetilde{\alpha}_6-\frac{3}{8}\alpha_9-\frac{1}{8}\widetilde{\alpha}_9+$ $\frac{3}{2}\alpha_{10}+\frac{1}{2}\widetilde{\alpha}_{10}-\alpha_{11}-\alpha_{12}+\alpha_{15}=0$ $\frac{1}{10}+\frac{1}{6}\widetilde{\alpha}_5-\frac{1}{6}\alpha_5-\frac{1}{2}\widetilde{\alpha}_6-\frac{1}{2}\alpha_6-\frac{3}{8}\widetilde{\alpha}_9-\frac{1}{8}\alpha_9\cdots$ $+\frac{3}{2}\widetilde{\alpha}_{10}+\frac{1}{2}\alpha_{10}-\widetilde{\alpha}_{11}-\widetilde{\alpha}_{12}+\widetilde{\alpha}_{15}=0$ $\frac{1}{60}-\frac{2}{3}\alpha_5-\frac{1}{3}\widetilde{\alpha}_5+\alpha_6+\widetilde{\alpha}_6+\frac{1}{4}(\alpha_9-\widetilde{\alpha}_9)\cdots$ $+(\widetilde{\alpha}_{10}-\alpha_{10})-\widetilde{\alpha}_{11}+2\alpha_{12}-\alpha_{16}=0$ $\frac{1}{60}-\frac{2}{3}\widetilde{\alpha}_5-\frac{1}{3}\alpha_5+\widetilde{\alpha}_6+\alpha_6+\frac{1}{4}(\widetilde{\alpha}_9-\alpha_9)\cdots$ $+(\alpha_{10}-\widetilde{\alpha}_{10})-\alpha_{11}+2\widetilde{\alpha}_{12}-\widetilde{\alpha}_{16}=0$ $\alpha_{17}=\frac{1}{120}+\frac{1}{8}(\alpha_9-\widetilde{\alpha}_9)-\frac{1}{2}(\alpha_{10}-\widetilde{\alpha}_{10})+(\alpha_{12}-\widetilde{\alpha}_{12})$ $\widetilde{\alpha}_{17}=\frac{1}{120}+\frac{1}{8}(\widetilde{\alpha}_9-\alpha_9)-\frac{1}{2}(\widetilde{\alpha}_{10}-\alpha_{10})+(\widetilde{\alpha}_{12}-\alpha_{12})$	$\beta_1=\widetilde{\beta}_1=\beta_2=\widetilde{\beta}_2=0,$ $\beta_3=-\frac{1}{12}+\frac{1}{3}\alpha_5,\ \widetilde{\beta}_3=-\frac{1}{12}+\frac{1}{3}\widetilde{\alpha}_5$ $\beta_4=-\frac{1}{24}-\frac{1}{3}\alpha_5+\alpha_6,$ $\widetilde{\beta}_4=-\frac{1}{24}-\frac{1}{3}\widetilde{\alpha}_5+\widetilde{\alpha}_6$ $\beta_5=\frac{3}{40}-\frac{1}{2}\alpha_5+\frac{1}{4}\alpha_9,$ $\widetilde{\beta}_5=\frac{3}{40}-\frac{1}{2}\widetilde{\alpha}_5+\frac{1}{4}\widetilde{\alpha}_9$ $\beta_6=\frac{3}{80}-\frac{1}{2}\alpha_6-\frac{1}{8}\alpha_9+\frac{1}{2}\alpha_{10},$ $\widetilde{\beta}_6=\frac{3}{80}-\frac{1}{2}\widetilde{\alpha}_6-\frac{1}{8}\widetilde{\alpha}_9+\frac{1}{2}\widetilde{\alpha}_{10}$ $\beta_7=-\frac{1}{60}+\frac{1}{3}\alpha_5+\frac{1}{6}\widetilde{\alpha}_5-\alpha_9+\frac{1}{4}\widetilde{\alpha}_9-\alpha_{10}+\alpha_{11}$ $\widetilde{\beta}_7=-\frac{1}{60}+\frac{1}{3}\widetilde{\alpha}_5+\frac{1}{6}\alpha_5-\widetilde{\alpha}_9+\frac{1}{4}\alpha_9-\widetilde{\alpha}_{10}+\widetilde{\alpha}_{11}$ $\beta_8=-\frac{1}{120}+\frac{1}{8}\alpha_9-\frac{1}{2}\alpha_{10}+\alpha_{12}$ $\widetilde{\beta}_8=-\frac{1}{120}+\frac{1}{8}\widetilde{\alpha}_9-\frac{1}{2}\widetilde{\alpha}_{10}+\widetilde{\alpha}_{12}$
5	4	$\alpha_1=\widetilde{\alpha}_1=1,\ \alpha_2=\widetilde{\alpha}_2=\frac{1}{2},\ \alpha_3=\widetilde{\alpha}_3=\frac{1}{3},\ \alpha_4=\widetilde{\alpha}_4=\frac{1}{6},$ $\alpha_5=\widetilde{\alpha}_5=\frac{1}{4},\ \alpha_6=\widetilde{\alpha}_6=\frac{1}{8}, \alpha_7=\widetilde{\alpha}_7=\frac{1}{12},\ \alpha_8=\widetilde{\alpha}_8=\frac{1}{24}$ $\frac{1}{4}\alpha_9-\alpha_{10}+\alpha_{13}=0, \frac{1}{4}\widetilde{\alpha}_9-\widetilde{\alpha}_{10}+\widetilde{\alpha}_{13}=0$ $\frac{1}{20}+\frac{3}{4}\widetilde{\alpha}_9-\frac{1}{4}\alpha_9-3\widetilde{\alpha}_{10}+3\alpha_{11}-\alpha_{14}=0,$ $\frac{1}{20}+\frac{3}{4}\alpha_9-\frac{1}{4}\widetilde{\alpha}_9-3\alpha_{10}+3\widetilde{\alpha}_{11}-\widetilde{\alpha}_{14}=0$ $\frac{1}{40}+\frac{3}{8}\alpha_9-\frac{1}{8}\widetilde{\alpha}_9-\frac{3}{2}\alpha_{10}-\frac{1}{2}\widetilde{\alpha}_{10}+\alpha_{11}+\alpha_{12}-\alpha_{15}=0$ $\frac{1}{40}+\frac{3}{8}\widetilde{\alpha}_9-\frac{1}{8}\alpha_9-\frac{3}{2}\widetilde{\alpha}_{10}-\frac{1}{2}\alpha_{10}+\widetilde{\alpha}_{11}+\widetilde{\alpha}_{12}-\widetilde{\alpha}_{15}=0$ $\frac{1}{60}+\frac{1}{4}(\alpha_9-\widetilde{\alpha}_9)-\alpha_{10}+\widetilde{\alpha}_{10}-\widetilde{\alpha}_{11}+2\alpha_{12}-\alpha_{16}=0$ $\frac{1}{60}+\frac{1}{4}(\widetilde{\alpha}_9-\alpha_9)-\widetilde{\alpha}_{10}+\alpha_{10}-\alpha_{11}+2\widetilde{\alpha}_{12}-\widetilde{\alpha}_{16}=0$ $\alpha_{17}=\frac{1}{120}+\frac{1}{8}(\alpha_9-\widetilde{\alpha}_9)-\frac{1}{2}(\alpha_{10}-\widetilde{\alpha}_{10})+(\alpha_{12}-\widetilde{\alpha}_{12})$ $\widetilde{\alpha}_{17}=\frac{1}{120}+\frac{1}{8}(\widetilde{\alpha}_9-\alpha_9)-\frac{1}{2}(\widetilde{\alpha}_{10}-\alpha_{10})+(\widetilde{\alpha}_{12}-\alpha_{12})$	$\beta_1=\widetilde{\beta}_1=\beta_2=\widetilde{\beta}_2=0,\ \beta_3=\widetilde{\beta}_3=\beta_4=\widetilde{\beta}_4=0$ $\beta_5=-\frac{1}{20}+\frac{1}{4}\alpha_9,\ \widetilde{\beta}_5=-\frac{1}{20}+\frac{1}{4}\widetilde{\alpha}_9$ $\beta_6=-\frac{1}{40}-\frac{1}{8}\alpha_9+\frac{1}{2}\alpha_{10},\ \widetilde{\beta}_6=-\frac{1}{40}-\frac{1}{8}\widetilde{\alpha}_9+\frac{1}{2}\widetilde{\alpha}_{10}$ $\beta_7=-\frac{1}{60}+\frac{1}{4}\alpha_9-\alpha_{10}+\alpha_{11}, \widetilde{\beta}_7=-\frac{1}{60}+\frac{1}{4}\widetilde{\alpha}_9-\widetilde{\alpha}_{10}+\widetilde{\alpha}_{11}$ $\beta_8=-\frac{1}{120}+\frac{1}{8}\alpha_9-\frac{1}{2}\alpha_{10}+\alpha_{12},\ \widetilde{\beta}_8=-\frac{1}{120}+\frac{1}{8}\widetilde{\alpha}_9-\frac{1}{2}\widetilde{\alpha}_{10}+\widetilde{\alpha}_{12}$

Table 4.6: Effective order q, classical order p conditions on α, $\widetilde{\alpha}$, β, and $\widetilde{\beta}$ for main and starting methods.

In order to obtain practical methods, we solve the equations given in Table 4.5. The first step is to obtain equations involving α_i and $\widetilde{\alpha}_i$ by determining β_i and $\widetilde{\beta}_i$ as linear combination of α_i and $\widetilde{\alpha}_i$. The resulting effective order conditions for the main methods M and $\widetilde{M}$ together with starting methods S and $\widetilde{S}$ are provided in Table 4.6 for all trees up to order 5. Table 4.6 provides us conditions under which the main methods M and $\widetilde{M}$ has classical order q and the effective order p.

4.3.1 Derivation of PRK methods with effective order 3 with 2 stages

By equating compositions $\beta\alpha$, $E\beta$ provided in Table 4.4 and $\widetilde{\beta}\widetilde{\alpha}$, $E\widetilde{\beta}$ given in Table 4.5, we get the following set of equations:

$$\alpha_1 = 1, \tag{4.5}$$

$$\widetilde{\alpha}_1 = 1, \tag{4.6}$$

$$\alpha_2 = \frac{1}{2}, \tag{4.7}$$

$$\widetilde{\alpha}_2 = \frac{1}{2}, \tag{4.8}$$

$$\alpha_3 = \frac{1}{3} + 2\beta_2, \tag{4.9}$$

$$\widetilde{\alpha}_3 = \frac{1}{3} + 2\widetilde{\beta}_2, \tag{4.10}$$

$$\alpha_4 + \widetilde{\beta}_2 = \frac{1}{6} + \beta_2, \tag{4.11}$$

$$\widetilde{\alpha}_4 + \beta_2 = \frac{1}{6} + \widetilde{\beta}_2. \tag{4.12}$$

We can eliminate β_2 and $\widetilde{\beta}_2$ from equations (4.8) and (4.10) as

$$\beta_2 = \frac{3\alpha_3 - 1}{6},$$

$$\widetilde{\beta}_2 = \frac{3\widetilde{\alpha}_3 - 1}{6}.$$

We used above values of β_2 and $\widetilde{\beta}_2$ in equations (4.11) and (4.12) to get the following equations in terms of α only:

$$\begin{aligned}
\alpha_1 =& 1,\\
\widetilde{\alpha}_1 =& 1,\\
\alpha_2 =& \frac{1}{2},\\
\widetilde{\alpha}_2 =& \frac{1}{2},\\
6\alpha_4 + 3\widetilde{\alpha}_3 - 3\alpha_3 =& 1,\\
6\widetilde{\alpha}_4 + 3\alpha_3 - 3\widetilde{\alpha}_3 =& 1.
\end{aligned} \tag{4.13}$$

The set of equations (4.13) in terms of their elementary weights are expressed as under:

$$\begin{aligned}
\sum b_i &= 1,\\
\sum \widetilde{b}_i &= 1,\\
\sum b_i \widetilde{c}_i &= \frac{1}{2},\\
\sum \widetilde{b}_i c_i &= \frac{1}{2},\\
6(\sum b_i \widetilde{a}_{ij} c_j) + 3(\sum \widetilde{b}_i c_i^2) - 3(\sum b_i \widetilde{c}_i^2) &= 1,\\
6(\sum \widetilde{b}_i a_{ij} \widetilde{c}_j) + 3(\sum b_i \widetilde{c}_i^2) - 3(\sum \widetilde{b}_i c_i^2) &= 1.
\end{aligned} \tag{4.14}$$

The above set of equations (4.14) are expanded in terms of coefficients of the following Butcher table

$$\begin{array}{c|cc} 0 & 0 & 0 \\ c_2 & a_{21} & 0 \\ \hline & b_1 & b_2 \end{array}, \qquad \begin{array}{c|cc} \widetilde{c}_1 & \widetilde{a}_{11} & 0 \\ \widetilde{c}_2 & \widetilde{a}_{21} & \widetilde{a}_{22} \\ \hline & \widetilde{b}_1 & \widetilde{b}_2 \end{array}.$$

For 2 stage method, we get the following set of equations in component form:

$$
\begin{aligned}
b_1+b_2 =&1,\\
\widetilde{b}_1+\widetilde{b}_2 =&1,\\
b_1\widetilde{c}_1+b_2\widetilde{c}_2 =&\frac{1}{2},\\
\widetilde{b}_2c_2 =&\frac{1}{2},\\
6b_2\widetilde{a}_{22}c_2+3\widetilde{b}_2c_2^2-3b_1\widetilde{c}_1^2-3b_2\widetilde{c}_2^2 =&1,\\
6\widetilde{b}_2c_2\widetilde{c}_1+3b_1\widetilde{c}_1^2+3b_2c_2^2-3\widetilde{b}_2c_2^2 =&1.
\end{aligned}
\tag{4.15}
$$

Now we have 6 equations in equations set (4.15) with 6 unknowns $b_1, b_2, \widetilde{b}_1, \widetilde{b}_2, \widetilde{a}_{22}, c_2$ after taking $\widetilde{c}_1, \widetilde{c}_2$ as free parameters. we get the following values:

$$
\begin{aligned}
b_1 &= \frac{-1+2\widetilde{c}_2}{2(-\widetilde{c}_1+\widetilde{c}_2)},\\
b_2 &= \frac{-1+2\widetilde{c}_1}{2(\widetilde{c}_1-\widetilde{c}_{2)}},\\
\widetilde{b}_1 &= \frac{7-18\widetilde{c}_1-6\widetilde{c}_2+12\widetilde{c}_1\widetilde{c}_2}{4-18\widetilde{c}_1-6\widetilde{c}_2+12\widetilde{c}_1\widetilde{c}_2},\\
\widetilde{b}_2 &= -\frac{3}{2(2-9\widetilde{c}_1-3\widetilde{c}_2+6\widetilde{c}_1\widetilde{c}_2)},\\
\widetilde{a}_{22} &= \frac{(-2+3\widetilde{c}_1)(\widetilde{c}_1-\widetilde{c}_2)}{(-1+2\widetilde{c}_1)(2-9\widetilde{c}_1-3\widetilde{c}_2+6\widetilde{c}_1\widetilde{c}_2)},\\
c_2 &= \frac{1}{3}(-2+9\widetilde{c}_1+3\widetilde{c}_2-6\widetilde{c}_1\widetilde{c}_2).
\end{aligned}
$$

The values of $\widetilde{a}_{11}, \widetilde{a}_{21}$ and a_{21} can be calculated by using consistency conditions $\sum a_{ij} = c_i$ as under:

$$
\begin{aligned}
\widetilde{a}_{11} &= \widetilde{c}_1,\\
\widetilde{a}_{21} &= \widetilde{c}_2-\widetilde{a}_{22},\\
&= \widetilde{c}_2-\frac{(-2+3\widetilde{c}_1)(\widetilde{c}_1-\widetilde{c}_2)}{(-1+2\widetilde{c}_1)(2-3\widetilde{c}_2+\widetilde{c}_1(-9+6\widetilde{c}_2))},\\
a_{21} &= c_2,\\
&= \frac{1}{3}(-2+9\widetilde{c}_1+3\widetilde{c}_2-6\widetilde{c}_1\widetilde{c}_2).
\end{aligned}
$$

After selecting $\widetilde{c}_1 = \frac{1}{3}$ and $\widetilde{c}_2 = \frac{2}{3}$, we get the following two Butcher tables for α and $\widetilde{\alpha}$ method, respectively:

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{5}{9} & \frac{5}{9} & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}, \qquad \begin{array}{c|cc} \frac{1}{3} & \frac{1}{3} & 0 \\ \frac{2}{3} & \frac{1}{15} & \frac{3}{5} \\ \hline & \frac{1}{10} & \frac{9}{10} \end{array}. \tag{4.16}$$

For starting methods β and $\widetilde{\beta}$, we have the following set of equations as given in Table 4.6:

$$\beta_1 = 0, \tag{4.17}$$

$$\widetilde{\beta}_1 = 0, \tag{4.18}$$

$$\beta_2 = \frac{1}{2}\alpha_3 - \frac{1}{6}, \tag{4.19}$$

$$\widetilde{\beta}_2 = \frac{1}{2}\widetilde{\alpha}_3 - \frac{1}{6}. \tag{4.20}$$

The values β_2 and $\widetilde{\beta}_2$ can be calculated by computing the values of α_3 and $\widetilde{\alpha}_3$ using coefficients given in tables (4.16):

$$\begin{aligned} \alpha_3 &= \sum b_i \widetilde{c}_i^2 = b_1 \widetilde{c}_1^2 + b_2 \widetilde{c}_2^2, \\ &= \frac{1}{2}(\frac{1}{9} + \frac{4}{9}), \\ &= \frac{5}{18}. \end{aligned}$$

$$\begin{aligned} \widetilde{\alpha}_3 &= \sum \widetilde{b}_i c_i^2 = \widetilde{b}_2 c_2^2, \\ &= \frac{9}{10}\left(\frac{5}{9}\right)^2, \\ &= \frac{5}{18}. \end{aligned}$$

We place these values of α_3 and $\widetilde{\alpha}_3$ in equation (4.19) and (4.20), we will have:

$$\beta_2 = -\frac{1}{36}, \tag{4.21}$$
$$\widetilde{\beta}_2 = -\frac{1}{36}. \tag{4.22}$$

By writing equations (4.17), (4.18), (4.21) and (4.22) in the form of their elementary weights as:

$$\begin{aligned} \sum B_i &= 0, \\ \sum \widetilde{B}_i &= 0, \\ \sum B_i\widetilde{C}_i &= -\frac{1}{36}, \\ \sum \widetilde{B}_i C_i &= -\frac{1}{36}. \end{aligned} \tag{4.23}$$

We write the above equations (4.23) in coefficient form for the following Butcher tables:

$$\begin{array}{c|cc} 0 & 0 & 0 \\ C_2 & A_{21} & 0 \\ \hline & B_1 & B_2 \end{array}, \qquad \begin{array}{c|cc} 0 & 0 & 0 \\ \widetilde{C}_2 & \widetilde{A}_{21} & 0 \\ \hline & \widetilde{B}_1 & \widetilde{B}_2 \end{array},$$

as,

$$\begin{aligned} B_1 + B_2 &= 0, \\ \widetilde{B}_1 + \widetilde{B}_2 &= 0, \\ B_2\widetilde{C}_2 &= -\frac{1}{36}, \\ \widetilde{B}_2 C_2 &= -\frac{1}{36}. \end{aligned} \tag{4.24}$$

The starting methods β and $\widetilde{\beta}$ can be obtained by solving set of equations (4.24). We can make choice for B_2 and $\widetilde{B}_2$. The choice $B_2 = \widetilde{B}_2$ will give $C_2 = \widetilde{C}_2$, $A_{21} = \widetilde{A}_{21}$, $B_1 = \widetilde{B}_1$ and this will lead us to following butcher table used for both β and $\widetilde{\beta}$ methods.

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{6} & \frac{1}{6} & 0 \\ \hline & \frac{1}{6} & -\frac{1}{6} \end{array}$$

After the calculation of starting method (β), main method (α), we need a finishing method which will cancel the effects of starting method. We call this method as beta inverse method (β^{-1}) and the composition with $\beta\alpha$ is $\beta\alpha\beta^{-1}$, which is represented in the following Butcher's table.

$$
\begin{array}{c|cccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{6} & \frac{1}{6} & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{6} & -\frac{1}{6} & 0 & 0 & 0 & 0 \\
\frac{5}{9} & \frac{1}{6} & -\frac{1}{6} & \frac{5}{9} & 0 & 0 & 0 \\
1 & \frac{1}{6} & -\frac{1}{6} & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\
1+\mathcal{A}_{21} & \frac{1}{6} & -\frac{1}{6} & \frac{1}{2} & \frac{1}{2} & \mathcal{A}_{21} & 0 \\
\hline
 & \frac{1}{6} & -\frac{1}{6} & \frac{1}{2} & \frac{1}{2} & \mathcal{B}_1 & \mathcal{B}_2
\end{array}
$$

The β^{-1} method of effective order 3 with 2-stage can be constructed by using Butcher table. The order conditions for this inverse method in their elementary weights form are:

$$
\begin{aligned}
\sum \mathcal{B}_i &= 1, \\
\sum \mathcal{B}_i \widetilde{\mathcal{C}}_i &= \frac{1}{2}, \\
\sum \mathcal{B}_i \widetilde{\mathcal{C}}_i^2 &= \frac{1}{3}, \\
\sum \mathcal{B}_i \widetilde{\mathcal{A}}_{ij} \mathcal{C}_j &= \frac{1}{6}.
\end{aligned} \tag{4.25}
$$

Now, the expansion of equations set (4.25) in components form for 2 stages will give us following set of equations:

$$\mathcal{B}_1 + \mathcal{B}_2 = 0, \tag{4.26}$$

$$\mathcal{B}_1 + \mathcal{B}_2 + \mathcal{B}_2\mathcal{A}_{21} = \frac{1}{36}, \tag{4.27}$$

$$\mathcal{B}_1 + \mathcal{B}_2 + \mathcal{B}_2(\mathcal{A}_{21}^2 + 2\mathcal{A}_{21}) = \frac{13}{216}, \tag{4.28}$$

$$\frac{17}{36}(\mathcal{B}_1 + \mathcal{B}_2) + \mathcal{B}_2\mathcal{A}_{21} = 1/36. \tag{4.29}$$

The finishing method β^{-1} can be calculated by solving equations (4.26) to (4.29) and is given in Butcher table as

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{6} & \frac{1}{6} & 0 \\ \hline & -\frac{1}{6} & \frac{1}{6} \end{array}.$$

As, $\beta = \widetilde{\beta}$, so we have, $\beta^{-1} = \widetilde{\beta}^{-1}$.

4.3.2 Derivation of PRK methods with effective order 4

PRK methods with classical order $p = 2$ and effective order $q = 4$ are obtained by considering the following equations from Table 4.6:

$$\alpha_1 = 1, \tag{4.30}$$

$$\widetilde{\alpha}_1 = 1, \tag{4.31}$$

$$\alpha_2 = \frac{1}{2}, \tag{4.32}$$

$$\widetilde{\alpha}_2 = \frac{1}{2}, \tag{4.33}$$

$$6\alpha_4 + 3\widetilde{\alpha}_3 - 3\alpha_3 = 1, \tag{4.34}$$

$$6\widetilde{\alpha}_4 + 3\alpha_3 - 3\widetilde{\alpha}_3 = 1, \tag{4.35}$$

$$-12\alpha_7 + 24\alpha_6 - 4\widetilde{\alpha}_5 - 8\alpha_5 + 12\widetilde{\alpha}_3 = 3, \tag{4.36}$$

$$-12\widetilde{\alpha}_7 + 24\widetilde{\alpha}_6 - 4\alpha_5 - 8\widetilde{\alpha}_5 + 12\alpha_3 = 3, \tag{4.37}$$

$$144\alpha_8 + 144\widetilde{\alpha}_6 - 144\alpha_6 - 48\widetilde{\alpha}_5 + 48\alpha_5 - 72\widetilde{\alpha}_3 + 72\alpha_3 = 6, \tag{4.38}$$

$$144\widetilde{\alpha}_8 + 144\alpha_6 - 144\widetilde{\alpha}_6 - 48\alpha_5 + 48\widetilde{\alpha}_5 - 72\alpha_3 + 72\widetilde{\alpha}_3 = 6. \tag{4.39}$$

In order to simplify these equations, we use $D(1)$ and $\widetilde{D}(1)$ simplifying assumptions. The $D(1)$ condition is

$$\begin{aligned} \sum_{j=1}^{s} d_j &= \sum_{i,j=1}^{s} \widetilde{b}_i a_{ij} + \sum_{j=1}^{s} b_j \widetilde{c}_j - \sum_{j=1}^{s} b_j, \\ &= \widetilde{\alpha}_2 + \alpha_2 - \alpha_1, \\ &= 0. \end{aligned}$$

Similarly, we have

$$\widetilde{\alpha}_2 + \alpha_2 - \alpha_1 = 0, \tag{4.40}$$

$$\alpha_2 + \widetilde{\alpha}_2 - \widetilde{\alpha}_1 = 0, \tag{4.41}$$

$$\widetilde{\alpha}_4 + \alpha_3 - \alpha_2 = 0, \tag{4.42}$$

$$\alpha_4 + \widetilde{\alpha}_3 - \widetilde{\alpha}_2 = 0, \tag{4.43}$$

$$\widetilde{\alpha}_7 + \alpha_5 - \alpha_3 = 0, \tag{4.44}$$

$$\alpha_7 + \widetilde{\alpha}_5 - \widetilde{\alpha}_3 = 0, \tag{4.45}$$

$$\widetilde{\alpha}_8 + \alpha_6 - \alpha_4 = 0, \tag{4.46}$$

$$\alpha_8 + \widetilde{\alpha}_6 - \widetilde{\alpha}_4 = 0. \tag{4.47}$$

Now from equation (4.38) and equation (4.35), we have

$$24\alpha_6 + 8\widetilde{\alpha}_5 - 8\alpha_5 = 3, \tag{4.48}$$

and from equation (4.39) and equation (4.34), we have

$$24\widetilde{\alpha}_6 + 8\alpha_5 - 8\widetilde{\alpha}_5 = 3. \tag{4.49}$$

Furthermore, from equation (4.48) and equation (4.34) and from equation (4.49) and equation (4.35), we get

$$24\alpha_6 + 8\widetilde{\alpha}_5 - 8\alpha_5 - 24\alpha_4 - 12\widetilde{\alpha}_3 + 12\alpha_3 = -1,$$
$$24\widetilde{\alpha}_6 + 8\alpha_5 - 8\widetilde{\alpha}_5 - 24c_3\widetilde{\alpha}_4 - 12c_3\alpha_3 + 12c_3\widetilde{\alpha}_3 = 3 - 4c_3.$$

Subtracting equation (4.36) from equation (4.37) and equation (4.36) from equation (4.48), we get

$$\widetilde{\alpha}_7 + \alpha_5 - \alpha_3 = 0,$$
$$\alpha_7 + \widetilde{\alpha}_5 - \widetilde{\alpha}_3 = 0.$$

Finally, using equation (4.43) in equation (4.34) and using equation (4.42) in equation (4.35), we get

$$\alpha_3 + \widetilde{\alpha}_3 = \frac{2}{3}.$$

Hence, there are 7 equations in 7 unknowns:

$$\alpha_1 = 1, \tag{4.50}$$
$$\widetilde{\alpha}_1 = 1, \tag{4.51}$$
$$\alpha_2 = \frac{1}{2}, \tag{4.52}$$
$$\widetilde{\alpha}_2 = \frac{1}{2}, \tag{4.53}$$
$$\alpha_3 + \widetilde{\alpha}_3 = \frac{2}{3}, \tag{4.54}$$
$$24\alpha_6 + 8\widetilde{\alpha}_5 - 8\alpha_5 - 24\alpha_4 - 12\widetilde{\alpha}_3 + 12\alpha_3 = -1, \tag{4.55}$$
$$24\widetilde{\alpha}_6 + 8\alpha_5 - 8\widetilde{\alpha}_5 - 24c_3\widetilde{\alpha}_4 - 12c_3\alpha_3 + 12c_3\widetilde{\alpha}_3 = 3 - 4c_3. \tag{4.56}$$

Writing equation (4.50) to equation (4.56) in the form of elementary weights, we have

$$\sum b_i = 1,$$
$$\sum \widetilde{b}_i = 1,$$
$$\sum b_i\widetilde{c}_i = \frac{1}{2},$$
$$\sum \widetilde{b}_i c_i = \frac{1}{2},$$
$$\sum b_i\widetilde{c}_i^2 + \sum \widetilde{b}_i c_i^2 = \frac{2}{3},$$
$$24\sum \widetilde{c}_i b_i \widetilde{a}_{ij} c_j + 8\widetilde{b}_i c_i^3 - 8b_i\widetilde{c}_i^3$$
$$-24\sum b_i\widetilde{a}_{ij}c_j - 12\sum \widetilde{b}_i c_i^2 + 12\sum b_i\widetilde{c}_i^2 = -1,$$
$$24\sum c_i\widetilde{b}_i a_{ij}\widetilde{c}_j + 8b_i\widetilde{c}_i^3 - 8\widetilde{b}_i c_i^3$$
$$-24c_3\sum \widetilde{b}_i a_{ij}\widetilde{c}_j - 12c_3\sum b_i\widetilde{c}_i^2 + 12c_3\sum \widetilde{b}_i c_i^2 = 3 - 4c_3.$$

Consider Butcher tableaux for main methods M and $\widetilde{M}$ as follows:

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ c_2 & a_{21} & 0 & 0 \\ c_3 & a_{31} & a_{32} & 0 \\ \hline & b_1 & b_2 & b_3 \end{array}, \quad \text{and} \quad \begin{array}{c|ccc} \widetilde{c}_1 & \widetilde{a}_{11} & 0 & 0 \\ \widetilde{c}_2 & \widetilde{a}_{21} & \widetilde{a}_{22} & 0 \\ 1 & \widetilde{a}_{31} & \widetilde{a}_{32} & \widetilde{a}_{33} \\ \hline & \widetilde{b}_1 & \widetilde{b}_2 & \widetilde{b}_3 \end{array}.$$

Thus, we get

$$b_1 + b_2 + b_3 = 1, \tag{4.57}$$
$$\widetilde{b}_1 + \widetilde{b}_2 + \widetilde{b}_3 = 1, \tag{4.58}$$
$$b_1\widetilde{c}_1 + b_2\widetilde{c}_2 + b_3\widetilde{c}_3 = \frac{1}{2}, \tag{4.59}$$
$$\widetilde{b}_2 c_2 + \widetilde{b}_3 c_3 = \frac{1}{2}, \tag{4.60}$$
$$b_1\widetilde{c}_1^2 + b_2\widetilde{c}_2^2 + b_3 + \widetilde{b}_2 c_2^2 + \widetilde{b}_3 c_3^2 = \frac{2}{3}, \tag{4.61}$$
$$\begin{aligned} &24b_2(\widetilde{c}_2\widetilde{a}_{22}c_2 - \widetilde{a}_{22}c_2) + \widetilde{b}_2 c_2^2(8c_2 - 12) \\ &+\widetilde{b}_3 c_3^2(8c_3 - 12) + b_1\widetilde{c}_1^2(12 - 8\widetilde{c}_1) + b_2\widetilde{c}_2^2(12 - 8\widetilde{c}_2) + 4b_3 = -1, \end{aligned} \tag{4.62}$$
$$\begin{aligned} &24\widetilde{b}_2(c_2^2\widetilde{c}_1 - c_3c_2\widetilde{c}_1) + b_1\widetilde{c}_1^2(8\widetilde{c}_1 - 12c_3) \\ &+b_2\widetilde{c}_2^2(8\widetilde{c}_2 - 12c_3) + b_3(8 - 12c_3) + \widetilde{b}_2 c_2^2(12c_3 - 8c_2) + 4\widetilde{b}_3 c_3^3 = 3 - 4c_3. \end{aligned} \tag{4.63}$$

We use consistency conditions $c_i{=}\sum a_{ij}$ and $\widetilde{c}_i{=}\sum \widetilde{a}_{ij}$ and take $c_2 = \frac{1}{4}, c_3 = \frac{1}{2}, \widetilde{c}_1 = 0, \widetilde{c}_2 = \frac{5}{16}$ to get the following M and $\widetilde{M}$ methods:

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{4} & \frac{1}{4} & 0 & 0 \\ \frac{1}{2} & \frac{23}{110} & \frac{16}{55} & 0 \\ \hline & \frac{13}{90} & \frac{256}{495} & \frac{67}{198} \end{array}, \quad \text{and} \quad \begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{5}{16} & 0 & \frac{5}{16} & 0 \\ 1 & \frac{44}{67} & -\frac{98}{67} & \frac{121}{67} \\ \hline & \frac{2}{9} & -\frac{4}{9} & \frac{11}{9} \end{array}.$$

To find the starting methods S and $\widetilde{S}$, we find the values of $\alpha_3, \widetilde{\alpha}_3, \alpha_5, \widetilde{\alpha}_5, \alpha_7$, and $\widetilde{\alpha}_7$. For example, the value of α_3 is obtained as

$$\alpha_3 = \sum b_i \widetilde{c}_i^2 = b_1 \widetilde{c}_1^2 + b_2 \widetilde{c}_2^2 + b_3 \widetilde{c}_3^2 = \frac{7}{18}.$$

From the Table 4.6, we have:

$$\beta_1 = \sum B_i = 0, \tag{4.64}$$

$$\widetilde{\beta}_1 = \sum \widetilde{B}_i = 0, \tag{4.65}$$

$$\beta_2 = \sum B_i \widetilde{C}_i = \frac{1}{2}\alpha_3 - \frac{1}{6} = \frac{1}{36}, \tag{4.66}$$

$$\widetilde{\beta}_2 = \sum \widetilde{B}_i C_i = \frac{1}{2}\widetilde{\alpha}_3 - \frac{1}{6} = -\frac{1}{36}, \tag{4.67}$$

$$\beta_3 = \sum B_i \widetilde{C}_i^2 = \frac{1}{12} - \frac{1}{2}\alpha_3 + \frac{1}{3}\alpha_5 = \frac{1}{144}, \tag{4.68}$$

$$\widetilde{\beta}_3 = \sum \widetilde{B}_i C_i^2 = \frac{1}{12} - \frac{1}{2}\widetilde{\alpha}_3 + \frac{1}{3}\widetilde{\alpha}_5 = -\frac{1}{144}, \tag{4.69}$$

$$\beta_4 = \sum B_i \widetilde{A}_{ij} C_j = -\frac{1}{24} - \frac{1}{4}\alpha_3 + \frac{1}{4}\widetilde{\alpha}_3 - \frac{1}{3}\alpha_5 + \alpha_6 = \frac{1}{144}, \tag{4.70}$$

$$\widetilde{\beta}_4 = \sum \widetilde{B}_i A_{ij} \widetilde{C}_j = -\frac{1}{24} - \frac{1}{4}\widetilde{\alpha}_3 + \frac{1}{4}\alpha_3 - \frac{1}{3}\widetilde{\alpha}_5 + \widetilde{\alpha}_6 = -\frac{1}{144}. \tag{4.71}$$

Solving these equation, we have the following starting methods S and $\widetilde{S}$:

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{2}{5} & \frac{2}{5} & 0 & 0 \\ \frac{4}{5} & \frac{12}{5} & -\frac{8}{5} & 0 \\ \hline & -\frac{3}{32} & \frac{5}{48} & -\frac{1}{96} \end{array}, \quad \text{and} \quad \begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ \frac{2}{3} & \frac{7}{3} & -\frac{5}{3} & 0 \\ \hline & \frac{95}{1152} & -\frac{55}{576} & \frac{5}{384} \end{array}.$$

Finally, the finishing methods S^{-1} and $\widetilde{S}^{-1}$ are reflections of S and $\widetilde{S}$ methods and are termed as inverse RK methods which can be calculated as given in [11].

4.4 Numerical testing

Consider Kepler's two body problem given as

$$\begin{aligned} y_1' &= z_1, & y_1(0) &= 1-e, \\ y_2' &= z_2, & y_2(0) &= 0, \\ z_1' &= \frac{-y_1}{r^3}, & z_1(0) &= 0, \\ z_2' &= \frac{-y_2}{r^3}, & z_2(0) &= \sqrt{\frac{1+e}{1-e}}, \end{aligned}$$

where $r = \sqrt{y_1^2 + y_2^2}$. The exact solution after half revolution is

$$y_1(\pi) = 1+e, \quad y_2(\pi) = 0, \quad z_1(\pi) = 0, \qquad z_2(\pi) = \sqrt{\frac{1-e}{1+e}}.$$

In order to verify the order behavior of effective order methods, we proceed as follows:

1. Apply the starting methods S and $\widetilde{S}$ to perturb initial values to $(\widetilde{y}_1)_0$, $(\widetilde{y}_2)_0$, and $(\widetilde{z}_1)_0$, $(\widetilde{z}_2)_0$, respectively.

2. Apply the main methods M and $\widetilde{M}$ for n number of iterations to $(\widetilde{y}_1)_0$, $(\widetilde{y}_2)_0$ and $(\widetilde{z}_1)_0$, $(\widetilde{z}_2)_0$, respectively, and obtain the numerical solutions $(\widetilde{y}_1)_n$, $(\widetilde{y}_2)_n$, and $(\widetilde{z}_1)_n$, $(\widetilde{z}_2)_n$ calculated at $x_n = x_0 + nh$ where h is the step-size.

3. Evaluate exact solutions at x_n to get $y_1(x_n)$, $y_2(x_n)$, and $z_1(x_n)$, $z_2(x_n)$ and perturb them using starting methods S and $\widetilde{S}$ to get $\widetilde{y}_1(x_n)$, $\widetilde{y}_2(x_n)$ and $\widetilde{z}_1(x_n)$, $\widetilde{z}_2(x_n)$.

4. Obtain global error by taking difference between numerical and exact solutions, i.e., $||\widetilde{y}_n - \widetilde{y}(x_n)||$.

4.4.1 Order verification and efficiency of Effective order PRK methods

Effective order 4 behavior is confirmed from Table 4.7. Here we have taken 400 iterations with step-size $\frac{\pi}{400}$ and calculated the global error. We then doubled the number of iterations and halved the step-size and calculated the global error again. We computed the ratio between two consecutive global errors and this confirms that it is approximately 2^p for method of order p [11].

h	n	Global error	Ratio
$\frac{\pi}{400}$	400	$1.2021829 \times 10^{-07}$	
			15.899
$\frac{\pi}{800}$	800	$7.5611756 \times 10^{-09}$	
			15.997
$\frac{\pi}{1600}$	1600	$4.7264462 \times 10^{-10}$	
			16.0486
$\frac{\pi}{3200}$	3200	$2.9450851 \times 10^{-11}$	

Table 4.7: Global errors and their comparison.

In order to check the efficiency and accuracy of the effective order 4 partitioned Runge–Kutta method (EPRK4), we compare it with the classical order 4 Runge–Kutta method (RK4). We solve the Kepler's problem using both methods with different step-sizes and calculate the number of function evaluations and global errors. It is evident from the Figure 4.1 that EPRK4 employs fewer number of function evaluations than RK4. We have constructed EPRK4 with fewer stages as compared to RK4 and this is the reason for fewer number of function evaluations. The Figure 4.2 depicts that RK4 has lesser global error than EPRK4. We have not optimized EPRK4 for least global error and this can be done in future.

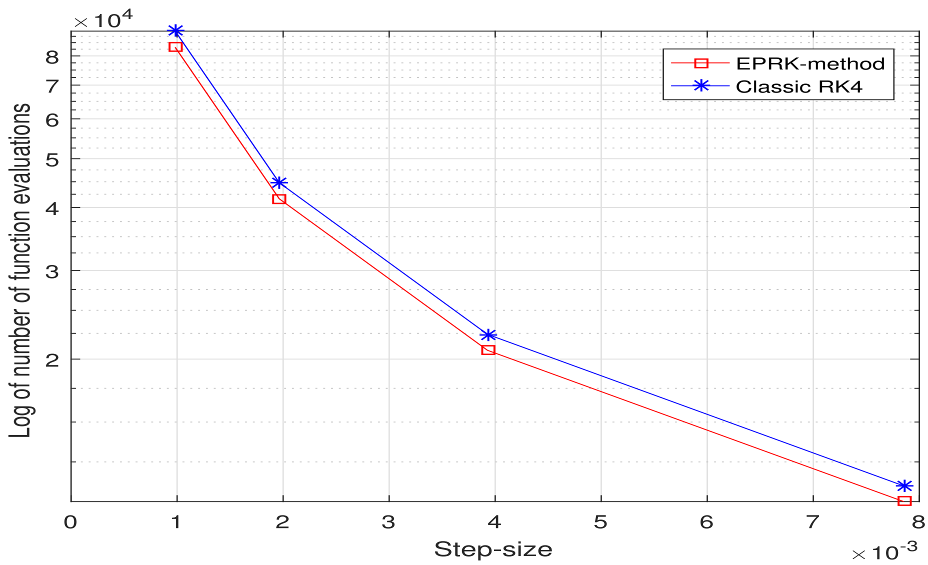


Figure 4.1: Comparison between step-size and the number of function evaluations.

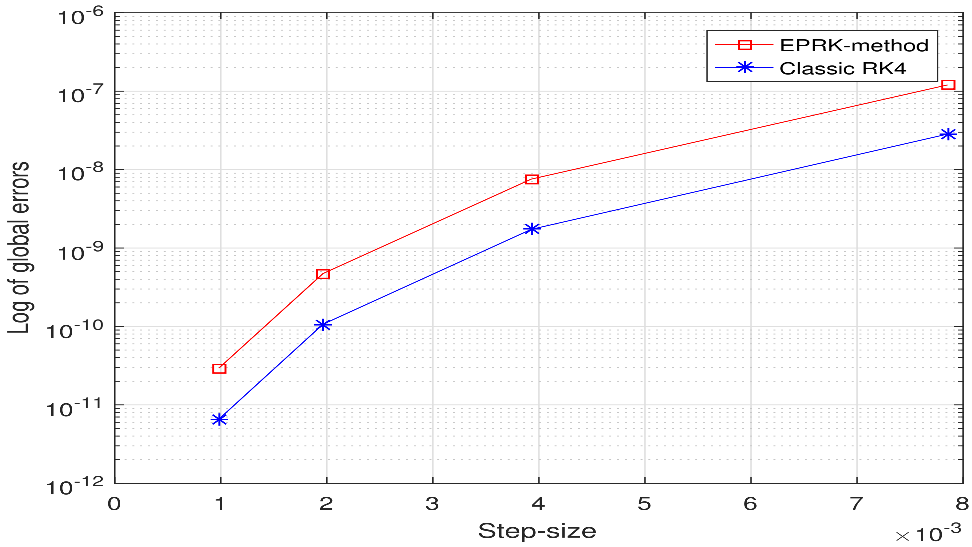


Figure 4.2: Comparison between step-size and global errors.

4.5 Conclusion

We have extended the idea of effective order to PRK methods. A complete classification of effective order up to 5 is provided. Moreover, effective order 4 methods are constructed with 3 stages which reduces the implementation cost as compared to classical order 4 method which requires 4 stages. The future work includes the construction of optimized effective order 5 PRK methods with five internal stages. We have already derived the conditions up to order 5 as given in Table 4.5. We believe that the simplifying assumptions $B(p)$, $C(\eta)$ and $D(\zeta)$ conditions will also be used in line with [6].

The type of differential equations we considered here have particular relevance to Hamiltonian systems and it is a well known fact that only symplectic methods can conserve quadratic invariants of the Hamiltonian systems. We have recently published a paper on symplectic effective order PRK methods [1].

Chapter 5

PRK methods for Hamiltonian systems

The PRK methods with symplectic property are only valid for separable systems, like, Hamiltonian systems. Due to this limited scope of applicable area, these methods look less interesting than symplectic RK methods but their explicit nature give an advantage over symplectic RK methods [35]. We start our discussion from symplectic PRk and then we shall move towards new developments.

5.1 Symplectic partitioned Runge-Kutta methods

The flow of Hamiltonian system is symplectic (4.1) and it is a well known fact that the discrete flow by symplectic Runge-Kutta methods is symplectic [33]. The PRK method M and $\widetilde{M}$ for separable Hamiltonian system (4.1) is symplectic if the following condition is satisfied [33].

$$\mathrm{diag}(b)\widetilde{a} + a^T \mathrm{diag}(\widetilde{b}) - b\widetilde{b} = 0. \tag{5.1}$$

Moreover, the composition of two symplectic RK methods is symplectic [16, 19]. We give the proof of this symlectic condition by using the quadratic invariants of PRK methods as

$$y^T D_1 g(y) =< y, g(y) >= 0, \quad \forall y,$$
$$z^T D_2 f(z) =< z, f(z) >= 0, \quad \forall z,$$

where D_1 and D_2 are symmetric matrices of square dimension. From PRK method, we know that

$$< Y_i, g(Y_i) > = 0,$$
$$< Z_i, f(Z_i) > = 0.$$

From equation (4.2), we hve

$$< y_n + \sum_{j=1}^{s} a_{ij} h f(Z_j), g(Y_i) >= 0,$$
$$< y_n, g(Y_i) >= -h \sum_{j=1}^{s} a_{ij} < f(Z_j), g(Y_i) >, \tag{5.2}$$

and also, we hve

$$< z_n + \sum_{j=1}^{s} \tilde{a}_{ij} h g(Y_j), f(Z_i) >= 0,$$
$$< z_n, f(Z_i) >= -h \sum_{j=1}^{s} \tilde{a}_{ij} < g(Y_j), f(Z_i) > . \tag{5.3}$$

And,

$$\begin{aligned} < y_{n+1}, z_{n+1} > &=< y_n + \sum_{i=1}^{s} b_i h f(z_i), z_n + \sum_{j=1}^{s} \tilde{b}_j h g(Y_j) >, \\ &=< y_n, z_n > +h \sum_{i=1}^{s} b_i < f(Z_i), z_n > +h \sum_{j=1}^{s} \tilde{b}_j \\ &\quad < y_n, g(Y_j) > +h^2 \sum_{i,j=1}^{s} b_i \tilde{b}_j < f(Z_i), g(Y_j) > . \end{aligned} \tag{5.4}$$

Equations (5.2), (5.3), and (5.4) are used to get

$$
\begin{aligned}
< y_{n+1}, z_{n+1} > =& < y_n, z_n > -h^2 \sum_{i,j=1}^{s} b_i \tilde{a}_{ij} < f(Z_i), g(Y_j) > -h^2 \sum_{i,j=1}^{s} \tilde{b}_j a_{ji} \\
& < f(Z_i), g(Y_j) > +h^2 \sum_{i,j=1}^{s} b_i \tilde{b}_j < f(Z_j), g(Y_j) >, \\
=& < y_n, z_n > -h^2 \sum_{i,j=1}^{s} (b_i \tilde{a}_{ij} + \tilde{b}_j a_{ji} - b_i \tilde{b}_j) < f(Z_i), g(Y_j) > .
\end{aligned}
$$

So, for

$$< y_{n+1}, z_{n+1} > = < y_n, z_n >,$$

we get

$$h^2 \sum_{i,j=1}^{s} (b_i \tilde{a}_{ij} + \tilde{b}_j a_{ji} - b_i \tilde{b}_j) < f(Z_i), g(Y_j) > = 0.$$

As

$$< f(Z_i), g(Y_j) > \neq 0,$$

so,

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

so it becomes symplectic condition for PRK methods as

$$\text{diag}(b)\widetilde{a} + a^T \text{diag}(\widetilde{b}) - b\widetilde{b} = 0.$$

5.2 Order conditions for symplectic partitioned Runge-Kutta methods

As we discussed in Chapter 2 that for symplectic RK methods, the trees related to order conditions can be divided into superfluous and non-superfluous bi-color trees and unlike RK methods, the superfluous bi-color trees of PRK methods also contribute one order condition together with one condition from non-superfluous bi-color tree [33]. In Partitioned Runge-Kutta methods, superfluous bi-colour trees provide one order condition and non-superfluous bi-colour trees provide two order conditions. The order conditions of these super and non-superfluous trees can be distinguished by using symplectic condition for PRK method as provided in equation (5.1). The bi-colour tree of order 2 is a superfluous. The symplectic condition can be rearranged to get a combination of such trees as

$$\sum_{i,j} b_i\tilde{a}_{ij} + \sum_{i,j} \tilde{b}_i a_{ji} - \sum_i b_i \sum_j \tilde{b}_j = 0,$$

$$(\sum_{i.j} b_i\tilde{a}_{ij} - \frac{1}{2}) + (\sum_{i,j} \tilde{b}_j a_{ji} - \frac{1}{2}) = 0,$$

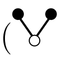
( $- \frac{1}{2}) + ($  $- \frac{1}{2}) = 0,$

Only one condition will involve as one is satisfied other will be satisfied automatically.

Similarly, in order 3 we have two non-superfluous trees, and we can find out their combinations order condition by multiplying symplectic condition with c_j as

$$\sum_{i,j} b_i\tilde{a}_{ij}c_j + \sum_{i,j} \tilde{b}_j c_j a_{ji} - \sum_i b_i \sum_j \tilde{b}_j c_j = 0,$$

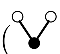
$$(\sum_{i,j} b_i\tilde{a}_{ij}c_j - \frac{1}{6}) + (\sum_{i,j} \tilde{b}_j c_j^2 - \frac{1}{3}) = 0,$$

( $- \frac{1}{6}) + ($  $- \frac{1}{3}) = 0.$

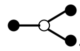
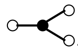
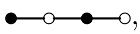
We shall include one above as one satisfied other. Now if we multiply $\tilde{c}_i$ to symplectic condition, we get

$$\sum_{i,j} b_i\tilde{c}_i\tilde{a}_{ij} + \sum_{i,j} \tilde{b}_j a_{ji}\tilde{c}_i - \sum_i b_i c_i \sum_j b_j = 0,$$

$$(\sum_{i,j} b_i\tilde{c}_i^2 - \frac{1}{3}) + (\sum_{i,j} \tilde{b}_j a_{ji}\tilde{c}_i - \frac{1}{6}) = 0,$$

( $- \frac{1}{3}) + ($  $- \frac{1}{6}) = 0.$

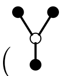
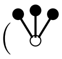
Therefore, we consider one order condition based on non-superfluous tree and also inclusion of one condition satisfies other automatically

Now we see the impact of symplectic condition on order 4 trees of PRK method. We see that there two non-superfluous and one superfluous trees are , , and , respectively. We can easily find out their relation with other pairs in the following way.
First, we multiply the symplectic condition by c_j^2 and will get

$$\sum_{i,j} b_i \tilde{a}_{ij} c_j^2 + \sum_{i,j} \tilde{b}_j c_j^2 c_j^2 a_{ji} - \sum_{j} \tilde{b}_j c_j^2 = 0,$$

$$\sum_{i,j} b_i \tilde{a}_{ij} c_j^2 + \sum_{i,j} \tilde{b}_j c_j^2 c_j - \frac{1}{3} = 0,$$

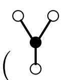
$$(\sum_{i,j} b_i \tilde{a}_{ij} c_j^2 - \frac{1}{12}) + (\sum_{i,j} \tilde{b}_j c_j^3 - \frac{1}{4}) = 0,$$

( $- \frac{1}{12}) + ($  $- \frac{1}{4}) = 0.$

So we include one of above for symplectic methods.
Secondly, we multiply $\tilde{c}_i^2$ to symplectic condition and will get

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

$$(\sum_{i} b_i \tilde{c}_i^3 - \frac{1}{4}) + (\sum_{i,j} \tilde{b}_j a_{ji} \tilde{c}_i^2 - \frac{1}{12}) = 0,$$

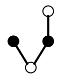
( $- \frac{1}{4}) + ($  $- \frac{1}{12}) = 0.$

Lastly, we multiply symplectic condition with $a_{jk}\tilde{c}_k$ to discuss the order conditions of superfluous trees for symplectic PRK method this comes out:

$$\sum_{i,j,k} b_i \tilde{a}_{ij} a_{jk} \tilde{c}_k + \sum_{i,j,k} \tilde{b}_j a_{ji} a_{jk} \tilde{c}_k - \sum_i b_i \sum_{j,k} \tilde{b}_j a_{jk} \tilde{c}_k = 0,$$

$$\sum_{i,j,k} b_i \tilde{a}_{ij} a_{jk} \tilde{c}_k + \sum_{j,k} \tilde{b}_j c_j a_{jk} \tilde{c}_k - \frac{1}{6} = 0,$$

$$(\sum_{i,j,k} b_i \tilde{a}_{ij} a_{jk} \tilde{c}_k - \frac{1}{24}) + (\sum_{j,k} \tilde{b}_j c_j a_{jk} \tilde{c}_k - \frac{1}{8}) = 0,$$

$\Big($  $- \frac{1}{24} \Big) + \Big($  $- \frac{1}{8} \Big) = 0.$

So after one tree satisfaction, we have no need of other tree. We use only one condition from above two. As we are using one order condition from pair of superfluous and non-superfluous trees so, we get less number of order conditions for symplectic PRK as compared to standard PRK methods. The Table 5.1 below provides the number of order conditions required for standard PRK and symplectic PRK for order up to 4.

order	PRK methods	symplectic PRK methods
1	2	2
2	4	3
3	8	5
4	16	8

Table 5.1: Number of order conditions for standard and symplectic PRK methods up to order 4.

5.3 Symplectic PRK methods with effective order 3

The effective order of PRK is constructed and tested in Chapter 4. We impose symplectic condition on the equations governing the effective order of PRK method for order three. Because the underlying bi-color tree of the rooted trees t_2 and $\widetilde{t_2}$ is superfluous, we can ignore the conditions (4.8), because it is automatically satisfied. Moreover, the underlying bi-color trees of t_3, t_4, $\widetilde{t_3}$, and $\widetilde{t_4}$ are non-superfluous, we can either take α_3 or $\widetilde{\alpha_4}$ and also α_4 or $\widetilde{\alpha_3}$ thus reducing the last two equations of set (4.13) to $\alpha_3 = \frac{1}{3}$ and $\widetilde{\alpha_3} = \frac{1}{3}$. Now consider the following Butcher table for methods M and $\widetilde{M}$ which satisfy the symplectic condition (5.1):

$$\begin{array}{c|ccc} 0 & 0 & & \\ b_1 & b_1 & & \\ b_1+b_2 & b_1 & b_2 & \\ \hline & b_1 & b_2 & b_3 \end{array}, \qquad \begin{array}{c|ccc} \widetilde{b_1} & \widetilde{b_1} & & \\ \widetilde{b_1}+\widetilde{b_2} & \widetilde{b_1} & \widetilde{b_2} & \\ \widetilde{b_1}+\widetilde{b_2}+\widetilde{b_3} & \widetilde{b_1} & \widetilde{b_2} & \widetilde{b_3} \\ \hline & \widetilde{b_1} & \widetilde{b_2} & \widetilde{b_3} \end{array}. \tag{5.5}$$

By using symplectic condition in (5.1) and the equations set (4.13) after simplification can be written in terms of elementary weights as:

$$\sum_{i=1}^{3} b_i = 1, \tag{5.6}$$

$$\sum_{i=1}^{3} \widetilde{b_i} = 1, \tag{5.7}$$

$$b_1\widetilde{b_1} + b_2(\widetilde{b_1}+\widetilde{b_2}) + b_3 = \frac{1}{2}, \tag{5.8}$$

$$\widetilde{b_1}^2 b_1 + b_2(\widetilde{b_1}+\widetilde{b_2})^2 + b_3(\widetilde{b_1}+\widetilde{b_2}+\widetilde{b_3})^2 = \frac{1}{3}, \tag{5.9}$$

$$\widetilde{b_2} b_1^2 + \widetilde{b_3}(b_1+b_2)^2 = \frac{1}{3}. \tag{5.10}$$

To get the values of 6 unknowns from 5 equations, we have one degree of freedom. Let us take $\widetilde{b_1} = \dfrac{2}{3}$ and solve the equation (4.57-4.61) to get main methods M and $\widetilde{M}$ methods as follows:

$$
\begin{array}{c|ccc}
 & 0 & 0 & 0 \\
 & \frac{13+\sqrt{205}}{12} & 0 & 0 \\
 & \frac{13+\sqrt{205}}{12} & \frac{5}{6} & 0 \\
\hline
 & \frac{13+\sqrt{205}}{12} & \frac{5}{6} & \frac{-11-\sqrt{205}}{12}
\end{array}
,\qquad
\begin{array}{c|ccc}
 & \frac{2}{3} & 0 & 0 \\
 & \frac{2}{3} & \frac{5+\sqrt{205}}{30} & 0 \\
 & \frac{2}{3} & \frac{5+\sqrt{205}}{30} & \frac{5-\sqrt{205}}{30} \\
\hline
 & \frac{2}{3} & \frac{5+\sqrt{205}}{30} & \frac{5-\sqrt{205}}{30}
\end{array}
.
$$

5.3.1 Derivation of starting method

For the starting method, we have the following equations:

$$\beta_1 = 0, \tag{5.11}$$

$$\widetilde{\beta}_1 = 0, \tag{5.12}$$

$$\beta_2 = \frac{1}{2}\alpha_3 - \frac{1}{6}, \tag{5.13}$$

$$\widetilde{\beta}_2 = \frac{1}{2}\widetilde{\alpha}_3 - \frac{1}{6}. \tag{5.14}$$

The starting methods should be symplectic [17]. The solution of (4.64-5.14) leads us to the following symplectic staring PRK methods S and $\widetilde{S}$ as:

$$
\begin{array}{c|ccc}
 & 0 & 0 & 0 \\
 & \frac{1}{3} & 0 & 0 \\
 & \frac{1}{3} & \frac{2}{5} & 0 \\
\hline
 & \frac{1}{3} & \frac{2}{5} & -\frac{11}{15}
\end{array}
,\qquad
\begin{array}{c|ccc}
 & \frac{1}{3} & 0 & 0 \\
 & \frac{1}{3} & -\frac{11}{18} & 0 \\
 & \frac{1}{3} & -\frac{11}{18} & \frac{5}{18} \\
\hline
 & \frac{1}{3} & -\frac{11}{18} & \frac{5}{18}
\end{array}
.
$$

5.4 Mutually adjoint symplectic effective order PRK methods

A separable Hamiltonian system remains unchanged by changing the role of kinetic and potential energies, position and momentum and also inverting the direction of time. For the two PRK method tableaux (5.5) being mutually adjoint, we have $b1 = \widetilde{b}_3$, $b2 = \widetilde{b}_2$ and $b3 = \widetilde{b}_1$ in equations (4.57–4.61) so that we have

$$\sum_{i=1}^{3} \widetilde{b}_i = 1, \tag{5.15}$$

$$\sum_{i=1}^{3} \widetilde{b}_i = 1, \tag{5.16}$$

$$\widetilde{b}_3\widetilde{b}_1 + \widetilde{b}_2(\widetilde{b}_1 + \widetilde{b}_2) + \widetilde{b}_1 = \frac{1}{2}, \tag{5.17}$$

$$\widetilde{b}_2\widetilde{b}_3^2 + \widetilde{b}_3(\widetilde{b}_3 + \widetilde{b}_2)^2 = \frac{1}{3}. \tag{5.18}$$

Sanz-Serna suggested in [33] to take $\widetilde{b}_3 = 0.91966152$, which leads us to the following main methods M and $\widetilde{M}$ with effective order 3 and with just 3 stages:

$$\begin{array}{c|ccc}
 & 0 & 0 & 0 \\
 & 0.91966152 & 0 & 0 \\
 & 0.91966152 & -0.18799162 & 0 \\
\hline
 & 0.91966152 & -0.18799162 & 0.26833010
\end{array}\;, \qquad
\begin{array}{c|ccc}
 & 0.26833010 & 0 & 0 \\
 & 0.26833010 & -0.18799162 & 0 \\
 & 0.26833010 & -0.18799162 & 0.91966152 \\
\hline
 & 0.26833010 & -0.18799162 & 0.91966152
\end{array}\;.$$

The starting methods S and $\widetilde{S}$ for mutually adjoint symplectic effective order PRK method are constructed by using $B_1 = \widetilde{B}_3$, $B_2 = \widetilde{B}_2$, $B_3 = \widetilde{B}_1$ in equations (4.64) to (4.65) to get

$$\widetilde{B}_1 + \widetilde{B}_2 + \widetilde{B}_3 = 0, \tag{5.19}$$

$$\widetilde{B}_1\widetilde{B}_3 + \widetilde{B}_2(\widetilde{B}_1 + \widetilde{B}_2) + \widetilde{B}_1(\widetilde{B}_1 + \widetilde{B}_2 + \widetilde{B}_3) \simeq 0. \tag{5.20}$$

By solving equations (5.19) and (5.20) with $\widetilde{B}_3 = \frac{1}{2}$, we get the following S and $\widetilde{S}$ methods:

$$\begin{array}{c|ccc} & 0 & 0 & 0 \\ & \frac{1}{2} & 0 & 0 \\ & \frac{1}{2} & -\frac{1}{4} & 0 \\ \hline & \frac{1}{2} & -\frac{1}{4} & -\frac{1}{4} \end{array} \quad \text{and} \quad \begin{array}{c|ccc} & -\frac{1}{4} & 0 & 0 \\ & -\frac{1}{4} & -\frac{1}{4} & 0 \\ & -\frac{1}{4} & -\frac{1}{4} & \frac{1}{2} \\ \hline & -\frac{1}{4} & -\frac{1}{4} & \frac{1}{2} \end{array}.$$

5.5 Numerical testing

The order of both symplectic and mutually adjoint symplectic effective PRK methods or order 3 is verified after applying these methods on Kepler's two body problem discussed in Chapter 4.

5.5.1 Order verification of symplectic effective order PRK methods

The effective order 3 behavior for symplectic and mutually adjoint symplectic PRK methods is confirmed from Table 4.7 and 5.3.

h	n	Global error	Ratio
$\frac{\pi}{225}$	225	$7.7741637102284 \times 10^{-04}$	
			8.927465
$\frac{\pi}{450}$	450	$8.7081425338124 \times 10^{-05}$	
			8.475956
$\frac{\pi}{900}$	900	$1.02739357736254 \times 10^{-05}$	
			8.063877
$\frac{\pi}{1800}$	1800	$1.27406905909534 \times 10^{-06}$	

Table 5.2: Global errors and their comparison: Symplectic effective order PRK methods.

h	n	Global error	Ratio
$\frac{\pi}{40}$	40	$4.635890382086 \times 10^{-03}$	
			7.963129
$\frac{\pi}{80}$	80	$5.82169473987045 \times 10^{-04}$	
			8.062262
$\frac{\pi}{160}$	160	$7.22091971134495 \times 10^{-05}$	
			7.836579
$\frac{\pi}{320}$	320	$9.21437776243649 \times 10^{-06}$	

Table 5.3: Global errors and their comparison: Mutually adjoint symplectic effective order PRK methods.

5.5.2 Energy conservation behaviour

Here, we applied both symplectic and mutually adjoint symplectic methods on kepler's two body problem and on Harmonic oscilator problem to verify the energy conservation behaviour of both methods.

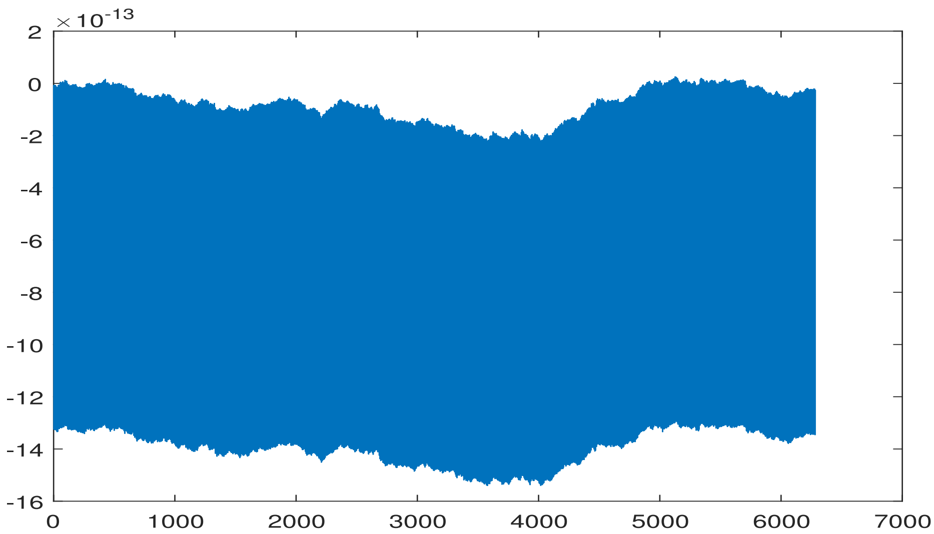


Figure 5.1: The error in energy of the Kepler's problem ($e = 0$) with symplectic effective PRK using step size $h = 2\pi/1000$ for 10^5 steps.

Kepler's problem

In this experiment, we used step-size $h = 2\pi/1000$ for 10^5 iterations. We obtained good energy conservation as shown in Figure 5.1 and Figure 5.2 using symplectic and mutually adjoint symplectic effective order PRK methods, respectively. It hs been observed that the error in the energy was bounded above by 10^{-13} and 10^{-14}, respectively.

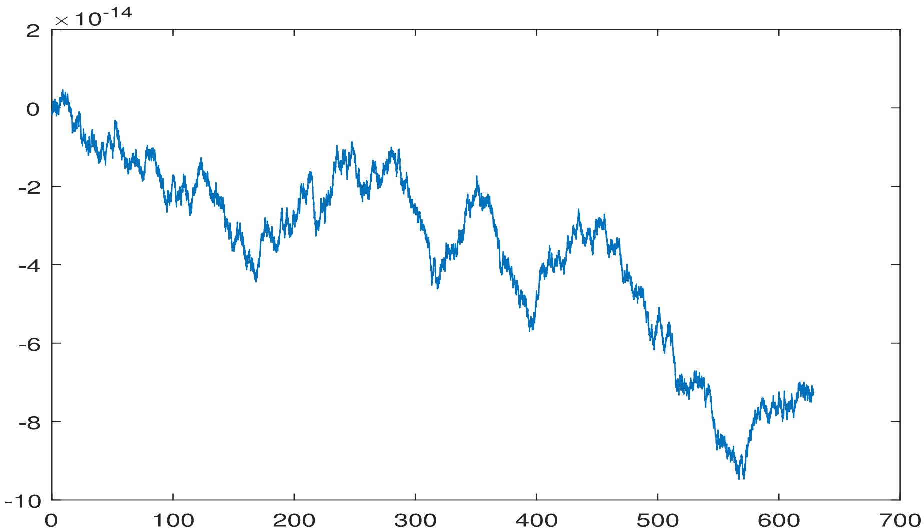


Figure 5.2: The error in energy of the Kepler's problem ($e = 0$) with mutually adjoint symplectic effective PRK using step-size $h = 2\pi/1000$ for 10^5 steps.

Harmonic Oscillator

The motion of a unit mass attached to a spring with momentum u and position co-ordinates v defines the Hamiltonian system

$$v^{'} = u, \qquad u^{'} = v.$$

The energy is given by

$$H = \frac{u^2}{2} + \frac{v^2}{2}.$$

The exact solution is

$$\begin{bmatrix} \mathrm{u(t)} \\ \\ \mathrm{v(t)} \end{bmatrix} = \begin{bmatrix} \cos(\mathrm{t}) & \text{-}\sin(\mathrm{t}) \\ \\ \sin(\mathrm{t}) & \cos(\mathrm{t}) \end{bmatrix} \begin{bmatrix} \mathrm{u(0)} \\ \\ \mathrm{v(0)} \end{bmatrix}.$$

We have applied symplectic PRK and mutually adjoint symplectic PRK methods with step-size $h = 2\pi/1000$ and 10^5 iteration in this experiment . We received good energy conservation as shown in Figure 5.3 and Figure 5.4 by symplectic effective order PRK and mutually adjoint symplectic effective order PRK methods, respectively.

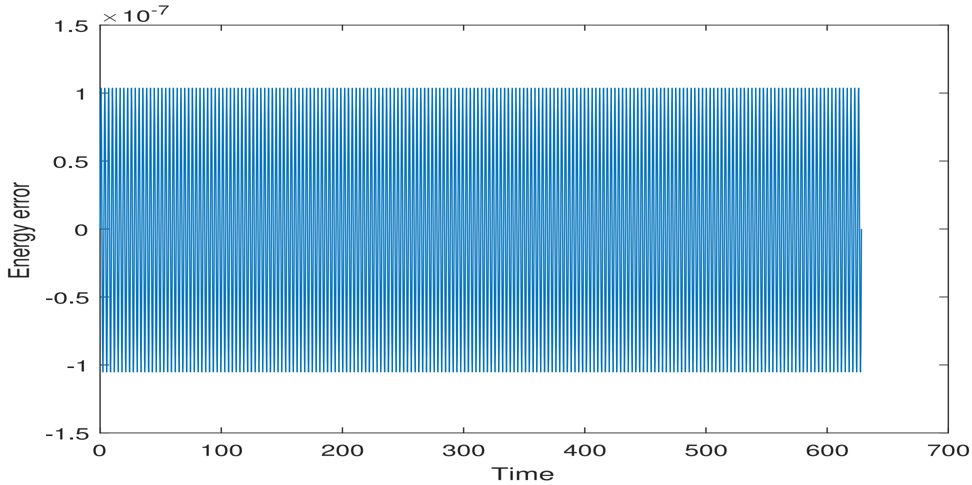


Figure 5.3: The error in energy of the Harmonic oscillator problem ($e = 0$) with symplectic effective PRK using step size $h = 2\pi/1000$ for 10^5 steps.

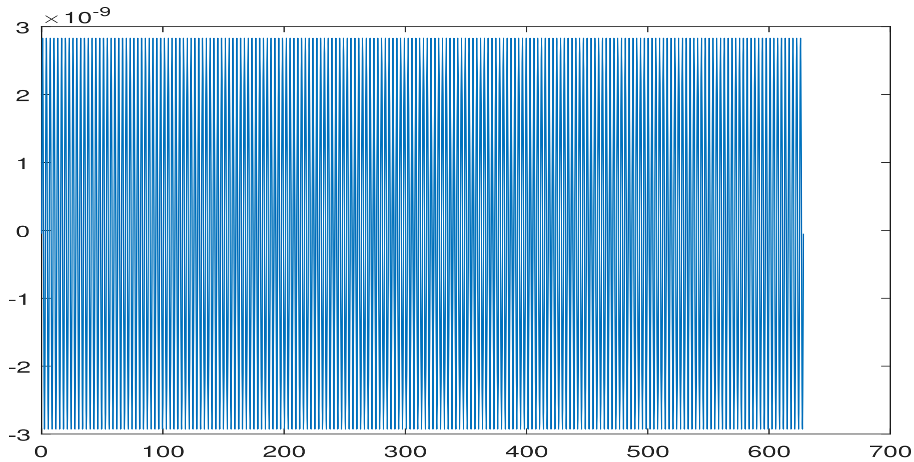


Figure 5.4: The error in energy of the Harmonic oscillator problem ($e = 0$) with mutually adjoint symplectic effective PRK using step size $h = 2\pi/1000$ for 10^5 steps.

5.6 Conclusions and future work

The type of differential equations we considered in this chapter have particular relevance to Hamiltonian systems and it is a well known fact that only symplectic methods can conserve quadratic invariant of the Hamiltonian systems. Keeping in view of this fact, we applied effective order techniques to symplectic and mutuallay adjoint symplectic PRK methods. We constructed 3 stage effective order 3 symplectic PRK methods and successfully applied to separable Hamiltonian systems with good energy conservation. It is worth mentioning that we are able to construct mutually adjoint symplectic effective order 3 PRK methods with just 3 stages, whereas an equivalent method of order 3 with 4 stages is given in [17]. For future work direction, we can go for construction of effective order symplectic and mutually adjoint methods for order 4 with 3 stages. Also, this work can be extended to non-separable systems of differential equations.

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