G-Symplectic Partitioned General Linear Methods for Hamiltonian Systems

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Declaration

I Muhammad Sarfraz Khan registration number **CIIT/FA16-RMT-022/LHR,** hereby declare that I have produced the work presented in this thesis, during the scheduled period of study. I also declare that I have not taken any material from any source except referred to wherever do that amount of plagiarism is within acceptable range. If a violation HEC rules has occurred in this thesis, I shall be liable to punishable action under the plagiarism rules of the HEC.

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Certificate

It is certified that Muhammad Sarfraz Khan (CIIT/FA16-RMT-022/LHR) has carried out all the work related to this thesis under my supervision at the Department of Mathematics, COMSATS University Islamabad, Lahore Campus, and the work fulfills the requirement for award of MS degree.

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DEDICATION

To
My Beloved Parents and Teachers.

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In the name of Allah, the Most Gracious and the Most Merciful
The Prophet (S.A.W) said:
"Seeking knowledge is obligatory for every Muslim"

First, I recognize the creator and finisher of my faith and in memorial of my life, I say thank ALLAH Almighty and Prophet Muhammad (S.A.W) for everything. I am grateful to Almighty ALLAH, without whose endowments it was difficult to finish this proposal.

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Abstract

The main aim of this thesis is to construct structure preserving numerical methods for Hamiltonian systems. General linear methods are a generalization of RK method and LMSM. G-symplectic GLM are suitable for numerical integration of Hamiltonian systems in a similar fashion as that of symplectic RK methods. Order 2 G-symplectic general linear methods were constructed by Butcher for numerically preserving Hamiltonian systems having invariants. After that, Order 4 G-symplectic general linear methods were constructed. We have constructed order 6 G-symplectic general linear methods that not only preserve energy of Hamiltonian systems but also show zero parasitism.

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Chapter 1

Introduction

Most physical wonders, similar to the movement of blood in veins, the conduct of electric circuits in machines, the development of stars in universes or the progression of offers in the stock exchange, can be comprehended through their numerical models. These models comprise of an arrangement of ordinary differential equations, that have time as the autonomous variable and the factors of physical frameworks as reliant factors. For the most part, these ODES joined by initial condition, constitute initial value problem.

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

Differential equations in which consist of both x and y are called non-autonomous differential equation, while those where f depends only on y are called as autonomous differential equations [1]. Autonomous differential equation is given below

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

Mostly physical phenomena are modeled by higher order differential equations. Differential equation having order n is given as

$$y^n(x) = f(x, y, y^{'}, y^{''}, \ldots, y^n)$$

1.1 Numerical methods

We have diverse numerical techniques [17] for the solution of our ODEs e.g. one step Euler method, Runge Kutta (RK) methods, multi-steps methods and general linear methods(GLM). Formula for one step Euler method is given below

$$y_i = y_{i-1} + hf(y_{i-1})$$

Despite the fact that the order of Euler method is one, higher order one step methods [4] are additionally accessible, one of which is RK methods. In RK methods first we need to compute the stages Y_i in the given interval $[x_{i-1}, x_i]$. After that, we can calculate required yield y_n

$$\begin{aligned} Y_i &= y_{n-1} + \sum_{j=1}^{s} ha_{ij} f(Y_j), \qquad\qquad i = 1, 2, 3 \ldots, s, \\ y_n &= y_{n-1} + \sum_{i=1}^{s} hb_i f(Y_i) \end{aligned}$$

where,

- h is step size
- a_{ij} is coefficients matrix
- b_i are quadrature weights

RK methods have always been considered as pricey because structure of these methods is multistage.

Multi-steps methods are multi-value in nature. It uses all previous information to obtain the desired output value. Formula for Linear Multi-steps methods are given below

$$\sum_{m=0}^{s} \alpha_m y_{n+m} = h \sum_{m=0}^{s} b_m f(x_{n+m}, y_{n+m})$$

if $\alpha_0 = \alpha_1 = \alpha_2 \ldots = \alpha_{s-2} = 0$, $\quad \alpha_{s-1} = -1$,$\alpha_s = 1$ $b_s = 0$

then we will have the follwing Adams Bashfroth method.

$$y_{n+s} = y_{n+s-1} + h \sum_{m=0}^{s-1} b_m f(x_{n+m}, y_{n+m})$$

If $\alpha_0 = \alpha_1 = \alpha_2 = \ldots = \alpha_{s-2} = 0, \quad \alpha_{s-1} = -1$ and $\alpha_s = 1$ and $b_s \neq 0$ we will have s-steps Adams-Moulton methods which is given below

$$y_{n+s} = y_{n+s-1} + h \sum_{m=0}^{s} b_m f(x_{n+m}, y_{n+m})$$

For Linear multi-steps methods, a starting method is required, which can be obtained by one step methods i.e either by Euler methods or RK methods. Linear Multi-step methods are cheap because they include a single function assessment for each step, however, due to $Dahlquist$ barrier; for stiff problems, the order should not be greater than 2 [12].

General linear methods(GLM) are the generalization of one step methods and multi-step mlethods [6]. The general form of (GLM) is

$$\begin{aligned} Y &= hAf(Y) + Uy^{[}n-1] \\ y^{[}n] &= hBf(Y) + Vy^{[}n-1] \end{aligned}$$

Here A, U, B, V are the matrices which represents our GLM.

where,

$$hf(Y) = \begin{bmatrix} h(Y_1^n) \\ hf(Y_2^n) \\ hf(Y_3^n) \\ \vdots \\ hf(Y_r^n) \end{bmatrix}, \quad y^{n-1} = \begin{bmatrix} y_1^{n-1} \\ y_2^{n-1} \\ y_3^{n-1} \\ \vdots \\ y_r^{n-1} \end{bmatrix}, \quad y^n = \begin{bmatrix} y_1^n \\ y_2^n \\ y_3^n \\ \vdots \\ y_r^n \end{bmatrix}$$

As GLM is multistage therefore it requires more than one input values to get output. In order to obtain the input values, we use starting methods for GLM [9]. A two stage two input value GLM is given as,

$$Y_1 = ha_{11}f(Y_1) + ha_{12}f(Y_2) + u_{11}y_1^0 + a_{12}y_2^0$$
$$Y_2 = ha_{21}f(Y_1) + ha_{22}f(Y_2) + u_{11}y_1^0 + a_{12}y_2^0$$
$$y_1^1 = hb_{11}f(Y_1) + hb_{12}f(Y_2) + v_{11}y_1^0 + v_{12}y_2^0$$

$$y_2^1 = hb_{21}f(Y_1) + hb_{22}f(Y_2) + v_{21}y_1^0 + v_{22}y_2^0$$

1.2 Hamiltonian systems

Hamiltonian systems depends upon equations of motion [4] in which we have generalized momentum **p** and generalized coordinates **q**, these equations of motion are called Hamiltonian systems. Hamiltonian differential equations are

$$\frac{d\mathbf{q}}{dt} = \frac{\partial H}{\partial \mathbf{p}} \qquad \frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{q}} \tag{1.3}$$

q=$[q_1, q_2 \ldots, q_n]$ and **p**=$[p_1, p_2 \ldots, p_n]$. where H is the function of **p**and **q** and it represents sum of its kinetic and potential energy.i.e

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

if write $y = (p, q)$ then we can write equation $eq(1.3)$ as

$$y^{'} = J^{-1}\nabla H \tag{1.4}$$

Where J is skew symmetric matrix and ∇ is gradient operator.

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

1.2.1 Conservation of energy

Numerous physical wonders in nature have some conserved quantities which do not change with time. We need to hold these features while integrating numerically the differential equations. e.g In case of Hamiltonian differential equations, total energy "H" remains constant [5]. Differentiate H(p,q) with respect to time

$$\frac{dH}{dt} = (\frac{\partial H}{\partial \mathbf{p}}\frac{d\mathbf{p}}{dt} + \frac{\partial H}{\partial \mathbf{q}}\frac{d\mathbf{q}}{dt}) = 0 \tag{1.5}$$

The energy of Hamiltonian systems is not conserved when we apply traditional numerical methods on them. In order to have conserve energy, symplectic methods have been constructed [15].

1.2.2 Symplecticity

The flow of Hamiltonian systems is $symplectic$ in nature. For $symplectic$ flow

$$< p_{i+1} \ \ , q_{i+1} >=< p_i \ \ , q_i >$$

Consider the transformation

$$\gamma : (p, q) \longrightarrow (\hat{p}, \hat{q})$$

The transformation γ will be $symplectic$ if,

$$(\gamma^{'})^T J\gamma^{'}\text{=J}$$

Let us consider the Jacobian "J" has unit determinant

$$\begin{vmatrix} \frac{\partial \hat{p}}{\partial \hat{p}} & \frac{\partial \hat{q}}{\partial p} \\ \frac{\partial \hat{p}}{\partial q} & \frac{\partial \hat{q}}{\partial q} \end{vmatrix} = \frac{\partial \hat{p}}{\partial p}\frac{\partial \hat{q}}{\partial q} - \frac{\partial \hat{q}}{\partial p}\frac{\partial \hat{p}}{\partial q} = I \tag{1.6}$$

Now,

$$\gamma^{'} = \begin{bmatrix} \frac{\partial \hat{p}}{\partial p} & \frac{\partial \hat{q}}{\partial p} \\ \frac{\partial \hat{p}}{\partial q} & \frac{\partial \hat{q}}{\partial q} \end{bmatrix}$$

$$(\gamma^{'})^T J \gamma^{'} = \begin{bmatrix} (\frac{\partial \hat{p}}{\partial p})(\frac{\partial \hat{q}}{\partial p}) - (\frac{\partial \hat{p}}{\partial p})(\frac{\partial \hat{q}}{\partial p}) & (\frac{\partial \hat{p}}{\partial p})(\frac{\partial \hat{q}}{\partial q}) - (\frac{\partial \hat{p}}{\partial q})(\frac{\partial \hat{q}}{\partial p}) \\ (\frac{\partial \hat{p}}{\partial q})(\frac{\partial \hat{q}}{\partial p}) - (\frac{\partial \hat{p}}{\partial p})(\frac{\partial \hat{q}}{\partial q}) & (\frac{\partial \hat{p}}{\partial q})(\frac{\partial \hat{q}}{\partial q})(\frac{\partial \hat{p}}{\partial q})(\frac{\partial \hat{q}}{\partial q}) \end{bmatrix}$$

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

Hence γ is $symplectic$.

1.2.3 Example: Harmonic Oscillator

Hamiltonian differential equations for Harmonic Oscillator are

$$p^{'} = -q, \qquad q^{'} = p$$

Total energy of Harmonic oscillator is

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

The flow of Harmonic Oscillator is symplectic

$$\gamma : \begin{pmatrix} p \\ q \end{pmatrix} \longrightarrow \begin{pmatrix} -q \\ p \end{pmatrix}$$

$$\gamma^{'} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

$$(\gamma^{'})^T J \gamma^{'} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \mathrm{J}$$

1.2.4 Example simple pendulum

The Hamiltonian Differential equations are

$$p^{'} = -sinq \quad q^{'} = p$$

Total energy of simple pendulum

$$H = \tfrac{p^2}{2} - cosq$$

$$\gamma : \begin{pmatrix} p \\ q \end{pmatrix} \longrightarrow \begin{pmatrix} -sinq \\ p \end{pmatrix}$$

$$\gamma^{'} = \begin{pmatrix} 0 & -cosq \\ 1 & 0 \end{pmatrix}$$

$$(\gamma^{'})^T J \gamma^{'} = J$$

1.2.5 Quadratic Invariants

Solution of Hamiltonian systems are Invariant.Consider

$$y^{'} = f(y) \quad y(x_0) = y_0 \tag{1.7}$$

Consider a quadratic function

$$I(y) = y^T C y$$

where C is symmetric matrix. It is invariant of (1.8) if

$$y^T C f(y) = 0$$

i.e

$$< y \ , f(Y) >= 0$$

Example : Consider Hamiltonian differential equations

$$p^{'} = -q \quad q^{'} = p \tag{1.8}$$

Then we may write energy of Hamiltonian systems

$$\begin{aligned} \tfrac{p^2}{2} + \tfrac{q^2}{2} &= \begin{pmatrix} p & q \end{pmatrix} \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} p \\ q \end{pmatrix} \\ &= y^T C y \end{aligned} \tag{1.9}$$

Now to check equation (1.9) is an invariant of (1.8)

$$\begin{aligned} y^T C f(y) &= \begin{pmatrix} p & q \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} -q \\ p \end{pmatrix} \\ &= -pq + pq = 0 \end{aligned}$$

1.3 Numerical methods for Hamiltonian systems

Standard numerical methods do not preserve the energy of Hamiltonian systems, Therefore our interest in those numerical methods which completely give us symplectic solution of Hamiltonian systems. These methods are known as structure preserving numerical methods in which we have one step methods and multi-steps methods [15]

Euler method and RK methods are example of one step methods. However, energy calculated by euler method was not conservative, therefore to obtain conservative solution of Hamiltonian systems, symplectic euler method [15] was introduced, which do energy preservation of Hamiltonian systems. General form of symplectic Euler method is

$$p_{n+1} = p_n + hf(q_n)$$
$$q_{n+1} = q_n + hg(p_{n+1})$$

Likewise euler method, RK method do not preserve energy of Hamiltonian systems. Therefore Lasagni [21], Sanz-Serna [4] and Suris [15] discovered the condition on the coefficients of RK methods that give us preserved solution of Hamiltonian system. If the coefficients of RK methods $[A,\ b^T\ , C]$ satisfy the relation

$$M = diag(b)A + A^T diag(b) - bb^T = 0$$

Then RK method will be symplectic that satisfy the property of linear and quadratic invariants. Energy calculated by implicit and explicit RK methods are also conservative which shows that implicit and explicit RK are energy preserving methods.

Multi-steps methods are multi-value in nature, therefore energy calculated by these methods are not symplectic. To obtain the symplectic solution of Hamiltonian systems by these methods Dahlquist introduced one-leg method [3,16] by which we can get energy preservation of Hamiltonian systems. For one-leg methods consider a matrix G with norm such that

$$\|y\|_G^2 = \sum_{i,j=1}^{r} g_{ij}\langle y_i,\ y_j\rangle$$

$$\text{for } y = \begin{pmatrix} y_1 \\ y_3 \\ \vdots \\ y_r \end{pmatrix}$$

such that numerical solution by one-leg methods is non dissipative under G-norm.
Another example of multi-step methods are GLM [6]. Similar to linear multi-steps methods these methods are also not symplectic. Energy preserving GLM for Hamiltonian system was introduced by Butcher [11] under G-norm, named as G-symplectic GLM. The first G-symplectic GLM was of order 2, after that order 4 G-symplectic GLM for Hamiltonian systems was constructed. In this thesis we have constructed order 6 G-symplectic GLM with invariants.

Chapter 2

Numerical methods for ordinary differential equations

2.1 Runge-Kutta methods

Runge-Kutta(RK) methods [4] belongs to family of one-step methods. Consider an initial value problem

$$y^{'} = f(y(x)), \qquad y(x_0) = y_0 \tag{2.1}$$

Then general form of RK methods to solve 2.1 is

$$k_i = y_{n-1} + \sum_{j=1}^{s} a_{ij} h f(k_j) \tag{2.2}$$

$$y_n = y_{n-1} + \sum_{i=1}^{s} b_i h f(k_i) \tag{2.3}$$

Eq(2.2) will give us the stages and from Eq(2.3) we will obtained out-put value of initial value problem.
RK methods can be represented by Butcher table given below

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

where b_i are quadrature weights, c_i are abscissas and a_{ij} is coefficient matrix of RK methods. RK methods are divided into two classes. One of which is explicit [4] and other is implicit [8] RK method. If $a_{ij} = 0$ for $i \leq j$ then it will become explicit otherwise implicit.
We prefer to use explicit RK method because it takes less time to obtained nu-

merical solution. But due to their limited stability region, explicit RK are not suitable.

2.1.1 Example

Explicit RK method of order 4

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

$k_1 = y_n$

$k_2 = y_n + \frac{h}{2}f(k_1)$

$k_3 = y_n + \frac{h}{2}f(k_2)$

$k_4 = y_n + hf(k_3)$

$y_{n+1} = y_n + \frac{h}{6}f(k_1) + \frac{h}{3}f(k_2) + \frac{h}{3}f(k_3) + \frac{h}{6}f(k_4)$

2.1.2 Example

Implicit RK method of order 4

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

2.2 Multi-step methods

Multi-step methods are multi-value in nature [17]. General form of multi-step methods are

$$\sum_{m=0}^{s} \alpha_m y_{n+m} = h \sum_{m=0}^{s} b_m f(x_{n+m}, y_{n+m}) \quad n = 0, 1, 2, \ldots \tag{2.4}$$

Expanding Eq(2.4)

$$\begin{aligned} &\alpha_0 y_n + \alpha_1 y_{n+1} + \alpha_2 y_{n+2} + \ldots + \alpha_{s-1} y_{n+s-1} + \alpha_s y_{n+s} \\ &= h[b_0 f(x_n, y_n) + b_1 f(x_{n+1}, y_{n+1}) + \ldots + b_s f(x_{n+s}, y_{n+s})] \end{aligned}$$

if $\alpha_0 = \alpha_1 = \alpha_2 = \ldots = \alpha_{s-2} = 0, \quad \alpha_{s-1} = -1$ and $\alpha_s = 1$ then we will have the following Adams-Bashforth(AB) methods.

$$y_{n+s} = y_{n+s-1} + h \sum_{m=0}^{s} b_m f(x_{n+m}, y_{n+m})$$

For explicit methods $b_s = 0$ and we have the following Adams-Bashforth methods

$$y_{n+s} = y_{n+s-1} + h \sum_{m=0}^{s-1} b_m f(x_{n+m}, y_{n+m}) \tag{2.5}$$

This is s-step Adams-Bashforth methods.

2.2.1 Derivation of s=1 step Adams-Bashforth methods

By putting $s = 1$ in eq(2.5) we have

$$\begin{aligned} y_{n+1} &= y_n + h b_0 f(x_n, y_n) \\ &= y(x_n) + h b_0 f(x_n, y_n) \end{aligned}$$

To calculate b_0, we compare the numerical solution with Taylor series of exact solution.

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

By comparing,
we get $b_0 = 1$ and we have the following

$$y_{n+1} = y_n + hf(x_n, y_n) \tag{2.6}$$

Derivation of s=2 Adams-Bashfroth methods

By putting $s = 2$ in eq(2.5) we have

$$y_{n+2} = y_{n+1} + hb_o f(x_n, y_n) + hb_1 f(x_{n+1}, y_{n+1}) \tag{2.7}$$

and
$y_{n+1} = y(x_n + h) = y(x_n) + hy^{'}(x_n) + \frac{h^2}{2!}y^{''}(x_n)$
$y_{n+2} = y(x_n + 2h) = y(x_n) + 2hy^{'}(x_n) + \frac{4h^2}{2}y^{''}(x_n)$
$f(x_{n+1}, y_{n+1}) = y^{'}_{n+1} = y^{'}(x_n + h) = y^{'}(x_n) + hy^{''}(x_n) + \frac{h^2}{2}y^{'''}(x_n)$
Putting values in Eq(2.7) and comparing powers of h, h^2 we have

$$b_0 = \frac{-1}{2}, \qquad b_1 = \frac{3}{2}$$

By putting b_0 and b_1 in Eq(2.7) we have

$$y_{n+2} = y_{n+1} - \frac{1}{2}hf(x_n, y_n) + \frac{3}{2}hf(x_{n+1}, y_{n+1})$$

Similarly we can find higher order Adams-Bashforth methods.

2.2.2 Adams-Moulton(AM) methods

By putting $\alpha_0 = \alpha_1 = \alpha_2 = \ldots = \alpha_{s-2} = 0, \quad \alpha_{s-1} = -1$ and $\alpha_s = 1$ and $b_s \neq 0$ in ea(2.4) we will have s-steps Adams-Moulton methods given below

$$y_{n+s} = y_{n+s-1} + h\sum_{m=0}^{s} b_m f(x_{n+m}, y_{n+m})$$

Coefficients of Adams-Moulton methods can be find in the same way like Adams-Bashforth methods.

Example: s=1 step Adams-Moulton methods is

$$y_{n+2} = y_{n+1} + h[\tfrac{1}{2}f(x_n, y_n) + \tfrac{1}{2}f(x_{n+1}, y_{n+1})]$$

2.3 General Linear Methods(GLM)

GLM are the generalization of one step methods and multi-step methods [6]. These methods are multi-value in nature. The general form of GLM is

$$Y = hAf(Y) + Uy^{n-1} \tag{2.8}$$

$$y = hBf(Y) + Vy^{n-1} \tag{2.9}$$

Eq(2.8) will give us stages and Eq(2.9) will give us required output value. Where A,U,B,V defines GLM. As one-step methods and multi-step methods can be written in the form of GLM.
Consider RK2

$$\begin{aligned} Y_1 &= ha_{11}f(Y_1) + ha_{12}f(y_2) + y_0 \\ Y_2 &= ha_{21}f(Y_2) + ha_{22}f(y_2) + y_0 \\ y_1 &= hb_1f(Y_1) + hb_2f(y_2) + y_2 \end{aligned}$$

As RK methods have only single input, therefore $U = 1$ and $V = 1$, and we can write RK methods as follows

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

2.3.1 Symmetric general linear methods

Symmetric general linear methods requires the condition that, it should be e-qual to its adjoint [6]. Consider the GLM

$$
\begin{aligned}
Y &= hAf(Y) + Uy^{n-1} \\
y^n &= hBf(Y) + Vy^{n-1}
\end{aligned}
$$

Introduce matrix L, such that $L^2 = I$ and $LV^{-1}L = V$ i.e

$$
L = \begin{pmatrix} 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & \dots & 1 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}
$$

We present a permutation matrix P so phases of the adjoint strategy is reordered to line up with phases of actual GLM.

$$
P = \begin{pmatrix} 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & \dots & 1 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}
$$

Now with the step size $-h$ adjoint GLM is

$$
\begin{aligned}
PY &= (-h)(PUBP - PAP)(Pf(Y)) + PUV^{-1}y^n \\
Ly^{n-1} &= (-h)(LPB)(PF(Y)) + V(LY^{n-1})
\end{aligned}
$$

and time reversal symmetry implies

$$
B = LBP \tag{2.10}
$$

$$A + PAP = PUBP \tag{2.11}$$

$$U = PUV^{-1} \tag{2.12}$$

Thus if a GLM satisfies (2.10),(2.11), (2.12) then it will be symmetric.

2.3.2 Pre-consistency and consistency conditon for GLM

A numerical method is said to be pre-consistent if it exactly solve the differential equation $y^{'}(x) = 0$. Thus for a GLM

$$Y = Uy^{n-1} = Uuy(x_{n-1}) + O(h),$$
$$y^n = Uy^{n-1} = Vuy(x_{n-1}) + O(h)$$

Hence Pre-consistency condition for GLM is

$$Uu = 1 \qquad Vu = u$$

Now if we talk about the consistency condition for numerical method then it should solve exactly the differential equations $y^{'}(x) = 1$. Thus for GLM

$$Y = A1hUy^{n-1} = A1hUuy(x_{n-1}) + hUvy^{'}(x_{n-1}) + O(h^2)$$
$$y^n = B1h + Vy^{n-1} = B1h + Vuy(x_{n-1}) + hVvy^{'}(x_{n-1}) + O(h^2)$$

Therefore consistency condition for GLM is

$$B1 + Vv = u + v$$

2.3.3 Starting method

As GLM are multi-value numerical methods, therefore they required more than one input values to start [11]. We have only one-put value as initial condition and remaining values are obtained by given by starting method. Consider an $(\bar{s}+r)\times(\bar{s}+1)$ starting method S given as

$$S = \left(\begin{array}{c|c} S_1 & S_2 \\ \hline S_3 & S_4 \end{array}\right)$$

where r and $\bar{s}$ are number of approximation and stages of GLM respectively. The pre-consistency conditions for this method are

$$S_4 = u \qquad S_2 = 1$$

When input vector is obtain by starting method then GLM 'M' is applid. The order of accuracy of GLM "M" is p if

$$M \circ S - S \circ E = O(h^{p+1})$$

2.4 Symplecticity of one step method

2.4.1 RK method

Here we will discuss the symplectic strategies for the numerical conservation of Hamiltonian systems [15]. The RK methods are symplectic if it full-fils the condition given below

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0$$

i.e

$$\langle y_1, y_1\rangle = \langle y_0, y_0\rangle$$

In general

$$\langle y_n, y_n\rangle = \langle y_n - 1, y_n - 1\rangle$$

Consider

$$Y_i = Y_0 + h\sum_{j=1}^{s} a_{ij} f(Y_j)$$

For conservative systems

$$\langle Y_i, f(Y_i)\rangle = 0$$

$$\langle Y_0, f(Y_i)\rangle + h\sum_{j=1}^{s} a_{ij}\langle f(Y_j), f(Y_i)\rangle = 0 \tag{2.13}$$

The out-put value is

$$y_1 = y_0 + h\sum_{i=1}^{s} b_i f(Y_i)$$

Now

$$\langle y_1, y_1\rangle = \langle y_0, y_0\rangle + h\sum_{i=1}^{s}\langle y_0, f(Y_i)\rangle + h\sum_{j=1}^{s} b_j\langle f(Y_j), y_0\rangle + h^2\sum_{i,j=1}^{s} b_i b_j\langle f(Y_j), f(Y_i)\rangle \tag{2.14}$$

From Eq(2.13) we have

$$\langle Y_0, f(Y_i\rangle = -h\sum_{j=1}^{s} a_{ij}\langle f(Y_j), f(Y_i)\rangle$$

and

$$\langle f(Y_j), y_0\rangle = -h\sum_{i=1}^{s} a_{ji}\langle f(Y_i), f(Y_j)\rangle$$

Putting these values in Eq(2.14) we have

$$\langle y_1, y_1\rangle = \langle y_0, y_0\rangle + h\sum_{i=1}^{s} b_i(-h\sum_{j=1}^{s} a_{ij} + \langle f(Y_j, f(Y_i)\rangle) +$$

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

$$\langle y_1, y_1\rangle = \langle y_0, y_0\rangle - h^2\sum_{i,j=1}^{s} b_i a_{ij}\langle f(Y_j, f(Y_i)\rangle - h^2\sum_{i,j=1}^{s} b_j a_{ji}\langle f(Y_i), f(Y_j)\rangle + h^2\sum_{i,j=1}^{s} b_i b_j\langle f(Y_j), f(Y_i)\rangle$$

$$\langle y_1, y_1\rangle = \langle y_0, y_0\rangle - h^2\sum_{i,j=1}^{s}(b_i a_{ij} + b_j a_{ji} - b_i b_j)\langle(f(Y_i), f(Y_j)\rangle$$

from above

$$\langle y_1, y_1\rangle = \langle y_0, y_0\rangle$$

is only possible if

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

and

$$\langle(f(Y_i), f(Y_j)\rangle \neq 0$$

therefore

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0$$

This is required condition for RK method to be symplectic.

2.4.2 Sypmlectic Euler's method

Symplectic Euler's method is a modification of Euler method for solving Hamiltonian equations of motion. This method gives us better approximation than traditional Euler method. We can apply this method on differential equations of the form.

$$\frac{dy}{dx} = f(x, y)$$
$$\frac{dw}{dx} = h(x, w)$$

where f and h are functions and y and w are either scalers or vectors. General form of symplectic Euler's method is

$$w_{n+1} = w_n + hf(x_n, y_n) \tag{2.15}$$

$$y_{n+1} = y_n + hf(x_n, w_{n+1}) \tag{2.16}$$

2.4.3 Symplecticity of multi-step methods

Long term conduct of multi-step techniques for the solution of Hamiltonian systems are unsuitable [12]. Not just multi-step techniques are not symplectic, they experience the effects of parasitic solution. Tang in [19] prove that multi-steps method cannot be symplectic.

2.4.4 Symplecticity of general linear methods

GLM is a greater class of methods containing RK techniques and multi-steps technique as common case. As a result of their multi-value nature, they can not be symplectic [11], in accordance with multi-step methods. The basic one-step method can drop light on symplectic behavior of GLM. We will give the criterion for the symplecticity of GLM in Chapter 3.

Chapter 3

General linear methods for ordinary differentials equations with invariants

GLM are multi-value in nature. Our main moto is, when we apply our GLM on Hamiltonian problems, it gives the same quality result similar to the exact solution of our Hamiltonian systems. Symplecticity and time reversal symmetry are major characteristics in the selection of numerical methods for solving Hamiltonian systems. Structure of our GLM for the solution of our Hamiltonian systems should show zero parasitism i.e it must avoid parasitic growth rate.

3.0.5 G-symplectic general linear methods

Purpose of G-symplectic GLM for Hamiltonian systems is to conserve energy and full-fill the property of linear and quadratic invariants [11]. When we construct our numerical method and do numerical testing on Hamiltonian systems, we came to know that our numerical method is capable of solving Hamiltonian problems over long time integration. GLM can be RK methods [14] if $r = 1$ and can be symplectic if it satisfies the symplectic conditions. Consider the GLM

$$Y = hAf(Y) + Uy^{n-1} \tag{3.1}$$

$$Y = hBf(Y) + Vy^{n-1} \tag{3.2}$$

We may produce the criterion of linear and quadratic invariants for these methods. Introduce the G-norm as we introduce it for non-linear stability of GLM. Consider $r \times r$ symmetric matrix G with element g_{ij}

$$\langle y, z\rangle_G = \textstyle\sum_{i,j=1}^{r} g_{ij}\langle y_i, z_j\rangle,$$

Where

$$y = \begin{bmatrix} y_1 \\ \vdots \\ y_r \end{bmatrix}, \quad z = \begin{bmatrix} z_1 \\ \vdots \\ z_r \end{bmatrix}$$

Now G-norm is

$$\| y \|_G^2 = \langle y, y \rangle$$

Choose a diagonal matrix $D = d_i$ i.e

$$\langle y^{n+1}, y^{n+1} \rangle_G = \langle y^n, y^n \rangle_G + 2h \textstyle\sum_{i=1}^{s} d_i \langle Y_i, F_i \rangle$$

Where $F_i = f(Y_i)$. If general linear methods solve conservative problems having the property

$$\langle y_i, f(y) \rangle = 0$$

which means

$$\langle y^{n+1}, y^{n+1} \rangle_G = \langle y^n, y^n \rangle_G \tag{3.3}$$

because the term 2h $\sum_{i=1}^{s} d_i \langle Y_i, F_i \rangle = 0$. Methods satisfying (1.3) are called G-symplectic general linear methods.

3.0.6 Theorem

A general linear method(A, U,B,V) is G-symplectic, if there exist a symmetric $r \times r$ matrix G and a diagonal $s \times s$ matrix D such that

$$\begin{aligned} G &= V^T G V \\ DU &= B^T G V \\ DA + A^T D &= B^T G B \end{aligned}$$

Proof. Take

$$\langle y^{n+1}, y^{n+1}\rangle_G - \langle y^n, y^n\rangle_G - 2h\sum_{i=1}^{s} d_i\langle Y_i, F_i\rangle$$

using equation (3.1) and (3.2) in above relation we have

$$=\sum_{ij=1}^{r} g_{ij}\langle BhF_i + Vy_i^n, BhF_j + Vy_j^n\rangle - \sum_{i,j=1}^{r} g_{ij}\langle y_i^n, y_j^n\rangle$$

$$-2h\sum_{i=1}^{s} d_i\langle AhF_i + Uy_i^n, F_i\rangle$$

Expanding and combining the similar terms of inner product we have

$$= g_{ij}\sum_{i,j=1}^{r}\langle BhF_i, BhF_j\rangle + g_{ij}\sum_{i,j=1}^{r}\langle BhF_i, vy_j^n\rangle + g_{ij}\sum_{i,j=1}^{r}\langle$$

$$vy_i^n, BhF_j\rangle + g_{ij}\sum_{i,j=1}^{r}\langle Vy_i^n, Vy_j^n\rangle - g_{ij}\sum_{i,j=1}^{r}\langle y_i^n,$$

$$y_j^n\rangle - d_i\sum_{i,j=1}^{r}\langle AhF_i, F_j\rangle - d_i\sum_{i,j=1}^{r}\langle AhF_i, F_j\rangle - d_i\sum_{i,j=1}^{r}\langle$$

$$Uy_i^n, F_j\rangle - d_i\sum_{i,j=1}^{r}\langle Uy_i^n, F_j\rangle$$

$$= -[GV^TGV]\langle y_i^n, y_j^n\rangle - 2[DU - B^TGV]\langle y_i^{n-1}, hF_j\rangle - [DA + A^TD - B^TGB]\langle hF_i, hF_j\rangle$$

To satisfy

$$\langle y, f(y)\rangle = 0$$

We have

$$\langle y^{n+1}, y^{n+1}\rangle_G = \langle y^n, y^n\rangle_G$$

Provided

$$\begin{aligned} G &= V^T G V \\ DU &= B^T G V \\ DA + A^T D &= B^T G B \end{aligned}$$

3.1 Parasitic solution

Parasitism is related to biological term parasites which means any extra thing that exist in any species and can have harmful effects on them. In a similar way when we talk about a numerical method i.e if there exists a term which disturbed our numerical method, then that term will refer to as parasitism and it must be removed in order to have good quality results. It has been observed that parasitic factor grow while solving general linear methods for Hamiltonian systems. We may study it as follows

Consider a GLM

$$\left[\begin{array}{c} Y_1 \\ Y_2 \\ \hline y_1^n \\ y_2^n \end{array}\right] = \left[\begin{array}{cc|cc} a_{11} & a_{11} & u_{11} & u_{12} \\ a_{21} & a_{22} & u_{21} & u_{22} \\ \hline b_{11} & b_{12} & 1 & 0 \\ b_{21} & b_{22} & 0 & -1 \end{array}\right] \left[\begin{array}{c} hF_1 \\ hF_2 \\ \hline y_1^{n-1} \\ y_2^{n-1} \end{array}\right],$$

where $F_i = f(Y_i)$. Here we have V is 1 and -1.
Stages:

$$Y_i = h\sum_{j=1}^{2} a_{ij}F_j + u_{i1}y_1^[n-1] + u_{i2}y_2^[n-1], \qquad i = 1, 2,$$

Output values:

$$\begin{aligned} y_1^{[n]} &= h\sum_{i=1}^{2} b_{1i}F_i + y_1^{[n-]}, \\ y_2^{[n]} &= h\sum_{i=1}^{2} b_{2i}F_i - y_2^{[n-1]}. \end{aligned}$$

Here y_1^n is approximate solution of our numerical method while y_2^n is parasitic solution. Now in order to have free parasitic solution we will make a little change i.e perturbation to y_2^n given below

$$y_2^{[n-1]} \longrightarrow y_2^{[n-1]} + (-1)^{n-1}\varphi_{n-1}.$$

There we have the following changes in Y_i as follows,

$$\begin{aligned} Y_i + \delta Y_i &= h\sum_{j=1}^{2} a_{ij}F_j + u_{i1}y_1^{[n-1]} + u_{i2}(y_2^{[n-1]} + (-1)^{n-1}\varphi_{n-1}), \\ \Rightarrow \delta Y_i &= (-1)^{n-1}u_{i2}\varphi_{n-1}. \end{aligned}$$

The stage derivatives F_i will become as follows,

$$\begin{aligned} F_i + \delta F_i &= f(Y_i + \delta Y_i) \\ &= f(Y_i) + \delta Y_i \frac{\partial f}{\partial y}, \\ \Rightarrow \delta F_i &= \delta Y_i \frac{\partial f}{\partial y} \\ &= (-1)^{n-1}\frac{\partial f}{\partial y}u_{i2}\varphi_{n-1}. \end{aligned}$$

By simplifying, we will have the following changes in second output value as follows

$$
\begin{aligned}
y_2^{[n]} + (-1)^n \varphi_n &= h \sum_{i=1}^{2} b_{2i}(F_i + \delta F_i) - (y_2^{[n-1]} + (-1)^{n-1}\varphi_{n-1}) \\
&= h \sum_{i=1}^{2} b_{2i} F_i - y_2^{[n-1]} + (-1)^{n-1} h \sum_{i=1}^{2} \frac{\partial f}{\partial y} b_{2i} u_{i2} \varphi_{n-1} - (-1)^{n-1}\varphi_{n-1}, \\
\Rightarrow \varphi_n &= \big(1 - h \sum_{i=1}^{2} \frac{\partial f}{\partial y} b_{2i} u_{i2}\big) \varphi_{n-1}.
\end{aligned}
$$

This represents Euler method solving the differential equation,

$$
\varphi' = \mu \frac{\partial f}{\partial y} \varphi, \tag{3.4}
$$

where $\mu = -\sum_{i=1}^{2} b_{2i} u_{i2}$ is the caure of Parasitic solution . We can find μ from the matrix product,

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

By putting $\mu = 0$ we can have our required soluion free from parasitism .

3.2 Order 2 G-symplectic general linear methods

G-symplectic general linear methods of order 2 was presented by Butcher in [6]. The purpose of this method was to obtain conservative solution of Hamiltonian problems. It is being observed while constructing the GLM having order 2 that parasitic factor grows and is unable to remove. we can only have parasitic free GLM having an order greater than 2. The GLM of order 2 has the following structure

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{cc|cc} a_{11} & 0 & 1 & u_{12} \\ a_{21} & a_{22} & 1 & u_{22} \\ \hline b_{11} & b_{12} & v_{11} & v_{12} \\ b_{21} & b_{22} & v_{21} & v_{22} \end{array}\right],$$

with,

$$G = \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix}, \qquad D = \begin{bmatrix} d_1 & 0 \\ 0 & d_2 \end{bmatrix}.$$

We can see that the structure of A matrix is lower triangular and the matrix U have elements $u_{11} = 1$ $u_{21} = 1$ because it will multiply with the input values while calculating the stages. As we have discuss above the G-symplectic conditions for general linear methods, here we will use these conditions in the construction of this method.

Consider

$$G = V^T G V,$$

By putting values in above relation we have

$$\begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix} = \begin{bmatrix} v_{11} & v_{12} \\ v_{21} & v_{22} \end{bmatrix} \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix} \begin{bmatrix} v_{11} & v_{12} \\ v_{21} & v_{22} \end{bmatrix},$$

$$g_{11} = v_{11}^2 g_{11} + v_{11}v_{12}g_{21} + v_{11}v_{12}g_{12} + v_{12}v_{21}g_{22},$$

$$g_{12} = v_{11}v_{12}g_{11} + v_{12}^2 g_{21} + v_{11}v_{22}g_{12} + v_{12}v_{22}g_{22},$$

$$g_{21} = v_{21}v_{11}g_{11} + v_{22}v_{11}g_{21} + v_{21}^2 g_{12} + v_{22}v_{21}g_{21}.$$

$$g_{22} = v_{21}v_{12}g_{11} + v_{22}v_{12}g_{12} + v_{21}g_{12}v_{22} + v_{22}^2 g_{12}$$

Now compare the above results on both sides

$$G = \begin{bmatrix} 1 & 0 \\ 0 & g \end{bmatrix}, \qquad V = \begin{bmatrix} 1 & 0 \\ 0 & v \end{bmatrix}.$$

Let $v = -1$

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

As we are constructing a symmetric method, stages and output values are,

$$\begin{aligned}
Y_1 &= ha_{11}F_1 + y_1^{[0]} + u_{12}y_2^{[0]}, \\
Y_2 &= ha_{21}F_1 + ha_{22}F_2 + y_1^{[0]} + u_{22}y_2^{[0]}, \\
y_1^{[1]} &= hb_{11}F_1 + hb_{12}F_2 + y_1^{[0]}, \\
y_2^{[1]} &= hb_{21}F_1 + hb_{22}F_2 - y_2^{[0]}.
\end{aligned}$$

Here the step size is h therefore Y_1 will be calculated at c_1 and that Y_2at c_2. But if we have a step size $-h$ then Y_1 will be calculated at c_2 and that of Y_2 at c_1. Here we will have our input values $[Y_1^1, Y_2^1]$ and out put value is

$$\begin{aligned}
y_1^{[0]} &= -hb_{11}F_2 - hb_{12}F_1 + y_1^{[1]}, \\
y_2^{[0]} &= -hb_{21}F_2 - hb_{22}F_1 - y_2^{[1]}.
\end{aligned}$$

This implies,

$$\begin{aligned}
y_1^{[1]} &= +hb_{11}F_2 + hb_{12}F_1 + y_1^{[0]}, \\
y_2^{[1]} &= -hb_{21}F_2 - hb_{22}F_1 - y_2^{[0]}.
\end{aligned}$$

As the method is symmetric therefore output values will be equal at step size h and -h.

$$b_{11} = b_{12}, \qquad b_{22} = -b_{21}.$$

Now consider the G-symplectic condition,

$$B^T G V = DU,$$
$$\begin{bmatrix} b_{11} & -gb_{21} \\ b_{11} & gb_{21} \end{bmatrix} = \begin{bmatrix} d_1 & d_1 u_{12} \\ d_2 & d_2 u_{22} \end{bmatrix}.$$

By comparing we get,

$$D = \begin{bmatrix} b_{11} & 0 \\ 0 & b_{11} \end{bmatrix}, \qquad U = \begin{bmatrix} 1 & -g\frac{b_{21}}{b_{11}} \\ 1 & g\frac{b_{21}}{b_{11}} \end{bmatrix}.$$

Let $x = b_{21}/b_{11}$, then the structure of the general linear method become,

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{cc|cc} a_{11} & 0 & 1 & -gx \\ a_{21} & a_{22} & 1 & gx \\ \hline b_{11} & b_{11} & 1 & 0 \\ b_{11}x & -b_{11}x & 0 & -1 \end{array}\right],$$

$$G = \begin{bmatrix} 1 & 0 \\ 0 & g \end{bmatrix}, \qquad D = \begin{bmatrix} b_{11} & 0 \\ 0 & b_{11} \end{bmatrix}.$$

Now consider the matrix product,

$$\begin{aligned} BU &= \begin{bmatrix} b_{11} & b_{11} \\ b_{11}x & -b_{11}x \end{bmatrix} \begin{bmatrix} 1 & -gx \\ 1 & gx \end{bmatrix} \\ &= \begin{bmatrix} 2b_{11} & 0 \\ 0 & -2gb_{11}x^2 \end{bmatrix}. \end{aligned}$$

To avoid parasitism we must have,

$$-2gb_{11}x^2 = 0.$$

Since, $g \neq 0$, $b_{11} \neq 0$, so the only option is $x^2 = 0$, which is impossible because if $x^2 = 0$ that second component of general linear method will fail to exist and our general linear method will become Runge-Kutta method. Hence we can not have general linear method free from parasitism with order two and two stages. The matrix B can be written as,

$$\begin{aligned} B &= \begin{bmatrix} b_{11} & b_{11} \\ b_{11}x & -b_{11}x \end{bmatrix} \\ &= \begin{bmatrix} 1 & 1 \\ x & -x \end{bmatrix} \begin{bmatrix} b_{11} & 0 \\ 0 & b_{11} \end{bmatrix} \\ &= XD. \end{aligned}$$

$$\begin{aligned} DA + A^T D &= B^T G B, \\ \begin{bmatrix} 2a_{11} & a_{21} \\ a_{21} & 2a_{22} \end{bmatrix} &= X^T G X D, \\ \begin{bmatrix} 2a_{11} & a_{21} \\ a_{21} & 2a_{22} \end{bmatrix} &= \begin{bmatrix} 1 & x \\ 1 & -x \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & g \end{bmatrix} \begin{bmatrix} 1 & 1 \\ x & -x \end{bmatrix} \begin{bmatrix} b_{11} & 0 \\ 0 & b_{11} \end{bmatrix} \\ &= \begin{bmatrix} b_{11}(1+gx^2) & b_{11}(1-gx^2) \\ b_{11}(1-gx^2) & b_{11}(1+gx^2) \end{bmatrix}. \end{aligned}$$

This implies,

$$\begin{aligned} a_{11} &= \frac{b_{11}}{2}(1+gx^2), \\ a_{21} &= b_{11}(1-gx^2), \\ a_{22} &= a_{11}. \end{aligned}$$

Relative order conditions are,

$$\begin{aligned} b_{11} + b_{11} &= 1, \\ \Rightarrow b_{11} &= \tfrac{1}{2}. \end{aligned}$$

The second order condition is,

$$b_{11}(c_1+c_2)=\tfrac{1}{2},$$
$$\Rightarrow c_1=1-c_2.$$

The third order condition is,

$$b_{11}(c_1^2+c_2^2)=\tfrac{1}{3},$$
$$c_1^2-c_1+\tfrac{1}{3}=0,$$
$$\Rightarrow c_1=\tfrac{3\pm\sqrt{3}}{6}.$$

Since $a_{11}=c_1$, we get,

$$gx^2=\tfrac{3+2\sqrt{3}}{3}.$$

Choose$c_1=\frac{3-\sqrt{3}}{6}$ $x=1$ and we have

$$b_{11}=b_{21}=\tfrac{1}{2}.$$

The GLM is,

$$N:\quad \left[\begin{array}{cc|cc} \frac{3-\sqrt{3}}{6} & 0 & 1 & -\frac{3-2\sqrt{3}}{3} \\ \frac{\sqrt{3}}{3} & \frac{3-\sqrt{3}}{6} & 1 & \frac{3-2\sqrt{3}}{3} \\ \hline \frac{1}{2} & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 & -1 \end{array}\right], \tag{3.5}$$

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

The GLM (3.5) have parasitism, and its parameter is

$$\mu_1=1-\tfrac{2}{\sqrt{3}}.$$

Starting method for GLM (3.5) is,

$$\left[\begin{array}{cc|c} \frac{3-\sqrt{3}}{6} & 0 & 1 \\ -\frac{3-\sqrt{3}}{3} & \frac{3-\sqrt{3}}{6} & 1 \\ \hline 0 & 0 & 1 \\ -\frac{\sqrt{3}+1}{8} & \frac{\sqrt{3}+1}{8} & 0 \end{array}\right]. \tag{3.6}$$

3.3 Order 4 G-symplectic general linear methods

Order 4 G-symplectic GLM was constructed by Y.Habib in [10]. The need for these methods were to obtain a symmetrical method that gives us the parasitic free solution which was not given by two stages general linear methods. The structure of this method given as

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{cccc|ccc} a_{11} & 0 & 0 & 0 & 1 & u_{12} & u_{13} \\ a_{21} & a_{22} & 0 & 0 & 1 & u_{22} & u_{23} \\ a_{31} & a_{32} & a_{33} & 0 & 1 & u_{32} & u_{33} \\ a_{41} & a_{42} & a_{43} & a_{44} & 1 & u_{42} & u_{43} \\ \hline b_{11} & b_{12} & b_{13} & b_{14} & 1 & 0 & 0 \\ b_{21} & b_{22} & b_{23} & b_{24} & 0 & z & 0 \\ \bar{b}_{21} & \bar{b}_{22} & \bar{b}_{23} & \bar{b}_{24} & 0 & 0 & \bar{z} \end{array}\right],$$

with,

$$G = \begin{bmatrix} 1 & 0 & 0 \\ 0 & g & 0 \\ 0 & 0 & g \end{bmatrix}, \qquad D = \begin{bmatrix} d_{11} & 0 & 0 & 0 \\ 0 & d_{22} & 0 & 0 \\ 0 & 0 & d_{33} & 0 \\ 0 & 0 & 0 & d_{44} \end{bmatrix}.$$

We can see that structure of A matrix is lower triangular similar to 2 stage method. The matrix U has elements in first column is all one i.e $u_{11} = 1$ $u_{21} = 1$, $u_{31} = 1$ and$u_{41} = 1$ because it will multiply with the input values while calculating the stages. For pre consistency vector u we have

$$Uu = \mathbf{1}, \qquad Vu = u.$$

B matrix have second and third row similar but they are conjugate complex of each other. The structure of V matrix is diagonal.The elements in V are conjugate complex of each other i.e one is z and other is $\bar{z}$. We will chose

$$z = e^{\frac{2\pi i}{3}}$$

We are using complex numbers here because we may convert it into real numbers via transformation. Vital role will done by Time reversal symmetry in the construction of GLM. Here we have stages

$$\begin{bmatrix} \widetilde{Y}_1 \\ \widetilde{Y}_2 \\ \widetilde{Y}_3 \\ \widetilde{Y}_4 \end{bmatrix} = P \begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \end{bmatrix},$$

where,

$$P = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

By using symplectic conditions we will have our required four stages three input value method(GLM). After getting our GLM we will convert it into real numbers via transformation which is given below

$$\gamma = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{i}{2} \\ 0 & \frac{1}{2} & -\frac{i}{2} \end{bmatrix}. \tag{3.7}$$

The GLM will be converted into real as

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] \longrightarrow \left[\begin{array}{c|c} A & U\gamma \\ \hline \gamma^{-1}B & \gamma^{-1}V\gamma \end{array}\right],$$

with,

$$G \longrightarrow \gamma^{*}G\gamma,$$

where,

$$\gamma^{*} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & -i & i \end{bmatrix}.$$

The general linear method thus become,

$$\left[\begin{array}{cccc|ccc}
0 & 0 & 0 & 0 & 1 & \frac{1}{4} & \frac{\sqrt{3}}{4} \\
-\frac{11}{72} & \frac{1}{4} & 0 & 0 & 1 & -\frac{1973}{29068}+\frac{2\sqrt{3}\sqrt{14595}}{7267} & -\frac{1973\sqrt{3}}{29068}-\frac{2\sqrt{14595}}{7267} \\
-\frac{2647}{72240} & \frac{1009}{1680} & \frac{1}{4} & 0 & 1 & \frac{1973}{29068}-\frac{2\sqrt{3}\sqrt{14595}}{7267} & \frac{1973\sqrt{3}}{29068}+\frac{2\sqrt{14595}}{7267} \\
-\frac{169}{1680} & \frac{113821}{283920} & \frac{473}{676} & 0 & 1 & -\frac{1}{4} & -\frac{\sqrt{3}}{4} \\
\hline
-\frac{169}{3360} & \frac{1849}{3360} & \frac{1849}{3360} & -\frac{169}{3360} & 1 & 0 & 0 \\
-\frac{169}{1680} & -\frac{84839}{283920} & \frac{84839}{283920} & \frac{169}{1680} & 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\
0 & -\frac{43\sqrt{14595}}{35490} & \frac{43\sqrt{14595}}{35490} & 0 & 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2}
\end{array}\right], \tag{3.8}$$

with,

$$G=\begin{bmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{4} & 0 \\ 0 & 0 & -\frac{1}{4} \end{bmatrix}, \qquad D=\begin{bmatrix} -\frac{169}{3360} & 0 & 0 & 0 \\ 0 & \frac{1849}{3360} & 0 & 0 \\ 0 & 0 & \frac{1849}{3360} & 0 \\ 0 & 0 & 0 & -\frac{169}{3360} \end{bmatrix}.$$

A suitable starting method for this GLM is

$$\left[\begin{array}{cccc|c}
0 & 0 & 0 & 0 & 1 \\
\frac{1}{2} & 0 & 0 & 0 & 1 \\
0 & \frac{1}{2} & 0 & 0 & 1 \\
0 & 0 & 1 & 0 & 1 \\
\hline
0 & 0 & 0 & 0 & 1 \\
\tilde{b}_1 & \tilde{b}_2 & \tilde{b}_3 & \tilde{b}_4 & 0 \\
\tilde{b}_5 & \tilde{b}_6 & \tilde{b}_7 & \tilde{b}_8 & 0
\end{array}\right], \tag{3.9}$$

where,

$$\begin{bmatrix} \tilde{b}_1 \\ \tilde{b}_2 \\ \tilde{b}_3 \\ \tilde{b}_4 \\ \tilde{b}_5 \\ \tilde{b}_6 \\ \tilde{b}_7 \\ \tilde{b}_8 \end{bmatrix} = \begin{bmatrix} -0.203599283611326 \\ 0.093013520189574 \\ 0.079026915254744 \\ 0.031558848167008 \\ -0.523240277404552 \\ 0.399628138816171 \\ 0.388537971512798 \\ -0.264925832924417 \end{bmatrix}.$$

3.4 Order 6 G-symplectic general linear methods

The structure of G-symplectic GLM with order 6 is given below

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{ccccc|cccc} a_{11} & 0 & 0 & 0 & 0 & 1 & u_{12} & u_{13} & u_{14} \\ a_{21} & a_{22} & 0 & 0 & 0 & 1 & u_{22} & u_{23} & u_{24} \\ a_{31} & a_{32} & a_{33} & 0 & 0 & 1 & u_{32} & u_{33} & u_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} & 0 & 1 & u_{42} & u_{43} & u_{44} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} & 1 & u_{52} & u_{53} & u_{54} \\ \hline b_1 & b_2 & b_3 & b_2 & b_1 & 1 & 0 & 0 & 0 \\ b_1\omega_1 & b_2\omega_2 & b_3\omega_3 & b_2\omega_4 & b_1\omega_5 & 0 & z & 0 & 0 \\ b_1\bar{\omega_1} & b_2\bar{\omega_2} & b_3\bar{\omega_3} & b_2\bar{\omega_4} & b_1\bar{\omega_5} & 0 & 0 & \bar{z} & 0 \\ b_1\gamma_1 & b_2\gamma_2 & b_3\gamma_3 & b_2\gamma_4 & b_1\gamma_5 & 0 & 0 & 0 & -1 \end{array}\right]$$

with

$$G = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & g & 0 & 0 \\ 0 & 0 & g & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \qquad D = \begin{bmatrix} d_{11} & 0 & 0 & 0 & 0 \\ 0 & d_{22} & 0 & 0 & 0 \\ 0 & 0 & d_{33} & 0 & 0 \\ 0 & 0 & 0 & d_{44} & 0 \\ 0 & 0 & 0 & 0 & d_{55} \end{bmatrix}$$

We can see that this method is categorized into four matrices (A, U, B, V). The matrix is lower triangular and all the entries in the first column of the matrix U are ones i.e $u_{11} = 1$ $u_{21} = 1$ $u_{31} = 1$ $u_{41} = 1$ $u_{51} = 1$ because it will multiply with the input values in order to calculate our stages. To analyze our solution of Hamiltonian problems with these methods, entries in

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right]$$

are complex because we may convert our complex entries into real via transformation. Structure of V is diagonal and two of its entries are a conjugate complex of each other. As we are constructing a symmetric and symplectic method so the method should satisfy the G-symplectic conditions given below,

$$\begin{aligned} G &= V^*GV && (3.10) \\ DU &= B^*GV && (3.11) \\ DA + A^TD &= B^*GB && (3.12) \end{aligned}$$

Here * is conjugate transpose.
We will choose value $z = e^{\frac{2\pi i}{3}}$, from equation(3.10) G is diagonal and we can assume it by [9]

$$G = diag(1, \pm\tfrac{1}{2}, \pm\tfrac{1}{2}, \pm 1)$$

In this method we will choose $G = diag(1, -\frac{1}{2}, -\frac{1}{2}, 1)$ To see the effect of Time reversal symmetry, consider the GLM as

$$\begin{aligned}
Y_1 &= ha_{11}f(y_1) + y_1^{[0]} + u_{12}y_2^{[0]} + u_{13}y_3^{[0]} + u_{14}y_4^{[0]} \\
Y_2 &= ha_{21}f(y_1) + ha_{22}f(y_2) + y_1^{[0]} + u_{22}y_2^{[0]} + u_{23}y_3^{[0]} + u_{24}y_4^{[0]} \\
Y_3 &= ha_{31}f(y_1) + ha_{32}f(y_2) + ha_{33}f(y_3) + y_1^{[0]} + u_{32}y_2^{[0]} + u_{33}y_3^{[0]} + u_{34}y_4^{[0]} \\
Y_4 &= ha_{41}f(y_1) + ha_{42}f(y_2) + ha_{43}f(y_3) + ha_{44}f(y_4) + y_1^{[0]} + u_{42}y_2^{[0]} + u_{43}y_3^{[0]} + u_{44}y_4^{[0]} \\
Y_5 &= ha_{51}f(y_1) + ha_{52}f(y_2) + ha_{53}f(y_3) + ha_{54}f(y_4) + y_1^{[0]} + u_{52}y_2^{[0]} + u_{53}y_3^{[0]} + u_{54}y_4^{[0]}
\end{aligned}$$

and

$$
\begin{aligned}
y_1^{[1]} = & \quad hb_1 f(y_1) + hb_2 f(y_2) + hb_3 f(y_3) + hb_2 f(y_4) + hb_1 f(y_5) + y_1^{[0]} \\
y_2^{[1]} = & \quad hb_1\omega_1 f(y_1) + hb_2\omega_2 f(y_2) + hb_3\omega_3 f(y_3) + hb_2\omega_4 f(y_4) + hb_1\omega_5 f(y_5) + zy_2^{[0]} \\
y_3^{[1]} = & \quad hb_1\bar{\omega_1} f(y_1) + hb_2\bar{\omega_2} f(y_2) + hb_3\bar{\omega_3} f(y_3) + hb_2\bar{\omega_4} f(y_4) + hb_1\bar{\omega_5} f(y_5) + \bar{z}y_3^{[0]} \\
y_4^{[1]} = & \quad hb_1\gamma_1 f(y_1) + hb_2\gamma_2 f(y_2) + hb_3\gamma_3 f(y_3) + hb_2\gamma_4 f(y_4) + hb_1\gamma_5 f(y_5) - y_4^{[0]} \\
\tilde{Y_1} = & \quad -ha_{11} f(y_1) + y_1^{[1]} + u_{12}y_2^{[1]} + u_{13}y_3^{[1]} + u_{14}y_4^{[1]}
\end{aligned}
$$

$= h(-a_{11} + b_1 + u_{12}b_1\omega_1 + u_{13}b_1\bar{\omega_1} + u_{14}b_1\gamma_1)f(y_1) + h(b_2 + u_{12}b_2\omega_2 + u_{13}b_2\bar{\omega_2} +$

$u_{14}b_2\gamma_2)f(y_2)$

$+h(b_3+u_{12}b_3\omega_3+u_{13}b_3\bar{\omega_3}+u_{14}b_3\gamma_3)f(y_3)+h(b_2+u_{12}b_2\omega_4+u_{13}b_2\bar{\omega_4}+u_{14}b_2\gamma_4)f(y_4)$

$+ h(b_1 + u_{12}b_1\omega_5 + u_{13}b_1\bar{\omega_5} + u_{14}b_1\gamma_5)f(y_5) + y_1^{[0]} + u_{12}zy_2^{[0]} + u_{13}\bar{z}y_3^{[0]} - u_{14}y_4^{[0]}$

Now

$\tilde{Y_5} = -ha_{51}f(y_5) - ha_{52}f(y_4) - ha_{53}f(y_3) - ha_{54}f(y_4) + y_1^{[1]} + u_{52}y_2^{[1]} + u_{53}y_3^{[1]} + u_{54}y_4^{[1]}$

$= h(b_1 + u_{12}b_1\omega_1 + u_{13}b_1\bar{\omega_1} + u_{14}b_1\gamma_1)f(y_1) + h(-a_{54} + b_2 + u_{52}b_2\omega_2 + u_{53}b_2\bar{\omega_2} +$

$u_{54}b_2\gamma_2)f(y_2) + h(b_3 - a_{53} + u_{52}b_3\omega_3 + u_{53}b_3\bar{\omega_3} + u_{54}b_3\gamma_3)f(y_3) + h(b_2 - a_{52} + u_{52}b_2\omega_4 +$

$u_{53}b_2\bar{\omega_4} + u_{54}b_2\gamma_4)f(y_4) + h(b_1 - a_{51} + u_{52}b_1\omega_5 + u_{53}b_1\bar{\omega_5} + u_{54}b_1\gamma_5)f(y_5) + y_1^{[0]} +$

$u_{52}zy_2^{[0]} + u_{53}\bar{z}y_3^{[0]} - u_{54}y_4^{[0]}$

Comparing Y_1 with $\tilde{Y_5}$ and $\tilde{Y_1}$ with Y_5we get

$$u_{52} = u_{12}, \qquad u_{53} = u_{13}, \qquad u_{54} = u_{14}$$

Similarly it can be shown that

$$u_{42} = u_{43}, \qquad u_{43} = u_{23}, \qquad u_{44} = u_{24}$$

and

$$u_{32} = u_{32}, \qquad u_{33} = u_{33}, \qquad u_{34} = u_{34}$$

now applying (3.11)

$$\text{DU=}\begin{bmatrix} d_{11} & 0 & 0 & 0 & 0 \\ 0 & d_{22} & 0 & 0 & 0 \\ 0 & 0 & d_{33} & 0 & 0 \\ 0 & 0 & 0 & d_{44} & 0 \\ 0 & 0 & 0 & 0 & d_{55} \end{bmatrix} \begin{bmatrix} 1 & u_{12} & u_{13} & u_{14} \\ 1 & u_{22} & u_{23} & u_{24} \\ 1 & u_{32} & u_{33} & u_{34} \\ 1 & u_{22} & u_{23} & u_{24} \\ 1 & u_{12} & u_{13} & u_{14} \end{bmatrix}$$

$$\text{DU=}\begin{bmatrix} d_{11} & d_{11}u_{12} & d_{11}u_{13} & d_{11}u_{14} \\ d_{22} & d_{22}u_{22} & d_{22}u_{23} & d_{22}u_{24} \\ d_{33} & d_{33}u_{32} & d_{33}u_{33} & d_{33}u_{34} \\ d_{44} & d_{44}u_{22} & d_{44}u_{23} & d_{44}u_{24} \\ d_{55} & d_{55}u_{12} & d_{55}u_{13} & d_{55}u_{14} \end{bmatrix}$$

$$B^*GV = \begin{bmatrix} b_1 & b_1\bar{\omega_1} & b_1\omega_1 & b_1\gamma_1 \\ b_2 & b_2\bar{\omega_2} & b_2\omega_2 & b_2\gamma_2 \\ b_3 & b_3\bar{\omega_3} & b_3\omega_3 & b_3\gamma_3 \\ b_2 & b_2\bar{\omega_4} & b_2\omega_4 & b_2\gamma_4 \\ b_1 & b_1\bar{\omega_5} & b_1\omega_5 & b_1\gamma_5 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & g & 0 & 0 \\ 0 & 0 & g & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & z & 0 & 0 \\ 0 & 0 & \bar{z} & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

$$B^*GV = \begin{bmatrix} b_1 & b_1\bar{\omega_1}gz & b_1\omega_1 g\bar{z} & -b_1\gamma_1 \\ b_2 & b_2\bar{\omega_2}gz & b_2\omega_2 g\bar{z} & -b_2\gamma_2 \\ b_3 & b_3\bar{\omega_3}gz & b_3\omega_3 g\bar{z} & -b_3\gamma_3 \\ b_2 & b_2\bar{\omega_4}gz & b_2\omega_4 g\bar{z} & -b_2\gamma_4 \\ b_1 & b_1\bar{\omega_5}gz & b_1\omega_5 g\bar{z} & -b_1\gamma_5 \end{bmatrix}$$

$equating\ \ DU\ \ and\ \ B^*GV\ \ we\ \ get$

D= $\begin{bmatrix} b_1 & 0 & 0 & 0 & 0 \\ 0 & b_2 & 0 & 0 & 0 \\ 0 & 0 & b_3 & 0 & 0 \\ 0 & 0 & 0 & b_2 & 0 \\ 0 & 0 & 0 & 0 & b_1 \end{bmatrix}$ and $U = \begin{bmatrix} 1 & \bar{\omega_1}gz & \omega_1 g\bar{z} & -\gamma_1 \\ 1 & \bar{\omega_2}gz & \omega_2 g\bar{z} & -\gamma_2 \\ 1 & \bar{\omega_3}gz & \omega_3 g\bar{z} & -\gamma_3 \\ 1 & \bar{\omega_4}gz & \omega_4 g\bar{z} & -\gamma_4 \\ 1 & \bar{\omega_5}gz & \omega_5 g\bar{z} & -\gamma_5 \end{bmatrix}$

as

B= $\begin{bmatrix} b_1 & b_2 & b_3 & b_2 & b_1 \\ b_1\omega_1 & b_2\omega_2 & b_3\omega_3 & b_2\omega_4 & b_1\omega_5 \\ b_1\bar{\omega_1} & b_2\bar{\omega_2} & b_3\bar{\omega_3} & b_2\bar{\omega_4} & b_1\bar{\omega_5} \\ b_1\gamma_1 & b_2\gamma_2 & b_3\gamma_3 & b_2\gamma_4 & b_1\gamma_5 \end{bmatrix}$

$$B = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ \omega_1 & \omega_2 & \omega_3 & \omega_4 & \omega_5 \\ \bar{\omega_1} & \bar{\omega_2} & \bar{\omega_3} & \bar{\omega_4} & \bar{\omega_5} \\ \gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 & \gamma_5 \end{bmatrix} \begin{bmatrix} b_1 & 0 & 0 & 0 & 0 \\ 0 & b_2 & 0 & 0 & 0 \\ 0 & 0 & b_3 & 0 & 0 \\ 0 & 0 & 0 & b_2 & 0 \\ 0 & 0 & 0 & 0 & b_1 \end{bmatrix}$$

=XD,

Now consider,

$$DA + A^*D = B^*GB$$

Now consider Lower triangular part of the follwing

$$L(DA + A^*D) = L(B^*GB)$$

$$L(DA + A^*D) = \begin{bmatrix} 2a_{11}b_1 & 0 & 0 & 0 & 0 \\ b_2a_{21} & 2a_{22}b_2 & 0 & 0 & 0 \\ b_3a_{31} & b_3a_{32} & 2a_{33}b_3 & 0 & 0 \\ b_2a_{41} & b_2a_{42} & b_2a_{43} & 2a_{44}b_2 & 0 \\ b_1a_{51} & b_1a_{52} & b_1a_{53} & b_1a_{54} & 2a_{55}b_1 \end{bmatrix}$$

$$= \begin{bmatrix} b_1 & 0 & 0 & 0 & 0 \\ 0 & b_2 & 0 & 0 & 0 \\ 0 & 0 & b_3 & 0 & 0 \\ 0 & 0 & 0 & b_2 & 0 \\ 0 & 0 & 0 & 0 & b_1 \end{bmatrix} \begin{bmatrix} 2a_{11} & 0 & 0 & 0 & 0 \\ a_{21} & 2a_{22} & 0 & 0 & 0 \\ a_{31} & a_{32} & 2a_{33} & 0 & 0 \\ a_{41} & a_{42} & a_{43} & 2a_{44} & 0 \\ a_{51} & a_{52} & a_{53} & a_{54} & 2a_{55} \end{bmatrix}$$

=DY Thus

$$DY = L(B^*GB) = L(DX^*GXD),$$

$$Y = L(X^*GXD) \tag{3.13}$$

From the relation (3.13)

$a_{11} = \frac{1}{2}(1 + 2\omega_1\bar{\omega_1}g + \gamma_1^2)b_1$

$a_{21} = (1 + \bar{\omega_2}\omega_1 g + \omega_2\bar{\omega_1}g + \gamma_2\gamma_1)b_1$

$a_{22} = \frac{1}{2}(1 + 2\bar{\omega_2}\omega_2 g + \gamma_2^2)b_2$

$a_{31} = (1 + \bar{\omega_3}\omega_1 g + \omega_3\bar{\omega_1} g + \gamma_3\gamma_1)b_1$

$a_{32} = (1 + \bar{\omega_3}\omega_2 g + \omega_3\bar{\omega_2} g + \gamma_3\gamma_2)b_2$

$a_{33} = \frac{1}{2}(1 + 2\bar{\omega_3}\omega_3 g + \gamma_3^2)b_3$

$a_{41} = (1 + \bar{\omega_4}\omega_1 g + \omega_4\bar{\omega_1} g + \gamma_4\gamma_1)b_1$

$a_{42} = (1 + \bar{\omega_4}\omega_2 g + \omega_4\bar{\omega_2} g + \gamma_4\gamma_2)b_2$

$a_{43} = (1 + \bar{\omega_4}\omega_3 g + \omega_4\bar{\omega_3} g + \gamma_4\gamma_3)b_3$

$a_{44} = \frac{1}{2}(1 + 2\bar{\omega_4}\omega_4 g + \gamma_4^2)b_2$

$a_{51} = (1 + \bar{\omega_5}\omega_1 g + \omega_5\bar{\omega_1} g + \gamma_5\gamma_1)b_1$

$a_{52} = (1 + \bar{\omega_5}\omega_2 g + \omega_5\bar{\omega_2} g + \gamma_5\gamma_2)b_2$

$a_{53} = (1 + \bar{\omega_5}\omega_3 g + \omega_5\bar{\omega_3} g + \gamma_5\gamma_3)b_3$

$a_{54} = (1 + \bar{\omega_5}\omega_4 g + \omega_5\bar{\omega_4} g + \gamma_5\gamma_4)b_2$

$a_{55} = \frac{1}{2}(1 + 2\omega_5\bar{\omega_5} g + \gamma_5^2)b_1$

above equations can also be written as

$$a_{ij} = b_j(1 - \alpha_i\alpha_j - \beta_i\beta_j + \gamma_i\gamma_j) \qquad j < i \tag{3.14}$$

$$a_{ij} = b_j(1 - \alpha_i\alpha_j - \beta_i\beta_j + \gamma_i\gamma_j) \qquad j = i \tag{3.15}$$

$$a_{ij} = 0 \qquad j > i \tag{3.16}$$

where $\omega_i = \alpha_i + \iota\beta_i$ and symmetry conditions $\alpha_3 = 0$,$\alpha_4 = -\alpha_2$,$\alpha_5 = -\alpha_1$,$\beta_4 = \beta_2$, $\beta_5 = -\beta_1$,$\gamma_4 = \gamma_2$,$\gamma_5 = \gamma_1$ will be assumed.
Select the abscissa vectors as $C = [0, c_2, 1-c_2, 1]$ and the vectors $b = [b_1, b_2, b_3, b_2, b_1]$ such that

$$b^T 1 = 1$$

$$b^T c^2 = \frac{1}{3}$$

$$b^t c^4 = \frac{1}{5}$$

Choose the abscissa vectors as $c = [0, \frac{1}{15}, \frac{1}{2}, \frac{14}{15}, 1]^T$ leading to

$b^T = [\frac{-17}{168}, \ \frac{3375}{9464}, \ \frac{248}{507}, \ \frac{3375}{9464}, \ \frac{-17}{168}]$

Now we will find the parasitism condition i.e by putting the diagonal elements

of BU=0 and we have the following

$$BU = \begin{bmatrix} b_1 & b_2 & b_3 & b_2 & b_1 \\ b_1\omega_1 & b_2\omega_2 & b_3\omega_3 & b_2\omega_4 & b_1\omega_5 \\ b_1\bar{\omega_1} & b_2\bar{\omega_2} & b_3\bar{\omega_3} & b_2\bar{\omega_4} & b_1\bar{\omega_5} \\ b_1\gamma_1 & b_2\gamma_2 & b_3\gamma_3 & b_2\gamma_4 & b_1\gamma_5 \end{bmatrix} \begin{bmatrix} 1 & \bar{\omega_1}gz & \omega_1 g\bar{z} & -\gamma_1 \\ 1 & \bar{\omega_2}gz & \omega_2 g\bar{z} & -\gamma_2 \\ 1 & \bar{\omega_3}gz & \omega_3 g\bar{z} & -\gamma_3 \\ 1 & \bar{\omega_4}gz & \omega_4 g\bar{z} & -\gamma_4 \\ 1 & \bar{\omega_5}gz & \omega_5 g\bar{z} & -\gamma_5 \end{bmatrix}$$

by simplifying and equating the diagonal elements to zero we have
$b_1 g(z+\bar{z})(\alpha_1^2+\beta_1^2) + b_2 g(z+\bar{z})(\alpha_2^2+\beta_2^2) + b_3 g(z+\bar{z})(\alpha_3^2+\beta_3^2) + b_2 g(z+\bar{z})(\alpha_4^2 + \beta_4^2) + b_1 g(z+\bar{z})(\alpha_5^2+\beta_5^2) - b_1\gamma_1^2 - b_2\gamma_2^2 - b_3\gamma_3^2 - b_2\gamma_4^2 - b_1\gamma_5^2 = 0$
Define a symmetric matrix of 5×5 such that

$$W_{ij} = \alpha_i\alpha_j + \beta_i\beta_j - \gamma_i\gamma_j, \quad i,j = 1,...,5 \tag{3.17}$$

such that

$$
\begin{aligned}
W_{11} &= 1 && (3.18)\\
b_1(1-W_{12}) &= \frac{1}{2}c_2 && (3.19)\\
b_2(1-W_{22}) &= c_2 && (3.20)
\end{aligned}
$$

$$
W_{ij} = W_{6-i,6-j}
$$

$$
(i,j) = (4,3),(4,4),(5,3),(5,4),(5,5) \qquad (3.21)
$$

$$
\begin{aligned}
b_3(1-W_{33}) &= c_2 && (3.22)\\
\sum_{j=1}^{i-1} b_j(1-W_{ij} + \frac{1}{2}b_i(1-W_{ii}) &= c_i, \quad i=3,4,5 && (3.23)\\
\sum_{j=2}^{i-1} b_jc_j(1-W_{ij}) + \frac{1}{2}b_ic_i(1-W_{ii}) &= \frac{1}{2}c_i^2 \quad i=3,4,5 && (3.24)
\end{aligned}
$$

By using equations (3.18), (3.19), (3.20), (3.21), (3.22), (3.23), (3.24) we have

$$
W=\begin{bmatrix}
1 & \frac{113}{85} & \frac{-5613}{85} & \frac{-466429841}{745875} & \frac{36703237}{18785} \\
\frac{113}{85} & \frac{41161}{50625} & \frac{-65239}{3375} & \frac{-466060571}{2278125} & \frac{36946367}{57375} \\
\frac{-5613}{85} & \frac{-65239}{3375} & \frac{1071}{1240} & \frac{-65239}{3375} & \frac{-5613}{85} \\
\frac{-466429841}{745875} & \frac{-466060571}{2278125} & \frac{-65239}{3375} & \frac{41161}{50625} & \frac{113}{85} \\
\frac{36703237}{18785} & \frac{36946367}{57375} & \frac{-5613}{85} & \frac{113}{85} & 1
\end{bmatrix}
$$

By using (3.14), (3.15), (3.16) we have

$$
A=\begin{bmatrix}
0 & 0 & 0 & 0 & 0 \\
\frac{1}{30} & \frac{1}{30} & 0 & 0 & 0 \\
\frac{691}{105} & \frac{29}{4} & \frac{1}{30} & 0 & 0 \\
\frac{-16684847}{263250} & \frac{8363191}{114075} & \frac{100688}{10125} & \frac{1}{30} & 0 \\
\frac{1310159}{6630} & \frac{-658732}{2873} & \frac{1413104}{43095} & \frac{-675}{5746} & 0
\end{bmatrix}
$$

From equation (3.17)

$$W = \alpha\alpha^T + \beta\beta^T - \gamma\gamma^T$$

Make two matrices which are symmetric

$$\hat{W} = \hat{\gamma}^T W \hat{\gamma}$$
$$\tilde{W} = \tilde{\gamma} W \tilde{\gamma}^T$$

where,

$$\hat{\gamma} = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \\ 0 & 0 \\ 0 & \frac{-1}{2} \\ \frac{-1}{2} & 0 \end{bmatrix} \text{ and } \tilde{\gamma} = \begin{bmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 1 \\ 0 & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 \end{bmatrix}$$

and

$$\hat{W} = \tilde{\alpha}\tilde{\alpha}^T \text{ ,} \quad \tilde{W} = \tilde{\beta}\tilde{\beta}^T - \tilde{\gamma}\tilde{\gamma}^T, \quad \hat{\alpha} = \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} \quad \tilde{\beta} = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} \quad , \tilde{\gamma} = \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \end{bmatrix}$$

leading to

$$\hat{W} = \begin{bmatrix} -\frac{18342226}{18785} & -\frac{198163}{49725} \\ -\frac{198163}{49725} & \frac{233956408}{2278125} \end{bmatrix}$$

and

$$\tilde{W}=\begin{bmatrix} \frac{18361011}{18785} & \frac{264268}{49725} & -\frac{5613}{85} \\ \frac{264268}{49725} & -\frac{232104163}{2278125} & -\frac{65239}{3375} \\ -\frac{5613}{85} & -\frac{65239}{3375} & \frac{1071}{1240} \end{bmatrix}$$

Thus we have our required GLM

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{ccccc|cccc}
0 & 0 & 0 & 0 & 0 & 1 & -\frac{1}{2}\iota\bar{\omega_1} & \frac{1}{2}\iota\omega_1 & -\gamma_1 \\
\frac{1}{30} & \frac{1}{30} & 0 & 0 & 0 & 1 & -\frac{1}{2}\iota\bar{\omega_2} & \frac{1}{2}\iota\omega_2 & -\gamma_2 \\
\frac{691}{105} & \frac{29}{4} & \frac{1}{30} & 0 & 0 & 1 & -\frac{1}{2}\iota\bar{\omega_3} & \frac{1}{2}\iota\omega_3 & -\gamma_3 \\
\frac{-16684847}{263250} & \frac{8363191}{114075} & \frac{100688}{10125} & \frac{1}{30} & 0 & 1 & -\frac{1}{2}\iota\bar{\omega_4} & \frac{1}{2}\iota\omega_4 & -\gamma_4 \\
\frac{1310159}{6630} & \frac{-658732}{2873} & \frac{1413104}{43095} & \frac{-675}{5746} & 0 & 1 & -\frac{1}{2}\iota\bar{\omega_5} & \frac{1}{2}\iota\omega_5 & -\gamma_4 \\
\hline
\frac{-17}{168} & \frac{3375}{9464} & \frac{248}{507} & \frac{3375}{9464} & \frac{-17}{168} & 1 & 0 & 0 & 0 \\
\frac{-17}{168}\omega_1 & \frac{3375}{9464}\omega_2 & \frac{248}{507}\omega_3 & \frac{3375}{9464}\omega_4 & \frac{-17}{168}\omega_5 & 0 & e^{\frac{2\pi i}{3}} & 0 & 0 \\
\frac{-17}{168}\bar{\omega_1} & \frac{3375}{9464}\bar{\omega_2} & \frac{248}{507}\bar{\omega_3} & \frac{3375}{9464}\bar{\omega_4} & \frac{-17}{168}\bar{\omega_5} & 0 & 0 & e^{\frac{-2\pi i}{3}} & 0 \\
\frac{-17}{168}\gamma_1 & \frac{3375}{9464}\gamma_2 & \frac{248}{507}\gamma_3 & \frac{3375}{9464}\gamma_4 & \frac{-17}{168}\gamma_5 & 0 & 0 & 0 & -1
\end{array}\right]$$

with

$$G=\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \qquad D=\begin{bmatrix} \frac{-17}{168} & 0 & 0 & 0 & 0 \\ 0 & \frac{3375}{9464} & 0 & 0 & 0 \\ 0 & 0 & \frac{248}{507} & 0 & 0 \\ 0 & 0 & 0 & \frac{3375}{9464} & 0 \\ 0 & 0 & 0 & 0 & \frac{-17}{168} \end{bmatrix}$$

Thus we have G-symplectic order 6 GLM, which is symmetric and free from parasitic solution. We can also find α_i, β_i, γ_i by using[9]. A starting method is required to implement this GLM and is the aim of ongoing research.

Chapter 4

Conclusion

This thesis discusses numerical methods that preserve the energy of Hamiltonian systems . Higher order G-symplectic general linear methods were explored in this thesis. In Chapter 1 we gave a brief introduction of Hamiltonian systems. We have also discussed some numerical methods that are suitable for this framework. Details of different numerical methods are given in Chapter 2, in which there are Runge-Kutta methods, Euler's methods, linear multi-steps methods and general linear methods. We have also given criterion for symplecticity of these numerical methods. Symplecticity of general linear methods was further explored in Chapter 3. General linear methods are multi-value in nature therefore we cannot expect symplectic behavior from these methods. G-symplectic general linear methods were first obtained by Butcher, to obtain conservative solution of Hamiltonian systems, but unfortunately these methods suffer from parasitism. Later higher order G-symplectic general linear methods having order 4 were constructed with a suitable structure free from parasitism. Order 6 G-symplectic GLM were first constructed by Butcher at. al [9] with $z = \iota$. We have constructed order 6 G-symplectic GLM with $z = e^{\frac{2\pi i}{3}}$ with zero parasitism.

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