HIGHER ORDER SYMPLECTIC METHODS FOR SEPARABLE HAMILTONIAN EQUATIONS

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ABSTRACT

HIGHER ORDER SYMPLECTIC METHODS FOR SEPARABLE HAMILTONIAN EQUATIONS

The higher order, geometric structure preserving numerical integrators based on the modified vector fields are used to construct discretizations of separable Hamiltonian systems. This new approach is called as modifying integrators. Modified vector fields can be used to construct high-order structure-preserving numerical integrators for both ordinary and partial differential equations. In this thesis, the modifying vector field idea is applied to Lobatto IIIA-IIIB methods for linear and nonlinear ODE problems. In addition, modified symplectic Euler method is applied to separable Hamiltonian PDEs. Stability and consistency analysis are also studied for these new higher order numerical methods. Von Neumann stability analysis is studied for linear and nonlinear PDEs by using modified symplectic Euler method. The proposed new numerical schemes were applied to the separable Hamiltonian systems.

ÖZET

AYRILABİLİR HAMİLTON DENKLEMLER İÇİN YÜKSEK MERTEBEDEN SİMPLEKTİK METODLAR

Yüksek mertebeden, modifiye edilmiş vektör alanını esas alan geometrik yapıyı koruyan nümerik integratörler, ayrılabilir Hamilton sistemlerin diskritizasyonu için kullanılmıştır. Bu yeni yaklaşım modifiye edilmiş integratör olarak adlandırılır. Modifiye vektör alanları tüm adi ve kısmi diferansiyel denklemler için yüksek mertebeden yapıyı koruyan nümerik integratörlerin oluşturulmasında kullanılabilir. Bu tezde, linear ve linear olmayan adi diferansiyel denklemler için Lobatto IIIA-IIIB metodlarına modifiye edilmiş vektör alanı uygulanmıştır. Ek olarak, modifiye edilmiş simplektik Euler metodu ayrılabilir Hamilton kısmi diferansiyel denklemlerine uygulandı. Ayrıca bu yeni yüksek mertebeden nümerik metodlar için kararlılık ve tutarlılık analizleri üzerine çalışıldı. Von Neumann kararlılık analizi linear ve linear olmayan Hamilton kısmi diferansiyel denklemlerine modifiye edilmiş simplektik Euler metodu kullanılarak çalışıldı. Sunulan yeni numerik şemalar ayrılabilir hamilton sistemlerine uygulandı.

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CHAPTER 1

INTRODUCTION

During the past decade there has been an increasing interest in studying numerical methods that preserve certain properties of some differential equations (Budd & Piggott, 2000). In recent years, geometric numerical integration methods have come to the fore, partly as an alternative to traditional methods such as Runge-Kutta methods. A numerical method is called *geometric integrator* if it preserves one or more physical/geometric properties of the system exactly (i.e up to round-off error). Examples of such geometric properties that can be preserved are (first) integrals, symplectic structure, symmetries and reversing-symmetries, phase-space volume, Lyapunov functions, foliations, e.t.c. Geometric methods have applications in many areas of physics, including celestial mechanics, particle accelerators, molecular dynamics, fluid dynamics, pattern formation, plasma physics, reaction-diffusion equations, and meteorology (Chartier et al., 2006).

The name symplectic integrator is usually attached to a numerical scheme that intends to solve such a hamiltonian system approximately, while preserving its underlying symplectic structure. Symplectic integrators tend to preserve qualitative properties of phase space trajectories: Trajectories do not cross, and although energy is not exactly conserved, energy fluctuations are bounded. Partitioned Euler method, Midpoint method are examples of symplectic integrators if they apply to the Hamiltonian system.

Symplectic integration technique have attracted more and more attention during the recent years. During numerical computations for Hamiltonian systems, the most standard numerical methods cannot produce excellent results simply because these methods usually neglect the important features of the dynamics in the Hamiltonian system and fail to preserve the symplectic property of the solution. The symplectic integration scheme has lots of advantages over these standard numerical methods. It can approximate the map of the exact dynamics in time direction to any desired order and still maintain the symplectic property for numerical solutions.

In the literature symplectic methods are generally constructed using generating functions, Runge Kutta methods, splitting methods and variational methods. One of the methods for constructing higher order symplectic integrators is developed by using modified vector fields. The primary work on this approach was developed by Philippe Chartier, Ernst Hairer and Gilles Vilmart (Hairer et al., 2002) and illustrated by the implicit midpoint rule applied to the full dynamics of the rigid body. The modified vector field is also used for the Kepler problem (Kozlov, 2007). This approach is developed by using the idea in backward error analysis while constructing modified equations by inverting the roles of the exact and numerical flows. In this case, we construct new higher order symplectic methods based on symplectic Euler method inspired by the theory of modified vector fields in combination with backward error analysis. Symplecticity is preserved by new higher order symplectic method which preserve structural properties of the differential equations was recently developed in (Hairer et al., 2002).

The outline of this thesis can be given as follows: After giving the idea of modified equations in combination with backward error analysis in Chapter 1, we explain the connection between backward error analysis and modifying integrators in Chapter 2, then we construct a new higher order symplectic numerical method in Chapter 3. In Chapter 4, the convergence properties of the modified fourth order Lobatto IIIA-IIIB method are analyzed using the concepts of stability, consistency and order. In Chapter 5, we study the analysis of modified symplectic Euler method for separable Hamiltonian PDE problems, as well. In Chapter 6, theoretical results and new numerical algorithms based on the modified vector field idea are verified on numerical test problems.

CHAPTER 2

BACKGROUND

In this section, for the sake of clarity of our thesis we have mainly explained the connection between backward error analysis and modifying numerical integrators. The concept of symplecticity is also explained and examples of symplectic integrators are given.

2.1. Backward Error Analysis

Modified differential equations in combination with backward error analysis, the monographs (Hairer, 1984), (Hairer & Stoffer, 1997) form an important tool for studying the long-time behaviour of numerical integrators for ordinary differential equations. The main idea of this theory is sketched in the following section. The detailed information related to the backward error analysis can be found in the book (Hairer et al., 2002).

2.1.1. Modified Equations for Backward Error Analysis

Consider an initial value problem

$$\dot{y} = f(y), \qquad y(0) = y_0 \tag{2.1}$$

with sufficiently smooth vector field $f(y)$, and a numerical one-step integrator $y_{n+1} = \Phi_{f,h}(y_n)$. The idea of backward error analysis is to search for a modified differential equation

$$\dot{z} = f_h(z) = f(z) + hf_2(z) + h^2 f_3(z) + \dots, \qquad z(0) = y_0, \tag{2.2}$$

which a formal series in powers of step size h, such that the numerical solution $\{y_n\}$ is formally equal to the exact solution of (2.2),

$$y_n = z(nh) \quad \text{for} \quad n = 0, 1, 2, \ldots . \tag{2.3}$$

The idea is explained in Figure 2.1.

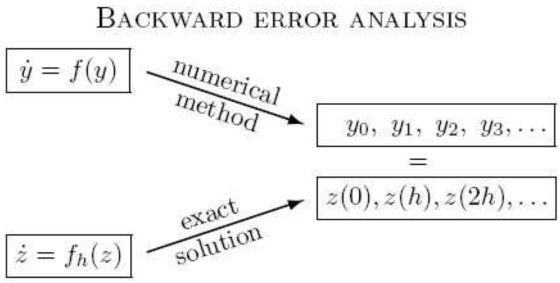

Figure 2.1. Idea of Backward Error Analysis.

To explain the above idea, we consider the following example which is taken from the book (Hairer et al., 2002).

Example 2.1 *Consider the scalar differential equation*

$$\dot{y} = y^2, \qquad y(0) = 1 \tag{2.4}$$

with exact solution $y(t) = \frac{1}{1-t}$. *It has a singularity at t=1. The exact solution exists for* $t < 1$. *We apply the explicit Euler method* $y_{n+1} = y_n + hf(y_n)$. *The one term modified differential equation is*

$$\dot{z} = f(z) - \frac{h}{2} f'(z) f(z) = z^2 - hz^3 \tag{2.5}$$

The system has an unstable equilibrium at $y = 0$ *and an asymptotically stable equilibrium at* $y = \frac{1}{h}$. *In particular a solution exists for all time. The Figure 2.2 shows the exact solution, the forward Euler solution and the modified equation solution for* $h = 0.1$

The modified equation is not much closer to the numerical solution than the exact solution is, but it does exist for all time.

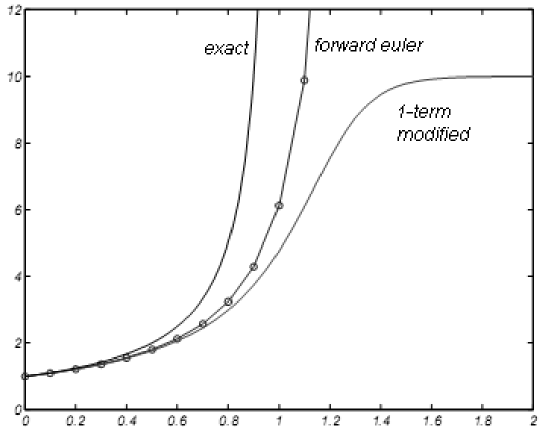

Figure 2.2. Exact, forward Euler and 1-term modified equation solutions to $\dot{y} = y^2,\ y(0) = 1$.

Continuing the procedure outlined above to determine higher order terms (and making use of symbolic mathematics software) gives the five term modified equation. Its output is

$$\dot{z} = z^2 - hz^3 + \frac{3}{2}h^2z^4 - \frac{8}{3}h^3z^5 + \frac{31}{6}h^4z^6 - \frac{157}{15}h^5z^7 \mp .... \tag{2.6}$$

The Figure 2.3 presents the exact solution, the forward Euler method and m-term modified equations for $m = 1, ..., 5$ plotted for $h = 2.10^{-2}$. We see that the modified equation solutions 'converge' to the numerical solution very quickly as h become smaller. We observe an excellent agreement of the numerical solution with the exact solution of the modified equation.

By the similar way the modified equation with respect to midpoint rule can be obtained given as below

$$\dot{z} = z^2 + \frac{1}{4}h^2z^4 + \frac{1}{8}h^4z^6 + \frac{11}{192}h^6z^8 + \frac{3}{128}h^8z^{10} + ... \tag{2.7}$$

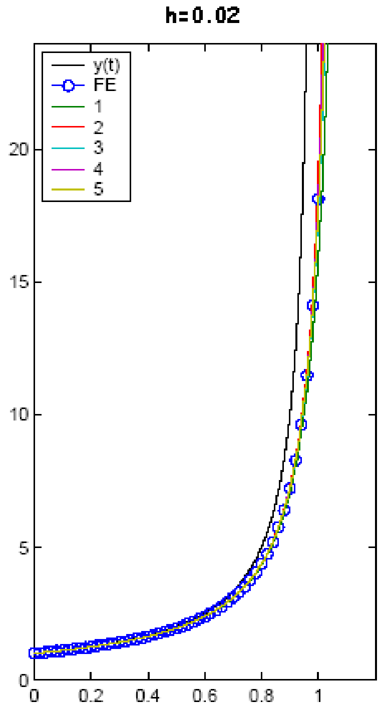

Figure 2.3. Exact, forward Euler and m-term modified equation solutions to $\dot{y} = y^2,\ y(0) = 1$ with step-size $h = 2.10^{-2}$.

For the classical Runge-Kutta method of order 4

$$\dot{z} = z^2 - \frac{1}{24}h^4 z^6 + \frac{65}{576}h^6 z^8 - \frac{17}{96}h^7 z^9 + \frac{19}{144}h^8 z^{10} \mp \ldots. \tag{2.8}$$

We observe that the perturbation terms in modified equation are of size $O(h^p)$, where p is the order of the method. This is true in general.

The error estimation committed by backward error analysis is stated in the following theorem.

Theorem 2.1 *Let $f(y)$ be analytic in a complex neighborhood of y_0 and that $||f(y)|| \leq M$ for $||y - y_0|| \leq 2R$ i.e., for all y of $\mathcal{B}_{2R}(y_0) := \{y \in \mathbb{C}^d; ||y - y_0|| \leq 2R\}$, let the coefficients $d_j(y)$ of the method be analytic and bounded in $\mathcal{B}_R(y_0)$. If $h < h_0/4$ where $h_0 = R/M$ then there exists $N = N(h)$ (namely N equal to the largest integer satisfying $hN \leq h_0$) such that the difference between the numerical solution $y_1 = \phi_h(y_0)$ and the* *exact solution $\tilde{\varphi}_{N,t}(y_0)$ of the truncated modified equation (2.28) satisfies*

$$||\phi_h(y_0) - \tilde{\varphi}_{N,h}(y_0)|| \leq h\gamma M e^{-h_0/h}. \tag{2.9}$$

Proof See (Hairer et al., 2002). □

Note that the local error does not grow exponentially with the time interval as like the forward error analysis.

2.2. Modifying Numerical Integrators

Backward error analysis is a purely theoretical tool that gives much insight into the long-term integration with geometric numerical methods. We shall show that by simply exchanging the roles of the numerical method and the exact solution, it can be turned into a means for constructing high order integrators that conserve geometric properties over long times. Let us be more precise: As before, we consider an initial value problem (2.1) and a numerical integrator. But now we search for a modified differential equation, again of the form (2.2), such that the numerical solution $\{z_n\}$ of the method applied with step size h to (2.2) yields formally the exact solution of the original differential equation (2.1), i.e.,

$$z_n = y(nh) \quad \text{for} \quad n = 0, 1, 2, \ldots . \tag{2.10}$$

The idea is explained in Figure 2.4.

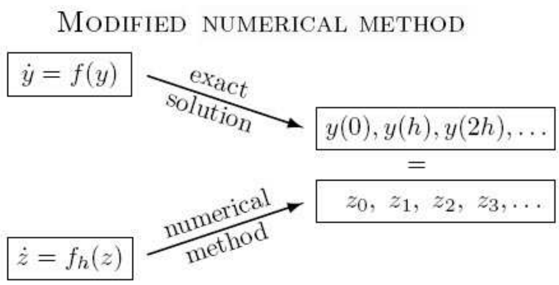

Figure 2.4. Idea of Modified Differential Equations.

Notice that this modified equation is different from the one considered before. However, due to the close connection with backward error analysis, all theoretical and practical results have their analogue in this new context. The modified differential equation is again an asymptotic series that usually diverges, and its truncation inherits geometric properties of the exact flow if a suitable integrator is applied. The coefficient functions $f_j(z)$ can be computed recursively by using a formula manipulation program like MAPLE. This can be done by developing both sides of $z(t+h) = \Phi_{f_h,h}(z(t))$ into a series in powers of h, and by comparing their coefficients. Once a few functions $f_j(z)$ are known, the following algorithm suggests itself:

Consider the truncation

$$\dot{z} = f_h^{[r]}(z) = f(z) + hf_2(z) + \ldots + h^{r-1}f_r(z) \tag{2.11}$$

of the modified differential equation corresponding to $\Phi_{f,h}(y)$. Then,

$$z_{n+1} = \Psi_{f,h}(z_n) := \Phi_{f_h^{[r]},h}(z_n) \tag{2.12}$$

defines a numerical method of order r that approximates the solution of (2.1). We call it modifying integrator, because the vector field $f(y)$ of (2.1) is modified into $f_h^{[r]}$ before the basic integrator is applied.

This is an alternative approach for constructing high order numerical integrators for ordinary differential equations (classical approaches are multistep, Runge Kutta, Taylor series, extrapolation, composition, and splitting methods). It is particularly interesting in the context of geometric integration because, as known from backward error analysis, the modified differential equation inherits the same structural properties as (2.1) if a suitable integrator is applied. This basic idea is explained in the following example.

Example 2.2 *For the numerical integration of (2.1) considering the midpoint rule*

$$y_{n+1} = y_n + h\ f\left(\frac{y_n + y_{n+1}}{2}\right). \tag{2.13}$$

We find the functions $f_j(y)$ *of the truncated modified vector field with respect to implicit midpoint rule.*
Consider the truncated modified differential equation (2.11)

$$\dot{\tilde{y}} = \underbrace{f_h^{[r]}(\tilde{y}) = f(\tilde{y}) + hf_2(\tilde{y}) + ... + h^{r-1}f_r(\tilde{y})}_{F} \tag{2.14}$$

and the Taylor expansion of exact solution $y(t)$ *for* h

$$y(t+h) = y(t) + h\dot{y}(t) + \frac{h^2}{2!}\ddot{y}(t) + \frac{h^3}{3!}y^3(t) + ..., \tag{2.15}$$

where $\ddot{y} = f'f$, $y^{(3)} = f'f'f + f''(f,f)$ *and* $\tilde{y}_{n+1} = \phi_{f_h^{[r]},h}(\tilde{y}_n)$ *where the method here is midpoint rule*

$$\tilde{y}_{n+1} = \tilde{y}_n + h\,F\left(\frac{\tilde{y}_n + \tilde{y}_{n+1}}{2}\right) \tag{2.16}$$

$$\tilde{y}_{n+1} = \tilde{y}_n + h\,F\left(\frac{\tilde{y}_n + \tilde{y}_n + h\,F(\frac{\tilde{y}_n+\tilde{y}_{n+1}}{2})}{2}\right) \tag{2.17}$$

$$\tilde{y}_{n+1} = \tilde{y}_n + h\,F\left(\tilde{y}_n + \frac{h}{2}\,F\left(\frac{\tilde{y}_n + \tilde{y}_{n+1}}{2}\right)\right) \tag{2.18}$$

$$\begin{aligned}\tilde{y}_{n+1} &= \tilde{y}_n + h\left[F(\tilde{y}_n) + \frac{h}{2}F\left(\frac{\tilde{y}_n + \tilde{y}_{n+1}}{2}\right)\ F'(\tilde{y}_n)\right. \\ &\quad \left. + \frac{h^2}{8}\,F^2\left(\frac{\tilde{y}_n + \tilde{y}_{n+1}}{2}\right)\ F''(\tilde{y}_n) + ...\right]\end{aligned} \tag{2.19}$$

$$\begin{aligned}\tilde{y}_{n+1} &= \tilde{y}_n + hf + h^2\left[f_2 + \frac{1}{2}ff'\right] \\ &\quad + h^3\left[f_3 + \frac{1}{2}f_2f' + \frac{1}{4}f'f'f + \frac{1}{8}f''(f,f)\right] + ...\end{aligned} \tag{2.20}$$

Now equating the terms of (2.20) to the terms of the exact solution (2.15) and expanding by Taylor series we get

$$\begin{aligned}
f_2 &= 0 && (2.21)\\
f_3 &= \frac{1}{12}\Big(-f'f'f+\frac{1}{2}f''(f,f)\Big) && (2.22)\\
f_4 &= 0 && (2.23)\\
f_5 &= \frac{h^4}{120}\Big(f'f'f'f'f-f''(f,f'f'f)+\frac{1}{2}f''(f'f,f'f)\Big)\\
&\quad+\frac{h^4}{120}\Big(-\frac{1}{2}f'f'f''(f,f)+f'f''(f,f'f)\\
&\quad+\frac{1}{2}f''(f,f''(f,f))-\frac{1}{2}f^{(3)}(f,f,f'f)\Big)\\
&\quad+\frac{h^4}{80}\Big(-\frac{1}{6}f'f^{(3)}(f,f,f)+\frac{1}{24}f^{(4)}(f,f,f,f)\Big) && (2.24)
\end{aligned}$$

Theorem 2.2 *Suppose that the method $y_{n+1}=\phi_{f,h}(y_n)$ is of order p, i.e.,*

$$\phi_{f,h}(y_n)=\varphi_h(y)+h^{p+1}\delta_{p+1}(y)+O(h^{p+2}) \tag{2.25}$$

where $\varphi_t(y)$ denotes the exact flow of $\dot{y}=f(y)$, and $h^{p+1}\delta_{p+1}(y)$ the leading term of the local truncation error. The modified equation then satisfies

$$\dot{\tilde{y}}=f(\tilde{y})+h^pf_{p+1}(\tilde{y})+h^{p+1}f_{p+2}(\tilde{y})+...,\qquad \tilde{y}(0)=y_0 \tag{2.26}$$

with $f_{p+1}(y)=\delta_{p+1}(y)$.

Proof The construction of the functions $f_j(y)$ (see the beginning of this section) shows that $f_j(y)=0$ for $2\le j\le p$ if and only if $\phi_{f,h}(y)-\varphi_h(y)=O(h^{p+1})$.

A first application of the modified equation (2.2) is the existence of an asymptotic expansion of the global error. Indeed by the nonlinear variation of constants formula, the difference between its solution $\tilde{y}(t)$ and the solution $y(t)$ of $\dot{y}=f(y)$ satisfies

$$\tilde{y}(t)-y(t)=h^pe_p(t)+h^{p+1}(t)+... \tag{2.27}$$

Since $y_n = \tilde{y}(nh) + O(h^N)$ for the solution of a truncated modified equation, this proves the existence of an asymptotic expansion in powers of h for the global error $y_n - y(nh)$.

In general, the series (2.2) diverges and the infinite order modified equation does not exist. Nonetheless, taking a finite number of terms of the series (2.2) yields a truncated modified equation that can still provide a good approximation to the behavior of the discrete dynamical system.

Consider the truncated modified differential equation

$$\dot{\tilde{y}} = F_N(\tilde{y}), \qquad F_N(\tilde{y}) = f(\tilde{y}) + hf_2(\tilde{y}) + ... + h^{N-1}(\tilde{y}) \tag{2.28}$$

There exists an optimal value of m, dependent on h and denoted by N for which the difference between the m-term modified equation and the numerical solution is minimized. N increases like $1/h$ as h tends to zero, and usually much larger than the order p of the numerical method. In other words, the modified equations are indeed a useful tool in understanding numerical methods. □

Next, we explain briefly symplecticity and the related theorems, in the next section.

2.3. Symplectic Integrators

A first property of Hamiltonian systems is that the Hamiltonian $H(q, p)$ is a first integral of the system $\dot{q}_i = \frac{\partial H}{\partial p_i}$ and $\dot{p}_i = -\frac{\partial H}{\partial q_i}$ where H is the Hamiltonian function (or just the Hamiltonian) of the system. In this section we shall study another important property: the *symplecticity* of its flow.

The basic objects to be studied are two-dimensional parallelograms lying in $\mathbb{R}^{2d}$. We suppose the parallelogram to be spanned by two vectors

$$\xi = \begin{pmatrix} \xi^q \\ \xi^p \end{pmatrix}, \qquad \eta = \begin{pmatrix} \eta^q \\ \eta^p \end{pmatrix} \tag{2.29}$$

in the (p, q) space ($\xi^q, \xi^p, \eta^q, \eta^p$ are in $\mathbb{R}^d$) as

$$P = \{t\xi + s\eta \,|\, 0 \le t \le 1, 0 \le s \le 1\}. \tag{2.30}$$

In the case $d = 1$ we consider the $oriented\, area$

$$Area(P) = det \begin{pmatrix} \xi^q & \eta^q \\ \xi^p & \eta^p \end{pmatrix} = \xi^q \eta^p - \xi^p \eta^q. \tag{2.31}$$

In higher dimensions, we replace this by the sum of the oriented areas of the projections of P onto the coordinate planes (p_i, q_i), i.e., by

$$\omega(\xi, \eta) := \sum_{i=1}^{d} det \begin{pmatrix} \xi_i^q & \eta_i^q \\ \xi_i^p & \eta_i^p \end{pmatrix} = \sum_{i=1}^{d} (\xi_i^q \eta_i^p - \xi_i^p \eta_i^q). \tag{2.32}$$

This defines a bilinear map acting on vectors of $\mathbb{R}^{2d}$, which will play a central role for Hamiltonian system. In matrix notation, this map has the form

$$\omega(\xi, \eta) = \xi^T J \eta \qquad \text{with} \qquad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{2.33}$$

where I is the identity matrix of dimension d (Hairer et al., 2002).

Definition 2.1 *A $linear\ mapping$ $A : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is called $symplectic$ if*

$$A^T J A = J \tag{2.34}$$

or, equivalently, if $\omega(A\xi, A\eta) = \omega(\xi, \eta)$ for all $\xi, \eta \in \mathbb{R}^{2d}$.

We can find it

$$\begin{aligned} \omega(A\xi, A\eta) = (A\xi)^T J (A\eta) &= \xi^T \underbrace{A^T J A}\eta \qquad (\text{since} \quad A^T J A = J) && (2.35) \\ &= \xi^T J \eta = \omega(\xi, \eta) && (2.36) \end{aligned}$$

Definition 2.2 *A differentiable map $g : U \to \mathbb{R}^{2d}$ (where $U \subset \mathbb{R}^{2d}$ is an open set) is* *called $symplectic$ if the Jacobian matrix $g'(q,p)$ is everywhere symplectic, i.e., if*

$$g'(q,p)^T J g'(q,p) = J \quad \text{or} \quad \omega(g'(q,p)\xi, g'(q,p)\eta) = \omega(\xi,\eta). \tag{2.37}$$

Lemma 2.1 *If ψ and φ are symplectic maps then $\psi \circ \varphi$ is symplectic.*

Proof Since ψ is symplectic

$$(\psi')^T J \psi' = J \quad , \quad \text{similarly} \qquad (\varphi')^T J \varphi' = J, \tag{2.38}$$

by using the equation (2.38), we get

$$\left[(\psi o \varphi)'\right]^T J(\psi o \varphi)' \quad = \quad (\psi' o \varphi')^T J(\psi' o \varphi') = (\varphi')^T o (\psi')^T J \psi' o \varphi' = J. \tag{2.39}$$

It gives the symplecticity of two maps. □

Theorem 2.3 *($Poincaré$ 1899). Let $H(q,p)$ be a twice continuously differentiable function on $U \subset \mathbb{R}^{2d}$. Then, for each fixed t, the flow φ_t is a symplectic transformation wherever it is defined.*

Proof Let φ_t be flow of the Hamiltonian system. φ_t' is a Jacobian matrix of the flow, then φ_t' satisfies the variational equation i.e.

$$\frac{d}{dt}\varphi_t' = J^{-1}H''\varphi_t' \qquad \text{where} \quad H'' = \begin{pmatrix} H_{pp} & H_{pq} \\ H_{qp} & H_{qq} \end{pmatrix} \quad \text{is symmetric.} \tag{2.40}$$

Hence

$$\frac{d}{dt}(\varphi_t'^T J \varphi_t') = [J^{-1}H''\varphi_t']^T J\varphi_t' + \varphi_t'^T \underbrace{JJ^{-1}}_{I} H''\varphi_t' \tag{2.41}$$

since $JJ^{-1} = I$, we get

$$\frac{d}{dt}(\varphi_t'^T J \varphi_t') = \varphi_t'^T H''^T (J^{-1})^T J \varphi_t' + \varphi_t'^T H'' \varphi_t' \tag{2.42}$$

now, we will use $(H'')^T = H''$ and $(J^{-1})^T J = -I$, let us prove it.

$$J^T \;\; = \;\; -J. \tag{2.43}$$

By using the equation (2.43), we get

$$\left[(J^{-1})^T J\right]^T \;\; = \;\; J^T \cdot J^{-1} = -J \cdot J^{-1} = -I, \tag{2.44}$$

then we finally find $(J^{-1})^T J = -I$. We put $(J^{-1})^T J = -I$ in the last equation

$$\frac{d}{dt}(\varphi_t'^T J \varphi_t') = -\varphi_t'^T H'' \varphi_t' + \varphi_t'^T H'' \varphi_t' = 0. \tag{2.45}$$

Since $\frac{d}{dt}(\varphi_t'^T J \varphi_t') = 0$ then $\varphi_t'^T J \varphi_t' = \mathbf{C}$. When $t = 0$, we have $\varphi_t'(t_0) = I \Rightarrow C = J$. $\square$

Theorem 2.4 *Let $f : U \to \mathbb{R}^{2d}$ be continuously differentiable. Then, $\dot{y} = f(y)$ is locally Hamiltonian if and only if its flow $\varphi_t(y)$ is symplectic for all $y \in U$ and for all sufficiently small t.*

Proof Assume that the flow φ_t is symplectic, and we have to prove the local existence of a function $H(y)$ such that $f(y) = J^{-1}\nabla H(y)$. Using the fact that $\frac{\partial \varphi_t}{\partial y_0}$ is a solution of the variational equation $\dot{\Psi} = f'(\varphi_t(y_0))\Psi$, we obtain

$$\frac{d}{dt}\left(\Big(\frac{\partial \varphi_t}{\partial y_0}\Big)^T J \Big(\frac{\partial \varphi_t}{\partial y_0}\Big)\right) = \Big(\frac{\partial \varphi_t}{\partial y_0}\Big)\Big(f'(\varphi_t(y_0))^T J + J f'(\varphi_t(y_0)\Big)\Big(\frac{\partial \varphi_t}{\partial y_0}\Big) = 0. \tag{2.46}$$

Putting $t = 0$, it follows from $J = -J^T$ that $Jf'(y_0)$ is a symmetric matrix for all y_0. $\square$

Definition 2.3 *A numerical one-step method is called symplectic if the one-step map $y_1 = \Phi_h(y_0)$ is symplectic whenever it is applied to a smooth Hamiltonian system. If the method is symplectic, we have*

$$\Phi_h'(y)^T \, J \, \Phi_h'(y) = J \tag{2.47}$$

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

2.3.1. Examples of the Symplectic Methods

One of the example of symplectic method is implicit midpoint method.

Example 2.3 *The implicit midpoint rule is symplectic.*

Proof The second order implicit midpoint rule is given as

$$U_{n+1} = U_n + hf\Big(\frac{U_n + U_{n+1}}{2}\Big). \tag{2.48}$$

Consider the Hamiltonian problem of the form

$$\dot{y} = J^{-1}\nabla H(y) \tag{2.49}$$

The application of the midpoint rule to the Hamiltonian system in (Hairer et al., 2002) yields

$$U_{n+1} = U_n + hJ^{-1}\nabla H\Big(\frac{U_n + U_{n+1}}{2}\Big) \tag{2.50}$$

Suppose $U_{n+1} = \psi_n(U_n)$, then we need to show

$$\psi_n'^T J \psi_n' = J. \tag{2.51}$$

First compute ψ_n' as follows

$$\begin{aligned} \psi_n' = \frac{\partial U_{n+1}}{\partial U_n} &= I + hJ^{-1}H''\Big(\frac{U_n + U_{n+1}}{2}\Big)\Big(\frac{1}{2}\Big)\Big(\frac{\partial U_{n+1}}{\partial U_n} + I\Big) && (2.52) \\ &= \Big(I - \frac{h}{2}J^{-1}H''\Big)^{-1}\Big(I + \frac{h}{2}J^{-1}H''\Big) && (2.53) \end{aligned}$$

Next, the symplecticity condition (2.51) can be written as

$$\Big(I+\frac{h}{2}J^{-1}H''\Big)J\Big(I+\frac{h}{2}J^{-1}H''\Big)^T=\Big(I-\frac{h}{2}J^{-1}H''\Big)J\Big(I-\frac{h}{2}J^{-1}H''\Big)^T. \quad (2.54)$$

By using the equalities $(H'')^T = H''$ (since H is symmetric) and $(J^{-1})^T = -J^{-1} = J$, we get

$$\Big(I+\frac{h}{2}J^{-1}H''\Big)^T = I-\frac{h}{2}H''J^{-1}, \quad \Big(I-\frac{h}{2}J^{-1}H''\Big)^T = I+\frac{h}{2}H''J^{-1}. \quad (2.55)$$

Inserting this into the equation (2.54), we get

$$\Big(IJ+\frac{h}{2}J^{-1}H''J\Big)\Big(I-\frac{h}{2}H''J^{-1}\Big)=\Big(IJ-\frac{h}{2}J^{-1}H''J\Big)\Big(I+\frac{h}{2}H''J^{-1}\Big). \quad (2.56)$$

After some manipulations of equation (2.56), we have

$$\begin{aligned}J+\frac{h}{2}J^{-1}H''J-\frac{h}{2}JH''J^{-1}-\frac{h^2}{4}J^{-1}H''JH''J^{-1} &= J+\frac{h}{2}JH''J^{-1}\\ &-\frac{h}{2}J^{-1}H''J-\frac{h^2}{4}J^{-1}H''JH''J^{-1}\end{aligned} \quad (2.57)$$

Finally, equation (2.57) implies the following result

$$hJH''J^{-1} = hJ^{-1}H''J \quad (2.58)$$

Since $J^{-1} = -J$ then $-JH''J = -JH''J$ completes the proof. □

The next example of symplectic method of order 1 is so-called symplectic method. If the partitioned Euler method is applied to the Hamiltonian system, the obtained method is called symplectic Euler method. Next example proves that symplectic euler method is a symplectic method.

Example 2.4 *The so-called symplectic Euler method*

$$u_{n+1} = u_n - h\frac{\partial H}{\partial v}(u_{n+1}, v_n), \quad v_{n+1} = v_n + h\frac{\partial H}{\partial u}(u_{n+1}, v_n) \tag{2.59}$$

is a symplectic method of order 1.

Proof Differentiation of (2.59) with respect to (u_n, v_n) yields

$$\begin{pmatrix} I + hH_{vu}^T & 0 \\ -hH_{uu} & I \end{pmatrix} \left(\frac{\partial(u_{n+1}, v_{n+1})}{\partial(u_n, v_n)}\right) = \begin{pmatrix} I & -hH_{vv} \\ 0 & I + hH_{vu} \end{pmatrix} \tag{2.60}$$

where the matrices $H_{vu}, H_{uu}, \ldots$ of partial derivatives are all evaluated at (u_{n+1}, v_n). This relation allows us to compute $\frac{\partial(u_{n+1}, v_{n+1})}{\partial(u_n, v_n)}$ and to check in a straightforward way the symplecticity condition

$$\frac{\partial(u_{n+1}, v_{n+1})}{\partial(u_n, v_n)}^T J \frac{\partial(u_{n+1}, v_{n+1})}{\partial(u_n, v_n)} = J. \tag{2.61}$$

The same proof shows that the adjoint method of (2.59),

$$u_{n+1} = u_n - h\frac{\partial H}{\partial v}(u_n, v_{n+1}), \quad v_{n+1} = v_n + h\frac{\partial H}{\partial u}(u_n, v_{n+1}) \tag{2.62}$$

is also symplectic. □

In the next section, we briefly explain the geometric properties which preserve by this construction.

2.4. Geometric Properties

The importance of backward error analysis in the context of geometric numerical integration lies in the fact that properties of numerical integrators are transferred to corresponding properties of modified equations.Because of the close relationship between backward error analysis and the approach of modifying integrators, it is not a surprise that most results can be extended to our situation. The most important properties of the modified equation can be collected given as below:

- If the numerical integrator $\Phi_{f,h}(y)$ has order p, i.e., the local error satisfies $\Phi_{f,h}(y) - \varphi_{f,h}(y) = O(h^{p+1})$, then we have $f_j = 0$ for $j = 2, ..., p$.
- If the numerical integrator $\Phi_{f,h}(y)$ is symmetric, i.e, $\Phi_{f,-h}(y) = \Phi^{-1}_{f,h}(y)$, then the modified differential equation has an expansion in even powers of h, i.e., $f_{2j} = 0$ for all j, and modifying integrator is symmetric.
- If the basic method $\Phi_{f,h}(y)$ exactly conserves a first integral $I(y)$ of (2.1), then the modified differential equation has $I(y)$ as first integral, and the modifying integrator exactly conserves $I(y)$.
- If the basic method is symplectic for Hamiltonian systems of the form

$$\dot{y} = J^{-1}\nabla \tilde{H}(y), \tag{2.63}$$

  the modifying integrator is also symplectic.
- If the basic method is reversible for reversible differential equations then the modified differential equation and the modifying integrator are reversible.

The proofs of these properties can be found in (Hairer et al., 2002). Here we are not concerned with these proofs.

In the next chapter, after giving a brief introduction about the symplecticity and examples of symplectic methods, we will construct a higher order symplectic methods by using modified vector field idea based on the Lobatto IIIA-IIIB method of order 2.

CHAPTER 3

CONSTRUCTION OF LOBATTO METHOD

We consider the initial value problem

$$\dot{y} = f(y), \qquad y(0) = y_0 \tag{3.1}$$

and a numerical one-step integrator $y_{n+1} = \Phi_{f,h}(y_n)$. We search for a modified differential equation

$$\dot{z} = f_h(z) = f(z) + hf_2(z) + h^2 f_3(z) + ..., \qquad z(0) = y_0 \tag{3.2}$$

such that the numerical solution $\{z_n\}$ of the method applied with step size h to (3.2) yields formally the exact solution of the original differential equation (3.1), i.e. $z_n = y(nh)$ for $n = 0, 1, 2, ...$ The coefficient functions $f_j(z)$ can be computed recursively.

Having found first functions $f_j(z)$, one can use the truncation

$$\dot{z} = f_h^{[r]}(z) = f(z) + hf_2(z) + ... + h^{r-1} f_r(z) \tag{3.3}$$

of the modified differential equation corresponding to $\Phi_{f,h}(y)$. A numerical method $z_{n+1} = \Phi_{f_h^{[r]},h}(z_n)$ approximates the solution of (3.1) with order r. It is called a *modifying integrator* because it applies to the modified vector field $f_h^{[r]}$ instead of $f(y)$.

We will consider partitioned systems

$$\begin{cases} y' = f(y, z) \\ z' = g(y, z) \end{cases} \tag{3.4}$$

and separable systems

$$\begin{cases} y' = f(z) \\ z' = g(y) \end{cases} \tag{3.5}$$

In particular, we will be interested in canonical Hamiltonian equations, which are generated by a Hamiltonian function $H(y,z)$:

$$f(y,z) = H_z(y,z), \qquad g(y,z) = -H_y(y,z). \tag{3.6}$$

Compact form of Hamiltonian system is given by where such system often arise in mechanical systems described by a Hamiltonian function

$$H = \frac{p^2}{2} + V(q) \tag{3.7}$$

which provides us

$$\begin{cases} q' = p \\ p' = -V_q(q). \end{cases} \tag{3.8}$$

with the Hamiltonian equations of motion.

3.1. Partitioned Runge-Kutta Methods

In this section we consider differential equations in the partitioned form

$$\dot{y} = f(y,z), \qquad \dot{z} = g(y,z), \tag{3.9}$$

where the variables y and z may be vectors of different dimensions.

The idea is to take two different Runge-Kutta methods, and to treat the y-variables with the first method (a_{ij}, b_i), and the z-variables with the second method $(\hat{a}_{ij}, \hat{b}_i)$.

Definition 3.1 *Let b_i,a_{ij} and $\hat{b}_i$,$\hat{a}_{ij}$ be the coefficients of two Runge-Kutta methods. A partitioned Runge-Kutta method for the solution of $\dot{y} = f(y, z)$ and $\dot{z} = g(y, z)$ are given by*

$$k_i = f\left(y_0 + h\sum_{j=1}^{s} a_{ij}k_j, z_0 + h\sum_{j=1}^{s} \hat{a}_{ij}l_j\right), \tag{3.10}$$

$$l_i = g\left(y_0 + h\sum_{j=1}^{s} a_{ij}k_j, z_0 + h\sum_{j=1}^{s} \hat{a}_{ij}l_j\right), \tag{3.11}$$

$$y_1 = y_0 + h\sum_{i=1}^{s} b_ik_i, \qquad z_1 = z_0 + h\sum_{i=1}^{s} \hat{b}_il_i. \tag{3.12}$$

Methods of this type were originally proposed by Hofer in 1976 and by Griepentrog in 1978 for problems with stiff and nonstiff parts. Their importance for Hamiltonian systems has been discovered only in the last decade. An interesting example is the Störmer/Verlet method is of the form (3.10),(3.11) and (3.12) with coefficients given in the following table.

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array} \qquad \begin{array}{c|cc} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 1/2 & 1/2 \end{array}$$

Definition 3.2 *A necessary and sufficient condition for a Runge-Kutta method to be symplectic is that for all $1 \leq i, j \leq s$*

$$b_ia_{ij} + b_ja_{ji} - b_ib_j = 0. \tag{3.13}$$

Definition 3.3 *If the coefficients of a partitioned Runge-Kutta method satisfy*

$$b_i\hat{a}_{ij} + \hat{b}_ja_{ji} - b_i\hat{b}_j = 0 \quad \text{for} \quad i, j = 1, \ldots, s, \tag{3.14}$$

and the following condition

$$b_i = \hat{b}_i \quad \text{for} \quad i = 1, \ldots, s, \tag{3.15}$$

then it is symplectic.

If the Hamiltonian is of the form $H(p, q) = T(p) + U(q)$, i.e., it is separable, then the condition (3.14) alone implies the symplecticity of the numerical flow.

3.2. Lobatto IIIA - IIIB Pairs

In this part of thesis we will construct higher order method corresponding to Lobatto IIIA-IIIB pair of method.

Definition 3.4 *The partitioned Runge-Kutta method composed of the s-stage Lobatto IIIA and the s-stage Lobatto IIIB method, is of order 2s-2.*

Lobatto IIIA - IIIB pair of order 2 is given as follows:

$$k_1 = f\left(y_0, z_0 + \frac{h}{2} l_1\right) \quad , \qquad k_2 = f\left(y_0 + \frac{h}{2}(k_1 + k_2), z_0 + \frac{h}{2} l_1\right), \tag{3.16}$$

$$l_1 = g\left(y_0, z_0 + \frac{h}{2} l_1\right) \quad , \qquad l_2 = g\left(y_0 + \frac{h}{2}(k_1 + k_2), z_0 + \frac{h}{2} l_1\right), \tag{3.17}$$

$$y_1 = y_0 + \frac{h}{2}(k_1 + k_2), \tag{3.18}$$

$$z_1 = z_0 + \frac{h}{2}(l_1 + l_2). \tag{3.19}$$

3-stage Lobatto IIIA-IIIB pair method is of the form (3.10),(3.11) and (3.12) with coefficients given in the following table.

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 1/2 & 5/24 & 1/3 & -1/24 \\ 1 & 1/6 & 2/3 & 1/6 \\ \hline & 1/6 & 2/3 & 1/6 \end{array} \qquad \begin{array}{c|ccc} 0 & 1/6 & -1/6 & 0 \\ 1/2 & 1/6 & 1/3 & 0 \\ 1 & 1/6 & 5/6 & 0 \\ \hline & 1/6 & 2/3 & 1/6 \end{array}$$

The Definition (3.1) together with the coefficients of 3-stage Lobatto IIIA-IIIB pair method given in the above table yields the Lobatto IIIA-IIIB method of order 4 are given by

$$
\begin{aligned}
k_1 &= f(y_0, z_0 + \frac{h}{6}(l_1 - l_2)), && (3.20)\\
k_2 &= f(y_0 + \frac{h}{24}(5k_1 + 8k_2 - k_3), z_0 + \frac{h}{6}(l_1 + 2l_2)), && (3.21)\\
k_3 &= f(y_0 + \frac{h}{6}(k_1 + 4k_2 + k_3), z_0 + \frac{h}{6}(l_1 + 5l_2)), && (3.22)\\
l_1 &= g(y_0, z_0 + \frac{h}{6}(l_1 - l_2)), && (3.23)\\
l_2 &= g(y_0 + \frac{h}{24}(5k_1 + 8k_2 - k_3), z_0 + \frac{h}{6}(l_1 + 2l_2)), && (3.24)\\
l_3 &= g(y_0 + \frac{h}{6}(k_1 + 4k_2 + k_3), z_0 + \frac{h}{6}(l_1 + 5l_2)), && (3.25)\\
y_1 &= y_0 + \frac{h}{6}(k_1 + 4k_2 + k_3), z_1 = z_0 + \frac{h}{6}(l_1 + 4l_2 + l_3). && (3.26)
\end{aligned}
$$

In the next section, we will construct a new fourth order modified Lobatto method. We will compare the method given in (3.26) with the new proposed method in the computational part.

3.3. Modified Lobatto Methods

We consider the modified differential equations which have the perturbated form given by

$$
\begin{cases} y' = f(y, z) + h^2 a(y, z), \\ z' = g(y, z) + h^2 b(y, z). \end{cases} \qquad (3.27)
$$

Our aim is to determine the functions $a(y, z)$ and $b(y, z)$. We simply follow the below procedures. The Taylor expansion of the exact solution of y for a fixed t is

$$
y_1 = y(t + h) = y(t) + hy'(t) + \frac{h^2}{2!}y''(t) + \frac{h^3}{3!}y'''(t) + \frac{h^4}{4!}y''''(t) + \dots . \qquad (3.28)
$$

Derivatives in the equation (3.28) for equation (3.4) are given by

$$\begin{aligned}
y' &= f && (3.29)\\
y'' &= f_y f + f_z g && (3.30)\\
y''' &= \Big(f_{yy} f + f_{yz} g\Big) f + f_y \Big(f_y f + f_z g\Big)\\
&\quad + \Big(f_{yz} f + f_{zz} g\Big) g + f_z \Big(g_y f + g_z g\Big) && (3.31)\\
&= 2 f_{yz}(f, g) + f_{yy}(f, f) + f_y f_y f + f_y f_z g + f_{zz}(g, g)\\
&\quad + f_z g_y f + f_z g_z g && (3.32)\\
y'''' &= \big[(f_{yyy} f + f_{yyz} g) f + f_{yy}(f_y f + f_z g) + (f_{yyz} f + f_{yzz} g) g + f_{yz}(g_y f + g_z g)\big] f\\
&\quad + 2(f_y f + f_z g)(f_{yy} f + f_{yz} g) + \big[(f_{yy} f + f_{yz} g) f + (f_y f + f_z g) f_y\\
&\quad + (f_{yz} f + f_{zz} g) g + f_z(g_y f + g_z g)\big] f_y + \ldots && (3.33)
\end{aligned}$$

Using Taylor series expansion and substituting (3.33) into (3.28), in equation (3.18), y_1 can be found as

$$\begin{aligned}
y_1 &= y(t+h) = y + hf + \frac{h^2}{2}(f_y f + f_z g) + \frac{h^3}{6}\Big(2 f_{yz}(f, g)\\
&\quad + f_{yy}(f, f) + f_y f_y f + f_y f_z g + f_{zz}(g, g) + f_z g_y f + f_z g_z g\Big)\\
&\quad + \frac{h^4}{24} y''''. && (3.34)
\end{aligned}$$

Next, the Lobatto method of order 2 to modified differential equation leads to below equation

$$\begin{aligned}
y_0 + \frac{h}{2}(k_1 + k_2) &= y + \frac{h}{2}\Big[2f + h\Big(f_y f + f_z(g + h^2 b)\Big) + \Big(\frac{h}{2}\Big)^2\\
&\quad \Big(f_{zz}(g, g) + 2(f_{yz}(f, g) + f_{yy}(f, f) + f_y f_y f\\
&\quad + f_y f_z g + f_z g_z g)\Big) + \ldots + h^2[2a + a_y h f + a_z h g]\Big]. && (3.35)
\end{aligned}$$

Finally, we compare the terms of (3.34) and (3.35) with respect to the powers of h,

$$\frac{1}{6}\Big(2f_{yz}(f,g)+f_{yy}(f,f)+f_yf_yf+f_yf_zg+f_{zz}(g,g)+f_zg_yf+f_zg_zg\Big)=$$
$$\frac{1}{4}\Big(f_{yz}(f,g)+f_{yy}(f,f)+f_yf_yf+f_yf_zg+\frac{1}{2}f_{zz}(g,g)+f_zg_zg\Big)+a(y,z) \quad (3.36)$$

we get

$$\begin{aligned} a(y,z) &= \frac{1}{12}\Big(-f_{yy}(f,f)+f_{yz}(f,g)+\frac{1}{2}f_{zz}(g,g) \\ &\quad -f_yf_yf-f_yf_zg+2f_zg_yf-f_zg_zg\Big) \end{aligned} \quad (3.37)$$

By the same procedure we can obtain the function $b(y,z)$ given by

$$\begin{aligned} b(y,z) &= \frac{1}{12}\Big(-g_{yy}(f,f)+g_{yz}(f,g)+\frac{1}{2}g_{zz}(g,g) \\ &\quad -g_yf_yf-g_yf_zg+2g_zg_yf-g_zg_zg\Big) \end{aligned} \quad (3.38)$$

If the original equations are Hamiltonian, then the modified differential equations (3.27) are generated by the Hamiltonian function

$$H^{[3]}=H+\frac{h^2}{12}\left(-H_{yy}(f,f)+H_{yz}(f,g)+\frac{1}{2}H_{zz}(g,g)\right), \quad (3.39)$$

where f and g are given by (3.6).

So far the calculations of the coefficient functions for the modified equations are more complex for the systems introduced in equation (3.27). So we choose separable systems after this section since the calculations of the coefficient functions become more easier. For separable systems the modified differential equations are

$$\left\{\begin{array}{l} y'=f(z)+h^2a(y,z), \\ z'=g(y)+h^2b(y,z), \end{array}\right. \quad (3.40)$$

where $f_y \equiv 0$ and $g_z \equiv 0$. Taking the derivatives of original system, for y we get

$$\begin{aligned}
y' &= f(z) && (3.41)\\
y'' &= f_z g && (3.42)\\
y''' &= f_{zz}(g,g) + f_z g_y f && (3.43)\\
y'''' &= \big(f_{zzz}(g,g,g) + 2f_{zz}(g_y f, g)\big) \\
&\quad + \big(f_{zz}(g_y f, g) + f_z g_{yy}(f,f) + f_z g_y f_z g\big) && (3.44)
\end{aligned}$$

for z we get

$$\begin{aligned}
z' &= g(y) && (3.45)\\
z'' &= g_y f && (3.46)\\
z''' &= g_{yy}(f,f) + g_y f_z g && (3.47)\\
z'''' &= \big(g_{yyy}(f,f,f) + 2g_{yy}(f_z g, f)\big) \\
&\quad + \big(g_{yy}(f_z g, f) + g_y f_{zz}(g,g) + g_y f_z g_y f\big). && (3.48)
\end{aligned}$$

Applying the third order approximation to k_1, k_2, l_1 and l_2, we have

$$\begin{aligned}
k_1 &= f + \frac{h}{2} f_z(g + h^2 b) + \frac{1}{2}\Big(\frac{h}{2}\Big)^2 f_{zz}(g,g) \\
&\quad + \frac{1}{6}\Big(\frac{h}{2}\Big)^3 (g,g,g) + h^2\Big[a + a_z \frac{h}{2} g\Big] + \mathcal{O}(h^4) && (3.49)
\end{aligned}$$

and k_2 as follows

$$\begin{aligned}
k_2 &= f + \frac{h}{2} f_z(g + h^2 b) + \frac{1}{2}\Big(\frac{h}{2}\Big)^2 f_{zz}(g,g) \\
&\quad + \frac{1}{6}\Big(\frac{h}{2}\Big)^3 (g,g,g) + h^2\Big[a + a_y h f + a_z \frac{h}{2} g\Big] + \mathcal{O}(h^4) && (3.50)\\
l_1 &= g + h^2\Big[b + b_z \frac{h}{2} g\Big] + \mathcal{O}(h^4) && (3.51)
\end{aligned}$$

and l_2 as follows

$$\begin{aligned} l_2 &= g + \frac{h}{2} g_y \Big[2f + hf_z g + \Big(\frac{h}{2}\Big)^2 f_{zz}(g,g) + h^2 a\Big] \\ &\quad + \frac{1}{2}\Big(\frac{h}{2}\Big)^2 g_{yy}(2f + hf_z g, 2f + hf_z g) \\ &\quad + \frac{1}{6}\Big(\frac{h}{2}\Big)^3 g_{yyy}(2f, 2f, 2f) + h^2\Big[b + b_y hf + b_z \frac{h}{2} g\Big] \\ &\quad + \mathcal{O}(h^4) \end{aligned} \tag{3.52}$$

Putting k_1 and k_2 into (3.18),

$$\begin{aligned} y_0 + \frac{h}{2}(k_1 + k_2) &= y + \frac{h}{2}\Big[2f + 2\Big(\frac{h}{2}\Big) f_z (g + h^2 b) + \Big(\frac{h}{2}\Big)^2 f_{zz}(g,g) \\ &\quad + \frac{1}{3}\Big(\frac{h}{2}\Big)^3 f_{zzz}(g,g,g) + h^2(2a + a_y hf + a_z hg)\Big] \\ &\quad + \mathcal{O}(h^5) \end{aligned} \tag{3.53}$$

and (3.41) into y_1,

$$\begin{aligned} y_1 &= y + hf + \frac{1}{2}h^2 f_z g + \frac{1}{6}h^3[f_{zz}(g,g) + f_z g_y f] + \frac{1}{24}h^4 \\ &\quad [f_{zzz}(g,g,g) + 3f_{zz}(g_y f, g) + f_z g_{yy}(f,f) + f_z g_y f_z g] \end{aligned} \tag{3.54}$$

Since (3.53) is equal to (3.54), $a(y,z)$ can be found easily.

$$a(y,z) = \frac{1}{12}\left(\frac{1}{2} f_{zz}(g,g) + 2 f_z g_y f\right). \tag{3.55}$$

Secondly, we put l_1 and l_2 into (3.19),

$$\begin{aligned} z_0 + \frac{h}{2}(l_1 + l_2) &= z + \frac{h}{2}\Big[2g + 2\Big(\frac{h}{2}\Big) g_y 2f + \Big(\frac{h}{2}\Big) g_y h f_z g \\ &\quad + \Big(\frac{h}{2}\Big)^3 g_y f_{zz}(g,g) + \Big(\frac{h}{2}\Big) g_y a h^2 + \frac{h^2}{2} g_{yy}(f,f) + \frac{h^3}{2} g_{yy}(f, f_z g) \\ &\quad + \frac{h^3}{6} g_{y,y,y}(f,f,f) + h^2(2b + b_y hf + b_z hg)\Big] + \mathcal{O}(h^5) \end{aligned} \tag{3.56}$$

and (3.45) into z_1,

$$\begin{aligned} z_1 &= z + hg + \frac{1}{2}h^2 g_y f + \frac{1}{6}h^3[g_{yy}(f,f) + g_y f_z g] + \frac{1}{24}h^4 \\ &\quad [g_{yyy}(f,f,f) + 3g_{yy}(f_z g, f) + g_y f_{zz}(g,g) + g_y f_z g_y f] \end{aligned} \tag{3.57}$$

Since (3.56) is equal to (3.57), $b(y,z)$ can be found easily as follows;

$$b(y,z) = -\frac{1}{12}(g_{yy}(f,f) + g_y f_z g). \tag{3.58}$$

If the original equations are Hamiltonian, the modified differential equations are generated by

$$H^{[3]} = H + \frac{h^2}{12}\left(-H_{yy}(f,f) + \frac{1}{2}H_{zz}(g,g)\right). \tag{3.59}$$

For mechanical system, equation (3.8) can read as

$$H^{[3]} = H + \frac{h^2}{12}\left(-V_{qq}(p,p) + \frac{1}{2}(V_q, V_q)\right). \tag{3.60}$$

Applying (3.55) and (3.58) into mechanical system

$$H = \frac{1}{2}p^2 + V(q) \tag{3.61}$$

where $\dot{q} = f(p) = p$, $\dot{p} = g(q) = -V(q)$, we get

$$a = \frac{1}{6}g_q p, \quad b = -\frac{1}{12}g_{qq}(p,p) - \frac{1}{12}g_q g. \tag{3.62}$$

The modified differential equations for separable systems are

$$\begin{cases} q' = f(p) + h^2 a(q,p), \\ p' = g(q) + h^2 b(q,p), \end{cases} \tag{3.63}$$

so the modified equations then take the following form

$$\begin{cases} q' = p + \frac{h^2}{6} g_q p = \left(I - \frac{h^2}{6} V_{qq}\right) p \\ \\ p' = -V_q(q) - \frac{h^2}{12}(g_{qq}(p,p) + g_q g). \end{cases} \tag{3.64}$$

After applying Lobatto IIIA - IIIB pair method of order 2 to (3.64), k_1, k_2, l_1 and l_2 can be given as follows

$$k_1 = \left(\mathrm{I} + \frac{h^2}{6} g_q(q_0)\right)\left(p_0 + \frac{h}{2} l_1\right), \tag{3.65}$$

$$k_2 = \left(\mathrm{I} + \frac{h^2}{6} g_q(q_1)\right)\left(p_0 + \frac{h}{2} l_1\right), \tag{3.66}$$

$$l_1 = g(q_0) - \frac{h^2}{12}\left(g_{qq}(q_0)\left(p_0 + \frac{h}{2} l_1, p_0 + \frac{h}{2} l_1\right) + g_q(q_0) g(q_0)\right), \tag{3.67}$$

$$l_2 = g(q_1) - \frac{h^2}{12}\left(g_{qq}(q_1)\left(p_0 + \frac{h}{2} l_1, p_0 + \frac{h}{2} l_1\right) + g_q(q_1) g(q_1)\right). \tag{3.68}$$

Combining the above equations with (3.18) and (3.19), we have

$$q_1 = q_0 + h\left(\mathrm{I} + \frac{h^2}{12}(g_q(q_0) + g_q(q_1))\right)\left(p_0 + \frac{h}{2} l_1\right), \tag{3.69}$$

$$\begin{aligned} p_1 = p_0 + \frac{h}{2}\Big(g(q_0) + g(q_1) - \frac{h^2}{12}\Big[& g_{qq}(q_0)(p_0 + \frac{h}{2} l_1, p_0 + \frac{h}{2} l_1) \\ & + g_{qq}(q_1)(p_0 + \frac{h}{2} l_1, p_0 + \frac{h}{2} l_1) + g_q(q_0) g(q_0) + g_q(q_1) g(q_1)\Big]\Big). \end{aligned} \tag{3.70}$$

these equations leads to a scheme which can be split into three stages:

$$p_{1/2} = p_0 + \frac{h}{2}\left(g(q_0) - \frac{h^2}{12}\left(g_{qq}(q_0)(p_{1/2}, p_{1/2}) + g_q(q_0) g(q_0)\right)\right), \tag{3.71}$$

$$q_1 = q_0 + h\left(I + \frac{h^2}{12}(g_q(q_0) + g_q(q_1))\right) p_{1/2}, \tag{3.72}$$

$$p_1 = p_{1/2} + \frac{h}{2}\left(g(q_1) - \frac{h^2}{12}\left(g_{qq}(q_1)(p_{1/2}, p_{1/2}) + g_q(q_1) g(q_1)\right)\right), \tag{3.73}$$

where we introduced an intermediate variable

$$p_{1/2} = p_0 + \frac{h}{2} l_1. \tag{3.74}$$

The equations (3.71) and (3.72) are implicit, the equation (3.73) is explicit.

CHAPTER 4

CONVERGENCE ANALYSIS

In this chapter after presenting the new numerical method, its convergence properties are analyzed using concepts familiar from numerical analysis of *stability*, *consistency* and *order*.

Definition 4.1 ***Consistency and order:*** *Suppose the numerical method is*

$$y_{n+k} = \phi(t_{n+k}; y_n, y_{n+1}, ..., y_{n+k-1}; h). \tag{4.1}$$

The local error of the method is the error committed by one step of the method. That is, it is the difference between the result given by the method, assuming that no error is made in earlier steps, and the exact solution:

$$\delta^h_{n+k} = \phi(t_{n+k}; y(t_n), y(t_{n+1}), ..., y(t_{n+k-1}); h) - y(t_{n+k}). \tag{4.2}$$

The method is said to be consistent if

$$\lim_{h\to 0} \frac{\delta^h_{n+k}}{h} = 0. \tag{4.3}$$

The method has order p if

$$\delta^h_{n+k} = \mathrm{O}(h^{p+1}) \ as \ h \to 0. \tag{4.4}$$

Hence a method is consistent if it has an order greater than 0. Most methods being used in practice attain higher order. Consistency is a necessary condition for convergence, but not sufficient; for a method to be convergent, it must be both consistent and stable.

A related concept is the global error, the error sustained in all the steps one needs to reach a fixed time t. Explicitly, the global error at time t is $y_N - y(t)$ with $N = (t - t_0)/h$

where N is the number of the discretization points and $y_N, y(t)$ represents the numerical solution and exact solution, respectively. The global error of a p^{th} order one-step method is $\mathcal{O}(h^p)$; in particular, such a method is convergent. This statement is not necessarily true for multi-step methods.

Proposition 4.1 *Application of the Lobatto IIIA - IIIB pair of the second order to the modified differential equations gives a numerical method of order 4.*

Proof For simplicity, we prove the theorem for mechanical system given by

$$\begin{aligned} \dot{q} &= p & (4.5) \\ \dot{p} &= -V_q(q). & (4.6) \end{aligned}$$

The application of Lobatto IIIA-IIIB pair method given in (3.16),(3.17),(3.18) and (3.19) to the above mechanical system yields

$$\begin{cases} q' = p + \dfrac{h^2}{6} g_q p = \left(I - \dfrac{h^2}{6} V_{qq} \right) p \\ \\ p' = -V_q(q) - \dfrac{h^2}{12} (g_{qq}(p,p) + g_q g). \end{cases} \tag{4.7}$$

Traditionally, local error analysis is done by comparing the Taylor expansions of exact solution and the numerical solution.

For one-step method it is useful to write these expansions in the form. The Taylor expansion of k_1, k_2, l_1, l_2 around the (q_0, p_0) are given in the below equations. For k_1, we have

$$\begin{aligned} k_1 &= f(q_0,p_0) + \frac{h}{2} l_1 \frac{\partial f}{\partial p}(q_0,p_0) + \frac{h^2}{2!} l_1^2 \frac{\partial^2 f}{\partial p^2}(q_0,p_0) + \ldots & (4.8) \\ &= (p_0 + \frac{h}{2} l_1)(1 - \frac{h^2}{6} g_q) + \frac{h}{2} l_1 f_p + \frac{h^2}{4} l_1^2 \underbrace{\frac{\partial^2 f}{\partial p^2}(q_0,p_0)}_{0} + \ldots & (4.9) \\ &= p_0 - \frac{h^2}{6} g_q p_0 + \frac{h}{2} l_1 - \frac{h^3}{12} l_1 g_q + \frac{h}{2} l_1 (1 - \frac{h^2}{6} g_q) & (4.10) \\ &= p_0 - \frac{h^2}{6} g_q p_0 + h l_1 - \frac{h^3}{6} l_1 g_q & (4.11) \end{aligned}$$

For l_1, we have

$$\begin{aligned} l_1 &= g(q_0, p_0 + \frac{h}{2}l_1) = g(q_0, p_0) + \frac{h}{2}l_1 g_q + \frac{h^2}{4}l_1^2 g_{qq} + ... \qquad (4.12) \\ &= -V_q(q_0) - \frac{h^2}{12}(g_{qq}(p_0, p_0) + g_q g) + \frac{h}{2}l_1[-V_{qq}(q_0) \\ &\quad -\frac{h^2}{12}(g_{qqq}(p_0, p_0) + g_{qq}g + g_q^2)] + ... \qquad (4.13) \end{aligned}$$

Since we will use the below equation which q_1 and q_0 are related in the next step

$$q_1 = q_0 + \frac{h}{2}(k_1 + k_2). \qquad (4.14)$$

Inserting k_1 and k_2 $(k_1 = k_2)$ into (4.14), we get

$$\begin{aligned} q_1 &= q_0 + \frac{h}{2}(k_1 + k_2) = q_0 + hp_0 - \frac{h^3}{6}g_q p_0 + h^2 l_1 - \frac{h^4}{6}l_1 g_q. \qquad (4.15) \\ &= q_0 + hp_0 - \frac{h^3}{6}g_q p_0 + h^2(-V_q(q_0) - \frac{h^2}{12}g_{qq}(p_0, p_0) - \frac{h^2}{12}g_q g + ...) \\ &\quad -\frac{h^4}{6}(-V_q(q_0) - \frac{h^2}{12}g_{qq}(p_0, p_0) - \frac{h^2}{12}g_q g + ...)g_q. \qquad (4.16) \end{aligned}$$

The Taylor expansion of the exact solution around the point t_0 is

$$q(t_0 + h) = q(t_0) + h\dot{q}(t_0) + \frac{h^2}{2!}\ddot{q}(t_0) + \frac{h^3}{3!}q^{(3)}(t_0) + \frac{h^4}{4!}q^{(4)}(t_0) + ... \qquad (4.17)$$

Next, we compute the derivatives of q in the Taylor expansion and substitute these derivatives into the equation (4.17), then the exact solution of

$$\dot{q} = p + \frac{h^2}{6}g_q p \qquad (4.18)$$

is

$$
\begin{aligned}
q(t_0+h) &= q_0 + h(p_0 - \frac{h^2}{6}g_q p_0) + \frac{h^2}{2!}(-V_q(q_0) - \frac{h^2}{6}g_{qq} - \frac{h^2}{6}g_q g) \\
&\quad + \frac{h^3}{3!}(-\frac{h^2}{6}g_{qqq} - ...) + \frac{h^4}{4!}(V_q(q_0) + \frac{h^2}{3}g_{qq}g_q + \frac{h^2}{3}g_q^2 g) + ... \quad (4.19)
\end{aligned}
$$

Substracting q_1 from $q(t_0+h)$, we get

$$
\frac{h^3}{3!}(-\frac{h^2}{6}g_{qqq} - ...) = C_1 h^5 \quad (4.20)
$$

This completes first part of proof.

For the second part of proof, we expand l_1 around (q_0, p_0),

$$
\begin{aligned}
l_1 &= g(q_0, p_0 + \frac{h}{2}l_1) = g(q_0, p_0) + \frac{h}{2}l_1 g_q + \frac{h^2}{4}l_1^2 g_{qq} + ... \quad (4.21) \\
&= -V_q(q_0) - \frac{h^2}{12}(g_{qq}(p_0, p_0) + g_q g) + \frac{h}{2}l_1[-V_{qq}(q_0) \\
&\quad -\frac{h^2}{12}(g_{qqq}(p_0, p_0) + g_{qq}g + g_q^2)] + ... \cong g \quad (4.22) \\
&= -V_q(q_0) - \frac{h^2}{12}(g_{qq}(p_0, p_0) + g_q g) + \frac{h}{2}g[-V_{qq}(q_0) \\
&\quad -\frac{h^2}{12}(g_{qqq}(p_0, p_0) + g_{qq}g + g_q^2)] + \frac{h^2}{4}g^2 g_{qq} + ... \quad (4.23) \\
&= -V_q(q_0) - \frac{h^2}{12}g_{qq}(p_0, p_0) - \frac{h^2}{12}g_q g - \frac{h}{2}g V_{qq}(q_0) \\
&\quad -\frac{h^3}{24}g_{qqq}g - \frac{h^3}{24}g_{qq}g^2 - \frac{h^3}{24}g_q^2 g + \frac{h^2}{4}g^2 g_{qq} + ... \quad (4.24)
\end{aligned}
$$

and

$$
\begin{aligned}
l_2 &= g(q_0 + \frac{h}{2}(k_1 + k_2), p_0 + \frac{h}{2}l_1) \quad (4.25) \\
&= -V_q(q_0 + hp_0 - \frac{h^3}{6}g_q p_0 + h^2 g - \frac{h^4}{6}g_q g) - \frac{h^2}{12}(g_{qq}(p_0, p_0) + g_q g) \\
&\quad + \frac{h}{2}g g_q + \frac{h^2}{4}g^2 g_{qq} + ... \quad (4.26)
\end{aligned}
$$

Since we will use the relation in the next step where q_1 and q_0 related with the below equation

$$p_1 = p_0 + \frac{h}{2}(l_1 + l_2) \tag{4.27}$$

Inserting l_1 and l_2 into (4.27), we get

$$\begin{aligned} &= p_0 - hV_q(q_0) - \frac{h^3}{12}g_{qq}(p_0,p_0) - \frac{h^3}{12}g_q g - \frac{h^2}{2}V_{qq}(q_0) \\ &\quad -\frac{h^4}{24}g_{qqq}(p_0,p_0) - \frac{h^4}{24}g_{qq}g - \frac{h^4}{24}g_q^2 - \frac{h^3}{6}V_{qqq} + ... \end{aligned} \tag{4.28}$$

Next, we compute the derivatives of p in the (4.17) and substitute these derivatives into the equation (4.17). The exact solution of

$$\dot{p} = -V_q(q) - \frac{h^2}{12}(g_{qq}(p,p) + g_q g) \tag{4.29}$$

is

$$\begin{aligned} p(t_0+h) &= p_0 + h(-V_q(q_0) - \frac{h^2}{12}g_{qq}(p_0,p_0) - \frac{h^2}{12}g_q g) \\ &\quad +\frac{h^2}{2!}(-V_{qq}(q_0) - \frac{h^2}{12}g_{qqq}(p_0,p_0) - \frac{h^2}{12}g_{qq}g - \frac{h^2}{12}g_q^2) \\ &\quad +\frac{h^3}{3!}(-V_{qqq}(q_0,q_0) - \frac{h^2}{12}g_{qqqq} - \frac{h^2}{12}g_{qqq}g - \frac{h^2}{12}g_{qq}g_q - ...) \\ &\quad +\frac{h^4}{4!}... \end{aligned} \tag{4.30}$$

Substracting p_1 from $p(t_0 + h)$, we get

$$\frac{h^3}{3!}(-\frac{h^2}{12}g_{qqqq} - \frac{h^2}{12}g_{qqq}g - \frac{h^2}{12}g_{qq}g_q - ...) = C_2 h^5, \tag{4.31}$$

and this completes second part of proof.

Therefore the difference between exact and numerical solution are estimated by

$$\|q(t_0 + h) - q_1\| \;\; \leq \;\; C_1 h^5 \tag{4.32}$$

and

$$\|p(t_0 + h) - p_1\| \;\; \leq \;\; C_2 h^5. \tag{4.33}$$

This inequality shows that the method is order four. Above inequality leads to the following corollary. □

Corollary 4.1 *The modified Lobatto method is consistent.*

Proof The consistency of the method is obvious since $\lim_{h\to 0} \frac{T_{n+1}}{h} = 0$ where T_{n+1} is truncation error of the method. □

Next, the theoretical findings are proven by the numerical test problem.

Example 4.1 *The errors of the modified Lobatto IIIA-IIIB method are given in Table 4.1. (Here an throughout this section the errors are given in the Euclidean norm.) We apparently have a fourth-order local error. In the following table the numbers in parantheses are the orders in which the error decreased in comparison with the error obtained with the previous step size.*

h	*Error* $(\mathcal{O}(h^{p+1}))$
1	*3.9382*
0.1	*0.0011 (3.5124)*
0.01	*3.3803e-007 (3.5539)*
0.001	*4.7164e-011 (3.8553)*

Table 4.1. The results for the modified Lobatto IIIA-IIIB method applied to Harmonic oscillation problem. The expected local order is 4.

As can be clearly seen that, when the step size decreased the error decreased in comparison with the error obtained with the previous step size. In Table 4.1, when the error decreased we got more regular results about the order of the modified Lobatto IIIA-IIIB method.

4.1. Stability Analysis

In this section we present the stability analysis for the new higher order symplectic methods which where constructed in the previous chapter.

So far we have examined stability theory only in the context of a scalar differential equation $y'(t) = f(y(t))$ for a scalar function $y(t)$. In this section we will look at how this stability theory carries over to systems of m differential equations where $y(t) \in \mathbb{R}^m$. For a linear system $y' = Ay$, where A is $m \times m$ matrix, the solution can be written as $y(t) = e^{At}y(0)$ and the behavior is largely governed by the eigenvalues of A. A necessary condition for stability is that $h\lambda$ be in the stability region for each eigenvalue of A. For general nonlinear systems $y' = f(y)$, the theory is more complicated, but a good rule of thumb is that $h\lambda$ should be in the stability region for each eigenvalue of the Jacobian matrix $f'(y)$. This may not be true if the Jacobian is rapidly changing with time, or even for constant coefficient linear problems in some highly nonnormal cases, but most of the time eigenanalysis is surprisingly effective.

Clearly the one-dimensional test equation

$$y'(t) = \lambda y(t),\ \lambda \in \mathbb{C},\ \ Re(\lambda) < 0,\ \ t \in [0, \infty) \tag{4.34}$$

is not suitable for the study of absolute stability of partitioned discretization methods as we emphasized in the previous subsection. Since we study mainly on separable systems we have to determine the stability condition of the new proposed methods applied to such systems.

Proposition 4.2 *The new symplectic methods applied to the separable systems given in (3.5) with test equations*

$$\dot{q} = \alpha p \tag{4.35}$$

$$\dot{p} = \beta q \tag{4.36}$$

that leads to the mapping $y_{n+1} = R(h)y_n$ said to be stable if $|Tr(R)| < 2$ where $R(h)$ is the linear stability matrix depending on the coefficients α,β and the time-step h.

Proof We have the equation in the form

$$\frac{d}{dt}y = Ay, \tag{4.37}$$

where

$$A = \begin{pmatrix} 0 & \alpha \\ \beta & 0 \end{pmatrix}. \tag{4.38}$$

The application of the new method leads to the mapping

$$y_{n+1} = R(h)y_n. \tag{4.39}$$

Consider the 2×2 matrix $R(h)$ such that

$$R(h) = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}. \tag{4.40}$$

A sufficient condition for stability is that the eigenvalues of method are (i) in the unit disc in the complex plane, and (ii) simple (not repeated) if on the unit circle. Since $R(h)$ is a symplectic map one of its properties is that its determinant is equal to 1.

The eigenvalues of the transformation are given by the characteristic equation

$$\begin{aligned} det\begin{pmatrix} a_{11}-\lambda & a_{12} \\ a_{21} & a_{22}-\lambda \end{pmatrix} &= ((a_{11}-\lambda)(a_{22}-\lambda)) - a_{12}a_{21} = 0 && (4.41)\\ &= \lambda^2 - \underbrace{(a_{11}+a_{22})}_{Tr(R)}\lambda + \underbrace{a_{11}a_{22}-a_{12}a_{21}}_{det(R)=1} = 0 && (4.42)\\ &= \lambda^2 - Tr(R)\lambda + 1 = 0. && (4.43) \end{aligned}$$

The eigenvalues of R are solutions of $\lambda^2 - Tr(R)\lambda + 1 = 0$.

Following Arnold's treatment of the stability of symplectic maps (Olver, 1993), if the two roots λ_1 and λ_2, of this equation are complex conjugates then

$$\lambda = \frac{Tr(R)}{2} \pm i\sqrt{1 - (\frac{Tr(R)}{2})^2}. \tag{4.44}$$

For stability $\lambda < 1$, hence $|Tr(R)| < 2$ is required. Because the norms of the eigenvalues given in the equation (4.39) are 1 it means that the roots are on the unit circle. For the stability condition the roots can not be multiple if they are on the unit circle. Since R depends explicitly on the step-size h, it is necessary to take the least positive solution of $|Tr(R)| = 2$ with respect to h in the calculation of stability criteria. $\square$

Since the general form of the Hamiltonian system is

$$\dot{q} = \alpha p \tag{4.45}$$

$$\dot{p} = \beta q. \tag{4.46}$$

Applying (4.45) and (4.46) to mechanical system given by the equations (3.16),(3.17),(3.18) and (3.19),

$$\begin{cases} q' = p + \dfrac{h^2}{6} g_q p = \left(I - \dfrac{h^2}{6} V_{qq}\right) p \\ \\ p' = -V_q(q) - \dfrac{h^2}{12}(g_{qq}(p,p) + g_q g), \end{cases} \tag{4.47}$$

we obtain the modified differential equations of the system (4.45) and (4.46) in the form

$$q' = \alpha p\left(1 - \frac{h^2}{6}\right) \tag{4.48}$$

$$p' = \beta q\left(1 + \frac{h^2}{12}\right). \tag{4.49}$$

Next proposition asserts the stability condition for the mechanical system.

Proposition 4.3 *The modified Lobatto method applied to the system (4.48) and (4.49) is stable for* $\left|2 + h^2\alpha\beta - \frac{h^4}{8}\alpha\beta - \frac{h^6}{72}\alpha\beta\right| < 2.$

Proof Applying (4.45) and (4.46) to the mechanical system, we get (4.48) and (4.49). Taking $\tilde{h} = \frac{h^2}{12}$, the modified system given in equations (4.48),(4.49) takes the form

$$q' = \alpha p(1 - 2\tilde{h}), \quad p' = \beta q(1 + \tilde{h}). \tag{4.50}$$

The application of the Lobatto IIIA-IIIB given in (3.16),(3.17),(3.18) and (3.19) yields expressions k_1,k_2,

$$k_1 = k_2 = f(q_0, p_0 + \frac{h}{2}l_1) = \Big[\alpha\big(p_0 + \frac{h}{2}(\beta q_0(1 + \tilde{h}))\big)\Big]\big(1 - 2\tilde{h}\big) \tag{4.51}$$

and l_1,l_2 below

$$l_1 = \beta q_0(1 + \tilde{h}), \;\; l_2 = \Bigg\{\beta\Big[q_0 + h\big(\alpha(p_0 + \frac{h}{2}(\beta q_0(1 + \tilde{h})))\big)\big(1 - 2\tilde{h}\big)\Big]\Bigg\}\big(1 + \tilde{h}\big) \tag{4.52}$$

Since

$$q_{n+1} = q_n + \frac{h}{2}(k_1 + k_2), \qquad p_{n+1} = p_n + \frac{h}{2}(l_1 + l_2), \tag{4.53}$$

then

$$\begin{aligned} q_{n+1} &= q_n + h\Big[\big(\alpha(p_n + \frac{h}{2}(\beta q_n(1 + \tilde{h})))\big)(1 - 2\tilde{h})\Big], & (4.54) \\ p_{n+1} &= p_n + \frac{h}{2}\Bigg\{\beta q_n(1 + \tilde{h}) + \Big[\beta\big(q_n + h(\alpha(p_n \\ &\quad + \frac{h}{2}(\beta q_n(1 + \tilde{h}))))(1 - 2\tilde{h})\big)\big(1 + \tilde{h}\big)\Big]\Bigg\}. & (4.55) \end{aligned}$$

As a result,

$$
\begin{aligned}
q_{n+1} &= q_n\left(1+\frac{h^2}{2}\alpha\beta-\frac{h^2\tilde{h}}{2}\alpha\beta-h^2\tilde{h}^2\alpha\beta\right)+p_n\left(h\alpha-2h\tilde{h}\alpha\right), && (4.56)\\
p_{n+1} &= p_n\left(1+\frac{h^2}{2}\alpha\beta-h^2\tilde{h}\alpha\beta-h^2\tilde{h}^2\alpha\beta\right)\\
&\quad +q_n\left(h\beta-\frac{3}{4}h^3\tilde{h}^2\alpha\beta^2+h\tilde{h}\beta+\frac{h^3}{4}\alpha\beta^2+\frac{h^2\tilde{h}}{2}\alpha\beta-\frac{h^3\tilde{h}^3}{2}\alpha\beta^2\right) && (4.57)
\end{aligned}
$$

Matrix form of our modified system is in the form $X_{n+1}=WX_n$:

$$
\begin{bmatrix} q_{n+1}\\ p_{n+1}\end{bmatrix}=\underbrace{\begin{bmatrix}1+\frac{h^2}{2}\alpha\beta-\frac{h^2\tilde{h}}{2}\alpha\beta-h^2\tilde{h}^2\alpha\beta & A\\ B & 1+\frac{h^2}{2}\alpha\beta-h^2\tilde{h}\alpha\beta-h^2\tilde{h}^2\alpha\beta\end{bmatrix}}_{W}\begin{bmatrix} q_n\\ p_n\end{bmatrix} \tag{4.58}
$$

where $A=h\alpha-2h\tilde{h}\alpha$, $B=h\beta-\frac{3}{4}h^3\tilde{h}^2\alpha\beta^2+h\tilde{h}\beta+\frac{h^3}{4}\alpha\beta^2+\frac{h^2\tilde{h}}{2}\alpha\beta-\frac{h^3\tilde{h}^3}{2}\alpha\beta^2$.

By using Proposition 4.2, we get

$$
Tr(W)=2+h^2\alpha\beta-\frac{3}{2}h^2\tilde{h}\alpha\beta-2h^2\tilde{h}^2\alpha\beta=2+h^2\alpha\beta-\frac{h^4}{8}\alpha\beta-\frac{h^6}{72}\alpha\beta. \tag{4.59}
$$

from the relation $\tilde{h}=\frac{h^2}{12}$. Since the characteristic polynomial for the 2x2 symplectic transformation is given by

$$
P(\lambda)=\lambda^2-(Tr(W))\lambda+1=0. \tag{4.60}
$$

The roots, λ_1 and λ_2, of this equation are complex conjugates then

$$
\begin{aligned}
\lambda_{1,2} &= \frac{Tr(W)}{2}\pm i\sqrt{1-\left(\frac{Tr(W)}{2}\right)^2}, && (4.61)\\
&= \frac{2+h^2\alpha\beta-\frac{h^4}{8}\alpha\beta-\frac{h^6}{72}\alpha\beta}{2}\\
&\quad \pm i\sqrt{1-\left(\frac{2+h^2\alpha\beta-\frac{h^4}{8}\alpha\beta-\frac{h^6}{72}\alpha\beta}{2}\right)^2} && (4.62)
\end{aligned}
$$

With the trace of the matrix W satisfies $|Tr(W)| < 2$, so

$$\left|2 + h^2\alpha\beta - \frac{h^4}{8}\alpha\beta - \frac{h^6}{72}\alpha\beta\right| < 2, \tag{4.63}$$

and

$$-2 < 2 + f(h)\alpha\beta < 2 \tag{4.64}$$

where $f(h) = h^2 - \frac{h^4}{8} - \frac{h^6}{72}$ and $\alpha\beta < 0$. Then

$$0 < \frac{f(h)}{|\alpha\beta|} < 4, \tag{4.65}$$

the method is stable ($\lambda < 1$) if the following conditions are satisfied

- $\alpha\beta < 0$
- $f(h) < 4|\alpha\beta|$.

□

4.1.1. The Behaviour of Stability of Modified Lobatto Method

We can obtain the stability conditions for Harmonic oscillation problem with different time-step h.

The following Figure 4.1 illustrates the stability conditions for the modified Lobatto method applied to Harmonic oscillation problem. The trace of the matrix W for the modified Lobatto method is $|Tr(W)| = \left|2 - h^2 + \frac{h^4}{8} + \frac{h^6}{72}\right|$.

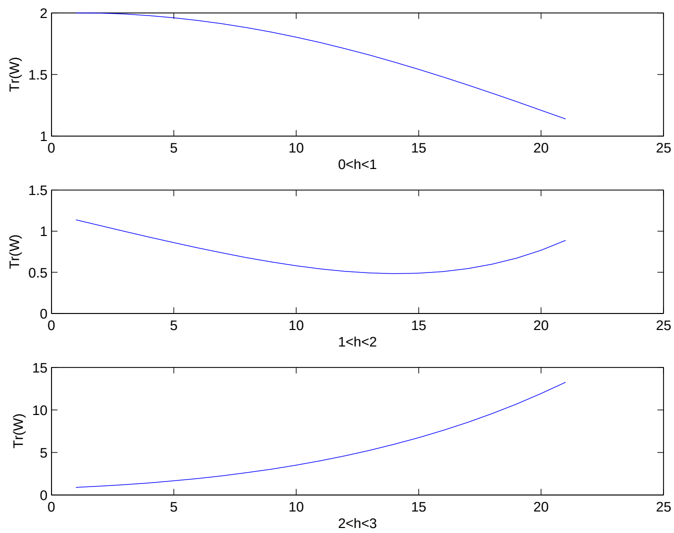

Figure 4.1. The relation between the parameter h and $Tr(W)$ for modified Lobatto method applied to Harmonic oscillation problem.

CHAPTER 5

MODIFIED SYMPLECTIC EULER METHOD FOR PDE PROBLEMS

The modified symplectic Euler method of order 2 and 3 were constructed in the thesis (Duygu Demir, 2009) by using the modified vector field idea. In this chapter, we apply these methods to linear and nonlinear PDE problems. In addition we present the Von-Neumann stability analysis of the differential equations we considered. The modified vector differential equations of 1-term modified symplectic Euler method are

$$\dot{q} = a(q,p) + hc(q,p) = F(q,p), \tag{5.1}$$

$$\dot{p} = b(q,p) + hd(q,p) = G(q,p). \tag{5.2}$$

where the functions $c = \frac{1}{2}(a_p b - a_q a)$ and $d = \frac{1}{2}(b_p b - b_q a)$, and 2-term modified symplectic Euler method are

$$\dot{q} = a(q,p) + hc(q,p) + h^2 e(q,p) = F(q,p) \tag{5.3}$$

$$\dot{p} = b(q,p) + hd(q,p) + h^2 f(q,p) = G(q,p) \tag{5.4}$$

where

$$c = \frac{1}{2}(a_p b - a_q a), \qquad d = \frac{1}{2}(b_p b - b_q a), \tag{5.5}$$

$$\begin{aligned} e = \frac{1}{6}(&a_{qq}(a,a) - a_{qp}(a,b) + a_{pp}(b,b) + a_q a_q a - 2a_q a_p b \\ &-2a_p b_q a + a_p b_p b), \end{aligned} \tag{5.6}$$

$$\begin{aligned} f = \frac{1}{6}(&b_{qq}(a,a) - b_{qp}(a,b) + b_{pp}(b,b) + b_q a_q a - 2b_q a_p b \\ &-2b_p b_q a + b_p b_p b). \end{aligned} \tag{5.7}$$

We choose separable systems since the calculations of the coefficient functions become more easier. For separable systems the coefficient functions can be given as follows

$$c = \frac{1}{2}a_p b, \qquad d = -\frac{1}{2}b_q a, \tag{5.8}$$

$$e = \frac{1}{6}(a_{pp}(b,b) - 2a_p b_q a), \qquad f = \frac{1}{6}(b_{qq}(a,a) - 2b_q a_p a). \tag{5.9}$$

If the original equations are Hamiltonian, we get

$$H^{[3]} = H + \frac{h}{2}(a,b) + \frac{h^2}{6}(H_{qq}(a,a) + H_{pp}(b,b)). \tag{5.10}$$

for separable systems.

5.1. Criteria of Linear Stability of Symplectic Algorithm

Here we will investigate the stability of the partial differential equations with Von Neumann approach (James E., Howard ,Holger R., & Dullin, 1998). In the approach taken here, it is not necessary to specify a spatial discretisation method. It suffices to know that there exist a spatial discretisation technique that can be applied to the resultant system of equation.

Let us consider the linear system of equation,

$$\begin{pmatrix} \frac{\partial u}{\partial t} \\ \frac{\partial v}{\partial t} \end{pmatrix} = \begin{pmatrix} L_1(u) \\ L_2(v) \end{pmatrix} \tag{5.11}$$

where L_1 and L_2 are linear and bounded operators $u = u(x,t)$ and $v = v(x,t)$. Suppose that we have a linear map resulting from the application of the 2nd order midpoint rule to the system (5.11) over one time step such that,

$$\begin{pmatrix} u'(x) \\ v'(x) \end{pmatrix} = \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} u_0(x) \\ v_0(x) \end{pmatrix} = A' \begin{pmatrix} u_0(x) \\ v_0(x) \end{pmatrix} \tag{5.12}$$

where A' is a matrix of linear operators, $u_0(x) = u(x,t_0)$, $v_0(x) = v(x,t_0)$ are the temporal initial conditions, and $u^{'}(x)$ and $v^{'}(x)$ are the approximations of u and v in function space at time $t = t_0 + \tau$.

The stability criterion for the linear map we need to check the eigenvalues of the matrix $A^{'}$. The eigenvalues of the $A^{'}$ are solutions of $\lambda^2 - Tr(A') + det(A') = 0$. Following the stability of the linear maps, if the roots λ_1 and λ_2 of the equation are complex conjugates then,

$$\lambda = \frac{Tr(A')}{2} \pm i\sqrt{det(A') - \left(\frac{Tr(A')}{2}\right)^2} \tag{5.13}$$

with $\mid Tr(A') \mid < 2\sqrt{det(A')}$ and $\lambda < 1$. In order to apply stability theory A' must be manipulated into a matrix of scalars. This is done by taking Fourier transforms of (5.12) as would be done in a Von-Neumann stability analysis. We will restrict this discussion to linear operators that are either spatial derivatives of at least first order or the identity multiplied by real or complex scalars. Given this restriction, applying a continuous Fourier transform to (5.12) according to the formula,

$$\hat{u}(w) = \frac{1}{\sqrt{2\pi}} \int_{\mathbf{R}} e^{-iwx} u(x) dx \tag{5.14}$$

we will yield,

$$\begin{pmatrix} \hat{u}^{'}(w) \\ \hat{v}^{'}(w) \end{pmatrix} = \begin{pmatrix} z_{11}(w) & z_{12}(w) \\ z_{21}(w) & z_{22}(w) \end{pmatrix} \begin{pmatrix} \hat{u}_0(w) \\ \hat{v}_0(w) \end{pmatrix} = A \begin{pmatrix} \hat{u}_0(w) \\ \hat{v}_0(w) \end{pmatrix} \tag{5.15}$$

where $z_{ij}(w)$ are complex scalars involving the frequency $w \in \mathbb{R}$ (Strehmel & Weiner, 1984), (Regan, 2000). This gives stability criteria in terms of the spectral variable w.

5.2. Von-Neumann Stability Analysis Applied to Hamiltonian PDEs

In this section, we briefly present Von-Neumann stability analysis for the linear PDE. The general PDE equation can be put into the matrix differential equation form with the help of the method of lines

$$\dot{u} = Bv \tag{5.16}$$

$$\dot{v} = Au \tag{5.17}$$

where A,B are constant matrices. The application of the modified symplectic Euler method of order 2 to the equation (5.16),(5.17) yields

$$u_{n+1} = u_n + h\left[v_{n+1} + \frac{h}{2}BAu_n\right] \tag{5.18}$$

$$v_{n+1} = v_n + h\left[Au_n - \frac{h}{2}ABv_{n+1}\right]. \tag{5.19}$$

The application of the modified symplectic Euler method of order 3 to the equation (5.16),(5.17) yields

$$u_{n+1} = u_n + h\left[v_{n+1} + \frac{h}{2}BAu_n - \frac{h^2}{3}BABv_{n+1}\right] \tag{5.20}$$

$$v_{n+1} = v_n + h\left[Au_n - \frac{h}{2}ABv_{n+1} - \frac{h^2}{3}ABAu_n\right]. \tag{5.21}$$

where $u,\ v \in \mathrm{R}^n$ and $A,\ B \in \mathrm{R}^n \times \mathrm{R}^n$. Next, we consider the following particular PDE problems.

5.2.1. Linear Wave Equation

Linear wave equation can be described as

$$u_{tt} - u_{xx} = 0 \tag{5.22}$$

for all $(x, t) \in \mathbf{R} \times (0, \infty)$.

Equation (5.22) can be written as an infinite dimensional Hamiltonian system by letting $u_t = v$ and $v_t = u_{xx}$,

$$u_t = -\frac{\delta H}{\delta v}(u, v), \quad v_t = \frac{\delta H}{\delta u}(u, v) \tag{5.23}$$

with Hamiltonian functional

$$H(u, v) = \frac{1}{2}\int_R (u_x^2 + v^2)\, dx. \tag{5.24}$$

The solution $(u(x,t), v(x,t))$, as a time-t map in the phase space, is symplectic. The equation (5.24) is discretized using central difference approximation for u_x with the Hamiltonian

$$H(u, v) = \frac{1}{2}\sum_{i=1}^{n}\left[\big(\frac{u_{i+1} - u_{i-1}}{2\Delta x}\big)^2 + v_i^2\right]. \tag{5.25}$$

From the general form of separable Hamiltonian PDEs (5.16) and (5.17), we take $B = \mathrm{I}$ for linear wave equation

$$\begin{aligned} \dot{u} &= \dot{q} = a(q, p) = v && (5.26)\\ \dot{v} &= \dot{p} = b(q, p) = \partial_{xx}u = Au && (5.27) \end{aligned}$$

where A is a linear operator. Application of 2nd order modified symplectic Euler method to linear wave equation yields

$$\begin{aligned} u_{n+1} &= u_n + h[v_{n+1} + \frac{h}{2}Au_n] && (5.28)\\ v_{n+1} &= v_n + h[Au_n - \frac{h}{2}Av_{n+1}]. && (5.29) \end{aligned}$$

The equations (5.28) and (5.29) may be put into the matrix equation as below

$$\begin{pmatrix} I & -hI \\ 0 & I + \frac{h^2}{2}A \end{pmatrix}\begin{pmatrix} u_{n+1} \\ v_{n+1} \end{pmatrix} = \begin{pmatrix} I + \frac{h^2}{2}A & 0 \\ hA & I \end{pmatrix}\begin{pmatrix} u_n \\ v_n \end{pmatrix}. \tag{5.30}$$

We take a fourier transform of (5.30) by using the Fourier transform formula

$$\hat{u}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{\mathrm{R}} e^{-i\omega x} u(x) dx \tag{5.31}$$

and Fourier transform formula gives

$$\underbrace{\begin{pmatrix} 1 & -h \\ 0 & 1-\frac{h^2}{2}\omega^2 \end{pmatrix}}_{D} \begin{pmatrix} \hat{u}_{n+1}(\omega) \\ \hat{v}_{n+1}(\omega) \end{pmatrix} = \begin{pmatrix} 1-\frac{h^2}{2}\omega^2 & 0 \\ -h\omega^2 & 1 \end{pmatrix} \begin{pmatrix} \hat{u}_n(\omega) \\ \hat{v}_n(\omega) \end{pmatrix}. \tag{5.32}$$

We take the inverse of D,

$$\begin{pmatrix} \hat{u}_{n+1}(\omega) \\ \hat{v}_{n+1}(\omega) \end{pmatrix} = \underbrace{\begin{pmatrix} 1-\frac{h^2}{2}\omega^2 - \frac{h^2\omega^2}{1-\frac{h^2}{2}\omega^2} & \frac{h}{1-\frac{h^2}{2}\omega^2} \\ -\frac{h\omega^2}{1-\frac{h^2}{2}\omega^2} & \frac{1}{1-\frac{h^2}{2}\omega^2} \end{pmatrix}}_{D'} \begin{pmatrix} \hat{u}_n(\omega) \\ \hat{v}_n(\omega) \end{pmatrix} \tag{5.33}$$

Note that $\det(D') = 1$ in (5.33) which gives the symplecticity condition. For stability we require

$$|Tr(D)| < 2 \quad \Rightarrow \left| 2 - \frac{h^2}{2}\omega^2 - \frac{\frac{h^2}{2}\omega^2}{1-\frac{h^2}{2}\omega^2} \right| < 2 \tag{5.34}$$

Now, we can find the stability condition for linear wave equation by using well-known Fourier method. Namely, we specify spatial discretisation method to see the value of ω and we see the stability condition more specifically. Application of the modified sypmlectic Euler method of order 2 to linear wave equation yields

$$u_m^{n+1} = u_m^n + hv_m^{n+1} + \frac{h^2}{2}\left[\frac{u_{m+1}^n - 2u_m^n + u_{m-1}^n}{(\Delta x)^2}\right] \tag{5.35}$$

$$v_m^{n+1} = v_m^n + h\left[\frac{u_{m+1}^n - 2u_m^n + u_{m-1}^n}{(\Delta x)^2}\right] - \frac{h^2}{2}\left[\frac{v_{m+1}^{n+1} - 2v_m^{n+1} + v_{m-1}^{n+1}}{(\Delta x)^2}\right] \tag{5.36}$$

We can take $u_m^n = g_1^n e^{im\theta}$ and $v_m^n = g_2^n e^{im\theta}$ and insert them in the equations (5.35) and

(5.36) respectively. The above equations become

$$\begin{aligned} g_1^{n+1}e^{im\theta} &= g_1^n e^{im\theta} + hg_2^{n+1}e^{im\theta} \\ &+\frac{h^2}{2}\left[\frac{g_1^n e^{i(m+1)\theta} - 2g_1^n e^{im\theta} + g_1^n e^{i(m-1)\theta}}{(\Delta x)^2}\right] \end{aligned} \tag{5.37}$$

$$\begin{aligned} g_2^{n+1}e^{im\theta} &= g_2^n e^{im\theta} + h\left[\frac{g_1^n e^{i(m+1)\theta} - 2g_1^n e^{im\theta} + g_1^n e^{i(m-1)\theta}}{(\Delta x)^2}\right] \\ &-\frac{h^2}{2}\left[\frac{g_2^{n+1} e^{i(m+1)\theta} - 2g_2^{n+1} e^{im\theta} + g_2^{n+1} e^{i(m-1)\theta}}{(\Delta x)^2}\right] \end{aligned} \tag{5.38}$$

Dividing both sides by $e^{im\theta}$, we have

$$g_1^{n+1} = g_1^n + hg_2^{n+1} + \frac{h^2}{2}\left[\frac{g_1^n e^{i\theta} - 2g_1^n + g_1^n e^{-i\theta}}{(\Delta x)^2}\right] \tag{5.39}$$

$$\begin{aligned} g_2^{n+1} &= g_2^n + h\left[\frac{g_1^n e^{i\theta} - 2g_1^n + g_1^n e^{-i\theta}}{(\Delta x)^2}\right] \\ &-\frac{h^2}{2}\left[\frac{g_2^{n+1} e^{i\theta} - 2g_2^{n+1} + g_2^{n+1} e^{-i\theta}}{(\Delta x)^2}\right] \end{aligned} \tag{5.40}$$

With the aid of $e^{i\theta} = \cos\theta + i\sin\theta$, the above equations can be rewritten as

$$g_1^{n+1} = g_1^n\left[1 - 2h^2\frac{\lambda}{1-h^2\lambda} - h^2\lambda\right] + g_2^n\frac{h}{1-h^2\lambda} \tag{5.41}$$

$$g_2^{n+1} = g_1^n\left[-\frac{2h\lambda}{1-h^2\lambda}\right] + g_2^n\frac{1}{1-h^2\lambda} \tag{5.42}$$

where $\lambda = \frac{\sin^2\frac{\theta}{2}}{(\Delta x)^2}$. One can put the equation (5.41) and (5.42) into the matrix form

$$\begin{pmatrix} g_1^{n+1} \\ g_2^{n+1} \end{pmatrix} = \begin{pmatrix} 1 - h^2\lambda - \frac{2h^2\lambda}{1-h^2\lambda} & \frac{h}{1-h^2\lambda} \\ -\frac{2h\lambda}{1-h^2\lambda} & \frac{1}{1-h^2\lambda} \end{pmatrix}\begin{pmatrix} g_1^n \\ g_2^n \end{pmatrix}. \tag{5.43}$$

Note that the determinant of the above matrix is 1 which gives the symplecticity. Trace of the matrix gives the stability condition,

$$\left|2 - h^2\lambda - \frac{h^2\lambda}{1 - h^2\lambda}\right| < 2. \tag{5.44}$$

Comparing (5.33) and (5.43) we observe that

$$\frac{\omega^2}{2} = \lambda \;\; \Rightarrow \;\; \omega^2 = 2\lambda = \frac{2\sin^2\frac{\theta}{2}}{(\Delta x)^2}. \tag{5.45}$$

By setting $\alpha = \frac{h^2}{2}\omega^2$, the equation (5.43) can be written in terms of ω.

$$\left|2 - \frac{h^2}{2}\omega^2 - \frac{\frac{h^2}{2}\omega^2}{1 - \frac{h^2}{2}\omega^2}\right| < 2. \tag{5.46}$$

Next, we define the following function in terms of α and we have

$$y(\alpha) = 2 - \alpha - \frac{\alpha}{1 - \alpha}. \tag{5.47}$$

In Figure 5.1, we exhibit the graph of the $y(\alpha)$ and $y = 2$, the inequality $y(\alpha) < 2$ holds for $0 < \alpha < \frac{1}{2}$.

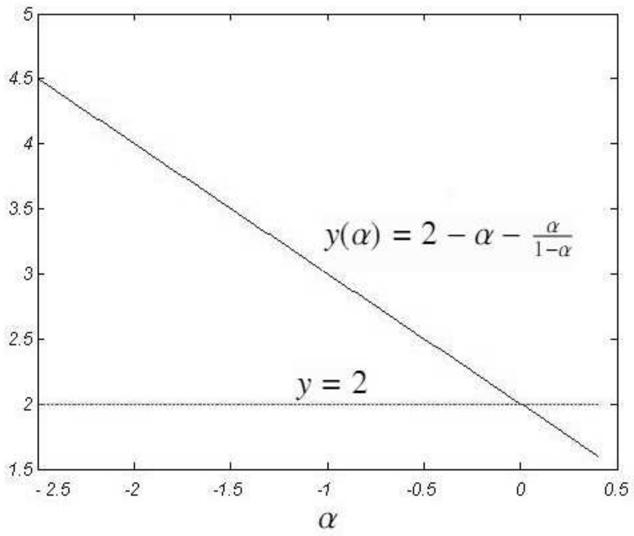

Figure 5.1. The graph of $y(\alpha) = 2 - \alpha - \frac{\alpha}{1-\alpha}$ and $y = 2$.

Finally, from the figure it is clear that the method is stable for $0 < \alpha < \frac{1}{2}$. We showed that $\omega^2 = \frac{2\sin^2\frac{\theta}{2}}{(\Delta x)^2}$. We can deduce the relation between h and Δx by inserting ω^2 into the equation (5.46).

$$\left| h^2 \frac{\sin^2 \frac{\theta}{2}}{(\Delta x)^2} \right| < \frac{h^2}{(\Delta x)^2} < \frac{1}{2} \quad \Rightarrow \quad \frac{h}{\Delta x} < \frac{1}{2}. \tag{5.48}$$

Note that, the method is in implicit form. By using the localization idea, we obtain the explicit form of the modified symplectic Euler method of order 2. For this purpose, we use the first order approximation of the variable v_n as follows

$$v_{n+1} = v_n + hAu_n \tag{5.49}$$

and put this into the equations (5.28) and (5.29), we get

$$u_{n+1} = \left[I + \frac{3}{2}h^2 A \right] u_n + hv_n \tag{5.50}$$

$$v_{n+1} = \left[hA - \frac{1}{2}h^3 AA \right] u_n + \left[I - \frac{1}{2}h^2 A \right] v_n. \tag{5.51}$$

The equations (5.50) and (5.51) may be put into the matrix equation as below

$$\begin{pmatrix} u_{n+1} \\ v_{n+1} \end{pmatrix} = \begin{pmatrix} I + \frac{3}{2}h^2 A & h \\ hA - \frac{1}{2}h^3 AA & I - \frac{1}{2}h^2 A \end{pmatrix} \begin{pmatrix} u_n \\ v_n \end{pmatrix}. \tag{5.52}$$

We take a fourier transform of (5.52),

$$\begin{pmatrix} \hat{u}_{n+1}(\omega) \\ \hat{v}_{n+1}(\omega) \end{pmatrix} = \begin{pmatrix} 1 - \frac{3}{2}h^2\omega^2 & h \\ -h\omega^2 - \frac{1}{2}h^3\omega^4 & 1 + \frac{1}{2}h^2\omega^2 \end{pmatrix} \begin{pmatrix} \hat{u}_n(\omega) \\ \hat{v}_n(\omega) \end{pmatrix} \tag{5.53}$$

Determinant of the above matrix gives the symplecticity of the explicit form of modified symplectic Euler method. Trace of the above matrix is $|2 - h^2\omega^2|$. By setting $2\alpha = h^2\omega^2$, we get $|2 - 2\alpha| < 2$. The method is stable for $0 < \alpha < \frac{1}{2}$. We can deduce the relation between h and Δx by inserting ω^2 into the equation (5.46).

$$\left| h^2 \frac{\sin^2 \frac{\theta}{2}}{(\Delta x)^2} \right| < \frac{h^2}{(\Delta x)^2} < \frac{1}{2} \quad \Rightarrow \quad \frac{h}{\Delta x} < \frac{1}{\sqrt{2}}. \tag{5.54}$$

Application of 3rd order modified symplectic Euler method to linear wave equation yields

$$u_{n+1} = u_n + h[v_{n+1} + \frac{h}{2}Au_n - \frac{h^2}{3}Av_{n+1}] \tag{5.55}$$

$$v_{n+1} = v_n + h[Au_n - \frac{h}{2}Av_{n+1} - \frac{h^2}{3}AAu_n]. \tag{5.56}$$

The equations (5.55) and (5.56) may be put into the matrix equation as below

$$\begin{pmatrix} I & -hI + \frac{h^3}{3}A \\ 0 & I + \frac{h^2}{2}A \end{pmatrix} \begin{pmatrix} u_{n+1} \\ v_{n+1} \end{pmatrix} = \begin{pmatrix} I + \frac{h^2}{2}A & 0 \\ hA - \frac{h^3}{3}AA & I \end{pmatrix} \begin{pmatrix} u_n \\ v_n \end{pmatrix}. \tag{5.57}$$

Taking a fourier transform of (5.57), we have

$$\begin{pmatrix} \hat{u}_{n+1}(\omega) \\ \hat{v}_{n+1}(\omega) \end{pmatrix} = \underbrace{\begin{pmatrix} 1 - \frac{h^2}{2}\omega^2 - \frac{\omega^2(h+\frac{h^3}{3}\omega^2)^2}{1-\frac{h^2}{2}\omega^2} & \frac{h+\frac{h^3}{3}\omega^2}{1-\frac{h^2}{2}\omega^2} \\ -\omega^2\frac{h+\frac{h^3}{3}\omega^2}{1-\frac{h^2}{2}\omega^2} & \frac{1}{1-\frac{h^2}{2}\omega^2} \end{pmatrix}}_{\acute{C}} \begin{pmatrix} \hat{u}_n(\omega) \\ \hat{v}_n(\omega) \end{pmatrix} \tag{5.58}$$

$\det(\acute{C}) = 1$ gives the symplecticity. For stability, we require

$$|Tr(\acute{C})| < 2 \quad \Rightarrow \left| \frac{2 - 2h^2\omega^2 - \frac{5}{12}h^4\omega^4 - \frac{1}{9}h^6\omega^6}{1 - \frac{1}{2}h^2\omega^2} \right| < 2. \tag{5.59}$$

with the above inequality.

5.2.2. Sine-Gordon Equation

Sine-Gordon equation can be described as

$$u_{tt} - u_{xx} + \sin u = 0 \tag{5.60}$$

for all $(x, t) \in \mathbf{R} \times (0, \infty)$.

Equation (5.60) can be written as an infinite dimensional Hamiltonian system by letting $u_t = v$ and $v_t = u_{xx} - \sin u$,

$$u_t = -\frac{\delta H}{\delta v}(u, v), \quad v_t = \frac{\delta H}{\delta u}(u, v) \tag{5.61}$$

with Hamiltonian functional

$$H(u, v) = \int_R [\frac{1}{2}(-u_x^2 - v^2) + \cos u] \, dx \tag{5.62}$$

where $\sin u$ is a smooth function of u. The solution $(u(x, t), v(x, t))$, as a time-t map in the phase space, is symplectic. The equation (5.62) is discretized using central difference approximation for u_x with the Hamiltonian

$$H(u,v)=\frac{1}{2}\sum_{i=1}^{n}\Big[-\frac{1}{2}\big(\frac{u_{i+1}-u_{i-1}}{2\Delta x}\big)^2-\frac{1}{2}v_i^2+\cos u_i\Big]. \tag{5.63}$$

Hamilton's equations for the Sine-Gordon equation in 1 space dimension are

$$\frac{\partial}{\partial t}u(x,t)=v(x,t), \quad \frac{\partial}{\partial t}v(x,t)=\frac{\partial^2}{\partial x^2}u(x,t)-\sin(u(x,t)). \tag{5.64}$$

A linearisation about the steady state $u=0$ gives the equations

$$\frac{\partial}{\partial t}u(x,t)=v(x,t), \quad \frac{\partial}{\partial t}v(x,t)=\frac{\partial^2}{\partial x^2}u(x,t)-(u(x,t))=Au \tag{5.65}$$

where $A=\partial_{xx}-\mathrm{I}$ is a linear operator.

Application of 2nd order modified symplectic Euler method to Sine-Gordon equation yields the same result with linear wave equation. The only difference between linear wave equation and Sine-Gordon equation is the linear operator. We have the matrix (5.30) and take the fourier transform of (5.30) with $A=\partial_{xx}-\mathrm{I}$,

$$\begin{pmatrix}\hat{u}_{n+1}(\omega)\\ \hat{v}_{n+1}(\omega)\end{pmatrix}=\begin{pmatrix}1-\frac{h^2}{2}(\omega^2+1)-\frac{h^2(\omega^2+1)}{1-\frac{h^2}{2}(\omega^2+1)} & \frac{h}{1-\frac{h^2}{2}(\omega^2+1)}\\ -\frac{h(\omega^2+1)}{1-\frac{h^2}{2}(\omega^2+1)} & \frac{1}{1-\frac{h^2}{2}(\omega^2+1)}\end{pmatrix}\begin{pmatrix}\hat{u}_n(\omega)\\ \hat{v}_n(\omega)\end{pmatrix} \tag{5.66}$$

and trace of the matrix satisfies the stability with the following condition

$$\left|2-\frac{h^2}{2}(\omega^2+1)-\frac{\frac{h^2}{2}(\omega^2+1)}{1-\frac{h^2}{2}(\omega^2+1)}\right|<2. \tag{5.67}$$

Application of 3rd order modified symplectic Euler method to Sine-Gordon equation yields the same result with linear wave equation. The only difference between (5.22) and (5.60) is the linear operator. We have the matrix (5.57) and take the fourier transform of (5.57) with $A = \partial_{xx} - \mathrm{I}$,

$$\begin{pmatrix} 1 - \frac{h^2}{2}(\omega^2+1) - \frac{(\omega^2+1)(h+\frac{h^3}{3}(\omega^2+1))^2}{1-\frac{h^2}{2}(\omega^2+1)} & \frac{h+\frac{h^3}{3}(\omega^2+1)}{1-\frac{h^2}{2}(\omega^2+1)} \\ -(\omega^2+1)\frac{h+\frac{h^3}{3}(\omega^2+1)}{1-\frac{h^2}{2}(\omega^2+1)} & \frac{1}{1-\frac{h^2}{2}(\omega^2+1)} \end{pmatrix} \tag{5.68}$$

and trace of the above matrix satisfies the stability

$$\left| \frac{2 - 2h^2(\omega^2+1) - \frac{5}{12}h^4(\omega^2+1)^2 - \frac{1}{9}h^6(\omega^2+1)^3}{1 - \frac{1}{2}h^2(\omega^2+1)} \right| < 2. \tag{5.69}$$

with the above condition.

5.2.3. Schrödinger Equation

Consider the linear time dependent Scrödinger equation

$$i\frac{\partial}{\partial t}\psi(x,t) = \Big(-\frac{1}{2\mu}\frac{\partial^2}{\partial t^2} + V(x) \Big)\psi(x,t) \tag{5.70}$$

with $V(x) = D(1 - e^{-\alpha x})^2$. It is separable in its kinetic and potential parts. The solution of the discretised equation is given by

$$i\frac{d}{dt}c(t) = \mathbf{H}c(t) \quad \Rightarrow \quad c(t) = e^{-it\mathbf{H}}c(0) \tag{5.71}$$

Consider $c = q + ip$ then $i\frac{d}{dt}(q+ip) = \mathbf{H}(q+ip)$, then the Hamiltonian system is

$$\mathcal{H} = \frac{1}{2}p^T\mathbf{H}p + \frac{1}{2}q^T\mathbf{H}q \tag{5.72}$$

and we have the separable system of Scrödinger equation

$$\dot{q} = \mathbf{H}p \quad \text{and} \quad \dot{p} = -\mathbf{H}q \tag{5.73}$$

with formal solution

$$O(t)=\begin{pmatrix} \cos(t\mathbf{H}) & \sin(t\mathbf{H}) \\ -\sin(t\mathbf{H}) & \cos(t\mathbf{H}) \end{pmatrix} \tag{5.74}$$

It is an orthogonal and symplectic operator.

Equation (5.70) can be written as an infinite dimensional Hamiltonian system by letting $u_t = (-v_{xx} + V(x))v$ and $v_t = (u_{xx} - V(x))u$.
The Hamiltonian functional

$$H(u,v)=\frac{1}{2}\int_R [u_x^2 + v_x^2 + V(x)(u^2+v^2)]\,dx. \tag{5.75}$$

Hamilton's equations for the Schrödinger equation are

$$\begin{aligned} \frac{\partial}{\partial t}u(x,t) &= \big(-\frac{\partial^2}{\partial x^2} + D(1-e^{-\alpha x})^2\big)v(x,t), && (5.76)\\ \frac{\partial}{\partial t}v(x,t) &= \big(\frac{\partial^2}{\partial x^2} - D(1-e^{-\alpha x})^2\big)u(x,t). && (5.77)\end{aligned}$$

Since $|V(x)| = |D(1-e^{-\alpha x})^2| \leq 1$ then $V(x) = 1$. Hamilton's equations can be taken as

$$\frac{\partial}{\partial t}u(x,t) = \big(-\frac{\partial^2}{\partial x^2}+1\big)v(x,t), \quad \frac{\partial}{\partial t}v(x,t) = \big(\frac{\partial^2}{\partial x^2}-1\big)u(x,t). \tag{5.78}$$

where $\mathbf{H} = -\partial_{xx} + 1$ is a linear operator.

$$\begin{aligned} \dot{q} &= \dot{u} = \big(-\frac{\partial^2}{\partial x^2} + D(1-e^{-\alpha x})^2\big)v = \mathbf{H}v && (5.79)\\ \dot{p} &= \dot{v} = \big(\frac{\partial^2}{\partial x^2} - D(1-e^{-\alpha x})^2\big)u = -\mathbf{H}u && (5.80)\end{aligned}$$

Application of 2nd order modified symplectic Euler method to Schrödinger equation yields

$$u_{n+1} = u_n + h[\mathbf{H}v_{n+1} - \frac{h}{2}\mathbf{H}^2 u_n] \tag{5.81}$$

$$v_{n+1} = v_n + h[-\mathbf{H}u_n + \frac{h}{2}\mathbf{H}^2 v_{n+1}]. \tag{5.82}$$

The equations (5.81) and (5.82) may be put into the matrix equation as below

$$\begin{pmatrix} I & -h\mathbf{H} \\ 0 & I - \frac{h^2}{2}\mathbf{H}^2 \end{pmatrix} \begin{pmatrix} u_{n+1} \\ v_{n+1} \end{pmatrix} = \begin{pmatrix} I - \frac{h^2}{2}\mathbf{H}^2 & 0 \\ -h\mathbf{H} & I \end{pmatrix} \begin{pmatrix} u_n \\ v_n \end{pmatrix}. \tag{5.83}$$

Fourier transform of (5.83) gives

$$\underbrace{\begin{pmatrix} 1 & -h(\omega^2+1) \\ 0 & 1 - \frac{h^2}{2}(\omega^2+1)^2 \end{pmatrix}}_{B} \begin{pmatrix} \hat{u}_{n+1}(\omega) \\ \hat{v}_{n+1}(\omega) \end{pmatrix} = \begin{pmatrix} 1 - \frac{h^2}{2}(\omega^2+1)^2 & 0 \\ -h(\omega^2+1) & 1 \end{pmatrix} \begin{pmatrix} \hat{u}_n(\omega) \\ \hat{v}_n(\omega) \end{pmatrix} \tag{5.84}$$

We take the inverse of B,

$$\begin{pmatrix} \hat{u}_{n+1}(\omega) \\ \hat{v}_{n+1}(\omega) \end{pmatrix} = \begin{pmatrix} 1 - \frac{h^2}{2}(\omega^2+1)^2 - \frac{h^2(\omega^2+1)^2}{1-\frac{h^2}{2}(\omega^2+1)^2} & \frac{h(\omega^2+1)}{1-\frac{h^2}{2}(\omega^2+1)^2} \\ -\frac{h(\omega^2+1)}{1-\frac{h^2}{2}(\omega^2+1)^2} & \frac{1}{1-\frac{h^2}{2}(\omega^2+1)^2} \end{pmatrix} \begin{pmatrix} \hat{u}_n(\omega) \\ \hat{v}_n(\omega) \end{pmatrix} \tag{5.85}$$

Since determinant of the above matrix is 1, it gives the symplecticity. For stability we require

$$\left| 2 - \frac{h^2}{2}(\omega^2+1)^2 - \frac{\frac{h^2}{2}(\omega^2+1)^2}{1 - \frac{h^2}{2}(\omega^2+1)^2} \right| < 2 \tag{5.86}$$

Application of 3rd order modified symplectic Euler method to linear wave equation yields

$$u_{n+1} = u_n + h[\mathbf{H}v_{n+1} - \frac{h}{2}\mathbf{H}^2 u_n + \frac{h^2}{3}\mathbf{H}^3 v_{n+1}] \tag{5.87}$$

$$v_{n+1} = v_n + h[-\mathbf{H}u_n + \frac{h}{2}\mathbf{H}^2 v_{n+1} - \frac{h^2}{3}\mathbf{H}^3 u_n]. \tag{5.88}$$

The equations (5.87) and (5.88) may be put into the matrix equation as below

$$\begin{pmatrix} I & -h\mathbf{H}-\frac{h^3}{3}\mathbf{H}^3 \\ 0 & I-\frac{h^2}{2}\mathbf{H}^2 \end{pmatrix}\begin{pmatrix} u_{n+1} \\ v_{n+1} \end{pmatrix}=\begin{pmatrix} I-\frac{h^2}{2}\mathbf{H}^2 & 0 \\ -h\mathbf{H}-\frac{h^3}{3}\mathbf{H}^3 & I \end{pmatrix}\begin{pmatrix} u_n \\ v_n \end{pmatrix}. \tag{5.89}$$

Taking a fourier transform of (5.89), we have the following matrix

$$\begin{pmatrix} 1-\frac{h^2}{2}(\omega^2+1)^2-\frac{(h(\omega^2+1)+\frac{h^3}{3}(\omega^2+1)^3)^2}{1-\frac{h^2}{2}(\omega^2+1)^2} & \frac{h(\omega^2+1)+\frac{h^3}{3}(\omega^2+1)^3}{1-\frac{h^2}{2}(\omega^2+1)^2} \\ -\frac{h(\omega^2+1)+\frac{h^3}{3}(\omega^2+1)^3}{1-\frac{h^2}{2}(\omega^2+1)^2} & \frac{1}{1-\frac{h^2}{2}(\omega^2+1)^2} \end{pmatrix} \tag{5.90}$$

For stability, we require

$$\left|\frac{2-2h^2(\omega^2+1)^2-\frac{5}{12}h^4(\omega^2+1)^4-\frac{1}{9}h^6(\omega^2+1)^6}{1-\frac{1}{2}h^2(\omega^2+1)^2}\right|<2. \tag{5.91}$$

CHAPTER 6

NUMERICAL EXPERIMENT

In this chapter, we make qualitative comparisons of fixed step symplectic integrators of separable Hamiltonian systems.

6.1. Numerical Results of Hamiltonian ODE Problems

In this section the modified Lobatto IIIA-IIIB pair method of order 4 (ML4) is applied to both linear and nonlinear Hamiltonian systems. The numerical results are compared with the classical method. For this purpose, Harmonic oscillation is chosen as linear test problem and Double Well is chosen as nonlinear test problem in order to show performance of the proposed method.

6.1.1. Applications to Harmonic Oscillator System

In this section we apply the modified differential equations based on the midpoint method and Lobatto IIIA-IIIB methods for the linear Hamiltonian system, particularly, Harmonic Oscillator system. Furthermore, the trajectory of motion (phase space), error in Hamiltonian and global error in the Hamiltonian $|H(q,p) - H(q_0,p_0)|$ are illustrated.

The Hamiltonian of this system can be given by

$$H(q,p) = \frac{1}{2}p^2 + \frac{1}{2}q^2 \tag{6.1}$$

so that the equations of motion become

$$\begin{aligned} \dot{q} &= H_p(q,p) = p && (6.2) \\ \dot{p} &= H_q(q,p) = -q && (6.3) \end{aligned}$$

6.1.2. Modified Equations Based on Lobatto IIIA-IIIB Methods

In this section we apply the modified differential equations of the system

$$\dot{q} = p = f(p) \tag{6.4}$$
$$\dot{p} = -q = -V_q(q) = g(q) \tag{6.5}$$

based on Lobatto IIIA-IIIB methods. Applying (6.4) and (6.5) to the modified equations

$$\begin{cases} q' = p + \dfrac{h^2}{6} g_q p = \left(I - \dfrac{h^2}{6} V_{qq} \right) p \\ \\ p' = -V_q(q) - \dfrac{h^2}{12}(g_{qq}(p,p) + g_q g). \end{cases} \tag{6.6}$$

we obtain the modified differential equations of the system (6.4) and (6.5) in the following form

$$q' = \left(1 - \frac{h^2}{6}\right) p \tag{6.7}$$
$$p' = -q\left(1 + \frac{h^2}{12}\right). \tag{6.8}$$

and we apply the methods in the following section.

6.1.3. Numerical Implementation for Harmonic Oscillation

In this section numerical methods are applied to the Harmonic oscillator system. We apply Lobatto IIIA-IIIB pair of order 2, Lobatto IIIA-IIIB pair of order 4, Runge Kutta method (order 4), modified Midpoint method (order 4), Gauss collocation method (order 4) to the system (6.4) and (6.5) and modified Lobatto method of order 4 to the system (6.7) and (6.8). We compare the methods for $(p_0, q_0) = (1, 0)$ with the step $h = 10^{-2}$ on the interval $[0, 1]$.

The Figures (6.1-6.6) illustrate errors in Hamiltonian and global errors in Hamiltonian (conservation of energy) obtained by Lobatto IIIA-IIIB pair of order 2, Lobatto IIIA-IIIB pair of order 4, Runge Kutta method (order 4), modified Midpoint method (order 4), Gauss collocation method (order 4) and proposed method (ML4) respectively. Since all of these methods are symplectic geometric integrators the shape of the trajectory preserved by these methods. Modified Lobatto method conserves the energy better than the other methods except Gauss collocation method.

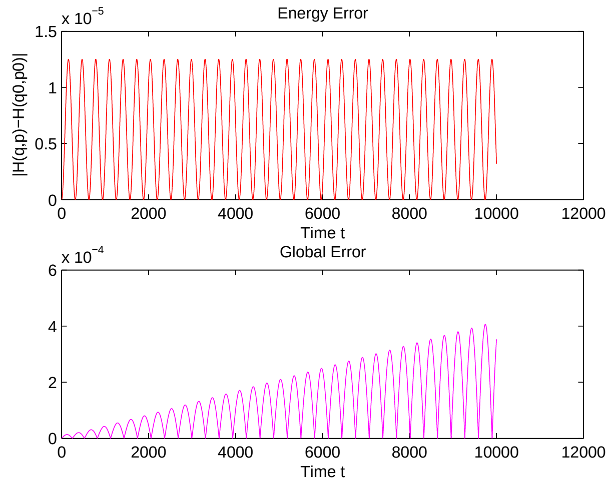

Figure 6.1. Error in Hamiltonian and global error in Hamiltonian by Lobatto IIIA-IIIB method of order 2.

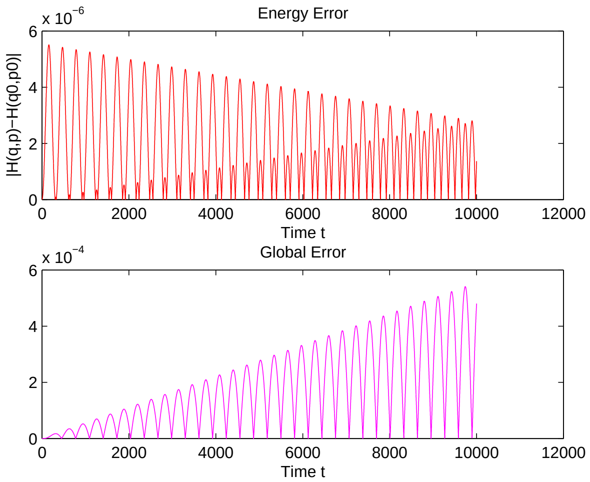

Figure 6.2. Error in Hamiltonian and global error in Hamiltonian by Lobatto IIIA-IIIB method of order 4.

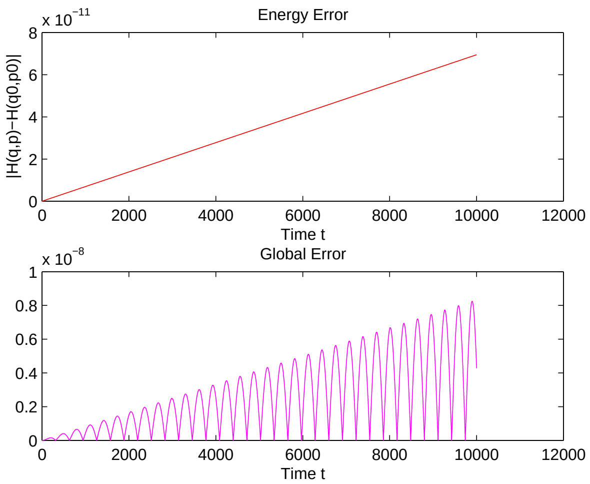

Figure 6.3. Error in Hamiltonian and global error in Hamiltonian by Runge Kutta method of order 4.

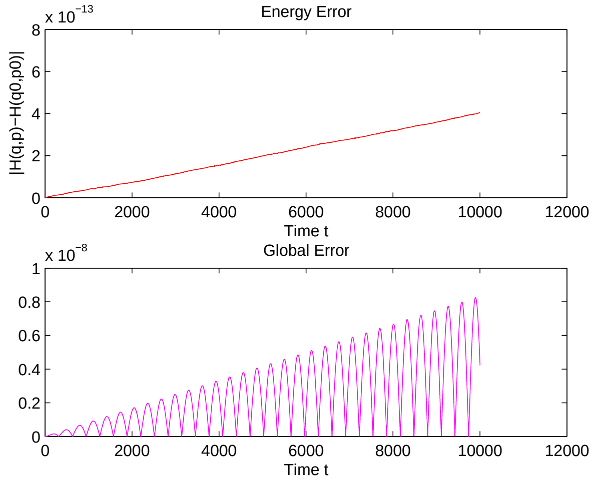

Figure 6.4. Error in Hamiltonian and global error in Hamiltonian by modified Midpoint method of order 4.

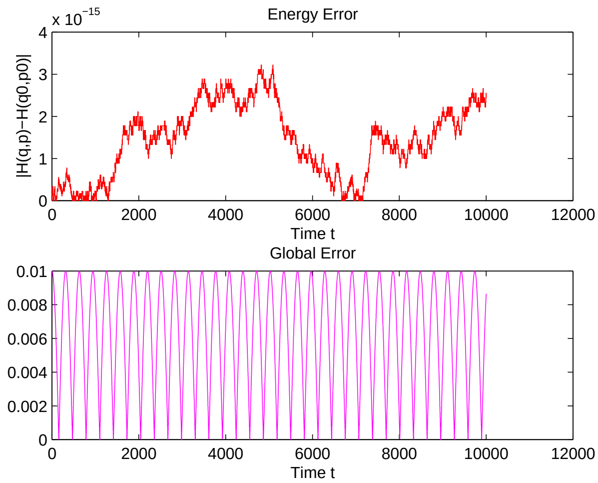

Figure 6.5. Error in Hamiltonian and global error in Hamiltonian by Gauss collocation method of order 4.

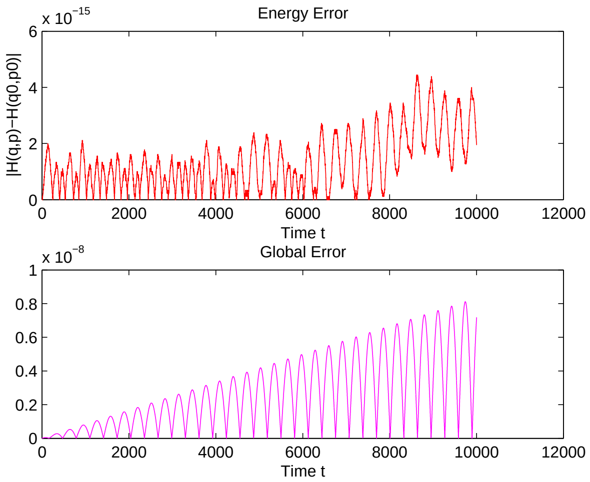

Figure 6.6. Error in Hamiltonian and global error in Hamiltonian by the proposed method (ML4).

6.1.3.1. Comparison of the Norm of Global Error, Norm of Error in Hamiltonian and CPU Time

In this section norm of global error, norm of error in Hamiltonian and CPU time are verified.

The Tables (6.1-6.3) illustrate the norm of global error, norm of error in Hamiltonian and CPU time (seconds) in Hamiltonian (conservation of energy) obtained by Lobatto IIIA-IIIB pair of order 2, Lobatto IIIA-IIIB pair of order 4, Runge Kutta method (order 4), modified Midpoint method (order 4), Gauss collocation method (order 4) and modified Lobatto method of order 4 respectively.

	Norm of global error
Lobatto method of order 2	0.0169
Lobatto method of order 4	0.0225
Runge Kutta method of order 4	3.4242e-007
Modified Midpoint of order 4	3.4245e-007
Gauss Collocation method of order 4	0.7056
Modified Lobatto method of order 4	3.3803e-007

Table 6.1. Comparison of the norm of global errors in Hamiltonian.

	Norm of error in Hamiltonian
Lobatto method of order 2	7.6744e-004
Lobatto method of order 4	2.5342e-004
Runge Kutta method of order 4	4.0099e-009
Modified Midpoint of order 4	2.2983e-011
Gauss Collocation method of order 4	1.6687e-013
Modified Lobatto method of order 4	1.6428e-013

Table 6.2. Comparison of the norm of errors in Hamiltonian.

	CPU time (seconds)
Lobatto method of order 2	0.874
Lobatto method of order 4	1.085
Runge Kutta method of order 4	0.577
Modified Midpoint of order 4	0.733
Gauss Collocation method of order 4	2.366
Modified Lobatto method of order 4	0.589

Table 6.3. Comparison of CPU times (seconds) in Hamiltonian.

The comparison of these six methods reveal that the proposed method (ML4) gives better performance with respect to the norm of global error, norm of error in Hamiltonian and CPU time.

6.2. Applications to Double Well System

In this section we determine the modified differential equations based on the Lobatto IIIA-IIIB, Gauss collocation methods for the nonlinear Hamiltonian system which is called Double Well system and illustrate the trajectory of motion (phase space) and the errors in Hamiltonian $|H(q,p) - H(q_0,p_0)|$. The Hamiltonian of this system can be given by

$$H(q,p) = \frac{1}{2}p^2 + \frac{1}{2}(q^2-1)^2, \tag{6.9}$$

so that the equations of motion become

$$
\begin{aligned}
\dot{q} &= H_p(q,p) = p && (6.10)\\
\dot{p} &= H_q(q,p) = -2q(q^2-1) && (6.11)
\end{aligned}
$$

We derive only the modified differential equations of the system (6.10) and (6.11) based on Lobatto IIIA-IIIB methods. Applying (6.10) and (6.11) to the modified equations

$$
\begin{cases}
q' = p + \dfrac{h^2}{6} g_q p = \left(I - \dfrac{h^2}{6} V_{qq} \right) p \\
\\
p' = -V_q(q) - \dfrac{h^2}{12} (g_{qq}(p,p) + g_q g).
\end{cases}
\tag{6.12}
$$

we obtain the modified differential equations of the system (6.10) and (6.11) in the form

$$
\begin{aligned}
q' &= \left[1 + \frac{h^2}{6} \big(-6q^2 + 2 \big) \right] p && (6.13)\\
p' &= -2q^3 + 2q + h^2 \left(qp^2 - q^5 + \frac{4}{3} q^3 - \frac{q}{3} \right). && (6.14)
\end{aligned}
$$

then we apply the methods in the below section.

6.2.1. Numerical Implementation for Double Well

In this part of thesis, numerical methods are applied to the Double Well system. We apply Gauss collocation method (order 4), Lobatto IIIA-IIIB pair of order 2, ODE 45 to the system (6.10) and (6.11), Lobatto IIIA-IIIB pair of order 4 to the system (6.13) and (6.14). We compare the methods for $(p_0, q_0) = (1, 0)$ with the step $h = 10^{-2}$ on the interval $[0, 1]$.

The Figures (6.7-6.10) illustrate the trajectory of motion and errors in Hamiltonian (conservation of energy) obtained by Gauss collocation method (order 4), Lobatto IIIA-IIIB pair of order 2, Lobatto IIIA-IIIB pair of order 4 and ODE 45 respectively. Since all of these methods are symplectic the shape of the trajectory preserved by these methods. ML4 method conserves the energy better than ODE 45 except Gauss collocation method.

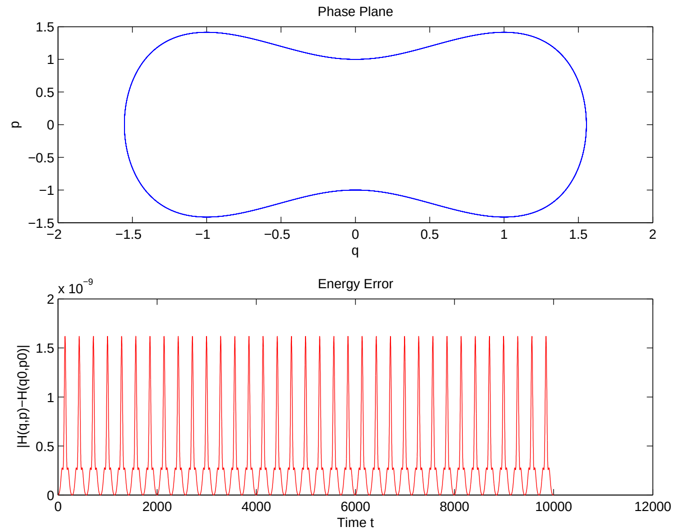

Figure 6.7. Trajectory of motion and error in Hamiltonian by 4th order Gauss collocation method.

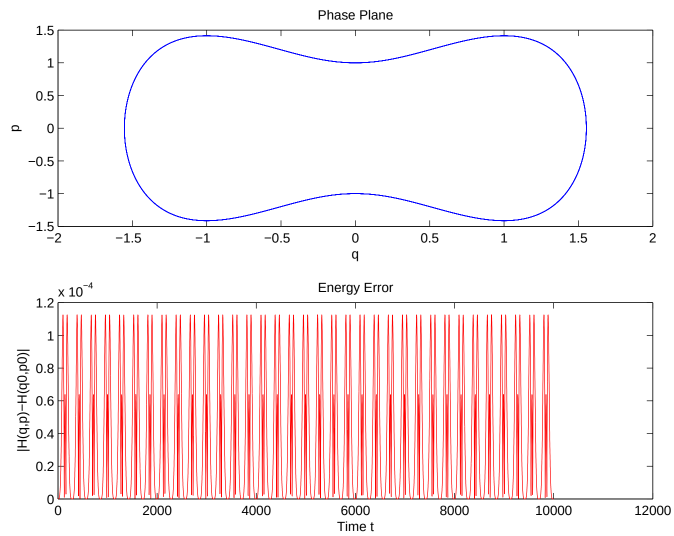

Figure 6.8. Trajectory of motion and error in Hamiltonian by 2nd order Lobatto IIIA-IIIB method.

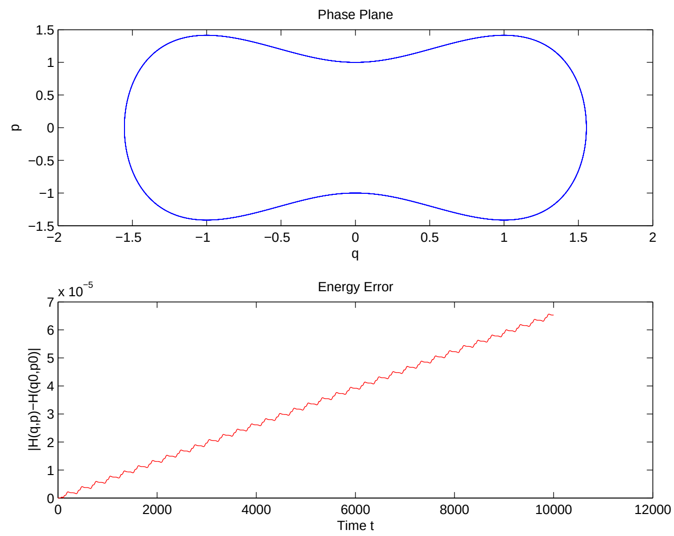

Figure 6.9. Trajectory of motion and error in Hamiltonian by 4th order modified Lobatto method.

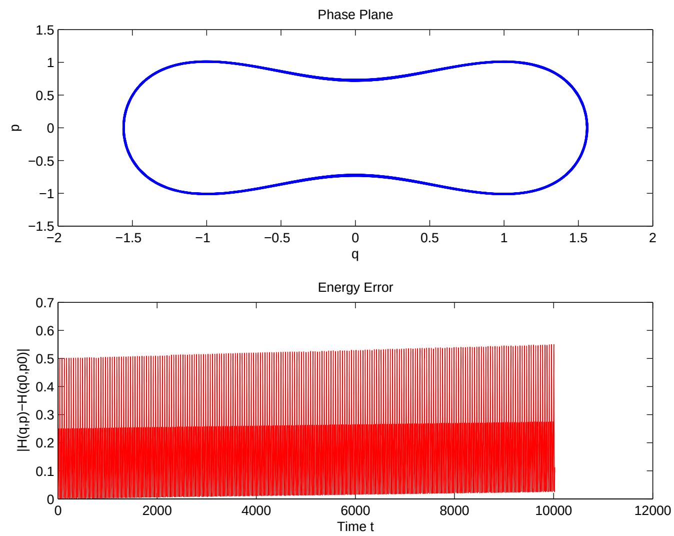

Figure 6.10. Trajectory of motion and error in Hamiltonian by ODE45.

The comparison of the four method reveals that proposed method conserves the energy better than ODE 45 except Gauss collocation method.

6.3. Numerical Results of Hamiltonian PDE Problems

In this section, modified symplectic Euler method is applied to PDE problems. Linear wave equation and Sine-Gordon equation are chosen as test problems.

6.3.1. Linear Wave Equation

Hamiltonian's equation for the 1-dimensional linear wave equation

$$u_{tt} - u_{xx} = 0 \tag{6.15}$$

in separable form,

$$\frac{\partial u(x,t)}{\partial t} = v(x,t) \tag{6.16}$$

$$\frac{\partial v(x,t)}{\partial t} = \frac{\partial^2 u(x,t)}{\partial x^2} = Au = \mathbf{F}(u) \tag{6.17}$$

with the initial conditions

$$u(x,0) = \sin \pi x, \quad u_t(x,0) = 0 \tag{6.18}$$

and boundary conditions

$$u(0,t) = 0, \quad u(1,t) = 0, \tag{6.19}$$

at $x = 0$ and $x = 1$.

We apply modified symplectic Euler method of order 2 to (6.16) and (6.17),

$$u^{n+1} = u^n + hv^{n+1} + \frac{h^2}{2}Au^n \tag{6.20}$$
$$v^{n+1} = v^n + hAu^n - \frac{h^2}{2}\left[\frac{\partial \mathbf{F}(u)}{\partial u}v^{n+1}\right] \tag{6.21}$$

where h is step size.

We apply central difference method to (6.17) and the linear wave equations given in (6.16), (6.17) get this form,

$$\dot{u_i} = v_i \quad \text{and} \quad \dot{v_i} = \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2} = Au \tag{6.22}$$

where A is a tridiagonal square matrix of the form

$$\begin{pmatrix} -2 & 1 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \cdots & \vdots \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & \cdots & 0 & 1 & -2 \end{pmatrix}, \tag{6.23}$$

$i = 1, \ldots, n$ and Δx is mesh size.

Modified symplectic Euler method of order 2 for the separable system (6.22) can be written in implicit form as

$$u_i^{n+1} = u_i^n + hv_i^{n+1} + \frac{h^2}{2}\left[\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2}\right] \tag{6.24}$$
$$v_i^{n+1} = v_i^n + h\left[\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2}\right] - \frac{h^2}{2}\left[\frac{v_{i+1}^{n+1} - 2v_i^{n+1} + v_{i-1}^{n+1}}{(\Delta x)^2}\right] \tag{6.25}$$

and explicit form as

$$u_i^{n+1} = u_i^n + hv_i^n + \frac{3}{2}h^2\left[\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2}\right] \tag{6.26}$$

$$\begin{aligned} v_i^{n+1} &= h\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} - \frac{1}{2}h^3\left[\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2}\right]^2 \\ &\quad + v_i^n - \frac{h^2}{2}\frac{v_{i+1}^n - 2v_i^n + v_{i-1}^n}{(\Delta x)^2} \end{aligned} \tag{6.27}$$

where $u = (u_0, u_1, \ldots, u_n)^T$,$v = (v_0, v_1, \ldots, v_n)^T$ are $n+1$ dimensional vectors, A is a tridiagonal $n+1 \times n+1$ dimensional matrix, h is step size and Δx is mesh size.

Now we can apply modified symplectic Euler method with given above equations on the space interval $[0,1]$ with boundary conditions $u(0,t) = 0,\ u(1,t) = 0$, at $x = 0$ and $x = 1$ using the following parameters set:

Space interval	$x = [0,1]$
Space discretization step	$\Delta x = 0.01/0.02/0.04$
Time discretization step	$\Delta t = 0.001$
Amount of time steps	$T = 1000$

We start with comparison of errors in linear wave problem after applying explicit and implicit form of modified symplectic Euler method with space discretization step $\Delta x = 0.01$, 0.02 and 0.04 and time discretization step $\Delta t = 0.001$ respectively.

The comparison of errors measured by L_∞ and L_1 are given in Table 6.4. The errors used in our computations are calculated by the following equations,

$$err_{L_\infty} := max(max(|u(x_i, t^n - u_{analy}(x_i, t^n)|)) \tag{6.28}$$

$$err_{L_1} := \sum_{i=1}^{m} \Delta x|u(x_i, t^n - u_{analy}(x_i, t^n)| \tag{6.29}$$

with respect to given parameters.

	Nx=100, Nt=1000	err_{L_∞}	err_{L_1}
SE		0.5001	0.2509
SV2		0.0392	0.0192
MSE2-IMP		0.0388	0.0192
MSE2-EXP		0.0315	0.0184
	Nx=50, Nt=1000	err_{L_∞}	err_{L_1}
SE		0.5149	0.2535
SV2		0.0756	0.0372
MSE2-IMP		0.0744	0.0371
MSE2-EXP		0.0660	0.0355
	Nx=25, Nt=1000	err_{L_∞}	err_{L_1}
SE		0.5310	0.2554
SV2		0.1522	0.0695
MSE2-IMP		0.1519	0.0695
MSE2-EXP		0.1383	0.0645

Table 6.4. Comparison of errors in linear wave problem measured by L_∞ norm and L_1 norm after applying symplectic Euler method (SE), Störmer Verlet method of order 2 (SV2), modified symplectic method of order 2 (MSE2) in implicit and explicit form respectively.

From the Table 6.4 we conclude that the number of space discretization point decreases, the accuracy of the solution obtained by the new proposed method increases. In other words, when the size of the matrix to be solved decreases, the accuracy of the solution obtained by the proposed increases. The accuracy of the solution obtained by the proposed and Störmer Verlet method are nearly equal. On the other hand, the explicit form of modified symplectic Euler method is more accurant for the small system than the methods we compared with.

6.3.2. Sine-Gordon Equation

Consider an IVP for the Sine-Gordon equation:

$$u_{tt} - u_{xx} + \sin(u) = 0 \tag{6.30}$$

on the interval $x \in [a, b]$ with initial conditions

$$u(x, 0) = f(x), \quad u_t(x, 0) = g(x), \tag{6.31}$$

and with, e.g., no-flux boundary conditions

$$\left.\frac{\partial u}{\partial x}\right|_{x=a,b} = 0. \tag{6.32}$$

Hamiltonian's equations for Sine-Gordon equation are

$$\begin{aligned}
\frac{\partial u(x,t)}{\partial t} &= v(x,t) && (6.33)\\
\frac{\partial v(x,t)}{\partial t} &= \frac{\partial^2 u(x,t)}{\partial x^2} - \sin(u(x,t)) = Au - \sin u = \mathbf{F}(u). && (6.34)
\end{aligned}$$

We apply modified symplectic Euler method of order 2 to (6.33) and (6.34),

$$\begin{aligned}
u^{n+1} &= u^n + hv^{n+1} + \frac{h^2}{2}\mathbf{F}(u^n) && (6.35)\\
v^{n+1} &= v^n + h\mathbf{F}(u^n) - \frac{h^2}{2}\big[\frac{\partial \mathbf{F}}{\partial u} v^{n+1}\big]. && (6.36)
\end{aligned}$$

We apply central difference method to (6.34) and Sine-Gordon equations get this form,

$$\dot{u}_i = v_i \quad \text{and} \quad \dot{v}_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2} - \sin u_i = Au - \beta \tag{6.37}$$

where A is a tridiagonal $n+1 \times n+1$ square matrix of the form

$$\begin{pmatrix} -2 & 1 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \cdots & \vdots \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & \cdots & 0 & 1 & -2 \end{pmatrix}, \tag{6.38}$$

$\beta = (\sin(u_0), \sin(u_1), \ldots, \sin(u_n))^T$ is a $n+1$-dimensional vector, and Δx is mesh size.

Modified symplectic Euler method of order 2 for the separable system (6.37) can be written as

$$u_i^{n+1} = u_i^n + hv_i^{n+1} + \frac{h^2}{2}\left[\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} - \sin(u_i^n)\right] \tag{6.39}$$

$$\begin{aligned} v_i^{n+1} &= v_i^n + h\left[\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} - \sin(u_i^n)\right] \\ &\quad -\frac{h^2}{2}\left[\frac{v_{i+1}^{n+1} - 2v_i^{n+1} + v_{i-1}^{n+1}}{(\Delta x)^2} - v_i^{n+1}\cos(u_i^n)\right] \end{aligned} \tag{6.40}$$

where h is step size and Δx is mesh size.

Now we can apply the given schemes (6.39) and (6.40) described above to eq. (6.31). Let us solve it on the interval $[-L, L]$ with no-flux boundary conditions using the following parameters set:

Space interval	$L = 20$
Space discretization step	$\Delta x = 0.1$
Time discretization step	$\Delta t = 0.05$
Velocity of the kink	$c = 0.2$

We use the different initial conditions for Sine-Gordon equation to simulate by using modified symplectic Euler method of order 2 and start with the numerical representation of kink and antikink solutions. The initial condition for the kink soliton is

$$f(x) = 4\arctan\left(\exp\left(\frac{x}{\sqrt{1-c^2}}\right)\right), \tag{6.41}$$

$$g(x) = -2\frac{c}{\sqrt{1-c^2}}\sec\mathrm{h}\left(\frac{x}{\sqrt{1-c^2}}\right). \tag{6.42}$$

Figure (6.11) shows the space-time plot of the numerical kink solution.

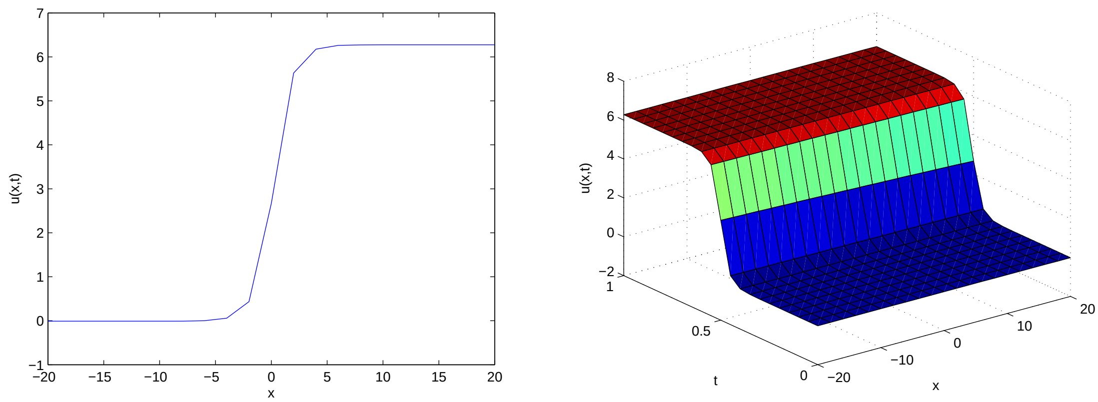

Figure 6.11. Numerical solution of (6.31), calculated with given schemes for the case of the kink solitons, moving with the velocity c = 0.2. Space-time information is shown.

For the antikink soliton, the initial condition reads

$$f(x) = 4\arctan\left(\exp\left(-\frac{x}{\sqrt{1-c^2}}\right)\right), \tag{6.43}$$

$$g(x) = -2\frac{c}{\sqrt{1-c^2}}\sec\mathrm{h}\left(\frac{x}{\sqrt{1-c^2}}\right). \tag{6.44}$$

Numerical solutions is shown on Figure (6.12).

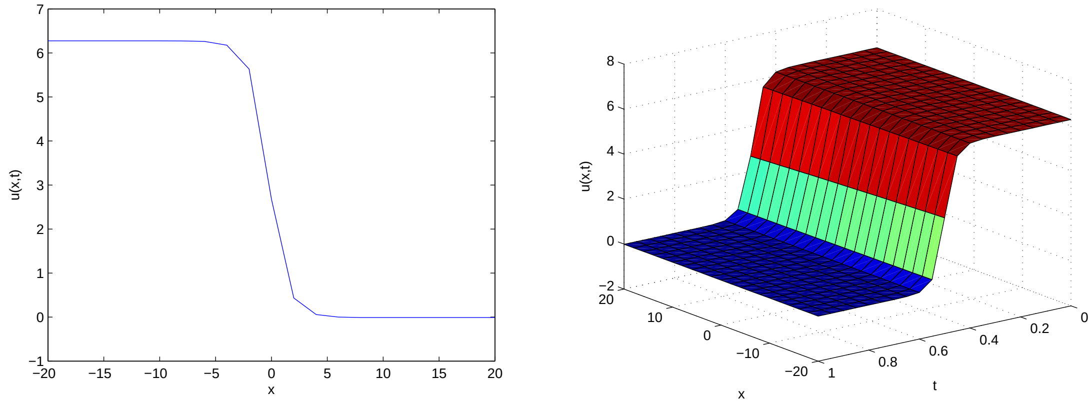

Figure 6.12. Numerical solution of (6.31), calculated with given schemes for the case of the antikink solitons, moving with the velocity c = 0.2. Space-time information is shown.

Now we are in position to find numerical solutions, corresponding to kink-kink and kink-antikink collisions. For the kink-kink collision we choose

$$f(x) = 4\arctan\left(\exp\left(\frac{x+L/2}{\sqrt{1-c^2}}\right)\right) + 4\arctan\left(\exp\left(\frac{x-L/2}{\sqrt{1-c^2}}\right)\right), \quad (6.45)$$

$$g(x) = -2\frac{c}{\sqrt{1-c^2}}\,\mathrm{sec\,h}\left(\frac{x+L/2}{\sqrt{1-c^2}}\right) + 2\frac{c}{\sqrt{1-c^2}}\,\mathrm{sec\,h}\left(\frac{x-L/2}{\sqrt{1-c^2}}\right), \quad (6.46)$$

whereas for the kink-antikink collision the initial conditions are

$$f(x) = 4\arctan\left(\exp\left(\frac{x+L/2}{\sqrt{1-c^2}}\right)\right) + 4\arctan\left(\exp\left(-\frac{x-L/2}{\sqrt{1-c^2}}\right)\right), \quad (6.47)$$

$$g(x) = -2\frac{c}{\sqrt{1-c^2}}\,\mathrm{sec\,h}\left(\frac{x+L/2}{\sqrt{1-c^2}}\right) - 2\frac{c}{\sqrt{1-c^2}}\,\mathrm{sec\,h}\left(\frac{x-L/2}{\sqrt{1-c^2}}\right). \quad (6.48)$$

Numerical solutions, corresponding to both cases is presented on Figure (6.13) and (6.14), respectively.

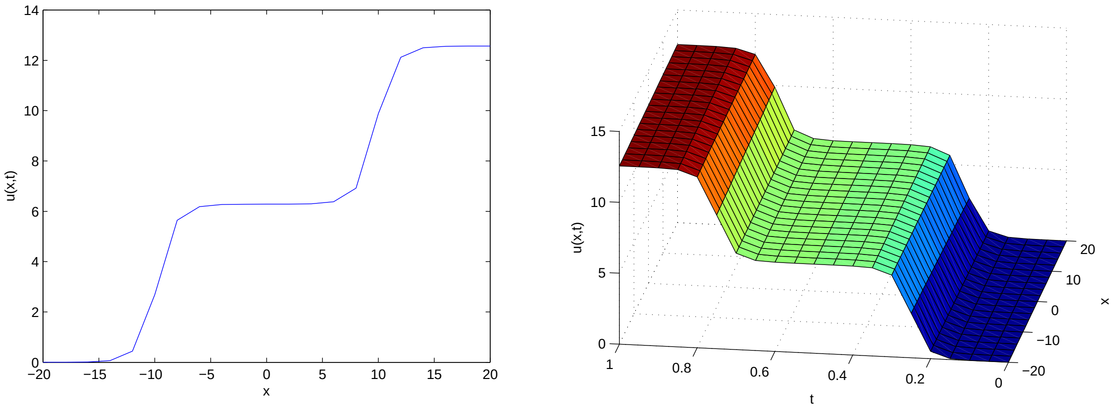

Figure 6.13. Space-time representation of the numerical solution of (6.31) for kink-kink collision.

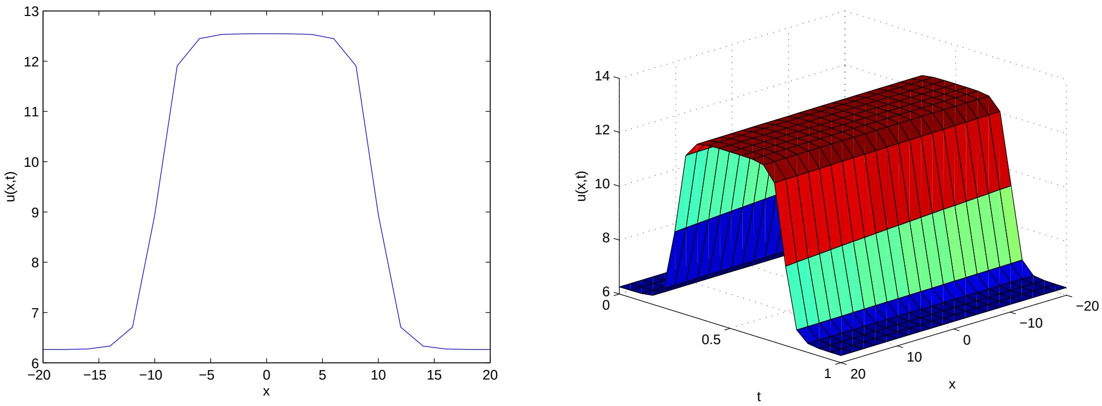

Figure 6.14. Space-time representation of the numerical solution of (6.31) for kink-antikink collision.

Finally, for the case of breather solution we choose

$$f(x) = 0, \tag{6.49}$$

$$g(x) = 4\sqrt{1-c^2}\,\mathrm{sec\,h}\big(x\sqrt{1-c^2}\big). \tag{6.50}$$

Corresponding numerical solution is presented on Figure (6.15).

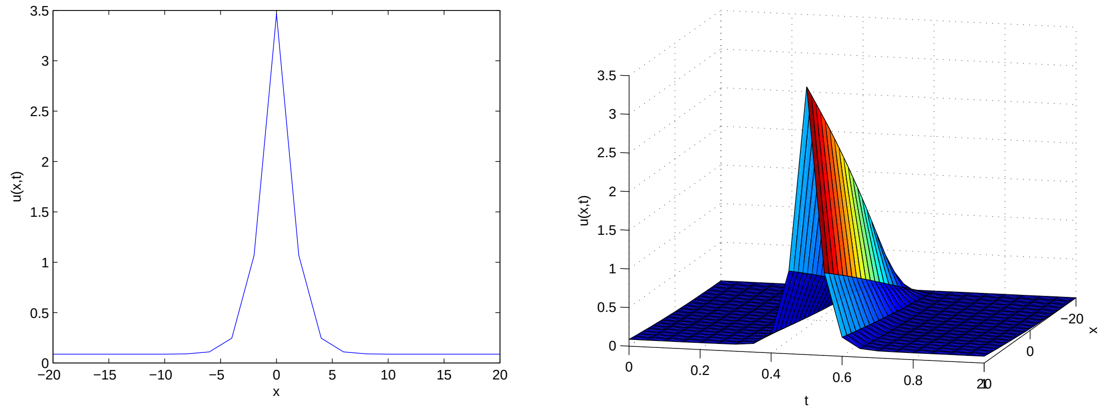

Figure 6.15. Space-time representation of the numerical solution of (6.31) for breather solution.

Modified symplectic Euler method is applied to Sine-Gordon equation with soliton solutions for various combinations of parameters under no-flux boundary conditions. We have different simulations for various combinations of parameters.

CHAPTER 7

CONCLUSION

Throughout this thesis we have used an approach that was developed by using the idea in backward error analysis while constructing modified equations by inverting the roles of the exact and numerical flows. In this case, we have constructed 4th order modified Lobatto IIIA-IIIB pair method (ML4) by using modified vector field idea.

After presenting this new method, its convergence properties are analyzed using concepts familiar from numerical analysis of *stability*, *consistency* and *order*.

In the next chapter, the modified symplectic Euler method of order 2 and 3 that were constructed by using the modified vector field idea are applied to linear and non-linear PDE problems. In addition we present the Von-Neumann stability analysis of the differential equations we considered.

In the numerical experiment section, first harmonic oscillation problem is examined as a first test problem. In particular error in Hamiltonian, global error and phase plane are investigated with respect to the six different algorithms for Harmonic oscillation problem. In our investigation of accuracy and efficiency of these algorithms we found the followings:

- The shape of the trajectories are preserved by these methods.
- Comparisons of the 4th order methods showed that ML4 method is more efficient with respect to the errors in Hamiltonian, global errors and computational times.

In addition, the Double Well problem is examined as a second test problem. Similar conclusions were drawn for the nonlinear ODE problem using ML4 method. ML4 method conserves the energy better than ODE45, except Gauss collocation method. The numerical results for this part show that not only linear ODE problem, but also nonlinear ODE problem can be high quality and efficient schemes for the long time behavior by using ML4 method.

Next, we make qualitative comparisons of fixed step symplectic integrators of separable Hamiltonian systems. We consider linear wave equation problem as a test problem, we presented the errors obtained by symplectic Euler method, Störmer-Verlet method of order 2, modified symplectic method of order 2 in implicit and explicit form measured by L_∞ and L_1. The numerical results indicate that

- The number of space discretization point decreases, the accuracy of the solution obtained by the new proposed method increases.

- The explicit form of modified symplectic Euler method is more accurant for the small system than the methods we compared with.

Finally, modified symplectic Euler method is applied to Sine-Gordon equation with soliton solutions for various combinations of parameters under no-flux boundary conditions. We have different simulations for various combinations of parameters.

Our computational results reveal that new proposed modified symplectic Euler and modified Lobatto method are efficient for whole linear ODE and PDE problems. Using the modified vector field idea, one can apply these symplectic methods for different Hamiltonian ODE and PDE systems as a future work.

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APPENDIX A

MATLAB CODES FOR NUMERICAL EXPERIMENTS

HIGHER ORDER SYMPLECTIC METHODS MATLAB CODE FOR HARMONIC OSCILLATION PROBLEM

```
%%%%% 2nd order Lobatto for harm. osc. problem %%%%%
clear all;
p4(1)= 1;
q4(1)= 0;
h=.01;
t=0:h:100;
n=100/h+1;
for i=1:n
ye(i)=sin(t(i));
end
tic
for i=1:n
H4(i)=.5*(p4(i).^2+q4(i).^2);
L1s(i)=-q4(i);
Ks(i)=p4(i)+h/2*L1s(i);
L2s(i)=-(q4(i)+h*(Ks(i)));
q4(i+1)=q4(i)+h*(Ks(i));
p4(i+1)=p4(i)+(h/2)*(L1s(i)+L2s(i));
e4(i)=abs(H4(i)-H4(1));
er(i)=abs(ye(i)-q4(i));
end
norm(er)
norm(e4)
toc
subplot(211);plot(e4,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
subplot(212);plot(t,er,'m');
```

```
title('Global Error');
xlabel('Time t');
%%%%% 4th order Lobatto for Harm. Osc. problem %%%%%
clear all;
p2(1)=1;
q2(1)=0;
h=.01;
t=0:h:100;
n=100/h+1;
for i=1:n
ye(i)=sin(t(i)); end
tic
for i=1:n
H2(i)=.5*(p2(i).^2+q2(i).^2);
L1(i)=-q2(i);
L2(i)=(-q2(i)-(h/2)*p2(i)-((h.^2)/12)*L1(i))
/(1+((h.^2)/24));
L3(i)=-q2(i)-(h/6)*(6*p2(i)+h*L1(i)-2*h*L2(i));
K1(i)=p2(i)+(h/6)*(L1(i)-L2(i));
K2(i)=p2(i)+(h/6)*(L1(i)+2*L2(i));
K3(i)=p2(i)+(h/6)*(L1(i)+5*L2(i));
q2(i+1)=q2(i)+(h/6)*(K1(i)+4*K2(i)+K3(i));
p2(i+1)=p2(i)+(h/6)*(L1(i)+4*L2(i)+L3(i));
e2(i)=abs(H2(i)-H2(1));
er2(i)=abs(ye(i)-q2(i));
end
norm(er2)
norm(e2)
toc
subplot(211);plot(e2,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
subplot(212);plot(t,er2,'m');
title('Global Error');
xlabel('Time t');
```

```
%%%%% Runge Kutta method of order 4 for Harm.
Osc. problem %%%%%
clear all;
Y=[1;0];
h=.01;
t=0:h:100;
n=100/h+1;
for i=1:n
ye(i)=cos(t(i));
end
tic
for i=1:n
p(i)=Y(1,1);
q(i)=Y(2,1);
H(i)=.5*(p(i).^2+q(i).^2);
C=[0 1;-1 0];
k1=C*Y;
Y1=Y+(1/3)*h*k1;
k2=C*Y1;
Y2=Y+(-1/3)*h*k1+h*k2;
k3=C*Y2;
Y3=Y+h*k1-h*k2+h*k3;
k4=C*Y3;
Y=Y+(1/8)*h*(k1+3*k2+3*k3+k4);
e(i)=abs(H(i)-H(1));
er(i)=abs(ye(i)-p(i));
end
norm(er)
norm(e)
toc
subplot(211);plot(e,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
subplot(212);plot(t,er,'m');
title('Global Error');
```

```
xlabel('Time t');
%%%%% Modified Midpoint of order 4 for harm. osc.
problem %%%%%
clear all;
p3(1)=1;
q3(1)=0;
h=.01;
t=0:h:100;
n=100/h+1;
K=(1+(h^2)/12);
A=((1-((h.^2)*K.^2)/4)/(1+((h.^2)*K.^2)/4));
B=((h*K)/(1+((h.^2)*K.^2)/4));
for i=1:n
ye(i)=cos(t(i));
end
tic
for i=1:n
H3(i)=(p3(i).^2+q3(i).^2);
e3(i)=(abs(H3(i)-H3(1)));
p3(i+1)=A*p3(i)+B*q3(i);
q3(i+1)=A*q3(i)-B*p3(i);
er3(i)=abs(ye(i)-p3(i));
end
norm(er3)
norm(e3)
toc
subplot(211);plot(e3,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
subplot(212);plot(t,er3,'m');
title('Global Error');
xlabel('Time t');
clear all;
%%%%% Gauss Collocation Method for Harm. Osc. problem %%%%%
p0= 1;
```

```
q0= 0;
h=.01;
t=0:h:100;
n=100/h+1;
a11=1/4;
a12=1/4-(sqrt(3)/6);
a21=1/4+(sqrt(3)/6);
a22=1/4;
q=q0;
p=p0;
k12p=feval('qpd',q,p,h);
k22p=feval('qpd',q,p,h);
H0 = .5*(p.^2 + q.^2);
for i=1:n
ye(i)=sin(t(i));
end
tic
for i=1:n
H=.5*(p.^2+q.^2);
for j=1:5
k11=p+h*(a11*k12p+a12*k22p);
k21=p+h*(a21*k12p+a22*k22p);
k12=feval('qpd',q+h*(a11*k11+a12*k21),p,h);
k22=feval('qpd',q+h*(a21*k11+a22*k21),p,h);
k12p=k12;
k22p=k22;
end
q1=q+h/2*(k11+k21);
p1=p+h/2*(k12+k22);
Q(:,i) = q1;
P(:,i) = p1;
q= q1;
p= p1;
er(i)=abs(ye(i)-q);
H(i)= .5*(p.^2+q.^2) ;
```

```
error_H(i)= abs(H(i)-H0)   ;
end
norm(er)
norm(error_H)
toc
subplot(211);plot(error_H,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
subplot(212);plot(t,er,'m');
title('Global Error');
xlabel('Time t');
%%%%% Modified Lobatto method of order 4 for
Harm. Osc. problem %%%%%
p1(1)= 1;
q1(1)= 0;
h=.01;
t=0:h:100;
n=100/h+1;
for i=1:n
ye(i)=sin(t(i));
end
tic
for i=1:n
H1(i)=.5*(p1(i).^2+q1(i).^2);
L11(i)=-q1(i)*(1+(h.^2)/12);
K(i)=(1-(h.^2)/6)*(p1(i)+(h/2)*L11(i));
L22(i)=-(1+(h.^2)/12)*(q1(i)+h*K(i));
q1(i+1)=q1(i)+h*(K(i));
p1(i+1)=p1(i)+(h/2)*(L11(i)+L22(i));
e1(i)=abs(H1(i)-H1(1));
er1(i)=abs(ye(i)-q1(i));
end
norm(er1)
norm(e1)
toc
```

```
subplot(211);plot(e1,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
subplot(212);plot(t,er1,'m');
title('Global Error');
xlabel('Time t');
```

HIGHER ORDER SYMPLECTIC METHODS MATLAB CODE FOR DOUBLE WELL PROBLEM

```
 %%%%% Gauss Collocation Method for Double Well %%%%%
clear all;
p0= 1;
q0= 0;
h=.01;
t=0:h:100;
n=100/h+1;
a11=1/4;
a12=1/4-(sqrt(3)/6);
a21=1/4+(sqrt(3)/6);
a22=1/4;
q=q0;
p=p0;
k12p=feval('qpdd',q,p,h);
k22p=feval('qpdd',q,p,h);
H0 = .5*(p.^2 + (q.^2-1).^2);
tic
for i=1:n
for j=1:10
k11=p+h*(a11*k12p+a12*k22p);
k21=p+h*(a21*k12p+a22*k22p);
k12=feval('qpdd',q+h*(a11*k11+a12*k21),p,h);
k22=feval('qpdd',q+h*(a21*k11+a22*k21),p,h);
k12p=k12;
k22p=k22;
end
```

```
q1=q+h/2*(k11+k21);
p1=p+h/2*(k12+k22);
Q(:,i) = q1;
P(:,i) = p1;
q= q1;
p= p1;
H(i)= .5*(p.^2+(q.^2-1).^2) ;
error_H(i)= abs(H(i)-H0)  ;
end
toc
subplot(111);plot(error_H,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
 %%%%% 2nd order Lobatto method for Double Well %%%%%
clear all;
p0= 1;
q0= 0;
h=.01;
t=0:h:100;
n=100/h+1;
q=q0;
p=p0;
H0 = .5*(p.^2 + (q.^2-1).^2);
L1p=feval('ppm',q,p,h);
tic
for i=1:n
% calculation of L1 implicitly
for j=1:5
L1=feval('ppm',q, p+h/2*L1p,h);
L1p=L1;
end
k2p=feval('qpm',q,p+(h/2)*L1,h);
k1=feval('qpm',q,p+h/2*L1,h);
% calculation of k2 implicitly
for j=1:5
```

```
k2=feval('qpm',q +(h/2)*(k1+ k2p),p+h/2*L1,h);
k2=k2p;
end
L2=feval('ppm',q + (h/2)*(k1+ k2), p+h/2*L1,h );
% Lobatto pair
q1=q+ (h/2)*(k1+ k2);
p1=p+(h/2)*(L1+L2);
Q(:,i) = q1;
P(:,i) = p1;
q= q1;
p= p1;
H(i)= .5*(p.^2+(q.^2-1).^2) ;
error_H(i)= abs(H(i)-H0)  ;
end
toc
subplot(111);plot(error_H,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
%%%%% Modified Lobatto order 4 for Double-Well
problem %%%%%
clear all;
p0= 1;
q0= 0;
h=.01;
t=0:h:100;
n=100/h+1;
q=q0;
p=p0;
H0 = .5*(p.^2 + (q.^2-1).^2);
L1p=feval('ppmm',q,p,h);
tic
for i=1:n
% calculation of L1 implicitly
for j=1:5
L1=feval('ppmm',q, p+h/2*L1p,h);
```

```
L1p=L1;
end
k2p=feval('qpmm',q,p+(h/2)*L1,h);
k1=feval('qpmm',q,p+h/2*L1,h);
% calculation of k2 implicitly
for j=1:5
k2=feval('qpmm',q +(h/2)*(k1+ k2p),p+h/2*L1,h);
k2=k2p;
end
L2=feval('ppmm',q + (h/2)*(k1+ k2), p+h/2*L1,h );
% Lobatto pair
q1=q+ (h/2)*(k1+ k2);
p1=p+(h/2)*(L1+L2);
Q(:,i) = q1;
P(:,i) = p1;
q= q1;
p= p1;
H(i)= .5*(p.^2+(q.^2-1).^2) ;
error_H(i)= abs(H(i)-H0)  ;
end
toc
subplot(111);plot(error_H,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
%%%%% ODE 45 for Double-Well problem %%%%%
options = odeset('RelTol',1e-4,'AbsTol',[1e-4 1e-4]);
[t,Y] = ode45(@rigid,[0 870],[-1 1.000001 ],options);
%  plot(t,Y(:,1),'-',t,Y(:,2),'-.');
q0=-1;
p0=1.000001;
q=Y(:,1);
p=Y(:,2);
n=size(p)
H0=  0.5* (p0.^2) - 0.5* (q0.^2- 1).^2;
tic
```

```
for i=1:n
P(i) = Y(i,2);
Q(i)= Y(i,1);
H(i) = ( P(i).^2 /2 ) + 0.5*(( Q(i).^2 ) -1 ).^2;
error(i)= H(i)- H0;
end
toc
subplot(111);plot(error,'r');
title('Energy Error');
xlabel('Time t');ylabel('|H(q,p)-H(q0,p0)|');
```