NUMERICAL SOLUTION OF HAMILTONIAN DIFFERENTIAL EQUATIONS

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JANUARY, 2023

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A PROJECT WORK SUBMITTED TO THE DEPARTMENT OF MATHEMATICS, FACULTY OF PHYSICAL SCIENCE, UNIVERSITY OF BENIN, BENIN CITY, IN PARTIAL FULFILMENT FOR THE AWARD OF THE DEGREE OF BACHELOR OF SCIENCE (B.Sc.) MATHEMATICS

JANUARY, 2023

CERTIFICATION

This is to certify that this project was carried out by ANTHONY COLLINS OGBEIDE with MAT NO: PSC1607466 of the Department of Mathematics, Faculty of Physical Sciences, University of Benin, Benin City, Edo State, Nigeria under the supervision of Prof M.N.O. IKHILE.

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PROF. M.N.O. IKHILE **Date**

(PROJECT SUPERVISOR)

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(HEAD OF DEPARTMENT)

DEDICATION

This project work is unreservedly dedicated to my late dad **Mr Anthony Egharevba** and my Almighty Father, my Lord and my God, by whose divine grace, might, knowledge and wisdom started and have bought to a successful conclusion the four years journey to this degree program and project write up.

DECLERATION

I hereby declare that this project work was carried out by me, **ANTHONY COLLINS OGBEIDE** with **MATRIC NO: PSC1607466** under the supervision of **Prof M.N.O. IKHILE.**

_____ _____

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ACKNOWLEDGEMENT

My sincere gratitude goes to God Almighty for giving me the moral, courage and enthusiasm to embark on this project.

I appreciate the efforts of my mother **Mrs. Violet Egharevba** for bringing me up morally and academically. I must register my profound gratitude to my in-law **Mr Igie** and my siblings for their guide, moral and financial supports.

The role of my supervisor, Prof M.N.O Ikhile is greatly appreciated.

I also wish to appreciate all my lecturers whose efforts have contributed to my knowledge base in Mathematics.

Special Mention to Code 123, Belle Boys, Bill Kahan Kapri (kodak Black) and also to my brother Japhet Throne. I want to say a big **Thank you**.

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ABSTRACT

Brief history, origin and relevant roles of some numerical methods in the solution of the Hamiltonian Differential Equation with the help of some definitions and theorem. Some important results, are incorporated in this work, extending, specifically the Runge-Kutta Methods. We study the application of Runge-Kutta schemes to Hamiltonian systems. Basic principles are illustrated by means of examples. This work has been selected carefully so that the work is useful for study in this area of research. Particularly, a survey of the effectiveness of the Runge-kutta Methods. The numerical methods developed are primarily intended for use with Hamiltonian systems, but many find uses in solving other forms of ordinary differential equations. Almost all the real conservative physical processes can be cast in suitable Hamiltonian formulation in phase spaces with symplectic structure, which has the advantages to make the intrinsic properties and symmetries of the underlying processes more explicit than in other mathematically equivalent formulations, so I choose the Hamiltonian formalism as the basis, together with the mathematical and physical motivations of our symplectic approach for the purpose of numerical simulation of dynamical evolutions.

CHAPTER ONE

INTRODUCTION

1.1 HAMILTONIAN DIFFERENTIAL EQUATIONS

Hamiltonian differential equations are a type of mathematical equation that describes the evolution of a physical system over time. These equations are named after William Rowan Hamilton, who developed the theory of classical mechanics that they are based on.

There are several methods for numerically solving Hamiltonian differential equations, including:

1. **Verlet Algorithm**: This method is based on the idea of approximating the position of a particle at a given time by using the positions at previous and subsequent times.
2. **Symplectic Euler Method**: This method is based on the idea of discretizing the time interval over which the equation is being solved, and then using the resulting discrete time steps to update the position and momentum of the system.
3. **Leapfrog Algorithm**: This method is similar to the Symplectic Euler method, but it uses a more accurate approximation of the position and momentum at each time step.
4. **Runge-Kutta Method**: This method involves approximating the solution to the differential equation by using a series of discrete time steps. It is a general-purpose method that can be used to solve a wide variety of differential equations.

There are also more specialized methods for solving specific types of Hamiltonian

differential equations, such as the Störmer-Verlet Algorithm for solving equations with periodic boundary conditions.

In general, the choice of numerical method for solving a Hamiltonian differential equation will depend on the specific characteristics of the equation and the desired level of accuracy.

Hamiltonian differential equations are based on the concept of the Hamiltonian, which is a mathematical function that represents the total energy of a physical system. The Hamiltonian is defined as the sum of the kinetic energy of the system and its potential energy. In classical mechanics, the evolution of a physical system is governed by the principles of energy conservation and the least action. These principles can be expressed mathematically using the Hamiltonian differential equations.

For example, consider a particle moving in one dimension under the influence of a force that is given by a potential energy function U(x). The Hamiltonian for this system is given by:

$$H(x,p) = \frac{p^2}{2m} + U(x)$$

where x is the position of the particle, p is its momentum, and m is its mass.

The Hamiltonian differential equations for this system are given by:

$$\frac{dx}{dt} = \frac{\partial H}{\partial p}$$

$$\frac{dp}{dt} = -\frac{\partial H}{\partial x}$$

These equations describe how the position and momentum of the particle change over time, given the potential energy function $U(x)$ and the initial conditions for the position and momentum of the particle.

1.2 ALTERNATIVE MODELS OF MECHANICS.

Questions concerning the evolution and stability of the solar system go back some 300 years. Mathematical theories prior to computers were based on asymptotic expansions. Euler, Lagrange and Laplace all made important contributions to the prediction of changing geometry and stability of orbits. Lagrange reformulated Newtonian mechanics in terms of a variational principle, which enhances the ability to analyze the behaviour of dynamical systems and readily extends to continuum mechanics.

Hamilton reformulated mechanics so that the dynamics was described by a momentum position phase space instead of the velocity-position phase space of Lagrange. There are two significant consequences of Hamilton's formalism. The first is that the phase space flow is volume preserving. The second is that if symmetries exist, then some of the generalized momenta may be conserved - effectively reducing the dimension of phase space.

Geometrical numerical integration methods

Geometric integration is the numerical integration of a differential equation, while preserving one or more of its geometric properties exactly, i.e., to within round-off error.

Many of these geometric properties are of crucial importance in physical applications: preservation of energy, momentum, volume, symmetries, time-reversal symmetry, dissipation, and symplectic structure being examples. The aim of this work is to present geometric numerical integration methods for ordinary differential equations. We concentrate mainly on Hamiltonian systems and on methods that preserve their symplectic structure, invariants, symmetries, or volume.

Structure preserving methods for Hamiltonian systems

Hamiltonian systems are an important class of differential equations with a geometric structure (their flow has the geometric property of being symplectic), whose preservation in the numerical discretization leads to substantially better methods, especially when integrating over long times.

Some of the reasons we are motivated to preserve structure are

1. It may yield methods that are faster, simpler, more stable, and/or more accurate for some types of ODEs;
2. It may yield more robust and quantitatively better results than standard methods for the long-time integration of Hamiltonian systems.

The standard problem in numerical ODEs to compute the solution to an initial value problem at a fixed time, to within a given global error, as efficiently as possible. The class of method, its order and local error, and choice of time steps are all tailored to this end. In contrast, a typical application of a geometric numerical method is to fix a (sometimes

moderately large) time step and compute solutions with perhaps many different initial conditions over very long time intervals.

1.3 DIFFERENTIAL EQUATIONS

Differential equations are among the most important mathematical tools used in producing models in the physical sciences, biological sciences, and engineering. In this project, we consider numerical methods for solving ordinary differential equations, that is, those differential equations that have only one independent variable. The differential equations we consider in most of this project are of the form

$$Y'(t) = f(t, Y(t)),$$

where $Y(t)$ is an unknown function that is being sought. The given function $f(t, y)$ of two variables defines the differential equation. This equation is called a first-order differential equation because it contains a first-order derivative of the unknown function, but no higher-order derivative. The numerical methods for a first-order equation can be extended in a straightforward way to a system of first-order equations. Moreover, a higher-order differential equation can be reformulated as a system of first-order equations. The simplest numerical method is the Euler's method. It is not an efficient numerical method, but it is an intuitive way to introduce many important ideas. More sophisticated and rapidly convergent methods, namely Runge–Kutta methods among others.

1.4 AIM AND SCOPE

In a wide range of mathematical problems the existence of numerical solution has been of great importance in solving Differential equations therefore of paramount importance in several areas of mathematics and other sciences. One advantage of the Hamiltonian formulation of mechanics is that the equations for arbitrarily complicated arrays of springs and masses can be obtained by simply finding the expression for the total energy of the system. Also Hamiltonian dynamical system is that it has a symplectic structure and one important consequence of this property is that an infinitesimal phase-space volume is preserved. In particular, Hamiltonian Systems have been applied in such diverse fields as Physics, Science and engineering.

1.5 OBJECTIVES

This project work is on some numerical techniques for solving the Hamiltonian systems or differential equation.

The objectives among other things are a review of the following;

- Deriving Hamilton's Equations
- Some numerical techniques for solving differential equations.
- Runge-kutta method.
- Definition, theorems and examples.
- Solutions to the Hamiltonian differential equation.

CHAPTER TWO

LITERATURE REVIEW

2.1 HISTORICAL BACKGROUND

The Hamilton equation, named after William Rowan Hamilton, is an alternative formulation of classical mechanics, equivalent to other formulations such as Newton's laws of motion, Lagrangian mechanics and Hamiltonian mechanics. The Hamilton equation is particularly useful in identifying conserved quantities for mechanical systems, which may be possible even when the mechanical problem itself cannot be solved completely.

The Hamilton equation is also the only formulation of mechanics in which the motion of a particle can be represented as a wave. In this sense, it fulfilled a long-held goal of theoretical physics (dating at least to Johann Bernoulli in the eighteenth century) of finding an analogy between the propagation of light and the motion of a particle.

William Rowan Hamilton was an Irish physicist/mathematician from Dublin. Born in 1806, He invented modern mechanics in his 60 years and laid the groundwork for the jump to quantum mechanics hundred years later. Two notable accomplishments bear his name, Hamilton's principle and Hamilton's equations. He also invented quaternians, an extension of complex numbers allowing an alternate representation of rotations in three dimensions, just as complex numbers can be used to represent rotations in two dimensions. Quaternians are closely related to the Pauli spin matrices that are used to

represent the spin angular momentum of electrons and other Fermions in quantum mechanics. They are also employed in the software underlying many modern computer games. Finally, Hamilton generalized the Langrangian approach to classical mechanics into the form we use today. (All these are referred to as Hamiltonian Mechanics).

2.2 HAMILTONIAN MECHANICS

Hamiltonian mechanics is a theory developed as a reformulation of classical mechanics and predicts the same outcomes as non-Hamiltonian classical mechanics. It uses a different mathematical formalism, providing a more abstract understanding of the theory. Historically, it was an important reformulation of classical mechanics, which later contributed to the formulation of statistical mechanics and quantum mechanics.

In Hamiltonian mechanics, a classical physical system is described by a set of canonical coordinates $r = (q, p)$, where each component of the coordinate q_i, p_i is indexed to the frame of reference of the system.

The time evolution of the system is uniquely defined by Hamilton's equations:

$$\dot{q} = \frac{\partial H}{\partial p}, \qquad \dot{p} = \frac{-\partial H}{\partial q} \tag{1}$$

Where $H = H(q, p, t)$ is the Hamiltonian, which often corresponds to the total energy of the system. For a closed system, it is the sum of the kinetic and potential energy in the system.

In Hamiltonian mechanics, the time evolution is obtained by computing the Hamiltonian of the system in the generalized coordinates and inserting it in Hamilton's equations. This

approach is equivalent to the one used in Lagrangian mechanics. The main motivation to use Hamiltonian mechanics instead of Lagrangian mechanics comes from the symplectic structure of Hamiltonian systems.

While Hamiltonian mechanics can be used to describe simple systems such as a bouncing ball, a pendulum, or an oscillating spring in which energy changes from kinetic to potential and back again over time, its strength is shown in more complex dynamic systems, such as planetary orbits in celestial mechanics.[3] .The more degrees of freedom the system has, the more complicated its time evolution is and, in most cases, it becomes chaotic.

2.3 BASIC PHYSICAL INTERPRETATION

A simple interpretation of the Hamiltonian mechanics comes from its application on a one-dimensional system consisting of one particle of mass m. The Hamiltonian represents the total energy of the system, which is the sum of kinetic and potential energy, traditionally denoted T and V, respectively. Here j is the space coordinate and n is the momentum, mv. Then

$$H = T + V,\ T = \frac{n^2}{2M},\ V = V(j) \qquad (2)$$

Note that T is a function of n alone, while V is a function of j alone (i.e., T and V are Scleronomic).

In this example, the time-derivative of the momentum n equals the Newtonian force, and so the first Hamilton equation means that the force equals the negative gradient of

potential energy. The time-derivative of j is the velocity, and so the second Hamilton equation means that the particle's velocity equals the derivative of its kinetic energy with respect to its momentum.

2.4 CALCULATING A HAMILTONIAN FROM A LAGRANGIAN

Given a Lagrangian in terms of the generalized coordinates q_i and generalized $\dot{q_i}$ velocities and time,

1. The momenta are calculated by differentiating the Lagrangian with respect to the (generalized) velocities:

$$p_i(q_i, \dot{q}_i) = \frac{\partial L}{\partial \dot{q}_i} . \qquad (3)$$

2. The velocities $\dot{q}_i$ are expressed in terms of the momenta p_i by inverting the expressions in the previous step.
3. The Hamiltonian is calculated using the usual definition of H as the Legendre transformation of L:

$$H = \sum_i q_i, \frac{\partial L}{\partial \dot{q}_i} - L = \sum_i \dot{q}_i, p_i - L \qquad (4)$$

Then the velocities are substituted for through the above results.

2.5 DERIVING HAMILTON'S EQUATIONS

Hamilton's equations can be derived by looking at how the total differential of the Lagrangian depends on time, generalized positions $q_{i,}$ and generalized velocities $\dot{q}_i$:

$$dL = \sum_i \left(\frac{\partial L}{\partial q_i}\mathrm{d}q_i + \frac{\partial L}{\partial \dot{q}_i}\mathrm{d}\dot{q}_i\right) + \frac{\partial L}{\partial t}\mathrm{dt}. \quad (5)$$

The generalized momenta is defined as

$$p_i = \frac{\partial L}{\partial \dot{q}_i}, \quad (6)$$

If this is substituted into the total differential of the Lagrangian (5), one gets

$$dL = \sum_i \left(\frac{\partial L}{\partial q_i}\mathrm{d}q_i + p_i\,\mathrm{d}\dot{q}_i\right) + \frac{\partial L}{\partial t}\mathrm{dt}. \quad (7)$$

This can be rewritten as

$$dL = \sum_i \left[\frac{\partial L}{\partial q_i}\mathrm{d}q_i + d(p_i\,\dot{q}_i) - \dot{q}_i\mathrm{d}p_i\right] + \frac{\partial L}{\partial t}\mathrm{dt}. \quad (8)$$

This after rearranging leads to

$$d\left(\sum_i p_i\,\dot{q}_i - L\right) = \sum_i \left(\frac{-\partial L}{\partial q_i}\mathrm{d}q_i + \dot{q}_i\mathrm{d}p_i\right) - \frac{\partial L}{\partial t}\mathrm{dt}. \quad (9)$$

The term on the left-hand side is just the Hamiltonian that was defined before, therefore

$$dH = \sum_i \left(\frac{-\partial L}{\partial q_i}\mathrm{d}q_i + \dot{q}_i\mathrm{d}p_i\right) - \frac{\partial L}{\partial t}\mathrm{dt}. \quad (10)$$

It is also possible to calculate the total differential of the Hamiltonian H with respect to time directly yielding:

$$dH = \sum_i \left(\frac{\partial H}{\partial q_i}\mathrm{d}q_i + \frac{\partial H}{\partial p_i}\mathrm{d}p_i\right) + \frac{\partial H}{\partial t}\mathrm{dt}. \quad (11)$$

It follows from the previous two independent equations that their right-hand sides are equal to each other. The result is

$$\sum_i \left(\frac{-\partial L}{\partial q_i}\mathrm{d}q_i + \dot{q}_i\mathrm{d}p_i\right) - \frac{\partial L}{\partial t}\mathrm{dt} = \sum_i \left(\frac{\partial H}{\partial q_i}\mathrm{d}q_i + \frac{\partial H}{\partial p_i}\mathrm{d}p_i\right) + \frac{\partial H}{\partial t}\mathrm{dt}.$$

Since this calculation was done off-shell, one can associate corresponding terms from both sides of this equation to yield:

$$\frac{\partial H}{\partial q_i} = \frac{-\partial L}{\partial q_i}, \quad \frac{\partial H}{\partial p_i} = \dot{q}_i \ , \quad \frac{\partial H}{\partial t} = \frac{-\partial L}{\partial t}$$

On shell, Lagrange's equations indicate that

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0$$

A rearrangement of this yield;

$$\frac{\partial L}{\partial q_i} = \dot{p}_i$$

Thus Hamilton's equations hold on shell:

$$\frac{\partial H}{\partial q_j} = -\dot{p}_j \ , \quad \frac{\partial H}{\partial pj} = \dot{q}_j \ , \qquad \frac{\partial H}{\partial t} = \frac{-\partial L}{\partial t}$$

CHAPTER THREE

SOME NUMERICAL METHODS

3.1 RUNGE-KUTTA METHOD

The Runge-Kutta method is a collection of different numeric integrators with versatile properties. One of the best-known examples is the Euler method.

3.1.1Definition

Given a constant step size h and a known starting point y_n of an iterative process, the next point is given by

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

in the explicit case. In the implicit case, it is given by

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

The straightforward solution of eq. (1), with initial condition y_n, is

$$y(t_{n+1}) = y_n + \int_{t_n}^{t_{n+1}} f(t, y)dt \tag{2}$$

which of course is far away from a practical solution since the integral above is generally not easy to solve. There are different ways to approximate the integral, one way is to construct "helping directions" k_i, which guide the method from y_n to y_{n+1}.

Using the trapezoid rule, results in:

$$y_{n+1} = y_n + \frac{h}{2}\big(f(t_n, y_n) + f(t_{n+1}, y_{n+1})\big). \tag{3}$$

So now, only the term $f(t_{n+1}, y_{n+1})$ needs to be approximated, which can be done with an explicit Euler step $f(t_{n+1}, y_{n+1}) \approx f\big(t_n + h, y_n + hf(y_n)\big)$. To summarize, three values have been calculated:

$$\begin{aligned} k_1 &= f(t_n, y_n) \\ k_2 &= f\big(t_n + h, y_n + hf(y_n)\big) \\ y_{n+1} &= y_n + \frac{h}{2}(k_1 + k_2) \end{aligned} \tag{4}$$

In the above example, two "helping directions" k_1 and k_2 have been used, making it a 2-stage Runge-Kutta method. The general case looks as follows:

3.1.2 Definition [s-Stage Runge-Kutta Method]

Let $b_i, a_{ij} i, j \in \{1, ..., s\}$ be real numbers and let $c_i = \sum_j^s a_{ij}$. The s-stage Runge-Kutta method is then given by

$$\begin{aligned} k_i &= f\left(t_n + c_i h, y_n + h\sum_{j=1}^{s} a_{ij} k_j\right),\ i = 1, ..., s \\ y_{n+1} &= y_n + h\sum_{i=1}^{s} b_i k_i \end{aligned} \tag{5}$$

The coefficients are concisely displayed in the Butcher-tableau

$$\begin{array}{cccc} c_1 & a_{11} & \dots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \dots & a_{ss} \\ & b_1 & \dots & b_s \end{array}$$

So for the above example equation (5), it looks as follows

$$\begin{array}{ccc} 0 & & \\ 1 & 1 & \\ & 1/2 & 1/2 \end{array}$$

Since the order of an integrator is an approximation of the local error, it would generally be favourable to use methods of a high order, but this leads to more and more difficult conditions for the integrator. This is why only conditions up to order 3 will be presented.

By computing a Taylor series of $y(t_0 + h)$ and y_1 around $h = 0$ we get the following conditions for the orders of $1,2\ and\ 3$:

1. $\sum_i b_i = 1$
2. order 1 and $\sum_i b_i c_i = 1/2$
3. order $2, \sum_i b_i c_i^2 = 1/3$ and $\sum_{i,j} b_i a_{ij} c_j = 1/6$

The Runge-Kutta method for Problem eq. (2) is given by the same approach, but combining two Runge-Kutta methods and thus having two kinds of "helping directions" k_i and ℓ_i, one for y and one for z. Again a_{ij} and b_i are coefficients for y and $\hat{a}_{ij}, \hat{b}_i$ are the ones concerning z.

$$k_i = f\left(y_n + h\sum_{j=1}^{s} a_{ij}k_j, z_n + h\sum_{j=1}^{s} \hat{a}_{ij}\ell_j\right)$$
$$\ell_i = g\left(y_n + h\sum_{j=1}^{s} a_{ij}k_j,\ z_n + h\sum_{j=1}^{s} \hat{a}_{ij}\ell_j\right)$$
$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i k_i,\ z_{n+1} = z_n + h\sum_{i=1}^{s} \hat{b}_i \ell_i$$

3.2 SYMPLECTIC RUNGE-KUTTA METHODS

(a) Symplecticity as a quadratic first integral.

Let $X(t) = \frac{\partial y(t)}{\partial y_0} = \varphi_t'(y_0)$ and consider the extended system

$$\begin{cases} \dot{y} = J^{-1}\nabla H(y) & y(0) = y_0 & \text{Hamiltonian system} \\ \dot{X} = J^{-1}\nabla^2 H(y)X & X(0) = I & \text{Variational equation} \end{cases}$$

Then, $X(t)^T JX(t)$ is a quadratic first integral of ($*$), because

$$X(t)^T JX(t) = \varphi_t'(y_0)^T J\varphi_t'(y_0) = J = X(0)^T JX(0)$$

(b) Runge-Kutta methods which preserve quadratic first integrals.

Every Runge-Kutta method

$$\begin{aligned} Y_i &= y_n + h\sum_{j=1}^{s} a_{ij} f\left(t_n + c_i h, Y_j\right) \\ y_{n+1} &= y_n + h\sum_{i=1}^{s} b_i f(t_n + c_i h, Y_i) \end{aligned}$$

for the ODE $\dot{y} = f(t,y)$ conserves all linear first integrals $I(y) = v^T y$, because then $v^T f(t,y) = 0$ for all y and hence

$$I(y_{n+1}) = v^T y_{n+1} = v^T y_n + h\sum_{i=1}^{s} b_i \underbrace{v^T f(t_n + c_i h, Y_i)}_{=0} = I(y_n).$$

However, quadratic first integrals are in general not conserved.

(c) Interchange the order of linearization and applying the method

Applying the Runge-Kutta method to the extended system

$$\begin{cases} \dot{y} = J^{-1}\nabla H(y) \\ \dot{X} = J^{-1}\nabla^2 H(y)X \end{cases}$$

yields approximations

$$y_n \approx y(t_n),\ X_n \approx X(t_n).$$

For the exact solution, we have

$$X(t) = \frac{\partial y(t)}{\partial y_0} = \varphi_t^{'}(y_0)$$

Is this still true for the numerical solution y_n and X_n ? Is $X_n = \frac{\partial y_n}{\partial y_0}$?

Examples.

- Explicit Euler: $a_{11} = 0, b_1 = 1 \longrightarrow$ not symplectic
- Implicit Euler: $a_{11} = 1, b_1 = 1 \longrightarrow$ not symplectic
- Trapezoidal rule: $a_{11} = a_{12} = c_1 = 0, c_2 = 1 \longrightarrow$ not symplectic

$$a_{21} = a_{22} = b_1 = b_2 = \frac{1}{2}$$

- Midpoint rule: $a_{11} = \frac{1}{2}, b_1 = 1 \longrightarrow$ symplectic

3.3 PARTITIONED RUNGE-KUTTA METHODS

This method is relevenat in solving an hamiltonian in terms of momentum and position variables. A partitioned Runge-Kutta method is given as

$$Y_i = y_n + h\sum_{j=1}^{s} a_{ij} f\left(Y_j, Z_j\right), \quad y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f(Y_i, Z_i)$$

$$Z_i = z_n + h\sum_{j=1}^{s} \hat{a}_{ij} g\left(Y_j, Z_j\right), \quad z_{n+1} = z_n + h\sum_{i=1}^{s} \hat{b}_i g(Y_i, Z_i)$$

CHAPTER FOUR

SOLUTION TO THE HAMILTONIAN DIFFERENTIAL EQUATION

Consider the Hamiltonian system

$$\begin{cases} \frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial H}{\partial q}(p,q), \\ \frac{\mathrm{d}q}{\mathrm{d}t} = \frac{\partial H}{\partial p}(p,q), \\ p(0) = p_0, q(0) = q_0, \end{cases} \tag{1}$$

where $p_0, q_0 \in \mathbb{R}^d$, and the Hamiltonian function $H: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a smooth function. Let $x = (p,q)^\top$. The Hamiltonian system of equations (1) can be rewritten as a first-order differential equation

$$\begin{cases} \frac{dx}{dt} = f(x) \\ x(0) = x_0 \in \mathbb{R}^{2d} \end{cases} \tag{2}$$

where $x_0 = (p_0, q_0)^\top$ and

$$\begin{aligned} f\colon \quad & \mathbb{R}^{2d} \to \mathbb{R}^{2d} \\ & x \mapsto J^{-1}\nabla H(x). \end{aligned}$$

4.1 RUNGE-KUTTA METHOD

Now we turn to Runge-Kutta method

$$\begin{cases} x_{i,k} = x^k + (\Delta t)\sum_{j=1}^{m} a_{ij} f\left(x_{j,k}\right) \\ x^{k+1} = x^k + (\Delta t)\sum_{i=1}^{m} b_i f\left(x_{i,k}\right) \end{cases} \tag{3}$$

for solving (2)

Theorem 4.1

(i) The Runge-Kutta method (3) preserve linear invariants;

(ii) The Runge-Kutta method (3) whose coefficients satisfy the condition

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0,\ i, j = 1, \ldots m, \tag{4}$$

preserves all quadratic invariants.

Proof:

Define $\Phi_{\Delta t}$ by $x^{k+1} = \Phi_{\Delta t}\left(x^k\right)$. Let $F(x) = d^{\top} x$, where $d \in \mathbb{R}^{2d}$. We compute

$$F\left(\Phi_{\Delta t}\left(x^k\right)\right) = d^{\top}\left(x^k + \Delta t \sum_{i=1}^{m} b_i f\left(x_{i,k}\right)\right) = d^{\top} x^k,$$

since $d^{\top} x$ is assumed to be an invariant of (2) hence $d^{\top} f\left(x_{i,k}\right) = 0$.

Next, let $F(x) = x^{\top} C x$, where C is a symmetric $2d \times 2d$ matrix. Assume that F is an invariant of (2). We have

$$x^{\top} C f(x) = 0 \text{ for all } x. \tag{5}$$

On the other hand, we have

$$\begin{aligned} F\left(\Phi_{\Delta t}(x^k)\right) = & \left(x^k + \Delta t \sum_{j=1}^{m} b_j f(x_{j,k})\right)^{\top} C \left(x^k + \Delta t \sum_{i=1}^{m} b_i f(x_{i,k})\right) \\ = & (x^k)^{\top} C x^k + (\Delta t) \sum_{i=1}^{m} (x^k)^{\top} C b_i f(x_{i,k}) + (\Delta t) \sum_{j=1}^{m} b_j f(x_{j,k})^{\top} C x^k \\ & + (\Delta t)^2 \sum_{i,j=1}^{m} b_i b_j f(x_{j,k})^{\top} C f(x_{i,k}) \end{aligned}$$

From (5), we obtain

$$(x_{i,k})^{\top} C f(x_{i,k}) = 0,$$

and hence, by writing

$$x^k = x^k + \Delta t \sum_{j=1}^{m} a_{ij} f(x_{j,k}) - \Delta t \sum_{j=1}^{m} a_{ij} f(x_{j,k}) = x_{i,k} - \Delta t \sum_{j=1}^{m} a_{ij} f(x_{j,k}),$$

we get

$$\begin{aligned} F\left(\Phi_{\Delta t}(x^k)\right) = & (x^k)^{\top} C x^k - (\Delta t)^2 \sum_{i,j=1}^{m} b_i a_{ij} f(x_{j,k})^{\top} C f(x_{i,k}) - (\Delta t)^2 \sum_{i,j=1}^{m} b_j a_{ji} f(x_{j,k})^{\top} C f(x_{i,k}) \\ & + (\Delta t)^2 \sum_{i,j=1}^{m} b_i b_j f(x_{j,k})^{\top} C f(x_{i,k}) \\ = & (x^k)^{\top} C x^k - (\Delta t)^2 \left(\sum_{i,j=1}^{m} (b_i a_{ij} + b_j a_{ji} - b_i b_j) f(x_{j,k})^{\top} C f(x_{i,k}) \right) \end{aligned}$$

Therefore, the Runge-Kutta method preserves the quadratic invariant F provided that

(4) holds.

Theorem 4.2

The Runge-Kutta method (3) for solving (2) whose coefficients satisfy condition (4) is symplectic.

Proof:

We know that the flow ϕ_t is a symplectic transformation (if H is smooth enough). Let $\Psi(t) := \frac{\partial \phi_t(x_0)}{\partial x_0} = \phi_t'$, where x_0 is the initial condition. We have

$$\begin{cases} \frac{d\Psi}{dt} = f'(x)\Psi \\ \Psi(0) = I \end{cases} \tag{6}$$

Apply a Runge-Kutta method satisfying (4) to (2) and (6) to obtain the approximations x^{k+1} and Ψ^{k+1} from x^k and Ψ^k. Since $\Psi^\top J\Psi$ is a quadratic invariant of the augmented system (6), we obtain

$$\left(\Psi^k\right)^\top J\Psi^k = J \text{ for all } k$$

Suppose for a moment that

$$\Psi^{k+1} = \frac{\partial x^{k+1}}{\partial x^k} \tag{7}$$

We obtain

$$\left(\frac{\partial x^{k+1}}{\partial x^k}\right)^\top J \frac{\partial x^{k+1}}{\partial x^k} = J$$

which means that the Runge-Kutta method for solving (2) whose coefficients satisfy condition (4) is symplectic.

In order to complete the proof, we prove (7) We want to show that the result of first applying $\Phi_{\Delta t}$ and then differentiating with respect to x^k is the same as applying the same Runge-Kutta method to (6).

In fact, on the one hand, by differentiating (3) with respect to x^k we obtain

$$\begin{cases} \frac{\partial x_{i,k}}{\partial x^k} & = I + (\Delta t)\sum_{j=1}^{m} a_{ij} f'\left(x_{j,k}\right)\frac{\partial x_{j,k}}{\partial x^k} \\ \frac{\partial x^{k+1}}{\partial x^k} & = I + (\Delta t)\sum_{i=1}^{m} b_i f'\left(x_{i,k}\right)\frac{\partial x_{i,k}}{\partial x^k} \end{cases} \tag{8}$$

Multiplying the first equation in (8) by $f'\left(x_{i,k}\right)$ yields the linear system in the unknowns $f'\left(x_{i,k}\right)\frac{\partial x_{i,k}}{\partial x^k}$

$$f'\left(x_{i,k}\right)\frac{\partial x_{i,k}}{\partial x^k} = f'\left(x_{i,k}\right)\left(I + (\Delta t)\sum_{j=1}^{m} a_{ij} f'\left(x_{j,k}\right)\frac{\partial x_{j,k}}{\partial x^k}\right), \tag{9}$$

$$\frac{\partial x^{k+1}}{\partial x^k} = I + (\Delta t)\sum_{i=1}^{m} b_i f'\left(x_{i,k}\right)\frac{\partial x_{i,k}}{\partial x^k}. \tag{10}$$

On the other hand, applying the same Runge-Kutta method to (8) yields

$$\Psi_{i,k} = f'\left(x^k + \Delta t\sum_{j=1}^{m} a_{ij} x_{j,k}\right)\left(I + (\Delta t)\sum_{j=1}^{m} a_{ij}\Psi_{j,k}\right) \tag{11}$$

$$\Psi^{k+1} = I + (\Delta t)\sum_{i=1}^{m} b_i \Psi_{i,k} \tag{12}$$

We conclude the proof by observing that (11) is the same system as (9) but in the unknowns $\Psi_{i,k}, i = 1, ..., m$. It is easily seen that this system has a unique solution for sufficiently small Δt, so it must be

$$\Psi_{i,k} = f'(x_{i,k})\frac{\partial x_{i,k}}{\partial x^k} \text{ for } i = 1, ..., m,$$

which, in view of (10) and 5ields (12). For arbitrary Hamiltonians, the only known symplectic one-step numerical methods are the symplectic Runge-Kutta methods of the form (12) that satisfy the symplectic condition (4).

4.2 LONG-TIME BEHAVIOUR OF NUMERICAL SOLUTIONS

As shown in the theorem below, the symplecticity of a one-step numerical method yields an approximate conservation of energy over very long times for general Hamiltonian systems.

Theorem 4.3

For an analytic Hamiltonian H and a symplectic one-step numerical method $\Phi_{\Delta t}$ of order n, if the numerical trajectory remains in a compact subset, then there exist $h > 0$ and $\Delta t^* > 0$ such that, for $\Delta t \leq \Delta t^*$,

$$H\left(p^k, q^k\right) = H(p^0, q^0) + O((\Delta t)^n),$$

for exponentially long times $k\Delta t \leq e^{\frac{h}{\Delta t}}$.

Here, $\left(p^{k+1}, q^{k+1}\right) = \Phi_{\Delta t}\left(p^k, q^k\right)$.

Theorem (4.3) is based on simplicticity. It can be proved via backward error analysis. The idea is to deduce the long-time behavior estimate from properties of the solution of the equation corresponding to an approximation $H_{\Delta t}$ of the Hamiltonian H.

CHAPTER FIVE

5.1 SUMMARY

In this project work, we have introduced the Hamiltonian system, Deriving the Hamilton's Equations, some numerical methods for solving differential equations. We have discussed various theorems and propositions. Later in the application of these methods in the solution of the Hamiltonian differential equation, we discussed on the concept of Runge-Kutta and its various types, e.g. Symplectic Runge-Kutta Method, Partitioned Runge-Kutta Method, s-Stage Runge-Kutta Method.

Finally, I discussed on the application of this to the solution of the Hamiltonian differential equation.

5.2 CONCLUSION

After all that was discussed on this concept of the numerical approach to the solution of the Hamiltonian differential equation. We hope that the content presented in the project work would be of immense help to the students who are beginners in the subject matter.

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