5-2017

Application of Symplectic Integration on a Dynamical System

William Frazier
East Tennessee State University

Application of Symplectic Integration on a Dynamical System

—————————

A thesis

presented to

the faculty of the Department of Mathematics

East Tennessee State University

In partial fulfillment

of the requirements for the degree

Master of Science in Mathematical Sciences

—————————

by

William Ty Frazier

May 2017

—————————

Jeff Knisley, Ph.D., Chair

Michele Joyner, Ph.D.

Robert Gardner, Ph.D.

Keywords: Lie algebra, Lie group, symplectic integration, molecular dynamics.

ABSTRACT

Application of Symplectic Integration on a Dynamical System

by

William Ty Frazier

Molecular Dynamics (MD) is the numerical simulation of a large system of interacting molecules, and one of the key components of a MD simulation is the numerical estimation of the solutions to a system of nonlinear differential equations. Such systems are very sensitive to discretization and round-off error, and correspondingly, standard techniques such as Runge-Kutta methods can lead to poor results. However, MD systems are conservative, which means that we can use Hamiltonian mechanics and symplectic transformations (also known as canonical transformations) in analyzing and approximating solutions. This is standard in MD applications, leading to numerical techniques known as symplectic integrators, and often, these techniques are developed for well-understood Hamiltonian systems such as Hills lunar equation. In this presentation, we explore how well symplectic techniques developed for well-understood systems (specifically, Hills Lunar equation) address discretization errors in MD systems which fail for one or more reasons.

DEDICATION

Dedicated to my friend, Tiara Charde Johnson (1991-2013), a friend who was always there and taken away from us too soon.

ACKNOWLEDGMENTS

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

1 INTRODUCTION

In the scientific world today – given the advancements made to computer processing power, memory storage, and data retrieval – many scientific experiments are performed on a computer. The experiments performed in computers are designed to be simulations of the real world scientific experiments. Numerical error plagues every algorithm, simulation, or otherwise when working with computers. Computers use floating point arithmetic, which means every simulation will have round-off error [17]. However, numerical error can be managed and that is the focus of this research.

1.1 Motivation

The motivation for this thesis originates from a research project in Spring 2014 in which we simulated the dynamics of a folded hen egg white lysozyme protein. We had a goal of destabilizing the protein. We were able to achieve our goal by removing certain disulfide bonds in the protein. This resulted in the protein losing its tertiary structure. We ran several simulations in attempts to replicate the results. However, we noticed during these simulations that the destabilization was due to the dynamics no longer being a Hamiltonian system. This is important because the molecular dynamics simulation package GROMACS [4] uses loss of Hamiltonicity to determine when a destabilization takes place. Specifically, GROMACS terminates a simulation when it detects exponential phase volume changes at a thermodynamic equilibrium (blow-up error). Typically, such destabilizations occur because of discretization error.

1.2   Numerical Error

The quantification of numerical error in a simulation indicates how much uncertainty exists in the results of the computer experiment [38]. If the amount of numerical error is substantial, then the amount of uncertainty is substantial. With a large amount of uncertainty the numerical simulation can start to produce "false-positives" [38], which can invalidate the results from the computational experiment. If the numerical error is significant enough during an update step of the algorithm for the simulation, then that error propagates into the model of the simulation [38]. These inaccuracies invalidate the numerical experiment; because it is no longer a representation of a real world experiment. The different types of error that can occur during a numerical experiment fall into three main categories: round-off error, iterative error, and discretization error [35, 38].

1.2.1   Round-off Error

The real numbers are a continuum [39]. Computers use floating-point arithmetic where numbers have a floating-point representation [17, 27, 44]. The complication with floating-point arithmetic is that the cardinality of the set of numbers accounted for by floating-point representation is a finite subset of the real numbers. Computers round numbers to give them a floating-point representation. Round-off error is the difference between the floating-point representation and the exact mathematical value [17, 27, 44]. There are a couple of ways to measure how much error is associated to round-off. Those measurements are called absolute error and relative error. For the

purposes of this thesis let x_{round} denote be a float-pointing representation of x and x be the exact value. We know by [17, 27] the absolute error is measured by

$$\left|x_{\text{round}} - x\right|.$$

We know by [17, 27] the relative error is

$$\frac{\left|x_{\text{round}} - x\right|}{|x|}.$$

The relative error tells us how big the inaccuracy of the approximate value is as a percentage of the exact value. The best solution to reduce round-off error is to increase the number of significant digits in the floating point representation[38].

1.2.2 Iterative Error

Iterative error is generated by iterative methods for solving linear and nonlinear problems. Iterative methods are successive refinements of an approximate solution [43]. In Subsection 1.2.2 let x be the exact solution and x^* be the approximate solution for some problem. We know from [23] that the error is

$$e = x - x^*.$$

In addition, [1, 23] tells us that iterative methods are commonly used on systems of linear equations that take the form

$$Ax = b.$$

2 DISCRETIZATION ERROR

Discretization error is the hardest type of numerical error to manage [17, 35, 36, 37, 38, 44]. Discretization error is produced in an attempt to estimate solutions to integral or differential equations using a partition or mesh of a geometric domain. Also, from those sources we know discretization error to be the difference between the exact solution to the discretized equations and the exact solution to the original ordinary differential or integral equations. Let $f_{\text{discretized}}$ be the solution to the discretized equation and f_{ODE} be the exact solution to the ordinary differential equations. According to [17, 38, 35, 44, 37, 36], discretization error is

$$f_{\text{Error}} = f_{\text{discretized}} - f_{\text{ODE}}$$

where f_{Error} is the amount of discretization error.

Let h be the width of an interval in a regular partition of $[a, b]$. If a method produces a discretization error that satisfies

$$\|f_{\text{Error}}\| < Ch^n$$

for some norm $\|\cdot\|$, for some $C \in \mathbb{R}$, and for some $n \in \mathbb{Z}^+$ then the method has an order of n, denoted by $O(h^n)$ with respect to that norm [17, 27, 44]. A numerical approximation with a order of n is called an n-th order (numerical) solution.

Managing discretization error can be very complicated, so methods are developed to better manage it. Some methods like Richardson extrapolation focus on getting very high orders of accuracy, but not preserving the manifold structure of the differential equations. Other methods like symplectic integration achieve high orders of accuracy while preserving the manifold structure of the differential equations.

14

2.1   Methods for Managing Discretization Error

2.1.1   Richardson Extrapolation Method

Richardson extrapolation, is the most prevalent and dependable method for managing error produced in the mesh grid in relation to the numerical solution of the differential equations [36, 37]. According to [33] and [34], Richardson extrapolation was developed by L.F. Richardson in the early 1900's in order to obtain a higher accuracy Taylor-Series derived approximations of solutions. Richardson started by taking two discrete second-order solutions and extrapolated them by means of algebraic operations, to achieve a solution with fourth-order accuracy. Richardson extrapolation comes from the realization that different discrete orders of accuracy solutions can be combined differently using algebraic expressions in order to extrapolate the original solutions to a higher order of accuracy solution than was previously attained. In addition, this method requires the refinement of each mesh to be uniform. According to [36, 37, 38], this method is a demanding process due to the number of grid points and strain on the computation tool that generates the meshes and does the systemic refinement of the meshes.

2.1.2   Method of Nearby Problems

The method that Roy et. al. [37] focuses on is the method of nearby problems, (MNP). MNP eliminates certain problems associated with the Richardson extrapolation. MNP requires two numerical solutions on the same grid. In addition MNP is a 6 step algorithm that is easy to follow. According to [37], the effectiveness of

MNP is due to the curve fit generated during the method. The curve fit is the exact solution to the nearby problem. The source terms of the curve fit indicate how close the nearby problem is to the original problem. If the source terms are small, then the nearby problem is close to the original problem, and if the source terms are large, then the nearby problem is far from the original problem. From [37] we know that the MNP works on the steady and unsteady Burgers' equations, the Euler equations, and the incompressible Navier-Stokes equations.

2.2 Simulations, Dynamics, and Errors

2.2.1 Newtonian Mechanics

From [32] we know that the theoretical basis comes from some of the greatest mathematical and physics minds in all of history: Newton, Euler, Lagrange, and Hamilton. When MD simulations are based on point particles, the dynamics are basically governed by Newton's second law [32]. Newton's second law is mathematically expressed as

$$F = m\mathbf{a} = m\left(\frac{d^2\mathbf{y}}{dt^2}\right)$$

where $\mathbf{y}$ is a distance function of time t [17]. According to [32] the force of an individual atom is

$$f = -\nabla u\left(r\right)$$

where $u\left(r\right)$ is the potential. By [32] the equations of motion corresponding to force are

$$mr_i'' = f_i = \sum_{\substack{j=1 \\ j\neq i}}^{N_m} f_{ij}$$

where the sum is over all N_m atoms, m is the atomic mass, and the equations are based upon Newton's second law. Newton's third law, which is for every action there is an equal and opposite reaction, implies that $f_{ji} = -f_{ij}$ [32]. This saves computation time and power as only half the interaction forces need to be calculated. Newtonian mechanics leads to systems of ordinary differential equations that often cannot be solved in closed form. Consequently, solutions must be approximated, and such approximations are often due to discretization of the time interval into a finite sequence of time steps.

2.2.2 Error in Molecular Dynamics

There are a few types of errors that can occur during a molecular dynamics simulation. A boundary error is when the protein in the simulation collides with the boundaries of the simulation. A time and space error is when at least two atoms have the same spatial and temporal coordinates. A time and space error can cause a blow up error, which is when the atoms of the protein splatter over the boundaries. This is a result of having at least two repelling atoms sitting on top of each other. This results in those atoms' velocities increasing exponentially. The last two errors are often due to discretization error. All of these types of errors are classified as mathematical errors.

The other types of errors are called physical errors. These types of errors are similar to the behavior a protein would depict in the real world. These errors include behaviors like the protein unfolding or unraveling, which in general is know as desta-bilization. Such errors are due to alterations to a protein's topology, where topology

17

refs to the geometry of the protein due to the connectivity within and between the amino acids that form the protein.

In this thesis we develop a novel numerical method that can be applied to any Newtonian system. The method will address the management of discretization error. The method will address this by using group theoretic splitting and composition methods for differential equations in general to develop novel symplectic integrators, which are numerical methods designed to preserve properties of Newtonian systems – properties like conservation of energy and conservation of momentum.

3   MOLECULAR DYNAMICS

Molecular Dynamics, (MD), is a computational tool designed to simulate inter-actions between molecules on an atomic scale. MD serves the purpose of allowing scientists to track the interactions and movements of the molecules [32]. MD models are systems of ordinary differential equations. Moreover MD is a dynamic simulation, which means it incorporates the laws of physics, chemistry, and biology in its models [17]. In the following subsections we will go over MD's origins, some of its internal structures, what it needs to simulate the dynamics of a protein, and the process of a simulation of the dynamics of a protein.

3.1   Origins

The theoretical mathematics and physics core of MD is constructed upon little more than Newton's Laws of motion. According to [32] it was not long after the invention of the first digital computer that MD came into existence. From [32] one of the biggest problems MD tries to address and solve numerically is the N-body problem. MD uses many different potentials in its models for those problems.

3.2   Lennard-Jones Potential

MD models become Newtonian models when the system is equilibrated and the energy is minimized. Newtonian models are defined by their potential energy. Poten-tials for MD are combinations of Coulomb potentials (inverse square law), Lennard-Jones potentials, and others as required by the MD model. From [32, 24, 50] the

19

Lennard-Jones potential, (LJ), is

$$U_{ij}^{\mathrm{LJ}} = k\varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^n - \left(\frac{\sigma}{r_{ij}} \right)^m \right]$$

with

$$k = \frac{n}{n-m} \left(\frac{n}{m} \right)^{\frac{m}{n-m}}$$

where n and m are parameters whose values determine the strength and range of the forces. In the model σ is the finite distance at which the inter-particle potential is 0, r_{ij} is the distance between atoms i and j, and ε is the strength of the interaction between atoms i and j. The model is constructed to be able to account for short range, repulsive overlap forces and longer range, attractive dispersion forces [24, 32]. This model is convenient for soft-sphere pair potentials, in which MD atoms are treated as soft-spheres and molecules are pairs of atoms bonded together. Furthermore, [24] tells us that n and m are used to determine the range and strength of those forces, where m is normally chosen to be 6 and n to be $2m = 12$. With the values of m and n chosen from [24, 32, 50], LJ is

$$U_{ij}^{\mathrm{LJ}} = 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right].$$

In MD simulations an assumption is made that if two atoms are more than a certain distance apart, then their potential is 0. From [24] this is done to shorten computer processing time. Consequently, LJ becomes a piecewise-defined function as

$$U_{ij}^{\mathrm{LJ}} = \begin{cases} 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right] & r_{ij} \leq r_c \\ \\ 0 & r_{ij} > r_c \end{cases}$$

20

where r_c is normally chosen to be 2.5σ. This implies that $U = -0.0163\varepsilon$, and when $r_{ij} = r_c$, the potential between atoms i and j is small [24].

3.3   Newtonian Model for Molecular Dynamics

From [32] MD mimics nature by basing its equations of motion on Newtonian mechanics. Even if Lagrange's equations of motion are being used, Newton's second law is incorporated into those equations. We will see this as we go through how MD uses Lagrange's equations of motion to control and vary temperature. From [32] a few new variables are introduced. A dynamical variable s is used as an equivalent to rescaling the unit of time t', the variable for real time, and t, the variable for scaled time. The relation between the variables is

$$dt = s\left(t'\right) dt'.$$

According to [32] the Lagrangian for an extended system is written as

$$\mathcal{L} = \frac{1}{2}ms^2 \sum_i \dot{r}_i^2 - \sum_{i<j} u\left(r_{ij}\right) + \frac{1}{2}M_s\dot{s}^2 - n_fT \log\left(s\right)$$

where T is the required temperature,

$$n_f = 3N_m + 1$$

is the number of degrees of freedom, M_s is the mass needed to assemble an equation of motion for coordinate s, and dots represent a derivative with respect to t. The Lagrangian is defined in terms of rescaled time t. The standard procedure for getting Lagrange's equations of motion are

$$\ddot{r}_i = \frac{1}{ms^2}f_i - \frac{2\dot{s}}{s}\dot{r}_i$$

21

and

$$M_s \ddot{s} = ms \sum_i \dot{r}_i^2 - \frac{n_f T}{s}.$$

Since the relationship between t and t' is

$$t = \int s\left(t'\right) dt'.$$

[32] it's easier if the equations are altered to use real time t'. The altered equations

are

$$\ddot{r}_i = \frac{1}{m} f_i - \frac{\dot{s}}{s} \dot{r}_i$$

and

$$\ddot{s} = \frac{\dot{s}^2}{s} + \frac{G_1 s}{M_s}$$

where

$$G_1 = m \sum_i \dot{r}_i^2 - n_f T$$

and dots represent the derivative with respect to t' [32]. As [32], states the first of

these equations of motion looks like the conventional Newtonian equation with an

extra term.

3.4 Protein Structure

The structure of a protein is mostly made up of a type of macromolecule called

polypeptides [22]. Polypeptides are made of α-amino acids. Each α-amino acid is

made of certain elements or atoms. Simulating the dynamics of a protein usually

entails inputting a protein data bank file and a molecular topology file. A protein

data bank file places all of the atoms of a protein on a grid system and gives the bonds and angle bonds between the atoms. A molecular topology file adds charges of the atoms and the nature of the interactions between all of the atoms in the simulation. The way MD interprets and combines the protein data bank and molecular topology files is by using a mathematical structure from graph theory called a network. In the network the vertices are the atoms, the edges are the bonds between atoms, and the cost functions are the strengths of the bonds. However, this cannot be thought of as a theoretical graph theory network because a sense of positions and angles needs to be incorporated. When a protein is folded in its tertiary structure [28, 48] the stabilization of the tertiary structure comes primarily from hydrophobic interactions between the nonpolar side chains, hydrogen bonds between polar side chains, and peptide bonds [28, 48]. A particular type of bond that helps stabilize the tertiary structure is disulfide bonds [28, 48]. For more information about proteins see the appendices.

3.4.1   The Protein Data Bank

X-ray crystallography is a technique used to determine the structure of proteins and biological marcomolecules [42]. X-ray crystallography was designed with the purpose of obtaining a three dimensional molecular structure from a crystal [42]. The Protein Data Bank, PDB, is a computer-based archival file for macromolecular structures [5]. PBD was established in 1971 with the purpose to gather, systematize, and distribute atomic coordinates and other data from crystallographic studies [5]. A PDB file has a uniform format of atomic coordinates and partial bond connectivities,

as derived from crystallographic studies [5]. In addition to these, each PBD file stores the structure factors and phases of a protein [5].

3.4.2 Molecular Topology

Molecular topology is the application of the mathematical field of graph theory applied to the study of molecular structures [14]. It is also referred to as chemical graph theory [14]. In addition to graph theory, molecular topology includes molecular descriptors that identity structural properties of the molecule, such as the characteristics of the bonds, interactive properties an atom has with the other atoms in the environment, and the overall charge of the molecule [14]. A root graph specifies heteroatoms or carbons with unshared electron(s) [14]. Heteroatoms are heavy atoms that are not carbon. The existence of a homeomoprh of graph is used to determine if a graph is planar or not. The following definitions are from [14].

Definition 3.4.2.1 *Chemical Graph* *is a model of a chemical system, used to characterize the interactions among its components: atoms, bonds, groups of atoms or molecules.*

Definition 3.4.2.2 *Molecular Graph* *is a graph that represents a structural formula of a chemical compound, where the vertices are atoms and edges are the covalent bonds.*

Definition 3.4.2.3 *A hydrogen depleted molecular graph is a graph where the hydrogen atoms are not depicted.*

Definition 3.4.2.4 *A reaction graph is a graph of a transformation of a molecule, chemical reaction, where vertices are chemical species and edges are reaction pathways.*

MD interprets these graphs computationally by using the adjacency matrices of the above graphs. For additional information about graph theory see the appendices.

3.5   GROMACS

GROMACS is a parallel message-passing execution software package for MD simulations [4]. GROMACS stands for GROningen MAchine for Chemcial Simulation [4]. GROMACS is made up of a preprocessor, procedures that simulate thermodynamic equilibration, and a MD runtime that can use one or multiple processors, an optional monitor, and tools analysis operations [4]. The MD runtime is implemented within GROMACS with the GROMOS package, which stands for GROningen MOlecular Simulation, as its basis [4]. The GROMOS package is useful for simulating bio(macro)molecules in solution [4].

3.6   Process of Simulation

There are five scripts and a tutorial from [25] that allows newcomers to molecular dynamics to be able to simulate the dynamics of a folded protein. Given a PBD file and molecular topology file the first script sets up the environment of a protein for the simulation. The first script also creates the "box" or boundaries of the environment for the protein [25]. In the first script, the user get to choose the force field, based on a combination of potentials, and the solvent, which is typically either water or saline [25]. After the first script runs, the molecular topology file has an overall net charge.

If the overall net charge is not 0, then Na^+ and Cl^- atoms need to be added [25]. The second script incorporates the Na^+ and Cl^- atoms into the environment of the protein making the overall net charge 0. It is possible before the second script to make other changes to the molecular topology file like breaking bonds or changing weights of atoms. The third script puts the environment into thermodynamic equilibrium and minimizes the energy [25]. For additional information on dynamic equilibrium see the appendices. Once the environment is in thermodynamic equilibrium, the environment becomes a Newtonian system. The fourth script simulates the dynamics of a protein [25]. In the fourth script the user gets to determine time of simulation, the size of time steps, and the type of time step integration to be used. If there were no errors, the fifth script creates a PBD file [25]. The PBD file produced contains the dynamics of the protein for each time step.

3.6.1 Hamiltonian Systems

In molecular dynamics when temperature reaches equilibrium, the environment becomes a Newtonian system, which is a special type of Hamiltonian system. For a system of m particles each with 3 spatial coordinates, the configuration space is the $n = 3m$ dimensional vector space $\mathbb{R}^n$. A Hamiltonian system is itself a special type of system of differential equations defined on a $2n$ dimensional *phase space*, where the first n components $q_1, \ldots, q_n$ are the configuration space coordinates and the next $p_1, \ldots, p_n$ components are the conjugate momenta corresponding to the configure space coordinates, respectively. Let $\mathbf{q} = (q_1, \ldots, q_n)$ and $\mathbf{p} = (p_1, \ldots, p_n)$. The Hamiltonian system itself is derived from a Hamiltonian function. A Hamiltonian

function is a smooth real-valued function. A Hamiltonian function is usually denoted either H or $H(\mathbf{q}, \mathbf{p})$. The Hamiltonian equations of motion are [2, 41]

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}.$$

A dynamical system with a phase space and conservation of energy is governed by the Hamiltonian equations of motion [2]. The following definition of a phase flow comes from [2].

Definition 3.6.1.1 *The phase flow is the one-parameter group of transformations of phase space*

$$g^t : \big(q\,(0)\,, p\,(0)\big) \mapsto \big(q\,(t)\,, p\,(t)\big),$$

where $q\,(t)$ and $p\,(t)$ are solutions of Hamilton's system of equations.

A particular type of phase flow is a Hamiltonian flow. We get the following definition of a Hamiltonian flow from [2].

Definition 3.6.1.2 *Hamiltonian flows are given by a Hamiltonian $H(\mathbf{q}, \mathbf{p})$ together with the Hamilton's equations of motion with the 2D phase space coordinates $(\mathbf{q}, \mathbf{p})$ split into the configuration space coordinates and the conjugate momenta of a Hamiltonian system with D degrees of freedom:*

$$\mathbf{q} = (q_1, q_2, \ldots, q_D), \quad \mathbf{p} = (p_1, p_2, \ldots, p_D).$$

In MD, numerical trajectories are approximate solutions to systems of differential equations [7, 26, 19]. A Hamiltonian flow moves along those trajectories or across those trajectories.

Theorem 3.6.1.1 *The energy, or the value of the Hamiltonian function at the state space point $(\mathbf{q}, \mathbf{p})$, is constant along the trajectory $\big(\mathbf{q}(t), \mathbf{p}(t)\big)$. So the trajectories lie on surfaces of constant energy, or level sets of the Hamiltonian $\{(q, p) : H(q, p) = E\}$.*

Proof Let H be a Hamiltonian function at the state space point $(\mathbf{q}, \mathbf{p})$. We take the derivative of H with respect to time, t, to get

$$
\begin{aligned}
\frac{d}{dt} H\big(\mathbf{q}(t), \mathbf{p}(t)\big) &= \frac{\partial H}{\partial q_i} \frac{dq_i(t)}{dt} + \frac{\partial H}{\partial p_i} \frac{dp_i(t)}{dt} \\
&= \frac{\partial H}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial H}{\partial q_i} = 0,
\end{aligned}
$$

Since $\frac{d}{dt} H\big(\mathbf{q}(t), \mathbf{p}(t)\big) = 0$, we know H is constant with respect to time. Hence $H(\mathbf{q}, \mathbf{p}) = E$ for E some constant.■

Hamiltonian flows preserve energy along trajectories. Hamiltonian flows are a particular type of phase flow. The reason phase flows are so important to a conservative system is due to Liouville's Theorem. We get the following theorem from [2].

Theorem 3.6.1.2 *Liouville's Theorem: The phase flow preserves volume in phase space: for any region D we have*

$$
\text{volume of } g^t D = \text{ volume of } D.
$$

Before we give the proof of Liouville's Theorem, we need to know what a Jacobian matrix is. We get the following definition of a Jacobian matrix from [16, 49].

Definition 3.6.1.3 *Given $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^m$ then*

$$
\mathbf{J} = \frac{d\mathbf{f}}{dx} = \begin{bmatrix} \dfrac{\partial \mathbf{f}}{\partial x_1} \cdots \dfrac{\partial \mathbf{f}}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \dfrac{\partial f_1}{\partial x_1} & \cdots & \dfrac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial f_m}{\partial x_1} & \cdots & \dfrac{\partial f_m}{\partial x_n} \end{bmatrix}
$$

28

is defined as the Jacobian matrix of **f**, *and furthermore if* $m = n$, *then its determinant is called the Jacobian determinant.*

From [12] the Jacobian J of a Hamiltonian flow satisfies

$$\left| \det(J) \right| = 1.$$

We get the following proof of Liouville's Theorem from [12].

Proof Let C be a region in phase space and $V(0)$ its volume. Denoting the flow of the Hamiltonian system by $f^t(x)$, the volume of C after a time t is $V(t) = f^t(C)$ and using the fact that the determinant of J is equal to 1, we get

$$V(t) = \int_{f^t(C)} dx = \int_C \left| \det\left(\frac{\partial f^t(x')}{\partial x} \right) \right| dx'$$

$$= \int_C \det(J)\, dx' - \int_C dx' = V(0),$$

Hamiltonian flows preserve phase space volumes.∎

4 LIE ALGEBRAS AND LIE GROUPS

Sophus Lie created Lie algebras and Lie groups in the late 1800's [18, 30]. He was inspired to do this after hearing a lecture from Peter Ludwig Mejdell Sylow in 1863 on Galios theory [18]. In the 1900s, mathematicans G. Birkhoff, I. Sedov, and L.V. Ovsiannikov exploited Lie algebras and Lie groups in applied mathematics and physics [30]. Lie algebras and Lie groups play a crucial role in the development of methods involving symplectic integration.

4.1 Lie Algebras

In about 1880 Wilhelm Killing classified all Lie algebras up to isomorphism [18]. He found that there are 9 classes of Lie algebras A_n, B_n, C_n, D_n, E_6, E_7, E_8, F_4, and G_2 [18]. However, his proofs were incomplete, but the proofs led to the discovery of exceptional groups. Elie Cartan managed to complete those proofs [18]. Cartan's biggest contributions came in the years after Sophus Lie's death [18]. As a result of Cartan's work, Lie algebras are very important in many fields of mathematics and physics [18]. We get the following definition of a Lie algebra from [20].

Definition 4.1.0.1 *A (real) Lie Algebra is a vector space g with a product $[\cdot, \cdot]$ which satisfies*

1. $[\lambda u, v] = \lambda [u, v]$ *for all* $u, v \in g$, $\lambda \in \mathbb{R}$

2. $[u + v, w] = [u, w] + [v, w]$ *for all* $u, v, w \in g$

3. $[u, u] = 0$ *for all* $u \in g$

4. $[u, v] = -[v, u]$ *for all* $u, v \in g$

5. *(Jacobi identity) If* $u_j \in g, j = 1, 2, 3$, *then*

$$\big[u_1, [u_2, u_3]\big] + \big[u_3, [u_1, u_2]\big] + \big[u_2, [u_3, u_1]\big] = 0$$

A Lie algebra need not be associative and often is not, in which case the Jacobi identity is in place of associativity.

According to [20] two Lie algebras, $\mathfrak{g}$ and $\mathfrak{g}'$, are isomorphic over a given field, $\mathbb{F}$, if there exists a vector space isomorphism $\varphi : \mathfrak{g} \to \mathfrak{g}'$ satisfying $\varphi\big([x, y]\big) = \big[\varphi(x), \varphi(y)\big]$. The mapping φ is called an isomorphism of Lie algebras. From [20] a Lie subalgebra of $\mathfrak{g}$ is a subspace K of $\mathfrak{g}$ if $[x, y] \in K$ for all $x, y \in K$. In particular, K is a Lie algebra in its own right relative to the inherited operations. For additional information about modern algebra see the appendices.

4.1.1   Examples of Lie Algebras

In this section, we consider 3 examples of Lie Algebras. The examples illustrate the use of a Lie bracket and of the properties of a Lie algebra. A tangible example of a Lie algebra is $\mathbb{R}^3$ under the cross product operation.

Example For $\mathbb{R}^3$ let the cross product be the Lie bracket. Let's consider the vector space $\mathbb{R}^3$ with $x, y, z \in \mathbb{R}^3$. For the first property let $\lambda \in \mathbb{R}$. So,

$$[\lambda x, y] \quad = \quad \lambda x \times y.$$

We apply distributive properties of the cross product to get

$$
\begin{aligned}
[\lambda x, y] &= \lambda\,(x \times y) \\
&= \lambda\,[x, y].
\end{aligned}
$$

For the second property consider

$$
[x + y, w] = (x + y) \times w.
$$

The distributive properties of the cross product give us

$$
\begin{aligned}
[x + y, w] &= x \times w + y \times w \\
&= [x, w] + [y, w].
\end{aligned}
$$

For the third property consider

$$
[x, x] = x \times x.
$$

From properties of the cross product we get

$$
[x, x] = 0.
$$

For the fourth property consider

$$
[x, y] = x \times y.
$$

The properties of the cross product give us

$$
\begin{aligned}
[x, y] &= -\,(y \times x) \\
&= -\,[y, x].
\end{aligned}
$$

For the fifth property consider

$$
\begin{aligned}
\big[x, [y, z]\big] + \big[z, [y, x]\big] + \big[y\,[x, z]\big] \;=\;& x \times (v \times w) + v \times (w \times u) + w \times (u \times v) \\
=\;& (u \cdot w)\, v - (u \cdot v)\, w + (v \cdot u)\, w - (v \cdot w)\, u \\
& + (w \cdot v)\, u - (w \cdot u)\, v.
\end{aligned}
$$

We get the above from properties of the cross product and it gives us

$$
\big[x, [y, z]\big] + \big[z, [y, x]\big] + \big[y\,[x, z]\big] \;=\; 0.
$$

The space $\mathbb{R}^{n \times n}$ with the ring commutator as the Lie bracket satisfies the first four properties of a Lie Algebra. For elements x and y the ring commutator is defined as $[x, y] = xy - yx$. Let $A, B, C, D \in \mathbb{R}^{n \times n}$. For the first property let $\lambda \in \mathbb{R}$. So,

$$
[\lambda A, B] \;=\; \lambda A B - B \lambda A.
$$

From the distributive properties of matrices we get

$$
[\lambda A, B] \;=\; \lambda (AB) - \lambda (BA).
$$

From the distributive properties of subtraction we get

$$
\begin{aligned}
[\lambda A, B] \;=\;& \lambda (AB - BA) \\
=\;& \lambda [A, B].
\end{aligned}
$$

For the second property consider

$$
[A + B, C] \;=\; (A + B)\, C - C\, (A + B).
$$

We use the distributive properties of matrices to get

$$
[A + B, C] \;=\; AC + BC - CA - CB.
$$

From the commutative of addition of matrices we get

$$[A+B,C] = AC - CA + BC - CB$$

$$= [A,C] + [B,C].$$

For the third property consider

$$[A,A] = AA - AA$$

$$= 0.$$

For the fourth property consider

$$[A,B] = AB - BA.$$

From the distributive properties of matrices we get

$$[A,B] = -(-AB + BA).$$

From the commutative of addition of matrices we get

$$[A,B] = -(BA - AB)$$

$$= -[B,A].$$

For elements of $\mathbb{R}^{n \times n}$ we need to only check the Jacobi Identity.

Example Consider $o(3) = \text{span}\{L_1, L_2, L_3\}$ where

$$L_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}, \quad L_2 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \quad L_3 = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

We just need to show the Jacobi identity. Notice the following relations.

$$[L_2, L_3] = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} - \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix} = -L_1$$

$$[L_1, L_2] = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix} - \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} = -L_3$$

$$[L_3, L_1] = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} - \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} = -L_2.$$

Thus, we have that $[L_i, L_k] = -L_j$. Combining properties 1 and 3 we get that

$$\begin{aligned} \big[L_1, [L_2, L_3]\big] + \big[L_3, [L_1, L_2]\big] + \big[L_2, [L_3, L_1]\big] &= 0 + 0 + 0 \\ &= 0. \end{aligned}$$

We note that the Lie algebras $\mathbb{R}^3$ under cross product and $o(3)$ are isomorphic.

Example Consider $su(2) = \text{span}\{E_1, E_2, E_3\}$ where $E_j = \frac{-i\sigma_j}{2}$ and

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

We just need to show the Jacobi identity. So,

$$\big[E_1, [E_2, E_3]\big] + \big[E_3, [E_1, E_2]\big] + \big[E_2, [E_3, E_1]\big] \;=\; \left[\frac{-i\sigma_1}{2}, \left[\frac{-i\sigma_2}{2}, \frac{-i\sigma_3}{2}\right]\right]$$

$$+ \left[\frac{-i\sigma_3}{2}, \left[\frac{-i\sigma_1}{2}, \frac{-i\sigma_2}{2}\right]\right]$$

$$+ \left[\frac{-i\sigma_2}{2}, \left[\frac{-i\sigma_3}{2}, \frac{-i\sigma_1}{2}\right]\right].$$

Applying the first property, which we proved for all n by n real matrix spaces, we get

$$\frac{1}{2}\left(\big[\sigma_1, [\sigma_2, \sigma_3]\big] + \big[\sigma_3, [\sigma_1, \sigma_2]\big] + \big[\sigma_2, [\sigma_3, \sigma_1]\big]\right).$$

Thus, we just need to show the Jacobi identity holds for

$$\big[\sigma_1, [\sigma_2, \sigma_3]\big] + \big[\sigma_3, [\sigma_1, \sigma_2]\big] + \big[\sigma_2, [\sigma_3, \sigma_1]\big].$$

Notice the following relations

$$[\sigma_2, \sigma_3] = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 2i \\ 2i & 0 \end{bmatrix} = 2i\sigma_1$$

$$[\sigma_1, \sigma_2] = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} - \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 2i & 0 \\ 0 & -2i \end{bmatrix} = 2i\sigma_3$$

$$[\sigma_3, \sigma_1] = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} - \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 2 \\ -2 & 0 \end{bmatrix} = 2i\sigma_2.$$

36

Thus, we have that $\left[\sigma_i, \sigma_j\right] = 2i\sigma_k$. Applying the first and third properties, which we proved for all n by n real matrix spaces, we get

$$
\begin{aligned}
\left[\sigma_1, \left[\sigma_2, \sigma_3\right]\right] + \left[\sigma_3, \left[\sigma_1, \sigma_2\right]\right] + \left[\sigma_2, \left[\sigma_3, \sigma_1\right]\right] &= 0 + 0 + 0 \\
&= 0.
\end{aligned}
$$

4.1.2   Vector Fields

Lie algebras are vector fields [20]. We get the following definition of a vector field from [15, 40].

Definition 4.1.2.1 *A vector field* **v** *may be identified with a linear partial differential operator of the form*

$$
\mathbf{v} = \sum_{i=1}^{n} v_i \frac{\partial}{\partial x_i}.
$$

Here $(x_1, \ldots, x_n)$ *are local coordinates on a manifold* M. *Each coefficient* v_i *is a smooth function on* M.

If V is a vector space, then a V-vector field on a manifold assigns a vector in V to each point on the manifold. Each point of the manifold is a vector space [40, 15]. We get the following theorem from [15, 40].

Definition 4.1.2.2 *If* z *is a smooth function on* M, *then the directional derivative of* z *along the vector* **v** *is*

$$
dz = \mathbf{v} \cdot z = \sum_{i=1}^{n} v_i \frac{\partial z}{\partial x_i}.
$$

The directional derivative of z along the vector field **v** is the differential operator **v** acting on z [15, 40]. Vector fields and systems of ordinary differential equations are related to each other [15, 40].

4.2 Lie Groups

According to [30] Sophus Lie created symmetry analysis of differential equations. His theory makes it possible to derive solutions to differential equations algorithmically [30]. In order to do this he created Lie groups. The following definition of a Lie group comes from [45].

Definition 4.2.0.1 *Let G be a topological group. Suppose there is an analytic structure on the set G, compatible with its topology, which converts it into an analytic manifold and for which the maps*

$$\begin{cases} (x, y) \mapsto xy & (x, y \in G) \\ \\ x \mapsto x^{-1} & (x \in G) \end{cases}$$

of $G \times G$ into G and of G into G, respectively, are both analytic. Then G together with this analytic structure, is called a Lie group.

In order to show how Lie groups allow a symmetry analysis of differential equations, we need a few definitions and theorems [30].

Definition 4.2.0.2 *Groups of transformations:* *Let us consider a domain $D \subseteq \mathbb{R}^N$ and a subset $S \subseteq \mathbb{R}$. The set of transformations*

$$z^* = Z(z; a), \quad Z : D \times S \to D$$

depending on the parameter a, forms a one-parameter group of transformations on D if:

1. *For each value of the parameter $a \in S$ the transformations are one-to-one from D onto D;*

2. *S with the law of composition μ is a group with identity e;*

3. *$Z(z; e) = z$, $\forall z \in D$;*

4. *$Z\big(Z(z; a); b\big) = Z\big(z; \mu(a, b)\big)$, $\forall z \in D$, $\forall a, b \in S$.*

Definition 4.2.0.3 ***Lie group of transformations:*** *The group of transformations defines a one-parameter Lie group of transformations if in addition to satisfying the axioms of the previous definition:*

1. *a is a continuous parameter, i.e., S is an interval in R;*

2. *Z is C^{∞} with respect to z in D and an analytic function of a in S.*

3. *$\mu(a, b)$ is an analytic function of a and b, $\forall a, b \in S$.*

Theorem 4.2.0.1 ***First Fundamental Theorem of Lie:*** *Solutions of the initial value problem for the system of first order differential equations*

$$\frac{dz^{*}}{da} = \zeta(z^{*}), \quad z^{*}(0) = z.$$

defines a 1 parameter Lie group of transformations.

Just like Sophus Lie, the Lie groups we are most concerned with are those involving differential equations. In general the Lie group of a differential equation or the system of differential equations, is the group that contains all mappings that map from solutions to solutions [8, 29, 30].

The tangent space to the identity of a Lie group is a Lie algebra [3, 52]. The elements of a Lie algebra are the generators for a Lie group. The elements of a Lie subalgebra are also generators for a Lie group. The Lie group generated by the elements of the Lie subalgebra is a subgroup of the Lie group generated the elements of the Lie algebra. In a section below, we will introduce the Baker-Campbell-Hausdorff formula. It is used to compose the solved parts of differential equations. Since the Baker-Campbell-Hausdorff formula is not well understand methods are used to take advantage of it. In this thesis a particular type of Verlet method, Strang method, is used.

4.2.1 Examples of Lie Groups

A particular type of Lie group that is useful in physics is the matrix Lie group, which can be defined using the general linear group, $GL\,(n;\mathbb{R})$ [52]. The following definitions come from [52].

Definition 4.2.1.1 *The general linear group over the real numbers, denoted by $GL\,(n;\mathbb{R})$ is the group of all $n \times n$ invertible matrices with real number entries. We can similarly define it over the complex numbers, $\mathbb{C}$ denoted by $GL\,(n;\mathbb{C})$.*

Definition 4.2.1.2 *A matrix Lie group is any subgroup H of $GL\,(n;\mathbb{C})$ with the following property: if A_n is any sequence of matrices in H, and A_n converges to some matrix A, then either $A \in H$, or A is not invertible. The condition on H amounts to saying that H is a closed subset of $GL\,(n;\mathbb{C})$. Thus, one can think of a matrix Lie group as simply a closed subgroup of $GL\,(n;\mathbb{C})$.*

Thus, the general linear groups are matrix Lie Groups as $GL(n; \mathbb{R})$ is a non-proper subgroup of itself. From [52] the special linear groups, $SL(n; \mathbb{R})$, are the groups of $n \times n$ invertible matrices having determinant 1. According to [52] special linear groups are an example of a matrix Lie group. From [52] the special orthogonal group, $SO(n)$, and the special unitary group, $SU(n)$, are examples of matrix Lie groups. According to [52] the solution space of a differential equation with dimension n and rotational symmetry, can be represented by $SO(n)$. For additional information about complex analysis see the appendices.

4.2.2   Baker-Campbell-Hausdorff

The splitting method for differential equations can be thought of as a two step process [6]. The first step is choosing the functions, f_i, for a differential equation, $\frac{dx}{dt} = f(x)$, such that [6]

$$f = \sum_{i=1}^{n} f_i.$$

The second step is solving either exactly or approximately each equation [6]

$$\frac{dx}{dt} = f_i(x).$$

The composition is composing the 1 parameter Lie groups of those solutions to construct an approximate solution of f [6].

The composition methods used for symplectic integration are constructed to take advantage of the Baker-Campbell-Hausdorff formula, (BCH). We need some additional information before getting to the BCH. We need to know about an exponential map, which connects a Lie algebra, $\mathfrak{g}$, to a Lie group, G. The homomorphism

$\varphi_X : \mathbb{R} \to G$ is called the one-parameter subgroup associated to $X \in \mathfrak{g}$. We get the following definition of an exponential map from [45, 13, 31].

Definition 4.2.2.1 *The exponential map, $\exp : \mathfrak{g} \to G$, is defined by $\exp(X) = \varphi_X(1)$.*

The BCH formula takes two elements of a Lie algebra and combines the exponential mappings of each element. The combining of the exponential mappings equals an exponential mapping of another element of the same Lie algebra. We get the following formula from [13, 31, 45].

Theorem 4.2.2.1 *Baker-Campbell-Hausdorff: Let $A, B, C \in \mathfrak{g}$. The BCH formula is*

$$\exp_A \exp_B = \exp_C$$

where

$$C = A + B + \frac{1}{2}[A, B] + \frac{1}{12}\left([A, [A, B]] - [B, [A, B]]\right) + \cdots.$$

There are a few types of composition methods designed to algebraically eliminate terms from BCH. The Verlet methods are a particular class of these methods. For this thesis we will be using a type of Verlet method called the Strang method. The Strang method is

$$x(t + dt) = \exp_A\left(\frac{dt}{2}\right)\exp_B(dt)\exp_A\left(\frac{dt}{2}\right)x(t).$$

4.2.3 Example of Splitting and Composition

For an illustration of how splitting and composition works, we will work with a simple nonlinear ordinary differential equation.

Example Consider the following nonlinear ordinary differential equation.

$$\frac{dx}{dt} = x + x^2. \tag{1}$$

First we will solve (1) the traditional way first by doing separation of variables.

$$\frac{dx}{x(1+x)} = dt.$$

From this point forward we will solve it using an integration factor. This is a very algorithmic process. First we algebraically rearrange the left side of our equation to get

$$\left(\frac{1}{x} - \frac{1}{1+x}\right) dx = dt.$$

Next, we integrate both sides and get

$$\ln(x) - (1+x) = t + c.$$

We apply a logarithmic property to get

$$\ln\left(\frac{x}{1+x}\right) = t + c.$$

After taking the exponential function of both sides we get

$$\frac{x}{1+x} = e^c e^t.$$

Let D represent the constant e^c. We substitute D into the equation and we get

$$\frac{x}{1+x} = De^t.$$

We solve for x to get

$$x = De^t(1+x)$$

$$\left(1 - De^t\right)x = De^t$$

$$x = \frac{De^t}{1 - De^t}.$$

43

To make a simplification for us we multiple the numerator and deminotar by $\frac{1}{D}$ to get

$$x = \frac{e^t}{\frac{1}{D} - e^t}.$$

Let K represent the constant $\frac{1}{D} = e^{-c}$. Substituting K into the equation gives us

$$x(t) = \frac{e^t}{K - e^t}.$$

We want to $x(t) = x_0$ when $t = 0$. So, first we calculate $x(t)$ when $t = 0$ to get

$$x(0) = \frac{1}{K - 1}.$$

Since we want $x(0) = x_0$ we get that

$$K - 1 = \frac{1}{x_0}.$$

We solve for K to get

$$K = 1 + \frac{1}{x_0}.$$

We plug in what K is equal to into the equation gives us

$$x(t) = \frac{e^t}{1 + \frac{1}{x_0} - e^t}$$
$$= \frac{x_0 e^t}{x_0 + 1 - x_0 e^t}.$$

This gives us a 1 parameter group, or flow, where for $t = 0$ we recovery our initial condition of $x(0) = x_0$.

Thus we have solved (1) using traditional techniques, where $x(0) = x_0$. Now we are going to illustrate splitting and composition. Let $A(x) = x$ and $B(x) = x^2$,

44

where A and B are vector fields. First we solve

$$\frac{dx}{dt} = A(x).$$

After putting in what A is equal to gives us

$$\frac{dx}{dt} = x.$$

We integrate both sides giving us the solution of A to be

$$x = e^t x_0.$$

Second we solve

$$\frac{dx}{dt} = B(x).$$

We substitute what B is equal to into the equation we get

$$\frac{dx}{dt} = x^2.$$

Doing a separation of variables on the equation results in

$$x^{-2} dx = dt.$$

We integrate both sides to get

$$-x^{-1} = t + c.$$

We solve for x to give us

$$\frac{1}{x} = -t - c$$

$$x = \frac{x_0}{1 - x_0 t}.$$

From here we use a composition method to solve the original equation. Let $G(t) = e^t x_0$ and $H(t) = \frac{x_0}{1 - x_0 t}$. Then

$$G(t) H\big(G(t)\big) = \frac{x_0 e^t}{x_0 + 1 - x_0 e^t}.$$

As we can see solving (1) using symplectic integration gives us the same answer as solving (1) the traditional way.

5 SYMPLECTIC INTEGRATION

According to [9] the best techniques for studying Hamiltonian dynamical systems,
are those that take advantage of the flow being symplectic. From [9] symplectic means
the motion of the phase-space points from time 0 to time t preserves the geometric
structure. We get the following definition of a symplectic transformation from [9].

Definition 5.0.0.1 *A symplectic transformation is one that satisfies*

$$f'^{T}\left(q,p\right)J\ \ f'\left(q,p\right)=J$$

*where f' is the Jacobian matrix of derivatives of the flow, $f\left(q,p\right)$, of phase space, q
and p are vectors of canonically conjugate coordinates, and J is the matrix*

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

with I the identity matrix.

A symplectic integration algorithm, (SIA), works with a Hamiltonian function,
H, preserving the geometric structure of a Hamiltonian system. The first step is
splitting H into easy to solve parts. If H cannot be split into easier to solve parts,
then new coordinates are substituted into H for the original coordinates. The new
coordinates have some sort of relation with the original coordinates that get rid of
certain complications in H.

Once H is split into parts, the equivalences given by the Hamiltonian flow trans-
form the parts into linear vector fields. Then each part is solved as a system of
differential equations. Next, we compose the solutions together. Now a geometric
preserving solution has been calculated.

5.1   Splitting of a Simple Hamiltonian System

Let $H(x,p) = \frac{1}{2}\left(x^2 + p^2\right) - x$ be our overall Hamiltonian. The split will be

$$A(x,p) = \frac{1}{2}\left(x^2 + p^2\right), \quad B(x,p) = -x.$$

To solve the full model with Hamiltonian H, we suppose $x(0) = u$, $p(0) = v$ and note that the Hamiltonian system is

$$\frac{dx}{dt} = p \quad \frac{dp}{dt} = -x + 1.$$

The solution is

$$x(t) = A\cos(t) + B\sin(t) + 1$$

and $x(0) = A + 1 = u$, so $A = u - 1$ or

$$x(t) = (u-1)\cos(t) + v\sin(t) + 1,$$

and

$$p(t) = -(u-1)\sin(t) + v\cos(t).$$

We use a projective representation to allow this in matrix form as

$$\begin{bmatrix} x(t) \\ p(t) \\ 1 \end{bmatrix} = \begin{bmatrix} \cos(t) & \sin(t) & 1 \\ -\sin(t) & \cos(t) & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u - 1 \\ v \\ 1 \end{bmatrix}.$$

Continuing projectively, we see that

$$\begin{bmatrix} x(t) \\ p(t) \\ 1 \end{bmatrix} = \begin{bmatrix} \cos(t) & \sin(t) & 1 \\ -\sin(t) & \cos(t) & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u \\ v \\ 1 \end{bmatrix}.$$

With $\mathbf{z}(t) = [x(t), p(t)]^T$, rotation matrix

$$R(t) = \begin{bmatrix} \cos(t) & \sin(t) \\ -\sin(t) & \cos(t) \end{bmatrix}$$

and $\mathbf{0}$, $\delta_1 = [1, 0]^T \in \mathbb{R}^2$, the solution is written in block form as

$$\begin{bmatrix} \mathbf{z}(t) \\ 1 \end{bmatrix} = \begin{bmatrix} R(t) & \delta_1 \\ \mathbf{0}^T & 1 \end{bmatrix} \begin{bmatrix} I & -\delta_1 \\ \mathbf{0}^T & 1 \end{bmatrix} \begin{bmatrix} \mathbf{z}(0) \\ 1 \end{bmatrix}$$

$$= \begin{bmatrix} R(t) & -R(t)\delta_1 + \delta_1 \\ \mathbf{0}^T & 1 \end{bmatrix} \begin{bmatrix} \mathbf{z}(0) \\ 1 \end{bmatrix}$$

$$= \begin{bmatrix} R(t) & (I - R(t))\delta_1 \\ \mathbf{0}^T & 1 \end{bmatrix} \begin{bmatrix} \mathbf{z}(0) \\ 1 \end{bmatrix}.$$

Thus, the phase space flow for the overall problem is

$$\exp_H(t) = \begin{bmatrix} R(t) & (I - R(t))\delta_1 \\ \mathbf{0}^T & 1 \end{bmatrix}.$$

The first split $A(x, p) = \frac{1}{2}(x^2 + p^2)$ leads to the harmonic oscillator $\ddot{x} + x = 0$,

whose solution (projectively) is

$$\begin{bmatrix} x(t) \\ p(t) \\ 1 \end{bmatrix} = \begin{bmatrix} \cos(t) & \sin(t) & 0 \\ -\sin(t) & \cos(t) & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u \\ v \\ 1 \end{bmatrix}$$

and in block form implies the 1 parameter flow

$$\exp_A(t) = \begin{bmatrix} R(t) & \mathbf{0} \\ \mathbf{0}^T & 1 \end{bmatrix}.$$

The second split $B(x, p) = -x$ leads to

$$\frac{dx}{dt} = 0, \quad \frac{dp}{dt} = 1$$

or $x(t) = u$, $p(t) = t + v$. Projectively, this is

$$\begin{bmatrix} x(t) \\ p(t) \\ 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & t \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u \\ v \\ 1 \end{bmatrix}$$

whose flow in block form is

$$\exp_B(t) = \begin{bmatrix} I & t\delta_2 \\ \mathbf{0}^T & 1 \end{bmatrix}$$

where $\delta_2 = [0, 1]^T$.

The reason this is a good sandbox for studying discretization error is that $\exp_A(t)$, $\exp_B(t)$, and $\exp_H(t) = \exp_{A+B}(t)$ are all subgroups of the 3 parameter group

$$G(\theta, \alpha, \beta) = \begin{bmatrix} \cos(\theta) & \sin(\theta) & \alpha \\ -\sin(\theta) & \cos(\theta) & \beta \\ 0 & 0 & 1 \end{bmatrix}.$$

If we let $\mathbf{t} = [\alpha, \beta]^T$, then in block form this is

$$G(\theta, \mathbf{t}) = \begin{bmatrix} R(\theta) & \mathbf{t} \\ \mathbf{0}^T & 1 \end{bmatrix}.$$

Notice that

$$G(0, \mathbf{t}) = \begin{bmatrix} I & t \\ \mathbf{0}^T & 1 \end{bmatrix}$$

and correspondingly,

$$G(0, \mathbf{s})\, G(0, \mathbf{t}) = \begin{bmatrix} R(\theta) & \mathbf{t} \\ \mathbf{0}^T & 1 \end{bmatrix} \begin{bmatrix} R(\theta) & \mathbf{t} \\ \mathbf{0}^T & 1 \end{bmatrix} = \begin{bmatrix} R(\theta) & \mathbf{s}+\mathbf{t} \\ \mathbf{0}^T & 1 \end{bmatrix} = G(0, \mathbf{s}+\mathbf{t}).$$

However, this sandbox is only useful for developing approaches to discretization error in linear Hamiltonian systems. Molecular dynamics is based on highly non-linear Hamiltonian systems with a varitey of potentials. Thus, we ultimately need a sandbox with exact solutions and group-theoretic properties similar to those here but for nonlinear systems similar to the n-body types of systems found in molecular dynamics.

5.2   Hill's Lunar Equation

The Hill's Lunar Equations are [46]

$$\ddot{x} - 2\dot{y} - 3x + xr^{-3} \ = \ 0 \tag{2}$$

$$\ddot{y} + 2\dot{x} + yr^{-3} \ = \ 0 \tag{3}$$

where x is the position coordinate, y is the momentum coordinate, dots denote derivative with respect to time, and $r = \sqrt{x^2 + y^2}$. From (2) and (3) we know the Jacobi integral exists and equals [46]

$$\frac{1}{2}\left(\dot{x}^2 + \dot{y}^2\right) - \frac{3}{2}x^2 - \frac{1}{r} = h. \tag{4}$$

Where h is the Jacobi constant. We are going to do a Levi-Civita regularization, which is a three step process [47]. The first step is to introduce a time substitute value τ according to the differential relation [46]

$$dt = \frac{r}{c} \cdot d\tau, \quad r = |x|.$$

The second step is to do a conformal squaring [47]. The third and final step is to fix the energy [47]. After doing a Levi-Civita's regularization procedure for removing the collision singularity at $x = y = 0$ and using the following coordinates and conjugated momenta

$$q_1 = x, \ q_2 = y, \ p_1 = \dot{q}_1 - q_2, \ p_2 = \dot{q}_2 + q_1,$$

we start to expand upon (4) in order to make it equivalent to the constant energy in a Hamiltonian system [46]. In order to do this we need to first add terms to the right side of the equation where terms cancel each other out. This process is similar

51

to completing the square, except the terms we are adding are being done to express the original coordinates of (3) in terms of the new coordinates that correspond to the Hamilton equation that represents the Hill's Lunar equations. Again the Jacobi integral is

$$h = \frac{1}{2}\left(\dot{x}^2 + \dot{y}^2\right) - \frac{3}{2}x^2 - \frac{1}{r}$$

$$= \frac{1}{2}\dot{x}\dot{x} + \frac{y^2}{2} + \frac{1}{2}\dot{y}\dot{y} + \frac{x^2}{2} - y^2$$

$$-x^2 - x^2 + \frac{1}{2}y^2 - \frac{1}{r}$$

$$= \frac{1}{2}\dot{x}\dot{x} - \dot{x}y + \frac{y^2}{2} + \frac{1}{2}\dot{y}\dot{y} + \dot{y}x + \frac{x^2}{2}$$

$$+\dot{x}y - y^2 - \dot{y}x - x^2 - x^2 + \frac{1}{2}y^2 - \frac{1}{r}.$$

With (4) expanded we start pairing like terms

$$h = \frac{1}{2}\left(\dot{x}\dot{x} - 2\dot{x}y + y^2 + \dot{y}\dot{y} + 2\dot{y}x + x^2\right)$$

$$+\dot{x}y - y^2 - \dot{y}x - x^2 - x^2 + \frac{1}{2}y^2 - \frac{1}{r}.$$

We group the original coordinates by means of factoring

$$h = \frac{1}{2}\left(\left(\dot{x} - y\right)^2 + \left(\dot{y} + x\right)^2\right) + \left(\dot{x} - y\right)y$$

$$-\left(\dot{y} + x\right)x - x^2 + \frac{1}{2}y^2 - \frac{1}{r}.$$

52

We substitute in the new coordinates to get

$$h = \frac{1}{2}\left(\left(\dot{q}_1 - q_2\right)^2 + \left(\dot{q}_2 + q_1\right)^2\right) + \left(\dot{q}_1 - q_2\right)q_2$$

$$- \left(\dot{q}_2 + q_1\right)q_1 - q_1^2 + \frac{1}{2}q_2^2 - \frac{1}{r}$$

and we put in the equivalence from above, to get a Hamiltonian that represents (2) and (3). The Hamiltonian is [46]

$$H\left(q,p\right) = \frac{1}{2}\|\mathbf{p}\|^2 + p_1 q_2 - p_2 q_1 - q_1^2 + \frac{1}{2}q_2^2 - \frac{1}{r}, \tag{5}$$

where $r = \|\mathbf{q}\|$, $\mathbf{p}$ is the momentum vector, and $\mathbf{q}$ is the position vector. What we want to do from here is make some kind of substitution that gets rid of the $\frac{1}{r}$ in (5) and thus making the linear vector fields produced during the symplectic integration easier to solve. Before we get to the substitution we must notice that during the first step of the Levi-Civita's regularization procedure a new independent variable, s, is introduced for the time variable, t [46]. The relation between s and t is [46]

$$dt = r\, ds$$

This relation also gives us a new Hamiltonian, K, based upon H and h. The new Hamiltonian is [46]

$$K = r\left(H - h\right).$$

The type of substitution we get from [46] on H is consistent with H's symplectic transformation. The substitution introduces two new vectors $\mathbf{u}$ and $\mathbf{v}$ with coordinates u_1, u_2, v_1, and v_2 with respect to the corresponding vectors and uses a complex

notation. The canonical transformation of the original coordinates are [46]

$$q_1 + iq_2 = (u_1 + iu_2)^2$$
$$= u_1^2 - u_2^2 + i2u_1u_2,$$

and

$$p_1 + ip_2 = \frac{v_1 + iv_2}{2(u_1 - iu_2)}.$$

Applying the reflection property to the above equations gives us

$$q_1 - iq_2 = (u_1 - iu_2)^2,$$

and

$$p_1 - ip_2 = \frac{v_1 - v_2}{2(u_1 + iu_2)}.$$

Now we use a property of complex numbers that says if two complex numbers are equal then their corresponding real and imaginary parts must also be equal. Using this knowledge we get that

$$q_1 = u_1^2 - u_2^2,$$

and

$$q_2 = 2u_1u_2.$$

From here we are going to apply the modulus, or absolute value, to $q_1 + iq_2$ to find what p_1 and p_2 must equal. After we apply the modulus we get the result below:

$$|q_1 + iq_2| = q_1^2 + q_2^2 = \left(u_1^2 + u_2^2\right)^2 = |u_1 + iu_2|^4$$

54

After applying the modulus again we get that

$$|u_1 + iu_2|^4 = u_1^2 + u_2^2 = \left\| q_1^2 + q_2^2 \right\| = r$$

Now, we have that q_1 and q_2 are expressed in terms of the new coordinates u_1 and u_2. In order to figure out what p_1 and p_2 are equal to, we need to simplify $p_1 + ip_2$. We cannot divide by complex numbers, so, we multiply the numerator and denominator by the conjugate of the denominator. As seen below this allows us to separate the fraction into real and imaginary parts:

$$p_1 + ip_2 = \frac{(v_1 + iv_2)(u_1 + iu_2)}{2\left(u_1^2 + u_2^2\right)} = \frac{(v_1 u_1 - v_2 u_2) + i(v_1 u_2 + v_2 u_1)}{2\left(u_1^2 + u_2^2\right)}.$$

At this point we can apply the same property we did in order to find q_1 and q_2 to get that:

$$p_1 = \frac{v_1 u_1 - v_2 u_2}{2\left(u_1^2 + u_2^2\right)}$$

and

$$p_2 = \frac{v_1 u_2 + v_2 u_1}{2\left(u_1^2 + u_2^2\right)}.$$

With the coordinates of H represented by v_1, v_2, u_1, and u_2, we start to transforming parts of H. First let us look at

$$\frac{1}{2}\left(p_1^2 + p_2\right) = \frac{1}{2}\left((p_1 - ip_2)(p_1 + ip_2)\right).$$

After substitution we get

$$\frac{1}{2}\left(p_1^2 + p_2\right) = \frac{1}{2}\left(\frac{v_1 - v_2}{2(u_1 + iu_2)} \frac{v_1 + v_2}{2(u_1 - iu_2)}\right).$$

We multiply everything out to give us

$$\frac{1}{2}\left(p_1^2 + p_2\right) = \frac{v_1^2 + v_2^2}{4\left(u_1^2 + u_2^2\right)}.$$

Next, we look at

$$p_1 q_2 - p_2 q_1 = \text{Im}\left((p_1 + ip_2)(q_1 - iq_2)\right).$$

We substitute $p_1 - ip_2$ and $q_1 + iq_2$ to get

$$p_1 q_2 - p_2 q_1 = \text{Im}\left(\frac{v_1 + v_2}{2\left(u_1 - iu_2\right)}(u_1 - u_2)^2\right).$$

We proceed by cancelling and multiplying everything out to get

$$p_1 q_2 - p_2 q_1 = \frac{1}{2}\text{Im}\left((v_1 + iv_2)(u_1 - iu_2)\right)$$

$$= \frac{1}{2}\text{Im}\left(v_1 u_1 + v_2 u_2 + i\left(u_1 v_2 - u_2 v_1\right)\right).$$

We take the imaginary part to get

$$p_1 q_2 - p_2 q_1 = \frac{1}{2}\left(u_1 v_2 - u_2 v_1\right).$$

The next term we look at is

$$-q_1^2 + \frac{1}{2}q_2^2 = -\left(u_1^2 - u_2^2\right)^2 + \frac{1}{2}\left(2u_1 u_2\right)^2.$$

After substituting what q_1 and q_2 are equal to. We multiply everything out to get

$$-q_1^2 + \frac{1}{2}q_2^2 = -u_1^4 + 2u_1^2 u_2^2 - u_2^4 + 2u_1^2 u_2^2$$

$$= -u_1^4 + 4u_1^2 u_2^2 - u_2^4.$$

We have transformed the individual parts of H to get

$$H = \frac{v_1^2 + v_2^2}{4\left(u_1^2 + u_2^2\right)} + \frac{1}{2}\left(v_1 u_2 - v_2 u_1\right) - u_1^4 + 4u_1^2 u_2^2 - u_2^4 - \frac{1}{u_1^2 + u_2^2}.$$

We substitute this in K to get

$$K = \left(u_1^2 + u_2^2\right)\left(\frac{v_1^2 + v_2^2}{4\left(u_1^2 + u_2^2\right)} + \frac{1}{2}\left(v_1 u_2 - v_2 u_1\right) - u_1^4 + 4u_1^2 u_2^2 - u_2^4 - \frac{1}{u_1^2 + u_2^2} - h\right).$$

After mulitply everyting out and reducing we get [46]

$$
\begin{aligned}
K\left(u, v\right) = {} & \frac{1}{8}\left(v_1^2 + v_2^2\right) + \frac{1}{2}\left(u_1^2 + u_2^2\right)\left(v_1 u_2 - v_2 u_1\right) - \left(u_1^2 + u_2^2\right)h - 1 \\
& + \left(u_1^2 + u_2^2\right)\left(-u_1^4 + 4u_1^2 u_2^2 - u_2^4\right).
\end{aligned}
$$

We split $K\left(u, v\right)$ into mixed and non-mixed terms equations $K_1\left(u, v\right)$ and $K_2\left(u\right)$ such that $K\left(u, v\right) = K_1\left(u, v\right) + K_2\left(u\right)$ [46].

$$K_1\left(u, v\right) = \frac{1}{8}\left(v_1^2 + v_2^2\right) - \left(u_1^2 + u_2^2\right)^2\left(\frac{1}{2}\left(u_1 v_2 - u_2 v_1\right) + h\right) - 1,$$

and

$$K_2\left(u\right) = \left(u_1^2 + u_2^2\right)\left(-u_1^4 + 4u_1^2 u_2^2 - u_2^4\right).$$

A substitution we made for the q_i and p_i coordinates for the Hamilitonian for Hill's Lunar equations are as follows:

$$q_i = \frac{u_i}{\|\mathbf{u}\|}$$

$$p_i = v_i\|\mathbf{u}\|.$$

Just like above we introduce new coordinates u_i and v_i and plugging those into H we

57

get

$$K(u,v) = \frac{1}{2}\left(\left(v_1^2 + v_2^2\right)\left(u_1^2 + u_2^2\right)\right) + v_1 u_2 + v_2 u_1 + \frac{\frac{1}{2}u_2^2 - u_1^2}{\|\mathbf{u}\|^2} + 1$$

$$= \frac{1}{2}\left(\left(v_1^2 + v_2^2\right)\left(u_1^2 + u_2^2\right)\right) + v_1 u_2 + v_2 u_1 + \frac{\frac{1}{2}u_2^2 - u_1^2 + \frac{1}{2}u_1^2 - \frac{1}{2}u_1^2}{\|\mathbf{u}\|^2} + 1$$

$$= \frac{1}{2}\left(\left(v_1^2 + v_2^2\right)\left(u_1^2 + u_2^2\right)\right) + v_1 u_2 + v_2 u_1 + \frac{1}{2} + \frac{-\frac{3}{2}u_1^2}{\|\mathbf{u}\|^2} + 1$$

$$= \frac{1}{2}\left(\left(v_1^2 + v_2^2\right)\left(u_1^2 + u_2^2\right)\right) + v_1 u_2 + v_2 u_1 - \frac{3}{2}\frac{u_1^2}{\|\mathbf{u}\|^2} + \frac{3}{2}.$$

Now, if we let $\mathbf{u}$ be an unit vector, or $\|\mathbf{u}\| = 1$, we get rid of the $\frac{1}{r}$ dilemma from earlier as desired and get:

$$K(u,v) = \frac{1}{2}\left(\left(v_1^2 + v_2^2\right)\left(u_1^2 + u_2^2\right)\right) + v_1 u_2 + v_2 u_1 - \frac{3}{2}u_1^2 + \frac{3}{2}.$$

This works really well for us because we get rid of the $\frac{1}{r}$ term and we can split the Hamiltonian into mixed terms and non-mixed terms. Specifically we make a split of

$$A = \frac{1}{2}\left(\left(v_1^2 + v_2^2\right)\left(u_1^2 + u_2^2\right)\right) + v_1 u_2 + v_2 u_1$$

$$B = -\frac{3}{2}u_1^2 + \frac{3}{2}.$$

6   RESULTS

Our hypothesis is that when solving systems with geometric properties, like a Hamiltonian system, it is better to use a method involving symplectic integration as opposed to Taylor polynomial based approaches when attempting to manage discretization error. We base this hypothesis on the fact that symplectic integration algorithms preserve geometric properties of conservative dynamical systems. For example over time, discretization error in solutions using Taylor polynomial based approaches grow to the point the numerical simulation is no longer valid. Whereas with symplectic integration, because it takes advantage of the geometric bound of constant energy in a Hamiltonian system, discretization error is far more manageable over longer periods of time.

In Section 5.1, we obtained the exact solution to the Hamiltonian system with Hamiltonian

$$H = \frac{1}{2}\left(x^2 + p^2\right) - x.$$

We compare the exact solution to the approximated solutions from symplectic integration, Euler, and Rung-Kutt methods. For the symplectic integration method we use a Strang method. We do $11,000$ cases of different initials values. Our initial values for x are 2, 10, 20, 30, 40, 50, 60, 70, 80, 90, and 100. Our initial values for p are $1,000$ evenly space numbers from 1 to 100. We combine each initial value of x with every initial value of p. We do 500 time steps with each method with the step equal to 0.1. We take the last 100 H values of each method and take the absolute difference between those values and the exact values. The difference in the values is

the error each method has for a given time step. Then we take the ℓ^2 norm of the error values and compare methods to each other in plots. The plots consist of one initial x value with every initial p value.

In Figure 1 we see the initial value of x being 2 with every initial value of p. We see that both the Strang and Runge-Kutta methods are far more accurate than the Euler method. We can see that the Strang and Runge-Kutta methods are comparable in accuracy to each other, but Runge-Kutta is more accurate at first. Even though the Runge-Kutta method is more accurate than the Strang method at first, the Runge-Kutta method has stability issues. Looking through the figures $1 - 11$ we see this trend continue. In those figures we see the Strang method is stable far longer than the Runge-Kutta method. When the Runge-Kutta method starts to become unstable its error grows exponentially. It is instability similar to that which causes blow-up errors in molecular dynamics. When a method becomes unstable in its error values, it is no longer a Hamiltonian system.

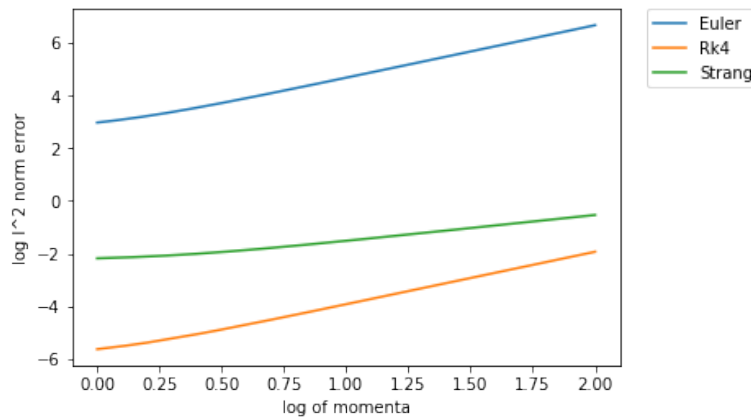Figure 1: $x = 2$
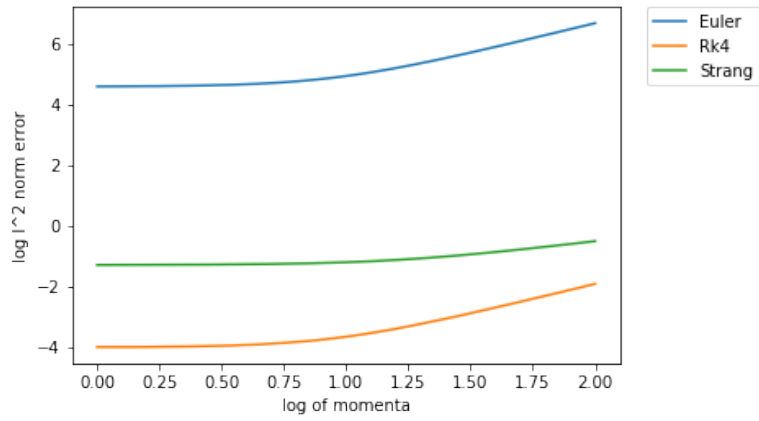
Figure 2: $x = 10$
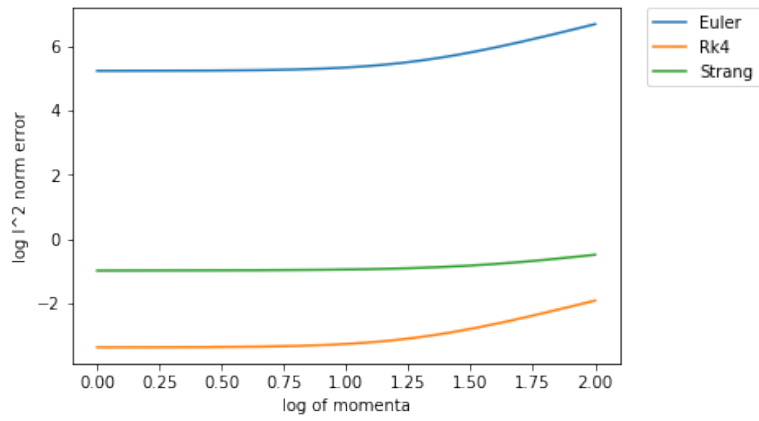

Figure 3: $x = 20$
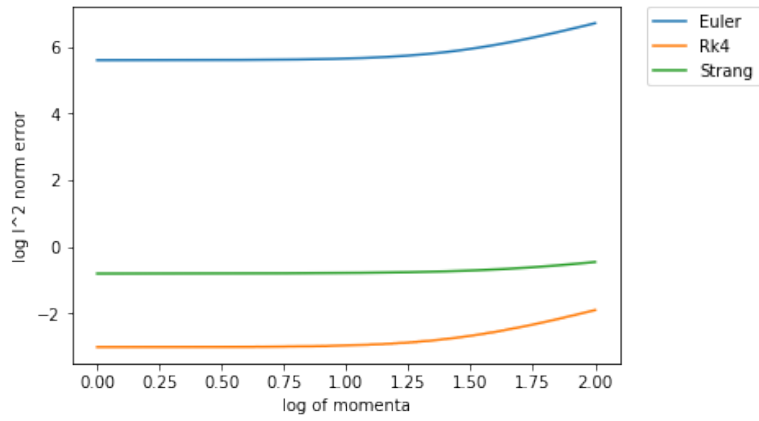
Figure 4: $x = 30$
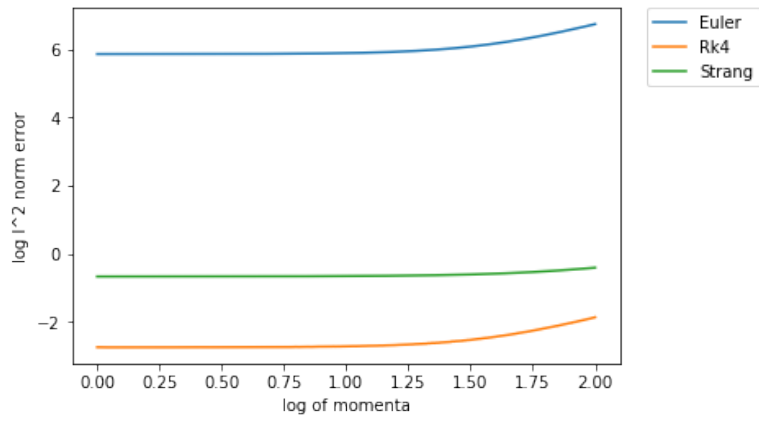
Figure 5: $x = 40$
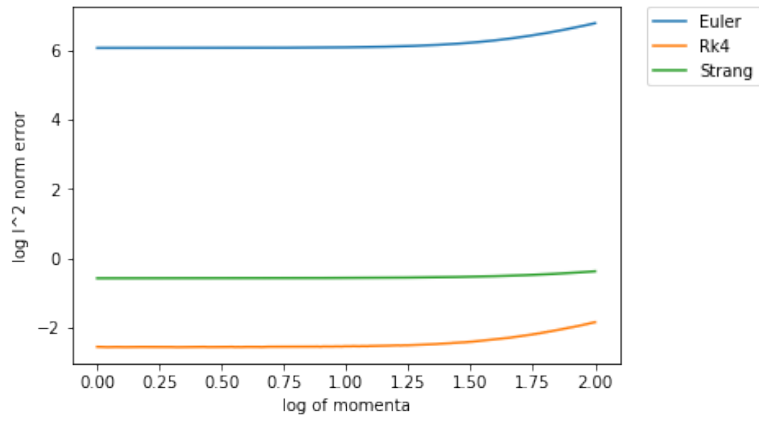
Figure 6: $x = 50$
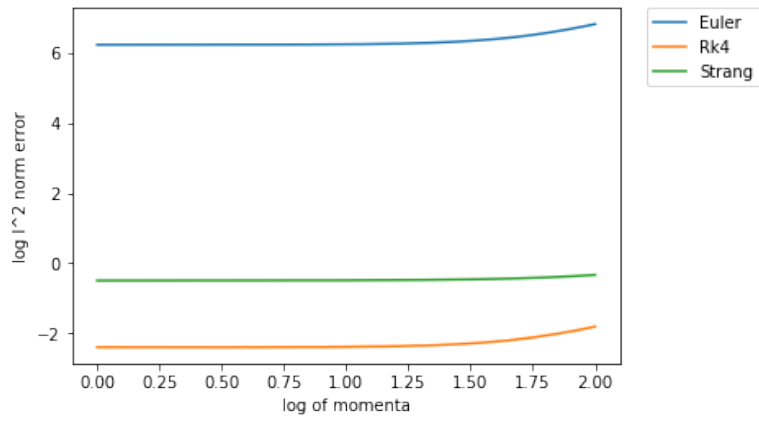
Figure 7: $x = 60$
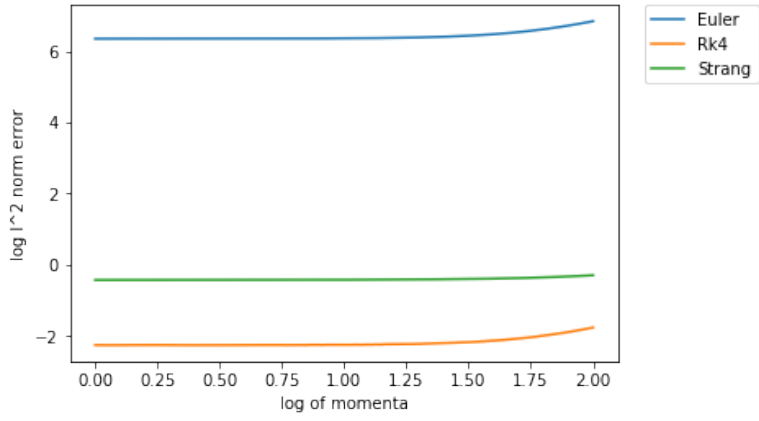
Figure 8: $x = 70$
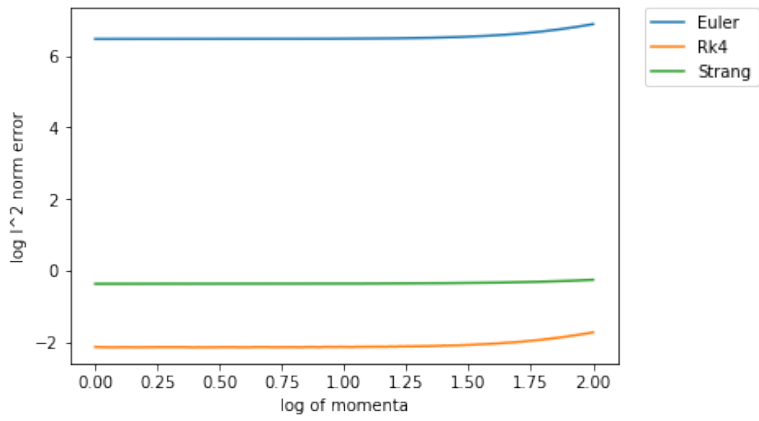
Figure 9: $x = 80$
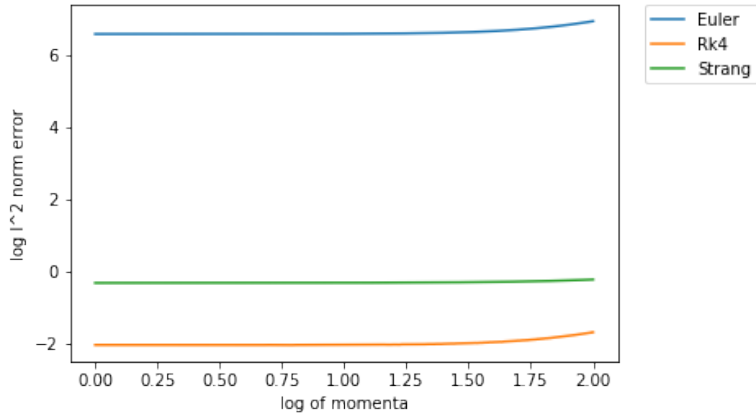
Figure 10: $x = 90$
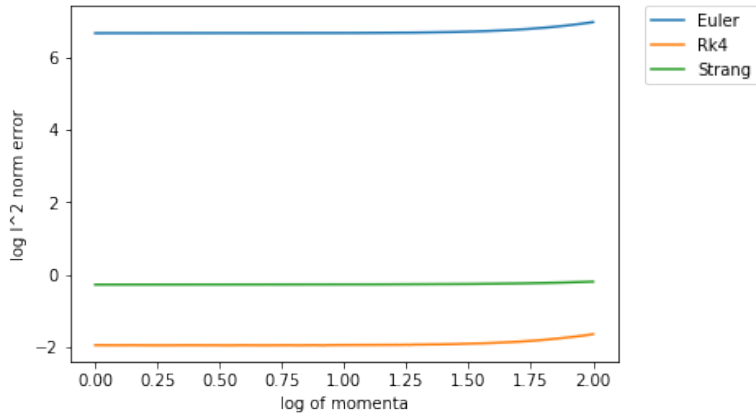
Figure 11: $x = 100$

Table 1 contains values for x and p from the exact solution with initial conditions of $x(0) = 2$ and $p(0) = 1$, a time step size of $t = 0.1$, and for 500 time steps.

Table 1: Exact x and p values

	x	p
0	2.000000	1.000000
1	2.094838	0.895171
2	2.178736	0.781397
3	2.250857	0.659816
4	2.310479	0.531643
⋮	⋮	⋮
496	1.169180	1.404058
497	1.308507	1.380153
498	1.444751	1.342459
499	1.576552	1.291351
500	1.702591	1.227341

We substitute those values into H and get

Table 2: Exact values of H

	H Values
0	0.500000000000000
1	0.500000000000000
2	0.499999999999999
3	0.500000000000000
4	0.499999999999999
⋮	⋮
496	0.499999999999939
497	0.499999999999939
498	0.499999999999939
499	0.499999999999938
500	0.499999999999939

We use our splitting and composition derived symplectic integration to the estimates of of x and p in Table 3.

Table 3: Symplectic x and p values

	x	p
0	2.000000	1.000000
1	2.094840	0.895212
2	2.178744	0.781480
3	2.250875	0.659939
4	2.310512	0.531805
⋮	⋮	⋮
496	1.169269	1.403800
497	1.308572	1.379930
498	1.444795	1.342272
499	1.576579	1.291202
500	1.702606	1.227232

After we substitute those values into H we get

Table 4: Symplectic Values

	H Values
0	0.500000000000000
1	0.500039528055413
2	0.500074498485053
3	0.500104561875947
4	0.500129417844628
⋮	⋮
496	0.499653761186814
497	0.499711820881950
498	0.499768597293063
499	0.499823523129022
500	0.499876049589031

In table 4, the reason all of the exact values are not 0.5 is due to round-off error. We take the absolute difference between the exact and symplectic x and p values to get

Table 5: Absolute difference between x and p values

	x	p
0	0.000000	0.000000
1	0.000002	0.000042
2	0.000008	0.000083
3	0.000019	0.000123
4	0.000033	0.000162
⋮	⋮	⋮
496	0.000089	0.000257
497	0.000065	0.000223
498	0.000044	0.000187
499	0.000028	0.000149
500	0.000015	0.000109

The mean of the differences in the x values is 0.000418 and the standard deviation is 0.000295. The mean of the differences in the p values is 0.000266 and the standard deviation is 0.000128. We take the absolute difference between the exact and symplectic values of H to get the values in Table 6. The mean difference of the H values is 0.000475 and the standard deviation is 0.000351.

Table 6: Absolute difference between H values

	H Values
0	0
1	3.95280554137400e-5
2	7.44984850538088e-5
3	0.000104561875946985
4	0.000129417844629387
⋮	⋮
496	0.000346238813124566
497	0.000288179117989396
498	0.000231402706875938
499	0.000176476870916042
500	0.000123950410907403

7 CONCLUSION

We have shown that for a conservative dynamical system that symplectic integration methods are more accuracte and stable than Euler methods. We showed that symplectic integration methods are comparable to Runge-Kutta methods in accuracy, but symplectic integration methods are far more stable. We have shown for a simple Hamiltonian that can be solved exactly, the differences between the exact and symplectic solutions are minimal at best. Thus, any Hamiltonian that can be solved exactly can be used as a sandbox for testing symplectic integration techniques. Since Hill's lunar equations can be solved exactly it can be used to test those techniques. Some alterations need to be made to K_1 from Section 5.2 to make it solvable. First symplectic techniques would be developed specifically for the H from Section 5.2. The goal however, is to determine symplectic techniques that are problem independent and increase the order of accuracy.

BIBLIOGRAPHY

[1] Amit Amritkar, Eric de Sturler, Katarzyna Świrydowicz, Danesh Tafti, and Kapil Ahuja. Recycling krylov subspaces for cfd applications and a new hybrid recycling solver. *Journal of Computational Physics*, 303:222–237, 2015.

[2] Vladimir Igorevich Arnol'd. *Mathematical methods of classical mechanics*, volume 60. Springer Science & Business Media, 2013.

[3] Michael Artin. *Algebra: Pearson New International Edition*. Pearson Higher Ed, 2013.

[4] Herman JC Berendsen, David van der Spoel, and Rudi van Drunen. Gromacs: a message-passing parallel molecular dynamics implementation. *Computer Physics Communications*, 91(1-3):43–56, 1995.

[5] Frances C Bernstein, Thomas F Koetzle, Graheme JB Williams, Edgar F Meyer, Michael D Brice, John R Rodgers, Olga Kennard, Takehiko Shimanouchi, and Mitsuo Tasumi. The protein data bank. *European Journal of Biochemistry*, 80(2):319–324, 1977.

[6] Sergio Blanes, Fernando Casas, and Ander Murua. Splitting and composition methods in the numerical integration of differential equations. *arXiv preprint arXiv:0812.0377*, 2008.

[7] Stephen D Bond and Benedict J Leimkuhler. Molecular dynamics and the accuracy of numerically computed averages. *Acta Numerica*, 16:1–65, 2007.

70

[8] BH Bradshaw-Hajek, MP Edwards, Philip Broadbridge, and GH Williams. Non-classical symmetry solutions for reaction–diffusion equations with explicit spatial dependence. *Nonlinear Analysis: Theory, Methods & Applications*, 67(9):2541–2552, 2007.

[9] PJ Channell and C Scovel. Symplectic integration of hamiltonian systems. *Nonlinearity*, 3(2):231, 1990.

[10] Gary Chartrand, Linda Lesniak, and Ping Zhang. *Graphs & digraphs*, volume 39. CRC Press, 2010.

[11] John B Conway. *Functions of one complex variable II*, volume 159. Springer Science & Business Media, 2012.

[12] Predrag Cvitanovic, Roberto Artuso, Ronnie Mainieri, Gregor Tanner, Gábor Vattay, Niall Whelan, and Andreas Wirzba. Chaos: classical and quantum. *ChaosBook. org (Niels Bohr Institute, Copenhagen 2005)*, 2005.

[13] Ashok Das and Susumu Okubo. *Lie Groups and Lie Algebras for Physicists*. World Scientific, 2014.

[14] Mircea V Diudea, Ivan Gutman, and Lorentz Jantschi. *Molecular topology*. Nova Science Publishers New York, 2001.

[15] William G Faris. Vector fields and differential forms. 2006.

[16] IM Gelfand and SV Fomin. Calculus of variations. 1963. *Revised English edition translated and edited by Richard A. Silverman.*

[17] Anne Greenbaum and Timothy P Chartier. *Numerical methods: design, analysis, and computer implementation of algorithms.* Princeton University Press, 2012.

[18] Sigurdur Helgason. Sophus lie and the role of lie groups in mathematics. 1990.

[19] David M Hernandez and Walter Dehnen. A study of symplectic integrators for planetary system problems: error analysis and comparisons. *arXiv preprint arXiv:1612.05329*, 2016.

[20] James Humphreys. *Introduction to Lie algebras and representation theory*, volume 9. Springer Science & Business Media, 2012.

[21] Thomas W Hungerford. Algebra. reprint of the 1974 original. *Graduate Texts in Mathematics*, 73, 1980.

[22] Neil D Jespersen and Alison Hyslop. *Chemistry: The Molecular Nature of Matter: The Molecular Nature of Matter.* Wiley Global Education, 2014.

[23] T KelleyC. Iterative methodsforlinearand nonlinear equations. *RaleighN. C.: NorthCarolinaStateUniversity*, 1995.

[24] Tu Cam Le. *Computational simulation of hyperbranched polymer melts under shear.* PhD thesis, Swinburne University of Technology, 2010.

[25] J Lemkul. Gromacs tutorial: Lysozyme in water. *Virginia Polytechnic Institute and State University, Virginia*, 2010.

[26] IV Likhachev, NK Balabaev, and OV Galzitskaya. Available instruments for analyzing molecular dynamics trajectories. *The open biochemistry journal*, 10:1, 2016.

[27] Charles F Van Loan. *Introduction to scientific computing: a matrix-vector approach using MATLAB*. Prentice Hall PTR, 1999.

[28] Harvey Lodish, David Baltimore, Arnold Berk, S Lawrence Zipursky, Paul Matsudaira, and James Darnell. *Molecular cell biology*, volume 3. Scientific American Books New York, 1995.

[29] Arash Mehraban. Non-classical symmetry solutions to the fitzhugh nagumo equation. 2010.

[30] Francesco Oliveri. Lie symmetries of differential equations: classical results and recent contributions. *Symmetry*, 2(2):658–706, 2010.

[31] Fatih Porikli, Oncel Tuzel, and Peter Meer. Covariance tracking using model update based on lie algebra. In *Computer Vision and Pattern Recognition, 2006 IEEE Computer Society Conference on*, volume 1, pages 728–735. IEEE, 2006.

[32] Dennis C Rapaport, Robin L Blumberg, Susan R McKay, Wolfgang Christian, et al. The art of molecular dynamics simulation. *Computers in Physics*, 10(5):456–456, 1996.

[33] Lewis F Richardson and J Arthur Gaunt. The deferred approach to the limit. part i. single lattice. part ii. interpenetrating lattices. *Philosophical Transactions*

of the Royal Society of London. Series A, containing papers of a mathematical or physical character, 226:299–361, 1927.

[34] Lewis Fry Richardson. The approximate arithmetical solution by finite differences of physical problems involving differential equations, with an application to the stresses in a masonry dam. *Philosophical Transactions of the Royal Society of London. Series A, Containing Papers of a Mathematical or Physical Character*, 210:307–357, 1911.

[35] Christopher Roy. Review of discretization error estimators in scientific computing. In *48th AIAA Aerospace Sciences Meeting Including the New Horizons Forum and Aerospace Exposition*, page 126, 2010.

[36] Christopher J Roy. Grid convergence error analysis for mixed-order numerical schemes. *AIAA journal*, 41(4):595–604, 2003.

[37] Christopher J Roy, Tyrone S Phillips, Matthew J Kurzen, Andrew J Sinclair, and Anil Raju. Discretization error estimation and exact solution generation using the method of nearby problems.

[38] Christopher J Roy and Andrew J Sinclair. On the generation of exact solutions for evaluating numerical schemes and estimating discretization error. *Journal of Computational Physics*, 228(5):1790–1802, 2009.

[39] Halsey Lawrence Royden and Patrick Fitzpatrick. *Real analysis*, volume 198. Macmillan New York, 1988.

[40] Siavash Shahshahani. *An Introductory Course on Differentiable Manifolds.* Courier Dover Publications, 2016.

[41] Joel A Shapiro. Classical mechanics, 2003.

[42] MS Smyth and JHJ Martin. x ray crystallography. *Journal of Clinical Pathology*, 53(1):8, 2000.

[43] Gilbert W Stewart. *Introduction to matrix computations*. Elsevier, 1973.

[44] Gilbert Strang. *Computational science and engineering*, volume 791. Wellesley-Cambridge Press Wellesley, 2007.

[45] Veeravalli Seshadri Varadarajan. *Lie groups, Lie algebras, and their representations*, volume 102. Springer Science & Business Media, 2013.

[46] J Waldvogel. Symplectic integrators for hill's lunar problem. Eidgenössische Technische Hochschule [ETH] Zürich. Seminar für Angewandte Mathematik, 1996.

[47] Jörg Waldvogel. Fundamentals of regularization in celestial mechanics and linear perturbation theories. In *Extra-Solar Planets: The Detection, Formation, Evolution and Dynamics of Planetary Systems*, pages 169–184. Taylor & Francis, 2010.

[48] William J Wedemeyer, Ervin Welker, Mahesh Narayan, and Harold A Scheraga. Disulfide bonds and protein folding. *Biochemistry*, 39(15):4207–4216, 2000.

[49] Robert Whitinger. An algorithm for the machine calculation of minimal paths. 2016.

[50] Mark R Wilson. Molecular dynamics simulations of flexible liquid crystal molecules using a gay-berne/lennard-jones model. *The Journal of chemical physics*, 107(20):8654–8663, 1997.

[51] Jay Yellen and Jonathan L Gross. *Handbook of Graph Theory (Discrete Mathematics and Its Applications)*. CRC press, 2003.

[52] JOO HEON YOO. Lie groups, lie algebras, and applications in physics. 2015.

A   Definition, Theorems, and Equations

A.1   Dynamic Equilibrium

Below we have chemistry and physics definitions and equations listed to understand the material in this thesis. The following definitions and equations are from [22].

Definition A.1.0.1 *Thermodynamics (Chemical Thermodynamics): The study of the role of engery in chemical change an din determining the behavior of material.*

Definition A.1.0.2 *Dynamic Equilibrium: a condition in which two opposing processes are occurring at equal rates.*

Definition A.1.0.3 *Enthalpy* (H)*: is the heat content of a system.*

Definition A.1.0.4 *Entropy* (S)*: s a thermodynamic quantity related to the number of equivalent ways the energy of a system can be distributed. The greater this number, the more probable is the state and the higher is the entropy.*

Definition A.1.0.5 *Gibbs Free Energy* (G)*: A thermodynamic quantity that relates enthalpy* (H)*, entropy* (S)*, and temperature* (T) *by the equation:*

$$G = H - TS$$

Definition A.1.0.6 *Enthalpy Change* (ΔH)*: The difference in enthalpy between the initial state and the final state for some change.*

Definition A.1.0.7 *Entropy Change* (ΔS)*: The difference in entropy between the initial state and the final state for some change.*

Definition A.1.0.8 *Gibbs Free Energy Change* (ΔG)*: The difference given by:*

$$\Delta G = \Delta H - T\Delta S.$$

Definition A.1.0.9 *Standard Heat of Reaction* (ΔH°)*: The enthalpy change of a reaction when determined with reactants and products at 25 °C and 1 atm and on the scale of the mole quantities given by the coefficients of the balanced equation.*

Definition A.1.0.10 *Standard Entropy Change* (ΔS°)*: The entropy change of a reaction when determined with reactants and products at 25 °C and 1 atm and on the scale of the mole quantities given by the coefficients of the balanced equation.*

Definition A.1.0.11 *Standard Free Energy Change* (ΔG°)*:*

$$\Delta G° = \Delta H° - T\Delta S°.$$

Definition A.1.0.12 *Gas Constant, Universal* (R)*: $R = 0.0821$ liter atm mol^{-1} K^{-1} or $R = 8.314J$ mol^{-1} K^{-1}.*

Mathematically a system is in a state of dynamic equilibrium if

$$G_{\text{products}} = G_{\text{reactants}} \quad \text{and } \Delta G = 0.$$

where G_{products} and $G_{\text{reactants}}$ are the Gibbs free energy of the products and reactants. The position of equilibrium in a reaction is determined by the sign and magnitude of $\Delta G°$. A mathematical way of relating ΔG and $\Delta G°$ is

$$\Delta G = \Delta G° + RT \ln(Q)$$

where Q is the reaction quotient. In terms of thermodynamics, a state is in dynamic equilibrium when $\Delta G = 0$ and $Q = K$, where K is the thermodynamic equilibrium constant. With $\Delta G = 0$ and $Q = K$ we get

$$\Delta G° = -RT \ln(K).$$

A.2   Protein

Below we have chemistry and biological definitions listed to understand to material in this thesis. The following definitions come from [22].

Definition A.2.0.1 *Compound: A substance consisting of chemically combined atoms from two or more elements and present in a definite ratio.*

Definition A.2.0.2 *Organic Compound: Any compound of carbon other than a carbonate, bicarbonate, cyanide, cyanate, carbide, or gaseous oxide.*

Definition A.2.0.3 *Atomic Mass: The average mass (in u) of the atoms of the isotopes of a given element as they occur naturally.*

Definition A.2.0.4 *Chemical Formula: A formula written using chemical symbols and subscripts that describes the composition of a chemical compound or element.*

**Definition A.2.0.5 *Formula Mass:* ** *The sum of the atomic mass (in u) of all of the atoms represented in a chemical formula. Often used with units of g mol^{-1} to represent masses of ionic substances.*

**Definition A.2.0.6 *Monomer:* ** *A substance of relatively low formula mass that is used to make a polymer.*

**Definition A.2.0.7 *Macromolecule:* ** *A molecule whose molecular mass is very large.*

**Definition A.2.0.8 α-*Amino Acid:* ** *One of about 20 monomers of polypeptides.*

**Definition A.2.0.9 *Polymer:* ** *A substance consisting of macromolecules that have repeating structural units.*

**Definition A.2.0.10 *Amide:* ** *An organic compound whose molecules have any one of the following groups:*

$$\underset{\overset{\|}{\overset{O}{}}}{\text{----CNH}_2} \qquad \underset{\overset{\|}{\overset{O}{}}}{\text{----CNHR}} \qquad \underset{\overset{\|}{\overset{O}{}}}{\text{----CNR}_2}$$
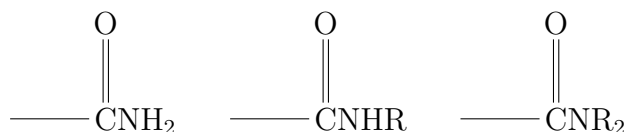
**Definition A.2.0.11 *Peptide Bond:* ** *The amide linkage in molecules of polypeptides.*

**Definition A.2.0.12 *Polypeptide:* ** *A polymer of α-amino acids that makes up all or most of a protein.*

**Definition A.2.0.13 *Protein:* ** *A macromolecular substance found in cells that consists wholly or mostly of one or more polypeptides that often are combined with an organic molecule or a metal ion.*

The following definition comes from [28].

Definition A.2.0.14 *Disulfide Bond:* *is a covalent type of bond derived from two thiol groups, takes either of the following groups:*

$$\text{———S———S———} \qquad \text{———SH+HS———}$$

Definition A.2.0.15 *Tertiary Structure:* *refers to the overall conformation of a polypeptide chain – that is, the three-dimensional arrangement of all its amino acid resides.*

A.3   Graph Theory

Below we have mathematical definitions listed to understand material in this thesis. Each of the following definitions come from [10].

Definition A.3.0.1 *A graph G is a finite nonempty set V of objects called vertices (the singular is vertex) together with a possibly empty set E of 2-element subsets of V called edges. Vertices are sometimes referred to as points or nodes, while edges are sometimes called lines or links.*

Definition A.3.0.2 *Let G be a graph and $u, v \in V(G)$. If uv is an edge of G, then u and v are adjacent vertices.*

Definition A.3.0.3 *The degree of a vertex v in a graph G is the number of vertices in G that are adjacent to v.*

Definition A.3.0.4 *The adjacency matrix of G is the $n \times n$ zero-one matrix $A(G) = \left[a_{ij}\right]$, or simply $A = \left[a_{ij}\right]$, where*

$$a_{ij} = \begin{cases} 1 & \text{if } v_i v_j \in E(G) \\ \\ 0 & \text{if } v_i v_j \notin E(G) \end{cases}$$

Definition A.3.0.5 *For an integer $n \geq 3$, the cycle C_n is a graph of order n and size n whose vertices can be labeled by $v_1, v_2, \ldots, v_n$ and whose edges are $v_1 v_n$ and $v_i v_{i+1}$ for $i = 1, 2, \ldots, n-1$.*

Definition A.3.0.6 *Two vertices u and v in a graph G are connected if G contains $u - v$ path. The graph G itself is connected if every two vertices of G are connected.*

Definition A.3.0.7 *An acyclic graph has no cycles. A tree is a connected acyclic graph.*

Definition A.3.0.8 *A directed graph or digraph D is a finite nonempty set of objects called vertices together with a (possibly empty) set of order pairs of distinct vertices of D called arcs or directed edges. As with graphs, the vertex set of D is denoted by $V(D)$ and the arc set (or directed edge set) of D is denoted by $E(D)$.*

Definition A.3.0.9 *A network N is a digraph D with two distinguished vertices u and v, called the source and the sink, respectively together with a nonnegative real valued function c on $E(D)$. The digraph D is called the underlying digraph of N and the function c is called the capacity function of N. The value $c(a) = c(x, y)$ of an arc $a = (x, y)$ of D is called the capacity of a. Any vertex of N distinct from u and v is called an intermediate vertex of N.*

Definition A.3.0.10 *Let D be a digraph and $u, v \in V(D)$. If $a = (u, v)$ is an arc of a digraph D, then a is said to join u and v. The vertex u is said to be adjacent to v and v is adjacent from u.*

Definition A.3.0.11 *For a vertex v in a digraph D, the outdegree od v of v is the number of vertices of D to which v is adjacent, while the indegree id v of v is the number of vertices of D from which v is adjacent.*

Definition A.3.0.12 *The adjacency matrix $A(D)$ of a diagraph D with $V(D) = \{v_1, v_2, \ldots, v_n\}$ is the $n \times n$ matrix $\left[a_{ij} \right]$ defined by $a_{ij} = 1$ if $\left(v_i, v_j \right) \in E(D)$ and $a_{ij} = 0$ otherwise.*

The following definitions come from [51].

Definition A.3.0.13 *The graph with a single vertex r (and no edges) is a tree with root r. Let (G, r) denote a tree with root r. Then $(G_1, r_1) \bigoplus (G_2, r_2)$ is a tree formed by taking the disjoint union of G_1 and G_2 and adding an edge (r_1, r_2). The root of this new tree is $r = r_1$.*

Definition A.3.0.14 *The underlying graph of a directed or partially directed graph G is the graph that results from removing all the designations of head and tail from the directed edges of G (i.e., deleting al the edge-directions).*

Definition A.3.0.15 *A directed tree is a digraph whose underlying graph is a tree.*

Definition A.3.0.16 *A root tree is a directed tree having a distinguished vertex r, called the root, such that for every other vertex v, there is a directed $r - v$ path.*

Definition A.3.0.17 *A surface is a 2-manifold, often taken in context to be connected.*

Definition A.3.0.18 *An imbedding of a graph G in an orientable surface S is a continuous one-to-one function $\rho : G \to S$ from a topological representation of the graph G into the surface S.*

Definition A.3.0.19 *The minimum genus $\gamma_{min}(G)$ (or simply the genus $\gamma(G)$) of a graph F is the minimum integer g such that there exists an imbedding of G into the orientable surface S_g of genus g.*

Definition A.3.0.20 *A graph of genus 0 is planar.*

Definition A.3.0.21 *The maximum genus $\gamma_{max}(G)$ of a graph G is the maximum integer g such that there exists a (cellular) imbedding of G into the orientable surface of genus g.*

Definition A.3.0.22 *Let G be a graph and let v be a degree-2 vertex with two neighbors u and w in G (u and w could be the same vertex). We say that a graph G' is obtained from G by smoothing the vertex v if G' is constructed from G by removing the vertex v then adding a new edge connecting the vertices u and w.*

Definition A.3.0.23 *Two graphs G_1 and G_2 are homeomorphic if they become isomorphic after smoothing all degree-2 vertices. It is easy to that two homeomorphic graphs have the same minimum genus and the same maximum genus.*

A.4   Modern Algebra

Below we have mathematical definitions listed to understand material in this thesis. The following definitions come from [21].

Definition A.4.0.1 *A semigroup is a nonempty set G together with a binary operation on G which is*

   (i) *associative: $a\,(bc) = (ab)\,c$ for all $a, b, c \in G$;*

a monoid is a semigroup G which contains a

   (ii) *(two-sided) identity element $e \in G$ such that $ae = ea = a$ for all $a \in G$.*

A group is a monoid G such that

   (iii) *for every $a \in G$ there exists a (two-sided) inverse element $a^{-1} \in G$ such that $a^{-1}a = aa^{-1} = e$.*

A semigroup G is said to be abelian or commutative if its binary operation is

   (iv) *commutative: $ab = ba$ for all $a, b \in G$.*

Definition A.4.0.2 *A ring is a nonempty set R together with two binary operations (usually denoted as addition $(+)$ and multiplication) such that:*

   (i) *$(R, +)$ is an abelian group;*

   (ii) *$(ab)\,c = a\,(bc)$ for all $a, b, c \in R$ (associative multiplication);*

   (iii) *$a\,(b + c) = ab + ac$ and $(a + b)\,c = ac + bc$ (left and right distributive laws).*

If in addition:

> (**iv**) $ab = ba$ *for all* $a, b \in R$,

then R is said to be a commutative ring. If R contains an element 1_R such that

> (**v**) $1_R a = a 1_R = a$ *for all* $a \in R$,

then R is said to be a ring with identity.

Definition A.4.0.3 *A nonzero element a in a ring R is said to be a left [resp. right] zero divisor if there exists a nonzero $b \in R$ such that $ab = 0$ [resp. $ba = 0$]. A zero divisor is an element of R which is both a left and a right zero divisor.*

Definition A.4.0.4 *An element a in a ring R with identity is said to be left [resp. right] invertible if there exists $c \in R$ [resp. $b \in R$] such that $ca = 1_R$ [resp. $ab = 1_R$]. The element c [resp. b] is called a left [resp. right] inverse of a. An element $a \in R$ that is both left and right invertible is said to be invertible or to be a unit.*

Definition A.4.0.5 *A commutative ring R wih identity $1_R \neq 0$ and no xero divisors is called an integral domain. A ring D with identity $1_D \neq 0$ in which every every nonzero element is a unit is called a division ring. A field is a commutative division ring.*

Definition A.4.0.6 *Let R be a ring. A (left) R-module is an additive abelian group A together with a function $R \times A \to A$ (the image of (r, a) being denoted by ra) such that for all $r, s \in R$ and $a, b \in A$:*

> (**i**) $r(a + b) = ra + rb$.

(ii) $(r + s)\, a = ra + sa$.

(iii) $r\,(sa) = (rs)\,a$.

If R has an identity element 1_R and

(iv) $1_R a = a$ *for all $a \in A$,*

then A is said to be a unitary R-module. If R is a division ring, then a unitary R-module is called a (left) vector space.

Definition A.4.0.7 *Let K be a commutative ring with identity. A K-algebra (or algebra over K) is a ring A such that*

(i) $(A, +)$ *is a unitary (left) K-module;*

(ii) $k\,(ab) = (ka)\,b = a\,(kb)$ *for all $k \in K$ and $a, b \in A$.*

A.5   Complex Analysis

Below we have mathematical definitions and proposition listed to understand the material in this thesis. The proof for the proposition is also listed for validity. The following definitions, proposition, and proof are from [11].

Definition A.5.0.1 *A metric space is a pair (X, d) where X is a set and d is function from $X \times X$ into $\mathbb{R}$, called a distance function or metric, which satisfies the following*

conditions for x, y, and z in X:

$$d(x, y) \geq 0$$

$$d(x, y) = 0$$

$$d(x, y) = d(y, x) \ \text{(symmetry)}$$

$$d(x, z) \leq d(x, y) + d(y, z) \ \text{(triangle ineqaulity)}$$

If x and r > 0 are fixed then define

$$B(x; r) = \{y \in X : d(x, y) < r\}$$

$$\overline{B}(x; r) = \{y \in X : d(x, y) \leq r\}.$$

$B(x; r)$ *and* $\overline{B}(x; r)$ *are called the open and closed balls, respectively, with center* x *and radius* r.

Definition A.5.0.2 *For a metric space* (X, d) *a set* $G \subset X$ *is open if for each* x *in* G *there is an* $\varepsilon > 0$ *such that* $B(x; \varepsilon) \subset G$.

Definition A.5.0.3 *A set* $F \subset X$ *is closed if its complement,* $X \backslash F$, *is open.*

Definition A.5.0.4 *Let* (X, d) *and* (Ω, ρ) *be metric spaces and let* $f : X \to \Omega$ *be a function. If* $a \in X$ *and* $\omega \in \Omega$, *then* $\lim_{x \to a} f(x) = \omega$ *if for every* $\varepsilon > 0$ *there is a* $\delta > 0$ *such that* $\rho(f(x), \omega) < \varepsilon$ *whenever* $0 < d(x, a) < \delta$. *The function* f *is continuous at the point* a *if* $\lim_{x \to a} f(x) = f(a)$. *If* f *is continuous at each point of* X *then* f *is a continuous function from* X *to* Ω.

Definition A.5.0.5 *If* G *is an open set in* $\mathbb{C}$ *and* $f : G \to \mathbb{C}$ *then* f *is differentiable at a poin* a *in* G *if*

$$\lim_{h \to 0} \frac{f(a + h) - f(a)}{h}$$

Proposition A.5.0.1 *If* $f : G \to \mathbb{C}$ *is differentiable at a point* a *in* G *then* f *is continuous at* a.

Proof In fact,

$$
\begin{aligned}
\lim_{z \to a} \left| f(z) - f(a) \right| & = \left[\lim_{z \to a} \frac{\left| f(z) - f(a) \right|}{\left| z - a \right|} \right] \cdot \left[\lim_{z \to a} \left| z - a \right| \right] \\
& = \left| f'(a) \right| \cdot 0 \\
& = 0. \blacksquare
\end{aligned}
$$

Definition A.5.0.6 *A function* $f : G \to \mathbb{C}$ *is analytic if* f *is continuously differentiable on* G.

Definition A.5.0.7 *A topological space is a pair* $(X, \mathcal{F})$ *where* X *is a set and* $\mathcal{F}$ *is a collection of subsets of* X *having the following properties:*

(a) $\varnothing \in \mathcal{F}$ *and* $X \in \mathcal{F}$;

(b) if $U_1, \ldots, U_n$ *are in* $\mathcal{F}$ *then* $\bigcap_{j=1}^{n} U_j \in \mathcal{F}$;

(c) if $\{U_i : i \in I\}$ *is any collection of sets in* $\mathcal{F}$ *then* $\bigcup_{i \in I} U_i$ *is in* $\mathcal{F}$.

The collection of sets $\mathcal{F}$ *is called a topology on* X, *and each member of* $\mathcal{F}$ *is called an open set.*

Definition A.5.0.8 *A subset* F *of a topological space* X *is closed if* $X \backslash F$ *is open. A point* a *in* X *is a limit point of a set* A *if for every open set* U *that contains* a *thre is a point* x *in* $A \bigcap U$ *such that* $x \neq a$.

Definition A.5.0.9 *A topological space $(X, \mathcal{F})$ is said to be a Hausdorff space if for any two distinct points a and b in X there are disjoint open sets U and V such that $a \in U$ and $b \in V$.*

Definition A.5.0.10 *A topological space $(X, \mathcal{F})$ is connected if the only nonempty subset of X which is both open and closed is the set X itself.*

Definition A.5.0.11 *Let X be a topological space; a coordinate patch on X is a pair (U, φ) where U is an open subset of X and φ is a homeomorphism of U onto an open subset of the plane. If $a \in U$ then the coordinate patch (U, φ) is said to contain a.*

Definition A.5.0.12 *An analytic manifold is a pair (X, Φ) where X is a Hausdorff connected topological space and Φ is a collection of coordinate patches on X such that: (i) each point of X is contained in at least one member of Φ, and (ii) if (U_a, φ_a), $(U_b, \varphi_b) \in \Phi$ with $U_a \bigcap U_b \neq \varnothing$ then $\varphi_a \circ \varphi_b^{-1}$ is an analytic function of $\varphi_b\left(U_a \bigcap U_b\right)$ onto $\varphi_a\left(U_a \bigcap U_b\right)$. The set Φ of coordinator patches is called an analytic structure on X. An analytic manifold is also called an analytic surface.*

VITA

WILLIAM TY FRAZIER

Education:	B.S. Mathematics, East Tennessee State University,
	Johnson City, Tennessee 2015
	M.S. Mathematical Sciences, East Tennessee State University
	Johnson City, Tennessee 2017
Professional Experience:	Graududate Assistant, East Tennessee State University,
	Johnson City, Tennessee, 2015–2017