Mathematical Methods of Classical Mechanics with Applications to Symplectic Integration

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1 Introduction

The main task of mechanics is the integration of the equations of motion (i.e. solving for the motion of particles as a function of time). Solving Newton's equations of motion is generally a hard problem, as the equations are coupled and non-linear. Standard approaches for solving the differential equations do not always work well. By recasting mechanics in a new framework, mathematicians and scientists have developed an extraordinarily powerful "tool set" to tackle problems in mechanics.

The purpose of this thesis is to investigate the mathematical tools needed to write mechanics in a more convenient and powerful form. These tools also find applications in the numerical study of mechanical systems, namely through numerical methods known as *symplectic integrators*. Unlike "standard" ODE initial value problem numerical methods, symplectic integrators are designed to respect some of the properties of exact solutions to equations of motion. Symplectic integrators have been used to study the motion of the outer planets of our Solar System over very large time spans [14].

1.1 Newtonian Mechanics

In Newtonian mechanics one studies the dynamics of a system of point masses by analyzing the forces acting on the masses in the system. The motions of particles are completely determined by a system of second-order ordinary differential equations and the positions and velocities of the particles at some given time; this is called *Newton's principle of determinacy* and is part of the foundation of classical mechanics [3]. The differential equations that describe the motion of the system, generically called the **equations of motion**, are determined by the forces on the system.

Let $\mathbf{x}_i$, $\dot{\mathbf{x}}_i = \mathrm{d}\mathbf{x}_i/\mathrm{d}t$, and $\ddot{\mathbf{x}}_i = \mathrm{d}^2\mathbf{x}_i/\mathrm{d}t^2$ be vectors of the positions, velocities, and accelerations of the i^{th} particle in a mechanical system in $\mathbb{R}^3$. In general, for particles of unit mass, Newton's equations of motion are

$$\ddot{\mathbf{x}}_i = \mathbf{F}_i(\mathbf{x}_1, ..., \mathbf{x}_N, \dot{\mathbf{x}}_1, ..., \dot{\mathbf{x}}_N, t), \tag{1.1}$$

where $\mathbf{F}_i$ is the familiar vector of forces on the i^{th} particle. The form of $\mathbf{F}$ is experimentally determined and verified; we consider $\mathbf{F}$ as defining the mechanical system. If there are N particles in the system, we require $6N$ initial conditions ($3N$ initial positions and $3N$ initial velocities) to solve Newton's $3N$ second-order equations of motion.

As an example, take the three-body problem, which is the study of the motion of three bodies interacting via Newton's law of universal gravitation. Newton's nine equations of motion are

$$\begin{aligned} m_1\ddot{\mathbf{x}}_1 &= -\frac{\partial}{\partial \mathbf{x}_1} U(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) \\ m_2\ddot{\mathbf{x}}_2 &= -\frac{\partial}{\partial \mathbf{x}_2} U(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) \\ m_3\ddot{\mathbf{x}}_3 &= -\frac{\partial}{\partial \mathbf{x}_3} U(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3), \end{aligned}$$

where the potential, which describes the forces between the particles, is

$$U(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = -\frac{Gm_2m_3}{||\mathbf{x}_2 - \mathbf{x}_3||} - \frac{Gm_3m_1}{||\mathbf{x}_3 - \mathbf{x}_1||} - \frac{Gm_1m_2}{||\mathbf{x}_1 - \mathbf{x}_2||},$$

and m_i is the mass of the i^{th} particle and G is Newton's universal gravitational constant. If a force on a particle can be written as the gradient of a scalar function, that force is said to be *conservative* and the scalar function a *potential*. In our studies of mechanical systems, we consider only conservative forces.

2 Vectors and Differential Forms

The goal of this section is to briefly describe manifolds, tangent vectors, and differential forms. For the reader who is "a bit rusty", this section will hopefully be a welcome refresher; readers that are already familiar with manifolds, differential forms, and the like need not spend their time reading this section. For a complete, formal treatment of these topics, the reader is recommended to Frankel [7].

2.1 Differentiable Manifolds

An n-dimensional **differentiable manifold** M^n is a topological space that is locally homeomorphic to $\mathbb{R}^n$ with differentiable overlap maps f_{VU}. More formally, the set M^n must be covered by subsets ($M^n = U \cup V \cup ...$) that are each in a $1:1$ correspondence $\phi_U : U \to \mathbb{R}^n$ to an open subset $\phi_U(U)$ of $\mathbb{R}^n$. Intersections of subsets U and V must also correspond to an open subset of $\mathbb{R}^n$. Finally, the overlap map

$$f_{VU} = \phi_V \circ \phi_U^{-1} : \phi_U(U \cap V) \to \phi_V(U \cap V),$$

must be differentiable. Note that both $\phi_U(U \cap V)$ and $\phi_V(U \cap V)$ are subsets of $\mathbb{R}^n$.

A subset U with a map ϕ_U give us a **coordinate patch** (U, ϕ_U) on the manifold M^n; the map $\phi_U^{-1} : \mathbb{R}^n \to U$ gives us coordinates x_U^i on the manifold. The differentiability of the overlap map $f_{VU} = \phi_V \circ \phi_U^{-1}$ allows us to smoothly transfer between coordinate patches. Instead of specifying with which coordinate patch and the associated coordinates we are working, we often denote x^i as "local coordinates" on M^n. Most importantly, the differentiable manifold structure allows us to do calculus on objects described solely on the manifold. Differentiable manifolds form the foundation of the more powerful methods of classical mechanics.

As an example of a differentiable manifold, let us take the case of a mechanical system with N particles in $\mathbb{R}^3$. In Newtonian mechanics, we track the positions $\mathbf{x}_i$ of the particles. Perhaps there are some constraints on the system that force the positions $\mathbf{x}_i$ to be restrained to a sphere. Then the set of all particle coordinates does not span all of $\mathbb{R}^{3N}$. Also, we cannot have two particles at the same point in space at the same time (this is known as a *singularity*). In any case, the set of all possible positions of the particles in a mechanical system describe an n-dimensional, differentiable manifold. This set of all the possible positions of particles in the system is called the **configuration space** of the mechanical system.

The configuration space, denoted M^n, describes every possible configuration of the system. Any possible set of positions of the particles is a point in M^n. The positions $\mathbf{x}_i$ of the particles in the mechanical system are really 3-tuples of coordinates on the configuration space (at least in our $1+3$ dimensional universe). Since one could describe equivalently the motion of each particle with respect to Cartesian coordinates, spherical coordinates, etc., we generally call the positions of particles **generalized coordinates**. We denote the i^{th} generalized coordinate by q^i.

Remark: *When working with a general manifold that is not necessarily related to a mechanical system, we use coordinates denoted x^i. When the manifold is the configuration space, we denote the coordinates by q^i (this is a common convention in the study of mechanics). In both the case of a general n-dimensional manifold and an n-dimensional configuration space, we denote the manifold by M^n.*

2.2 Vectors

Consider a differentiable manifold M^n. We can form a curve (a one-parameter, connected subset of points) $\boldsymbol{\gamma} = \boldsymbol{\gamma}(t) \in M^n$. In some coordinate patch (U, ϕ_U) with coordinates x^i_U in a neighborhood of $\boldsymbol{\gamma}(0)$, the curve is given by n component functions $x^i = x^i(t)$ such that $\boldsymbol{\gamma}(t) = (x^1(t), ..., x^n(t))$. The "velocity vector" $\dot{\boldsymbol{\gamma}}(0)$ of the curve at the point $\boldsymbol{\gamma}(0)$ has components

$$\dot{\boldsymbol{\gamma}}(0) = \left(\left.\frac{\mathrm{d}x^1}{\mathrm{d}t}\right|_{t=0}, ..., \left.\frac{\mathrm{d}x^n}{\mathrm{d}t}\right|_{t=0} \right).$$

Suppose that the curve $\boldsymbol{\gamma}$ is described in another coordinate patch (V, ϕ_V) with coordinates x^i_V in a neighborhood of the point $\boldsymbol{\gamma}(0)$: $\boldsymbol{\gamma}(t) = (y^1(t), ..., y^n(t))$; the curve should be the same object in both coordinate systems, although it might have different component functions. By applying the chain rule to the overlap map taking coordinates in U to coordinates in V, we can find the components of the "velocity vector" $\dot{\boldsymbol{\gamma}}(0)$ in the coordinate patch (V, ϕ_V):

$$\left.\frac{\mathrm{d}y^i}{\mathrm{d}t}\right|_{t=0} = \sum_{j=1}^{n} \left.\frac{\partial x^i_V}{\partial x^j_U}\right|_{\boldsymbol{\gamma}(0)} \left.\frac{\mathrm{d}x^j}{\mathrm{d}t}\right|_{t=0}$$

Here $\partial x^i_V / \partial x^j_U$ is the (i, j) component of the Jacobian of the transition function between (V, ϕ_V) and (U, ϕ_U); the Jacobian is evaluated at the point $\boldsymbol{\gamma}(0)$. In order to compute this Jacobian, we must know that the derivatives exist and are continuous; this differentiability is exactly the assumed differentiability of the overlap map from Section 2.1.

Physical laws should be coordinate independent. We should be able to freely transfer from the (U, ϕ_U) coordinate patch to the (V, ϕ_V) coordinate patch; the results of any calculations should be independent of the coordinate patch we used. Whenever a definition is made using a coordinate system, it must always be shown that the definition is coordinate independent. Coordinate independence can be shown by showing that the structure transforms linearly (e.g. like the "velocity vector"), or by defining the structure without the use of coordinates. Since the "velocity vector" of a curve transforms in a linear manner, we can more rigorously define a vector.

Definition 2.1: *A **(tangent) vector** $\mathbf{X}$ at a point $\mathbf{x} \in M^n$ is an n-tuple of real numbers*

$$(X^1_U, ..., X^n_U)$$

in some coordinate patch (U, ϕ_U) with coordinates x^i_U containing the point $\mathbf{x}$. If $\mathbf{x} \in U \cap V$, then components of the vector must transform to coordinates x^i_V in the following manner:

$$X^i_V = \sum_{j=1}^{n} \left.\frac{\partial x^i_V}{\partial x^j_U}\right|_{\mathbf{x}} X^j_U. \tag{2.1}$$

Notice that (2.1) *is exactly a change of basis for the vector $\mathbf{X}$. Any coordinate system on M^n naturally defines a basis for vectors.*

Definition 2.2: *The **tangent space** to M^n at some point $\mathbf{x} \in M^n$, denoted $TM^n_{\mathbf{x}}$, is the real vector space consisting of all the vectors $\mathbf{X}$ based at the point $\mathbf{x}$. $TM^n_{\mathbf{x}}$ is an n-dimensional differentiable manifold.*

The vector space operations act on the components of vectors just like the operations in the vector space $\mathbb{R}^n$. Note that these operations are not defined for vectors from tangent spaces over different points! We break this rule and add vectors located at different points all the time when we the base manifold is $\mathbb{R}^n$. We can add vectors from different tangent spaces when $M^n = \mathbb{R}^n$ only because the tangent spaces to $\mathbb{R}^n$ are the same at each point of $\mathbb{R}^n$. For a general differentiable manifold, however, the tangent spaces at different points are different.

Suppose we have some function $f = f(x_U^1, ..., x_U^n)$ on the manifold M^n in some coordinate patch (U, ϕ_U). We could then look at the derivative of f along the curve $\boldsymbol{\gamma}(t)$ evaluated at $t = 0$. This derivative is

$$\left.\frac{\mathrm{d}f}{\mathrm{d}t}\right|_{t=0} = \sum_{j=1}^{n} \left.\frac{\partial f}{\partial x_U^j}\right|_{\boldsymbol{\gamma}(0)} \left.\frac{\mathrm{d}x^j}{\mathrm{d}t}\right|_{t=0}.$$

Consider a first-order, linear, differential operator $\mathbf{X}$ with components X_U^j such that

$$\mathbf{X} = \sum_{j=1}^{n} X_U^j \left.\frac{\partial}{\partial x_U^j}\right|_{\boldsymbol{\gamma}(0)}.$$

The derivative of f along $\boldsymbol{\gamma}$ can be expressed as

$$\mathbf{X}(f) = \sum_{j=1}^{n} X_U^j \left.\frac{\partial f}{\partial x_U^j}\right|_{\boldsymbol{\gamma}(0)},$$

where we choose $X_U^j = dx^j/dt$. It can be shown that this first-order, linear, differential operator transforms between coordinate patches exactly like a vector. Thus, *vectors are in a* $1:1$ *correspondence with first-order, linear, differential operators.* It is quite usual to ignore the distinction; we usually write vectors as

$$\mathbf{X} = \sum_{j=1}^{n} X_U^j \left.\frac{\partial}{\partial x_U^j}\right|_{\boldsymbol{\gamma}(0)}.$$

It is also quite common to drop the subscripts reminding us of the coordinate patch we are using; the notation might re-appear if we need to show how an object transforms between coordinates (primes might also be used). Since vectors are always defined at a point, it is also common to drop the notation that reminds us where derivatives are evaluated at. With these conventions, vectors take the form

$$\mathbf{X} = \sum_{j=1}^{n} X^j \frac{\partial}{\partial x^j}. \tag{2.2}$$

Remark: *Another common notational convenience (that has already been used!) is the use of bold glyphs to represent an n-tuple of quantities. An example we've already seen quite a bit of is the point* $\mathbf{x} \in M^n$. *This quantity is, of course, an n-tuple of the values of the coordinate functions at that point. We will use indexed and/or bold quantities in this paper whenever convenient.*

The local coordinates x^i form a natural basis, also called *frame*, for the tangent space $TM_{\mathbf{x}}^n$:

$$\left(\frac{\partial}{\partial x^1}, ..., \frac{\partial}{\partial x^n}\right).$$

Recall that these operators act at the point $\mathbf{x}$. In the vector space $\mathbb{R}^n$, we (improperly) add vectors based from different points; this works only because $T\mathbb{R}_{\mathbf{x}}^n = \mathbb{R}^n$ is the same at every point. On a general manifold, the operation of addition of vectors from two different tangent spaces cannot be done as the vectors exist at different points on the manifold and the tangent spaces are not generally the same at each point; the notation describing at which point a differential operator acts makes this clear, but we have dropped this notation for convenience.

2.3 Lagrangian Mechanics

A mechanical system consisting of N particles has an n-dimensional configuration space M^n whose elements contain every possible position of the particles in the system (no singularities, however). The configuration space has the structure of a differentiable manifold. If we know Newton's equations of motion, we can use those same coordinates to introduce coordinate patches on M^n. Coordinates on the configuration

space are typically denoted q^i.

Since Newton's equations of motion give us differentiable motion, we expect that the trajectories of the particles in the system give us a corresponding differentiable curve on M^n. The tangent vector $\dot{\mathbf{q}}$ to the curve (at some point) has components that are the components of the instantaneous generalized velocities. A generalized velocity does not have to correspond to the velocity in "x" direction. A common generalized coordinate/velocity pair is angle/angular velocity, which of course has a physical meaning.

With the notion of the tangent space, we can now say that the generalized velocities of particles in the system, grouped together as $(\dot{q}^1, ..., \dot{q}^n)$ in the coordinates q^i, form a vector $\dot{\mathbf{q}} \in TM^n_{\mathbf{x}}$, where M^n is the configuration space. We then have a generalized velocity vector along each point in the trajectory of the system.

On a general manifold M^n, we have tangent spaces $TM^n_{\mathbf{x}}$ at every point $\mathbf{x} \in M^n$. Instead of being restricted to vectors at a single point, we would like to have a vector *field*, which would be a single object that defines a vector at each point of M^n. A vector field should intrinsically group every tangent space $TM^n_{\mathbf{x}}$ together; thus, we have the following definition.

Definition 2.3: *The **tangent bundle** TM^n of M^n is the union of all the tangent spaces $TM^n_{\mathbf{x}}$, $\mathbf{x} \in M^n$:*

$$TM^n = \bigcup_{\mathbf{x} \in M^n} TM^n_{\mathbf{x}}.$$

If x^i are some local coordinates on M^n, the $\partial/\partial x^i$ form a local basis of $TM^n_{\mathbf{x}}$, and X^i are the components a vector $\mathbf{X} \in TM^n_{\mathbf{x}}$. The $(x^1, ..., x^n, X^1, ..., X^n)$ then form a set of $2n$ local coordinates on TM^n. We also have a projection map $\pi : TM^n \to M^n$ that picks off the coordinates $(x^1, ..., x^n)$. The tangent bundle TM^n is naturally a $2n$-dimensional differentiable manifold.

Remark: *There is much more structure to the tangent bundle, but we don't need it for this paper.*

The notion of a vector field can now be expressed in terms of the tangent bundle. A vector field $\mathbf{X} : M^n \to TM^n$ is a map from the manifold to the tangent bundle. At each point $\mathbf{x} \in M^n$, the vector field $\mathbf{X}$ defines a vector in the tangent space $TM^n_{\mathbf{x}}$. Thus, at each point in the manifold, a vector field is a vector, just as we wanted.

In a *Lagrangian* mechanical system, we construct a function $L : TM^n \to \mathbb{R}$ that gives us equations of motion that are compatible with Newton's equations of motion. If Newton's equations of motion (in Cartesian coordinates) are of the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(m_i \mathbf{x}_i\right) = -\frac{\partial}{\partial \mathbf{x}_i} U,$$

then the *Lagrangian function* of the system is of the form $L = T - U$, where T is the kinetic energy and U is the potential energy of the system. A *motion* of the system $\boldsymbol{\gamma}(t)$ is a curve on the configuration space M^n given by the solution of the equations of motion of the system. *Hamilton's principle of least action* states that the motion of the system $\boldsymbol{\gamma}(t)$ is the extremal that minimizes the *action* functional

$$S[\boldsymbol{\gamma}] = \int_{t_0}^{t_1} L \, \mathrm{d}t.$$

If the motion $\boldsymbol{\gamma}(t)$ and Lagrangian function $L = L(\mathbf{q}, \dot{\mathbf{q}})$ are expressed in local coordinates q^i, then the coordinates evolve with time via the Euler-Lagrange equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i} = 0. \tag{2.3}$$

The Euler-Lagrange equations of motion are, in essence, nothing more than a generalization of Newton's equations of motion. They are found by constructing a variational principle that is consistent with Newton's

equations of motion.

By considering particle motion as motion on the configuration space and introducing the Lagrangian function L, we have described the dynamical system in terms of the tangent bundle TM^n instead of just M^n. The methods in Lagrangian mechanics are quite powerful, but are not the focus of this paper. Hamiltonian mechanics is, in a sense, the "dual" of Lagrangian mechanics; the goals are the same, but the structure is different. Instead of using (only) the language of vectors, Hamiltonian mechanics is written in the language of differential forms.

2.4 Differential 1-Forms

Recall that any vector $\mathbf{X} \in TM^n_{\mathbf{x}}$ is in a $1:1$ correspondence with a first-order, linear differential operator. In some local coordinates x^i on M^n, $\mathbf{X}$ acts on a function $f : M^n \to \mathbb{R}$ and returns a real number:

$$\mathbf{X}(f) = \sum_{i=1}^{n} X^i \frac{\partial f}{\partial x^i}. \tag{2.4}$$

In a calculus class, one may have studied the total derivative of a function of multiple variables; given $f(x^1, ..., x^n)$, the *total derivative* is

$$\mathrm{d}f = \sum_{i=1}^{n} \frac{\partial f}{\partial x^i}\mathrm{d}x^i = \frac{\partial f}{\partial x^1}\mathrm{d}x^1 + ... + \frac{\partial f}{\partial x^n}\mathrm{d}x^n. \tag{2.5}$$

With the exception of the components of the vector in (2.4), the total derivative (2.5) has a similar action on f. It is possible to relate the two objects in a coordinate invariant manner.

Definition 2.4: *The **differential** of some function $f : M^n \to \mathbb{R}$ at a point $\mathbf{x} \in M^n$, is the linear functional $\mathrm{d}f : TM^n_{\mathbf{x}} \to \mathbb{R}$ defined by*

$$\mathrm{d}f(\mathbf{X}) = \mathbf{X}(f). \tag{2.6}$$

This definition does not utilize a coordinate patch on M^n. This definition is then "automatically" coordinate invariant. If we were to define *df* in terms of some coordinates, coordinate invariance must be shown in order that *df* be well defined.

The differential of f at a point is a map that takes a *vector* and returns a real number. If x^i are local coordinates for M^n, then

$$\mathrm{d}f = \sum_{i=1}^{n} \frac{\partial f}{\partial x^i}\mathrm{d}x^i.$$

is a proposed form for $\mathrm{d}f$. With this form, the left-hand side of (2.6) is

$$\mathrm{d}f(\mathbf{X}) = \sum_{i=1}^{n} \frac{\partial f}{\partial x^i}\mathrm{d}x^i \left(\sum_{j=1}^{n} X^j \frac{\partial}{\partial x^j} \right).$$

The "dual vector" $\mathrm{d}x^i$ is a linear functional that acts on the natural basis vectors $\partial/\partial x^j$ of the local coordinate system x^i via

$$\mathrm{d}x^i \left(\frac{\partial}{\partial x^j} \right) = \delta^i_j,$$

where δ^i_j is the **Kronecker delta symbol**:

$$\delta^i_j = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}.$$

Using the linearity of the $\mathrm{d}x^i$, we can write (2.6) in coordinates as

$$\mathrm{d}f(\mathbf{X}) = \sum_{i=1}^{n} \frac{\partial f}{\partial x^i} \sum_{j=1}^{n} X^j \delta^i_j = \sum_{i=1}^{n} X^i \frac{\partial f}{\partial x^i} = \mathbf{X}(f).$$

In coordinates x^i, the set of vectors of the form $\partial/\partial x^i$ form a basis for the tangent space at a point. The $\mathrm{d}x^i$ are linear functionals that act on the basis vectors $\partial/\partial x^i$ and return a Kronecker delta symbol. The $\mathrm{d}x^i$ form a basis for the "dual" of the tangent space at a point.

Definition 2.5: *The **dual space** of a real vector space V is the real vector space V^* whose elements are linear functionals $\alpha : V \to \mathbb{R}$ on the vector space V. Linearity gives us the following property:*

$$\alpha(a\mathbf{X} + b\mathbf{Y}) = a\alpha(\mathbf{X}) + b\alpha(\mathbf{Y}) \qquad \mathbf{X}, \mathbf{Y} \in V, \quad \alpha \in V^*, \quad a, b \in \mathbb{R}.$$

Vector addition and scalar multiplication in V^* are

$$(\alpha + \beta)(\mathbf{X}) = \alpha(\mathbf{X}) + \beta(\mathbf{X}) \qquad \mathbf{X} \in V, \quad \alpha, \beta \in V^*$$
$$(c\alpha)(\mathbf{X}) = c\alpha(\mathbf{X}) \qquad \mathbf{X} \in V, \alpha \in V^*, c \in \mathbb{R}.$$

The dual space to $TM^n_{\mathbf{x}}$ is a vector space, so we can form dual vectors α as linear combinations of the dual basis vectors $\mathrm{d}x^i$. We can choose the coefficients of the dual vector at $\mathbf{x} \in M^n$ to be those of a differential evaluated at $\mathbf{x}$. In fact, we can choose any real coefficients we like.

Definition 2.6: *A **differential 1-form**, **1-form**, or **covector** α^1 at a point $\mathbf{x} \in M^n$ is an n-tuple of real numbers*

$$(a^U_1, ..., a^U_n)$$

in some coordinate patch (U, ϕ_U) with coordinates x^i_U containing $\mathbf{x}$. If $\mathbf{x} \in U \cap V$, then components of the differential 1-form must transform to coordinates x^i_V in the following manner:

$$a^V_i = \sum_{j=1}^{n} \left.\frac{\partial x^i_U}{\partial x^j_V}\right|_{\mathbf{x}} a^U_j. \tag{2.7}$$

In some local coordinate system x^i on M^n, α^1 can be expressed in the dual basis $\mathrm{d}x^i$ as

$$\alpha^1 = \sum_{i=1}^{n} a_i \mathrm{d}x^i. \tag{2.8}$$

The linear combination (2.8) is the most general 1-form. Note that the superscript 1 on α^1 is not a coordinate or component index, but a reminder that α^1 is a 1-form (later on, we will see how to join 1-forms together to build higher-order differential forms).

Since we use the dual of $TM^n_{\mathbf{x}}$ quite frequently, we will give it a special name.

Definition 2.7: *The **cotangent space** $T^*M^n_{\mathbf{x}}$ at a point $\mathbf{x} \in M^n$ is the dual space to the tangent space $TM^n_{\mathbf{x}}$. Just as vectors at $\mathbf{x}$ are elements of $TM^n_{\mathbf{x}}$, differential 1-forms α^1 at $\mathbf{x}$ are elements of the cotangent space: $\alpha^1 \in T^*M^n_{\mathbf{x}}$. In some local coordinates x^i for M^n, the dual vectors dx^i form a basis of the dual space $T^*M^n_{\mathbf{x}}$. The union of all of the cotangent spaces over all points in the manifold form the **cotangent bundle***

$$T^*M^n = \bigcup_{\mathbf{x} \in M^n} T^*M^n_{\mathbf{x}}.$$

If $\alpha^1 \in T^*M^n_{\mathbf{x}}$ is given by components a_i in some local coordinates x^i, then local coordinates on T^*M^n are $\big(x^1, ..., x^n, a_1, ..., a_n\big)$. We also have a projection map $\pi : T^*M^n \to M^n$ that picks off the coordinates $(x^1, ..., x^n)$. Just like the tangent space $TM^n_{\mathbf{x}}$ and tangent bundle TM^n, the cotangent space $T^*M^n_{\mathbf{x}}$ is an n-dimensional differentiable manifold and the cotangent bundle T^*M^n is a $2n$-dimensional differentiable

manifold.

As one might expect, this "local product" structure of T^*M^n is very similar to TM^n. Just like the tangent bundle TM^n, the cotangent bundle T^*M^n has a lot of structure that we will not need for our purposes. However, the cotangent bundle plays a crucial role in the formulation of Hamiltonian mechanics. It is in this context that we will study the cotangent bundle in further detail in the next few sections.

2.5 Exterior Product of Differential Forms

It turns out that we can extend the idea of the differential of functions to derivatives of 1-forms. In this generalization, we think of functions as 0-forms, and this derivative would take 0-forms to 1-forms, so that it is consistent with the differential. In fact, this derivative is based on the differential of 0-forms. The extension of the differential requires a product structure that allows us to build higher degree forms. Although this product structure can be generalized to more than just differential forms, *we will consider only the case of differential forms.*

As a start, this product should take two 1-forms and give back what we will call a "2-form". The "2-form", let us denote it ω^2, will thus be built of two 1-forms, will take two vectors as arguments, and will return a scalar. This "2-form" ω^2 (at some point $\mathbf{x} \in M^n$) is a mapping

$$\omega^2 : TM^n_{\mathbf{x}} \times TM^n_{\mathbf{x}} \to \mathbb{R},$$

where the superscript 2 on ω^2 reminds us that ω^2 is a "2-form".

Definition 2.8: *A **k-form** is a k-linear, skew-symmetric functional of k vectors* $\mathbf{X}_i \in TM^n_{\mathbf{x}}$

$$\omega^k : \underbrace{TM^n_{\mathbf{x}} \times ... \times TM^n_{\mathbf{x}}}_{k \text{ copies}} \to \mathbb{R}.$$

The k-linearity of ω^k is

$$\omega^k(a\mathbf{X}'_1 + b\mathbf{X}''_1, \mathbf{X}_2, ..., \mathbf{X}_k) = a\omega^k(\mathbf{X}'_1, \mathbf{X}_2, ..., \mathbf{X}_k) + b\omega^k(\mathbf{X}''_1, \mathbf{X}_2, ..., \mathbf{X}_k),$$

for the first argument. The remaining arguments are also linear. The skew-symmetry of ω^k is

$$\omega^k(\mathbf{X}_{i_1}, ..., \mathbf{X}_{i_k}) = (-1)^\nu \omega^k(\mathbf{X}_1, ..., \mathbf{X}_k),$$

where

$$\nu = \begin{cases} 0 & \text{if the permutation } (i_1, ..., i_k) \text{ is even} \\ 1 & \text{if the permutation } (i_1, ..., i_k) \text{ is odd} \end{cases}$$

If we apply ω^p a linearly dependent set of vectors (e.g. $\mathbf{X}_1, \mathbf{X}_1, \mathbf{X}_2, ..., \mathbf{X}_{i_{k-1}}$), we must have $\omega^p(\mathbf{X}_1, \mathbf{X}_1, \mathbf{X}_2, ..., \mathbf{X}_{i_{k-1}}) = 0$.

As both an example of a higher degree form and an introduction to the product structure for differential forms, we now present a special case of the product structure.

Definition 2.9: *The **exterior product**, or **Grassman product** of two 1-forms $\alpha^1, \beta^1 \in T^*M^n_{\mathbf{x}}$ is the quantity*

$$\omega^2 = \alpha^1 \wedge \beta^1,$$

where $\wedge$ is also called the wedge product. *If $\mathbf{X}, \mathbf{Y} \in TM^n_{\mathbf{x}}$,*

$$\omega^2(\mathbf{X}, \mathbf{Y}) = \alpha^1(\mathbf{X})\beta^1(\mathbf{Y}) - \alpha^1(\mathbf{Y})\beta^1(\mathbf{X}).$$

This "product of monomials" has some nice properties:

Theorem 2.1: *The product $\omega^2 = \alpha^1 \wedge \beta^1$, where $\alpha^1, \beta^1 \in T^*M^n_{\mathbf{x}}$, has the following properties:*

- *ω^2 is a 2-form (2-linear and antisymmetric)*
- *distributivity:* $\left(\alpha^1 + \beta^1\right) \wedge \gamma^1 = \alpha^1 \wedge \gamma^1 + \beta^1 \wedge \gamma^1 \qquad a, b \in \mathbb{R}$
- *associativity:* $\left(\alpha^1 \wedge \beta^1\right) \wedge \gamma^1 = \alpha^1 \wedge \left(\beta^1 \wedge \gamma^1\right)$

Note that the product of 1-forms is anticommutative:

$$\alpha^1 \wedge \beta^1 = -\beta^1 \wedge \alpha^1,$$

which implies

$$\alpha^1 \wedge \alpha^1 = 0 \quad \forall \alpha^1 \in T^*M^n_{\mathbf{x}}.$$

From the exterior product of 1-forms, we can build up any k-form we like. If the x^i are a local coordinate system on M^n, then the $\mathrm{d}x^i$ form a natural basis for $T^*M^n_{\mathbf{x}}$ for any $\mathbf{x}$ in the coordinate patch. A k-form ω^k in the coordinates x^i is of the form

$$\omega^k = \sum_{i_1,\ldots,i_k} a_{i_1,\ldots,i_k} \mathrm{d}x^{i_1} \wedge \ldots \wedge \mathrm{d}x^{i_k},$$

where the $a_{i_1,\ldots,i_k}$ are the components of ω^k. We also know that the *basic forms* $\mathrm{d}x^{i_1} \wedge \ldots \wedge \mathrm{d}x^{i_k}$ form a basis for the k-forms on $T^*M^n_{\mathbf{x}}$.

From the skew-commutativity and associativity of the exterior product, we know that there are

$$\binom{n}{k} = \frac{n!}{k!(n-k)!}$$

basis k-forms. Thus, all of the k-forms with $k > n$ are identically zero.

The exterior product of a k-form and a l-form is now given.

Definition 2.10: *The **exterior product**, or **Grassman product** of a k-form ω^k and a l-form ω^l is the $(k+l)$-form $\omega^k \wedge \omega^l$ whose value on the vectors $\mathbf{X}_1, \ldots, \mathbf{X}_{k+l} \in TM^n_{\mathbf{x}}$ is*

$$\omega^k \wedge \omega^l(\mathbf{X}_1, \ldots, \mathbf{X}_{k+l}) = \sum (-1)^\nu \omega^k(\mathbf{X}_{i_1}, \ldots, \mathbf{X}_{i_k}) \omega^l(\mathbf{X}_{j_1}, \ldots, \mathbf{X}_{j_l}), \tag{2.9}$$

where $i_1 < \ldots < i_k$, $j_1 < \ldots < j_l$, and

$$\nu = \begin{cases} 0 & \text{if the permutation } (i_1, \ldots, i_k, j_1, \ldots, j_l) \text{ is even} \\ 1 & \text{if the permutation } (i_1, \ldots, i_k, j_1, \ldots, j_l) \text{ is odd} \end{cases}.$$

Again, we have skew-commutativity, distributivity, and associativity:

$$\begin{aligned}\omega^k \wedge \omega^l &= (-1)^{kl}\omega^l \wedge \omega^k \\ \left(a\omega^k + b\rho^k\right) \wedge \omega^l &= a\omega^k \wedge \omega^l + b\rho^k \wedge \omega^l \qquad a, b \in \mathbb{R} \\ \left(\omega^k \wedge \omega^l\right) \wedge \omega^r &= \omega^k \wedge \left(\omega^l \wedge \omega^r\right).\end{aligned}$$

In the case of the exterior product of two 1-forms α^1 and β^1, the factor $(-1)^\nu$ puts the action of the product $\alpha^1 \wedge \beta^1$ on two vectors into the form the determinant of a 2×2 matrix. This generalizes to the case of the exterior product of a k-form and an l-form, where we would be taking the determinant of a $(k+l) \times (k+l)$ matrix. It should be noted that we do not always think of the exterior product in terms of determinants; the properties of the exterior product allow us to work with higher degree forms without relying on their action of a set of vectors.

In Hamiltonian mechanics, the exterior product is used quite frequently. There is a 2-form that naturally appears on the configuration space of a mechanical system and is based on the momenta and generalized coordinates of the particles in the mechanical system. We will see what this 2-form is in Section 3.2.

2.6 Exterior Derivative of Differential Forms

Now that we can construct k-forms, we can generalize the differential of 0-forms (i.e. functions). In local coordinates x^i, a 1-form $\alpha^1 \in T^*M$ can be expressed as

$$\alpha^1 = \sum_{i=1}^{n} a_i \mathrm{d}x^i,$$

where the a_i are functions of the x^i since $\alpha^1 \in T^*M^n$. The a_i can really be though of as 0-forms, and with the exterior product,

$$\alpha^1 = \sum_{j=1}^{n} a_i \wedge \mathrm{d}x^i.$$

We do not usually write the $\wedge$ when we take the exterior product of a 0-form with another form, even though that is actually what is being done. We know how to take differentials of 0-forms (functions), and we know how to take exterior products; thus, we can generalize the differential.

Definition 2.11: *The* ***exterior derivative*** d *is the unique operator that takes k-forms to $k+1$-forms and satisfies*

- d *is additive:* $\mathrm{d}(\alpha^k + \beta^k) = \mathrm{d}\alpha^k + \mathrm{d}\beta^k$
- $\mathrm{d}\alpha^0$ *is the usual differential of the function* α^0
- $\mathrm{d}(\alpha^k \wedge \beta^l) = \mathrm{d}\alpha^k \wedge \beta^l + (-1)^k \alpha^k \wedge \mathrm{d}\beta^l$
- $\mathrm{d}^2(\alpha^k) = \mathrm{d}\left(\mathrm{d}\alpha^k\right) = 0$ *for all* α^k

For some k-form in local coordinates x^i, where the basic forms $\mathrm{d}x^{i_1} \wedge ... \wedge \mathrm{d}x^{i_k}$ form a basis for $T^*M^n_{\mathbf{x}}$, the k-form can be expressed as

$$\alpha^k = \sum a_{i_1,...,i_k} \mathrm{d}x^{i_1} \wedge ... \wedge \mathrm{d}x^{i_k}.$$

In those same local coordinates,

$$\mathrm{d}\alpha^k = \sum \mathrm{d}a_{i_1,...,i_k} \wedge \mathrm{d}x^{i_1} \wedge ... \wedge \mathrm{d}x^{i_k}. \tag{2.10}$$

The properties of d can be shown to be coordinate independent, and the form of $\mathrm{d}\alpha^k$ in Equation (2.10) is well defined. When changing coordinates, each $\mathrm{d}x^{i_k}$ changes according to the transformation (2.7).

Definition 2.12: *A differential k-form α^k is called **closed** if $\mathrm{d}\alpha^k = 0$. A differential k-form β^k is called **exact** if there exists a differential $(k-1)$-form ω^{k-1} such that $d\omega^{k-1} = \beta^k$.*

Every exact k-form is closed, since $\omega^k = \mathrm{d}\omega^{k-1} \implies \mathrm{d}\omega^k = \mathrm{d}^2\omega^{k-1} = 0$. However, not every closed k-form is exact, since one cannot always find α^{k-1} such that $\mathrm{d}\alpha^{k-1} = \omega^k$.

A differential 1-form α^1 is exact if there exists a function $f : M^n \to \mathbb{R}$ such that $df = \alpha^1$; this is analogous to a vector field in $\mathbb{R}^3$ being the gradient of some function. It turns out that we can write every bit of vector analysis in $\mathbb{R}^3$, in any coordinate system, very efficiently in the language of differential forms.

Thus far, we have encountered a lot more structure for differential forms than for vectors. This is not an accident! There is a substantial amount of structure that comes from using differential forms. Every differentiable manifold has a cotangent bundle and thus a vector space of differential forms at every point; this includes the configuration space of a mechanical system. As we will see in the next few sections, working with *covector fields* (like vector fields, covector fields define a differential form at every point on the manifold) can be much "nicer" than working with vector fields.

2.7 Flows

When we defined vectors $\mathbf{X} \in TM^n_{\mathbf{x}}$ in Section 2.2, we considered "velocity vectors" of curves on M^n. Instead of constructing a curve through $\mathbf{x} \in M^n$, we can smoothly map M^n into itself and construct vectors from this mapping.

Definition 2.13: *A **diffeomorphism** $g : M^n \to N^n$ is a mapping of the n-dimensional differentiable manifold M^n to the n-dimensional differentiable manifold N^n such that both g and g^{-1} are differentiable mappings. A differentiable mapping takes coordinates on M^n and maps them to coordinates on N^n in a differentiable manner.*

In a mechanical system, we express the position of the particles by generalized coordinates $\mathbf{q} = \left(q^1, ..., q^n\right)$. The equations of motion of the system tell us how the positions $\mathbf{q}$ evolve with time. From this, we constructed curves that allowed us to define generalized velocity vectors. We would like to consider the evolution of $\mathbf{q}$ forward in time by some amount τ as being a diffeomorphism $g^\tau : M^n \to M^n$. There is nothing special about our choice of τ; we would like to be able to pick any $\tau \in \mathbb{R}$, as it would move our coordinates $\mathbf{q}$ forward or backward in time. These "flows" of points would then completely describe the evolution of the mechanical system.

Definition 2.14: *A **one-parameter group of transformations** is a family of mappings $\{g^t\}$ that map a set M into itself and is indexed by $t \in \mathbb{R}$ such that*

$$g^{s+t} = g^s g^t \quad \forall s, t \in \mathbb{R},$$

and g^0 is the identity mapping that leaves every element of M fixed.

Due to the commutativity of the group $(\mathbb{R}, +)$, we know that a one-parameter group of transformations must be commutative.

In the context of a mechanical system, a certain one-parameter group of transformations of the configuration space M^n moves the generalized coordinates of the particles forward (or backward) in time according to the equations of motion. From Newton's principle of determinacy (see Section 1.1), we know that motions of a mechanical system are deterministic. Therefore, the description of the motion of a mechanical system by a one-parameter (commutative) group of transformations of the configuration space is consistent with Newton's principle of determinacy.

Remark: *Later on, we will see exactly how these groups of transformations are related to our new, first-order equations of motion, and more generally, systems of first-order ordinary differential equations. Arnold gives a geometric treatment of the theory of first-order ODE in [2], in which Arnold spends a great deal of time working with* flows*, as they are in a* $1:1$ *correspondence with first-order systems of ODE.*

For a mechanical system obeying some differential equations of motion, the group of transformations of the configuration space should also be a differentiable mapping.

Definition 2.15: *A* ***one-parameter group of diffeomorphisms****, or* ***(phase) flow*** *is a one-parameter group of transformations* $\{g^t\}$ *of a manifold* M^n*:*

$$g : \mathbb{R} \times M^n \to M^n \qquad g(t, \mathbf{x}) = g^t \mathbf{x} \quad t \in \mathbb{R},\ \mathbf{x} \in M^n.$$

The mapping $g : \mathbb{R} \times M^n \to M^n$ *is a differentiable mapping (but not a diffeomorphism). The mapping* $g^t : M^n \to M^n$ *is a diffeomorphism for each* $t \in \mathbb{R}$*. The inverse mapping* $(g^t)^{-1}$ *is* g^{-t}*.*

Remark: *In other texts the flow is denoted* (M^n, g^t)*. The distinction is that the flow is always given in terms of the manifold that the mapping acts on. For notational convenience, we commonly denote a flow* $\{g^t\}$ *by an* element g^t *of the flow.*

Let $g^t : M^n \to M^n$ be an element of a one-parameter group of diffeomorphisms of M^n. We can define a curve $\boldsymbol{\gamma}$ going through some point $\mathbf{x}$ as being the set of image points $g^t\mathbf{x}$ where $t \in \mathbb{R}$:

$$\boldsymbol{\gamma}(t) = g^t \mathbf{x} \qquad \mathbf{x} \in M^n, \quad t \in \mathbb{R}.$$

Also note that $\boldsymbol{\gamma}(0) = g^0\mathbf{x} = \mathbf{x}$ exactly as before. From this, we get an equivalent definition of a vector $\mathbf{X} \in TM^n_{\mathbf{x}}$:

$$\mathbf{X} = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \left(g^t \mathbf{x}\right). \tag{2.11}$$

From this, we can see that the correspondence between vector fields $\mathbf{X}$ and flows g^t is one-to-one, and flows are in a one-to-one correspondence with first-order, linear, differential operators.

2.8 Push-forwards and Pull-backs

A flow g^t takes points $\mathbf{x} \in M^n$ to points $\mathbf{y} \in M^n$ in a differentiable manner. We can define a vector $\mathbf{X} \in TM^n_{\mathbf{x}}$ and a vector $\mathbf{Y} \in TM^n_{\mathbf{y}}$ using the flow g^t and (2.11). It turns out that a curve defined by g^t that connects $\mathbf{x}$ and $\mathbf{y}$ with velocity vector $\mathbf{X}$ at $\mathbf{x}$ and velocity vector $\mathbf{Y}$ at $\mathbf{y}$ is unique. It turns out that we can construct a mapping between $TM^n_{\mathbf{x}}$ and $TM^n_{\mathbf{y}}$ using the flow g^t.

Instead of constructing a mapping between tangent spaces of the same manifold, we can "do one better". If we have a differentiable mapping between a manifold M^n and another manifold N^r, we can construct a mapping from tangent spaces $TM^n_{\mathbf{x}}$ to tangent spaces $TN^r_{f(\mathbf{x})}$; this will, of course, work for the case where $M^n = N^r$.

Definition 2.16: *The* ***differential*** *of the differentiable mapping* $f : M^n \to N^r$*, or* ***push-forward*** *at a point* $\mathbf{x} \in M^n$ *is the linear mapping of the tangent spaces*

$$f_{*\mathbf{x}} : TM^n_{\mathbf{x}} \to TN^r_{f(\mathbf{x})}.$$

If x^i *are coordinates for* M^n *in a coordinate patch containing* $\mathbf{x}$ *and* y^m *are coordinates in a coordinate patch containing* $f(\mathbf{x})$*, then the linear transformation* $f_{*\mathbf{x}}$ *is given by the Jacobian* $\partial y^m / \partial x^i$*.*

Remark: *One must be careful with the push-forward: Let $f : M^n \to N^r$ and $\mathbf{X} \in TM^n$. It is very well possible that, under the map f, two points $\mathbf{x}, \mathbf{x}' \in M^n$ get mapped to the same point $\mathbf{y} \in N^r$. The vector field $\mathbf{X}$ at some point $\mathbf{x}$ is denoted $\mathbf{X}(\mathbf{x})$.*

The push-forward takes $\mathbf{X}(\mathbf{x})$ to $f_{*\mathbf{x}}\mathbf{X}(\mathbf{x})$ and $\mathbf{X}(\mathbf{x}')$ to $f_{*\mathbf{x}'}\mathbf{X}(\mathbf{x}')$. But these two new vectors are based over the same point $\mathbf{y} = f(\mathbf{x}) = f(\mathbf{x}')$. Thus, the push-forward does not take vector fields to vector fields, even though it maps tangent spaces to tangent spaces! We can fix this by instead mapping differential forms.

If $\mathbf{X} \in TM^n_{\mathbf{x}}$, $n = r$, and f is $1:1$ (so f^{-1} exists locally), then the differential map $f_{*\mathbf{x}}$ takes $\mathbf{X}$ to a *vector* $\mathbf{Y} \in TN^r_{f(\mathbf{x})}$ given by the components

$$Y^m = \sum_{i=1}^{n} \frac{\partial y^m}{\partial x^i} X^i \quad m = 1, ..., r. \tag{2.12}$$

The assumptions on the dimension of N^r and the $1:1$ nature of f allow us to map vectors to vectors. We could just as easily construct the differential map of elements of a flow; then the conditions $n = r$ and the $1:1$ nature of the map are satisfied (since g^t is a diffeomorphism for all $t \in \mathbb{R}$). These mappings would then map tangent spaces of M^n to other tangent spaces of M^n. Further, we can construct a mapping between tangent bundles:

$$f_*\mathbf{X} = f_{*\mathbf{x}}\mathbf{X} \text{ for } \mathbf{X} \in TM^n_{\mathbf{x}},$$

where $f_{*\mathbf{x}} : TM^n_{\mathbf{x}} \to TN^r_{f(\mathbf{x})}$ and $f_* : TM^n \to TN^r$. We have the following commutative diagram for the push-forward:

$$\begin{array}{ccc} TM^n & \xrightarrow{f_*} & TN^r \\ \downarrow{\scriptstyle \pi_M} & & \downarrow{\scriptstyle \pi_N} \\ M^n & \xrightarrow{f} & N^r \end{array}$$

Recall that π_M and π_N are the projection mappings for the tangent bundles TM^n and TN^r, respectively (see Section 2.3).

There also a way of mapping cotangent spaces of M^n to cotangent spaces of N^r.

Definition 2.17: *Let $f : M^n \to N^r$ be a differentiable map, $\mathbf{x} \in M^n$, $\mathbf{y} = f(\mathbf{x}) \in N^r$, and $f_{*\mathbf{x}} : TM^n_{\mathbf{x}} \to TN^r_{f(\mathbf{x})}$ be the differential of f at $\mathbf{x}$. The **pull-back** $f^*_{f(\mathbf{x})}$ is the linear transformation taking $T^*N^r_{f(\mathbf{x})}$ to $T^*M^n_{\mathbf{x}}$ defined by*

$$f^*_{f(\mathbf{x})}(\alpha^1)(\mathbf{X}) = \alpha^1(f_{*\mathbf{x}}\mathbf{X}) \tag{2.13}$$

for all 1-forms $\alpha^1 \in T^*N^r_{f(\mathbf{x})}$ and vectors $\mathbf{X} \in TM^n_{\mathbf{x}}$.

In some coordinates x^i on M^n in a coordinate patch containing $\mathbf{x}$ and coordinates y^i on N^r in a coordinate patch containing $f(\mathbf{x})$, we can write down the components of $f^*_{f(\mathbf{x})}\alpha^1$ in terms of the components of α^1. Let

$$\alpha^1 = \sum_{m=1}^{r} a_m \mathrm{d}y^m,$$

and $\beta^1 = f^*_{f(\mathbf{x})}\alpha^1$ with components b_i such that

$$\beta^1 = \sum_{i=1}^{n} b_i \mathrm{d}x^i.$$

Under the pull-back, the components of α^1 transform as

$$b_i = \sum_{m=1}^{r} \frac{\partial y^m}{\partial x^i} a_m. \tag{2.14}$$

Most of the time, we write the pull-back of a differential form α as $f^*\alpha$, where we drop the notation reminding us which cotangent space α is from. Similarly, we usually write the push-forward as f_*. These operations are defined for the cotangent bundle and tangent bundle respectively. In exactly the same manner as the differential for the tangent bundle, we can construct the pull-back for the cotangent bundle T^*N^r, and we have the commutative diagram:

$$\begin{array}{ccc} T^*M^n & \xleftarrow{f^*} & T^*N^r \\ \downarrow{\scriptstyle \pi_M} & & \downarrow{\scriptstyle \pi_N} \\ M^n & \xrightarrow{f} & N^r \end{array}$$

We can also pull-back higher degree forms:

$$f^*(\alpha^k)(\mathbf{X}_1, ..., \mathbf{X}_k) = \alpha^k(f_*\mathbf{X}_1, ..., f_*\mathbf{X}_k).$$

The pull-back of higher degree forms is crucial in integration of forms over manifolds; the interested reader is recommended to read Frankel [7].

Remark: *The major difference between the push-forward and the pull-back, besides mapping vectors and covectors (1-forms), is that* the pull-back of a covector field is always defined*! This is one of the most attractive features of working with differential forms, especially since we do not have this property for the push-forward of vector fields.*

The pull-back of differential forms can be used to develop integration of differential forms over differentiable manifolds. We already know how to compute integrals of functions over *oriented* subsets $(U, o) \subset \mathbb{R}^n$:

$$\int_{(U,o)} u(x^1, ..., x^n) \mathrm{d}x^1 \wedge ... \wedge \mathrm{d}x^n = o(\mathbf{x}) \int_U u(x^1, ..., x^n) \mathrm{d}x^1 ... \mathrm{d}x^n,$$

where $o = o(\mathbf{x}) = \pm 1$ is $+1$ if the orientation of the coordinate basis

$$\left(\frac{\partial}{\partial x^1}, ..., \frac{\partial}{\partial x^n} \right)$$

matches the orientation of o. If we have a mapping $f : U \to M^n$, we can use the pull-back of this map to define the integral of differential forms over subsets of M^n. The following is just a sketch of what can be done. For a more rigorous, complete treatment of the integration of differential forms, see Frankel [7].

Define an **oriented, parameterized k-subset** of a manifold M^n as the pair $(U, o; f)$ where (U, o) is an oriented subset of $\mathbb{R}^k$ and

$$f : U \to M^n$$

is a differentiable map. In the case $k = 1$, we have a curve on M^n with a specific parameterization. In any case, the push-forward f_* might take a vector field and map it to the zero vector at a point (we can call this "rank deficient"); such a point is called a *singular point*. It turns out that in most important cases, the push-forward f_* has "rank" k "almost everywhere".

We can define the integral of some k-form field α^k on M^n, defined in coordinate patches covering $f(U)$, over the oriented, parameterized k-subset $(U, o; f)$ as

$$\int_{(U,o;f)} \alpha^k = \int_{(U,o)} f^* \alpha^k.$$

If we have another map $\phi : M^n \to N^r$, we can map the k-subset $(U, o; f)$ to a k-subset $(U, o; \phi \circ f)$ of N^r. If we let $\sigma = (U, o; f)$ and $\phi(\sigma) = (U, o; \phi \circ f)$, then the above definition of the integral of a k-form can be generalized. If ω^k is a k-form on N^r, we can pull ω^k back to M^n and compute the integral:

$$\int_{\phi(\sigma)} \omega^k = \int_\sigma \phi^* \omega^k.$$

Finally, we state Stokes's Theorem. It highlights the structure that has been developed for differential forms.

Stokes's Theorem: *Let $V^k \subset M^n$ be a compact, oriented submanifold of M^n with boundary $\partial V^k \subset M^n$. If ω^{k-1} is a $(k-1)$-form on M^n, then*

$$\int_{\partial V^k} \omega^{k-1} = \int_{V^k} \mathrm{d}\omega^{k-1}.$$

In the case $k = 1$, Stokes's Theorem simplifies to the Fundamental Theorem(s) of calculus!

By now, we hope the reader is sufficiently comfortable with vector fields and differential forms on manifolds. For much more detail and formality, the reader is recommended to Frankel [7]. In the following section on Hamiltonian mechanics, the "language" of vector fields and differential forms is quite prevalent. In Newtonian mechanics, the geometry underlying the problem is not always apparent; this is most definitely not the case in Hamiltonian mechanics.

3 Hamiltonian Mechanics

Hamiltonian mechanics is geometry in phase space – V.I. Arnold [3].

3.1 Hamilton's Equations of Motion

In Section 2.3 we briefly explained how Lagrangian mechanics can be developed from Newtonian mechanics. Consider the configuration space M^n of some mechanical system. In Lagrangian mechanics, one constructs the *Lagrangian* $L : TM^n \to \mathbb{R}$ such that

$$L = T - V,$$

where T is the total kinetic energy and V is the total potential energy. Hamilton's principle of least action states the motion $\boldsymbol{\gamma}$ of a mechanical system in configuration spaces minimizes the action functional

$$S[\boldsymbol{\gamma}] = \int_{t_0}^{t_1} L \, \mathrm{d}t.$$

In general $L = L(\mathbf{q}, \dot{\mathbf{q}}, t)$, where the q^i are generalized coordinates on M^n and $\mathbf{q} = \left(q^1, ..., q^n\right)$. Note that we treat $\mathbf{q}$ and $\dot{\mathbf{q}}$ as $2n$ *independent* variables. If we consider a motion of the system, then we will have $\mathbf{q} = \mathbf{q}(t)$ and $\dot{\mathbf{q}} = d\mathbf{q}/dt$ will be determined from that motion; until we have defined the motion, however, we treat $\mathbf{q}$ and $\dot{\mathbf{q}}$ as being independent.

In the autonomous case where $L = L(\mathbf{q}, \dot{\mathbf{q}})$, a necessary condition for the motion $\boldsymbol{\gamma}$ of a Lagrangian mechanical system to minimize the action functional S is that the generalized coordinates evolve according to the n second-order Euler-Lagrange equations:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{\mathbf{q}}}\right) - \frac{\partial L}{\partial \mathbf{q}} = 0. \tag{3.1}$$

The Euler-Lagrange equations are the equations of motion in Lagrangian mechanics. Note that derivatives with respect to a bold quantity represent a "gradient" operation: $\partial L/\partial \mathbf{q}$ denotes the n equations $\partial L/\partial q^i$. Even if we have *holonomic* constraints and/or a non-autonomous Lagrangian, the appropriate Euler-Lagrange equations are still a necessary condition for the motion $\boldsymbol{\gamma}$ to minimize the action functional S.

A **natural** mechanical system is one where the total kinetic energy of the system is given as a quadratic form of the generalized velocities $\dot{q}^i$:

$$T = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(q^1, ..., q^n)\dot{q}^i\dot{q}^j.$$

As the reader might know from experience, quadratic kinetic energy terms appear quite frequently in our models of nature. For mechanical systems that are natural in Cartesian coordinates, the momentum of the i^{th} particle is given by $p_i = \partial L/\partial \dot{q}^i$. For simple systems in Cartesian coordinates, the Euler-Lagrange equations are *exactly* Newton's equations of motion; this is expected since Lagrangian mechanics is designed to be equivalent to Newtonian mechanics.

For any Lagrangian mechanical system, we can define the **generalized momentum** $\mathbf{p}(\mathbf{q}, \dot{\mathbf{q}})$ as

$$\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}}. \tag{3.2}$$

We assume that this mapping is a diffeomorphism, so that the inverse exists (for the conditions required to invert this mapping, see Section 4.4 in [7]). In local coordinates q^i, (3.2) is

$$p_i = \frac{\partial L}{\partial \dot{q}^i},$$

where p_i is the generalized momentum corresponding to the i^{th} generalized velocity q^i. The reader should note that each generalized momentum p_i is given a *subscripted* index, which is how we denote components of a differential 1-form. Let us see why this is by determining how the p_i transform to another coordinate system.

Let $Q^i = Q^i(q^1, ..., q^n)$ be another set of local coordinates on M^n. Then $\dot{Q}^i$ are the components of the coordinate basis vectors in the Q^i coordinates and are given by

$$\dot{Q}^i = \sum_{j=1}^{n} \frac{\partial Q^i}{\partial q^j} \dot{q}^j. \tag{3.3}$$

The reader may want to check that this agrees with the transformation (2.1). We can write the Lagrangian L, assumed to be autonomous, in either coordinate system: $L = L(\mathbf{q}, \dot{\mathbf{q}}) = L(\mathbf{Q}, \dot{\mathbf{Q}})$. The generalized momentum P_i is given by the chain rule:

$$P_i = \frac{\partial L}{\partial \dot{Q}^i} = \sum_{j=1}^{n} \left[\frac{\partial L}{\partial q^j} \frac{\partial q^j}{\partial \dot{Q}^i} + \frac{\partial L}{\partial \dot{q}^j} \frac{\partial \dot{q}^j}{\partial \dot{Q}^i} \right].$$

We consider the coordinates $\mathbf{q}$ as being independent of the generalized velocities $\dot{\mathbf{q}}$ (in any coordinate system). This means that

$$\frac{\partial q^j}{\partial \dot{Q}^i} = 0.$$

From the vector transformation rule (3.3), we have

$$\frac{\partial \dot{q}^j}{\partial \dot{Q}^i} = \frac{\partial q^j}{\partial Q^i},$$

so that

$$P_i = \sum_{j=1}^{n} \frac{\partial q^j}{\partial Q^i} p_i. \tag{3.4}$$

Thus, the generalized momenta $\mathbf{p}$ are the components of a differential 1-form field, which is an element of the cotangent bundle T^*M^n! The definition given by (3.2) is really a mapping $\mathbf{p} : TM^n \to T^*M^n$ that gives us the components p_i. In the context of a mechanical system, the cotangent bundle of the configuration space is called the **phase space**, and is given by the local coordinates $(q^1, ..., q^n, p_1, ..., p_n)$. The Euler-Lagrange equations give us equations of motion in terms of $\mathbf{q}$ and $\dot{\mathbf{q}}$ that are equivalent to Newton's equations of motion. What are the equations of motion of the mechanical system in terms of $\mathbf{q}$ and $\mathbf{p}$ that are equivalent to the Euler-Lagrange equations of motion?

Theorem 3.1: *Lagrange's equations of motion* (3.1) *in* TM^n *transform to* ***Hamilton's equations of motion*** *in* T^*M^n

$$\dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}} \qquad \dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}, \tag{3.5}$$

where the ***Hamiltonian*** *is defined by*

$$H(\mathbf{q}, \mathbf{p}, t) = \mathbf{p}\dot{\mathbf{q}} - L(\mathbf{q}, \dot{\mathbf{q}}, t). \tag{3.6}$$

The generalized velocities $\dot{\mathbf{q}}$ *are written in terms of* $\mathbf{q}$ *and* $\mathbf{p}$ *using the inverse of* (3.2) *(The Hamiltonian* $H(\mathbf{q}, \mathbf{p}, t) = \mathbf{p}\dot{\mathbf{q}} - L(\mathbf{q}, \dot{\mathbf{q}}, t)$ *is the Legendre transform of the Lagrangian* $L(\mathbf{q}, \dot{\mathbf{q}}, t)$ *viewed as a function of* $\dot{\mathbf{q}}$*).*

Proof: *Since we assumed that the mapping* $\mathbf{p} : TM^n \to T^*M^n$ *given by* (3.2) *was a diffeomorphism, the inverse mapping exists and is a differentiable mapping. Locally, we can write the generalized velocities as* $\dot{\mathbf{q}} = \dot{\mathbf{q}}(\mathbf{q}, \mathbf{p})$.

The total derivative of H *must be the same when* $H = H(\mathbf{q}, \mathbf{p}, t)$ *and when* $H = H(\mathbf{q}, \dot{\mathbf{q}}, t)$. *In the first case, we have*

$$\mathrm{d}H = \frac{\partial H}{\partial \mathbf{p}}\mathrm{d}\mathbf{p} + \frac{\partial H}{\partial \mathbf{q}}\mathrm{d}\mathbf{q} + \frac{\partial H}{\partial t}\mathrm{d}t.$$

In the second case, we have

$$\mathrm{d}\left(\mathbf{p}\dot{\mathbf{q}} - L(\mathbf{q}, \dot{\mathbf{q}}, t)\right) = \dot{\mathbf{q}}\ \mathrm{d}\mathbf{p} - \frac{\partial L}{\partial \mathbf{q}}\mathrm{d}\mathbf{q} - \frac{\partial L}{\partial t}\mathrm{d}t.$$

Both expressions for $\mathrm{d}H$ *must be equivalent, and so we have*

$$\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}} \qquad -\frac{\partial L}{\partial \mathbf{q}} = \frac{\partial H}{\partial \mathbf{q}} \qquad -\frac{\partial L}{\partial t} = \frac{\partial H}{\partial t}.$$

From the Euler-Lagrange equations (3.1), *we know* $\dot{\mathbf{p}} = \partial L/\partial \mathbf{q}$, *and we have Hamilton's equations of motion:*

$$\dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}} \qquad \dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}} \qquad \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t} \qquad \square$$

Lagrange's equations of motion (3.1) are *equivalent* to Hamilton's equations of motion (3.5). Disregarding any complexities in transforming the Lagrangian into the Hamiltonian, we have complete freedom to choose which equations of motion we want to solve. Due to the geometry of the cotangent bundle (e.g. we can *always* pull back forms), Hamiltonian mechanics allows us to find complete solutions to problems that do not yield solutions by other means, such as Lagrangian and Newtonian mechanics.

3.2 Symplectic Manifolds

As we just saw, we can rewrite the n second-order equations of motion in Lagrangian mechanics as a system of $2n$ first-order equations of motion using coordinates on the phase space. The second n-tuple of coordinates on the phase space is given by the components $p_i = \partial L/\partial \dot{q}^i$ of a 1-form. On the phase space, there exists a structure, analogous to a Riemannian metric, that gives us an isomorphism between tangent spaces and cotangent spaces. As we will see, this isomorphism relates phase flows on T^*M^n with functions on T^*M^n, and (naturally) gives us Hamilton's equations of motion in terms of the geometry of the phase space!

Definition 3.1: *Let* M^{2n} *be an even-dimensional differentiable manifold. A* ***symplectic structure*** *on* M^{2n} *is a closed, non-degenerate differential* 2*-form* ω^2 *on* M^{2n}*:*

$$\mathrm{d}\omega^2 = 0$$
$$\forall \mathbf{X} \in TM^{2n}_{\mathbf{x}} \quad \exists \mathbf{Y} \in TM^{2n}_{\mathbf{x}} \quad s.t. \quad \omega^2(\mathbf{X}, \mathbf{Y}) \neq 0.$$

The pair (M^{2n}, ω^2) *is called a* ***symplectic manifold****.*

The word *symplectic* comes from an Ancient Greek *συμπλεκτικός*, which translates, roughly, to "braided together" (think of how Hamilton's equations of motion (3.5) are "braided together"). The introduction of the term symplectic into mathematics is attributed to Herman Weyl.

Theorem 3.2: *The cotangent space T^*M^n of an n-dimensional differentiable manifold M^n has a natural symplectic structure. In local coordinates $(x^1, ..., x^n, a_1, ..., a_n)$ on T^*M^n, this structure can be written as*

$$\omega^2 = \sum_{i=1}^{n} \mathrm{d}a_i \wedge \mathrm{d}x^i. \tag{3.7}$$

Recall that the phase space T^*M^n of a mechanical system is a $2n$-dimensional differentiable manifold. The phase space can be given local coordinates $(q^1, ..., q^n, p_1, ..., p_n)$, where the q^i are generalized coordinates and the p_i are generalized momenta. By Theorem 3.2, *the phase space of a mechanical system is a symplectic manifold.*

In Arnold's proof of Theorem 3.2, it is shown that $\omega^2 = \mathrm{d}\omega^1$, where $\omega^1 = \mathbf{a}\ \mathrm{d}\mathbf{x}$. This guarantees that ω^2 is closed [3]. In the context of a mechanical system, $\omega^1 = \mathbf{p}\ \mathrm{d}\mathbf{q}$ is called the **Poincaré 1-form**; the symplectic structure of the phase space is occasionally called the *Poincaré 2-form.*

The reader who is familiar with Riemannian geometry may recall that the Riemannian metric induces an isomorphism between the tangent and cotangent spaces of the manifold. The symplectic structure induces a similar isomorphism on symplectic manifolds.

Definition 3.2: *To each vector $\mathbf{X}$ tangent to a symplectic manifold (M^{2n}, ω^2) at a point $\mathbf{x}$, there is a 1-form $\omega^1_{\mathbf{X}}$ associated to $\mathbf{X}$ by*

$$\omega^1_{\mathbf{X}}(\mathbf{Y}) = \omega^2(\mathbf{Y}, \mathbf{X}) \quad \forall \mathbf{Y} \in TM^{2n}_{\mathbf{x}}.$$

This association induces an isomorphism between $TM^{2n}_{\mathbf{x}}$ and $T^*M^{2n}_{\mathbf{x}}$. Due to its role in taking total derivatives of functions to vector fields, we usually use the isomorphism $I : T^*M^{2n} \to TM^{2n}$. If we let H be a function on M^{2n}, the isomorphism I takes $\mathrm{d}H$ to a vector field $I\ \mathrm{d}H$ on M^{2n}.

Definition 3.3: *The vector field $I\ \mathrm{d}H$ on M^{2n} is called a **Hamiltonian vector field**; the function H is called a **Hamiltonian function**.*

By computing $\mathrm{d}H$ and mapping it to a Hamiltonian vector field $I\ \mathrm{d}H$, we can associate H to a phase flow with elements g^t defined by

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} g^t\mathbf{x} = I\ \mathrm{d}H(\mathbf{x}),$$

where the group of elements g^t is called a **Hamiltonian phase flow** with Hamiltonian function H.

In the case of a mechanical system, the symplectic manifold is (T^*M^n, ω^2). The Hamiltonian function H is found from the Lagrangian function L. The phase flow g^t of a mechanical system is exactly the solution to Hamilton's equations of motion (3.5), which are in a $1:1$ correspondence with the Hamiltonian vector field $I\ \mathrm{d}H$. Note that the phase space T^*M^n does not include time t as a coordinate; we must have $\partial H/\partial t = 0$. The non-autonomous case will be handled in the next subsection.

3.3 Canonical Transformations

Hamiltonian functions define a one-parameter group of diffeomorphisms (phase flows) of symplectic manifolds (notably the phase space of a mechanical system). How do flows change a symplectic manifold?

Definition 3.4: *Let $g : M^{2n} \to M^{2n}$ be a differentiable mapping. A differential p-form ω^p is an **(absolute) integral invariant** of the map g if*

$$\int_{g\sigma} \omega^p = \int_{\sigma} \omega^p,$$

for any oriented, parameterized p-subset σ of M^{2n}.

The following theorems highlight some of the beautiful structure that comes from the cotangent bundle.

Theorem 3.3: *A p-form ω^p on M^{2n} is an absolute integral invariant of the map g if and only if the map preserves ω^p:*

$$g^*\omega^p = \omega^p.$$

Theorem 3.4: *If ω^p and ω^q are absolute integral invariants of the map g, then*

$$\omega^p \wedge \omega^q$$

is also an absolute integral invariant of g.

Theorem 3.5: *A Hamiltonian phase flow g^t on a symplectic manifold (M^{2n}, ω^2) preserves the symplectic structure:*

$$(g^t)^*\omega^2 = \omega^2. \tag{3.8}$$

From Theorem 3.3, we know that Theorem 3.5 is equivalent to stating that the symplectic form is an absolute integral invariant of Hamiltonian phase flows. Note that this is true both for the case of a general symplectic manifold and for the phase space of a mechanical system. This means that *solutions to Hamilton's equations* (i.e Hamiltonian phase flows with Hamiltonian function H) *must preserve the symplectic structure.* We will deal with this fact in Section 4.

Definition 3.5: *A differentiable map $g : M^{2n} \to M^{2n}$ is called* ***canonical****, a* ***canonical transformation****, or a* ***symplectomorphism*** *if it preserves the symplectic structure.*

In these terms, Theorem 3.5 states that every Hamiltonian phase flow is a canonical transformation. However, not every canonical transformation is a Hamiltonian phase flow.

Consider a mechanical system with configuration space M^n. The phase space T^*M^n is a $2n$-dimensional manifold. On the phase space, we can only have conservative (i.e. autonomous) Hamiltonian functions $H = H(\mathbf{q}, \mathbf{p})$. We can, however, extend phase space to include the time parameter. Define the **extended phase space** to be $T^*M^n \times \mathbb{R}$. Local coordinates on the extended phase space are $(q^1, ..., q^n, p_1, ..., p_n, t)$, and we can now have non-autonomous Hamiltonian functions $H = H(\mathbf{q}, \mathbf{p}, t)$.

By considering the 1-form $\omega^1 = \mathbf{p}\mathrm{d}\mathbf{q} - H\mathrm{d}t$ on the extended phase space M^{2n+1}, it can be shown that the *vortex lines* of ω^1 are the trajectories of the phase flow given by Hamilton's equations of motion (3.5). Vortex lines are the integral curves of the *vortex directions* $\mathbf{X} \in TM^{2n+1}_{\mathbf{x}}$ given by

$$\mathrm{d}\omega^1(\mathbf{X}, \mathbf{Y}) = 0 \quad \forall \mathbf{Y} \in TM^{2n+1}_{\mathbf{x}}.$$

It turns out that $\mathrm{d}\omega^1$ is non-degenerate; $\mathrm{d}\omega^1$ is also closed, since $\mathrm{d}^2\omega^1 = 0$.

Since ω^1 gives us Hamilton's equations of motion via the vortex lines of ω^1, we expect that in some new coordinates $(\mathbf{Q}, \mathbf{P}, T)$ on M^{2n+1}, the vortex lines of ω^1 in the new coordinate patch are exactly the vortex lines of ω^1 in the original coordinates $(\mathbf{q}, \mathbf{p}, t)$. In particular, we can choose $T = t$, so we are only changing coordinates $(\mathbf{q}, \mathbf{p}) \to (\mathbf{Q}, \mathbf{P})$.

Theorem 3.6: *In the new coordinates $(\mathbf{Q}, \mathbf{P}, t)$ on M^{2n+1}, Hamilton's equations of motion* (3.5) *have the same form:*

$$\dot{\mathbf{P}} = -\frac{\partial K}{\partial \mathbf{Q}} \qquad \dot{\mathbf{Q}} = \frac{\partial K}{\partial \mathbf{P}},$$

where $K(\mathbf{Q}, \mathbf{P}, t) = H(\mathbf{q}, \mathbf{p}, t)$. Note that the time derivatives are with respect to t.

If the transformation $g : (\mathbf{q}, \mathbf{p}) \to (\mathbf{Q}, \mathbf{P})$ is canonical, then the form of the equations of motion is preserved. This gives us quite a bit of freedom in how we can solve problems. There are a number of techniques for generating canonical coordinate transformations that result in a more easily integrable problem. One of the most notable methods is called the *Hamilton-Jacobi method* for constructing generating functions for coordinate transformations.

3.4 Lie Algebras in Hamiltonian Mechanics

We can define a binary operation on the tangent space of a differentiable manifold that takes two vectors and returns a vector. If the manifold is symplectic, this vector operation can be limited to Hamiltonian vector fields and induce closure. A compatible operation can be written in terms of Hamiltonian functions on the symplectic manifold. This new operation on Hamiltonian functions is related to conserved quantities of a Hamiltonian mechanical system. In Section 4 we will see how this operation can be used to develop numerical methods for approximating solutions to the equations of motion of a Hamiltonian mechanical system.

Definition 3.6: *A* ***Lie algebra*** $\mathfrak{g}$ *is a vector space* V *together with a bilinear, skew-symmetric operation* $[\cdot, \cdot] : V \times V \to V$ *that satisfies the* Jacobi identity

$$[[\mathbf{X}, \mathbf{Y}], \mathbf{Z}] + [[\mathbf{Y}, \mathbf{Z}], \mathbf{X}] + [[\mathbf{Z}, \mathbf{X}], \mathbf{Y}] = 0 \quad \forall\, \mathbf{X}, \mathbf{Y}, \mathbf{Z} \in V.$$

The operation $[\cdot, \cdot]$ *is usually called the* ***Poisson bracket****, or* ***commutator****.*

Remark: *One may be asking, "where is the Lie* group*?" The Lie group, in the case where the vectors in the Lie algebra are Hamiltonian vector fields on* (M^{2n}, ω^2)*, is, roughly speaking, the space of all diffeomorphisms of the symplectic manifold. We have been regularly using elements of this Lie group, but we have not (explicitly) needed the structure of the Lie group for our purposes thus far; it is for this reason that we do not call the commutator a Lie bracket. The Lie group "under" the Lie algebra of Hamiltonian vector fields will make a brief appearance in Section 4.2.*

Let M^n be a differentiable manifold and $TM^n_{\mathbf{x}}$ the tangent space at $\mathbf{x} \in M^n$. We know that the tangent space is a vector space, whose elements are the tangent vectors based at the point $\mathbf{x}$. Thus, for vectors, which we write as first-order, linear differential operators, we can define the commutator operation. Let $\mathbf{X}, \mathbf{Y} \in TM^n_{\mathbf{x}}$ be given in some coordinates x^i so that $\mathbf{X}$ and $\mathbf{Y}$ are given by the components X^i and Y^j, respectively.

The commutator of tangent vectors is defined by its action on a smooth function f:

$$[\mathbf{X}, \mathbf{Y}](f) = \mathbf{X}(\mathbf{Y}(f)) - \mathbf{Y}(\mathbf{X}(f)).$$

At first sight, this looks like a *second*-order, bilinear differential operator, but upon inspection of the components of $[\mathbf{X}, \mathbf{Y}]$ it is clear that it is a first-order, bilinear differential operator. The components of $[\mathbf{X}, \mathbf{Y}]$ are

$$[\mathbf{X}, \mathbf{Y}]^j = \sum_{i=1}^{n} \left(X^i \frac{\partial Y^j}{\partial x^i} - Y^i \frac{\partial X^j}{\partial x^i} \right). \tag{3.9}$$

It is clear that the commutator operation is skew-symmetric: $[\mathbf{X}, \mathbf{Y}] = -[\mathbf{Y}, \mathbf{X}]$. Note that some authors, Arnold in particular, define the commutator to be $-[\mathbf{X}, \mathbf{Y}]$. The commutator also satisfies the Jacobi identity.

Together with the commutator defined above, each tangent space $TM^n_{\mathbf{p}}$ of a differentiable manifold is a Lie algebra. In the case of a symplectic manifold, the Lie algebra of Hamiltonian vector fields is a sub-algebra of the Lie algebra of all vector fields.

We already know that vector fields $\mathbf{X}$ are related to flows g^t:

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} g^t\mathbf{x} = \mathbf{X}(\mathbf{x}).$$

As the reader might suspect, the degree of commutativity of vector fields is also intimately related to the degree of commutativity of the associated flows.

Theorem 3.7: *Let* $\mathbf{X}$ *and* $\mathbf{Y}$ *be the vector fields associated to the flows* g^t *and* h^s*. The flows* g^t *and* h^s *commute if and only if commutator* $[\mathbf{X}, \mathbf{Y}]$ *is equal to zero.*

Everything previously in this section is defined for any differentiable manifold M^n. Let us now move to the case in which the manifold is symplectic.

Let (M^{2n}, ω^2) be a symplectic manifold. The symplectic structure allows us to determine a Hamiltonian vector field $I\ \mathrm{d}H$ and Hamiltonian phase flow g^t_H from a Hamiltonian function $H : M^{2n} \to \mathbb{R}$. Each element of the flow g^t_H is a canonical transformation of M^{2n}.

Definition 3.7: *Let* $F : M^{2n} \to \mathbb{R}$ *be another Hamiltonian function. The* ***Poisson bracket*** $\{F, H\}$ *is the derivative of* F *in the direction of the flow of* H*:*

$$\{F, H\}(\mathbf{x}) = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} F(g^t_H\mathbf{x}). \tag{3.10}$$

The Poisson bracket $\{F, H\}$ is also a function on M^{2n}. From the definition of the Poisson bracket (3.10), we know that F is a first integral (integral invariant) of the phase flow g^t_H if and only if $\{F, H\} = 0$.

If we use the isomorphism $I : T^*M^{2n} \to TM^{2n}$ defined in Section 3.2, we can write the Poisson bracket of F and H using the symplectic structure:

$$\{F, H\} = \omega^2(I\ \mathrm{d}F, I\ \mathrm{d}H).$$

This shows that the Poisson bracket is bilinear and skew-symmetric:

$$\{\lambda_1 F_1 + \lambda_2 F_2, H\} = \lambda_1\{F_1, H\} + \lambda_2\{F_2, H\} \qquad \lambda_1, \lambda_2 \in \mathbb{R}$$
$$\{F, H\} = -\{H, F\}.$$

By looking at the Hamiltonian vector fields associated to the Hamiltonian functions F, H, and G, one can show that the Poisson bracket obeys the Jacobi identity:

$$\{\{F, H\}, G\} + \{\{H, G\}, F\} + \{\{G, H\}, F\} = 0.$$

Therefore, the vector space of Hamiltonian functions on a symplectic manifold (M^{2n}, ω^2) with the Poisson bracket form a Lie algebra.

If we have two first integrals F_1 and F_2 of a system with Hamiltonian H, then we can construct a third, not necessarily new, first integral $\{F_1, F_2\}$. From this, if we know that the first two angular momenta of a mechanical system in $\mathbb{R}^3$ are conserved, then the third component must also be conserved.

Finally, let us state a generalization of Noether's Theorem, which relates symmetries of the Lagrangian to first integrals of the equations of motion. This generalization, which we still attribute to Noether, is instead written in terms of a Hamiltonian system.

Noether's Theorem: *If a Hamiltonian function* H *on the symplectic manifold* (M^{2n}, ω^2) *is preserved by the one-parameter group of canonical transformations given by a Hamiltonian function* F*, then* F *is a first integral of the equations of motion of the mechanical system with Hamiltonian* H*.*

3.5 The Hamilton-Jacobi Method

The Hamilton-Jacobi method is a set of techniques for finding coordinate transformations that yield more easily integrable equations of motion. The method relies on the fact that both the Hamiltonian and the form of Hamilton's equations of motion are preserved under a canonical transformation (Theorem 3.6). Therefore, if we "somehow" succeed in finding a "good" coordinate transformation, we know that the solution to the new equations of motion satisfies the original problem.

In Section 2.3 we defined the *action* functional

$$S[\boldsymbol{\gamma}] = \int_{\boldsymbol{\gamma}} L \, \mathrm{d}t,$$

where the motion of a mechanical system is the extremal $\boldsymbol{\gamma}$ and L is the Lagrangian function. The action S is defined with some starting position and time $(\mathbf{q}_0, t)$, from which we integrate following the path of the extremal $\boldsymbol{\gamma}$. It turns out that the differential of the action is

$$\mathrm{d}S = \mathbf{p} \, \mathrm{d}\mathbf{q} - H \, \mathrm{d}t,$$

where $\mathbf{p} = \partial L / \partial \dot{\mathbf{q}}$ and $H = \mathbf{p}\dot{\mathbf{q}} - L$ are defined with the help of the terminal velocity $\dot{\mathbf{q}}$ of the extremal $\boldsymbol{\gamma}$. From this, we arrive at the **Hamilton-Jacobi equation**. Note that $\mathbf{p} = \partial S / \partial \mathbf{q}$.

Theorem 3.8: *The action function S satisfies the single, non-linear partial differential equation*

$$\frac{\partial S}{\partial t} + H\left(\mathbf{q}, \frac{\partial S}{\partial \mathbf{q}}, t\right) = 0, \tag{3.11}$$

with Cauchy data $S(\mathbf{q}, t_0) = S_0(\mathbf{q})$.

The Hamilton-Jacobi equation gives us yet another equation of motion. Our "primary" equations of motion are still Hamilton's equations of motion, however. We will soon see the utility of the Hamilton-Jacobi equation for finding canonical transformations.

Suppose that the $2n$ functions $\mathbf{Q}(\mathbf{q}, \mathbf{p})$ and $\mathbf{P}(\mathbf{q}, \mathbf{p})$ define a canonical transformation $g : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$. From Theorem 3.6, it can be shown that there exists a function $S(\mathbf{q}, \mathbf{p})$ such that

$$\mathrm{d}S(\mathbf{q}, \mathbf{p}) = \mathbf{p} \, \mathrm{d}\mathbf{q} - \mathbf{P} \, \mathrm{d}\mathbf{Q}, \tag{3.12}$$

is an exact differential form. Also, if the form $\mathbf{p} \, \mathrm{d}\mathbf{q} - \mathbf{P} \, \mathrm{d}\mathbf{Q}$ is exact, then the transformation it induces is canonical.

If we assume that in a neighborhood of the point $(\mathbf{q}_0, \mathbf{p}_0)$ the Jacobian determinant

$$\det \frac{\partial(\mathbf{Q}, \mathbf{q})}{\partial(\mathbf{p}, \mathbf{q})} = \det \frac{\partial \mathbf{Q}}{\partial \mathbf{p}} \neq 0$$

then we can take $(\mathbf{Q}, \mathbf{q})$ as independent coordinates. Such a transformation is called *free*. Locally S can be expressed as

$$S(\mathbf{q}, \mathbf{p}) = S_1(\mathbf{q}, \mathbf{Q}).$$

The function S_1 is called a **generating function** of the canonical transformation g. From (3.12), we have

$$\mathbf{p} = \frac{\partial S_1}{\partial \mathbf{q}} \qquad \mathbf{P} = -\frac{\partial S_1}{\partial \mathbf{Q}}. \tag{3.13}$$

As long as

$$\det \left. \frac{\partial^2 S_1}{\partial \mathbf{q} \partial \mathbf{Q}} \right|_{(\mathbf{q}_0, \mathbf{Q}_0)} \neq 0,$$

S_1 is a generating function for some free canonical transformation. It should be noted that a general canonical transformation is given in terms of $2n$ functions of $2n$ variables. In the case of the generating function S_1, we can find a canonical transformation in terms of *one* function of $2n$ variables!

We now know that if we somehow construct a function S_1, we can generate a canonical transformation (with the above assumption on the determinant). However, what makes a good canonical transformation? Clearly, we want to transform the coordinates to some where the equations of motion are easily integrated!

Notice that if $H(\mathbf{q}, \mathbf{p}, t) = K(\mathbf{Q}, t)$ depends only on $\mathbf{Q}$ (in the new coordinates), Hamilton's equations are

$$\dot{\mathbf{P}} = -\frac{\partial K}{\partial \mathbf{Q}} \qquad \dot{\mathbf{Q}} = 0.$$

The solution is

$$\mathbf{P}(t) = \mathbf{P}(0) - \int_0^t \left. \frac{\partial K}{\partial \mathbf{Q}} \right|_{\mathbf{Q}(0)} \mathrm{d}t \qquad \mathbf{Q}(t) = \mathbf{Q}(0).$$

Now we need a way of transforming $(\mathbf{q}, \mathbf{p})$ such that $H(\mathbf{q}, \mathbf{p}, t) = K(\mathbf{Q}, t)$.

Using (3.13), we want to find $S(\mathbf{q}, \mathbf{Q})$ such that

$$H\left(\mathbf{q}, \frac{\partial S}{\partial \mathbf{q}}, t\right) = K(\mathbf{Q}, t), \tag{3.14}$$

where the derivatives $\partial S / \partial \mathbf{q}$ are taken and then the substitution $\mathbf{q} = \mathbf{q}(\mathbf{Q}, \mathbf{P})$ is made. The reader should note the similarity of (3.14) and the Hamilton-Jacobi equation (3.11). Finally, we have the following theorem which states that if we can find such an S, then we can completely solve the original problem.

Jacobi's Theorem: *If a solution $S(\mathbf{q}, \mathbf{Q})$ of* (3.14) *is found that depends on the n parameters $\mathbf{Q}$ such that $\det \partial^2 S / \partial \mathbf{q} \partial \mathbf{Q} \neq 0$, then Hamilton's equations*

$$\dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}} \qquad \dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}$$

can be solved explicitly in terms of integrals.

Jacobi's Theorem has proven itself to be one of the most powerful methods for solving Hamilton's equations of motion using exact integration. Using Jacobi's Theorem, many problems have been completely solved that have yet to be solved by other means [3].

Not every canonical transformation is *free*, however. Thus, the "type 1" generating function S_1 will not work. There are, however, a multitude of other types generating functions. For instance, the "type 2" generating functions S_2:

$$S_2(\mathbf{q}, \mathbf{P}) = \mathbf{P}\mathbf{Q} + S(\mathbf{q}, \mathbf{p}),$$

where $\mathbf{Q} = \mathbf{Q}(\mathbf{q}, \mathbf{P})$ and $\mathbf{p} = \mathbf{p}(\mathbf{q}, \mathbf{P})$. For S_2, we have

$$\mathbf{p} = \frac{\partial S_2}{\partial \mathbf{q}} \qquad \mathbf{Q} = \frac{\partial S_2}{\partial \mathbf{P}}.$$

Just as in the "type 1" case, we have a local condition on the determinant of the Hessian of S_2. The identity transformation $\mathbf{q} = \mathbf{Q}$, $\mathbf{p} = \mathbf{P}$ is given by the "type 2" generating function

$$S_2(\mathbf{q}, \mathbf{P}) = \mathbf{P}\mathbf{q}.$$

Finally, consider a generating function that is close to the identity transformation (τ is "small"):

$$S_\tau(\mathbf{q}, \mathbf{P}) = \mathbf{P}\mathbf{q} + \tau S(\mathbf{q}, \mathbf{P}; \tau), \tag{3.15}$$

where again $\mathbf{Q} = \mathbf{Q}(\mathbf{q}, \mathbf{P})$ and $\mathbf{p} = \mathbf{p}(\mathbf{q}, \mathbf{P})$. For this generating function,

$$\mathbf{p} = \mathbf{P} + \tau \frac{\partial S}{\partial \mathbf{q}} \qquad \mathbf{Q} = \mathbf{q} + \tau \frac{\partial S}{\partial \mathbf{P}}. \tag{3.16}$$

Such a transformation is called an *infinitesimal canonical transformation*. This type of generating function is used in the construction of symplectic integrators, as we will see in the next section.

4 Symplectic Integrators

Symplectic integrators are numerical methods for approximating solutions to the equations of motion of Hamiltonian mechanical systems. They are called *symplectic* because they preserve the symplectic structure (up to machine precision). Symplectic integrators have been shown to be extraordinarily powerful in long-time numerical integrations of Hamiltonian systems.

Consider a time independent Hamiltonian function $H = H(\mathbf{q}, \mathbf{p})$. Solutions to Hamilton's equations of motion (3.5) are canonical maps from $(\mathbf{q}, \mathbf{p})$ at time $t = 0$ to $(\mathbf{Q}, \mathbf{P})$ at time $t = \tau$ for any $\tau \in \mathbb{R}$. From Theorem 3.2, we know that the symplectic structure on the phase space can be written as $\omega^2 = \mathrm{d}\mathbf{p} \wedge \mathrm{d}\mathbf{q}$. We know that the solutions preserve the Hamiltonian (i.e. energy is conserved) since H is time independent. In summary, exact solutions to time independent Hamiltonians

1. are exactly symplectic: $\mathrm{d}\mathbf{p} \wedge \mathrm{d}\mathbf{q} = \mathrm{d}\mathbf{P} \wedge \mathrm{d}\mathbf{Q}$
2. conserve the energy: $H(\mathbf{q}, \mathbf{p}) = H(\mathbf{Q}, \mathbf{P})$.

When developing numerical integration methods for Hamiltonian systems, we would like the numerical method to obey those two properties of true solutions. Unfortunately, we cannot have both in any numerical method; if we did, the method must necessarily give the flow of the exact solution (perhaps up to a reparameterization of time) [8]. Nevertheless, we can develop numerical methods that preserve the symplectic structure (again, up to round-off errors). Also, for arbitrarily many time steps, the errors in the Hamiltonian are bounded (which generally does not occur for "standard" numerical integration methods) when a symplectic integrator is used.

The methods included in this section were developed in the 1980's and 1990's. Since that time, these methods have been improved (e.g. individual time stepping [12]) and other methods have been developed. Still, the methods studied in this section are a modern application of the methods of classical mechanics.

4.1 Construction of Explicit Methods

As a first case, consider a time independent, *separable* Hamiltonian function $H(\mathbf{q}, \mathbf{p}) = T(\mathbf{p}) + V(\mathbf{q})$. Hamilton's equations of motion are

$$\dot{\mathbf{p}} = -\frac{\partial V}{\partial \mathbf{q}} \qquad \dot{\mathbf{q}} = \frac{\partial T}{\partial \mathbf{q}}. \tag{4.1}$$

Consider the infinitesimal canonical transformation given by the generating function (3.15):

$$S_\tau = \mathbf{P}\mathbf{q} + \tau S(\mathbf{q}, \mathbf{P}), \tag{4.2}$$

where $\tau > 0$. From Section 3.5, we know

$$\mathbf{p} = \mathbf{P} + \tau \frac{\partial S}{\partial \mathbf{q}} \qquad \mathbf{Q} = \mathbf{q} + \tau \frac{\partial S}{\partial \mathbf{P}}. \tag{4.3}$$

Our symplectic integrator should be a canonical transformation that moves the coordinates $(\mathbf{q}, \mathbf{p})$ at time $t = t_0$ forward in time to the new coordinates $(\mathbf{Q}, \mathbf{P})$ at time $t = t_0 + \tau$. We choose $S(\mathbf{q}, \mathbf{P}) = T(\mathbf{P}) + V(\mathbf{q})$ so that the transformation coincides with the exact solution to (4.1) up to $O(\tau)$ (see [9] for more details on this choice). We now have the mapping $g^\tau(\mathbf{q}, \mathbf{p}) = (\mathbf{Q}, \mathbf{P})$ given by

$$\begin{aligned} \mathbf{P} &= \mathbf{p} - \tau \frac{\partial V}{\partial \mathbf{q}} \\ \mathbf{Q} &= \mathbf{q} + \tau \frac{\partial T}{\partial \mathbf{P}}. \end{aligned} \tag{4.4}$$

Note that this transformation is consistent with the first-order approximation of (4.1). In the limit as $\tau \to 0$, the transformation matches the Taylor series of (4.1), and this method said to be *consistent*.

If we break the solution time interval into an *evenly spaced* mesh t_k and denote the approximation to the coordinates $(\mathbf{q}(t_k), \mathbf{p}(t_k))$ at time $t = t_k$ by $(\mathbf{q}_k, \mathbf{p}_k)$, then this simple, explicit symplectic integrator for separable Hamiltonians is

$$\begin{aligned} \mathbf{p}_{k+1} &= \mathbf{p}_k - \tau \left.\frac{\partial V}{\partial \mathbf{q}}\right|_{\mathbf{q}_k} \\ \mathbf{q}_{k+1} &= \mathbf{q}_k + \tau \left.\frac{\partial T}{\partial \mathbf{p}}\right|_{\mathbf{p}_{k+1}} . \end{aligned} \tag{4.5}$$

Remark: *The coordinates $\mathbf{q}_k$ and $\mathbf{p}_k$ are the numerical approximations to the exact solution coordinates $\mathbf{q}(t_k)$ and $\mathbf{p}(t_k)$, respectively. It is common to denote the approximation to an exact quantity by another symbol (usually a larger glyph). As this notation a bit cumbersome (but precise), we put some of the burden of tracking the exact and approximate quantities on the reader.*

The method (4.5) is know as *symplectic Euler's method*, since it is first-order accurate, explicit, and consists of only one stage. If the difference between the approximate solution $(\mathbf{q}_{k+1}, \mathbf{p}_{k+1})$ and the exact solution, Taylor expanded about $t = t_k$, is of order τ^{N+1}, we say the method is N^{th} *order accurate*.

The reader might suspect that we can choose another S_τ so that the approximate solution matches the exact solution up to $O(\tau^2)$ or higher. Higher order methods usually consist of multiple stages (i.e. multiple steps between t_k and t_{k+1}). We denote these intermediate times as $t_{k,i}$. Similarly, we denote the approximate solution at time $t = t_{k,i}$ as $(\mathbf{q}_{k,i}, \mathbf{p}_{k,i})$. Ruth found that the following two stage method is second-order accurate [11]; we call this *Ruth's second-order method*:

$$\begin{aligned} \mathbf{p}_{k,1} &= \mathbf{p}_k & \mathbf{q}_{k,1} &= \mathbf{q}_k + \frac{\tau}{2} \left.\frac{\partial T}{\partial \mathbf{p}}\right|_{\mathbf{p}_{k,1}} \\ \mathbf{p}_{k+1} &= \mathbf{p}_{k,1} - \tau \left.\frac{\partial V}{\partial \mathbf{q}}\right|_{\mathbf{q}_{k,1}} & \mathbf{q}_{k+1} &= \mathbf{q}_{k,1} + \frac{\tau}{2} \left.\frac{\partial T}{\partial \mathbf{p}}\right|_{\mathbf{p}_{k+1}} . \end{aligned} \tag{4.6}$$

Note that we make the identifications $\mathbf{p}_k = \mathbf{p}_{k,0}$, $\mathbf{p}_{k+1} = \mathbf{p}_{k,2}$, $\mathbf{q}_k = \mathbf{q}_{k,0}$, and $\mathbf{q}_{k+1} = \mathbf{q}_{k,2}$ for the two stage method. These generating function techniques work not only for explicit methods, but also for deriving implicit methods, which will be handled in Section 4.4.

A more general iteration than (4.6) is the s-stage method

$$\begin{aligned} \mathbf{p}_{k,i+1} &= \mathbf{p}_{k,i} - d_i \tau \left.\frac{\partial V}{\partial \mathbf{q}}\right|_{\mathbf{q}_{k,i}} \\ \mathbf{q}_{k,i+1} &= \mathbf{q}_{k,i} + c_i \tau \left.\frac{\partial T}{\partial \mathbf{p}}\right|_{\mathbf{p}_{k,i+1}} . \end{aligned} \tag{4.7}$$

The coefficients $c_i, d_i \in \mathbb{R},\ i = 1, ..., s$ are determined such that the method achieves the desired order using $s - 1$ intermediate time steps. For a single stage method, the analysis is trivial. Determining the coefficients for multi-stage methods can become prohibitively hard.

Written in terms of the c_i and d_i, Ruth's second-order method is given by

$$\begin{aligned} c_1 &= \frac{1}{2} \quad d_1 = 0 \\ c_2 &= \frac{1}{2} \quad d_2 = 1. \end{aligned}$$

Ruth also found a three stage, third-order method given by the coefficients

$$\begin{aligned} c_1 &= \frac{2}{3} \qquad d_1 = \frac{7}{24} \\ c_2 &= -\frac{2}{3} \quad d_2 = \frac{3}{4} \\ c_3 &= 1 \qquad d_3 = -\frac{1}{24}. \end{aligned}$$

It is interesting to note that some of the intermediate steps *move backward in time* to achieve third order! This is not a coincidence; every symplectic integrator of the form (4.7) of order at least three must have a stage where $c_i < 0$ and/or $d_i < 0$ [16]!

Remark: *We will use Ruth's second-order method* (4.6) *in Section 4.5. Although it is a simple, explicit method, it is fast and accurate enough for a qualitative calculation of the orbits of the outer planets and Pluto.*

4.2 Higher Order Explicit Methods

Deriving equations to achieve higher order methods is a difficult procedure [4]. A Lie algebraic perspective on multi-stage methods yields a different method for deriving the coefficients c_i and d_i for certain types of higher order methods. Following Yoshida, let $\mathbf{z}$ be the pair of coordinates $\mathbf{z} = (\mathbf{q}, \mathbf{p})$ [16]. Hamilton's equations can be written using the Poisson bracket:

$$\dot{\mathbf{z}} = \{H(\mathbf{z}), \mathbf{z}\},$$

where, in the coordinates $(\mathbf{q}, \mathbf{p})$, the Poisson bracket is

$$\{F, H\} = \frac{\partial F}{\partial \mathbf{p}} \frac{\partial H}{\partial \mathbf{q}} - \frac{\partial F}{\partial \mathbf{q}} \frac{\partial H}{\partial \mathbf{p}}.$$

Note that the possible difference in sign convention can be "fixed" by the ordering $(\mathbf{q}, \mathbf{p})$ versus $(\mathbf{p}, \mathbf{q})$.

Since the action of the Poisson bracket is just that of a first-order, linear, differential operator, we can also write Hamilton's equations as $\dot{\mathbf{z}} = \mathcal{L}_H \mathbf{z}$, where

$$\mathcal{L}_H = \frac{\partial H}{\partial \mathbf{p}} \frac{\partial}{\partial \mathbf{q}} - \frac{\partial H}{\partial \mathbf{q}} \frac{\partial}{\partial \mathbf{p}}. \tag{4.8}$$

Formally, the exact solution to Hamilton's equations of motion at time τ is simply

$$\mathbf{z}(\tau) = e^{\tau \mathcal{L}_H} \mathbf{z}(0).$$

Remark: *From Section 3.4 we know that both $\mathcal{L}_T$ and $\mathcal{L}_V$ are elements of the Lie algebra $\mathfrak{g}$ of all Hamiltonian vector fields on the phase space. The underlying Lie group G is, roughly, the set of all Hamiltonian phase flows (diffeomorphisms) of the phase space. The exponential map $\exp : \mathfrak{g} \to G$ takes the first-order, linear, differential operator $\mathcal{L}_H$ and returns the associated phase flow $e^{t\mathcal{L}_H}$.*

If we still have a separable Hamiltonian $H = T + V$, then the operator $\mathcal{L}_H$ also separates. We then have the formal solution in terms of the *non-commuting* operators $\mathcal{L}_T$ and $\mathcal{L}_V$:

$$\mathbf{z}(\tau) = e^{\tau(\mathcal{L}_T + \mathcal{L}_V)} \mathbf{z}(0), \tag{4.9}$$

where

$$\mathcal{L}_T = \frac{\partial T}{\partial \mathbf{p}} \frac{\partial}{\partial \mathbf{q}} \qquad \mathcal{L}_V = -\frac{\partial V}{\partial \mathbf{q}} \frac{\partial}{\partial \mathbf{p}}.$$

We already have (4.5), which approximates the flows $e^{\mathcal{L}_T}$ and $e^{\mathcal{L}_V}$. We cannot simply apply such a simple symplectic integrator, however. If we formally define the operator $e^{\mathcal{L}_T+\mathcal{L}_V}$ by its power series, we have non-commuting operators $\mathcal{L}_T$ and $\mathcal{L}_V$ acting on each other. Therefore, we know

$$e^{\mathcal{L}_T+\mathcal{L}_V} \neq e^{\mathcal{L}_T}e^{\mathcal{L}_V},$$

in general [16]. To find a computable method, we look for real coefficients c_i and d_i such that

$$e^{\tau(\mathcal{L}_T+\mathcal{L}_V)} = \prod_{i=1}^{s} e^{c_i\tau\mathcal{L}_T}e^{d_i\tau\mathcal{L}_V} + O(\tau^{N+1}). \tag{4.10}$$

Although (4.10) is written slightly differently, it is the same as the s-stage method (4.7) if we use the basic symplectic method (4.5). Each term in the product of (4.10) is a canonical transformation, so the product of the mappings must also be canonical (just like (4.7)). The method (4.10) is not only computable, but gives rise to an explicit method for separable Hamiltonians.

Before we attempt to find any such c_i and d_i, we present the Baker-Campbell-Hausdorff (BCH) formula. Note that while we only consider the case of the Lie algebra of Hamiltonian vector fields, the BCH formula exists for other Lie algebras. Let X and Y be elements of a Lie algebra $\mathfrak{g}$. In general, X and Y will not commute, so let their commutator be $[X,Y] = XY - YX$. The BCH formula allows one to write the product e^Xe^Y as a single exponential

$$e^Xe^Y = e^Z,$$

where

$$\begin{aligned} Z =& X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}\left([X,[X,Y]] + [Y,[Y,X]]\right) + \frac{1}{24}[X,[Y,[X,Y]]] \\ &- \frac{1}{720}\left([Y,[Y,[Y,[Y,X]]]] + [X,[X,[X,[X,Y]]]]\right) \\ &+ \frac{1}{360}\left([Y,[X,[X,[X,Y]]]] + [X,[Y,[Y,[Y,X]]]]\right) \\ &+ \frac{1}{120}\left([X,[X,[Y,[Y,X]]]] + [Y,[Y,[X,[X,Y]]]]\right) \\ &+ \dots . \end{aligned} \tag{4.11}$$

Consider the second-order method given by (4.6). Written in the form of (4.10) and denoted by $S_2(\tau)$, this method is

$$S_2(\tau) = e^{\frac{\tau}{2}\mathcal{L}_T}e^{\tau\mathcal{L}_V}e^{\frac{\tau}{2}\mathcal{L}_T}.$$

If we apply the BCH formula twice, we find the method takes the form [15]

$$S_2(\tau) = e^{\tau\alpha_1+\tau^3\alpha_3+\tau^5\alpha_5+\cdots}, \tag{4.12}$$

where

$$\alpha_1 = \mathcal{L}_T + \mathcal{L}_V \qquad \alpha_3 = \frac{1}{24}\left(2[\mathcal{L}_V,[\mathcal{L}_V,\mathcal{L}_T]] - [\mathcal{L}_T,[\mathcal{L}_T,\mathcal{L}_V]]\right) \qquad \frac{7}{5760}[\mathcal{L}_T,[\mathcal{L}_T,[\mathcal{L}_T,[\mathcal{L}_T,\mathcal{L}_V]]]] + \dots .$$

We note that the method (4.6) is *symmetric* and *time reversible*:

$$S(-\tau)S(\tau) = S(\tau)S(-\tau) = \text{identity}.$$

Note that there are no even powers of τ in (4.12). Yoshida showed that every symplectic integrator of the form (4.10) that is time reversible has no even powers of τ when expanded as

$$S(\tau) = e^{\tau\beta_1+\tau^2\beta_2+\tau^3\beta_3+\tau^4\beta_4+\tau^5\beta_5+\cdots}.$$

In terms of the β_j, we must have $\beta_2 = \beta_4 = ... = 0$. Note that these powers of τ give the order of the method: for consistency, we must have $\beta_1 = 1$; the order of the method (plus one) is given by the next non-zero β_i. Thus, time reversible, symmetric methods are always of even order.

Using Ruth's second-order, symmetric, time reversible method given by (4.6), we can build a fourth-order method by finding coefficients $x_1, x_2 \in \mathbb{R}$ such that the method given by

$$S_4(\tau) = S_2(x_2\tau)S_2(x_1\tau)S_2(x_2\tau),$$

is fourth-order accurate. Using the BCH formula, $S_4(\tau)$ can be written as a single exponential:

$$S_4(\tau) = e^{\tau(x_1+2x_2)\alpha_1+\tau^3(x_1^3+2x_2^3)\alpha_3+\tau^5(x_1^5+2x_2^5)\alpha_5+\cdots}.$$

The condition for $S_4(\tau)$ to be fourth-order accurate is

$$x_1 + 2x_2 = 1 \qquad x_1^3 + 2x_2^3 = 0.$$

In general, if a symmetric, time reversible method of order $2N$ is known, then the method given by

$$S_{2N+2}(\tau) = S_{2N}(x_1\tau)S_{2N}(x_2\tau)S_{2N}(x_1\tau)$$

is of order $2N + 2$ if

$$x_1 + 2x_2 = 1 \text{ and } x_1^{2N+1} + 2x_2^{2N+1} = 0$$

are satisfied. The real solution to these equations is

$$x_1 = -\frac{2^{1/(2N+1)}}{2 - 2^{1/(2N+1)}} \qquad x_2 = \frac{1}{2 - 2^{1/(2N+1)}}.$$

The above symmetric, time reversible methods can easily be of high order, but at the expense of a *large* number of function evaluations. Using a similar approach, Yoshida found sixth and eighth order methods that use fewer function evaluations than the standard composition method [15]. In the same year, Suzuki developed a similar "fractal" composition method with much fewer function evaluations [13]. The algebraic manipulations involved in using the BCH formula with many terms is quite cumbersome. Simply deriving equations for coefficients becomes very difficult for high order methods [4].

4.3 Backward Error Analysis

By starting from the generating function (4.2) and composing the resulting symplectic integrators, we can develop higher order symplectic integrators. We briefly mentioned that the Hamiltonian is not and cannot be conserved by symplectic integrators [8]. However, symplectic integrators *bound* the errors in (smooth) Hamiltonians. To understand why this happens, we will turn to backward error analysis.

Turning away from Hamiltonian systems for a brief moment, consider the single ODE (initial value problem)

$$\dot{x} = f(x) \qquad x(0) = x_0.$$

Suppose we also have some numerical method $L_\tau(x_k)$ that produces the approximations

$$x_{k+1} = L_\tau(x_k)$$

of the original system at the time $t = t_{k+1}$. The standard *forward error analysis* of the method consists of studying the local errors $x_1 - L_\tau(x_0)$ and global errors $x_k - L_{k\tau}(x_0)$. The idea of a *backward error analysis* is to search for a *modified equation* $\dot{\xi} = f_\tau(\xi)$ of the form

$$\dot{\xi} = f_\tau(\xi) = f(\xi) + \tau F_2(\xi) + \tau^2 F_3(\xi) + \dots, \tag{4.13}$$

where $x_k = \xi(t_k)$ [9]. The next step is to study the differences between the flows induced by $f(x)$ and $f_\tau(x)$. It is common to truncate the series in (4.13) and so we will not worry about its convergence. The search for a modified equation is also common in the analysis of finite difference methods for partial differential equations (e.g. Beam-Warming and Lax-Friedrichs).

Suppose we know that $x(t_0) = \xi(t_0) = \xi$ at some time $t = t_0$. We can expand the solution to the modified equation (4.13) at $t = t_0$ into a Taylor series about t_0:

$$\begin{aligned}\xi(t_0 + \tau) = &\xi + \tau\left(f(\xi) + \tau F_2(\xi) + \tau^2 F_3(\xi) + \dots\right) \\ &\frac{\tau^2}{2}\left(f'(\xi) + \tau F_2'(\xi) + \tau^2 F_3'(\xi) + \dots\right)\left(f(\xi) + \tau F_2(\xi) + \tau^2 F_3(\xi) + \dots\right) + \dots .\end{aligned} \tag{4.14}$$

We are searching for the (smooth) functions F_i such that the numerical method L_τ, which we assume can be expanded as

$$L_\tau(x) = x + \tau f(x) + \tau^2 G_2(x) + \tau^3 G_3(x) + \dots, \tag{4.15}$$

"exactly" solves the modified equation (4.13) (i.e. $x_k = \xi(t_k)$). The coefficients of the powers of τ in (4.14) and (4.15) must match, which give the following recurrence relations for the F_i in terms of the method L_τ:

$$F_2 = G_2 - \frac{1}{2} f' f$$

$$F_3 = G_3 - \frac{1}{2}\left(f' F_2 + F_2' f\right) - \frac{1}{6}\left(f'' f f + f' f' f\right)$$

$$\vdots$$

These recurrence relations give us exactly the modified equation for which we were searching. Through various numerical experiments, Hairer shows that symplectic Euler and various other numerical integration methods approximate the exact solutions to their (truncated) modified equations very well [9]. He also notices that the lowest order of τ in the modified equation yields exactly the order of the method and proves the following theorem.

Theorem 4.1: *Suppose the method $x_{k+1} = L_\tau(x_k)$ is of order N so that*

$$L_\tau(x) = g^\tau(x) + \tau^{N+1}\delta_{N+1}(x) + O(\tau^{N+2}),$$

where g^t denotes the exact flow of $\dot{x} = f(x)$ and $\tau^{N+1}\delta_{N+1}(x)$ is the leading term of the local truncation error. The modified equation satisfies

$$\dot{\xi} = f(\xi) + \tau^N F_{N+1}(\xi) + \tau^{N+1} F_{N+2}(\xi) + \dots$$

where $\xi(t_0) = x(t_0)$ and $F_{N+1} = \delta_{N+1}$.

This theorem shows us that the more accurate the method, the "closer" the modified equation is to the actual equation we are trying to solve.

All of the above work was for a general, sufficiently differentiable function f. We can apply a backward error analysis to Hamilton's equations of motion to find a set of modified equations of motion. It turns out that we can do even better; we can (at least locally) find a Hamiltonian function that gives us the modified equations of motion. To to this, we must truncate the modified equation at the r^{th} term. This gives us with a modified Hamiltonian function $H^{[r]}$ of the form

$$H^{[r]} = H + \tau^N H_{N+1} + ... + \tau^{r-1} H_r. \tag{4.16}$$

We can always find a *globally* defined, truncated, modified Hamiltonian in some open subset U of phase space (on which the original Hamiltonian function is defined). The constructive proof of this assertion gives us a method for finding generating functions of the form that are used in the next section on implicit symplectic integrators [9].

We are now in a position to state a theorem on the boundedness of errors in the original Hamiltonian function H. The theorem and a sketch of the proof are from [9].

Theorem 4.2: *Consider a Hamiltonian mechanical system with a smooth Hamiltonian function $H : U \to \mathbb{R}$, configuration space M^n, and $U \subset T^*M^n$. Apply a symplectic integrator S_τ of order N with step size τ and assume the truncated, modified Hamiltonian $H^{[r]}$ is globally defined on U. If the numerical solution $\mathbf{z}_k$ stays in the compact set $K \subset U$, then we have asymptotically for $\tau \to 0$*

$$H^{[r]}(\mathbf{z}_k) = H^{[r]}(\mathbf{z}_0) + O(t\tau^r)$$
$$H(\mathbf{z}_k) = H(\mathbf{z}_0) + O(\tau^N)$$

over time intervals of size $t = k\tau \leq C\tau^{N-r}$.

Proof: *Let g_r^t be the flow of the truncated, modified Hamiltonian. The effect of the truncation is that $||\mathbf{z}_{k+1} - g_r^\tau(\mathbf{z}_k)|| \leq C\tau^{r+1}$ for some norm equivalent to the 2-norm. Let the Lipschitz constant $K_L \in \mathbb{R}$ be the minimum value, independent of τ, such that*

$$|H(\mathbf{x}) - H(\mathbf{y})| \leq K_L||\mathbf{x} - \mathbf{y}|| \quad \forall\, \mathbf{x}, \mathbf{y} \in K.$$

The error in $H^{[r]}$ at time $t = t_k$ is

$$H^{[r]}(\mathbf{z}_k) - H^{[r]}(\mathbf{z}_0) = \sum_{j=0}^{k-1} H^{[r]}(\mathbf{z}_{j+1}) - H^{[r]}(\mathbf{z}_j).$$

Since g_r^τ is the exact flow of $H^{[r]}$ we know it conserves $H^{[r]}$ exactly. Namely, we have $H^{[r]}(g_r^\tau(\mathbf{z}_j)) = H^{[r]}(\mathbf{z}_j)$ at each time t_j. The summand becomes

$$H^{[r]}(\mathbf{z}_{j+1}) - H^{[r]}(g_r^\tau(\mathbf{z}_j)) \leq K_L||\mathbf{z}_{j+1} - g_r^\tau(\mathbf{z}_j)||.$$

Now we have

$$H^{[r]}(\mathbf{z}_k) - H^{[r]}(\mathbf{z}_0) \leq \sum_{j=0}^{k-1} K_L C\tau^{r+1} = O(k\tau^{r+1}) = O(t\tau^r).$$

Because $H_{N+1}(\mathbf{z}) + ... + \tau^{r-N-1} H_r(\mathbf{z})$ is uniformly bounded, independent of τ and r, on K, and $N \leq r$,

$$H(\mathbf{z}_k) - H(\mathbf{z}_0) = O(\tau^N). \qquad \square$$

Essentially, Theorem 4.2 states that if we apply an N^{th} order symplectic integrator to a smooth Hamiltonian that has motions restricted to a compact domain of phase space, the error in the modified Hamiltonian will grow linearly with time, but *the error in the true Hamiltonian will oscillate inside of a constant bound*. It is for this reason that symplectic integrators are said to *nearly* conserve the Hamiltonian. Also note that the error in the true Hamiltonian will oscillate inside of its bound for all time (disregarding numerical errors).

The property of long-time Hamiltonian error boundedness is one of the chief attractions to symplectic integrators; symplectic integrators very nearly obey both of the properties of exact solutions listed at the beginning of this section. Kinoshita applied various symplectic integrators and a classical fourth-order Runge-Kutta (RK) method to the Kepler problem for both short and long-time spans. As one might expect, given Theorem 4.2, the symplectic integrators performed much better than the Runge-Kutta method for *long* time spans. However, for shorter time spans, the Runge-Kutta method produced more accurate results [10].

Yoshida also compared a symplectic method and Runge-Kutta method to the Kepler problem [16]. It is quite common to use an adaptive step size in numerical integration to obtain better accuracy (perhaps set by some absolute or relative tolerance). Yoshida demonstrated how (naively) using an adaptive time step *destroys* the Hamiltonian error boundedness of the symplectic integrator; as is expected, the same (naive) adaptive time stepper *improves* the accuracy of the classical Runge-Kutta method. At least in the context of gravitational n-body problems with a large central mass, a working method of *individual* time stepping has been introduced [12].

4.4 Construction of Implicit Methods

In many Hamiltonian systems, one cannot separate the Hamiltonian function as $H(\mathbf{q},\mathbf{p}) = T(\mathbf{p}) + V(\mathbf{q})$. None of the previously considered (explicit) methods will work. However, using the same generating function idea with generating function (4.2), one can derive *implicit* symplectic integrators. The analog of the symplectic Euler method, which is generically called the one step method, is given by the transformation

$$\begin{aligned} \mathbf{p}_{k+1} &= \mathbf{p}_k - \tau \frac{\partial H}{\partial \mathbf{q}}\bigg|_{(\mathbf{q}_k,\mathbf{p}_{k+1})} \\ \mathbf{q}_{k+1} &= \mathbf{q}_k + \tau \frac{\partial H}{\partial \mathbf{p}}\bigg|_{(\mathbf{q}_k,\mathbf{p}_{k+1})} \end{aligned}. \tag{4.17}$$

Note that in (4.17), one can solve the evolution for $\mathbf{p}_{k+1}$ using a simple fixed-point iteration (or more sophisticated methods), and then explicitly find $\mathbf{q}_{k+1}$ once $\mathbf{p}_{k+1}$ is known. This one step method gives a first-order, *implicit* method. Using a backward error analysis, one can show that this method, if it satisfies the conditions of Theorem 4.2, nearly conserves the Hamiltonian function [16].

If we instead use the infinitesimal generating function

$$S_\tau(\mathbf{q},\mathbf{P}) = \mathbf{q}\mathbf{P} + \tau H + \frac{\tau^2}{2}\frac{\partial H}{\partial \mathbf{P}}\frac{\partial H}{\partial \mathbf{q}},$$

where $H = H(\mathbf{q},\mathbf{P})$, we arrive at the second-order, one stage, implicit method

$$\begin{aligned} \mathbf{p}_{k+1} &= \mathbf{p}_k - \tau \frac{\partial H}{\partial \mathbf{q}}\bigg|_{(\mathbf{q}_k,\mathbf{p}_{k+1})} - \frac{\tau^2}{2}\left(\frac{\partial^2 H}{\partial \mathbf{q}\partial \mathbf{p}}\frac{\partial H}{\partial \mathbf{q}} + \frac{\partial H}{\partial \mathbf{p}}\frac{\partial^2 H}{\partial \mathbf{q}^2}\right)\bigg|_{(\mathbf{q}_k,\mathbf{p}_{k+1})} \\ \mathbf{q}_{k+1} &= \mathbf{q}_k + \tau \frac{\partial H}{\partial \mathbf{p}}\bigg|_{(\mathbf{q}_k,\mathbf{p}_{k+1})} + \frac{\tau^2}{2}\left(\frac{\partial^2 H}{\partial \mathbf{p}^2}\frac{\partial H}{\partial \mathbf{q}} + \frac{\partial H}{\partial \mathbf{p}}\frac{\partial^2 H}{\partial \mathbf{p}\partial \mathbf{q}}\right)\bigg|_{(\mathbf{q}_k,\mathbf{p}_{k+1})} \end{aligned}. \tag{4.18}$$

Again, we note that the evolution of $\mathbf{p}_{k+1}$ is the implicit part of the integrator. We can solve for $\mathbf{p}_{k+1}$ using any one of a variety of methods, and once $\mathbf{p}_{k+1}$ is known, $\mathbf{q}_{k+1}$ is given explicitly by its evolution equation.

To obtain higher order symplectic integrators, one must find a generating function S_τ of the form of (4.2) such that the transformation given by (4.3) agrees with the Taylor expansion of the solution up to τ^N. Simply finding the generating function can be quite difficult; deriving the symplectic integrator becomes a "mess" of derivatives and algebra; and finally coding the integrator becomes extraordinarily difficult. Channell and Scovel developed a preprocessor to write FORTRAN code for up to sixth order methods derived from generating functions [4].

Another implicit, second-order method is the Störmer-Verlet method, which is given by

$$\begin{aligned}
\mathbf{p}_{k,1} &= \mathbf{p}_k - \frac{\tau}{2}\left.\frac{\partial H}{\partial \mathbf{q}}\right|_{(\mathbf{q}_k,\mathbf{p}_{k,1})} \\
\mathbf{q}_{k+1} &= \mathbf{q}_k + \frac{\tau}{2}\left(\left.\frac{\partial H}{\partial \mathbf{p}}\right|_{(\mathbf{q}_k,\mathbf{p}_{k,1})} + \left.\frac{\partial H}{\partial \mathbf{p}}\right|_{(\mathbf{q}_{k+1},\mathbf{p}_{k,1})}\right) \\
\mathbf{p}_{k+1} &= \mathbf{p}_{k,1} - \frac{\tau}{2}\left.\frac{\partial H}{\partial \mathbf{q}}\right|_{(\mathbf{q}_{k+1},\mathbf{p}_{k,1})}.
\end{aligned} \tag{4.19}$$

Note that we must solve for $\mathbf{p}_{k,1}$, then solve for $\mathbf{q}_{k+1}$, and then $\mathbf{p}_{k+1}$ is given explicitly in terms of $\mathbf{p}_{k,1}$ and $\mathbf{q}_{k+1}$. This method was successfully used in the study of the Fermi-Pasta-Ulam problem in the early 1950's. The Fermi-Pasta-Ulam problem has connections to the Korteweg-de Vries equation, appears in the study of shallow water waves.

We now consider Runge-Kutta methods. For general ODE initial value problems, Runge-Kutta methods have become very popular, and are implemented in many software packages. These methods can perform quite well if they are coupled with adaptive time stepping, paired with a higher order Runge-Kutta method (e.g. Dormand-Prince pairs), etc. In general, an s-stage Runge-Kutta method for the problem $\dot{x} = f(t,x)$ is of the form

$$x_{k+1} = x_k + \tau \sum_{k=1}^{s} b_i k_i \qquad k_i = f\left(t_0 + c_i\tau, x_k + \tau \sum_{j=1}^{s} a_{ij} k_j\right).$$

In order to have a consistent method, we must have $c_i = \sum_{j=1}^{s} a_{ij}$. It is common to list the a_{ij}, b_i, and c_i in a *Butcher table*:

$$\begin{array}{c|cccc}
c_1 & a_{11} & a_{12} & \dots & a_{1s} \\
c_2 & a_{21} & a_{22} & \dots & a_{2s} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
c_s & a_{s1} & a_{s2} & \dots & a_{ss} \\
\hline
 & b_1 & b_2 & \dots & b_s
\end{array} \tag{4.20}$$

Note that the Runge-Kutta method given by (4.20) is explicit if A is strictly lower triangular, where A is the matrix of a_{ij}. When A is not strictly lower triangular, the method is implicit. Also note that $b_j \neq \sum_{i=1}^{s} a_{ij}$ in general.

Just as the c_i and d_i of (4.10) are parameters of the method, the a_{ij} and b_j are parameters of a Runge-Kutta method. Similarly, there are consistency restraints on the a_{ij}. The parameters that remain are used to build a method with certain properties, such as the order of accuracy of the method, its stability region, possible pairing with a slightly different Runge-Kutta method (e.g. Dormand-Prince pairs).

A further desirable property that we might want in a Runge-Kutta method is that the method preserve the symplectic structure of a Hamiltonian mechanical system. However, Runge-Kutta methods do not in general preserve the symplectic structure and so are not in general symplectic integrators. Therefore, instead of being bounded, the error in the Hamiltonian grows in time [10]. Symplectic Runge-Kutta methods do exist, and there is a formula used to determine if a Runge-Kutta method is symplectic [9].

Theorem 4.3: *If the coefficients of a consistent Runge-Kutta method satisfy*

$$b_i a_{ij} + b_j a_{ji} = b_i b_j \quad \forall i \, \forall j,$$

then the method is symplectic.

A simple, second-order, symplectic Runge-Kutta method is given by the following Butcher table:

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

The above method is called the *implicit midpoint method*. A fourth-order symplectic Runge-Kutta method is given by:

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

Remark: *Perhaps the reader who is already quite familiar with Runge-Kutta methods will recognize this as the fourth-order collocation method based on the points of Gauss-Legendre quadrature (i.e. Gaussian quadrature using Legendre polynomials). The Gauss-Legendre method based on s points has order $2s$ and is symplectic. However, these methods aren't regularly used due to prohibitive computational cost [9].*

Finally, we turn our attention to a motivating example for studying Hamiltonian mechanics and symplectic integrators: the motion of the outer planets and Pluto for one billion years!

4.5 Example: The Outer Planets for One Billion Years

The gravitational N-body problem is a classic problem in mechanics. In this example, we study the motion of $N-1$ massive particles interacting via Newton's law of universal gravitation; one of the masses is significantly larger the rest. The method that we briefly describe was developed by Wisdom and Holman as part of Holman's dissertation [14]. Wisdom and Holman successfully used their new *symplectic map* to confirm and extend the integrations performed with the Digital Orrery [1].

In (heliocentric) Cartesian coordinates, the Hamiltonian for the N-body problem is

$$H = \sum_{i=0}^{N-1} \frac{||\mathbf{p}_i||^2}{2m_i} - \sum_{i<j} \frac{G m_i m_j}{r_{ij}}, \tag{4.21}$$

where $||\mathrm{p}_i||$ is the 2-norm of the i^{th} momentum, m_i is the mass of the i^{th} particle, G is Newton's gravitational constant, and $r_{ij} = ||\mathbf{x}_i - \mathbf{x}_j||$, and $\mathbf{x}_i$ is the position of the i^{th} particle. One approach to solving Hamilton's equations of motion for the Hamiltonian (4.21) would be to apply a symplectic integrator directly to the problem. This is a good test for the performance of a symplectic integrator, but by changing coordinates, Wisdom and Holman were able to utilize the integrability of the Kepler problem (i.e. the two body problem) to greatly improve the speed and accuracy of their integrations.

A Hamiltonian function is called *Keplerian* if it can be written as

$$H_K = \frac{||\mathbf{p}||^2}{2m} - \frac{GMm}{||\mathbf{r}||}$$

or a sum of Keplerian Hamiltonians. The Hamiltonian (4.21), as a whole, is not Keplerian, although we can separate the Keplerian portions of the Hamiltonian; if we were to do so, the remaining terms would would still make up a significant portion of the total Hamiltonian. If we write the N-body Hamiltonian in the well known Jacobi coordinates, the Hamiltonian becomes the sum of Keplerian Hamiltonians (in Jacobi coordinates) plus much smaller interaction terms (conveniently written in mixed Cartesian and Jacobi coordinates).

Let the first Jacobi coordinate be the center of mass $\mathbf{x}'_0$. The remaining $N-1$ Jacobi coordinates are

$$\mathbf{x}'_i = \mathbf{x}_i - \mathbf{X}_{i-1},$$

where $\mathbf{X}_i$ is the center of mass of the particles with with indexes up to i:

$$\mathbf{X}_i = \frac{1}{\eta_i}\sum_{j=0}^{i} m_j \mathbf{x}_j \qquad \eta_i = \sum_{j=0}^{i} m_j.$$

Note that $\mathbf{X}_{N-1} = \mathbf{x}'_0$. When deriving the Jacobi requirements, we require that the transformed kinetic energy portion of the Hamiltonian be a diagonal sum of squared-norms of the momenta; that is, we do not want cross-terms between the momenta. We also require that $\mathbf{p}'_i = m'_i \mathbf{v}'_i$, where $\mathbf{v}'_i$ is the time derivative of $\mathbf{x}'_i$ and the new mass factors are $m'_i = \eta_{i-1} m_i / \eta_i$ for $1 \leq i \leq (N-1)$ and $m'_0 = \eta_{N-1}$. Note that $\eta_{N-1} = M$ is the total mass of the system.

The transformation from Jacobi coordinates to Cartesian coordinates is given by

$$\mathbf{x}_i = \mathbf{x}'_i + \sum_{j<i} \frac{m_j \mathbf{x}'_j}{\eta_j}.$$

The transformation from Cartesian coordinates to Jacobi coordinates can be written as a matrix transformation, which will inherently depend on how the positions are stored in the code. The inverse transformation can then be realized with a linear system solver. We index the particles in order of increasing distance from the center of mass with one exception; we put Pluto in the first index after the Sun. This reduces high frequency oscillations in the Jacobi coordinates of Pluto due to the motion of planets interior to Pluto.

In mixed Cartesian and Jacobi coordinates, the N-body Hamiltonian becomes

$$H = \frac{||\mathbf{p}'_0||^2}{2M} + \sum_{i=1}^{N-1}\left(\frac{||\mathbf{p}'_i||^2}{2m'_i} - \frac{Gm_i m_0}{r_{i0}}\right) - \sum_{0<i<j} \frac{Gm_i m_j}{r_{ij}}.$$

The second term of the Hamiltonian is "half" of a Keplerian Hamiltonian in Jacobi coordinates. If we add and subtract the "missing" quantity

$$\sum_{i=1}^{N-1} \frac{Gm_i m_0}{r'_i},$$

where $r'_i = ||\mathbf{x}'_i||$, the Hamiltonian becomes

$$H = \frac{||\mathbf{p}'_0||^2}{2M} + \sum_{i=1}^{N-1}\left(\frac{||\mathbf{p}'_i||^2}{2m'_i} - \frac{Gm_i m_0}{r'_i}\right) + \sum_{i=1}^{N-1}\left(\frac{Gm_i m_0}{r'_i} - \frac{Gm_i m_0}{r_{i0}}\right) - \sum_{0<i<j} \frac{Gm_i m_j}{r_{ij}}. \tag{4.22}$$

The N-body Hamiltonian is now of the form

$$H = H_{\text{Kepler}} + H_{\text{Interaction}},$$

where $H_{\text{Interaction}} << H_{\text{Kepler}}$.

Up to this point, no approximations have been made, and the Hamiltonian (4.22) is equivalent to (4.21). The motions induced by $H_{\text{Interaction}}$ are highly oscillatory and have a small amplitude. By the averaging principle, which essentially states that the long term motion of a Hamiltonian system is not greatly affected by highly oscillatory terms (which tend to average to zero), Wisdom and Holman argue that the modified Hamiltonian

$$H_{\text{Map}} = H_{\text{Kepler}} + 2\pi\delta_{2\pi}(\Omega t)H_{\text{Interaction}} \tag{4.23}$$

produces nearly the same motion as (4.21) [14, 3]. Ω is the constant mapping frequency, and is chosen to be on the order of the orbital frequencies. The 2π periodic δ "function" comes about by adding in progressively higher frequency cosine terms [14]:

$$\frac{1}{2\pi}\sum_{n=-\infty}^{\infty}\cos(nt) = \sum_{n=-\infty}^{\infty}\delta(t-2\pi n) = \delta_{2\pi}(t).$$

The mapping Hamiltonian (4.23) has a particularly simple interpretation: for the times when the delta "function" is "off", the system evolves according to only H_{Kepler}; for the times when the delta "function" is "on", the system receives a "kick" from the terms in $H_{\text{Interaction}}$ with no contributions from H_{Kepler}. The Keplerian Hamiltonian is separately integrable, and can be handled with its own method; the interaction terms can similarly be handled with their own numerical method. The whole integration method becomes "evolve according to H_{Kepler} for some amount of time", "evolve according to $H_{\text{Interaction}}$ for some amount of time", and repeat.

Let $\mathbf{z}' = (\mathbf{x}', \mathbf{p}')$ be the pair of generalized coordinates and momenta in Jacobi coordinates. Let $\mathcal{L}_K$ and $\mathcal{L}_I$ be the operators based on the Kepler and interaction Hamiltonians such that $\mathbf{z}'(\tau) = e^{\tau\mathcal{L}_K}\mathbf{z}'(0)$ and $\mathbf{z}'(\tau) = e^{\tau\mathcal{L}_I}\mathbf{z}'(0)$ give the exact flows for the Kepler and interaction Hamiltonians, respectively. The problem of integration is now very similar to that of Section 4.2: we can split the Hamiltonian and evolve each part forward (and sometimes backward, depending on the method!) in time by itself.

Combining the Kepler and interaction mappings together in the form of (4.10), we have a symplectic integrator given by

$$e^{\tau(\mathcal{L}_K+\mathcal{L}_I)} = \prod_{i=1}^{s} e^{c_i\tau\mathcal{L}_K}e^{d_i\tau\mathcal{L}_I} + O(\tau^{N+1}).$$

We can choose any of the high order integrator coefficients discussed in Section 4.2 and the references therein, but Wisdom and Holman suggest that using Ruth's second-order method (4.6) is good enough for a "qualitatively accurate" integration. Thus, we used Ruth's second-order method in all of our integrations.

Instead of integrating the Keplerian motion using derivatives of H_{Kepler} like one might normally do with a symplectic integrator, we can efficiently integrate the motion "exactly" using the f and g functions of orbital mechanics [5, 6]. Note that we do this entirely in Jacobi coordinates with the appropriate masses and gravitational parameter (the Jacobi version of Gm_0); there is no need to compute all of the orbital elements at each time step! Efficient algorithms for moving Keplerian orbits forward in time using the f and g functions can be found in [6].

The interaction Hamiltonian is handled in the usual manner. Therefore, we need to know the derivatives of $H_{\text{Interaction}}$ with respect to the Jacobi coordinates $\mathbf{x}'_i$ to update the momenta $\mathbf{p}'_i$. The necessary derivatives of $H_{\text{Interaction}}$ are given in [12].

Initial conditions for the Solar system were taken from Applegate et al. [1]; these are the same initial conditions used by Wisdom and Holman in their integrations. We integrated the motion of the Sun, Jupiter, Saturn, Uranus, Neptune, and Pluto. Since Jupiter has the shortest period, its orbit restricted our time step to *one year*. The Digital Orrery integrations used a different numerical method which required a time step of 40 days [1]; it is no wonder that Wisdom and Holman's symplectic mappings (with a low order symplectic integrator) were significantly faster than those of Applegate et al. The orbits of the Sun and outer planets were integrated for one billion years; positions and velocities of the planets and Sun were recorded every 1000 years.

Figure 1 shows Pluto's orbital element $h = e\sin(\omega+\Omega)$ and the relative error in the Hamiltonian function (4.21). Initial conditions were chosen to be *slightly* different than Applegate's initial conditions. The plot of h over one billion years is very nearly the same as Applegate's and Wisdom and Holman's, but there are *slight* differences. The plot of the relative error in the Hamiltonian function clearly shows the constant bound (recall Theorem 4.2). The relative error is bounded on the order of 10^{-5}, which matches Wisdom and Holman's results [14].

Both Applegate et al. and Wisdom found that the modulation of h had a period of about 137 Myr and a basic oscillation period of 3.69 Myr. In our integrations, we found that the basic oscillation period was 3.69 ± 0.01 Myr; the longer period modulation had a period of 133 ± 10 Myr. The errors given here are rough estimates to impart on the reader a sense of the width of the peak in the power spectrum of h.

Figure 2 shows Pluto's h and the relative error in the Hamiltonian for an integration starting with initial conditions based on Jet Propulsion Laboratory Development Ephemeris 200 (DE 200). These initial orbits of the Sun, outer planets, and Pluto are not as close to those used by Applegate as the initial conditions used to create Figure 1. The slight differences in the initial conditions manifests itself as the differences between Figure 2 and Figure 1. Again, the relative error in the Hamiltonian is bounded on the order of 10^{-5}.

For the different initial conditions, we found the basic oscillation period to be 3.68 ± 0.01 Myr. The larger modulation period was not very well defined in the power spectrum, as we expect from Figure 2; however, there was a wide peak in the spectrum from 130 Myr to 170 Myr.

It is quite clear from the figures that the error in the Hamiltonian is bounded for at least one billion time steps. We could use a more accurate symplectic integrator for the $H_{\text{Interaction}}$ term, which would decrease the bound for the errors in the Hamiltonian. Integrations of the Solar system modeled as a Hamiltonian mechanical system are not usually carried past one billion years due to the accumulation of non-gravitational and non-conservative forces.

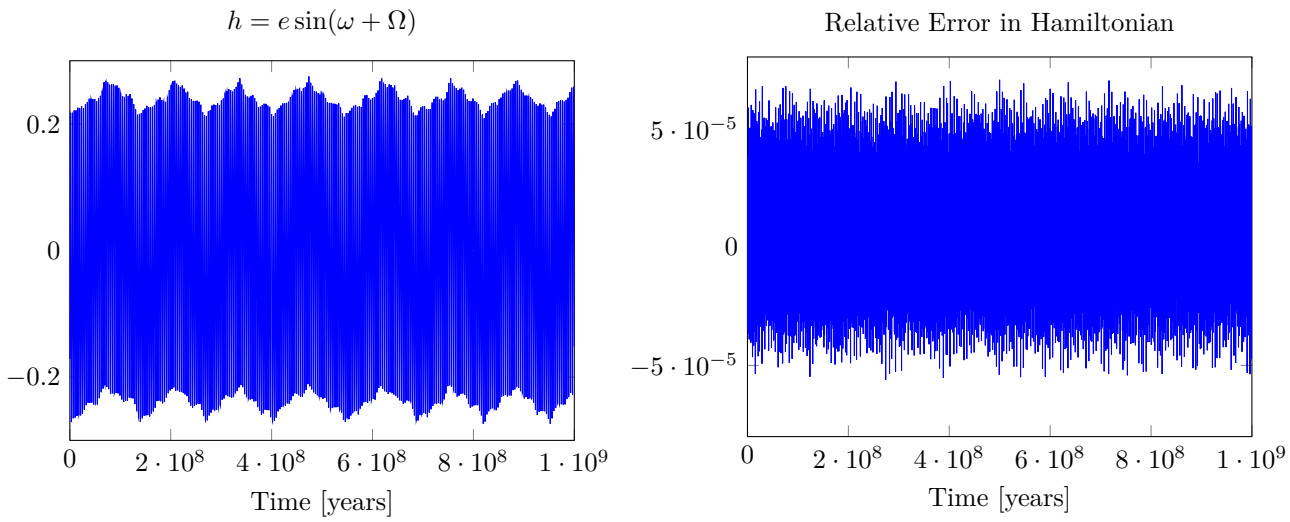

Figure 1: Orbital element h and relative error in Hamiltonian for initial conditions very close to Wisdom and Holman's.

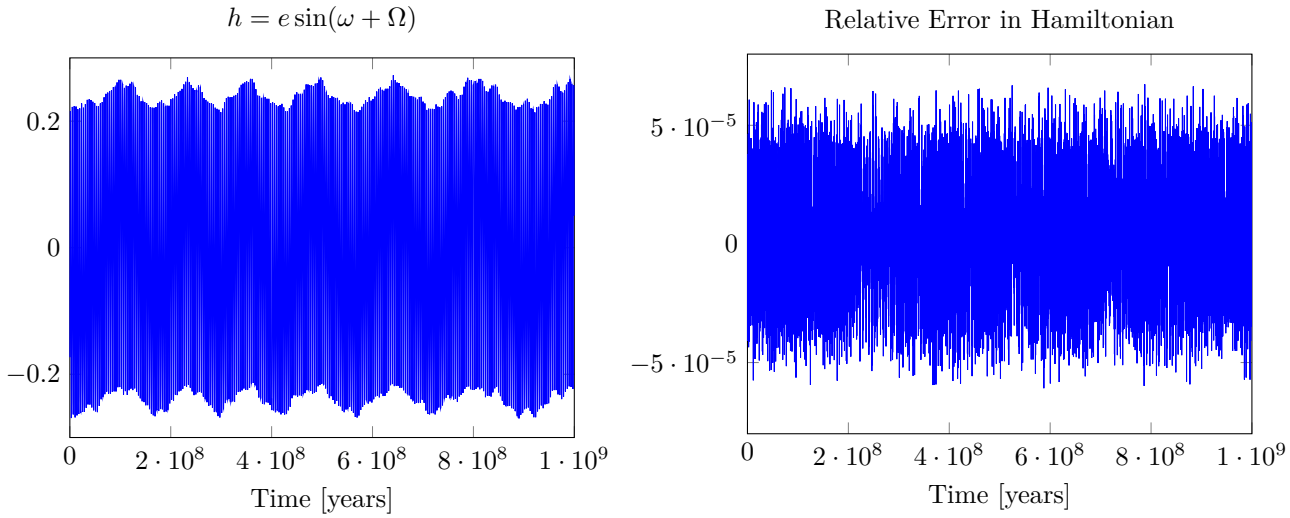

Figure 2: Orbital element h and relative error in Hamiltonian for initial conditions not as close to Wisdom and Holman's.

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References

[1] J. Applegate, M. Douglas, Y. Gürsel, G. Sussman, and J. Wisdom, *The outer solar system for 200 million years*, The Astronomical Journal, (1986).

[2] V. I. Arnold, *Ordinary Differential Equations*, The MIT Press, 1973.

[3] ——, *Mathematical Methods of Classical Mechanics*, Springer, 1989.

[4] P. J. Channell and C. Scovel, *Symplectic integrators for hamiltonian systems*, Nonlinearity, (1990).

[5] H. Curtis, *Orbital Mechanics for Engineering Students*, Elsevier, 2010.

[6] J. Danby, *Fundamentals of Celestial Mechanics*, Willmann-Bell, 2 ed., 2003.

[7] T. Frankel, *The Geometry of Physics: An Introduction*, Cambridge University Press, 2 ed., 2003.

[8] Z. Ge and J. Marsden, *Lie-poisson hamilton-jacobi theory and lie-poisson integrators*, Physical Letters A, (1988).

[9] E. Hairer, *Geometric numerical integration - lecture notes*. http://www.unige.ch/ hairer/polycop.html, 2010.

[10] H. Kinoshida, H. Yoshida, and H. Nakai, *Symplectic integrators and their application to dynamical astronomy*, Celestial Mechanics and Dynamical Astronomy, (1991).

[11] R. Ruth, *A canoncial integration technique*, IEEE Transactions on Nuclear Science, (1983).

[12] P. Saha and S. Tremaine, *Long-term planetary integration with individual time steps*, astro-ph/9403057, (1994).

[13] M. Suzuki, *Fractal decomposition of exponential operators with applications to many-body theories and monte carlo simulations*, Physical Letters A, (1990).

[14] J. Wisdom and M. Holman, *Symplectic maps for the n-body problem*, The Astronomical Journal, (1991).

[15] H. Yoshida, *Construction of higher order symplectic integrators*, Physics Letters A, (1990).

[16] ——, *Recent progress in the theory and application of symplectic integrators*, Celestial Mechanics and Dynamical Astronomy, (1993).