

Hamiltonian Mechanics on Discrete Manifolds

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Abstract

The mathematical/geometric structure of discrete models of systems, whether these models are obtained after discretization of a smooth system or as a direct result of modeling at the discrete level, have not been studied much. Mostly one is concerned regarding the nature of the solutions, but not much has been done regarding the structure of these discrete models. In this paper we provide a framework for the study of discrete models, specifically we present a Hamiltonian point of view. To this end we introduce the concept of a discrete calculus.

1 Introduction

The modeling of physical systems using differential equations (ordinary or partial) is well-established. Solutions of most models are extremely difficult to derive analytically. For this reason the models are discretized, various methods exist for this, such that they are *suitable* for numerical simulation on computers. Hence, one starts with a system for which the spatial and time variables live in smooth spaces, and ends up with a system whose spatial and time variables live in discrete spaces (more precisely the set of floating point numbers). But *what is the structure of the final system?* To the knowledge of the authors very little has been done regarding this question. Mostly one is interested in the nature of the solutions, not the structure itself. Some researchers address questions such as energy/momentum conservation - but very few answers have been given regarding the complete structure of the system.

In [1] there has been an novel and very interesting attempt to formalize *discrete mechanical systems*, Basically the well-known concepts of differential calculus are placed in an algebraic setting using tools from algebraic geometry. Two of the basic ideas in [1] are: replacing the field of reals by an arbitrary commutative ring, the use of the algebraic definition of a derivation as an analogue to a vector field. There are two problems with this theory. Firstly in a fully discrete setting, derivations are not the correct analogues of vector fields. We will argue that twisted derivations are the appropriate analogues of vector fields, and this has nontrivial consequences. Moreover, in general, computers use floating point numbers for computations, and most of the research in numerical simulation uses floating point numbers. But the set of floating point numbers is not a ring, and without this most basic property trying to define any sort of formal structure is a seemingly hopeless task. Also note that numerical simulations employ many tools, from forward differences to Runge-Kutta methods and so

on. What do such methods mean in the context of discrete physical systems? The basic motivations of the paper are essentially to provide answers to the above raised issues. Moreover in this paper we formalize discrete physical systems in a Hamiltonian framework. To this end we also introduce a discrete calculus, the concept of discrete manifolds and so on. The outline of this paper may be summarized as follows: to define a discrete calculus, to relate various integration techniques to the discrete calculus, and to define discrete-Hamiltonian dynamics. Our basic motivation is to give a formal structure for discrete physical systems.

2 The algebraic structure of the set of floating point numbers

Differentiable manifolds locally look like, loosely speaking, Euclidean \mathbb{R}^n . If we want to extend this definition to more general manifolds, we need to replace the field \mathbb{R} by a general ring. In the case of discrete manifolds, defined later on, we would like to replace \mathbb{R} with the set of floating point numbers \mathbb{F} . The reason for this is very simple, since most computers work with floating point numbers, from our point of view this is the most obvious choice. However, unlike \mathbb{R} , \mathbb{F} does not have an algebraic structure - as one usually understand it. \mathbb{F} is a finite set, algebraic operations defined on \mathbb{F} usually have results that are truncated (because of the finite precision of floating point numbers [2, 3]), and hence some of the basic algebraic properties like associativity and distributivity are destroyed. Hence \mathbb{F} is *not even a ring* (c.f. [3] for more details), and then it seems that there is simply no way that we can use it as a replacement for \mathbb{R} in the discrete setting. However since we would like to extend the concepts of differential geometry to the discrete setting, we have to endow \mathbb{F} with some *new* algebraic structure.

The properties of floating point numbers have been very well researched, c.f. [2, 3] among others. For the purpose of studying discrete mechanics the algebraic structure of the set of floating point numbers is straightforward to deal with, as will be obvious from latter sections. The algebraic structure is itself quite simple. \mathbb{F} is an example of what is called a *quasi-ring*, c.f. [4]. Loosely speaking, a quasi-ring is a *finite* set closed under two special operations denoted by $+$, \cdot s.t. in general the set does not have the associativity and distributivity properties of ordinary rings. $+$, \cdot are called 'special' because in \mathbb{F} all operations are truncated, unless they fall within a certain finite precision range, - for example: $2 + 10^{-15} = 2$ in many computer architectures. Hence one can loosely think of $+$, \cdot being the usual operations in \mathbb{R} followed by a truncation process.

Example 1 *Floating point numbers \mathbb{F} are examples of quasi-rings. The properties¹ of the set of floating point numbers are:*

¹Note that the properties of \mathbb{F} are not being defined formally. The reason for this is that these properties are very well known, and one would need to introduce many entities in order to formally define this, which we cannot do due to space constraints. In [4] we have formally

<i>Closure under addition and multiplication</i>	<i>Yes.</i>
<i>Associativity/distributivity of addition and multiplication</i>	<i>No.</i>
<i>Additive and multiplicative commutativity</i>	<i>Yes.</i>
<i>Unique identity element w.r.t. +, ·</i>	<i>Yes.</i>
<i>Unique additive and multiplicative inverse</i>	<i>Yes.</i>

Hence \mathbb{F} is a quasi-ring, this will be our discrete analogue of the reals (which is a field, i.e. a ring with a multiplicative inverse). In our approach space and time are considered as discrete, and importantly our system variables take their values in \mathbb{F} , the same goes for the independent variables space and time. So for example systems do not evolve in integer time steps, rather they evolve in floating-point time steps.

The point spacings in \mathbb{F} are not constant, and it is in this respect that our approach is fundamentally different from the usual lattice approach to discretization.

3 Non regular lattices

We are interested in modeling mechanical systems at the discrete level in order to be able to represent those models on a computer. We require discreteness because computers are not able to represent continuous variables, since they can only handle floating point numbers. The set of floating point numbers \mathbb{F} is quite 'similar' to regular lattices, but it exhibits an important difference: *the spacing between two consecutive elements is not constant*. Let us now revisit floating point numbers from a slightly different viewpoint.

Definition 1 *A floating point number corresponds to a sequence of bits in the form:*

$$SE \cdots EF \cdots F \implies (-1)^S \times 1.F \cdots F \times 2^{E \cdots E - B}$$

where S determines the sign (as $(-1)^S$), $E \cdots E$ represent the exponent, which is biased by B to allow negative values, and $F \cdots F$ represent the mantissa which fixes the precision.

Compared to the real numbers, \mathbb{F} is not dense, but yet the variation (in the point spacings) is not random, since it depends on the range of numbers represented by the exponent. Hence, for numbers with the same value of the exponent, the spacing is constant and equal to 2^{e-n_m} where e is the value of the exponent and n_m is the number of digits of the mantissa. It is easy to see:

Lemma 1 *The set of floating point numbers is only continuous for a representation with an infinite number of bits in the mantissa.*

A very important issue to be taken into account is that the cardinality of the set of floating point numbers depend on the computer we work on: the larger defined quasi-rings and the properties of \mathbb{F} .

the memory, the larger and denser the set. Therefore, continuum limit is also a natural goal in the process.

In this sense, we can write:

Lemma 2 *Consider the floating point numbers scheme with a varying number of digits N , and denote the resulting set as \mathbb{F}_N . Then, the limit when $N \rightarrow \infty$ are the real numbers, i.e.:*

$$\lim_{N \rightarrow \infty} \mathbb{F}_N = \mathbb{R}$$

As we are interested in modeling physical systems, it is enough to be able to recover a subset of the reals \mathbb{R}^n , which without loss of generality can be considered to be $V = [0, 1]^n \subset \mathbb{R}^n$.

Definition 2 *Consider a **non-regular discrete space** \mathbb{F}_N^n to be any discrete set of V such that, for any two consecutive points in one direction, the euclidian distance between them is an element of \mathbb{F}_N .*

Obviously, the cardinality of the set \mathbb{F}_N corresponds to the number of real numbers which can be defined by using N bits in the representation. It is exactly 2^N , as in the case of the integers.

Definition 3 *Let A and B be two discrete spaces. We shall call **discrete mapping** to any bijection between the sets $\Psi : A \rightarrow B$.*

Asking the discrete mapping to be a bijection only is not sufficient, for example in the smooth setting one asks for differentiability also. In fact in our discrete setting we demand the discrete mapping to be also *discrete-differentiable*, a concept we introduce in Section 4.1.

3.0.1 A 'basis' for \mathbb{F}_N^n

In the following, it will be quite useful to define the analogue of basis for floating point numbers. It is trivial to see:

Lemma 3 *The elements $\overbrace{(1, 0, \dots, 0)}^n, \overbrace{(0, 1, 0, \dots, 0)}^n, \dots, \overbrace{(0, \dots, 0, 1)}^n$ generate the elements in \mathbb{F}_N^n with linear combinations of \mathbb{F}_N elements. We will refer to this as the **canonical set of generators** or **canonical basis** of \mathbb{F}_N^n .*

Proof. In each dimension, the property is trivial, since the value of the element of \mathbb{F}_N itself defines the suitable coefficient, i.e.

$$(\lambda_1, \dots, \lambda_n) = \lambda_1(1, 0, \dots, 0) + \lambda_2(0, 1, 0, \dots, 0) + \dots + \lambda_n(0, \dots, 0, 1) \quad \lambda_i \in \mathbb{F}_N$$

The system does not define a basis, though, because the representation is not unique. Any element $\mu_i \in \mathbb{F}_N$ such that $\lambda_i \cdot \mu_i = 0$ (truncation errors) allows to define a set as $(1, \mu_2, 0, \dots)$, with the same coefficients. In spite of this, with respect to this 'basis', the decomposition is unique, because the element $1 \in \mathbb{F}_N$ is the identity element for the product. ■

Note that even though we should not be using the word 'basis' (since this is meant only for vector spaces), we will stick to this abuse of notation.

3.1 Calculus on \mathbb{F}^n

In this section we study a discrete analogue of calculus on what we call non-regular discrete spaces, [4], (an example of such a space being the space of floating point numbers). We argue in Remark (1) why such an approach is preferable to developing a discrete calculus on regular lattices. Now we take the following approach to developing a discrete calculus on \mathbb{F}^n : first we define discrete functions, then discrete vectors and discrete covectors. Using these we define global objects like discrete tensors, discrete vector fields and discrete forms. Towards the end of the section we touch upon an important aspect of our discrete mechanics - the relation between various integration techniques and different 'types' of discrete vectors. Finally we present the concept of discrete differentiability.

3.1.1 Functions:

The most obvious step would be to consider functions in the natural way, i.e as mappings from a regular discrete vector space onto the elements of \mathbb{F} (the one dimensional discrete space):

$$A(\mathbb{F}^n) = \{f^\epsilon : \mathbb{F}^n \rightarrow \mathbb{F}\} \quad (1)$$

It is trivial to see that the set $A(\mathbb{F}^n)$ can be endowed with an additive structure which makes of it a group. Also we can choose as scalars the elements of \mathbb{F} itself. The product by scalars is closed in \mathbb{F} .

In any case, from the set theoretical point of view, it is trivial to see that the continuum limit of the set above becomes the set of functions of \mathbb{R}^n , i.e.

Lemma 4 $\lim_{N \rightarrow \infty} A(\mathbb{F}_N^n) = A(\mathbb{R}^n)$

3.1.2 Discrete Vectors

Definition 4 A discrete vector at the point $p \in \mathbb{F}^n$ is a pair (p, q) where $q \in \mathbb{F}^n$. We will denote by $T_p\mathbb{F}^n$ the set defined as the union of all possible vectors defined at the point x , i.e.

$$T_p\mathbb{F}^n = \{(p, q) \in \mathbb{F}^n \times \mathbb{F}^n\} \sim \mathbb{F}^n$$

$T_p\mathbb{F}^n$ is called the tangent space at p . A simple example of a discrete vector can be given as follows. Let $c : [0, T] \rightarrow \mathbb{F}^n$ be a discrete curve on \mathbb{F}^n , with $c(0) = p$ and $[0, T] \subset \mathbb{F}$. We define a tangent vector $\frac{\Delta c(t)}{\Delta t}$ at $c(t)$ as follows:

$$\frac{\Delta}{\Delta t} c(t) = \frac{c(t + \delta) - c(t)}{\delta} \quad (2)$$

where $\delta \in \mathbb{F}$. In other words the tangent vector at $c(t)$ is defined by two points $(c(t), c(t + \delta))$. There are various definitions of vectors in the discrete setting. We shall encounter such definitions in Section WHAT? where we also present,

in detail, the algebraic and geometric properties of discrete vectors. For now we shall use the definition of vectors as given above.

We can consider the effect of discrete mappings at the level of vectors:

Lemma 5 *Let A and B be \mathbb{F}^n -spaces and $\Psi : A \rightarrow B$ be a discrete mapping. Then, the mapping $\Phi_{p*} : T_p A \rightarrow T_{\Psi(p)} B$ defined as:*

$$\Psi_{p*}(p, q) = (\Psi(p), \Psi(q)),$$

defines a one-to-one correspondence of the tangent spaces at the point $p \in A$ and $\Psi(p) \in B$.

We demand for Φ_{p*} to be discrete differentiable, see Section 4.1. Again, at any point of the lattice, we can consider as many discrete vectors as points, i.e. the cardinality of the space of discrete vectors is 2^N .

We have shown in [4] that from the analysis done in terms of the tangent groupoid on \mathbb{F}^n , that the limit when $N \rightarrow \infty$ of a sequence of vectors at a point $p \in [0, 1)$ defined on the family of lattices corresponds to an element of $T_p \mathbb{R}^n$, thus validating our definition of discrete vector.

We can take linear combinations of elements of $T_p \mathbb{F}^n$ with coefficients in \mathbb{F} , and then we can claim that an arbitrary linear combination of the form:

$$\lambda_1 v_1 + \lambda_2 v_2 + \cdots + \lambda_k v_k \equiv (p, \lambda_1 q_1 + \cdots + \lambda_k q_k) \quad \lambda_i \in \mathbb{F}, v_i \in T_p \mathbb{F}^n,$$

belongs to $T_p \mathbb{F}^n$. And now, this structure can be taken, in the continuum limit, to the usual vector space structure of \mathbb{R}^n , since the elements λ_i belong to \mathbb{F}_N , and this set goes to \mathbb{R} in the limit. If we consider the canonical basis of \mathbb{F}^n , we see that each element $v \in T_p \mathbb{F}^n$ has, as coordinates,

$$v = v_1(1, 0, \cdots, 0) + \cdots + v_n(0, \cdots, 0, 1)$$

if $v = (v_1, \cdots, v_n) \in \mathbb{F}^n$. Summarizing, *any system of coordinates used to parameterize the points of \mathbb{F} do define a coordinate system for the tangent space.* Another equivalent way of defining the coordinate system for the tangent space is explained, using the concept of discrete-differentiability, in Proposition 1.

When representing vectors, we will denote the canonical basis as:

$$(0, \cdots, 0, \overbrace{1}^i, 0, \cdots, 0) \equiv v_i$$

Remark 1 *There are certain fundamental limitations in using the usual regular lattice approach towards a discrete mechanics. We present now a highly condensed summary of one particular problem (among many). Just the way we have defined tangent spaces on nonregular spaces in Definition 4., we can do exactly the same on regular lattices.*

It is clear then that, in principle, an arbitrary combination of discrete vectors at a point p on the regular lattice with integer coefficients makes sense and it

is closed in the tangent space denoted by $T_p\mathcal{R}_\epsilon^n$, where \mathcal{R}_ϵ^n denotes the regular lattice i.e.

$$\lambda_1 v_1 + \lambda_2 v_2 + \cdots + \lambda_k v_k \equiv (p, \lambda_1 q_1 + \cdots + \lambda_k q_k) \quad \lambda_i \in \mathbb{Z}, v_i \in T_p\mathbb{R}_\epsilon^n,$$

belongs to $T_p\mathbb{R}_\epsilon^n$, as long as the combination $\lambda_1 q_1 + \cdots + \lambda_k q_k$ belongs to \mathbb{R}_ϵ^n . The problem of this construction is that it does not define a proper continuum limit, since even though in the limit it does provide linear combinations of real vectors, but it does so only with integer coefficients, since the scalars λ_i must belong to \mathbb{Z} for the combination above to be closed. So we end up with the conclusion that the discrete structure defined on regular lattices does not go to the corresponding smooth structure on \mathbb{R}^n in the continuum limit.

3.1.3 Discrete Covectors

Definition 5 Consider the discrete space \mathbb{F}^n . A **discrete covector** α at the point $p \in \mathbb{F}^n$ is defined as a mapping from any pair of points of the form (p, q) , where $q \in \mathbb{F}^n$ to the discrete space \mathbb{F} . It can be represented as the link connecting p and q with the value of the function associated to the link. Since we can take a collection of vectors at a particular point, dual to this, we take the collection of discrete covectors and this collection is denoted by $T_p^*\mathbb{F}^n$ also called the cotangent space at p .

Now we can study the analogue of the usual duality for real numbers. We can use the linear structure we defined for the vectors to define again the analogue of the duality product of the real case. Hence, we claim that the action of a vector $v_p \in T_p\mathbb{F}^n$ on a covector $\alpha \in T_p^*\mathbb{F}^n$ gives as a result a \mathbb{F} -number which is associated to the point p , i.e. we define a function. And now, unlike for a regular lattice case, this function is a \mathbb{F} function, and hence goes to the limit to define the proper \mathbb{R}^n function associated to the action of the smooth vector on the smooth covector.

3.1.4 Tensors

We now have vectors and covectors, so the definition of general tensors is completely straightforward:

Definition 6 We shall call **discrete tensor contravariant of order r and covariant of order s** to the elements t_s^r of the vector space

$$(\mathcal{T}_p)_s^r = \{t \in T_p\mathbb{F}_N^n \times \cdots \text{ (r times) } \cdots \times T_p\mathbb{F}_N^n \times T_p^*\mathbb{F}_N^n \times \cdots \text{ (s times) } \cdots \times T_p^*\mathbb{F}_N^n\}$$

As in the smooth case, completely symmetric and completely skew-symmetric tensors will be particularly important, particularly the last (because we need k -forms and multivectors to represent our mechanical objects).

3.2 Global objects

Definition 7 We shall call **discrete tensor field contravariant of order r and covariant of order s** to the mapping which assigns to each point of the discrete space \mathbb{F}^n a discrete tensor of order r and covariant of order s :

$$\mathcal{T} : \mathbb{F}^n \rightarrow \text{set}(\mathcal{T}_p)_s^r$$

The particular case of vector fields is then defined as:

Definition 8 We shall call **discrete vector field** to the mapping X which assigns to each point $p \in \mathbb{F}^n$ a discrete vector:

$$X(p) \in T_p\mathbb{F}^n \quad \forall p \in \mathbb{F}^n \Rightarrow X(p) = (p, q) \quad q \in \mathbb{F}^n$$

From the representation we chose for the vectors, it is quite obvious that we can define the analogue of the flow of vector fields in a very straightforward manner:

Definition 9 Let X be a discrete vector field. We shall call the **flow** of X to the sequence of points in \mathbb{F}^n

$$p_0, p_1, p_2, \dots$$

such that:

$$X(p_i) = (p_i, p_{i+1})$$

It is also possible to extend the additive structure that we defined on $T_p\mathbb{F}^n$ to the space of discrete vector fields in the natural way: given two discrete vector fields X, Y , their sum $X + Y$ is defined as the vector field whose value at the point $p \in \mathbb{F}^n$ is given by the vector $X(p) + Y(p) \in T_p\mathbb{F}^n$.

Definition 10 We shall call a **discrete k -form** to any mapping α which assigns to each point of the discrete space $p \in \mathbb{F}^n$ an oriented hypersurface of dimension k whose perimeter contains p and a \mathbb{F}_N -value. We will represent that object as $\alpha(p \rightarrow p_1 \rightarrow \dots \rightarrow p_n)$.

We will denote by $\bigwedge^k(\mathbb{F}^n)$ the set of discrete k -forms of the discrete space \mathbb{F}^n , and by $\bigwedge^\bullet(\mathbb{F}^n)$ the set of discrete forms of any order.

This definition allows us to consider functions trivially as 0-forms, since according to the definition it defines a hypersurface of dimension 0 (i.e. one point).

Then we define the wedge product:

Definition 11 Let $\alpha \in \bigwedge^j(\mathbb{F}^n)$ and $\beta \in \bigwedge^k(\mathbb{F}^n)$. Then, we define the product $\alpha \wedge \beta$ to be the $(j+k)$ -discrete form which assigns, at each point, of the discrete space, the hypersurface defined by the union of the $j+1$ -points which define the j -dimensional hypersurface associated to α and the $k+1$ points which define the k -dimensional hypersurface associated to β . If the union of the points does not define a hypersurface of dimension $j+k$ the wedge product is zero.

The discrete exterior differential is a mapping:

$$\Delta : \bigwedge^k(\mathbb{F}^n) \rightarrow \bigwedge^{k+1}(\mathbb{F}^n)$$

defined in the following way. Consider, for instance, a function $f \in A(\mathbb{F}^n)$. The function corresponds to the assignment of an element of \mathbb{F} at each point of the discrete space. The definition of a discrete one-form implies that we must construct a covector at each point. We can do that in many different ways, but if we want to preserve at the discrete level the smooth property:

$$X(f) = \langle X, \Delta f \rangle,$$

the definition of the exterior differential must take into account the type of action that vector fields have on functions. For the forward difference method, this leads us to a definition of the exterior differential such as to define the one-form $\Delta f \in \bigwedge^1(\mathbb{F}^n)$ which assigns to the link connecting each pair of points (p, q) the value $f(q) - f(p)$. Hence, in the natural basis, we would obtain as a representation:

$$\Delta f(p) = \sum_i (f(p + \epsilon_i) - f(p)) dx^i$$

Analogously, given a one form $\alpha \in \bigwedge^1(\mathbb{F}^n)$, we define the two form $\Delta\alpha$ to be the mapping which assigns to every point $p \in \mathbb{F}^n$ one surface defined by a triplet of points (p, q, r) (where $q, r \in \mathbb{F}^n$) and the value

$$\Delta\alpha(p \rightarrow q \rightarrow r) = \alpha(p \rightarrow q) + \alpha(q \rightarrow r) + \alpha(r \rightarrow p)$$

Lemma 6 *From the definition above, d is nilpotent:*

$$\Delta^2 = 0$$

Proof. It is completely analogous to the usual proof of the boundary operator of simplicial homology being nilpotent. For instance, in the case of functions we have, for any $p, q, r \in \mathbb{F}^n$

$$\begin{aligned} \Delta^2 f(p \rightarrow q \rightarrow r) &= \Delta f(p \rightarrow q) + \Delta f(q \rightarrow r) + \Delta f(r \rightarrow p) \\ &= f(q) - f(p) + f(r) - f(q) + f(p) - f(r) = 0 \end{aligned}$$

■

4 A class of discrete vectors

Let $A(\mathbb{F}^n)$ be the algebra of functions on \mathbb{F}^n . The functions in $A(\mathbb{F}^n)$ are considered to be \mathbb{F} -valued functions. In the smooth setting in order to define the concept of a tangent vector at a certain point, one considers functions defined in a neighborhood (i.e. an open set) of that point. In the discrete setting however the concept of 'locality' is a bit different. What should be the radius

of this open set in our discrete case? It cannot be of arbitrary radius, because then the continuum limit would make no sense. This obviously means that the discrete tangent vector in an n -dimensional discrete regular space must be defined only by points that are *immediate neighbors*. Then we can consider functions $f \in A_p(\mathbb{F}^n)$ defined on such an open set around the point $p \in \mathbb{F}^n$. We have seen before that one particular way to explicitly define a discrete vector is as in 2. Then we have discrete vectors $v_i := (p, p + \epsilon_i)$ defined as follows:

Definition 12 (The Euler discrete vector)

Define elements $v_1, \dots, v_n \in T_p \mathbb{F}^n$ by letting:

$$v_i(f(p)) = \frac{f(p + \epsilon_i) - f(p)}{\epsilon_i} \quad (3)$$

where $\epsilon_i = \epsilon \cdot 1_i$, and where $1_i = [0, \dots, 1, 0, \dots]^T$. v_i is called a discrete vector and it has the following very important property:

A Euler discrete vector at a point p is a linear map $v_i : A_p(\mathbb{F}^n) \rightarrow \mathbb{F}$ which satisfies the following **modified Leibniz rule**:

$$v_i(f \cdot g) = v_i(f) \cdot g(p) + Aut_{v_i}(f(p)) \cdot v_i(g), \quad \forall f, g \in A_p \quad (4)$$

where Aut_{v_i} is an automorphism which is a linear map $Aut_{v_i} : A_p(\mathbb{F}^n) \rightarrow \mathbb{F}$, corresponding to the discrete vector v_i , defined as:

$$Aut_{v_i}(f(p)) := f(p + \epsilon_i), \quad p \in \mathbb{F}^n \quad (5)$$

such that $Aut_{v_i}(f \cdot g) = Aut_{v_i}(f) \cdot Aut_{v_i}(g); \forall f, g \in A$

Let us now see (4) in an example: consider two discrete functions $f, g \in A(\mathbb{F}^n)$. Then (dropping all indices):

$$\begin{aligned} v(f \cdot g) &= \frac{f(p + \epsilon) \cdot g(p + \epsilon) - f(p) \cdot g(p)}{\epsilon} \\ &= v(f(p)) \cdot g(p) + f(p + \epsilon) \cdot v(g(p)) \\ &= v(f) \cdot g + Aut(f) \cdot v(g) \end{aligned}$$

In fact *every* discrete vector, see Section (4) for definitions of other discrete vectors, has the fundamental property (4). An arbitrary Euler discrete vector $v := (p, p + \bar{\epsilon})$ in $T_p \mathbb{F}^n$ is written as:

$$v(f(p)) = \frac{f(p + \bar{\epsilon}) - f(p)}{\bar{\epsilon}}$$

s.t. the modified Leibniz rule is satisfied and where $Aut_v(f(p)) = f(p + \bar{\epsilon})$.

To summarize, we have that a Euler discrete vector $v : A_p(\mathbb{F}^n) \rightarrow \mathbb{F}$ is a linear mapping satisfying a modified Leibniz rule (4). From an algebraic geometric viewpoint such an object would be defined by the action of a *twisted derivation*, c.f. [5], on a point p . We define on our discrete regular space \mathbb{F}^n :

Definition 13 Discrete vector field

A discrete vector field is a linear mapping $X : A(\mathbb{F}^n) \rightarrow A(\mathbb{F}^n)$ which assigns to every point $p \in \mathbb{F}^n$ a Euler discrete vector v_p of $T_p\mathbb{F}^n$ as follows:

$$X_p(f) := v(f(p))$$

and is a twisted derivation, i.e. it satisfies the following property; $X : A(\mathbb{F}^n) \rightarrow A(\mathbb{F}^n)$ s.t. $\forall f, g \in A(\mathbb{F}^n)$

$$X(f \cdot g) = X(f) \cdot g + \text{Aut}_X(f) \cdot X(g)$$

where $\text{Aut}_X : A(\mathbb{F}^n) \rightarrow A(\mathbb{F}^n)$ s.t.

$$\text{Aut}_{X_p}(f(p)) = f(p + \epsilon), \quad \forall p \in \mathbb{F}^n$$

where $(p, p + \epsilon)$ of course corresponds to discrete vectors at every point $p \in \mathbb{F}^n$.

In the smooth setting there is a *unique* definition of vectors. Due to the lack of a limiting process, it turns out that (3) is just *one particular representation* of the smooth vector. Or from a discrete mechanics viewpoint, it is only a single element of a class of discrete vectors. (3) is called the Euler discrete vector because it represents both the forward difference and the backward difference methods, the backward difference is expressed differently, i.e. as

$$\frac{f(p) - f(p - \epsilon_i)}{\epsilon_i}$$

where f, p and ϵ_i are as defined in (3). but it has a similar structure as for (3). Similarly (3) can be rewritten to represent a central difference method, i.e.

$$\frac{f(p + \epsilon_i) - f(p - \epsilon_i)}{2\epsilon_i}$$

One of main strengths of numerical analyses has been the large number of integration techniques available - for example, Euler techniques Runge-Kutta, Verlet, Leap-frog among others. Each of these techniques is used heavily in practice, and there is a large amount of theoretical studies also done, [6].

A fundamental question arises here - to what type of geometrical/mathematical entity in our framework do these various integration techniques correspond to? We start off with investigating the second order Runge-Kutta method. We denote a second order Runge-Kutta discrete vector by *rk2*. Below we are going to do roughly the following: given a discrete curve $y : [0, T] \rightarrow \mathbb{F}^n$, $[0, T] \subset \mathbb{F}$ and we want to define a *rk2* discrete vector at the point $y(t)$: first we use the Euler method to compute $y(t + \delta)$. Using this we *recompute* $y(t + \delta)$ by finding a point halfway across the time interval and using a midpoint discrete vector (to be made clear below) across the full width of the interval. Formally we proceed as follows; let $\frac{\Delta y(t)}{\Delta t}$ be a Euler discrete-vector, then first we compute $y(t + \delta)$ as follows:

$$\frac{\Delta y(t)}{\Delta t} =: f(y, t), \quad \Rightarrow y(t + \delta) = y(t) + \delta \cdot f(y, t)$$

$$\text{Let } k_1 = \delta \cdot f(y, t)$$

Then we recompute $y(t + \delta)$ as:

$$y_{rk2}(t + \delta) = y(t) + \delta \cdot f(y(t) + k_1/2, t + \delta/2)$$

So now we have a new value for y at $t + \delta$ which we denote by $y_{rk2}(t + \delta)$. Then we have a new kind of discrete vector $\frac{\Delta}{\Delta t}_{rk2}$:

$$\left. \frac{\Delta y(t)}{\Delta t} \right|_{rk2} = \frac{y_{rk2}(t + \delta) - y(t)}{\delta}$$

which we call the $rk2$ discrete vector. Note that the $rk2$ discrete vector can also be called a midpoint discrete vector (since it is nothing more than a midpoint derivative!). We can extend the above idea to Runge-Kutta methods of *any order*, see [4] for more details. Now consider the $rk2$ discrete vector. A collection of such objects (when we consider an equivalence class of discrete curves, [4]) forms a free module structure (like we have seen before for the Euler discrete vector). This is the tangent space formed by $rk2$ discrete vectors. This tangent space is different from the tangent space formed by Euler vectors. We use the usual notation $T_p \mathbb{F}^n$, it should be clear from the context what type of elements are used to define the tangent spaces. Now consider functions $f \in A_p(\mathbb{F}^n)$. Then we have

Definition 14 From (3) let $k = \epsilon_i \cdot v_i(f(p))$. Define elements $v_1|_{rk2}, \dots, v_n|_{rk2} \in T_p \mathbb{F}^n$ by letting:

$$v_i|_{rk2}(f(p)) = \frac{f_{rk2}(p + \epsilon_i) - f(p)}{\epsilon_i} \quad (6)$$

where

$$f_{rk2}(p + \epsilon) = f(p) + \epsilon_i \cdot v_i(f(p) + k/2)$$

$v_i|_{rk2}$ is called a $rk2$ discrete vector and it satisfies the modified Leibniz rule, i.e.

$$v_i|_{rk2}(f \cdot g) = v_i|_{rk2}(f) \cdot g + \text{Aut}_{v_i|_{rk2}}(f(p)) \cdot v_i|_{rk2}(g), \forall f, g \in A_p$$

A similar definition can be written for Runge-Kutta vectors of any order. Hence a Runge-Kutta vector is also a discrete vector. Further more one can easily show that the Leapfrog method can also be incorporated into our setting, thereby giving us a Leapfrog discrete vector. Hence one can see how a wide variety of integration techniques turn out simply to be nothing more than just discrete vectors in our setting.

4.1 Discrete Differentiability

The notion of a discrete differentiability is crucial. In the smooth setting the concept of differentiability is used to distinguish between various functions. Likewise it is possible to do so in the discrete setting, and also our definition will, in the limit, correspond to the usual definition of differentiability in the smooth case. We first adapt the definition of the smooth case here:

Definition 15 A function $f : \mathbb{F}^n \rightarrow \mathbb{F}$ is said to be **discrete-differentiable** at $p \in \mathbb{F}^n$ iff there exists a mapping $G : A(\mathbb{F}^n) \rightarrow \mathbb{F}^n$ s.t.

$$\frac{f(p + \epsilon_i) - f(p) - G(f(p)) \cdot \epsilon_i}{\epsilon_i} = 0$$

where $\epsilon_i = \epsilon \cdot 1_i$, $1_i = [0, \dots, 1, 0, \dots]$.

Remark 2 From the above definition it might seem that any, and every, discrete function on \mathbb{F}^n is discrete-differentiable!, after all we are not demanding a limiting process. The only things that we need are the values of f at the points $p + \epsilon_i$ and at p . So it seems that the definition is of no formal use. Fortunately this is not the case in general. Indeed, since we are working with floating point numbers it can very easily happen that $f(p + \epsilon_i) - f(p)$ gives a result which is too large to be contained in \mathbb{F} , and hence we have what is usually called an overflow situation, c.f. [2]. In this case the above definition is not satisfied. A lot of such overflow, or underflow, situations can happen - and hence there are many discrete functions that are not discrete differentiable! Moreover note that, in the continuum limit we recover the usual definition of differentiability, and then $L \in \mathbb{F}$ would correspond to the ∞ element of the reals.

To formalize the above remark we need an extra notion - that of discrete 'smoothness'.

Definition 16 Discrete Smoothness

A function $f : \mathbb{F}^n \rightarrow \mathbb{F}$ is said to be smooth, in a discrete sense, around a point $p \in \mathbb{F}^n$, if in an open set around the point p we have that:

$$|f(p + \epsilon) - f(p)| < L$$

where L is the largest number in \mathbb{F} .

We explain in detail the discrete differentiability of a two-dimensional function $g : \mathbb{F}^2 \rightarrow \mathbb{F}$. The one-dimensional case $f : \mathbb{F} \rightarrow \mathbb{F}$ is straightforward; define

$$G(f(p)) \cdot \epsilon = v(f(p)) \cdot \epsilon$$

where $v(f)$ is as defined in (3). This satisfies the definition of discrete differentiability (by direct substitution) for one-dimensional functions $f : \mathbb{F} \rightarrow \mathbb{F}$.

For the two (and higher) dimensional case things are a bit different because, as we will make clear soon, there is more than one *path* along which the discrete differentiability of the function can be defined. We want to know when $f : \mathbb{F}^2 \rightarrow \mathbb{F}$ is differentiable at a point $p \in \mathbb{F}^2$. On \mathbb{F}^2 we first define the *path vectors*. At a point $p \in \mathbb{F}^2$ define the path vectors v_1 and v_2 , see Figure 1, as:

$$v_1(f(p)) = \frac{f(p + (\epsilon, 0)) - f(p)}{\epsilon}, \quad v_2(f(p)) = \frac{f(p + (0, \epsilon)) - f(p)}{\epsilon}$$

Note that in the above we have assumed that the point spacings are the same, and hence we used a single ϵ to indicate the equal spacing. This result holds in

the general case also, but notationally it is much simpler to assume equal point spacings. Then define the *concatenation* of these path vectors as follows:

$$(v_2 \ominus v_1)(f(p)) := \frac{f(p + (\epsilon, 0)) - f(p)}{\epsilon} + \frac{f(p + (\epsilon, \epsilon)) - f(p + (\epsilon, 0))}{\epsilon} \quad (7)$$

However in the discrete case, since we do not have a limiting process as in the smooth case we obtain an *equivalence class of concatenations* depending on the path taken to define the vectors, see Figure 1. In the smooth case we do not

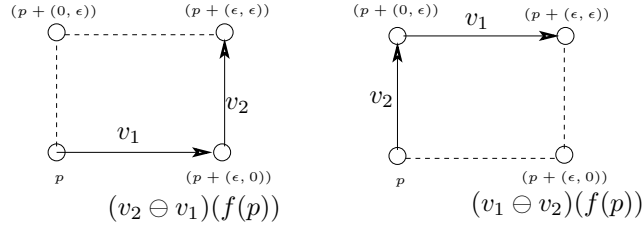


Figure 1: Path vectors of a two-dimensional function.

have such a situation, because in the limit all points (that are an ϵ distance from p) converge to p , implying that *in the limit* there is no such thing as a *path*. What the above equation implies is that any discrete vector v_p at a point p on the lattice \mathbb{F}^2 can be written as a concatenation of two path vectors, v_1 and v_2 . Now we come to the differentiability of the two dimensional function. Define

$$\begin{aligned} G(f) &= \frac{f(p + (\epsilon, 0)) - f(p)}{\epsilon} + \frac{f(p + (\epsilon, \epsilon)) - f(p + (\epsilon, 0))}{\epsilon} \\ &\Rightarrow G(f) \cdot \epsilon_i = f(p + (\epsilon, 0)) - f(p) + f(p + (\epsilon, \epsilon)) - f(p + (\epsilon, 0)) \end{aligned}$$

With this choice for G , we have differentiability for the two dimensional case, this can be checked by direct substitution of G into Definition 15. Note that the differentiability of functions is *independent* of the path taken, as can be easily seen when we substitute the above choices of G (i.e. $v_1 \ominus v_2$ or $v_2 \ominus v_1$) into the definition of discrete differentiability. G is called the gradient of the function and our definition of G is coordinate free. Extending this idea to higher dimensional discrete vectors, an n -dimensional discrete vector v_p at the point p on the n -dimensional lattice \mathbb{F}^n , can be written as the concatenation of n path vectors, i.e.

$$v_p = c_1 v_1 \ominus c_2 v_2 \ominus \cdots \ominus c_n v_n \quad (8)$$

or any other $n!$ -linear combination of the above elements. Hence we have an equivalence class, of representations, with $n!$ elements. Using this in the next section we will define the set of linear independent elements generating the tangent spaces on discrete manifolds.

5 Discrete Manifolds, Tangent and Cotangent spaces

Discrete manifolds locally look like, loosely speaking, the space of floating point numbers \mathbb{F}^n . To do anything further we need a topological structure and a metric for \mathbb{F}^n . \mathbb{F}^n does have a topological structure, which is inherited from \mathbb{R}^n . Likewise with the metric. So what we have on \mathbb{F}^n are a relative topology and a relative metric, see [4]. Now let \mathcal{Z} be a discrete set which is also a topological manifold. Suppose that for any $l \in \mathcal{Z}$ there exists an open set U containing l , and a bijection ψ mapping U onto some open subset of \mathbb{F}^n for some fixed n . \mathbb{F}^n is a special kind of a *free module* over \mathbb{F} of finite rank n , see [4, 7] for more details. Hence we have on \mathbb{F}^n the natural coordinate functions (i.e. basis elements) denoted by $r_i, i := \{1, \dots, n\}$. Then by composition with ψ we obtain coordinate functions $z_i, i := \{1, \dots, n\}$ on U by letting $z_i = r_i \circ \psi$. (U, ψ) is called a coordinate chart. As we have seen in Definition 15., there exists a notion of *discrete differentiability* on \mathbb{F}^n , and of course we would then like to transfer this notion onto \mathcal{Z} also. In order to do this we impose the conditions that the coordinate chart mappings ψ be homeomorphisms and that the corresponding coordinate transformation maps $S = \psi \circ \phi^{-1} : \phi(U \cap V) \rightarrow \psi(U \cap V)$ be discrete differentiable. The second condition is known as *compatibility of coordinate charts*. The collection of compatible coordinate charts is said to be an **atlas**, and we define that there exists a maximal atlas if any coordinate chart (U, θ) , that is compatible with any coordinate chart of the atlas, also belongs to the atlas.

Definition 17 *Let \mathcal{Z} be a discrete topological set² (so it automatically Hausdorff) Then \mathcal{Z} is a discrete differentiable manifold if it has a maximal atlas.*

We have introduced tangent spaces in Section 3.1. Now we have all the necessary ingredients to define the basis of a tangent space. Note that since we are not dealing with vector spaces, it is not correct to use the terminology 'basis' - however for this paper we stick to this abuse of notation. Denote discrete vectors (either ordinary or mixed) in $T_p \mathbb{F}^n$ by v_{ip} . Then

$$v_{ip}(\bar{r}_j) = \delta_j^i, \quad i, j \in \{1, \dots, n\}$$

where \bar{r}_j are the coordinate functions on \mathbb{F}^n . Since \bar{r}_j are independent natural coordinates on \mathbb{F}^n , it follows that $\{v_{1p}, \dots, v_{np}\}$ are independent module elements in $T_p \mathbb{F}^n$. The following proposition shows that these independent elements are actually the basis of the tangent space.

Proposition 1 *$\{v_{1p}, \dots, v_{np}\}$ form a basis of the tangent space $T_p \mathbb{F}^n$.*

Proof. We have seen that on the lattice \mathbb{F}^n , any discrete vector v_p is written as the concatenation of path vectors. So for an n -dimensional tangent space we can write v_p by a concatenation of n -path vectors as in (7). This directly

²Since \mathcal{Z} is a finite set, it is second countable.

implies that for any function $f \in A_p(\mathbb{F}^n)$, the action of an arbitrary discrete vector v_p on f can be written as

$$v_p(f) = c_1 v_1(f) \circ c_2 v_2(f) \circ \cdots \circ c_n v_n(f) = \sum_{i=1}^n c_i v_{i_p}(f)$$

Hence $\{v_{1_p}, \dots, v_{n_p}\}$ form a basis of the tangent space. ■

Now we move onto discrete manifolds \mathcal{Z} . For any point $l \in \mathcal{Z}$ we associate a coordinate chart (U, Ψ) , where U is a neighborhood of the point l , and the map $\psi : U \subset \mathcal{Z} \rightarrow Y \subset \mathbb{F}^n$ is a homeomorphism. Now we define the **tangent map** between \mathcal{Z} and \mathbb{F}^n . Let $T_l \mathcal{Z}$ be the tangent space of \mathcal{Z} at the point l , and denote its elements by $\partial|_l$. Given $\psi : \mathcal{Z} \rightarrow \mathbb{F}^n$, the tangent map(at l) is a linear mapping $\psi_*|_l : T_l \mathcal{Z} \rightarrow T_{\psi(l)} \mathbb{F}^n$ defined as

$$[\psi_*|_l(\partial|_l)](f) = \partial|_l(f \circ \psi), \quad \forall f \in A_{\psi(l)}(\mathbb{F}^n) \quad (9)$$

Once this is done we then have a **basis for the tangent space** $T_l \mathcal{Z}$:

$$\partial_1|_l, \dots, \partial_n|_l$$

by letting $\partial_i|_l := \psi_*^{-1}(v_{i_{\psi(l)}})$, since ψ is an homeomorphism we can do this.

The analogous concept of a *vector field* on configuration space is a discrete vector field which we already encountered in 13. And the analogous concept to a *one form* is a discrete one form which we have encountered in Definition 10. These concepts can be easily extended onto discrete manifolds, see [4].

We have defined discrete covectors on \mathbb{F}^n in Definition 5. We now define this on the discrete manifold. Since the tangent space $T_l \mathcal{Z}$ is a free-module, there exists a dual free-module, of the same dimension, defined as:

Definition 18 *Let ∂_{z_i} be the basis of the tangent space $T_l \mathcal{Z}$, corresponding to the coordinate functions z_i of the algebra A . Then we denote the set of basis elements of the dual free-module $T_l^* \mathcal{Z}$, called the cotangent space, by $\{\Delta z_i|_l\}$ such that*

$$\Delta z^i|_l(\partial_{z_j}|_l) = \delta_j^i$$

Since the tangent space is a free-module, hence the cotangent space is also a free-module and so any discrete covector can be written as $\sum_{i=1}^n \alpha_i \Delta z_i|_l$.

Proceeding along such lines we can define tangent/cotangent bundles and their associated structure, see [4] for further details.

6 Discrete Hamiltonian mechanics

In the following subsection we give a brief description of how we represent system dynamics in our discrete setting. Then we restrict ourselves to Hamiltonian dynamics.

6.1 Discrete Dynamics

Systems are described by an algebra $A(\mathcal{Z})$ on a manifold \mathcal{Z} . In the smooth case this is just the algebra of functions (with the continuity degree we wish to impose) of the corresponding manifold. In our discrete case we have the algebra of discrete functions of the corresponding discrete manifold. These functions represent the set of positions of the system. The algebra $A(\mathcal{Z})$ is generated by a finite set of generators z^i . In the discrete case we also need a second copy of the algebra to describe the velocities. The velocities have some type of finite-difference representation, hence by considering two copies of the algebra we can represent both the position and the velocity of the system.

The dynamics are described as follows: since time is discrete, the evolution is described by several copies of A , one for each time instant:

$$h = A_0 \times A_\delta \times A_{2\delta} \times \cdots \times A_{t\delta} \cdots \times A_{T\delta}$$

where $t \in [0, 1, 2, \dots, T] \in \mathbb{F}$, and δ is the integration time step. Hence if the system starts from A_0 at time 0 we must provide an algorithm Φ to define elements of the next copies of A in h . h is called as the space of histories. The evolution of a function $f \in A_0$ is then represented by the point

$$(f, \Phi(f), \Phi(\Phi(f)), \dots, \Phi^T(f), \dots) \in h$$

Note that if the discrete system is the result of a discretization of a continuous system, this corresponds to, roughly speaking, an **integrator**. There are several ways to define the algorithm describing the system evolution. [8, 1] have developed the algorithm for the Lagrangian framework, although this has been developed on lattices. In this paper we develop the algorithm for the Hamiltonian framework. There are two ways we can proceed from here - the symplectic approach or the Poisson approach.

6.2 Poisson manifolds

In the smooth case, the Poisson structure is usually defined in two ways. One is by the generalization of the symplectic structure i.e.: If (M, w) be a symplectic manifold, $f, g \in C^\infty(M)$ and $X_f, X_g \in \mathfrak{X}(M)$ be the corresponding vector fields, then the Poisson bracket is the function $\{f, g\} = w(X_f, X_g)$. In our formulation we are unable to do the above, as yet, since we do not know how to define a canonical symplectic form. The other way is to use a completely anti-symmetrical tensor field of order $(2, 0)$, whose action on a pair of exact one-forms defines a Poisson bracket. We proceed in this latter setting.

Definition 19 *Let \mathcal{Z} be a discrete manifold and consider the algebra of discrete differentiable functions $A(\mathcal{Z})$ on \mathcal{Z} . Consider a skew-symmetric $(2, 0)$ tensor $J : \Omega^1(A) \times \Omega^1(A) \rightarrow A(\mathcal{Z})$. J defines a Poisson bracket by its action on a pair of exact one-forms as follows:*

$$\{f, g\} := J(df, dg) \tag{10}$$

such that $\{\cdot, \cdot\}$ is a skew-symmetric bilinear operation on $A(\mathcal{Z})$ with the property

- $\{, \}$ is a twisted derivation in each factor, i.e. it satisfies the following modified Leibniz rule:

$$\{f, g \cdot h\} = \{f, g\} \cdot h + \text{Aut}_{X_f}(g) \cdot \{f, h\}$$

J is called a *discrete Poisson-tensor*. A discrete manifold \mathcal{Z} whose algebra of functions $A(\mathcal{Z})$ is endowed with a Poisson bracket is called a *discrete Poisson manifold*.

$\{, \}$ as defined above should actually be called *almost Poisson*, since we are not asking of it to satisfy any kind of Jacobi-identity. We discuss a *fully Poisson* bracket later on in this section. We claim that to compute the Poisson bracket of any pair of functions in a given set of local coordinates, it suffices to know the Poisson brackets between the coordinate functions themselves - we will see towards the end of this section how this works out. The brackets between the coordinate functions:

$$J^{ij}(z) = \{z^i, z^j\} \quad (11)$$

are called the *structure functions* of the discrete Poisson manifold relative to the given local coordinates and uniquely determine the Poisson structure itself. The structure functions can be given a skew-symmetric matrix representation, $J(z)$, whose coefficients are in \mathbb{F} , and is called the structure matrix of $A(\mathcal{Z})$. Then we define:

$$\{f, g\} = \nabla f \cdot J \nabla g = \sum_{ij} \partial_{z^i} f J^{ij} \partial_{z^j} g \quad (12)$$

where $\nabla(f) = (\partial_{z^i} f)$ is the gradient of the function f , it is a column of discrete vectors. We want to know which matrices $J(z)$ are the structure matrices for almost-Poisson brackets.

Proposition 2 *Let $J(z) = J^{ij}(z)$ be an $m \times m$ matrix of functions of $z = (z^1, \dots, z^n)$ defined over an open subset $P \subset \mathbb{F}^n$. Then $J(z)$ is the structure matrix for an almost-Poisson bracket over $A(P)$ if it has the properties of Bilinearity, Skew-symmetry and Modified Leibniz rule:*

Proof. Note that the almost-Poisson bracket as in (12) automatically satisfies bilinearity. For the modified Leibniz rule we have:

$$\{f, g \cdot h\} = \sum_{ij} \partial_{z^i} f J^{ij} \partial_{z^j} (g \cdot h) = \sum_{ij} \partial_{z^i} f J^{ij} \left(\partial_{z^j} g \cdot h + \text{Aut}(g) \cdot \partial_{z^j} h \right)$$

The Poisson bracket (10) is skew-symmetric due to the Poisson tensor J . Then the skew-symmetry of the structure matrix is equivalent to the skew-symmetry of the bracket (10). ■

Note that any constant skew symmetric matrix (whose coefficients belong to \mathbb{F}) trivially satisfies the above requirement and thus determines a Poisson bracket. Next we look at a special case of the structure matrices. We consider a J for which the Poisson bracket (12) looks as follows:

$$J = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \Rightarrow \{f, g\} = \partial_{z^i} f \partial_{z^j} g - \partial_{z^j} g \partial_{z^i} f$$

Now let us check the properties of this simple bracket. Skew-symmetry and bilinearity are obvious. The modified Leibniz rule is :

$$\begin{aligned}\{f, g \cdot h\} &= \partial_{z^i} f \partial_{z^j} (g \cdot h) - \partial_{z^j} f \partial_{z^i} (g \cdot h) \\ &= \partial_{z^i} f \partial_{z^j} g \cdot h + \partial_{z^i} f \partial_{z^j} h \cdot \text{Aut}(g) - [\partial_{z^j} f \partial_{z^i} g \cdot h + \partial_{z^j} f \partial_{z^i} h \cdot \text{Aut}(g)] \\ &= \{f, g\} \cdot h + \text{Aut}(g) \cdot \{f, h\}\end{aligned}$$

A manifold \mathcal{Z} , where $A(\mathcal{Z})$ is equipped with a Poisson bracket, is called a **Poisson manifold**, the bracket defining a Poisson structure on $A(\mathcal{Z})$. Let \mathcal{Z} be a Poisson manifold, then w.r.t the bilinearity and modified Leibniz properties of the Poisson bracket, note that given a function $H \in A(\mathcal{Z})$ the map

$$f \mapsto \{f, H\}$$

defines a discrete vector field on $A(\mathcal{Z})$.

Definition 20 *Let \mathcal{Z} be a Poisson manifold and $H \in A(\mathcal{Z})$. The **Hamiltonian discrete vector field**³ associated with H is the unique discrete vector field X_H satisfying*

$$X_H(f) = \{f, H\} = -\{H, f\} \quad (13)$$

for every $f \in A(\mathcal{Z})$.

It is easy to show, see [4], that to compute the Poisson bracket of any pair of functions in a given set of local coordinates it suffices to know the Poisson bracket between the coordinate functions themselves - i.e. it suffices to know the structure functions.

Remark 3 {Hamiltonian dynamics on Poisson manifolds}

We have a canonical mapping from the algebra $A(\mathcal{Z})$ onto the space of discrete vector fields $\text{Der}(A)$ of the algebra:

$$f \mapsto X_f = \{f, \cdot\}, \quad \forall f \in A(\mathcal{Z}) \quad (14)$$

This means that our system is represented by the algebra $A(\mathcal{Z})$ which denotes the positions of the system, moreover the algebra is endowed with a canonical mapping $A(\mathcal{Z}) \rightarrow \text{Der}(A)$. The dynamics in the smooth case are given by the equations governing the flow of X_H and are called as Hamiltons equations for the Hamiltonian function H . The discrete dynamics are defined as: For any $f \in A(\mathcal{Z})$:

$$\frac{\Delta f(t)}{\Delta t} = \{f, H\} \Rightarrow f_{n+\delta} = f_n + \delta X_H(f_n) \quad (15)$$

So in the limit as $\delta \rightarrow 0$ we recover the definition of dynamics in the smooth case: $\dot{f} = \{H, f\} = X_H(f)$. The discrete dynamics as we defined above, gives a mapping $A_n \rightarrow A_{n+\delta}$, and this is the algorithm we desire.

³discrete analog of a Hamiltonian vector field.

The form of equation (15) is very special. Indeed, it implies energy conservation, i.e.

$$\frac{\Delta H}{\Delta t} = \{H, H\} = 0$$

However most integration techniques are *not* energy conserving. This would necessitate in a modification of the definition of dynamics as in (15). For our purposes energy conservation is very important, indeed in future work we aim at extending the discrete framework developed in this paper to Port-Hamiltonian systems [9, 10], and then energy conservation is certainly the most important first integral that needs to be conserved. *In our definition of discrete Poisson dynamics (15), we assume that we have integration algorithms which are energy conserving.*

Remark 4 Invariance of Poisson Brackets

We now show that canonical transformations leave the Poisson brackets invariant. The basic idea is as follows: let $\eta = [q \ p]^T$ and $\xi = [Q \ P]^T$ be two different coordinate representations of the set of generators of $A(\mathcal{Z})$. Then define a matrix M

$$M = \begin{bmatrix} \partial_p Q & \partial_q Q \\ \partial_p P & \partial_q P \end{bmatrix}$$

s.t. $\dot{\xi} = M\dot{\eta}$. The equations of motion are in the form $\dot{\eta} = J \cdot \nabla H$ where J is a skew-symmetric matrix. With this choice for M we one can easily show

$$J = M \cdot J \cdot M^T$$

Now consider η and ξ to be n -dimensional vectors of, say, the type $\eta = [q_1, \dots, q_n, p_1, \dots, p_n]^T$. Now for any pair of functions $f, g \in A(\mathcal{Z})$ we have defined $\{f, g\}$ as in (12). Then

$$\begin{aligned} \{f, g\}_\eta &= (\nabla_\eta f)^T \cdot J \cdot \nabla_\eta g = (\nabla_\xi f)^T \cdot M \cdot J \cdot M^T \cdot \nabla_\xi g = (\nabla_\xi f)^T \cdot J \cdot (\nabla_\xi g) \\ &= \{f, g\}_\xi \end{aligned}$$

Let us now see, in the following very simple example, the energy behavior w.r.t. to two different types of integration algorithms.

Example 2 *Consider a discrete model of an LC-circuit, the Hamiltonian will have the form $H(q, \phi) = \frac{1}{2}(q^2 + \phi^2)$, where $q(t), \phi(t)$ are discrete curves on a discrete manifold \mathcal{Z} . First we consider the usual Euler forward difference approach, i.e. we have difference equations of the type: $q(t + \delta) = q(t) + \delta \cdot \phi(t)$ and $\phi(t + \delta) = \phi(t) - \delta \cdot q(t)$. Then the energies at times t and $t + \delta$ are given by:*

$$\begin{aligned} H(t) &= \frac{1}{2} \left(q^2(t) + \phi^2(t) \right) \\ H(t + \delta) &= \frac{1}{2} \left([q(t) + \delta \cdot \phi(t)]^2 + [\phi(t) - \delta \cdot q(t)]^2 \right) \end{aligned}$$

Obviously $H(t + \delta) \neq H(t)$. And what this means is that our formal definition of Poisson dynamics (15) does not capture this non-conservation of energy, i.e. (15) implies $\{H, H\} = 0$ which is of course not true as we have shown above. Our definition of Poisson dynamics assume energy conservation, but this is not so when using most integration techniques. Hence in the discrete setting we need to define a more general type of Poisson dynamics. We do not attempt to do that in this paper. There are many ways of exactly conserving energy, c.f. [11] and the references therein. Now we introduce an Euler integration technique that does conserve energy. The basic idea is adopted from [11]. Consider the modified Euler dynamics:

$$q(t + \delta) = q(t) + \delta \cdot \phi(t), \quad \phi(t + \delta) = \phi(t) - \delta \cdot q(t) + f(t)$$

where $f(t)$ is s.t. $H(t + \delta) - H(t) = 0$. Such an $f(t)$ is easy to obtain, indeed we have:

$$H(t + \delta) - H(t) = \delta f^2 + 2\phi f - 2\delta q f + \delta(\phi^2 + q^2)$$

and solving the above for $H(t + \delta) - H(t) = 0$ we obtain the desired $f(t)$. Hence we can easily design energy conserving algorithms. However this means that formally we must change the definition of the Poisson dynamics (15). So in the Hamiltonian framework, given two discrete curves $q(t)$ and $\phi(t)$, for energy conservation we cannot define $\dot{q} = \{q, H\}$ and $\dot{\phi} = \{\phi, H\}$. Rather we should, for example, define the dynamics as:

$$\dot{q} = \{q, H\}, \quad \dot{\phi} = \{\phi, H\} + f(t)$$

where $f(t)$ is s.t. $\frac{\Delta H}{\Delta t} = 0$. In essence we have changed one part of the dynamics i.e. $\phi(t)$. Of course one could also change $q(t)$, it makes no difference for energy conservation.

The above analysis extends to other integration techniques as well, like Runge-Kutta, Leap-frog etc.

Note a fundamental problem in the above energy-conserving algorithm, the Poisson structure is destroyed due to this additional term. Of course an alternative is to consider adaptive time steps, but here too the geometric structure is destroyed. We shall see in [12] how such problems are avoided.

7 Conclusions

In this paper we have formalized discrete physical systems in an Hamiltonian framework. Moreover we also investigated the relationship between different choices of integration techniques and the corresponding discrete vector, in other words we showed that many integration techniques are nothing more than discrete vectors. Finally we presented discrete Hamiltonian dynamics on discrete Poisson manifolds with an example.

However already one can see certain fundamental problems with the energy conserving approaches that are used, either the one we showed above or any of the other well-known ones. The basic problem is that it destroys the Hamiltonian

geometric structure at the discrete level. We show in future work, [12], how this problem which exists for Hamiltonian systems is avoided in the framework of port-Hamiltonian systems.

References

- [1] John C. Baez and James W. Gilliam. An algebraic approach to discrete mechanics. *Lett. Math. Phys.* 31, pages 205–212, 1994.
- [2] John R. Hauser. Handling floating-point exceptions in numeric programs. *ACM Transactions on Programming Languages and Systems*, 18:2, pages 139–174, March 1996.
- [3] User-Notes. User notes on fortran programming - an open cooperative practical guide, 1996. <http://www.ibiblio.org/pub/languages/fortran/>.
- [4] V. Talasila, J.Clemente-Gallardo, and A.J. van der Schaft. Mechanics on discrete manifolds. *Technical Report, Department of Applied Mathematics, University of Twente, To be submitted*, 2004.
- [5] R. Hartshorne. *Algebraic Geometry*. Springer Verlag, 1999.
- [6] Samuel Daniel Conte and Carl W. De Boor. *Elementary Numerical Analysis: An Algorithmic Approach, 3rd edition*. McGraw-Hill Higher Education, 1980.
- [7] S. MacLane and G. Birkhoff. *Algebra*. The MacMillan Company, 1967.
- [8] James W. Gilliam. Lagrangian and symplectic techniques in discrete mechanics. *Ph.D. thesis, University of California, Riverside*, August, 1996.
- [9] A.J. van der Schaft and B.M. Maschke. The hamiltonian formulation of energy conserving physical systems with external ports. *Archiv fur Elektronik und Ubertragungstechnik*, pp. 362-371, 49:362–371, 1995.
- [10] A.J. van der Schaft and B.M. Maschke. Hamiltonian formulation of distributed-parameter systems with boundary energy flow. *Journal of Geometry and Physics*, Vol.42, pages 166–194, 2002.
- [11] B. A. Shadwick, Walter F. Buell, and John C. Bowman. Structure preserving integration algorithms. *Institute for Advanced Physics, Report Number 10*, 2000.
- [12] V. Talasila, J.Clemente-Gallardo, and A.J. van der Schaft. Port hamiltonian systems - a discrete approach. *In preperation*.