# Using Extended Interval Algebra in Discrete Mechanics

Fulvio Tonon
*Department of Civil Engineering, University of Texas, Austin (USA), tonon@mail.utexas.edu*

**Abstract:** Discrete mechanics deals with discrete mechanical systems, such as cellular automata, in which time proceeds in integer steps and the configuration space is discrete. Directly modeling discrete mechanical systems is a well known alternative to starting from a continuous setting, discretizing the model, and finally force the model to the finite alphabet of a computer. The time evolution of discrete dynamical systems, however, can be calculated exactly. In order to take into account imprecision in the input data and the need to accommodate a finite alphabet, extended interval analysis is introduced in the discrete mechanical systems formulation developed by Baez and Gilliam. It is shown how the Euler-Lagrange equation must be modified when working with interval input.

**Keywords:** Discrete mechanical systems, cellular automata, interval analysis.

## 1. Introduction

Baez and Gilliam (1994) and Gilliam (1996) developed an algebraic approach to the mechanics of discrete mechanical systems, that is, systems such as cellular automata (CA) (von Neumann, 1951), in which time evolution proceeds in integer steps and the state space is a finite set. By substituting algebraic geometry concepts for differential geometry concepts, the authors derived an analog for the Euler-Lagrange equation, a version of Noether's theorem, and symplectic techniques applicable to this context. They also gave a definition of complete integrability for a smooth mechanical system on a smooth real affine algebraic variety, and gave a criterion for the complete integrability of such systems. Additionally, they showed that, as the time steps of a discrete system decrease to zero, a solution of the discrete system converges uniformly to a solution of the corresponding continuous system. These Lagrangian and symplectic techniques allow one to use computers for *exactly* simulating discrete mechanical systems that take values in a commutative ring, $k$, as opposed to approximately simulating physical systems by numerically solving differential equations: let us expand on this crucial point.

One of the first uses of digital computers was to approximately simulate physical systems by numerically solving differential equations. This approach leads to numerical computation that is at least three levels removed from the physical world represented by those differential equations:

1) As a first step, one models a physical phenomenon using a differential equation (or a system of differential equations) or a variational principle.

2) Then, one obtains the algebraic forms of the differential equation(s) or variational principle by forcing them into the mold of discrete time and space; and
3) Finally, in order to commit those algebraic forms to algorithms, one projects real-valued variables onto finite computer words, thus introducing round-off during computation and truncation.

Since at one end of the chain is the original physical system and at the other end is another physical system (a computer), physicists wondered whether there was a less roundabout approach to modeling physics (Toffoli, 1984; Toffoli and Margolus, 1987). Indeed, the moment one gives up symbolic manipulation as a major motive for using differential equations, one starts wondering whether one should keep them as a starting point for numerical modeling altogether. Adopting a totally different approach, CA have been proposed as a modeling tool that is isomorphic to the available and foreseeable computational resources (e.g., Toffoli and Margolus, 1987) and that is prototypical for complex interacting systems. Because of the intrinsic discreteness of CA, numerical integration is an *exact* process (there are no truncation or round-off errors), and thus the results that one obtains have the force of theorems. In other words, any properties that one discovers through simulation are guaranteed to be properties of the model itself rather than a simulation artifact (Toffoli, 1984). However, the lack of a rational and physics-based way to define evolution rules for CAs hindered their application to mechanics. Baez's and Gilliam's algebraic approach to discrete mechanical systems for the first time provides for this rational and physics-based way to define evolution rules, and shows how CAs can be seen as a subset of discrete mechanical systems.

A large body of literature has been devoted to estimating the errors introduced in Step 2 above. For example, Dow (1998), Oden *et al*. (2005) and a recent issue of the journal *Computer Methods in Applied Mechanics and Engineering* (2006) give a recent overview of results in the finite element discretization method. Peraire and coworkers have started developing algorithms for calculating guaranteed bounds on these errors (Sauer-Budge *et al*., 2004; Xuan *et al*., 2006); however (based on the published literature), their calculations are performed in floating-point arithmetic. Errors involved in step 3 have been vigorously attacked by the "reliable computing" community using interval analysis started by Warmus (1956) and Moore (1966); the reader I referred to the journal *Reliable Computing* (formerly *Interval Computations*) and to the web site (www.cs.utep.edu/interval-comp/main.html) for up-to-date information. Both types of errors are to be addressed during verification and validation of numerical models (Oberkampf *et al*., 2003).

Discrete mechanical systems avoid these issues associated with Steps 2 and 3. On the other hand uncertainty may affect the available information on initial and boundary conditions, as well as information on a system's parameters. Moreover, when using finite computer words for a physical quantity (even if it is known exactly), real values must be truncated. Therefore, it seems worthwhile to *exactly* extend such uncertain information to a system's behavior: if this is not possible, guaranteed bounds on the system's evolution should be calculated. In this paper, it is

assumed that information on a physical quantity of interest is given as an interval on $k$; we will refer to this assumption as *imprecision*. Generalized interval arithmetic (Dimitrova *et al*. 1992, Gardenes *et al*., 1980a and 1980b, 1981, 1982, 1986, 2001; Kaucher, 1973; Kaucher *et al*., 1977, 1980, 1977; Markov 1992, 1995, 1997, Ortolf, 1969; Popova 1994, 2000, 2001, 2005; Popova and Ullrich, 1996, 1998; Ratschek, 1970, 1971; Spaniol, 1970) is used to extend information in a validated way because generalized interval arithmetic is an algebraically closed system.

For completeness, Talasila *et al*. (2004a, 2004b) have attempted to extend Baez's and Gilliam's work to floating point numbers, but have eventually developed a different theory based on discrete calculus. Finally, a note of caution: the term "discrete mechanics" is also adopted in the literature to denote mechanical systems whose configuration space is continuous and whose evolution proceeds in finite time steps (e.g., Marsden and West, 2001 and references therein); these systems are frequently used to develop structure-preserving and numerically stable time integrators.

In the following sections, some basic notions of discrete mechanics are recalled with more background definitions and explanation than in the available literature, so that these notions can be more easily grasped by an engineering audience. A simple example of a linear harmonic oscillator is used to highlight the properties of a discrete mechanical system. Likewise, the basic algebra of generalized intervals is reviewed. Subsequently, the discrete Euler-Lagrange equation is modified in order to work with generalized intervals and the harmonic oscillator example is extended to accommodate imprecise input values.

## 2. Basic Notions in Discrete Mechanics (Gilliam, 1996; Lang, 2002)

The configuration space of discrete mechanical systems is required to be no more than a ring or a group, without specific topological or analytical properties that allow for the use of the common concepts of tangent and cotangent vectors, spaces, bundles, etc. Since algebraic analogs for these concepts will be needed, let us review some basic definitions from abstract algebra.

Recall that a group $G$ is a set with an associative law of composition $(x, y) \rightarrow xy$, having a unit element, and such that for every element $x \in G$, there exists an inverse element $y \in G$ such that $xy = yx = e$. If the law of composition is also commutative, a commutative group is obtained. A homomorphism $f : G \rightarrow G'$ is a mapping between two groups, $G$ and $G'$, that preserves the product, i.e. $f(xy) = f(x)\, f(y)$, and that maps the unit element of $G$ into that of $G'$. An isomorphism is a bijective homomorphism: if there is an isomorphism between $G$ and $G'$, then one writes $G \cong G'$ to indicate that $G$ and $G'$ are isomorphic.

A ring $R$ is a set, together with two laws of composition called multiplication and addition, respectively, and written as a product and sum respectively, satisfying the following conditions:

– With respect to addition, *R* is a commutative group (zero denotes the additive unit element).
– The multiplication is associative, and has a unit element (denoted as "1").
– For all *x, y, z* in *R* one has (distributivity)

$$(x + y)z = xy + yz \tag{1}$$

Also recall that a module *M* over a ring *R* is a commutative group, usually written additively, together with an operation of *R* on *M*, such that, for all $a, b \in R$ and $x, y \in M$ one has

$$(a+b)x = ax + bx \text{ and } a(x+y) = ax + ay \tag{2}$$

Finally, an algebra is a module *M* with a bilinear map (product) $g : M \times M \to M$

Let $\{E^i\}$ be family of commutative groups. Their direct sum $G = \bigoplus_{i=0}^{\infty} E^i$ is the set of all sequences ($\sigma_1$, $\sigma_2$,…, $\sigma_p$,…) where $\sigma_i \in E_i$, and all but a finite number of $\sigma_i$'s are zero. The direct sum becomes a group when the sum of two elements is defined componentwise. A graded algebra is an algebra that can be written as $G = \bigoplus_{i=0}^{\infty} E^i$, and such that for $s = (\sigma_0, \sigma_1, ...)$ and $r = (\rho_0, \rho_1, ...)$ in *G*, the product in *G* is defined as $sr = \left(\sigma_0\rho_0, \sigma_0\rho_1 + y_0\rho_1, ..., \sum_{i+j=p} \sigma_i\rho_j, ...\right)$, in such a way that if $\sigma_p \in E^p$ and $\rho_q \in E^q$, then the product $\sigma_p\rho_q \in E^{p+q}$. Tensor algebras (e.g., [**Error! Reference source not found.**], page 76) are examples of graded algebras in which the product $\sigma_p\rho_q$ is the outer product of tensors $\sigma_p$ and $\rho_q$ of order *p* and *q*, respectively. Another example of graded algebra is the algebra of polynomial functions described below, in which the product $\sigma_p\rho_q$ is the product of polynomials $\sigma_p$ and $\rho_q$ of order *p* and *q*, respectively.

In discrete mechanics, rather than working directly with configuration space, one works with the algebraic functions on the configuration space, which form a commutative algebra *A* over configuration space. For example, if the configuration space is an *n*-dimensional vector space over a field *k*, then one would use the algebra of polynomial functions in *n* variables over *k*, $k[x_1, ..., x_n] = \bigoplus_{i=0}^{\infty} E^i$, where $E^i = \left\{ \sum_{j=1}^{n} \lambda_j x_j^{n_j} : \sum_{j=1}^{n} n_j = i \right\}; \lambda_j \in k$. The analog of a vector field on configuration space is then a derivation on *A*, that is, a *k*-linear map $v : A \to A$ such that

$v(ab) = av(b) + bv(a)$ for all *a*, *b* ∈ *A*. In order to define differential forms on *A*, let us introduce the concept of differential.

Let $\Omega = \oplus_{i=0}^{\infty} \Omega^i$ be a graded algebra. The differential of $\Omega$ is a map $d : \Omega \to \Omega$ such that if $\omega \in \Omega^p$, then

$$d(\omega\mu) = d(\omega)\mu + (-1)^p \omega d(\mu) \tag{3}$$

$$dd(\omega) = 0 \tag{4}$$

Let *A* be a commutative *k*-algebra (e.g., the algebraic functions on the configuration space). The algebraic differential forms $\Omega(A) = \oplus_{i=0}^{\infty} \Omega^i(A)$ are the graded algebra, in which $\Omega^0(A) = A$, in which the product is written as a wedge product, and which are generated by *A* and by the elements *da*, where $a \in A$, with the relations:

$$d(\lambda a) = \lambda da, \qquad d(a+b) = da + db$$

$$d(ab) = da \wedge b + a \wedge db, \qquad a \wedge db = db \wedge a$$

$$da \wedge db = -db \wedge da \qquad da \wedge da = 0$$

for all *a*, *b* ∈ *A*, λ ∈ *k*, with the last necessary only if 2 has no multiplicative inverse in *k*. A *p*-form is an element of $\Omega^p(A)$.

Since *A* is the equivalent of the configuration space, the space of histories is the algebra $H = A^{\otimes(T+1)} = A_0 \otimes \ldots \otimes A_T$ , where the algebras $A_i$ are simply copies of *A* with $A_i$ thought of as the functions on configuration space at time *i*. The Lagrangian for the system, $\mathscr{L}$, is a fixed element of *A* ⊗ *A*. In the algebra *H*, the discrete analog for the action functional in classical mechanics is

$$S = \sum_{i=0}^{T-1} \mathscr{L}_i \tag{5}$$

where $\mathscr{L}_i = 1 \otimes \ldots \otimes \mathscr{L} \otimes \ldots \otimes 1$, with $\mathscr{L}$ occupying the *i*th and (*i*+1)th slots.

In order to derive Lagrange equations from *S*, one needs to differentiate *S*, and thus one needs 1-forms on the space of histories *H*. Since for any algebra, *A*, one has that: $\Omega^1(A\otimes A) = A\otimes\Omega^1(A)\oplus\Omega^1(A)\otimes A$, by induction:

$$\Omega^1(H) = \bigoplus_{i=1}^{T} A_0\otimes\ldots\otimes\Omega^1(A_i)\otimes\ldots\otimes A_T \tag{6}$$

Let $d_i = p_i d$ where $p_i$: $\Omega^1(H)\to\Omega^1(H)$ is the projection on the *i*th summand. The variation of *S* is effected by the operator $\delta = \sum_{i=1}^{T-1} d_i$, which keeps the first and the second summand of *H* fixed. Now, since $\mathscr{L} = a\otimes b$ with $a, b \in A$:

$$\begin{aligned} d_i\mathscr{L}_i &= p_i d\left(1\otimes\ldots\otimes\mathscr{L}\otimes\ldots\otimes 1\right) = p_i\left(0\otimes\ldots\otimes d\mathscr{L}\otimes\ldots\otimes 0\right) \\ &= p_i\left(\left(0\otimes\ldots\otimes \underset{i}{da}\otimes \underset{i+1}{b}\otimes\ldots\otimes 0\right)\oplus\left(0\otimes\ldots\otimes \underset{i}{a}\otimes \underset{i+1}{db}\otimes\ldots\otimes 0\right)\right) \\ &= \left(0\otimes\ldots\otimes \underset{i}{da}\otimes 0\otimes\ldots\otimes 0\right)\oplus\left(0\otimes\ldots\otimes \underset{i}{a}\otimes 0\otimes\ldots\otimes 0\right) \end{aligned} \tag{7}$$

and

$$\begin{aligned} d_i\mathscr{L}_{i-1} &= p_i\left(\left(0\otimes\ldots\otimes \underset{i-1}{da}\otimes \underset{i}{b}\otimes\ldots\otimes 0\right)\oplus\left(0\otimes\ldots\otimes \underset{i-1}{a}\otimes \underset{i}{db}\otimes\ldots\otimes 0\right)\right) \\ &= \left(0\otimes\ldots\otimes 0\otimes \underset{i}{b}\otimes\ldots\otimes 0\right)\oplus\left(0\otimes\ldots\otimes 0\otimes \underset{i}{db}\otimes\ldots\otimes 0\right) \end{aligned} \tag{8}$$

with $d_j\mathscr{L}_i = 0$ for $j \neq i, j \neq i$-1.

The variation of *S* is thus:

$$\delta S = \delta\sum_{i=0}^{T-1}\mathscr{L}_i = \sum_{i=0}^{T-1}\delta\mathscr{L}_i = \sum_{i=1}^{T-1} d_i\mathscr{L}_i + d_i\mathscr{L}_{i-1} \tag{9}$$

Finally, Eqs. (7) and (8) indicate that the last sum in Eq. (9) is actually a direct sum. Thus:

$$\delta S = 0 \Rightarrow d_i\mathscr{L}_i + d_i\mathscr{L}_{i-1} = 0 \tag{10}$$

Eq. (10) is the Euler-Lagrange equation for discrete systems. This 1-form does not vanish on the whole space of histories *H*, but only on the trajectories that satisfy the equations of motion. Since the Lagrangian is an element of $A \otimes A$, the equations of motion give the configuration at

the *i*-th time step as a function of the previous two time steps *i*-1 and *i*-2. This is formalized as a homomorphism $\varphi : A_2 \to A_0 \otimes A_1$, which defines a homomorphism $\Phi : A_1 \otimes A_2 \to A_0 \otimes A_1$: $a \otimes 1 \mapsto 1 \otimes a$ and $1 \otimes a \mapsto \varphi(a)$. One says that $\varphi$ or $\Phi$ satisfies the equation of motion provided

$$\Phi_* \mathrm{d}_i \mathscr{L} + \mathrm{d}_i \mathscr{L}_{i-1} = 0; \tag{11}$$

where $\Phi_* : \Omega^1(A_1 \otimes A_2) \to \Omega^1(A_0 \otimes A_1)$ is the map induced by $\Phi$, and $d_i$ is the restriction of $d_i$ on *H* to its sub-algebras $A_1 \otimes A_2$ and $A_0 \otimes A_1$.

EXAMPLE (modified from Baez and Gilliam, 1994). Let the base ring *k* be the ring of rational numbers, $\mathbb{Q}$, so that, in particular, 2 has an inverse. Consider the case of a particle in a polynomial potential constrained to move along a line with coordinate *q*. The algebra of functions on configuration space is $A \cong k[q] = \{\lambda_0, \lambda_0 + \lambda_1 q, \lambda_0 + \lambda_2 q^2, \lambda_0 + \lambda_1 q + \lambda_2 q^2 : \lambda_0 + \lambda_3 q^3, ...\}$, so that $A \otimes A \cong k[q_1, q_2]$, the polynomials in 2 variables over *k*, and $H \cong k[q_0, ..., q_T]$, the polynomials in *T*+1 variables over *k*. Consider the Lagrangian $\mathscr{L}_i$ (written here as a polynomial function) for a particle in a polynomial potential *V* as a function of consecutive positions $q_i$ and $q_{i+1}$ of the particle:

$$\mathscr{L}_i = \mathscr{L}(q_i, q_{i+1}) = \frac{1}{2} m \dot{q}_i^{\,2} - V(q_i) \tag{12}$$

where one defines $\dot{q}_i = q_{i+1} - q_i$, and where *m* is in *k*, and represents the mass of the particle. Since $\mathrm{d}_i \mathscr{L} = \partial_{q_i} \mathscr{L}(q_1, q_2)\, \mathrm{d}q_i$, *i* = 1, 2, one obtains:

$$d_i \mathscr{L}_i = -m(q_{i+1} - q_i) - V'(q_i)\, dq_i = m \dot{q}_i dq_i \tag{13}$$

Likewise

$$d_i \mathscr{L}_{i-1} = m(q_i - q_{i-1}) = m \dot{q}_{i-1} dq_i \tag{14}$$

The Euler-Lagrange equation is thus:

$$m(\dot{q}_i - \dot{q}_{i-1}) = -V'(q_i), \tag{15}$$

which is the discrete analog for Newton's law, and yields the time evolution map

$$\varphi(q_2) = q_1 + \dot{q}_0 - m^{-1}V'(q_1) = 2q_1 - q_0 - m^{-1}V'(q_1) \tag{16}$$

and homomorphism Φ

$$\Phi(q_1) = q_1,\ \Phi(q_2) = \varphi(q_2) = 2q_1 - q_0 - m^{-1}V'(q_1) \tag{17}$$

$$\Phi_*(\mathrm{d}q_1) = \mathrm{d}q_1,\ \Phi_*(\mathrm{d}q_2) = 2\mathrm{d}q_1 - \mathrm{d}q_0 - m^{-1}V''(q_1)\mathrm{d}q_1 \tag{18}$$

Let us check that the time evolution map satisfies the equation of motion:

$$\begin{aligned}
&\Phi_*\mathrm{d}_1\mathscr{L}_1 + \mathrm{d}_1\mathscr{L}_0 = \Phi_*\partial_{q_1}\mathscr{L}(q_1, q_2)\mathrm{d}q_1 + \partial_{q_1}\mathscr{L}(q_0, q_1)\mathrm{d}q_1 = \\
&= \Phi_*\left(\left(-m(q_2 - q_1) - V'(q_1)\right)\mathrm{d}q_1\right) + m(q_1 - q_0)\mathrm{d}q_1 \\
&= \left(-m\left(2q_1 - q_0 - m^{-1}V'(q_1) - q_1\right) - V'(q_1)\right)\mathrm{d}q_1 + m(q_1 - q_0)\mathrm{d}q_1 = 0
\end{aligned}$$

It can be seen that homomorphism $\Phi_*$ pulls back $\mathrm{d}_1\mathscr{L}_1$ from $\Omega^1(A_1 \otimes A_2)$ to $\Omega^1(A_0 \otimes A_1)$. In this simple case, this entails substituting the expression for the time evolution map (16) into the expression Euler-Lagrange equation (15).

Figure 1 shows the evolution of a linear harmonic oscillator with: $m$ = 1, $q_0$ = 8; $q_1$ = 16; $V$= ½$sq^2$ (where $s$ is the spring stiffness), $s$ = 1. The mass takes positions: {8, 16, 8, -8, -16, -8, 8, 16, 8, -8…}, and the mass revisits the same location in space after 6 steps. Notice that this time integration is *exact*, and can be *exactly* reversed.

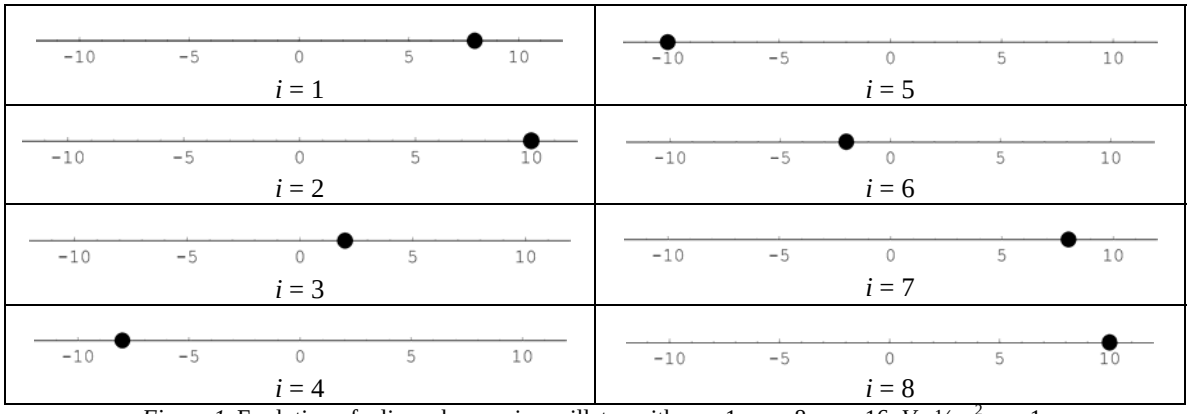
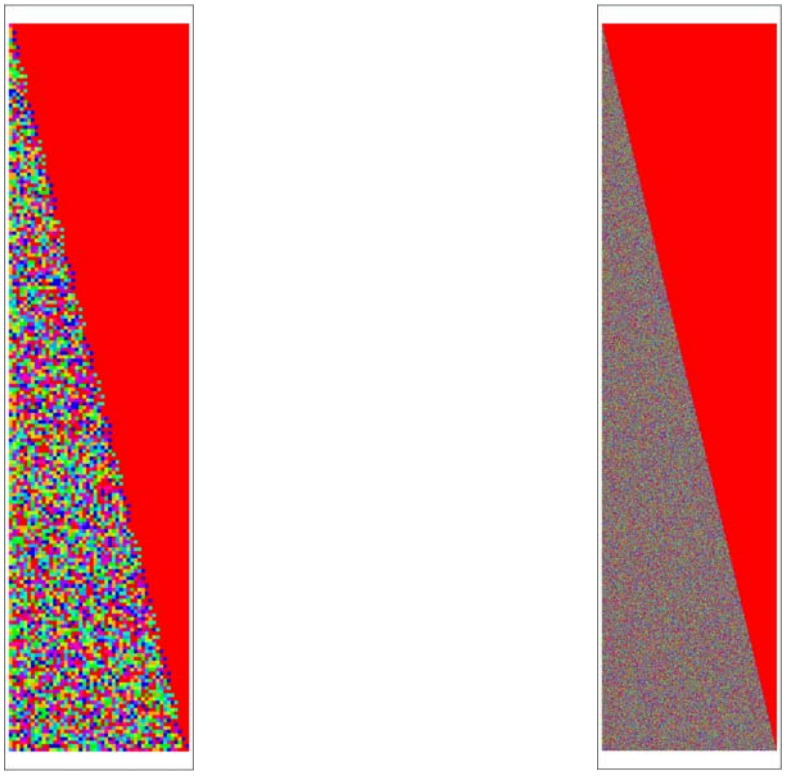



*Figure 1*. Evolution of a linear harmonic oscillator with $m$ = 1, $q_0$ = 8; $q_1$ = 16; $V$= ½$sq^2$, $s$ = 1.

However, if the ratio $s/m$ is not an integer, then the mass never revisits the same location twice; for example, for $s/m$ = 1/3, the coordinates of the particle are (all calculations in this paper were carried out using Mathematica exact arithmetic): {8, 16, 56/3, 136/9, 176/27, -344/81, -3304/243, -13424/729, -37384\/2187, -66104/6561, 5936/19683, 624616/59049, 3069656/177147…}. The numbers of digits in the numerator and denominator keep increasing at each time step as shown in Figure 2. In Figure 2, each digit in the [0, 9] range is assigned a color. Each digit of the numerator occupies a cell, and numerator digits for the $i$-th step occupy the first cells from the left of the (2$i$-1)-th row. Likewise, denominator digits for the $i$-th step occupy the first cells from the left of the 2$i$–th row.



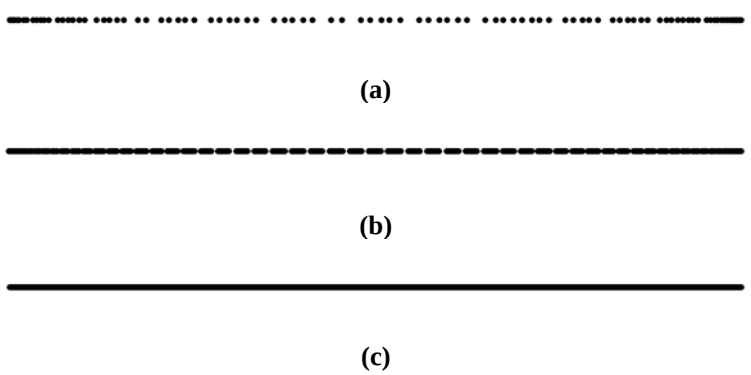
**(a)** **(b)**

*Figure 2*. Graphical representation of the digits in the numerator and denominator of a particle coordinates. The particle is a linear harmonic oscillator with $m$ = 1, $q_0$ = 8; $q_1$ = 16; $V$= ½$sq^2$, $s$ = 1/3.
(a) First 100 time steps; (b) First 1,000 time steps.

Since there is no periodicity in the pattern of digits, the CA depicted in Figure 2 belongs to the third CA class in the following Wolfram's classification (Wolfram, 1985a, 1985b):

1) Class 1: All components attain the same state; the final state is unique and unaffected by any change to the initial state;
2) Class 2: Simple stable states or periodic and separated structures emerge; small changes in the initial state only affect a fixed finite region around the area in which the values were changed;
3) Class 3: Chaotic non-periodic patterns are generated; a minimal perturbation to the initial state affects arbitrarily large regions; or
4) Class 4: Complex, localized, propagating structures are formed; some perturbations to some initial configurations appear to propagate arbitrarily far, whereas others die out.

Figures 3a through 3c show all the positions occupied by the particle after 100, 1,000, and 10,000 time steps. It can be seen that these positions are closer one to the other around the extremes of the current oscillation range (Figures 3a and 3b), where the particle velocity is smaller. The particle positions form clusters separated by empty segments (Figure 3b). After the first two steps and within 10,000 time steps, the particle never occupies a position having an integer coordinate: it is an open question whether it will eventually occupy integer coordinate positions. Another open question is whether the particle will visit all positions between the extremes reached, say, after 1,000 iterations, or there will always be "holes" in between.



**(a)**

**(b)**

**(c)**

*Figure 3*. Cumulative positions occupied by a linear harmonic oscillator with $m = 1$, $q_0 = 8$; $q_1 = 16$; $V = \frac{1}{2}sq^2$, $s = 1/3$ (same as in Figure 2). (a) First 100 time steps; (b) First 1,000 time steps; (c) First 10,000 time steps (positions are indistinguishable at this scale).

Additionally, it is not possible to determine *a priori* the maximum and minimum coordinates reached by the particle for an infinite number of time steps. For any finite number of time steps,

the maximum and minimum coordinates are not symmetric about zero. For example, the maximum (minimum, resp.) coordinate after 100 time steps is approximately equal to 18.682435719981747 (-18.68289250959053), after 1,000 time steps it is approximately equal to 18.683060458305423 (-18.68289250959053), after 10,000 time steps it is approximately equal to 18.6839719940311 (-18.683972612054987). The maximum coordinate increases steadily, but the minimum coordinate remains constant between 100 and 1,000 time steps, and then it decreases further. Thus, even for a very simple linear harmonic oscillator without any forcing, it is impossible to find a shortcut to its range of oscillation: all we can do is to sit back and watch it evolve.

Let us now introduce some basic concepts of extended interval algebra and then see how the discrete mechanics formulation described in this section must be modified in the presence of imprecision.

## 3. Ordering of *k* and generalized interval arithmetic

In order to work with intervals, we need to introduce the concept of ordering. Let $k$ be a ring. An ordering of $k$ is a subset $P$ of $k$ having the following properties (Lang, 2002):

1) Given $x \in k$, either $x \in P$ or $x = 0$, or $-x \in P$, and these possibilities are mutually exclusive. In other words, $k$ is a disjoint union of $P$, $\{0\}$, and $-P$.
2) If $x, y \in P$, then $x + y$ and $xy \in P$.

One also says that $k$ is ordered by $P$ and one calls $P$ the set of positive elements. Let $x, y \in k$. Define $x < y$ (or $y > x$) to mean that $y\text{-}x \in P$; define $x \le y$ to mean $x < y$ or $x = y$. Define $|x| = x$ if $x>0$, and $|x| = -x$ if $x<0$.

In generalized interval arithmetic, the set of proper intervals $\{[x^-, x^+] \,|\, x^- \le x^+; x^-, x^+ \in k\}$ is extended by the set $\{[x^-, x^+] \,|\, x^- \ge x^+; x^-, x^+ \in k\}$ of improper intervals, thus obtaining the set $\mathscr{D} = \{\mathbf{x} = [x^-, x^+] |; x^-, x^+ \in k\} \cong k^2$ of all ordered couples called generalized intervals (strictly speaking, generalized interval arithmetic is defined over the reals, but it is easy to see that the operations and properties used below are valid over any ordered ring, $k$). Denote the set of generalized intervals that involve zero by $\mathscr{T} = \{\mathbf{x} \in \mathscr{D} \,|\, x^- x^+ \le 0\}$. In this paper, intervals are written in boldface type.

From a physical viewpoint, a proper interval, **x**, can also be seen as a set $\mathbf{x} = [x^-, x^+] = \left\{ x \in k \mid x^- \le x \le x^+; x^-, x^+ \in k \right\}$ of possible values of a physical quantity of interest, say $\mathcal{X}$. Improper intervals are introduced to make interval algebra closed: if, at the end of a calculation sequence, $\mathcal{X}$ turns out to be an improper interval, then this means that the possible set of values of $\mathcal{X}$ is the empty set (more refined semantics has been developed in modal interval analysis (Gardenes *et al.*, 2001), but this is beyond the scope of this paper).
The "dual" is an important operator that reverses the endpoints of the intervals. Let $\mathbf{x} = [x^-, x^+] \in \mathscr{D}$; its dual is defined as *Dual*(**x**) = $\mathbf{x}_- = [x^+, x^-] \in \mathscr{D}$. In order to simplify the formulae below, we use the functional notation introduced by Popova (2001). Define Λ = {+, -}, and, for $\mu$ and $\nu \in \Lambda$, define the (commutative) product $\lambda = \mu\nu \in \Lambda$ by $\lambda$ = {+, if $\mu = \nu$, - otherwise}.
For $\lambda \in \Lambda$, define:

$$x^\lambda = \begin{cases} x^+ \text{ if } \lambda = + \\ x^- \text{ if } \lambda = - \end{cases} \quad \text{and} \quad \mathbf{x}_\lambda = \begin{cases} \mathbf{x} \text{ if } \lambda = + \\ \mathbf{x}_- \text{ if } \lambda = - \end{cases}. \tag{19}$$

The direction of an interval, $\tau(\mathbf{x})$, its sign, $\sigma(\mathbf{x})$, and its relative magnitude, $\nu(\mathbf{x})$, are defined as, respectively:

$$\tau(\mathbf{x}) = \begin{cases} + \text{ if } x^- < x^+ \\ - \text{ if } x^- > x^+ \\ \pm \text{ if } x^- = x^+ \end{cases} \quad \sigma(\mathbf{x}) = \begin{cases} + \text{ if } x^{-\tau(\mathbf{x})} > 0 \\ - \text{ if } x^{\tau(\mathbf{x})} < 0 \end{cases} \quad \nu(\mathbf{x}) = \begin{cases} + \text{ if } \left|x^+\right| > \left|x^-\right| \\ - \text{ if } \left|x^+\right| < \left|x^-\right| \\ \pm \text{ if } \left|x^+\right| = \left|x^-\right| \end{cases} \tag{20}$$

Addition, multiplication, and subtraction of intervals are defined as follows:

$$\mathbf{x} + \mathbf{y} = \left[ x^- + y^-, x^+ + y^+ \right], \text{ for } \mathbf{x}, \mathbf{y} \in \mathscr{D} \tag{21}$$

$$\mathbf{xy}=\begin{cases}\left[x^{-\sigma(\mathbf{y})}y^{-\sigma(\mathbf{x})},x^{\sigma(\mathbf{y})}y^{\sigma(\mathbf{x})}\right] & \mathbf{x},\mathbf{y}\in\mathscr{D}\setminus\mathscr{T}\\ \left[x^{\sigma(\mathbf{x})\tau(\mathbf{y})}y^{-\sigma(\mathbf{x})},x^{\sigma(\mathbf{x})\tau(\mathbf{y})}y^{\sigma(\mathbf{x})}\right] & \mathbf{x}\in\mathscr{D}\setminus\mathscr{T},\ \mathbf{y}\in\mathscr{T}\\ \left[x^{-\sigma(\mathbf{y})}y^{\sigma(\mathbf{y})\tau(\mathbf{x})},x^{\sigma(\mathbf{y})}y^{\sigma(\mathbf{y})\tau(\mathbf{x})}\right] & \mathbf{x}\in\mathscr{T},\ \mathbf{y}\in\mathscr{D}\setminus\mathscr{T}\\ \left[\min\left\{x^{-}y^{+},x^{+}y^{-}\right\},\max\left\{x^{-}y^{-},x^{+}y^{+}\right\}\right] & \mathbf{x},\mathbf{y}\in\mathscr{T},\ \tau(\mathbf{x})=\tau(\mathbf{y})\\ 0 & \mathbf{x},\mathbf{y}\in\mathscr{T},\ \tau(\mathbf{x})=-\tau(\mathbf{y})\end{cases} \tag{22}$$

$$\mathbf{x}-\mathbf{y}=\mathbf{x}+(-1)\mathbf{y}=\left[x^{-}-y^{+},x^{+}-y^{-}\right],\ \text{for } \mathbf{x},\ \mathbf{y}\in\mathscr{D};$$

$$-1 \text{ is the additive unit of } 1\in k \tag{23}$$

Addition and multiplication are commutative and associative, and have unit elements, namely [0, 0] for addition and [1, 1] for multiplication. Any element $\mathbf{x}\in\mathscr{D}$ has a unique inverse element for addition, namely $-\mathbf{x}_{\_}$: $\mathbf{x}-\mathbf{x}_{\_}=0$. Additionally, conditional distributivity laws hold and have been summarized by Popova (2001). To illustrate, let us introduce a law, which will be used in the examples that follow. Denote $\hat{\mu}(\mathbf{x})=\begin{cases}\sigma(\mathbf{x})\ if\ \mathbf{x}\in\mathscr{D}\setminus\mathscr{T}\\ \nu(\mathbf{x})\tau(\mathbf{x})\ if\ \mathbf{x}\in\mathscr{T}\setminus\{0\}\end{cases}$. For $\mathbf{x}_1,\mathbf{x}_2\in\mathscr{D}\setminus\{0\}$ and $\mathbf{s}=\mathbf{x}_1+\mathbf{x}_2$, if $\mathbf{s}\in\mathscr{D}\setminus\mathscr{T}$, $\mathbf{y}\in\mathscr{D}\setminus(\mathscr{T}\cup k)$, then

$$(\mathbf{x}_1+\mathbf{x}_2)\mathbf{y}=\mathbf{x}_1\mathbf{y}_{\hat{\mu}(\mathbf{x}_1)\hat{\mu}(\mathbf{s})}+\mathbf{x}_2\mathbf{y}_{\hat{\mu}(\mathbf{x}_2)\hat{\mu}(\mathbf{s})}\ \text{iff} \tag{24}$$

either $\mathbf{x}_1,\mathbf{x}_2\in\mathscr{D}\setminus\mathscr{T}$, or

$\mathbf{x}_i\in\mathscr{T}\setminus\{0\}$ for some $i\in\{1,2\}$ and either $x^{-}=0$ or $x^{+}=0$ for all $\mathbf{x}_i\in\mathscr{T}\setminus\{0\}$.

Thus, $\mathscr{D}$ is a conditional ring, and one could be tempted to blindly use all results derived by Baez and Gilliam (1994) using $\mathscr{D}$ as the ring in which the system takes values. However, since the addition unit of $\mathbf{x}$ is $-\mathbf{x}_{\_}$, $\mathbf{x}-\mathbf{x}\neq 0$ unless $\mathbf{x}$ is degenerate, i.e. $\tau(\mathbf{x})=\pm$, and only conditional distributivity applies. Finally, we will use the following properties:

- An element $\mathbf{x}\in\mathscr{D}/\mathscr{T}$ is a multiplication unit in $\mathscr{D}$ iff all $x\in\mathbf{x}$ are units in $k$; the multiplicative inverse of $\mathbf{x}$ is then $\mathbf{x}_{\_}^{-1}$ with

$$1/\mathbf{x}=\left[1/x^{+},1/x^{-}\right];1/\mathbf{x}_{\_}=\left[1/x^{-},1/x^{+}\right]$$

- The dual operator is distributive with respect to finite addition ($Dual(\mathbf{x}+\mathbf{y}) = Dual(\mathbf{x}) + Dual(\mathbf{y})$) and multiplication ($Dual(\mathbf{xy}) = Dual(\mathbf{x})\,Dual(\mathbf{y})$) and is an automorphism.

Let $f(x): k \to k$ be a rational function. The generalized rational interval extension of *f* is the interval function $fR(\mathbf{x}): \mathscr{D} \to \mathscr{D}$ defined by the syntactic expression of *f*, where the variables in *k* are replaced by generalized intervals, and operations on *k* are replaced by the operations between generalized intervals described above. Likewise, the derivative $R_f'(\mathbf{x}): \mathscr{D} \to \mathscr{D}$, if it exists, is defined by the syntactic expression of *f'*, only replacing the argument *x* by its interval counterpart **x**, and its operations on *k* by their corresponding interval operations. The united extension, $R_f$, is defined as the range of function values

$$R_f(\mathbf{x}) = \left[\min_{x\in\mathbf{x}} f(x), \max_{x\in\mathbf{x}} f(x)\right]$$

In general, $fR(\mathbf{x}) \supseteq R_f(\mathbf{x})$. Similar definitions apply for multi-dimensional cases.

Since calculating the united extension is an NP-hard problem involving global optimization, generalized interval arithmetic will be used to carry out symbolic manipulations, and an algorithm due to Popova (2005) will be used to calculate interval extensions for the rational functions of interest in such a way that $fR(\mathbf{x}) = R_f(\mathbf{x})$. The following thus rewrites Baez's and Gilliam's results using $\mathscr{D}$ as the ring in which the system takes values. Time evolution still proceeds in integer steps: if one is interested in the evolution of a system in the interval of time [*i*, *i*+*n*], such evolution is just the union of the results at each time step in [*i*, *i*+*n*]. Imprecision in time measurement is accounted for by allowing time-related quantities to be intervals, e.g., the initial velocity. Future research will deal with the case in which such physical quantities are measured in a time interval, e.g., the initial velocity measured between time steps *i*, and *i*+*n*.

## 4. Euler-Lagrange equation

As in Section 2, let *A* be a commutative algebra over $\mathscr{D}$ and let $\Omega(A) = \bigoplus_{i=1}^{\infty} \Omega^i(A)$ be the graded-commutative differential graded algebra on *A* with differential *d*, and product written as a wedge product. Let time take value in the discrete set {0, …, *T*} and $A_i$ be a copy of *A* representing the system at time *i*. In order to satisfy Newton's first and second laws, the Euler-

Lagrange equation on the space of histories $H = A^{\otimes(T+1)} = A_0 \otimes ... \otimes A_T$ must be modified as follows:

$$Dual\left(d_i \mathscr{L}_i\right) + d_i \mathscr{L}_{i-1} = 0 \tag{25}$$

where $\mathscr{L} \in A \otimes A$ is the Lagrangian, $\mathscr{L}_i = 1 \otimes ... \otimes \mathscr{L} \otimes ... \otimes 1$ (in which $\mathscr{L}$ occupies the *i*th and (*i*+1)th slots); $p_i$: $\Omega^1(H) \to \Omega^1(H)$ is the projection on the *i*th summand of $\Omega^1(H) = \bigoplus_{i=1}^{T} A_0 \otimes ... \otimes \Omega^1(A_i) \otimes ... \otimes A_T$, and $d_i = p_i d$. The example that follows illustrates why the *Dual* operator is necessary in Eq. (25).

Recall that the time evolution map is formalized as a homomorphism $\Phi : A_1 \otimes A_2 \to A_0 \otimes A_1 :\ a \otimes 1 \mapsto 1 \otimes a$ and $1 \otimes a \mapsto \varphi(a)$, where $\varphi : A_2 \to A_0 \otimes A_1$ is a homomorphism that formalizes the equation of motion. Similarly to Section 2, $\varphi$ or $\Phi$ satisfies the equation of motion provided

$$Dual\left(\Phi_* \mathrm{d}_1 \mathscr{L}_1\right) + \mathrm{d}_1 \mathscr{L}_0 = 0; \tag{26}$$

where $\Phi_* : \Omega^1(A_1 \otimes A_2) \to \Omega^1(A_0 \otimes A_1)$ is the map induced by $\Phi$.

The *Dual* operator in Eq. (26) is necessary in order to ensure that distributivity be a necessary condition for the evolution map to satisfy the equation of motion, as shown in the following example.

EXAMPLE (modified from Baez and Gilliam, 1994). Suppose 2 is a unit in *k* and that the algebra $A \cong \mathscr{D}[q]$, so that $A \otimes A \cong \mathscr{D}[q_1, q_2]$ and $H \cong \mathscr{D}[q_0, ..., q_T]$, the polynomials in *T*+1 variables over $\mathscr{D}$. Consider the Lagrangian $\mathscr{L}_i$ (written here as a polynomial function) for a particle in a polynomial potential **V** as a function of consecutive positions $\mathbf{q}_i$ and $\mathbf{q}_{i+1}$ of the particle:

$$\mathscr{L}_i = \mathscr{L}(\mathbf{q}_i, \mathbf{q}_{i+1}) = \frac{1}{2}\mathbf{m}\dot{\mathbf{q}}_i^{\,2} - \mathbf{V}(\mathbf{q}_i)_- \tag{27}$$

where one defines $\dot{\mathbf{q}}_i = \mathbf{q}_{i+1} - \mathbf{q}_{i\_}$ (so that $\dot{\mathbf{q}}_i = 0$ iff $\mathbf{q}_{i+1} = \mathbf{q}_i$), and where **m** is a unit in $\mathscr{D}$ representing the mass of the particle. Notice that $\mathscr{L}_i = 0$ iff $\frac{1}{2}\mathbf{m}\dot{\mathbf{q}}_i^{\,2} = \mathbf{V}(\mathbf{q}_i)$. Since

$\mathrm{d}_i\mathscr{L} = \partial_{q_i}\mathscr{L}\left(\mathbf{q}_1, \mathbf{q}_2\right)\mathrm{d}q_i$ , $i$ = 1, 2 and the *Dual* operator is distributive with respect to sum and product, one obtains:

$$\begin{aligned} Dual\left(d_i\mathscr{L}_i\right) &= Dual\left(-\mathbf{m}\left(\mathbf{q}_{i+1} - \mathbf{q}_{i\_}\right) - \mathbf{V}'\left(\mathbf{q}_i\right)_-\right)dq_i = \\ &= -\mathbf{m}_-\left(\mathbf{q}_{i+1} - \mathbf{q}_{i\_}\right)_- dq_i - \mathbf{V}'\left(\mathbf{q}_i\right)dq_i = -\mathbf{m}_-\dot{\mathbf{q}}_{i\_}dq_i - \mathbf{V}'\left(\mathbf{q}_i\right)dq_i = \\ &= -\left(\mathbf{m}\dot{\mathbf{q}}_i\right)_- dq_i - \mathbf{V}'\left(\mathbf{q}_i\right)dq_i \end{aligned}$$

Likewise

$$d_i\mathscr{L}_{i-1} = \mathbf{m}\left(\mathbf{q}_i - \mathbf{q}_{i-1\_}\right) = \mathbf{m}\dot{\mathbf{q}}_{i-1}dq_i$$

The Euler-Lagrange equation is thus:

$$\left(\mathbf{m}\dot{\mathbf{q}}_i\right)_- - \mathbf{m}\dot{\mathbf{q}}_{i-1} + \mathbf{V}'\left(\mathbf{q}_i\right) = 0\,, \tag{28}$$

which correctly yields $\mathbf{V}'\left(\mathbf{q}_i\right) = 0$ iff $\dot{\mathbf{q}}_i = \dot{\mathbf{q}}_{i-1}$ (compare with Eq. (10)).

The discrete analog for Newton's second law is immediately derived:

$$\begin{aligned} \left(\mathbf{m}\dot{\mathbf{q}}_i\right)_- - \mathbf{m}\dot{\mathbf{q}}_{i-1} + \mathbf{V}'\left(\mathbf{q}_i\right) = 0 &\Leftrightarrow \left(\mathbf{m}\dot{\mathbf{q}}_i\right)_- = \left(\mathbf{m}\dot{\mathbf{q}}_{i-1}\right)_- - \mathbf{V}'\left(\mathbf{q}_i\right)_- \\ &\Leftrightarrow \dot{\mathbf{q}}_{i\_} = \dot{\mathbf{q}}_{i-1\_} - \mathbf{m}^{-1}\mathbf{V}'\left(\mathbf{q}_i\right)_- \\ &\Leftrightarrow \dot{\mathbf{q}}_{i\_} - \dot{\mathbf{q}}_{i-1} = -\mathbf{m}^{-1}\mathbf{V}'\left(\mathbf{q}_i\right)_- \\ &\Leftrightarrow \dot{\mathbf{q}}_i - \dot{\mathbf{q}}_{i-1\_} = -\mathbf{m}_-^{-1}\mathbf{V}'\left(\mathbf{q}_i\right) \end{aligned},$$

which yields the time evolution map (compare with Eq. (16))

$$\varphi\left(\mathbf{q}_2\right) = \mathbf{q}_1 + \dot{\mathbf{q}}_0 - \mathbf{m}^{-1}\mathbf{V}'\left(\mathbf{q}_1\right)_- = 2\mathbf{q}_1 - \mathbf{q}_{0-} - \mathbf{m}_-^{-1}\mathbf{V}'\left(\mathbf{q}_1\right) \tag{29}$$

and homomrphism Φ (compare with Eqs. (17) and (18))

$$\Phi\left(\mathbf{q}_1\right) = \mathbf{q}_1,\ \Phi\left(\mathbf{q}_2\right) = \varphi\left(\mathbf{q}_2\right) = 2\mathbf{q}_1 - \mathbf{q}_{0-} - \mathbf{m}_-^{-1}\mathbf{V}'\left(\mathbf{q}_1\right) \tag{30}$$

$$\Phi_*\left(\mathrm{d}q_1\right) = \mathrm{d}q_1\,,\ \Phi_*\left(\mathrm{d}q_2\right) = 2\mathrm{d}q_1 - \mathrm{d}q_0 - \mathbf{m}_-^{-1}\mathbf{V}''\left(\mathbf{q}_1\right)\mathrm{d}q_1 \tag{31}$$

Let us check that the time evolution map satisfies the equation of motion:

$$Dual\left(\Phi_* \mathrm{d}_1 \mathscr{L}_1\right) + \mathrm{d}_1 \mathscr{L}_0 = Dual\left(\Phi_* \partial_{q_1} \mathscr{L}\left(\mathbf{q}_1, \mathbf{q}_2\right) \mathrm{d}q_1\right) + \partial_{q_1} \mathscr{L}\left(\mathbf{q}_0, \mathbf{q}_1\right) \mathrm{d}q_1 =$$
$$= Dual\left(\Phi_*\left(\left(-\mathbf{m}\left(\mathbf{q}_2 - \mathbf{q}_{1-}\right) - \mathbf{V}'\left(\mathbf{q}_1\right)_-\right) \mathrm{d}q_1\right)\right) + \mathbf{m}\left(\mathbf{q}_1 - \mathbf{q}_{0-}\right) \mathrm{d}q_1$$
$$= \left(\left(-\mathbf{m}\left(2\mathbf{q}_1 - \mathbf{q}_{0-} - \mathbf{m}_-^{-1} \mathbf{V}'\left(\mathbf{q}_1\right) - \mathbf{q}_{1-}\right) - \mathbf{V}'\left(\mathbf{q}_1\right)_-\right) \mathrm{d}q_1\right)_- + \mathbf{m}\left(\mathbf{q}_1 - \mathbf{q}_{0-}\right) \mathrm{d}q_1$$
$$= \left(\left(-\mathbf{m}\left(\mathbf{q}_1 - \mathbf{q}_{0-} - \mathbf{m}_-^{-1} \mathbf{V}'\left(\mathbf{q}_1\right)\right) - \mathbf{V}'\left(\mathbf{q}_1\right)_-\right) \mathrm{d}q_1\right)_- + \mathbf{m}\left(\mathbf{q}_1 - \mathbf{q}_{0-}\right) \mathrm{d}q_1$$

whether or not this quantity is equal to zero depends on the actual input data, as the two following numerical examples of a harmonic oscillator show (assume $k = \mathbb{Q}$):

1. Example 2a: assume $\mathbf{q}_0 = [40, 45]$, $\mathbf{q}_1 = [50, 65]$; $\mathbf{V}\left(\mathbf{q}_1\right) = \frac{1}{2}\mathbf{s}\mathbf{q}_1^{\,2}$; $\mathbf{s}$ = [1/25, 6/25]; $\mathbf{V}'\left(\mathbf{q}_1\right) = \mathbf{s}\mathbf{q}_1$; $\mathbf{m}$ = [1, 2]. Then $-\mathbf{m}\left(\mathbf{q}_1 - \mathbf{q}_{0-} - \mathbf{m}_-^{-1} \mathbf{V}'\left(\mathbf{q}_1\right)\right) - \mathbf{V}'\left(\mathbf{q}_1\right)_-$ = [-38, -13] $\subset$ $-\mathbf{m}\left(\mathbf{q}_1 - \mathbf{q}_{0-}\right)$ = [-40, -10] because only sub-distributivity holds. As a result, $Dual\left(\Phi_* \mathrm{d}_1 \mathscr{L}_1\right) + \mathrm{d}_1 L_0$ = [-3, 2], and thus generalized interval arithmetic leads to the conclusion that the time evolution map does not satisfy the equation of motion.
2. Example 2b: assume $\mathbf{q}_0 = [11{,}000, 11{,}100]$, $\mathbf{q}_1 = [10{,}000, 11{,}000]$; $\mathbf{V}\left(\mathbf{q}_1\right) = \frac{1}{2}\mathbf{s}\mathbf{q}_1^{\,2}$; $\mathbf{s}$ = [1/5000, 3/5500]; $\mathbf{V}'\left(\mathbf{q}_1\right) = \mathbf{s}\mathbf{q}_1$; $\mathbf{m}$ = [1, 2]. Then $-\mathbf{m}\left(\mathbf{q}_1 - \mathbf{q}_{0-} - \mathbf{m}_-^{-1} \mathbf{V}'\left(\mathbf{q}_1\right)\right) - \mathbf{V}'\left(\mathbf{q}_1\right)_-$ = [100, 2000] = $-\mathbf{m}\left(\mathbf{q}_1 - \mathbf{q}_{0-}\right)$ = [100, 2000] and the time evolution map satisfies the equation of motion.

More in general, if Eq. (24) applies, then the time evolution map is satisfied using generalized interval arithmetic iff $\hat{\mu}\left(\mathbf{x}_1\right)\hat{\mu}\left(\mathbf{s}\right) = +$ AND $\hat{\mu}\left(\mathbf{x}_2\right)\hat{\mu}\left(\mathbf{s}\right) = +$, with $\mathbf{x}_1 = \mathbf{q}_1 - \mathbf{q}_{0-}$, $\mathbf{x}_2 = -\mathbf{m}_-^{-1}\mathbf{V}'\left(\mathbf{q}_1\right)$, and $\mathbf{y} = -\mathbf{m}$. If one defines the momentum as $\mathbf{p}_i = \mathbf{m}\dot{\mathbf{q}}_i = \mathbf{m}\left(\mathbf{q}_{i+1} - \mathbf{q}_{i\_}\right)$, then these conditions are equivalent to the momentum having the same sign, $\sigma$ (Eq. (20)), as the spring force $-\mathbf{V}'\left(\mathbf{q}_{i+1}\right)$. If the time evolution map does not satisfy the equation of motion because only subdistributivity holds, then $\Phi_*$ pulls $d_i \mathscr{L}_i$ back to a subset of $-d_i \mathscr{L}_{i-1}$.

This shows that the imprecision in the input data together with subdistributivity may lead to a time evolution map that does not satisfy the equation of motion, which is nevertheless satisfied when no imprecision exists. In other terms, the time evolution map may not satisfy the equation

of motion in $\mathscr{D}$ even if it is always satisfied for every ring *k*. It may also happen that the time evolution map ceases to satisfy the equation of motion after a finite number of time steps: this occurs, for example, in Example 1b for $i = 13$. Let us analyze this crucial point in more detail.

What is happening is overestimation caused by the multi-incidence of some variables in the expressions to be evaluated: a well known problem in interval analysis. Since the evolution map is always defined in terms of the previous two time steps (e.g., Eq. (29)), multi-incidence occurs in the computation of the flow as well. The dependency problem in range computation over a domain of proper intervals is eliminated using the algorithm developed by Popova (2005), which applies to rational functions such as those arising here by working on a polynomial configuration space. Within the Mathematica environment, this is efficiently accomplished by transforming the function to be evaluated using the `IntervalComputations`Range` package (2005), which takes into account the function's monotonicity properties in each incidence.

In the Example above, the described algorithm leads $Dual\left(\Phi_* \mathrm{d}_1 L_1\right) + \mathrm{d}_1 L_0$ to be identically equal to zero. As for the flow, steps 3 to 15 of the flow for Example 2b are given below as a way to exemplify:

$$\left(\begin{array}{ll}
\frac{97840}{11} & \frac{109989}{10} \\
\frac{23547324}{3025} & \frac{1099670011}{100000} \\
\frac{27741730507}{4159375} & \frac{10993400549989}{1000000000} \\
\frac{126999172635479}{22876562500} & \frac{109890016499230011}{10000000000000} \\
\frac{557422553635612563}{125821093750000} & \frac{1098350384969200989989}{100000000000000000} \\
\frac{2288250850107591605311}{692016015625000000} & \frac{1097690769907604949879 0011}{10000000000000000000} \\
\frac{830186235115590485285 5067}{3806088085937500000000} & \frac{1096921385769018149274 01429989}{10000000000000000000000000} \\
\frac{220759920599068396061894 21799}{2093348447265625000000000} & \frac{1096042309491854446854100098350011}{10000000000000000000000000000} \\
-\frac{836165143967060664960070522639 7}{1151341645996093750000000000} & \frac{1095053628983741558989500486800 1869989}{100000000000000000000000000000000} \\
-\frac{759751840694239559412888964794437809}{6332379052978515625000000000000000} & \frac{1093955443112730296969001925201682979 10011}{10000000000000000000000000000000000000} \\
-\frac{810205103606451658371311861274592333 5573}{3482808479138183593750000000000000000} & \frac{1092747861697407761918806463410658791002309989}{100000000000000000000000000000000000000000} \\
-\frac{661157620626007421988532741993351751990462 81}{1915544663526000976562500000000000000000} & \frac{1091431005495915486092419120973293537025409747 0011}{10000000000000000000000000000000000000000000000} \\
-\frac{481987991561468735303467618334524740762828702157}{1053549564939300537109375000000000000000000000} & \frac{1090005006193873618717422536623830953694806964027 49989}{100000000000000000000000000000000000000000000000000}
\end{array}\right)$$

These ranges exactly correspond to those computed using the Mathematica global optimization functions `Maximize` and `Minimize`, thus confirming that $fR(\mathbf{x}) = R_f(\mathbf{x})$. However, when using Mathematica global optimization functions, computational times are over

$13 \cdot 10^3$ times higher, and they could be impractically higher for more complex problems. As a way to interpret these results, recall that the time evolution map (Eq. (16)) is continuous in $q_1$, $q_0$, $m$ and $s$. As a consequence, the meaning of interval $\mathbf{q}_i$ calculated at the $i$-th step is as follows: the actual position of the particle at the $i$-th time step is a rational number in the interval $\mathbf{q}_i$. In a non-degenerate interval $\mathbf{q}_i$ there are infinite (albeit countable) possible positions.

Similarly to the example in Section 2, the numbers of digits in the numerator and denominator increase at each time step. As time steps proceed, the shift to the left of the upper bound (slowest possible particle) is much smaller (1%) than the shift to the left undergone by the left bound (146%), which becomes negative at the 11th time step (fastest possible particle). At the 15th time step, the width of the position interval is equal to about 15,475, whereas at the 1st time step it was equal to 1,000. Thus, the width has increased by about 150%. Figure 4 illustrates this behavior using some snapshots of the evolution of the configuration space. Notice that when the fastest particle bounces back to the right after the 80th step, the lower bound remains constant. The upper bound keeps decreasing because the slowest particle keeps marching to the left, until the fastest particle (which is now marching to the right) overcomes the slowest particle between $i$ = 140 and $i$ = 160, and makes the upper bound increase again.

After the 160th time step, the interval never decreases because the fastest possible particle is always "much faster" than the slower possible particle. Similarly to the precise case of Section 2, it is impossible to determine the asymptotic values for the smallest and largest coordinates reached by the particle. Despite the fact that it is unknown whether the particle will actually visit all rational coordinate positions between the reached extremes (see Section 2), the continuity of the evolution map ensures that the particle may occupy *any* of the rational coordinate positions in the intervals depicted in Figure 4.

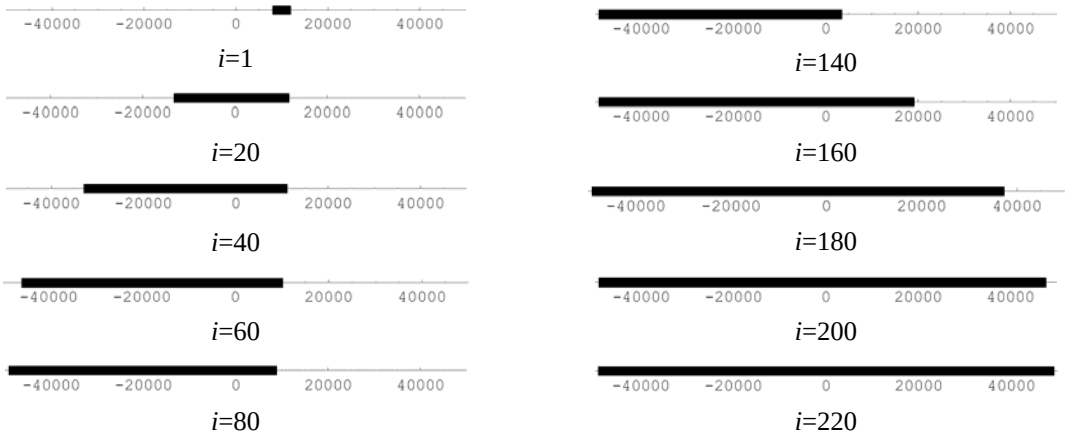



*Figure 4.* Snapshots of the evolution of the configuration interval for the harmonic oscillator in Example 2a.

When the function's monotonicity properties cannot be exploited because the hypotheses in (Popova, 2005) are not fulfilled, validated bounds on the system's evolutions can be calculated by a discrete version of Taylor models. Taylor models have proven very effective in reducing overestimation in validated calculations of the flow for continuous systems (e.g., Makino, K. and Berz, 2004 and Berz and Makino, 1998 and references therein). The extension of Taylor models to discrete mechanics is the subject of current study.

## 5. Conclusions

Discrete dynamical systems that take values in a ring *k* allow for an exact integration of their time evolution. When the ring *k* is the ring of rational numbers, it may be impossible to determine *a priori* the evolution of even the simpler linear systems.

When discrete dynamical systems take values in $\mathbb{D}$ (the set of extended intervals defined on a ring *k*), one finds that:

- The definition of the Euler-Lagrange equation and of satisfaction of the equation of motion for the time evolution map must be modified by introducing the *Dual* operator for extended intervals.
- When monotonicity can be exploited, exact bounds on the system evolution can be calculated very efficiently at each time step without the use of global optimization. When monotonicity cannot be exploited, validated bounds can be calculated, but more research is needed in this field, where Taylor models look very promising.

Two interpretations of directed intervals have been used, namely directed interval as an ordered couple of elements of *k* and as a set of elements of *k*. The interpretation of directed intervals in terms of modal logic (Gardenes, 1986) opens the way to logical interpretations of mechanical systems (including cellular automata) and vice versa; this aspect will be investigated in the future.

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