Space-Discretized Verlet-Algorithm from a Variational Principle

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A form of the Verlet-algorithm for the integration of Newton's equations of motion is derived from Hamilton's principle in discretized space and time. It allows the computation of exactly time-reversible trajectories on a digital computer, offers the possibility of systematically investigating the effects of space discretization, and provides a criterion as to when a trajectory ceases to be physical.

For three decades, the Verlet algorithm [1, 2] is the method of choice in molecular dynamics simulations (MDS in short) [3, 4]. Newton's equation of motion are hereby integrated numerically via

$$x(t+\Delta t) = 2x(t) - x(t-\Delta t) + (\Delta t)^2 F(x(t)). \quad (1)$$

For simplicity, only one degree of freedom is considered; $x(t)$ is the position of a particle at time t, Δt is the time step, and F is the force term that governs the motion. From a numerical point of view (1) is the simplest third-order algorithm for the task. The Verlet-algorithm, therefore, suggests itself naturally for use in the simulations of large systems like, e. g., the motion of proteins in solution [4]. By deriving the Verlet algorithm from Hamilton's principle [5], Gillilan and Wilson [6] recently demonstrated that this algorithm also has a deep physical foundation. A justification for and an intuitive understanding of Hamilton's principle, i. e. the principle that classical trajectories are those of extremal action, comes from the path integral description of quantum mechanics [7].

One of the outstanding properties of (1) is its time-reversibility [2, 8, 9]. That is, the form of (1) is invariant under an exchange of $x(t+\Delta t)$ by $x(t-\Delta t)$. It therefore is equally appropriate for computing the forward and the backward time evolution.

Nevertheless, in an actual implementation on a digital computer, the exact time-reversibility of the Verlet-algorithm is broken due to roundoff errors. This generates problems – for example, when investigating the origin of irreversibility and checking the validity of Boltzmann's entropy concept [10] in many-particle systems by means of MDS. It has been known for a long time that MDS-results in the context of investigating irreversibility in the evolution of Boltzmann's entropy have to be taken with a grain of salt since velocity inversion does not generate an exactly time-reversed behavior [11]. Spurious effects due to roundoff errors occur also in dissipative dynamical systems [12], where numerical dissipation is superimposed on the dynamics at hand.

Roundoff errors occur because real numbers are represented as finite-size floating point numbers in digital computers [13]. This representation introduces an uncontrollable nonlinear discretization which gives rise to a slighly incorrect, machine-dependent arithmetic. Integer arithmetic, in contrast, is exact and machine-independent on digital computers. In a seminal but not widely known paper, Wolff and Huberman [14] made use of this property to systematically investigate the effects of discretization on the logistic map, a generic dissipative system which exhibits chaotic behavior. Rather than discretizing a continuous equation, they started out from the concept of a granular state space and looked at the behavior of integer maps that resemble the logistic one.

Similarly, a large class of algorithms, among them the Verlet-algorithm, can be implemented on a computer using integer arithmetic in order to make these algorithms exactly invertible [8]. Levesque and Verlet [2] applied this integer representation of the state space to solve the problem of generating a reliable time evolution of the Boltzmann entropy in an MDS. Rather than representing the force term in (1) by the closest integer (i. e., the ROUND function), Levesque and Verlet chose to represent it by the integer part

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of the real number (i. e., the INT function) which is less optimal as we shall see. In the following, it will be shown that Wolff and Huberman's concept of spatial discretization together with Gillilan and Wilson's time-discrete Hamiltonian principle provide the starting point for moving any arbitrariness in an exactly time-reversible algorithm for computing Newtonian trajectories. Moreover, the same approach simultaneously produces a criterion for the validity of the computed trajectory.

Our starting point for the application of Hamilton's principle is the action integral of a trajectory $q(t)$,

$$S[q(t)] = \int_{t_i}^{t_f} \left\{ \frac{1}{2}\dot{q}(t)^2 - V[q(t)] \right\} \,\mathrm{d}t. \tag{2}$$

Discretization of time and space via $t = t_i + k\Delta t$, and $q = q_0 + x\Delta q$ with $k, x \in \mathbf{Z}$, changes (2) into an action sum for the discretized trajectory $\{x_k\}$. Specifically, the representation of the action integral in granular state space and time corresponding to (2) is

$$\begin{aligned} S[\{x_k\}] = \frac{1}{2}\Delta t \sum_{k=0}^{N-1} \left[\frac{x_{k+1} - x_k}{\Delta t} \right]^2 (\Delta q)^2 \\ - \Delta t \sum_{k=0}^{N-1} V(q_0 + x_k \Delta q). \end{aligned} \tag{3}$$

In deriving (3), the representation of the momentum introduced by Gillilan and Wilson [6] was chosen [15].

A classical trajectory in granular state space and time is one that obeys Hamilton's principle, i. e., it extremalizes the action sum (3). When dealing with functions defined on discretized space, we cannot resort to the usual technique of looking for the zeros of appropriate derivatives in order to find extremal points. Nevertheless, it is immediately clear that a function $S(x)$, defined on the integers, is extremal for a particular value of x if the sign of the difference in S obtained by varying x to $x-1$ is the same as that for varying x to $x+1$. If one uses the following notation for a variation of the action S at x_k in the + and – directions, respectively,

$$\begin{aligned} \partial S_{\pm}(x_k) = S(x_0, \ldots, x_k, \ldots, x_N) \\ - S(x_0, \ldots, x_k + 1, \ldots, x_N), \end{aligned} \tag{4}$$

the discretized extremality condition discussed above assumes the simple form

$$\partial S_{-}(x_k) \partial S_{+}(x_k) > 0. \tag{5}$$

Insertion of the discretized action (3) into expression (5) results in an inequality condition which any triple (x_{k-1}, x_k, x_{k+1}) that is part of a physical trajectory on granular space has to obey:

$$\begin{aligned} &\left\{ x_{k+1} - 2x_k + x_{k-1} + 1 \right. \\ &\quad \left. + (\Delta t)^2 \frac{V(q_0 + x_k \Delta q) - V(q_0 + (x_k - 1)\Delta q)}{(\Delta q)^2} \right\} \\ &\left\{ x_{k+1} - 2x_k + x_{k-1} - 1 \right. \\ &\quad \left. + (\Delta t)^2 \frac{V(q_0 + (x_k + 1)\Delta q) - V(q_0 + x_k \Delta q)}{(\Delta q)^2} \right\} < 0. \end{aligned} \tag{6}$$

Equation (6) can be used for the derivation of a time-reversible integration algorithm. That is, once x_{k-1} and x_k are specified, we seek an x_{k+1} which fulfills that criterion. The lhs of (6) is a simple second-degree polynomial in x_{k+1} with a minimum at

$$\begin{aligned} x_{k+1}^{\min} = 2x_k - x_{k-1} \\ -\Delta t^2 \frac{V(q_0 + (x_k + 1)\Delta q) - V(q_0 + (x_k - 1)\Delta q)}{2\Delta q^2}. \end{aligned} \tag{7}$$

Since $x_{k+1}^{\min}$ is not integer-valued in general, the most promising candidate for a solution in the discretized state space is the one integer number which lies closest to it, namely

$$x_{k+1}^{\min} = 2x_k - x_{k-1} - \mathrm{ROUND}(a), \text{ where} \tag{8}$$

$$a = \Delta t^2 \frac{V(q_0 + (x_k + 1)\Delta q) - V(q_0 + (x_k - 1)\Delta q)}{2\Delta q^2}$$

The existence and uniqueness of this solution to (6) remains to be discussed. The two zeros in x_{k+1} of the lhs of (6) – which may be denoted by $x_{k+1}^{(1)}$ and $x_{k+1}^{(2)}$, with $x_{k+1}^{(1)} \le x_{k+1}^{(2)}$ – define an interval $\left[x_{k+1}^{(1)}, x_{k+1}^{(2)}\right]$ in which the sought-for integer value of x_{k+1} lies. Three cases need to be distinguished. First, if there is only one integer enclosed in that interval, then it is the one already found by (8). Second, if the interval encloses more than one integer number, one can convince oneself easily that the solution (8) has found is the only one relevant. This is because all other possible solutions that satisfy the extremality condition can be considered to be spurious: in the limit $\Delta t \to 0$ the parabola defined by the lhs. of (6) is contracted and the interval $\left[x_{k+1}^{(1)}, x_{k+1}^{(2)}\right]$ shrinks, so that those other solutions vanish, leaving only that of (8). Third, there is the interesting case to consider that no integer lies in the interval $\left[x_{k+1}^{(1)}, x_{k+1}^{(2)}\right]$. In that case, the value of x_{k+1} defined by (8) violates the extremality condition (6). It is then impossible to find a value of x_{k+1} so that the trajectory obeys Hamilton's principle: the trajectory ceases to be physical. This case is easily recognizable and a finer discretization has then to be used if a viable trajectory is desired beyond the point in time reached so far.

Equation (8) therefore represents an algorithmic formula for the exactly time-reversible computation of a physical trajectory in granular space. It bears a close resemblance to the original Verlet algorithm, eq. (1), but supplements the latter with a rule of how to avoid arbitrariness in the definition of the force term in granular space. In addition, a numerical criterion for the physical acceptability of the calculated trajectory is provided. Extension to higher dimensions is straightforward.

It is worth pointing out that momentum is exactly preserved by the algorithm (8) under a rather general condition, namely, whenever V is a sum of distance-dependent pair potentials, as is usually the case in MDS [16]. This conservation property avoids the vexing problem of a secular drift of momentum in MDS. Actually this property is not specific to algorithm (8), but holds true for any integer representation of the force term. On the other hand, total energy is not exactly conserved in the algorithm (8), and hence it usually fluctuates. However, time reversibility ensures that there is no secular drift in energy [17].

To conclude, we have derived a new variant to Verlet's algorithm appropriate for use in MDS. It is derived from the fundamental physical principle of least action, applicable in discretized state space and time. It can be regarded as a quasi-Newtonian equation of motion. It is exactly time-reversible. There is no secular drift in total energy. Therefore, the new algorithm is highly appropriate for applications, for example, in investigating the validity of Boltzmann's deterministic entropy concept, in far from equilibrium systems. The most important property of the new algorithm appears to be that it provides a criterion (automatically checked concomitantly) as to whether the computed trajectory is physically acceptable.

The algorithm will be especially useful for the planned setting-up of an exactly time-invertible deterministic artificial Newtonian universe.

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[15] A more symmetric choice of the discretized representation of the momentum, i. e. $(x_{n+1} - x_{n-1})/2h$, as originally suggested by Verlet [1], leads to the same final algorithm (8).
[16] Total momentum is no longer conserved in some cases of non-pair potentials (like wall potentials).
[17] An algorithm-dependent secular drift in energy should also appear in the time-reversed direction. However, from the time-reversibility property of an algorithm it can be concluded that such a drift must vanish. Apparently, this argument is due to J.-M. Caillol, as cited in [2].