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Newton's algorithm for discrete classical dynamics

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ABSTRACT

A recent article in J. Chem. Phys. argues that the two algorithms, the velocity-Verlet and position-Verlet integrators, commonly used in Molecular Dynamics (MD) simulations, are different [L. Ni and Z. Hu, J. Chem. Phys. **161**, 226101 (2024)]. However, not only are the two algorithms just different formulations of the same discrete algorithm, but also are other simple discrete algorithms used in MD simulations in the natural sciences. They are all reformulations of the discrete algorithm derived by Newton in 1687 in *Proposition I* in the very first part of his book *Principia*. The different reformulations of Newton's algorithm for discrete dynamics lead to identical discrete dynamics with the same invariances, momentum, angular momentum, and energy as Newton's analytical dynamics. Hundreds of thousands of MD simulations with Newton's discrete dynamics have appeared but unfortunately with many recorded errors for energies, potential energies, temperatures, and heat capacities. The public software for MD should be corrected.

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I. INTRODUCTION

A recent article in *J. Chem. Phys.* argues that the two simple discrete algorithms, the velocity-Verlet and position-Verlet integrators, are different.[1] However, not only are the two algorithms just different formulations of the same discrete algorithm, but also are other simple discrete algorithms used in Molecular Dynamics (MD) simulations in the natural sciences. They are all reformulations of the discrete algorithm derived by Newton in 1687 in *Proposition I* in the very first part of his book *Principia*.[2,3]

The new position of an object in Newton's discrete dynamics, $\mathbf{r}_i(t+\delta t)$, at time $t+\delta t$ i with the mass m_i is determined by the force $\mathbf{f}_i(t)$ acting on the object at the discrete position $\mathbf{r}_i(t)$ at time t together with the position $\mathbf{r}_i(t-\delta t)$ at time $t-\delta t$ as

$$m_i \frac{\mathbf{r}_i(t+\delta t)-\mathbf{r}_i(t)}{\delta t} = m_i \frac{\mathbf{r}_i(t)-\mathbf{r}_i(t-\delta t)}{\delta t} + \delta t \mathbf{f}_i(t), \tag{1}$$

where the velocities $\mathbf{v}_i(t+\delta t/2) = (\mathbf{r}_i(t+\delta t)-\mathbf{r}_i(t))/\delta t$ and $\mathbf{v}_i(t-\delta t/2) = (\mathbf{r}_i(t)-\mathbf{r}_i(t-\delta t))/\delta t$ and the corresponding momenta are constant in the time intervals in between the discrete positions.

II. NEWTON'S DISCRETE ALGORITHM

Newton begins *Principia* by postulating Eq. (1) in *Proposition I* and with Fig. 1. The English translation of *Proposition I* is

*Of the Invention of Centripetal Forces.*Proposition I. Theorem I.

The areas, which revolving bodies describe by radii drawn to an immovable centre of force do lie in the same immovable planes, and are proportional to the times in which they are described.

For suppose the time to be divided into equal parts, and in the first part of time let the body by its innate force describe the right line AB. In the second part of that time, the same would (by Law I.), if not hindered, proceed directly to c, along the line Bc equal to AB; so that the radii AS, BS, cS, drawn to the centre, the equal areas ASB, BSc, would be described. But when the body is arrived at B, ***suppose that a centripetal force acts at once with a great impulse****, and, turning aside the body from the right line Bc, compels it afterwards to continue its motion along the right line BC. Draw cC parallel to BS meeting BC in C; and at the end of the second part of the time, the body (by Cor. I of Laws) will be found in C, in the same plane with the triangle ASB. Join SC, and, because SB and Cs are parallel, the triangle SBC will be equal to the triangle SBc, and therefore also to the triangle SAB. By the like argument, if the centripetal force acts successively in C, D, E, & c., and makes the body, in each single particle of time, to describe the right lines CD, DE, EF, & c., they will all lie in the same*

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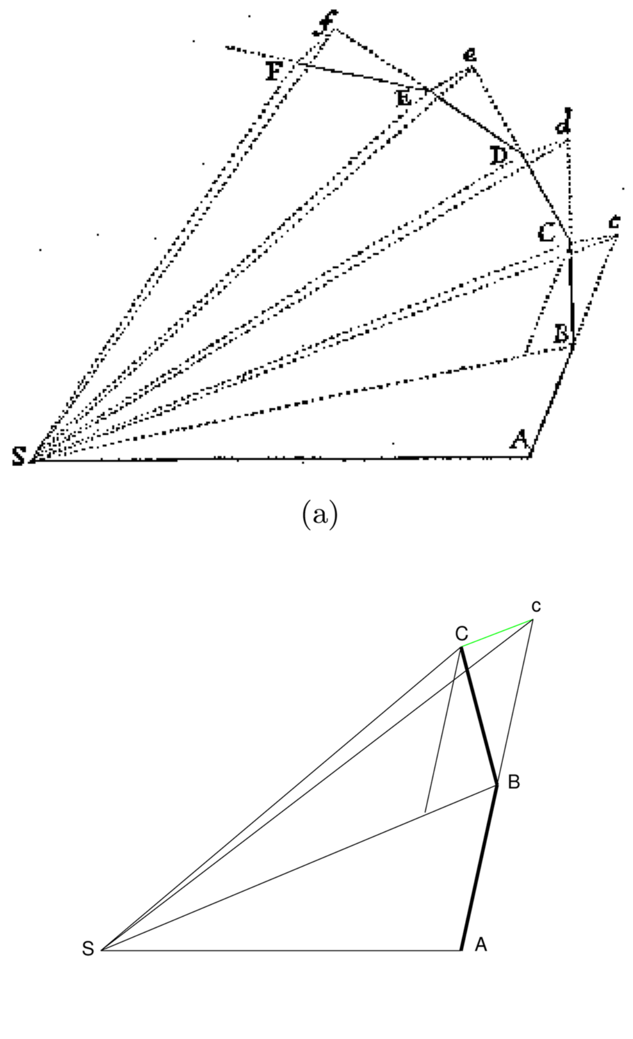

(b)

FIG. 1. Newton's figure at *Proposition I*. (a) A Newton's figure at *Proposition I* in *Principia*, with the formulations of the discrete dynamics. (b) Central part: A: $\mathbf{r}_i(t-\delta t)$; B: $\mathbf{r}_i(t)$; C: $\mathbf{r}_i(t+\delta t)$, etc. The deviation cC (green) from the straight line ABc (Newton's first law) is caused by the force $\mathbf{f}_i(t)$ with direction $\overrightarrow{\mathrm{BS}}$ at time *t*.

plane; and the triangle SCD will be equal to the triangle SBC, and SDE to SCD, and SEF to SDE. And therefore, in equal times, equal areas are described in on immovable plane: and, by composition, any sums SADS, SAFS, of those areas, are one to the other as the times in which they are described. Now let the number of those triangles be augmented; and their breadth diminished in infinitum; and (by Cor. 4, Lem III) their ultimate perimeter ADF will be a curve line: and therefore the centripetal force, by which the body is perpetually drawn back from the tangent of this curve, will act continually; and any described areas SADS, SAFS, which are always proportional to the times of description, will, in this case also, be proportional to those times. Q. E. D.

The central assumption … ***suppose that a centripetal force acts at once with a great impulse*** in *Proposition I* is highlighted here. The forces change the momenta only at discrete times, and the dynamics is solely determined by the positions and the forces at these discrete times. The positions with constant velocities and momenta in between the discrete times are changed with $\overrightarrow{\mathrm{AB}} = \mathbf{r}_i(t) - \mathbf{r}_i(t-\delta t) = \overrightarrow{\mathrm{Bc}}$ (Newton's first law) to $\overrightarrow{\mathrm{BC}} = \mathbf{r}_i(t+\delta t) - \mathbf{r}_i(t)$. The change of position is caused by the force $\mathbf{f}_i(t)$ in the direction $\overrightarrow{\mathrm{BS}}$. Within the next times from t to $t+\delta t$, the force changes the momentum with a total amount $\delta t \mathbf{f}_i(t)$ and the position to C with $\overrightarrow{\mathrm{cC}} = \delta t^2 \mathbf{f}_i(t)/m_i$, i.e.,

$$\overrightarrow{\mathrm{BC}} = \overrightarrow{\mathrm{AB}} + \overrightarrow{\mathrm{cC}}, \tag{2}$$

with is equal to Eq. (1). Reference 3 is a review of Newton's discrete dynamics.

Newton obtained his second law for classical analytic dynamics as the limit $\lim_{\delta t \to 0}$ of Eq. (1). At present, Newton's second law is formulated as an equality between the mass times the acceleration being equal to the force acting on the object, but this formulation is due to Euler in 1736 after Newton died in 1727.[4]

III. REFORMULATIONS OF NEWTON'S DISCRETE ALGORITHM

The algorithm, Eq. (1), is usually presented as the leapfrog algorithm,

$$\begin{aligned} \mathbf{v}_i(t+\delta t/2) &= \mathbf{v}_i(t-\delta t/2) + \frac{\delta t}{m_i}\mathbf{f}_i(t), \\ \mathbf{r}_i(t+\delta t) &= \mathbf{r}_i(t) + \delta t \mathbf{v}_i(t+\delta t/2), \end{aligned} \tag{3}$$

where the new values $\mathbf{v}_i(t+\delta t/2)$ and $\mathbf{r}_i(t+\delta t)$ are obtained from the corresponding old values $\mathbf{v}_i(t-\delta t/2)$ and $\mathbf{r}_i(t)$. The rearrangement of Eq. (1) gives the Verlet algorithm,[5,6]

$$\mathbf{r}_i(t+\delta t) = 2\mathbf{r}_i(t) - \mathbf{r}_i(t-\delta t) + \frac{\delta t^2}{m_i}\mathbf{f}_i(t). \tag{4}$$

The velocity-Verlet algorithm[7]

$$\mathbf{r}_i(t+\delta t) = \mathbf{r}_i(t) + \delta t \mathbf{v}_i(t) + \frac{\delta t^2}{2m_i}\mathbf{f}_i(t), \tag{5}$$

$$\mathbf{v}_i(t+\delta t) = \mathbf{v}_i(t) + \frac{\delta t}{2m_i}[\mathbf{f}_i(t) + \mathbf{f}_i(t+\delta t)], \tag{6}$$

with

$$\mathbf{v}_i(t) = \frac{\mathbf{v}_i(t+\delta t/2) + \mathbf{v}_i(t-\delta t/2)}{2} = \frac{\mathbf{r}_i(t+\delta t) - \mathbf{r}_i(t-\delta t)}{2\delta t} \tag{7}$$

is a reformulation of Newton's discrete algorithm. It can be seen by rearranging Eq. (5),

$$\mathbf{v}_i(t) = \frac{\mathbf{r}_i(t+\delta t) - \mathbf{r}_i(t)}{\delta t} - \frac{\delta t}{2m_i}\mathbf{f}_i(t), \tag{8}$$

and inserting Eq. (8) in Eq. (6),

$$\mathbf{v}_i(t+\delta t) = \frac{\mathbf{r}_i(t+\delta t) - \mathbf{r}_i(t)}{\delta t} + \frac{\delta t}{2m_i}\mathbf{f}_i(t+\delta t), \tag{9}$$

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or

$$\frac{\mathbf{r}_i(t+2\delta t)-\mathbf{r}_i(t)}{2\delta t}=\frac{\mathbf{r}_i(t+\delta t)-\mathbf{r}_i(t)}{\delta t}+\frac{\delta t}{2m_i}\mathbf{f}_i(t+\delta t), \tag{10}$$

which by a rearrangement is the Verlet algorithm,

$$\mathbf{r}_i(t+2\delta t)=2\mathbf{r}_i(t+\delta t)-\mathbf{r}_i(t)+\frac{\delta t^2}{m_i}\mathbf{f}_i(t+\delta t). \tag{11}$$

The position-Verlet algorithm, Eq. (2.22) in Ref. 8, is

$$\mathbf{v}_i(t+\delta t)=\mathbf{v}_i(t)+\frac{\delta t}{m_i}\mathbf{f}_i(\mathbf{r}_i(t+\delta t/2)), \tag{12}$$

$$\mathbf{r}_i(t+\delta t)=\mathbf{r}_i(t)+\frac{\delta t}{2}[\mathbf{v}_i(t)+\mathbf{v}_i(t+\delta t)], \tag{13}$$

and the algorithm differs from the other discrete algorithms by that the forces are calculated at the positions

$$\mathbf{r}_i(t+\delta t/2)=\mathbf{r}_i(t)+\frac{\delta t}{2}\mathbf{v}_i(t) \tag{14}$$

after a half time step in between the positions $\mathbf{r}_i(t)$ and $\mathbf{r}_i(t+\delta t)$. However, Newton's discrete dynamics depends solely on the momenta $m_i\mathbf{v}_i(\tilde{t})$ at the time $\tilde{t}$ where the forces act, so we need to compare different algorithms with changes in velocities and momenta at the time where they change and to change the time when one compares the position-Verlet algorithm with the other reformulations of Newton's discrete algorithm. Doing so,

$$\tilde{t}\equiv t+\delta t/2, \tag{15}$$

and

$$\mathbf{r}_i(\tilde{t})=\mathbf{r}_i(t+\delta t/2), \tag{16}$$

$$\mathbf{v}_i(t)=\mathbf{v}_i(\tilde{t}-\delta t/2), \tag{17}$$

and Eq. (14) is

$$\mathbf{r}_i(\tilde{t})=\mathbf{r}_i(t)+\frac{\delta t}{2}\mathbf{v}_i(t). \tag{18}$$

The change in velocities in Eq. (12) is

$$\mathbf{v}_i(\tilde{t}+\delta t/2)=\mathbf{v}_i(\tilde{t}-\delta t/2)+\frac{\delta t}{m_i}\mathbf{f}_i(\tilde{t}). \tag{19}$$

The change in the discrete positions is obtained by inserting Eq. (18) in Eq. (13),

$$\mathbf{r}_i(\tilde{t}+\delta t/2)=\mathbf{r}_i(\tilde{t})+\frac{\delta t}{2}\mathbf{v}_i(\tilde{t}+\delta t/2), \tag{20}$$

and the velocities and momenta are constant in between the changes at the discrete times, so Eq. (20) is equivalent to

$$\mathbf{r}_i(\tilde{t}+\delta t)=\mathbf{r}_i(\tilde{t})+\delta t\mathbf{v}_i(\tilde{t}+\delta t/2), \tag{21}$$

and Eqs. (19) and (21) are the leapfrog formulation of Newton's discrete algorithm.[9]

MD simulations with Newton's discrete dynamics start at time $t = 0$ with the following two sets of start data:

$\mathbf{r}_i(-\delta t)$ and $\mathbf{r}_i(0)$ (Verlet),

$\mathbf{r}_i(0)$ and $\mathbf{v}_i(-\delta t/2) = (\mathbf{r}_i(0) - \mathbf{r}_i(-\delta t)/\delta t)$ (leapfrog, velocity-Verlet),

and if the position-Verlet algorithm is compared with the other algorithms with their start data for the force actions at time zero, one shall start the position-Verlet algorithm with

$\mathbf{r}_i(\tilde{t}=0)=\mathbf{r}_i(\delta t/2)$ and $\mathbf{v}_i(\tilde{t}-\delta t/2)=\mathbf{v}_i(-\delta t/2)$. However, the simulations in Ref. 1 were started at $x_0 = y_0(\equiv\mathbf{r}_i(-\delta t))$ and $x_1 = y_1(\equiv\mathbf{r}_i(0))$ for both the velocity-Verlet and position-Verlet algorithms.[10]

IV. NEWTON'S DISCRETE DYNAMICS

Newton's discrete dynamics have the same qualities and invariances as his analytic dynamics. It is time reversible, symplectic, and with the exact conservation of momentum, angular momentum, and energy for a conservative system. Newton's third law ensures the first two invariances by which pairs of force actions between two objects cancel. The exact energy conservation, which is not obvious, can be seen by comparing the work done by the forces in time intervals with the corresponding change in the kinetic energy. The proof is given in Refs. 3 and 11 and in the Appendix. The derivation of the discrete energy conservation is in fact in close analogy with the way energy conservation is derived for Newton's analytic dynamics[12] and to the formulation of the first law of thermodynamics.

There is probably a remarkable connection between Newton's analytic and discrete dynamics: the existence of a *shadow Hamiltonian*, H_{shadow}, nearby the Hamiltonian H for the corresponding analytic dynamic. If the analytic dynamics with the shadow Hamiltonian starts at the same phase point at $t = t_0$ as Newton's discrete dynamics, then the discrete points $\mathbf{r}_i(t_n)$ at $t_0, t_0+\delta t, \ldots, t_0+n\delta t, \ldots$ are located on the analytic trajectory $\mathbf{r}_i(t)$ for H_{shadow}.[3,13,14] The existence of H_{shadow} means no qualitative differences exist between the two kinds of dynamics. However, if one starts the force calculation at another position corresponding to the position at a later time for the analytic dynamics, then the discrete dynamics is with another nearby shadow Hamiltonian except for monotonic forces. The linear extrapolation in the position-Verlet dynamics of the positions from $\mathbf{r}(t_n)$ to $\mathbf{r}(t_n+\delta t/2)$ before the forces are calculated is only valid for H_{shadow} for the analytic dynamics from $t = t_0$ for forces which also depend linearly on the positions. For all other force fields, the trajectories will be different. There are small numerical differences between positions obtained by different algorithms for Newton's discrete dynamics due to the accumulation of different round-off errors,[15] which could be removed by performing the simulations with integer arithmetics.[16]

When discussing the qualities of different reformulations of Newton's discrete dynamics, one must compare the dynamics from the same starting point for force actions, as with analytic dynamics. The exact conservation of energy implies that the discrete dynamics are propagating on an energy shell in the microcanonical phase space. The trajectories for starting points with different force actions deviate, and this is also closely analogous to what happens if one starts with different Hamiltonians for analytic dynamics.

Hundreds of thousands of articles with MD, and in all subdisciplines of natural sciences, have been published since Verlet published his MD simulations in 1967. Almost all the simulations are with Newton's discrete algorithm and with the same qualities

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as Newton's analytic dynamics. Feynman gave in 1982 a keynote speech *Simulating Physics with Computers*[17] in which he talked "...about the possibility...that the computer will do exactly the same as nature," and his conclusion was that it is not possible. Newton's discrete dynamics is exact in the same sense as his analytic dynamics, but computer simulations are not exact simulations of real systems dynamics, they contain many approximations. The physical world is not known exactly, and it is far more complex than any simulated systems, and no real systems have been simulated exactly. Hence, more than forty years later, and after hundreds of thousands of computer simulations of the physical system's dynamics, the answer to Feynman's question is still negative. Although it is not possible to simulate the dynamics exactly for any real systems, simulations with Newton's discrete algorithm have been and will be of great use in the natural sciences.

AUTHOR DECLARATIONS

Conflict of Interest

The author has no conflicts to disclose.

Author Contributions

Søren Toxvaerd: Formal analysis (equal); Investigation (equal); Writing – original draft (equal); Writing – review & editing (equal).

DATA AVAILABILITY

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

APPENDIX: THE ENERGY INVARIANCE IN DISCRETE NEWTONIAN DYNAMICS

Newton's classical discrete dynamics between N spherically symmetrical objects with masses $m^N = m_1, m_2, \ldots, m_i, \ldots, m_N$ and positions $\mathbf{r}^N(t) = \mathbf{r}_1(t), \mathbf{r}_2(t), \ldots, \mathbf{r}_i(t), \ldots, \mathbf{r}_N(t)$ is obtained by Eq. (1). Let the force, $\mathbf{f}_i(t)$, on object i be a sum of pairwise forces $\mathbf{f}_{ij}(t)$ between pairs of objects i and j,

$$\mathbf{f}_i(t) = \sum_{j\neq i}^{N} \mathbf{f}_{ij}(t). \tag{A1}$$

Newton's algorithm is a symmetrical time-centered difference, whereby the dynamics is time reversible and symplectic. The conservation of momentum and angular momentum for a conservative system follows directly from Newton's third law for the conservative system with $\mathbf{f}_{ij}(t) = -\mathbf{f}_{ji}(t)$, but the energy invariance is not so obvious.

The energy in analytic dynamics is the sum of potential energy $U(\mathbf{r}^N(t))$ and kinetic energy $K(t)$, and it is a time-invariance for a conservative system. However, the kinetic energy in the discrete dynamics with a force action at time t is not well-defined. Traditionally, one uses Verlet's first-order expression for the velocity at time t,

$$\mathbf{v}_{0,i}(t) = \frac{\mathbf{v}_i(t+\delta/2) + \mathbf{v}_i(t-\delta/2)}{2} = \frac{\mathbf{r}_i(t+\delta/2) - \mathbf{r}_i(t-\delta/2)}{2\delta t}, \tag{A2}$$

obtained by his time symmetric Taylor expansion,[18] and

$$K_0(t) = \sum_i^N \frac{1}{2} m_i \mathbf{v}_{0,i}(t)^2, \tag{A3}$$

$$E_0(t) = U(\mathbf{r}^N(t)) + K_0(t). \tag{A4}$$

The energy $E_0(t)$ obtained by using the approximation equations (A3) and (A4) with $K(t) = K_0(t)$ for the kinetic energy and $U(\mathbf{r}^N(t))$ for the potential energy of analytic dynamics fluctuates with time, although it is constant averaged over long time intervals.[19]

The velocities in Newton's discrete dynamics are, however, constant in between the discrete times with force actions, and the energy invariance can be obtained by dividing time into time intervals $[t_n - \delta t/2, t_n + \delta t/2]$ with force actions at t_n ($n = 1, 2, \ldots$) and with sub-intervals $[t_n - \delta t/2, t_n]$ and $[t_n, t_n + \delta t/2, t]$. The energy invariance, E_{D}, in Newton's discrete dynamics (D) can then be obtained by considering the change in kinetic energy δK_{D}, the work W_{D} done by the forces, and the change in the discrete values of the potential energy $\delta U_{\mathrm{D}} \equiv -W_{\mathrm{D}}$ in a time interval $[t - \delta t/2, t + \delta t/2]$ with $t = t_n$.

The loss in potential energy, $-\delta U_{\mathrm{D}}$, is defined as the work done by the forces at a move of the positions.[12] The discrete force at time t changes the position from $(\mathbf{r}_i(t) + (\mathbf{r}_i(t-\delta t))/2$ at $t - \delta t/2$ to $(\mathbf{r}_i(t+\delta t) + \mathbf{r}_i(t))/2$ at $t + \delta t/2$, and with the change $\delta \mathbf{r}_i$ of the position $\delta \mathbf{r}_i = (\mathbf{r}_i(t+\delta t) - \mathbf{r}_i(t-\delta t))/2$ and with

$$\begin{aligned} -\delta U_{\mathrm{D}} \equiv W_{\mathrm{D}} &= \sum_i^N \mathbf{f}_i(t)\delta \mathbf{r}_i \\ &= \sum_i^N \mathbf{f}_i(t)((\mathbf{r}_i(t+\delta t) - \mathbf{r}_i(t-\delta t))/2. \end{aligned} \tag{A5}$$

By rewriting Eq. (4) as

$$\mathbf{r}_i(t+\delta t) - \mathbf{r}_i(t-\delta t) = 2(\mathbf{r}_i(t) - \mathbf{r}_i(t-\delta t)) + \frac{\delta t^2}{m_i}\mathbf{f}_i(t) \tag{A6}$$

and inserting it in Eq. (A5), one obtains the following expression for the total work in the time interval:

$$-\delta U_{\mathrm{D}} = W_{\mathrm{D}} = \sum_i^N \left[\mathbf{f}_i(t)((\mathbf{r}_i(t) - \mathbf{r}_i(t-\delta t)) + \frac{\delta t^2}{2m_i}\mathbf{f}_i(t)^2\right]. \tag{A7}$$

The mean kinetic energy K_{D} of the discrete dynamics in the time interval $[t - \delta t/2, t + \delta t/2]$ is

$$\begin{aligned} K_{\mathrm{D}} &= \frac{1}{2}\sum_i^N \frac{1}{2} m_i \left[\frac{(\mathbf{r}_i(t+\delta t/2) - \mathbf{r}_i(t))^2}{\delta(t/2)^2} + \frac{(\mathbf{r}_i(t) - \mathbf{r}_i(t-\delta t/2))^2}{\delta(t/2)^2}\right] \\ &= \frac{1}{2}\sum_i^N \frac{1}{2} m_i \left[\frac{(\mathbf{r}_i(t+\delta t) - \mathbf{r}_i(t))^2}{\delta t^2} + \frac{(\mathbf{r}_i(t) - \mathbf{r}_i(t-\delta t))^2}{\delta t^2}\right], \end{aligned} \tag{A8}$$

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and with the change

$$\delta K_{\rm D} = \sum_i^N \frac{1}{2} m_i \left[\frac{(\mathbf{r}_i(t+\delta t) - \mathbf{r}_i(t))^2}{\delta t^2} - \frac{(\mathbf{r}_i(t) - \mathbf{r}_i(t-\delta t))^2}{\delta t^2} \right]. \tag{A9}$$

By rewriting Eq. (4) as

$$\mathbf{r}_i(t+\delta t) - \mathbf{r}_i(t) = \mathbf{r}_i(t) - \mathbf{r}_i(t-\delta t) + \frac{\delta t^2}{m_i}\mathbf{f}_i(t) \tag{A10}$$

and inserting the squared expression for $\mathbf{r}_i(t+\delta t) - \mathbf{r}_i(t)$ in Eq. (A9), the change in kinetic energy is

$$\delta K_{\rm D} = \sum_i^N \left[\mathbf{f}_i(t)(\mathbf{r}_i(t) - \mathbf{r}_i(t-\delta t)) + \frac{\delta t^2}{2m_i}\mathbf{f}_i(t)^2 \right]. \tag{A11}$$

The energy invariance at a discrete change of time from $t - \delta t/2$ to $t + \delta t/2$ in Newton's discrete dynamics is expressed by Eqs. (A7) and (A11) as[3]

$$\delta E_{\rm D} = \delta(U_{\rm D} + K_{\rm D}) = 0. \tag{A12}$$

Unfortunately, the energy E_D in the MD simulations is recorded with systematic errors. The systematic errors are partly caused by the use of the analytical expressions for the potential energies of the discrete forces,[19] by truncating the potentials and not the forces,[20] and partly by using the incorrect expression K_0 for the kinetic energy. However, the errors are typically of a few percent or less.[11]

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