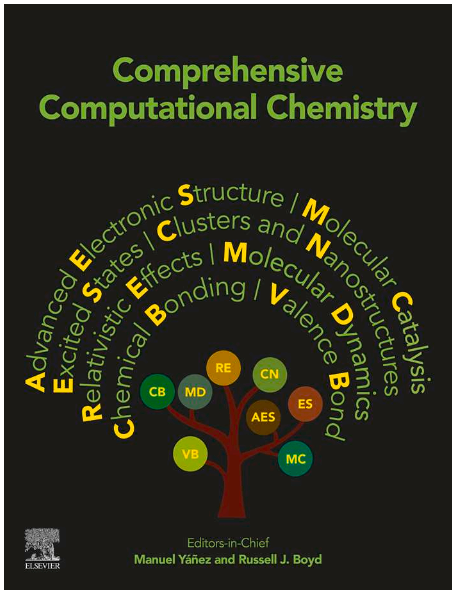

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Discrete Molecular Dynamics

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Abstract

Computer simulation of the time evolution in a classical system is a standard numerical method, used in numerous scientific articles in Natural Science. Almost all the simulations are performed by discrete Molecular Dynamics (MD). The algorithm used in MD was originally formulated by I. Newton at the beginning of his book *Principia*. Newton's discrete dynamics is exact in the same sense as Newton's analytic counterpart Classical Mechanics. Both dynamics are time-reversible, symplectic, and have the same dynamic invariances. There is no qualitative difference between the two kinds of dynamics. This is due to the fact, that there exists a "shadow Hamiltonian" nearby the Hamiltonian $H(\mathbf{q},\mathbf{p})$ for the analytic dynamics, and where its dynamics can be obtained by an asymptotic expansion from $H(\mathbf{q},\mathbf{p})$, and where the positions generated by MD are located on the analytic trajectories for the shadow Hamiltonian.

It is only possible to obtain the solution of Newton's classical differential equations for a few simple systems, but the exact discrete Newtonian dynamics can be obtained for almost all complex classical systems. Some examples are given here: The emergence and evolution of a planetary system. The emergence and evolution of planetary systems with inverse forces. The emergence and evolution of galaxies in the expanding Universe.

The fact that there exist two equally valid formulations of classical dynamics raises the question: What is the classical limit of quantum mechanics? Discrete molecular dynamics is mathematically different from analytic dynamics. The Heisenberg uncertainty between the concurrent values of positions and momenta is an inherent property of the discrete dynamics, but the analytic quantum electrodynamics (QED) is in all manner fully appropriate, and there is a lack of justification for preferring discrete quantum mechanics.

Key Points

- Newton's discrete Classical Mechanics.
- Invariances in Discrete Molecular Dynamics.
- Discrete Molecular Dynamics and discrete Quantum Mechanics.
- Discrete dynamics of planetary systems.
- Discrete dynamics of galaxies in an expanding Universe.

1 Introduction

In Molecular Dynamics (MD) the movements of atoms and molecules are obtained by Newtonian dynamics[1]. The trajectories of atoms and molecules are determined by numerically solving Newton's equations of motion for a system of interacting particles, where forces between the particles and their potential energies are calculated using interatomic potentials or molecular mechanics force fields. The method is widely applied in physics, chemistry, materials science, biophysics, and biochemistry.

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Almost all MD simulations are performed using a simple discrete algorithm, mostly named the *Verlet algorithm* (Appendix A)[2]. But the algorithm also appears under a variety of other names e.g. Leap frog, and in textbooks for MD [3,4] the algorithm is presented as a third-order predictor of the positions of the objects in the system. It was, however, Isaac Newton who first formulated the *Discrete Molecular Dynamics* algorithm, when he in PHILOSOPHIÆ NATURALIS PRINCIPIA MATHEMATICA. (*Principia*)[1] derived his second law for classical mechanics. The discrete algorithm is not only time-reversible and symplectic, but it has also the same dynamic invariances for a conservative system (momentum, angular momentum, and energy) as Newton's analytic dynamics. So the dynamics obtained by the algorithm is exact in the same sense as an exact solution for Newton's analytic Classical Mechanics. Furthermore, the dynamics obtained by Newton's analytic classical mechanics and his discrete molecular dynamics are qualitatively equal, because there exists a *shadow Hamiltonian* nearby the Hamiltonian for the analytic dynamics, and for which the discrete positions are placed on the analytic trajectories for the shadow Hamiltonian[5].

In the chapter on Discrete Molecular Dynamics we first in Section 2 present Newton's formulation of the analytic classical dynamics and the discrete dynamics in *Principia*. The proof that the two complementary formulations of classical dynamics, the analytic dynamics, and the discrete dynamics have the same dynamical invariances, is given in Section 3.1. The connection between the two kinds of dynamics, given by the existence of a shadow Hamiltonian, is given in Section 3.2. The mathematical difference between the two formulations and the connections with discrete quantum mechanics is presented in Section 3.3. In Section 4 there are three examples of exact discrete molecular dynamics for complex systems. The examples are Section 4.1. The emergence and evolution of a planetary system. 4.2. The emergence and evolution of planetary systems with inverse forces. Section 4.3. The emergence and evolution of galaxies in the expanding Universe. The article ends with a conclusion in Section 5.

2 Newtonian Dynamics

Isaac Newton (1643–1727) published PHILOSOPHIÆ NATURALIS PRINCIPIA MATHEMATICA (*Principia*)[1] in 1687, where he formulated the equations for the classical analytic dynamics of objects. *Principia* was reprinted in 1713 with errors of the 1687 edition corrected, and in an improved version in 1726.

2.1 Principia

The first edition of *Principia* contains 510 pages, many with figures and geometrical proofs of the dynamics of a celestial object. *Principia* starts with *DEFINITIONES*, where Newton defines *matter* (mass) *motion* (momentum) and *force*, and in the next section Newton's three laws are postulated in *AXIOMATA sive LEGES MOTUS* on page 12–25, and with detailed explanations in *Corollary I-VI*. The English translation[6] of the Latin formulation of Newton's second law is.

The alteration of motion(momentum) *is ever proportional to the motive force impressed; and is made in the direction of the right line in which that force is impressed.*

Expressed with Newton and Leibniz's algebra the second law for the differential change of the momentum **p** of a mass center due to a force **F** is

$$\frac{d\mathbf{p}(t)}{dt} = \mathbf{F}(\mathbf{r}(t)) \tag{1}$$

After the section with the axioms of his three laws and the corollaries follows a section on pages 26–36, *De MOTU CORPORUM* (OF THE MOTION OF BODIES), where Newton in eleven lemmas treats the connections between infinitesimals and the limiting procedure for analytic curves.

Newton's second law for classical analytic mechanics as well as his discrete dynamics are presented in the succeeding section in *Proposition I* at page 37 and *Proposition VI* at page 44.

2.2 Proposition I and Proposition VI

Newton's classical mechanics with the two *Propositions* starts with the heading *Of the Invention of Centripetal Forces. Proposition I* is a derivation/illustration of Newton's second law and how to obtain the analytic orbit of a mass center by Newton's discrete dynamics. *Proposition I* is the central point in *Principia*, although it is presented as a geometrical proof of some equalities between areas in his discrete dynamics. The text was illustrated by a figure (**Fig. 1**). Newton supplemented the proof in a succeeding proposition, *Proposition VI*, by considering the change of the position of a mass center on an analytic orbit caused by an analytic centripetal force.

The English translation of *Proposition I* is:

PROPOSITION I. Theorem I.

The areas, which revolving bodies describe by radii drawn to an immovable center 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 center, 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

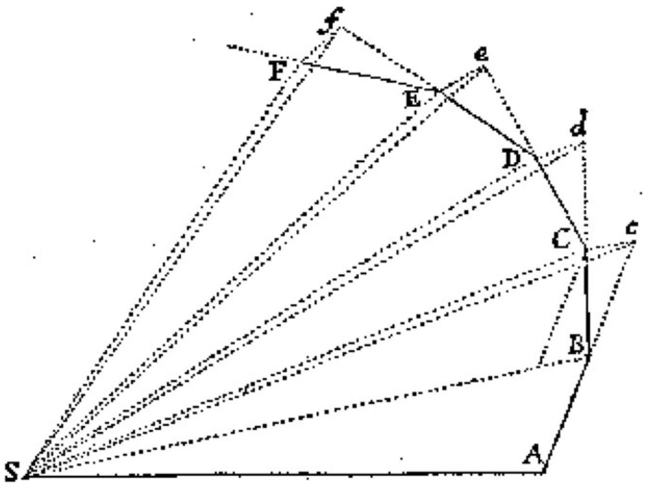

Fig. 1 Newton's figure at *Proposition I* in Principia, with the formulation of the discrete dynamics. The discrete positions are A: $\mathbf{r}(t-\delta t)$; B: $\mathbf{r}(t)$; C: $\mathbf{r}(t+\delta t)$, etc. The deviation cC from the straight line, ABc (Newton's first law) is caused by a force from the position S at time t.

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 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 text can be expressed with Newton's and Leibniz's algebra. The time is changed with a discrete and constant time increment δt. The body with mass m is at the position A: $\mathbf{r}(t-\delta t)$ at time $t-\delta t$, at position B: $\mathbf{r}(t)$ at time t and position C: $\mathbf{r}(t+\delta t)$ at time $t+\delta t$. The momenta $\mathbf{p}(t+\delta t/2)=m(\mathbf{r}(t+\delta t)-\mathbf{r}(t))/\delta t$ and $\mathbf{p}(t-\delta t/2)=m(\mathbf{r}(t)-\mathbf{r}(t-\delta t))/\delta t$ are constant in the time intervals in between the discrete positions. In vector notation *Proposition I* is

$$\vec{BC}=\vec{Bc}+\vec{cC}, \tag{2}$$

and the momentum is changed at B by (**Fig. 1**)

$$m\frac{\mathbf{r}(t+\delta t)-\mathbf{r}(t)}{\delta t}=m\frac{\mathbf{r}(t)-\mathbf{r}(t-\delta t)}{\delta t}+\delta t\mathbf{f}(t). \tag{3}$$

One obtains the Verlet algorithm by a rearrangement of Eq. (3) (see Appendix A)

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

The corresponding "Leap-frog" algorithm is

$$\mathbf{p}(t+\delta t/2)=\mathbf{p}(t-\delta t/2)+\delta t\mathbf{f}(t)$$

$$\mathbf{r}(t+\delta t)=\mathbf{r}(t)+\frac{\delta t}{m}\mathbf{p}(t+\delta t/2). \tag{5}$$

Newton notices that the relation, Eq. (3) for the dynamics holds for any value of δt, and the differential equation for the change in momentum of a mass m on a classical analytic orbit (Eq. (1)) is obtained as the limit $lim_{\delta t\to 0}$ of Eq. (3).

Newton published the two new editions of *Principia* with corrections and additions, but he never changed anything in the formulation of *Proposition I*. There are, however, several things to note about the formulation:

1. The equality of the areas of the triangles is a consequence of the conservation of the angular momentum,[7] and Newton was aware of this fact. In astronomy, it is Kepler's second law for the Solar system, but Newton did not mention this important fact in *Proposition I*.
2. The equality of the areas plays no role in obtaining the analytic dynamics.
3. The formulation is for discrete dynamics. But the discreteness is not only in time, space, and momentum, but also the force acts discrete: *..suppose that a centripetal force acts at once with a great impulse*,...(Notice *at once*).

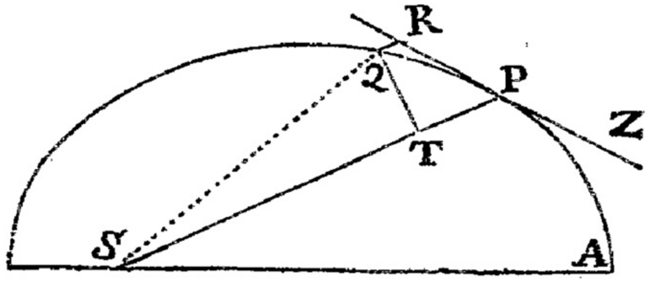

Fig. 2 Figure in *Principia* illustrating *Proposition VI*.

When Newton formulated the second law, he must immediately have realized that his discrete relation Eq. (3) at least explains Kepler's second law. But he did not mention it at the derivation of the second law, nor in his second- or third editions of *Principia*. An explanation for this omission could be, that Newton believed that the exact classical dynamics first is achieved in the analytic limit with continuous time and space. But this is in fact not the case, his discrete dynamics have the same invariances as his analytic dynamics (see Section 3).

Newton returned in *Proposition VI* to the determination of the analytic orbit of an object exposed to a centripetal force. The figure at *Proposition VI* in *Principia* (**Fig. 2**) shows the analytic orbit (APQ) of a mass center continuously attracted by a centripetal force from a force center at S. Newton proved that a tangential deviation $\overrightarrow{RQ}$ from the analytic orbit after a time increment δt is proportional to δt^2 and thus vanishes in the limit $lim_{\delta t \to 0}$.[8]
Proposition I is the central point in *Principia*, although it is presented as a geometrical proof of some equalities between areas in discrete dynamics. *Proposition I* and the relation with *Proposition VI* have played a crucial role in the history of *Principia* and classical mechanics. The prehistory and genesis of *Principia* is given in a recent and excellent review article by Michael Nauenberg.[9] The present article concerns the actual difference between the two formulations of classical dynamics.

In Summary: *Proposition I* is Newton's discrete dynamics and *Proposition VI* is for Newton's Classical Mechanics. As will be shown in the next section both dynamics are exact and the two dynamics are qualitatively equal despite the fact that they mathematically are different.

2.3 The Emergence and History of Proposition I and Proposition VI and Newton's Second Law

Newton submitted in 1684–1685 a draft, *De Muto Corporum* of Principia to Edmond Halley and the Royal Society, and he and Robert Hooke used in the period 1679–1684 the geometrical construction of discrete dynamics to obtain the orbits of mass centers exposed to a discrete centripetal force.[9] The relationship between Newton and Hooke and the emergence of Propostition I and Newton's second law have given rise to an extensive debate right up to our time.[10–15] Robert Hooke has without any doubt inspired Newton according to M. Nauenberg, although Newton not acknowledged Hooke's role in the formulation of Propostition I and Newton's second law.

Propostition I is the algorithm for Discrete Molecular Dynamics, whereas Propostition VI expresses the first-order deviation of the position by a discrete move from the analytic orbit. The equivalence of Propostition I and Propostition VI was debated already shortly after the publication of Principia among leading scientists (e.g. Leibniz and Huygens).[16,17]

Newton's second law is traditionally not given by Eq. (1), but as an equality between the acceleration **a** and force

$$\mathbf{F}(t) = m\mathbf{a}(t) = m\frac{d^2\mathbf{r}(t)}{dt^2}. \tag{6}$$

This algebraic formulation of Newton's second law was, however, first given after Newton's dead 1727 by Euler in 1736[18].

3 Newton's Discrete and Analytic Dynamics

Newton's Classical Mechanics is the exact formulation of the classical analytic dynamics of objects exposed to forces. The dynamics are obtained by solving the second-order differential equations Eq. (6) for N objects. The ''exactness'' is given by some qualities: the analytic dynamics is time reversible, symplectic, and with three invariances for a conservative system of N objects. The total momentum, angular momentum, and energy of a conservative system are conserved. Here we shall first show (Subsection 3.1), that Newton's discrete dynamics, obtained by solving the corresponding discrete equations, Eq. (3), has the same quality and thus is exact in the same sense as his analytic classical mechanics.

The analytic and the discrete dynamics is, however, most likely connected by the existence of a shadow Hamiltonian for analytic dynamics,[5] where the positions obtained by discrete dynamics are on the trajectories for the shadow Hamiltonian. The indication of an existence of a shadow Hamiltonian is given in Subsection 3.2. An existence implies that the classical dynamics obtained by analytic and discrete dynamics, respectively, are qualitatively similar. But the discrete dynamics and the analytic dynamics are, however, mathematically different and fundamentally with different physics. The difference between the two kinds of dynamics and the relation with quantum mechanics is given in Subsection 3.3.

3.1 Newton's Discrete Dynamics

Newton's discrete dynamics for a simple system of N spherically symmetrical objects with masses $m^N \equiv m_1, m_2, .., m_i, .., m_N$ and positions $\mathbf{r}^N(t) \equiv \mathbf{r}^1(t), \mathbf{r}^2(t), .., \mathbf{r}^i(t), ..\mathbf{r}_N(t)$ is obtained by Eq. (3). Let the force, $\mathbf{F}_i$ on object No i be a sum of pairwise forces $\mathbf{f}_{ij}$ between pairs of objects i and j

$$\mathrm{F}_i = \sum_{j \neq i}^{N} \mathrm{f}_{ij}. \tag{7}$$

Newton's discrete dynamics, Eq. (3) is a central difference algorithm and it is time symmetrical, so the discrete dynamics is time reversible and symplectic.[19]

The momentum for a conservative system of the N objects is conserved since (Eq. (3))

$$\sum_i^N m_i \frac{\mathbf{r}_i(t+\delta t/2) - \mathbf{r}_i(t)}{\delta t} = \sum_i^N \mathbf{p}_i(t+\delta t/2) = \tag{8}$$

$$\sum_i^N \mathbf{p}_i(t-\delta t/2) + \delta t \sum_{i,j\neq i}^N \mathbf{f}_{ij}(t) = \sum_i^N \mathbf{p}_i(t-\delta t/2).$$

($\sum_{i,j\neq i}^N \mathbf{f}_{ij}(t) = 0$ with $\mathbf{f}_{ij}(t) = -\mathbf{f}_{ji}(t)$ due to Newton's third law).

The discrete positions and momenta are not known simultaneously. An expression for the angular momentum of the conservative system is

$$\mathbf{L}(t) = \sum_i^N \mathbf{r}_i(t) \times (\mathbf{p}_i(t+\delta t/2) + \mathbf{p}_i(t-\delta t/2))/2$$

$$= \sum_i^N \mathbf{r}_i(t) \times (m_i\mathbf{r}_i(t+\delta t) - m_i\mathbf{r}_i(t-\delta t))/2\delta t. \tag{9}$$

The angular momentum is conserved since (using $\mathbf{r}_i(t) \times (\mathbf{f}_{ij}(t) + \mathbf{f}_{ji}(t)) = 0$, $\mathbf{a} \times \mathbf{a} = 0$, $\mathbf{a} \times \mathbf{b} = -\mathbf{b} \times \mathbf{a}$ and Eq. (4))

$$2\delta t\mathbf{L}(t) = \sum_i^N \mathbf{r}_i(t) \times (m_i\mathbf{r}_i(t+\delta t) - m_i\mathbf{r}_i(t-\delta t))$$

$$= \sum_i^N m_i\mathbf{r}_i(t) \times (2\mathbf{r}_i(t) - 2\mathbf{r}_i(t-\delta t)) = \sum_i^N m_i\mathbf{r}_i(t-\delta t) \times (\mathbf{r}_i(t) + \mathbf{r}_i(t))$$

$$= \sum_i^N m_i\mathbf{r}_i(t-\delta t) \times (\mathbf{r}_i(t) - \mathbf{r}_i(t-2\delta t)) = 2\delta t\mathbf{L}(t-\delta t). \tag{10}$$

The energy in analytic dynamics is the sum of potential energy $U(r^N(t))$ and kinetic energy $K(t)$, and it is an invariance for a conservative system. The kinetic energy in the discrete dynamics is, however, ill-defined since the velocities at time t are not known. Traditionally one uses the expressions

$$\mathbf{v}_i(t) = \frac{\mathbf{r}_i(t+\delta t) - \mathbf{r}_i(t-\delta t)}{2\delta t} \tag{11}$$

$$K_0(t) = \sum_i^N \frac{1}{2} m_i \mathbf{v}_i(t)^2 \tag{12}$$

$$E_0(t) = U(\mathbf{r}^N(t)) + K_0(t) \tag{13}$$

for the velocity, kinetic energy $K(t)$, potential energy $U(\mathbf{r}^N(t))$ and energy $E(t)$ in MD. But the total energy obtained by using Eq. (13) with $K(t) = K_0(t)$ for the kinetic energy fluctuates with time although it remains constant, averaged over long time intervals. This is due to the fundamental quality of Newton's discrete dynamics, where the positions and momenta appear asynchronous.

The energy invariance, E_D in the discrete dynamics can, however, be seen by considering the change in kinetic energy, δK_D, potential energy, δU_D, and the work done by the force in the time interval $[t-\delta t/2, t+\delta t/2]$. The loss in potential energy, $-\delta U_D$ is defined as the work done by the forces at a move of the positions .[20] An expression for the work, W_D done in the time interval by the discrete dynamics from the position $(\mathbf{r}_i(t) + (\mathbf{r}_i(t-\delta t))/2$ at $t-\delta t/2$ to the position $(\mathbf{r}_i(t+\delta t) + \mathbf{r}_i(t))/2$ at $t+\delta t/2$ with the change in position $(\mathbf{r}_i(t+\delta t) - \mathbf{r}_i(t-\delta t))/2$ is [21]

$$-\delta U_D = W_D = \sum_i^N \mathbf{f}_i(t)(\mathbf{r}_i(t+\delta t) - \mathbf{r}_i(t-\delta t))/2. \tag{14}$$

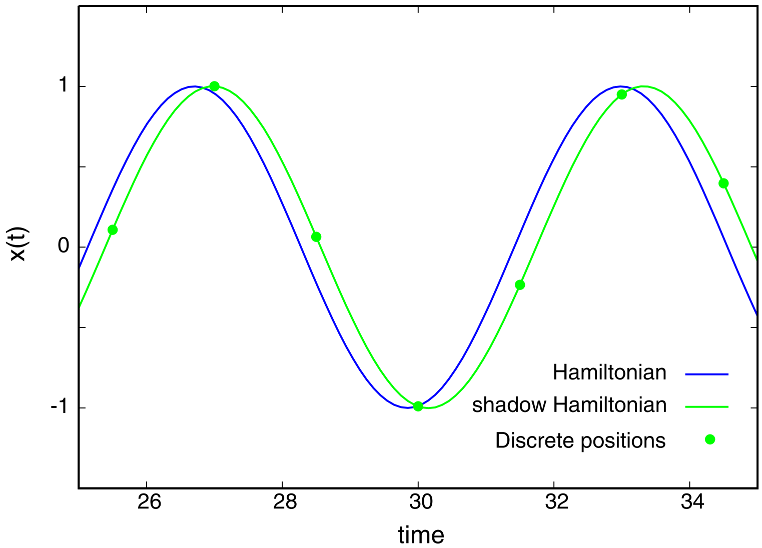

Fig. 3 The dynamics for a one dimensional oscillator. In blue is the analytic curve, Eq. (21), and the green curve is for the shadow Hamiltonian, Eq. (24). The discrete positions with green dots are generated by Eq. (23) for a big time increment with $\approx$ four discrete positions per oscilllations.

By rewriting Eq. (4) to

$$\mathbf{r}_i(t+\delta t) - \mathbf{r}_i(t-\delta t) = 2(\mathbf{r}_i(t) - \mathbf{r}_i(t-\delta t)) + \frac{\delta t^2}{m_i}\mathbf{f}_i(t), \tag{15}$$

and inserting in Eq. (14) one obtains an expression for the total work in the time interval

$$-\delta U_D = W_D = \sum_i^N \left[(\mathbf{r}_i(t) - \mathbf{r}_i(t-\delta t))\mathbf{f}_i(t) + \frac{\delta t^2}{2m_i}\mathbf{f}_i(t)^2\right]. \tag{16}$$

The change in kinetic energy in the time interval $[t-\delta t/2, t+\delta t/2]$ is

$$\delta K_D = \sum_i^N \frac{1}{2} m_i \left[\frac{(\mathbf{r}_i(t+\delta t) - \mathbf{r}_i(t))^2}{\delta t^2} - \frac{(\mathbf{r}_i(t) - \mathbf{r}_i(t-\delta t))^2}{\delta t^2}\right]. \tag{17}$$

(In time intervals without forces the dynamics follow Newton's first law.) By rewriting Eq. (4) to

$$\mathbf{r}_i(t+\delta t) - \mathbf{r}_i(t) = \mathbf{r}_i(t) - \mathbf{r}_i(t-\delta t) + \frac{\delta t^2}{m_i}\mathbf{f}_i(t) \tag{18}$$

and inserting the squared expression for $\mathbf{r}_i(t+\delta t) - \mathbf{r}_i(t)$ in Eq. (17), the change in kinetic energy is

$$\delta K_D = \sum_i^N \left[(\mathbf{r}_i(t) - \mathbf{r}_i(t-\delta t))\mathbf{f}_i(t) + \frac{\delta t^2}{2m_i}\mathbf{f}_i(t)^2\right]. \tag{19}$$

The energy invariance in Newton's discrete dynamics is expressed by Eqn. (16), and Eq. (19) as[21]

$$\delta E_D = \delta U_D + \delta K_D = 0, \tag{20}$$

where the difference in energies, $\sum_i^N \frac{\delta t^2}{2m_i}\mathbf{f}_i(t)^2$, between the analytic and the discrete energies at time t only depends on the square of the forces and time increment.

In summary: Newton's discrete dynamics is time reversible and symplectic, and the discrete dynamics for a conservative system has the same invariances as the corresponding analytic dynamics. Newton's discrete dynamics is exact in the same sense as Classical Mechanics.

3.2 The Connection Between the Discrete and the Analytic Dynamics

The classical analytic dynamics, determined by the second order differential equation Eq.(6) can only be solved for a few systems, e.g., a harmonic oscillator

$$x(t) = A\sin(\omega t). \tag{21}$$

The corresponding difference equation for a discrete harmonic oscillator can, however, also be solved and the solution reveals the existence of a *shadow Hamiltonian*, $\tilde{H}$.[5] The discrete positions are located on a harmonic curve

$$x(t) = \tilde{A}\sin(\tilde{\omega} t). \tag{22}$$

The solution in[5] was obtained directly from the discrete points and without any use of an expansion of an analytic Hamiltonian $H(\mathbf{r},\mathbf{p})$ by noticing that if the discrete dynamics

$$x(t+\delta t)=2x(t)-x(t-\delta t)-\omega^2\delta t^2 x(t)=\alpha x(t)-x(t-\delta t), \tag{23}$$

with $\alpha=2-\omega^2\delta t^2$ is started with positions $x(0)=0$ and $x(\delta t)=A\sin(\omega\delta t)$, then the generated discrete points lie on a harmonic curve Eq. (22), with the frequency $\tilde{\omega}$ and amplitude $\tilde{A}$ given by

$$\tilde{\omega}=\cos^{-1}\left(1-\frac{(\omega\delta t)^2}{2}\right)/\delta t$$

$$\tilde{A}=\frac{A\sin(\omega\delta t)}{\sin(\tilde{\omega}}\delta t), \tag{24}$$

i.e. with the harmonic shadow Hamiltonian, $\tilde{H}(\tilde{\omega})$ with $x(t)=\tilde{A}sin(\tilde{\omega}t)$ and the energy $\tilde{E}=(\tilde{A}\tilde{\omega})^2/2$. Eq. (24) sets, however, a limit to the discrete dynamics, given by δt. The discrete dynamics are stable for

$$\left|1-\frac{\omega^2\delta t_{max}^2}{2}\right|\leq 1. \tag{25}$$

or

$$\delta t_{max}\leq\frac{2}{\omega}. \tag{26}$$

Fig. 3 shows the positions of the one-dimensional harmonic oscillations in the time interval $t\in[25,35]$ after $\approx$ six oscillations from $x(0)=0$ at the start at $t=0$. The solution is for $A=\omega=1$ and a big time increment, for which $\tilde{A}=1.00119889$ and $\tilde{\omega}=0.98983513$, and the energies are $E=0.5$ and $\tilde{E}=0.49106$, respectively. The discrete positions (green dots) are obtained by the discrete dynamics Eq. (23), and the green curve is $x(t)=\tilde{A}sin(\tilde{\omega})$ for the shadow Hamiltonian $\tilde{H}(\tilde{\omega})$. The blue curve is the harmonic solution Eq. (21). The discrete dynamics only generates $\approx$ 4 positions per oscillation.

The existence of a shadow Hamiltonian is a general property of discrete symplectic dynamics. Mathematical investigations have established[22–25] that, if a discrete algorithm is symplectic, then there exists a shadow Hamiltonian, $\tilde{H}(\mathbf{r},\mathbf{p})$ for sufficient small δt such that the discrete positions $\mathbf{r}(n\delta t)$, for an object, generated by the symplectic algorithm, lie on the analytic trajectory for the object obtained by $\tilde{H}(\mathbf{r}(t),\mathbf{p}(t))$.

Newton's discrete algorithm, Eq. (3), is symplectic and the first non-trivial term in the asymptotic expansion was obtained for the LJ system in.[5] The term was obtained from consecutive sets of positions using the expression obtained from the expansion of H for a one-dimensional harmonic oscillator. Ref. 26 gives the general expression for the first term in the expansion using the method of modified equations derived in Refs. 22–25. The Hessian, $\partial^2U(\mathbf{r}^N)/\partial\mathbf{r}^2$, of the potential energy function $U(\mathbf{r}^N)$ is denoted by $\mathbf{J}$, the velocities of the N particles by $\mathbf{v}^N\equiv(\mathbf{v}_1,...,\mathbf{v}_N)$, and the force at positions $\mathbf{r}^N$ by $\mathbf{F}^N(\mathbf{r}^N)\equiv(\mathbf{f}_1(r^N),...,\mathbf{f}_N(\mathbf{r}^N))$. Using Eq. (13) for v^N, the first term in the asymptotic expansion at the n'th time step can be expressed as [27]

$$\begin{aligned}\tilde{E}(t_n)&\simeq E_0(t)+\frac{\delta t^2}{12}(\mathbf{v}_n^N)^T\mathbf{J}(\mathbf{r}_n^N)\mathbf{v}_n^N-\frac{\delta t^2}{24m}\mathbf{F}_n^N(\mathbf{r}_n^N)^2\\&=E_0(t)+E_1(t)\end{aligned} \tag{27}$$

for the the energy, E_0+E_1, at time $t=n\delta t$. The zero-order term is the discrete energy E_0 (Eq. (13)) used in MD. The detailed expression for the first order term E_1 in the asymptotic expansion for a system with pair interactions is given in.[27]

The existence of a shadow Hamiltonian for classical dynamics can be demonstrated by MD for a system of particles with Lennard-Jones (LJ) pair interactions

$$u(r_{ij})=4\epsilon\left[\left(r_{ij}/\sigma\right)^{-12}-\left(r_{ij}/\sigma\right)^{-6}\right]. \tag{28}$$

The energy conservation in discrete dynamics for a system of N particles with LJ interactions is shown in **Fig. 4**. The energies are for a system of $N=2048$ particles in a liquid state with the number density $\rho=0.80$ and temperature $T=1.00$ (for units of length, time, and energy in MD see[28]). The energies in the figure are for 150 time steps with $\delta t=$ 0.005 and shown from a configuration (at $t=t_0$) where $E_0(t_0)\approx E_0(t_0)+E_1(t_0)$. The energy estimate $E_0(t)$ used in almost all MD simulations is shown in blue. The first order expression Eq. (27)[5,27]) is shown in green, and the constant energy $\tilde{E}(t)=\tilde{E}(t_0)+\Sigma_n\delta E(n\delta t)$ of the shadow Hamiltonian for the discrete dynamics[21] is with red. (The shadow energy $\tilde{E}(t_0)$ is not known, and $\tilde{E}(t)$ in the figure is $E_0(t_0)+E_1(t_0)+\delta E(n\delta t)$ with $\delta E(n\delta t)$ given by Eqs. (14) and (17)). The first order correction $E_1(t)$ of the energy decreases the fluctuations in the energy with a factor of hundred[5,27] and the difference $\delta(\tilde{E}(t)-(E_0(t)+E_1(t)))$ from the energies of the higher-order term in the expansion can not be seen in the figure but is visible in the inset.

Simulations for different state points and time increments indicate, that the energy at the asymptotic expansion rapidly converges towards $\tilde{E}(\rho,T)$ for time increments used in MD.[27] In **Fig. 5** the means of the energy amplitudes $<|E(t_n)-<E(t_n)>|>$ in the LJ system, (the amplitudes for $\delta t=0.005$ are shown in **Fig. 4**) are plotted as a function of the time increment δt. The green dots are the amplitudes for $E(t_n)=E_0(t_n)+E_1(t_n)$ and the blue dots are for $E(t_n)=E_0(t_n)$. Systems of liquids of LJ particles or mass units in molecules for e.g. carbon atoms in organic molecules have "vibration times" of the order $\approx 10^{-12}$ sec, and the maximum

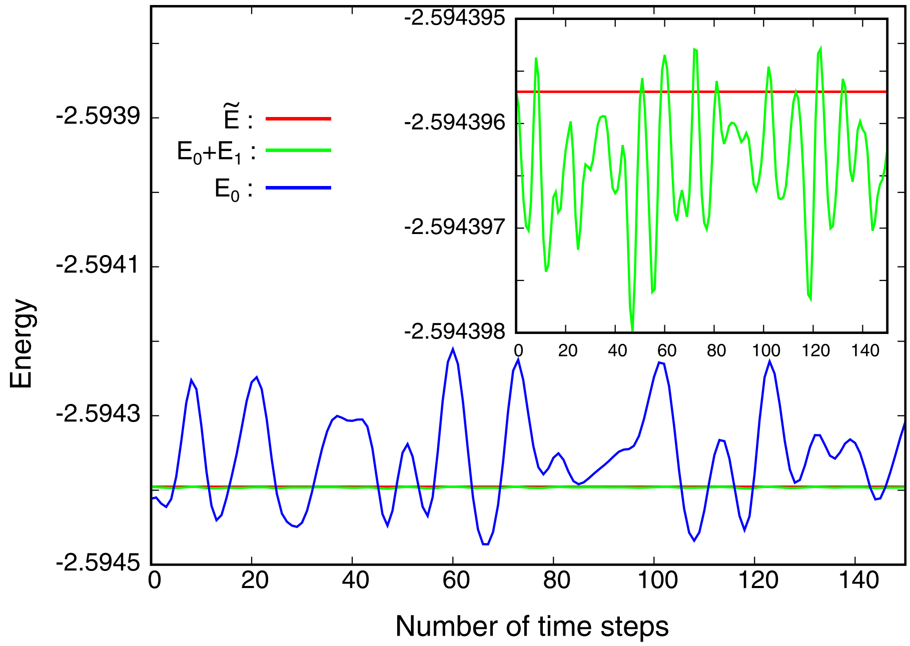

Fig. 4 Energies at 150 time steps with the discrete dynamics for a system of Lennard-Jones particles. The traditional energy $E_0(t)$ used in MD simulations is shown in blue. The first order expression for the shadow energy $E_0(t)+E_1(t)$, Eq. (27), is shown in green, and the constant shadow energy energy $\tilde{E}(t_0)+\Sigma_n\delta E(n\delta t)$, Eq. (20), is shown with red. The energies $E_0(t)+E_1(t)$ and $\tilde{E}(t_0)+\delta E(t)$ are enlarged in the inset.

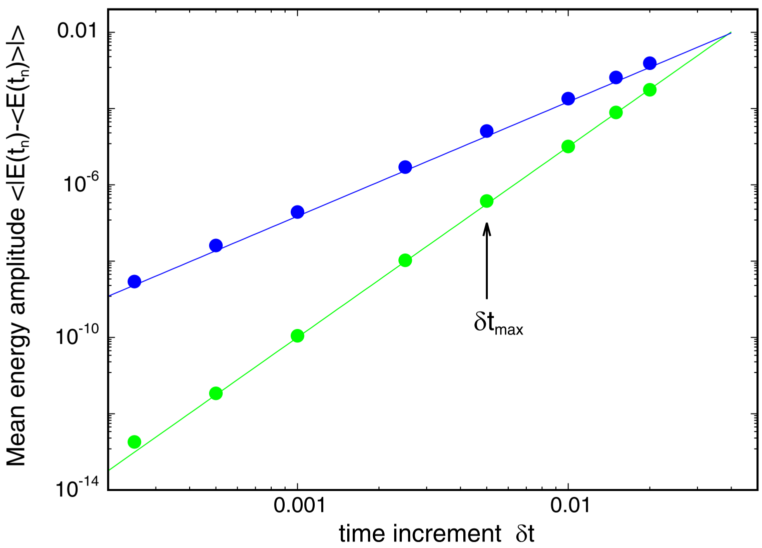

Fig. 5 The mean amplitudes, $<|E(t_n)-<E(t_n)>|>$, of the energy in a LJ system at $\rho=0.80$ and $T=1.00$ as a function of the time-increment δt in a $log-log$ plot[29]. The green dots are for the first order estimate, Eq. (27), of the shadow energy E_0+E_1 and blue dots are for E_0. The lines through the green and blue dots have slopes of five and three, respectively. $\delta t_{max}=0.005$ is used in the first discrete Newtonian MD simulation in 1967 by L. Verlet[2].

time increment used in these MD simulations are $\delta t_{max} \approx 0.005 \approx 10^{-14}$ sec, used by L. Verlet in 1967 in the first discrete Newtonian MD[2]. It corresponds to of the order a hundred discrete positions for a typical "vibration"; but most MD simulations are, however, with smaller time increments. The data in **Figs. 4** and **5** indicate that the asymptotic expansion is rapidly converging for these values of the time increment and that the energies are well determined by $E_0(t_n)+E_1(t_n)$ as well as by $E_0(t_n)$.

In summary: There exists most likely a shadow Hamiltonian for discrete molecular dynamics, and the asymptotic expansion is rapidly converging for the time increments used in discrete molecular dynamics. The existence of a shadow Hamiltonian implies that there is no qualitative difference between the analytic Classical Mechanics and the discrete Newtonian dynamics. The two kinds of dynamics are, however, mathematically different (see next subsection).

3.3 The Difference Between Classical Mechanics and Discrete Newtonian Dynamics

The dynamics obtained by Classical Mechanics or discrete Newtonian dynamics are qualitatively equal, despite the fact that they mathematically are fundamentally different. The difference between the two dynamics can perhaps best be seen by rewriting *Proposition I*

$$\mathbf{r}(t+\delta t)-\mathbf{r}(t)=\mathbf{r}(t)-\mathbf{r}(t-\delta t)+\delta t^2\mathbf{f}(\mathbf{r}(t))/m, \tag{29}$$

and

$$\mathbf{r}(t+\delta t)=\mathbf{r}(t)+\delta t(\mathbf{r}(t+\delta t)-\mathbf{r}(t)) \tag{30}$$

where the new position $\mathbf{r}(t+\delta t)$ is obtained from the old position $\mathbf{r}(t)$ by that the difference with the previous positions is adjusted by a force quantum $\delta t^2\mathbf{f}(\mathbf{r}(t))/m$. Or as Newton expressed it: *..suppose that a centripetal force acts at once with a great impulse*. The time and space are discretized in *Proposition I* and connected by a quant of the square of the time quant and the ratio between the force and the mass.

It is only the positions, the time, and the force that appear in the dynamics, Eqs. (29) and (30). *The momenta are not dynamic variables in discrete dynamics*.

Although Newton starts *Principia* with his first law for momenta and refers to the law in the formulation of *Proposition I*, the momenta do not enter into the dynamics, but they play a role as a ’’bookkeeping" registration during the time evolution. In Newton’s analytic dynamics, the momenta are, however, also dynamic variables, and due to this fact, the analytic dynamics can be reformulated to Lagrangian mechanics.[30]

Classical Mechanics is the analytic limit dynamics of nonrelativistic quantum mechanics,[31] and the question is: Could the discrete Newtonian dynamics be a corresponding limit dynamics of discrete nonrelativistic quantum mechanics? Noble Laureate T. D. Lee wrote in 1983 a paper entitled, "Can Time Be a Discrete Dynamical Variable?".[32] The article led to a series of publications by Lee and collaborators on the formulation of fundamental dynamics in terms of difference equations, but with exact invariance under continuous groups of translational and rotational transformations. Quoting Lee,[33] he "wish to explore an alternative point of view: that physics should be formulated in terms of difference equations and that these difference equations could exhibit all the desirable symmetry properties and conservation laws". Lee’s analysis covers not only classical mechanics,[32] but also non-relativistic quantum mechanics and relativistic quantum field theory,[34] and Gauge theory and Lattice Gravity.[33] Lee’s discrete dynamics is obtained by treating only the positions but not the momenta as discrete dynamical variables, as is the case in discrete Newtonian dynamics.

The discrete nonrelativistic quantum mechanics is obtained by Lee using Feynman’s path integration formalism, but for discrete positions and a corresponding discrete action,

$$\mathcal{A}_D=\sum_{n=1}^{\mathcal{N}+1}(t_n-t_{n-1})\left[\frac{1}{2}\frac{(\mathbf{r}_n^N-\mathbf{r}_{n-1}^N)^2}{(t_n-t_{n-1})^2}+\overline{V(n)}\right], \tag{31}$$

where $\mathbf{r}_{\mathcal{N}+1}^N$ is the end-positions at time $t_{\mathcal{N}+1}$ and the minimum of $\mathcal{A}_D$ determines the classical path. According to Lee, the action is a sum over products of time increments and energies with "kinetic energies" and $\overline{V(n)}$, for the average of "potential energy" in the time intervals $[t_{n-1}, t_n]$. In discrete Newtonian dynamics, it is the action sum over products of time intervals and with the classical limit energies given by the shadow Hamiltonians in the time intervals

$$\tilde{E}(t)=\left[\frac{1}{2}\frac{(\mathbf{r}_n^N-\mathbf{r}_{n-1}^N)^2}{(t_n-t_{n-1})^2}+\overline{V(n)}\right]. \tag{32}$$

In Lee’s formulation of discrete mechanics, "there is a *fundamental length* l or time t_l (in natural units). Given any time interval $T=t_f-t_0$, the total number $\mathcal{N}$ of discrete points that define the trajectory is given by the integer nearest T/l." The classical discrete trajectory is the classical limit path for discrete quantum mechanics with $\delta t=t_l$, as the classical analytic trajectory is for traditional quantum mechanics. There is, however, one important difference between analytic and discrete dynamics. The momenta *for all the paths* in the discrete quantum dynamics aŕe not dynamic variables. They are obtained by a difference between discrete sets of positions and they are all *asynchronous* with the positions. So the Heisenberg uncertainty principle is a trivial consequence of Lee’s discrete quantum dynamics. The fundamental length and time in quantum electrodynamics (QED) are the Planck length $l_P\approx 1.6\times 10^{-35}$m and Planck time $t_P\approx 5.4\times 10^{-44}$ s,[35] and they are immensely smaller than the length unit and time increments used in MD to generate the classical discrete dynamics. But the analogy implies that the discrete Newtonian dynamics is the classical limit of the Lee’s discrete non-relativistic quantum mechanics.

In Newton’s discrete dynamics, the contributions from the forces are also discretized. T. Regge and R. M. Williams have analyzed the dynamical implications of a discretized gravitational force[36].

In summary: Newton’s discrete and analytic dynamics are mathematically different. The fact that the positions and momenta are asynchronous implies, that it could be that discrete dynamics in principle is the correct classical limit dynamics of a discrete quantum dynamics. But the energy difference, Eq. (20), between the two kinds of classical dynamics are, however, proportional to t_P^2 and incredibly small, and since there is no qualitative difference between the two classical dynamics, there is a lack of justification for preferring the discrete quantum mechanics.

4 Discrete Molecular Dynamics

Almost all MD simulations are performed with Newton's discrete algorithm, Eq. (3). The MD algorithm is, however, hardly mentioned in the simulations. The simulations are stable at the time propagation, and the focus in the articles is on the physics of the MD systems rather that on the computational method. And with good reason because the algorithm offers an exact time propagation of the MD models provided that the time step is not too big so that the asymptotic expansion no longer converges. The data of the simulated models depends primarily on the quality of the expressions for the forces and the molecular mechanics force fields used in the simulations, and not on the discrete dynamics.

There are, however, some factors that can affect the exactness of the time propagation. The positions are in the best cases given in ''double-precision" with the order $\approx 10^{-16}$ relative accuracy, and the round-off errors in long simulations generate cumulative errors in the numerical integration. The accumulations will, however, normally not affect the results obtained by the simulation,[37] and the round-off errors can optionally be avoided by performing the MD simulation with integer arithmetic.[38]

Most MD simulations contain approximations of the forces and the size of the systems with the result, that the simulations no longer are exact, but have to be adjusted e.g. for energy conservation. The range of the interactions is often set to zero at a sufficiently large distance, and this approximation causes a small drift in the energy. The interactions are usually restricted at these large distances by a ''cut and shift" of the potentials, but since it is the forces that enter into the algorithm it is much better to cut and shift the range of the forces.[39] A cut in the potentials introduces new ''Delta function" forces in the systems and they perform a work on the system according to Eq. (16). This will affect the energy conservation and show up as a small drift in the temperatures of the systems unless one uses a thermostat, which one, however, usually do.

The MD computational method is described in.[3,4] This section is ended by showing some examples where the exactness of the dynamics is used to obtain the exact dynamics of complex systems. The differential equation(s) for the analytic dynamics in Classical Mechanics can only be solved for a few simple systems, but the discrete Newtonian dynamics with the algorithm, Eq. (3), offers a general method for obtaining exact discrete solutions, e.g. regular solutions of complex systems of celestial objects. Three examples are given here: 4.1 The emergence and evolution of planetary systems. 4.2 The emergence and evolution of planetary systems with inverse forces. 4.3 The emergence and evolution of galaxies in the expanding Universe.

4.1 The Emergence and Evolution of a Planetary System

According to Newton's shell theorem[40] the force, $\mathbf{F}_i$, on a spherically symmetrical object i with mass m_i is a sum over the forces, $\mathbf{f}(r_{ij})$, caused by the other spherically symmetrical objects j with mass m_j, and it is solely given by their center of mass distance r_{ij} to i

$$\mathbf{F}_i(r_{ij}) = \sum_{j \neq i}^{N} \mathbf{f}(r_{ij}) = -\sum_{j \neq i}^{N} \frac{G m_i m_j}{r_{ij}^2} \hat{\mathbf{r}}_{ij}. \tag{33}$$

Newton's discrete algorithm can be extended to include a ''perfect" fusion of mass objects.[41] Let all the spherically symmetrical objects have the same (reduced) number density $\rho = (\pi/6)^{-1}$ by which the diameter σ_i of the spherical object i is

$$\sigma_i = m_i^{1/3} \tag{34}$$

and the collision diameter

$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2}. \tag{35}$$

If the distance $r_{ij}(t)$ at time t between two objects is less than σ_{ij} the two objects merge into one spherical symmetrical object with mass

$$m_\alpha = m_i + m_j, \tag{36}$$

and diameter

$$\sigma_\alpha = (m_\alpha)^{1/3}, \tag{37}$$

and with the new object α at the position

$$\mathbf{r}_\alpha = \frac{m_i}{m_\alpha}\mathbf{r}_i + \frac{m_j}{m_\alpha}\mathbf{r}_j, \tag{38}$$

at the center of mass of the two objects before the fusion. (The object α at the center of mass of the two merged objects i and j might occasionally be near another object k by which more objects merge, but after the same laws.) Let the center of mass of the system of the N objects be at the origin, i.e.

$$\Sigma_k m_k \mathbf{r}_k(t) = \mathbf{0}. \tag{39}$$

The momenta of the objects in the discrete dynamics just before the fusion are $\mathbf{p}^N(t - \delta t/2)$ and the total momentum of the system is conserved at the fusion if

$$\mathbf{v}_\alpha(t - \delta t/2) = \frac{m_i}{m_\alpha}\mathbf{v}_i(t - \delta t/2) + \frac{m_j}{m_\alpha}\mathbf{v}_j(t - \delta t/2), \tag{40}$$

which determines the velocity $\mathbf{v}_\alpha(t - \delta t/2)$ of the merged object.

The invariances in the classical Newtonian dynamics are for a conservative system with Newton's third law, i.e with

$$\mathbf{f}_{kl}(t) = -\mathbf{f}_{lk}(t) \tag{41}$$

for the forces between two objects k and l, and with no external forces. An object k's forces with i and j before the fusion are $\mathbf{f}_{ik}(t)$ and $\mathbf{f}_{jk}(t)$, and these forces must be replaced by calculating the force $\mathbf{f}_{\alpha k}(\mathbf{r}_{\alpha k}(t))$. The total force after the fusion is zero due to Newton's third law for a conservative system with the forces $\mathbf{f}_{\alpha k} = -\mathbf{f}_{k\alpha}$ between pairs of objects, and the total momentum

$$\begin{aligned}\Sigma_k \mathbf{p}_k(t_n + \delta t/2) &= \Sigma_k \mathbf{p}_k(t_n - \delta t/2) + \delta t \Sigma_k \mathbf{f}_k(t_n) \\ &= \Sigma_k \mathbf{p}_k(t_n - \delta t/2),\end{aligned} \tag{42}$$

and the position of the center of mass, Eq. (39), is conserved for the discrete dynamics with fusion.

The determination of the position, $\mathbf{r}_\alpha(t)$, and the velocity, $\mathbf{v}_\alpha(t-\delta t/2)$, of the new object from the requirement of conserved center of mass and conserved momentum determines the discrete dynamics of the $N-1$ objects.

The total angular momentum is also not affected by the fusion. The angular momentum of the system of spherically symmetrical objects consist of two terms

$$\mathbf{L}(t) = \mathbf{L}_G(t) + \mathbf{L}_S(t) \tag{43}$$

where $\mathbf{L}_G(t)$ is the angular momentum of the objects in their orbits, due to the dynamics obtained from the gravitational (G) forces between their centers of mass, and $\mathbf{L}_S(t)$ is the angular momentum due to the spin (S) of the objects. Without fusion $\mathbf{L}_G(t)$ is conserved for Newtons discrete dynamics, Eq. (10). $\mathbf{L}_S(t)$ is, however, also conserved according to the shell theorem,[40] where Newton proves that no net gravitational force is exerted by a shell on any object inside, regardless of the object's location within the uniform shell, by which the spin of the object is not affected by any force and is therefore constant. But at a fusion $\mathbf{L}_G$ changes by

$$\delta\mathbf{L}_G(t) = \mathbf{r}_\alpha(t) \times m_\alpha \mathbf{v}_\alpha(t-\delta t/2) - \mathbf{r}_i(t) \times m_i \mathbf{v}_i(t-\delta t/2) - \mathbf{r}_j(t) \times m_j \mathbf{v}_j(t-\delta t/2). \tag{44}$$

and $\mathbf{L}_S$ changes by

$$\begin{aligned}\delta\mathbf{L}_S(t) &= (\mathbf{r}_i(t) - \mathbf{r}_\alpha(t)) \times m_i \mathbf{v}_i(t-\delta t/2) + (\mathbf{r}_j(t) - \mathbf{r}_\alpha(t)) \times m_j \mathbf{v}_j(t-\delta t/2) \\ &= \mathbf{r}_i(t) \times m_i \mathbf{v}_i(t-\delta t/2) + \mathbf{r}_j(t) \times m_j v_j(t-\delta t/2) - \mathbf{r}_\alpha(t) \times m_\alpha \mathbf{v}_\alpha(t-\delta t/2) \\ &= -\delta\mathbf{L}_G(t).\end{aligned} \tag{45}$$

So without fusion, the angular momenta $\mathbf{L}_S(t)$ and $\mathbf{L}_G(t)$ with Newton's discrete dynamics are conserved separately, and at a fusion, the total angular momentum is still conserved but with an exchange of angular momentum with $\delta\mathbf{L}_S(t) = -\delta\mathbf{L}_G(t)$.

The exact classical discrete dynamics with a fusion of colliding objects can be used to explore the self-assembly at the emergence of planetary systems and to investigate the stability of a planetary system. The emergence and stability of planetary systems were investigated in,[41] and **Fig. 6** shows the orbits of the four innermost planets at the end of the simulation in a planetary system with 21 planets in regular orbits around a heavy gravity center. The emergence of the simple planetary system was obtained from thousand objects relatively close to each other and with a Maxwell Boltzmann distribution of the velocities and with the dynamics given by the Eqs. (5),(34)-(38) and (40). For the setup and details see,[41].

4.2 The Emergence and Evolution of Planetary Systems With Inverse Forces

Newton was aware that the extension of an object can affect the gravitational force between two objects, and in *Theorem XXXI* in *Principia*[40] he solved this problem for the gravitational inverse square forces (ISF), Eq. (33), between spherically symmetrical objects. Newton's

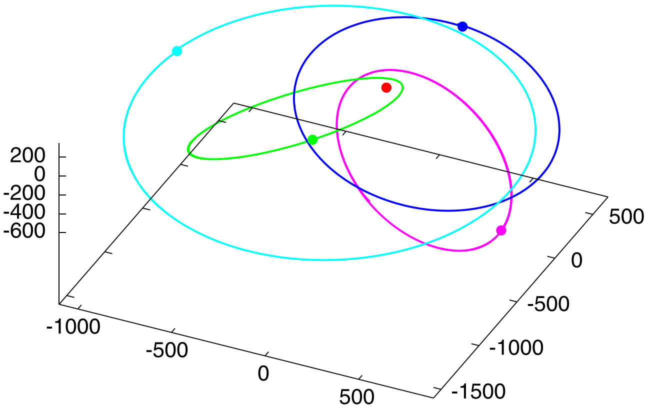

Fig. 6 The regular orbits of the four innermost planets in a planetary system. The planetary system contains 21 planets in regular orbits[41]. The orbit times (MD time unit) t_{orbit} and eccentricity ϵ are: light blue: $t_{orbit} = 818$, $\epsilon = 0.835$; green: $t_{orbit} = 300$, $\epsilon = 0.327$; blue $t_{orbit} = 463$, $\epsilon = 0.586$; magenta $t_{orbit} = 313$, $\epsilon = 0.768$. The green planet has circulated more than four thousand times around the Sun (red).

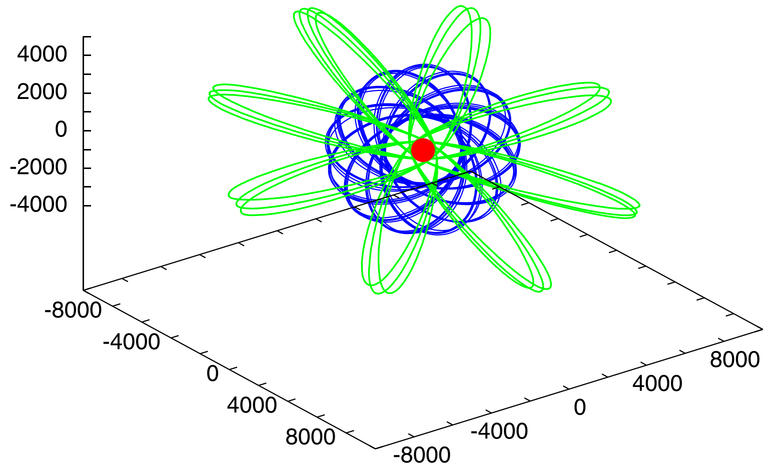

Fig. 7 Regular orbits for two of the 38 planets in a planetary system with inverse force attraction[42]. The orbits with green are for twenty-five ''revolving orbits'' of one of the planets in the system, and the orbits in blue are correspondingly sixty-three revolving orbits of another planet. With red is the (enlarged) center of mass of the planetary system.

theorem is, however, only valid for ISF. But for inverse gravitational forces (IF) and inverse cubic gravitational forces (ICF) one can expand the contributions in powers of the ratio σ/r between the diameters of the objects and their mutual distance. The result is.[42]

For the IF gravitational forces:

$$\mathbf{f}_{ij}(r_{ij}) \simeq -\frac{G_1 m_i m_j}{r_{ij}}\left(1 - \frac{\sigma_i^2 + \sigma_j^2}{5r_{ij}^2}\right)\hat{\mathbf{r}}_{ij} + \mathcal{O}(r_{ij}^{-4}) \tag{46}$$

For ISF one obtains the usual expression for the gravitational forces which do not depend on the extensions of the two spherically symmetrical objects and is given by Eq. (33).

For the ICF gravitational forces:

$$\mathbf{f}_{ij}(r_{ij}) = -\frac{G_3 m_i m_j}{r_{ij}^3}\left(1 + \frac{2\sigma_i^2 + 2\sigma_j^2}{5r_{ij}^2}\right)\hat{\mathbf{r}}_{ij} + \mathcal{O}(r_{ij}^{-6}). \tag{47}$$

Planetary systems with IF attractions were created in the same way as for the usual ISF attractions,[42] and the systems were even easier to create. There is, however, a remarkable difference between the regular orbit in an ordinary planetary system and the regular orbits of objects in a planetary system with IF forces. Whereas the orbits of the planets in e.g. our Solar system are regular with elliptical orbits, the orbits in an IF planetary system is what Newton probably would have called ''revolving orbits". An example is shown in **Fig. 7**. The figure shows the orbits at the end of the simulation ($t = 2.5 \times 10^6$) of two of the planets in a planetary system with 38 planets. All the planets have performed many orbits around the common center of gravity (the ''Sun" enlarged and with red in the figure), but none of the orbits were elliptical. They showed different kinds of revolving orbits where the ''orientation" of the regular orbit was changed when the planet passed the ''Perihelion". The orientation of the ''principal axis" was then changed with $\approx$ fractions of 2π. For details see.[42]

The Moon exhibits apsidal precession, which is called Saroscyclus and it has been known since ancient times. Newton shows in Proposition 43–45 in *Principia*, that the added force on a single object from a fixed mass center which can cause its apsidal precession must be a central force between the planet and a mass point fixed in space (the Sun). In Proposition 44 he shows that an inverse-cube force (ICF) might cause the revolving orbits, and in Proposition 45 Newton extended his theorem to arbitrary central forces by assuming that the particle moved in a nearly circular orbit.[8] The Moon's apsidal precession is explained by flattering by the rotating Earth with tide waves, which causes an ICF on the Moon. For Newton's analysis of the Moon's apsidal precession see.[43]

It was, however, not possible to obtain stable regular orbits for systems with pure ICF, but systems with the gravitational ISF attraction, perturbed by additional ICF showed revolving orbits in qualitative accordance with the dynamics of the Moon.

The conclusion from the investigation in[42] is that the gravitational ISF is the limit of attraction, $-G_n m_i m_j / r^n$ with respect to the power n. A system of N objects can only have regular orbits for $n \leq 2$.

4.3 The Emergence and Evolution of Galaxies in the Expanding Universe

The dynamics of galaxies in an expanding universe are often obtained for gravitational and dark matter in an Einstein-de Sitter universe,[44] or alternatively, by modifying the weak accelerations from gravitation long-range attractions (MOND)[45]. But the time evolution of galaxies can also be determined for galaxies with pure gravitational forces by discrete Newtonian dynamics.[46] The time-reversible algorithm for the formation and aging of gravitational systems by self-assembly of baryonic objects in Section 4.1 is extended to include the Hubble expansion of the space.[47] The algorithm is stable for billions of time steps without any adjustments. The algorithm was used to simulate simple models of the Milky Way with the Hubble expansion of the universe, and the galaxies were simulated for times that correspond to more than 25 Gyr.

The expansion of the space during the discrete Newtonian time propagation of a galaxy was obtained by comparing it with the Hubble expansion of the Universe. A galaxy, l, far away in the universe moves away from the Earth at a speed proportional to its ''proper distance", $Hr_{kl}(t)$, to the Earth, k, measured at the ''cosmological time" t, and this behavior is explained by an expanding universe. The Hubble constant H is the expansion coefficient in Hubble's law[47,48]

$$\mathbf{v}^H(\mathbf{r}_{kl}(t)) = H\mathbf{r}_{kl}(t) \tag{48}$$

for the velocity, $\mathbf{v}^H(\mathbf{r}_{kl}(t))$ of a galaxy k a distance $\mathbf{r}_{kl}(t)$ from the Earth l. The Hubble expansion can be obtained by an intensive expansion of the space independently of the baryonic matter in the universe

$$\mathbf{v}^H(\mathbf{r}(t)) = H\mathbf{r}(t), \tag{49}$$

by which the distance between pairs of positions $\mathbf{r}_k(t), \mathbf{r}_l(t)$, or $\mathbf{r}_k(t), \mathbf{r}_k(t+\delta t)$ increases with the Hubble velocity. Eq. (49) fulfills the *Cosmological principle* and the *Copernican principle* for expansion of the universe.[49] The Cosmological principle, which was first formulated by Newton[1] demands, that no place in the universe is preferred, and the Copernican principle demands, that no direction in the universe is preferred. Eq. (49) will accelerate the expansion of the universe, and observations of galaxies indicate, that the distances between the galaxies accelerate (dark energy).[50,51]

The Hubble constant H is quoted in km $s^{-1}Mpc^{-1}$, for the velocity in kms^{-1} of a galaxy 1 megaparsec (3.09×10^{19} km) away. Its value is[52]

$$H = 72.1 \pm 2.0 \text{ km s}^{-1}\text{Mpc}^{-1}. \tag{50}$$

The Hubble velocity has no effect on the orbits of the planets and the stability of the Solar system, but it affects the stability of galaxies.

The Hubble expansion is included in the discrete Newtonian dynamics.[46] Newton's discrete dynamics changes the position of an object k. If the space expands monotonously over time with the Hubble velocity $\mathbf{v}^H$, then the expansion also changes the distance between two positions. The new position $r_k(t+\delta t)$ is the sum of the change due to the gravitational force on k and the contribution from the Hubble expansion. The mean location of an object changes from $r_k(t-\delta t/2) = (r_k(t-\delta t) + \mathbf{r}_k(t))/2$ at $t \in [t-\delta t, t]$ to $\mathbf{r}_k(t+\delta t/2) = (\mathbf{r}_k(t) + \mathbf{r}_k(t+\delta t))/2$ at $t \in [t, t+\delta t]$. The Hubble expansion changes the distance between the two positions by the Hubble velocity

$$\begin{aligned}
\mathbf{v}^H &= H\delta\mathbf{r}_k = H(\mathbf{r}_k(t+\delta t/2) - \mathbf{r}_k(t-\delta t/2)) \\
&= \delta t H \frac{\mathbf{r}_k(t+\delta t) - \mathbf{r}_k(t)}{2\delta t} + \delta t H \frac{\mathbf{r}_k(t) - \mathbf{r}_k(t-\delta t)}{2\delta t} \\
&= \frac{\delta t H}{2}\mathbf{v}_k(t+\delta t/2) + \frac{\delta t H}{2}\mathbf{v}_k(t-\delta t/2).
\end{aligned} \tag{51}$$

By including the Hubble velocity, Eq. (51), in the Newtons algorithm, Eq. (5), and after a re-arrangement, one obtains the algorithm for the classical mechanics with a Hubble expansion of the space included in the Newtonian dynamics

$$\begin{aligned}
\mathbf{v}_k(t+\delta t/2) &= \frac{(1+\delta t H/2)\mathbf{v}_k(t-\delta t/2) + \delta t/m_k \mathbf{f}_k(t)}{1-\delta t H/2}, \\
\mathbf{r}(t+\delta t) &= \mathbf{r}(t) + \delta t \mathbf{v}(t+\delta t/2).
\end{aligned} \tag{52}$$

The discrete classical dynamics with Hubble expansion, Eq. (52), is still time-reversible, but it increases the velocities, the momenta, and the angular momenta.

A galaxy, including the Milky Way, contains hundred of billion of stars, and a substantial amount of baryonic gas[53,54] and it is not possible directly to obtain the Newtonian dynamics of a galaxy with this number of objects. Instead, models of small ''galaxies" of hundred of objects in orbits around their center of gravity were simulated in,[46] and in an expanding universe with various strengths of the expansion. If these MD systems shall simulate the dynamics of a galaxy in the expanding universe, then one must relate *distances*, *times*, and *Hubble expansion* in the MD systems with the corresponding distances, times and Hubble expansion in a galaxy. Doing so the value of the Hubble constant in the MD units for the models in[46] of the Milky Way in the expanding universe was $H = 5. \times 10^{-8\pm1}$ in MD units.

Models of galaxies with $H = 0$, $5. \times 10^{-8}$, $5. \times 10^{-7}$ and $5. \times 10^{-6}$, respectively, were simulated over a very long time with many billion of time steps and corresponding to more than 25 billion years in cosmological time. **Fig. 8** shows the number of objects in the central part of the galaxies with a mean distance $\bar{r}(t) < 15000 \approx 15$ kg parsec to the center of gravity of the MD system as a function of time. The galaxies with with $H \leq 5. \times 10^{-8}$ contained twice as many bound objects in the ''halos" with distances $15000 < \bar{r}(t) < 100000$. The models of the Milky Way with $H \leq 5. \times 10^{-8}$ were rather stable even for times which corresponds to more than twice the age of the Universe in contrast to galaxies with $H > 5. \times 10^{-8}$. The release of the last bound object in a galaxy with $H = 5. \times 10^{-7}$ is shown in **Fig. 9**. The last bound object escaped the gravitational center, but first after $t = 7.5 \times 10^6$ (3 billion MD time steps) or what corresponds to ≈ 13 billion years after the galaxy was created. The rotating galaxies with $H \leq 5. \times 10^{-8}$ released an object from time to time, but they contained still many bound objects at the end of the simulations corresponding to more than 25 Gyr (**Fig. 8**).

The dynamics of galaxies in an expanding universe are often determined by gravitational and dark matter in an Einstein-de Sitter universe,[44] or alternatively by modifying the gravitational long-range attractions in the Newtonian dynamics (MOND).[45] The Milky Way has, however, only performed ≈ 60 rotations after its creation and the galaxy is hardly in any kind of a steady state,

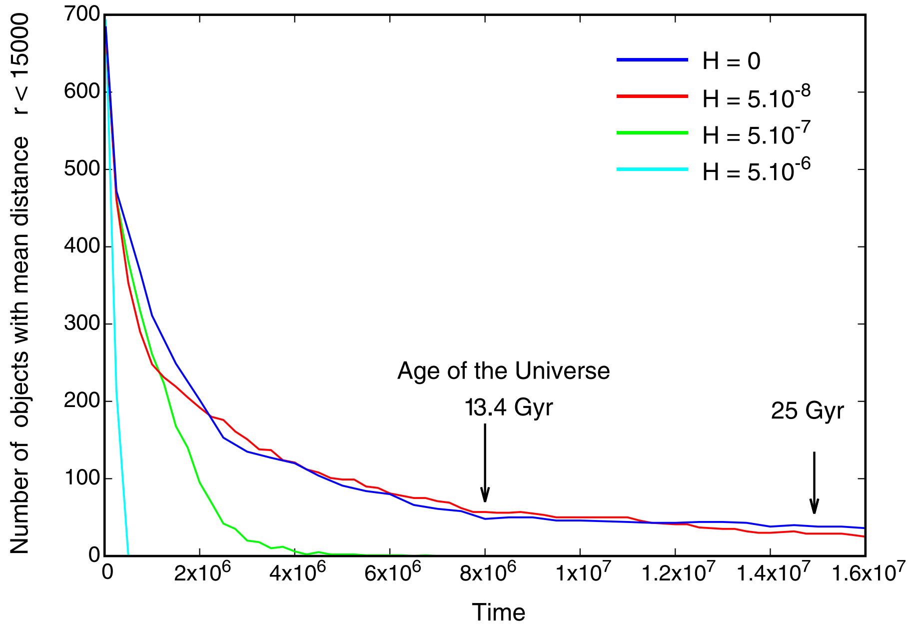

Fig. 8 Number of objects in the ''disk'' in the galaxies with mean distances to the mass centers of the galaxies as a function of time. The systems were exposed to different strengths of Hubble expansions given in the figure.

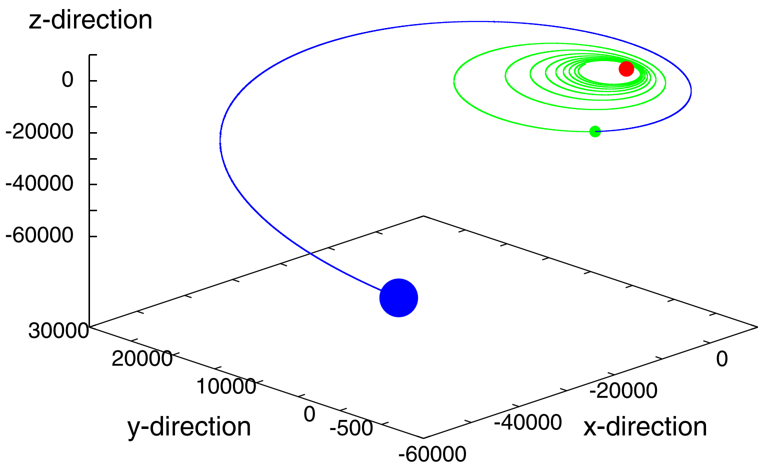

Fig. 9 The last bound object in an unstable galaxy in a fast expanding universe with $H = 5. \times 10^{-7}$. The object escaped the gravitational center (enlarged red sphere) after what corresponds to $\approx$ 13 billion years after the galaxy was created. The first part of its dynamics ($0 < t < 6.5 \times 10^6 \approx 10.9$ Gyr) is shown with green, and the escape from the center of gravity is shown with blue. The galaxies are, however, stable for a Hubble expansion ten times weaker and equal to the Hubble expansion of our Universe.

and the simulations in[46] with pure gravitational forces indicate, that the explanation for the dynamics of galaxies may be that the Universe is very young in cosmological times. Although the models of the Milky Way release objects from time to time they still contained many bound objects at 25 Gyr, which is almost twice the age of the Universe. The Hubble expansion will, however, sooner or later release the objects in the galaxies, but the simulations indicate that this will first happen in a faraway future.

5 Conclusion

Computer simulation of the time evolution in a complex classical system, Molecular Dynamics (MD), is a standard method, and it is used in numerous scientific articles in Natural Science. Newton's discrete algorithm, Eq. (3) is used in almost all the simulations, albeit it is not acknowledged nor known that it was Newton who proposed it at the beginning of his book *Principia* (Section 2). Usually, the computational algorithm in the MD simulations is even not mentioned in the articles. MD is a standard tool and the algorithm is a ''black box". MD with Newton's discrete algorithm from Propostion *I* is, however, exact in the same sense as

Newton's analytic counterpart, the Classical Mechanics. The discrete dynamics is time reversible, symplectic, and has the same invariances as the analytic dynamics (Section 3.1).

There is, however, no qualitative difference between the two dynamics. This is due to the fact, that there exists a "shadow Hamiltonian" nearby the Hamiltonian for the analytic dynamics. The shadow Hamiltonian can be obtained by an asymptotic expansion, and the positions generated by the discrete Newtonian dynamics are located on the analytic trajectories for the shadow Hamiltonian (Section 3.2).

It is only possible to obtain the solution of Newton's classical differential equations for a few simple systems, e.g. for a harmonic oscillator. But the discrete Newtonian dynamics can be obtained for almost all classical systems without any problems, e.g. for complex celestial systems (Sections 4.1, 4.2, and 4.3).

The fact that there exist two equally valid formulations of classical dynamics, the discrete Newtonian dynamics and the analytic Classical Mechanics raises the question: What is the classical limit of quantum mechanics? Classical Mechanics and analytic quantum mechanics are connected by the Wigner expansion,[31] and Lee and coworkers have formulated a discrete nonrelativistic quantum mechanics,[32–34] where Newton's discrete dynamics is the classical limit (Section 3.3). The difference in the energy between the analytic energy and the energy obtained by Eq. (20) for a time quant t_p is of the order t_p^2. With t_p equal to Plank's time quant the difference is absolute marginal. The Heisenberg uncertainty between positions and momenta is of the order t_p and this uncertainty is an inherent quality of discrete dynamics. But the analytic quantum electrodynamics (QED) is in all manner fully appropriate and there is a lack of justification for preferring discrete quantum mechanics.

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Appendix A Verlet algorithm

The first Molecular Dynamics simulation of systems of particles with analytic potentials was published in 1964 by A. Rahman,[55] where he used a higher-order predictor-corrector algorithm for the determination of the new positions $\mathbf{r}^N(t+\delta t)$ from the previous discrete positions. Loup Verlet (1931–2019) published in 1967 the article *Computer "Experiments" on Classical Fluids. I. Themodynamical Properties of Lennard-Jones Molecules*,[2] where his algorithm, Eq. (4),

$$\mathbf{r}(t+\delta t) = 2\mathbf{r}(t) - \mathbf{r}(t-\delta t) + \frac{\delta t^2}{m}\mathbf{f}(t) \tag{A.1}$$

was introduced without any explanation. Loup Verlet was in the mid-nineteen hundred and sixties affiliated with J. L. Lebowith at Yeshiva University, NY. Lebowith gave a preliminary report of Verlet's simulation at a conference in Copenhagen in 1966, where I became acquainted with the Verlet algorithm and Discrete Molecular Dynamics. According to my supervisor at Copenhagen University Eigil L. Prae stgaard, who was a postdoc at Yeshiva University in the same period, the algorithm was derived by a forward and backward Taylor expansion

$$\begin{aligned}\mathbf{r}(t+\delta t) &= \mathbf{r}(t) + \delta t\frac{\partial \mathbf{r}(t)}{\partial t} + \frac{1}{2}\delta t^2\frac{\partial^2 \mathbf{r}(t)}{\partial t^2} + \frac{1}{6}\delta t^3\frac{\partial^3 \mathbf{r}(t)}{\partial t^3} + \mathcal{O}(\delta t^4)\\ \mathbf{r}(t-\delta t) &= \mathbf{r}(t) - \delta t\frac{\partial \mathbf{r}(t)}{\partial t} + \frac{1}{2}\delta t^2\frac{\partial^2 \mathbf{r}(t)}{\partial t^2} - \frac{1}{6}\delta t^3\frac{\partial^3 \mathbf{r}(t)}{\partial t^3} + \mathcal{O}(\delta t^4),\end{aligned} \tag{A.2}$$

and the algorithm was obtained from the sum $\mathbf{r}(t+\delta t) + \mathbf{r}(t-\delta t)$ and $\delta t^2\partial^2\mathbf{r}(t)/\partial t^2 = \frac{\delta t^2}{m}\mathbf{f}(t)$. All the odd terms in A.2 cancel, and the Verlet algorithm is a four-order time symmetric predictor of the positions at the analytic trajectories. The scientific community and Verlet were first much later aware, that it actually was Newton who first published the geometric formulation of the algorithm in *Proposition I*.[56]

Today almost all MD simulations in physics and chemistry are performed with the algorithm, which appears under a variety of different names.

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