Time Reversibility and the Logical Structure of the Universe

Hans H. Diebner, Thomas Kirner,
and Otto E. Rössler

Institut für Theoretische Chemie, Universität Tübingen,
Auf der Morgenstelle 8, D-72076 Tübingen, Germany

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Both Fredkin's findings on the reversibility of logical operations and the novel capability to integrate Newton's equation of motion in an exactly reversible manner enables one to perform a gedankenexperiment in the form of a molecular dynamics simulation of the universe. This leads to a new validation of the reversible structure of the universe. Alternatively, the role of information needs to be upgraded in accordance with a recent proposal by Stonier.

The aim of this note is to throw a new light on the fundamental character of time reversibility which is related to the logical structure of the universe, as will be shown. Starting with a concrete example from the field of molecular dynamics simulations (MDS), an unexpected relation of physical reversible computation arises. To be specific, we rely on exactly reversible integration algorithms as recently investigated in [1, 2] and applied in [3, 4]. The idea is to employ such algorithm for an MDS of the universe in combination with Fredkin's results on "conservative logic" [5]. This enables a new hypothesis which may be called the extended Church-Turing-hypothesis. This Boltzmannian hypothesis can be put into the form "the world is a differential equation". Two alternative consequences arise, either Stonier's proposal to treat "information" on an equal footing as mass and energy, resulting in an equivalence of these three entities, acquires now importance or, time reversibility becomes more fundamental than previously thought.

Even though time reversal symmetry is accepted by most physicists, today there is still some confusion about its meaning. Most recently, there have been some interesting "computer experiments" [3, 4] designed to destroy this confusion. The intention of such simulations is to give a consistent description of many-particle systems with a view to the micro-macro transition. In this context the development of an exactly reversible integration algorithm for Newton's equation of motion, based on the frequently used Verlet algorithm [6], marks a giant step forward. With the aid of such an algorithm the microscopic equations of motion can be integrated under conservation of time reversal symmetry. As shown by Nadler et al. [2], a variant of Verlet's algorithm can be obtained by transposing the fundamental Hamiltonian principle from a continuous to a spatiotemporally discretized state space. This algorithm can be regarded as the spatiotemporal discretized analog to Newton's equations of motion. Since digital computers are an unrenounceable tool especially in the natural sciences, this result may acquire importance.

Using a reversible algorithm, Levesque and Verlet [3] performed a simulation of a purely diffusive many-particle system. They showed that it is possible to give a consistent description of time symmetric systems on the micro level exhibiting a decreasing (macroscopic) Boltzmann H-function which can be interpreted as a measure of lost information.

Extending this idea to reaction-diffusion systems, Diebner and Rössler [4] imposed "chemical" identities on the particles in a simplified 2D-model of point-particles with smooth $1/r$-pair-potentials. On the mechanical level the time evolution of the particles is determined by the use of the above-mentioned discrete Newtonian equation of motion. The reactions according to a given set of chemical reaction channels were governed by the following rules: After each time step there is a check of whether the mutual potential energy of a given pair of particles exceeds a certain threshold. If so, the chemical identities are changed according to the reaction rules. This procedure mimics the action of the activation energy. The advantage of such an MDS is that no a priori assumptions on probabilities and homogeneity have to be made, as is always the case when mass action kinetics is applied to derive macroscopic rate equations. Thus, a consistency check becomes possible. In the above-mentioned simulation, [4], a non-chaotic recurrent macrostructure has been reproduced. A simulation showing chaotic behavior will follow soon.

When at a given instant of time the particles' momenta are all reversed, the mechanical trajectory can be traced back exactly. But how to treat the non-mechanical entities, namely, the chemical identities? When the particles reach the potential thresholds on their way back, how are the mostly commutative algebraic

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terms that represent the corresponding reactions to be treated? For example, after an autocatalytic reaction, say

$$A + B \rightarrow 2A\,, \tag{1}$$

information about the pre-reaction identities is ordinarily lost.

At this stage Fredkin's results [5] on reversible computation can be brought in. As it was stressed by Bennett and Landauer [7], computation is a physical process which underlies the laws of physics. The essential point here is that on the one hand, on thermodynamical grounds the erasure of one bit of information must be accompanied by the thermalization of the hardware of an amount $kT/2$ of energy. The hardware has to be brought in a new physical state by dissipating free energy. On the other hand this erasure of information can be circumvented when one uses "Fredkin gates" as they are called. They perform reversible computations when combined in a suitable manner. In computer engineering the dissipation of energy in computational processes is of special interest because, the more one approaches a minimum of dissipated energy, the more the processor size can be reduced. Extrapolating this idea to the exactly reversible case leads to the result that the hardware has to be present only to carry the logical structure. To keep the computational process independent of the energetic state of the hardware while subsequent logical operations are performed, a corresponding amount of memory bits has to be reserved for every allowed state.

Note that a realization of a reversible Fredkin gate is given by means of a billiard system, as was shown in [5]. In a chemical MDS case, the logical operations can be reduced to those of a purely mechanical system in a natural sense if the problem is treated while taking into account all the internal degrees of freedom of "realistic" molecules. This is because on the level of elementary particles the problem of changing identities vanishes. In fact, we might have started our description of the chemical MDS on this level from the beginning. But then it would have been impossible to see the reversed argument. It states that the physical world can be regarded as a computational process. Matter then works as hardware that carries the logical structure.

This point of view is perhaps not novel. But what this indirect approach – via a virtual universe – shows is that the possibility that the universe could be irreversible has to be discarded. For otherwise (if it were irreversible), there would have to be a thermalization of the hardware. Since the hardware, too, is simulated when a whole universe is simulated, there is no space for such a process left. For a simulated universe includes all the physical processes on the hardware level. Thus we have arrived at a contradiction.

An alternative way out is to assume that information is a natural basic entity equivalent to mass and energy in the sense of Einstein (cf. [8]). Then the above contradiction can be overcome because it is then no longer possible to simulate a universe on a purely logical basis. We are not in favour of this solution, however. Levesque and Verlet's experiment seems to rule out this possibility. Although the loss of information is captured by a function of the arrangement of the particles, expressed via a decreasing H-function, the total energy could be held almost constant. The small increase in energy is due to the approximation incurred by discretization. Noether's theorem does not hold in discrete simplectic dynamics. A discrete structure of the universe therefore becomes unlikely. In the present context, however, it suffices to refer to the continuum limit. In this limit the digital computer becomes an analog computer while the original Church-Turing-hypothesis changes over into the "extended Church-Turing-hypothesis" mentioned above.

To conclude, a new step in the direction of a consistent description of the world has been done. Consistency relies on reversibility. Of course, the currently favored big-bang model of cosmology is believed to be dissipative, although this is an open issue [9]. The present considerations therefore are of a more general kind and may eventually have to be incorporated into more specific models. If one considers the human operator as an information processing device [10] an exactly reversible simulation becomes an indispensable tool in the field of endophysics [11, 12]. The proposed gedankenexperiment need not remain in the thought domain when one is content with a simplified model universe as we hope to show soon. We express our gratitude to Werner Pabst for his fruitful criticism. For J. O. R.

[1] H. H. Diebner, Investigations of exactly reversible algorithms for dynamics-simulations (in German). Master's thesis, University of Tübingen 1993.
[2] W. Nadler et al., Space-discretized Verlet-algorithm from a variational principle, preprint 1995.
[3] D. Levesque and L. Verlet, Molecular dynamics and time reversibility, J. Stat Phys. **72,** 519 (1993).
[4] H. H. Diebner and O. E. Rössler, Z. Naturforsch. **50 a,** 1139 (1995).
[5] E. Fredkin and T. Toffoli, Int. J. Theo. Phys. **21,** 219 (1982).
[6] L. Verlet, Phys. Rev. **159,** 159 (1967).
[7] C. Bennett and R. Landauer, The fundamental physical limits of computation, Sci. Amer **253,** (7/1985).
[8] T. Stonier, Information and the internal structure of the universe, Springer Verlag, London 1990.
[9] S. W. Hawking, A brief history of time: from big bang to black holes, Bantam Books, Toronto 1988.
[10] L. Szilard, Über die Entropieverminderung in einem thermodynamischen System bei Eingriffen intelligenter Wesen, Z. Physik **53,** 56 (1928).
[11] O. E. Rössler, Endophysics (in German), Merve Verlag, Berlin 1992.
[12] O. E. Rössler, A chaotic 1-D gas: Some implications. In: The Physics of Phase Space, Y. S. Kim and W. W. Zachary, ed., Lect. Not. Phys. **278,** 9 (1987).