Noise-Driven Numerical Irreversibility in Time-Reversible Molecular Dynamics Simulation

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Abstract (written in Japanese): 不可逆性の問題は，Chaos 理論に基づき数値的に盛んに研究されているが，現在も未解決である。しかし，従来の数値解析は，丸め誤差による不可逆性を回避できないため，ミクロな力学法則の可逆性を厳密には模擬していない。即ち，現在まで，このような微小ノイズが不可逆性に与える影響を考慮せずに，不可逆性の問題が研究されてきた。従って，本研究では，厳密な時間可逆性を有する Bit 可逆アルゴリズムを新たに用いて，非平衡度／系の不安定性の観点から，従来研究に内在する数値的不可逆性を検討し，その特性を明らかにした。

Recently, irreversibility on macroscopic systems has been investigated based on the chaos theory, by using Molecular Dynamics (MD) methods. However, the MD methods can not avoid the numerical irreversibility due to round-off errors. For example, Loschmidt's reversibility paradox was investigated by Orban and Bellemans[1]. In their simulation, a time-reversal operation is realized by a velocity-inversion technique. That is, all velocities of the particles are reversed suddenly at a certain time in the middle of the equilibrium state. As a result, irreversibility appeared in the simulation, i.e., Boltzmann's H-function didn't return to the initial value after the time-reversal operation. Accordingly, it is still unclear whether the irreversibility of the system can be investigated properly, even if the stability has some relation to the irreversibility.

Therefore, to study the characteristic of this numerical irreversibility, we employ the *bit-reversible algorithm*[2] as a test bed. The bit-reversible algorithm (Bit MD) is completely time-reversible and is free from any round-off error and, therefore, any irreversibility can be detected definitely[3] (Fig. 1). This is because Bit MD employs Verlet's algorithm for time derivatives but, unlike the standard MD, employs a discrete coordinate-space, instead of a continuous coordinate-space. This complete time-reversibility suggests that, if a quantitatively-controlled noise is added to Bit MD, it may be possible to quantitatively investigate numerical irreversibility in the

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[2] D. Levesque and L. Verlet, J. Stat. Phys. **72**, 519(1993).
[3] N. Komatsu, T. Abe, Physica D **195**, 391(2004). N. Komatsu, T. Abe, Conference on Computational Physics, Italy, Europhysics conference abstracts **28D**, 105(2004). N. Komatsu, Ph.D. thesis, University of Tokyo, 2004.

standard MD. Based on this idea, we investigate the irreversibility by means of the following controlled noise which is added to Bit MD. The controlled noise is a deliberate displacement of the particles; that is, the particles change their position suddenly by a certain amount, in a random direction in the discrete coordinate-space.

Through this study, it is clearly demonstrated that, other than the extent of the stability of the system, the appearance of irreversibility is related to the '*quantity*' of the controlled noise (See Fig. 2). By means of the bit-reversible simulation added to the controlled noise of an appropriate '*quantity*', the characteristic of the numerical irreversibility in the standard MD is revealed. Note that, to measure the numerical irreversibility properly, a recovery rate of Boltzmann's H-function, R_R, is newly defined by

$$R_R \equiv \frac{\mathrm{dH}}{\Delta\mathrm{H}} = \frac{H(2t_{\mathrm{rev}}) - H(t_{\mathrm{rev}})}{H(0) - H(t_{\mathrm{rev}})}. \tag{1}$$

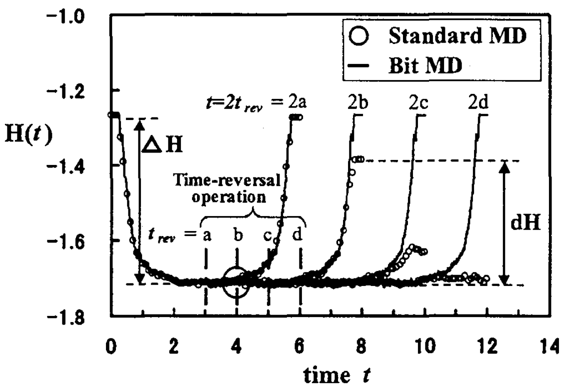

Fig. 1

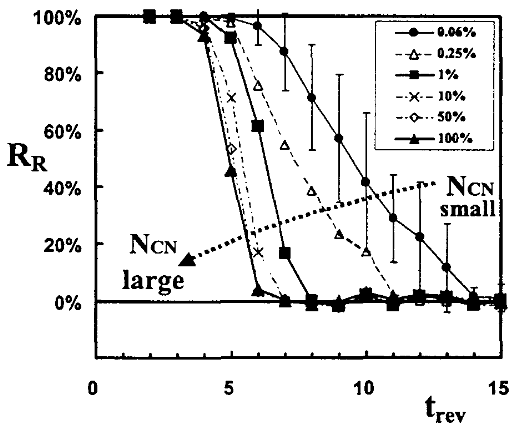

Fig. 2

Fig. 1: Time evolution of Boltzmann's H-function obtained by time-reversible simulations. Time-reversal operations are executed at the timings designated by a, b, c and d. The H-functions in Bit MD return to the initial value exactly after a passage of time from the time-reversal operations, which is equal to a time interval from 0 to t_{rev}. On the other hand, in the standard MD, the time evolution of the H-function is influenced by the timings t_{rev} of the time-reversal operation, and the H-functions don't return to the initial state completely. In this figure, for Eq. 1, dH and ΔH at t_{rev} =b are also shown.

Fig. 2: Effects of the number of particles to which the controlled noise is added, N_{CN}. Arbitrary N_{CN} particles are chosen to be displaced by the minimum lattice distance in the discrete coordinate-space, only once at the timing t_{rev} of the time-reversal operation. In this study, N_{CN}/N is varied ranging from 0.06% to 100%. Here, the total number of particles N is set to be 1600. As shown in Fig. 2, the number N_{CN} has a significant influence on the appearance of irreversibility. The more the ratio N_{CN}/N increases, the more quickly the irreversibility starts to appear, and the more rapidly the irreversibility prevails.