

# A Deterministic Entropy Based on the Instantaneous Phase Space Volume

Hans H. Diebner and Otto E. Rössler

Division of Theoretical Chemistry, University of Tübingen,  
Auf der Morgenstelle 8, D-72076 Tübingen

Z. Naturforsch. **53 a**, 51–60 (1998); received September 10, 1997

A deterministic entropic measure is derived for the time evolution of Newtonian N-particle systems based on the volume of the instantaneously occupied phase space (IOPS). This measure is found as a natural extension of Boltzmann's entropy. The instantaneous arrangement of the particles is exploited in the form of spatial correlations. The new entropy is a bridge between the time-dependent Boltzmann entropy, formulated on the basis of densities in the one-particle phase space, and the static Gibbs entropy which uses densities in the full phase space. We apply the new concept in a molecular dynamics simulation (MDS) using an exactly time reversible "discrete Newtonian equation of motion" recently derived from the fundamental principle of least action in discretized space-time. The simulation therefore is consistent with micro-time-reversibility. Entropy becomes an exact momentary observable in both time directions in fulfillment of a dream of Boltzmann.

Reprint requests to H. H. Diebner; Fax: +49 7071 296919, [E-mail: diebner@uni-tuebingen.de](mailto:diebner@uni-tuebingen.de)