Abstract Submitted
for the DFD06 Meeting of
The American Physical Society

Recurrence Analysis of Fluid Molecular Dynamics Simulation[1]
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— We present a Recurrence Quantification Analysis (RQA) of instantaneous temperature records obtained using molecular dynamics simulations of Lennard-Jones fluids. Simulations were performed at various system (temperature and density) states. The instantaneous temperature was recorded as function of time and consequently analyzed using Recurrence Quantification Analysis. We calculated several RQA variables such us determinism, maximum line, trapping time as functions of the system temperature and density. By comparison with other time series analysis methods it is demonstrated that RQA is useful in extracting significant characteristics of the system dynamics. The existence of vibrational and diffusional motion of the fluid atoms are reflected on the results of the recurrence analysis and related to physical quantities such as Mean Square Displacement (MSD) of the atoms. White bands represent diffusion events and thus are larger at low system densities. Determinism (%deter) becomes smaller as temperature or density increases since collisions of atoms are then more frequent.

[1]Acknowledgements.This research has been partially supported by the program PYTHAGORAS-EPEAK II jointly funded by the European Community and the Greek Ministry of Education.

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Date submitted: 02 Aug 2006 Electronic form version 1.4