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Short-Time Dynamical Behavior of Fluids at the Atomic Scale

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In this paper we discuss fundamental aspects of the dynamical behaviour of fluids at the atomic scale using Molecular Dynamics simulation. We present time-series analyses of instantaneous temperature and pressure using linear and non-linear methods. Within the framework of the linear analysis methods, power spectra show evidence of a two-regime power-law (1/fa) behaviour with a large exponent at the high frequency region and a smaller exponent at low frequencies. The dependence of exponent a on system density and temperature is discussed. All time-series exhibit essentially the same characteristics for short times (high frequencies). In contrast, at low frequencies, pressure shows a faster loss of memory. Extracted characteristic times are consistent with results obtained from mean square displacements calculations. Rescaled range analysis reveals also a two-regime behavior. In the framework of nonlinear time series analysis, mutual information is employed for the determination of the optimal embedding delay leading to phase space reconstruction.

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