

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Molasses Tail in Dense Hard Core Fluids MASAHARU ISOBE, Nagoya Institute of Technology, BERNI ALDER, Lawrence Livermore National Laboratory — The long slow decaying potential part of the shear-stress autocorrelation function has been called the “molasses tail” to differentiate it from the hydrodynamic origin of the long time tail in the velocity autocorrelation function and to emphasize its relation to the highly viscous glassy state [1]. Some twenty years ago, the molasses tail in dense liquids near the solid-fluid transition point was speculated to be due to transient crystal nuclei formation [2]. This slow decaying process of the OACF and its decomposition (pair, triplet, and quadruplet) is a key factor in understanding the onset of the glass transition. With additional computer power, we are now investigating the origin of the molasses tail using a modern fast algorithm based on event-driven Molecular Dynamics (MD) simulation. We confirm the non-algebraic decay (stretched exponential) at intermediate times corresponding to the existence of various cluster sizes a solid cluster at high densities. The decay in dense systems thus consists of a three stage relaxation process, which are the kinetic regime, the molasses regime and the diffusional power regime[3]. [1] B. J. Alder, in *Molecular Dynamics Simulation of Statistical-mechanical Systems*, G. Ciccotti and W. G. Hoover, eds.(North-Holland, Amsterdam, 1986) 66. [2] A. J. C. Ladd, and B. J. Alder, *J. Stat. Phys.* 57, 473 (1989). [3] M. Isobe and B. J. Alder, *Mol. Phys.*, 107, 609 (2009).

Masaharu Isobe
Nagoya Institute of Technology

Date submitted: 18 Dec 2009

Electronic form version 1.4