

## **67e Novel Computational Probes of Diffusive Motion**

*M. Scott Shell, Frank H. Stillinger, Thomas Lombardo, and Pablo G. Debenedetti*

Recently we proposed new theoretical expressions for the self-diffusion coefficient and the shear viscosity [1]. The equation for the diffusion coefficient emphasizes how initial particle momentum biases the long-time mean displacement. We present numerical calculations for two model systems: a binary Lennard-Jones mixture and the Van Beest-Kramer-Van Santen (BKS) potential for liquid silica. The primary conceptual tool is the joint probability distribution of single particles as a function of initial velocity and positional displacement at a given later instant. In the supercooled regime there appears a marked deviation of the momentum-integrated displacement distribution away from single-Gaussian behavior. We investigate the possible connection of this observation with the appearance of "dynamic heterogeneity" [2], whereby different regions of a supercooled liquid exhibit markedly different dynamics.

[1] Stillinger, F.H., and Debenedetti, P.G., *J.Phys.Chem. B*, 109, 6604 (2005).

[2] Ediger, M.D., *Annu. Rev. Phys. Chem.*, 51, 99 (2000)