Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Diffusion in Crowded Environments: Monte Carlo and Molecular Dynamics Studies[1] ROBIN SELINGER, PRITHVIRAJ NANDIGRAMI, ANDREW KONYA, Kent State University, JENNIFER TOTH, Grove City College — Anomalous diffusion is sometimes, but not always, observed in dense multicomponent mixtures, e.g. in diffusion of proteins in a lipid membrane [1]. To investigate this phenomenon, we carry out 2-d simulation studies using both on-lattice Monte Carlo and off-lattice Molecular Dynamics. "Tracer" particles are emitted from a source along one side of the simulation cell and absorbed by a sink along the other side, diffusing through a chamber containing "crowder" particles whose number remains constant. On-lattice Monte Carlo studies show that equilibrium tracer flux drops linearly with crowder density, showing non-Fickian behavior well below the percolation threshold. Molecular dynamics studies in the same geometry also show non-Fickian behavior, but tracer flux is a nonlinear function of crowder density. We compare our results with analytical calculations and experimental studies, and discuss implications for understanding diffusion-mediated processes in cell membranes.

[1] J. A. Dix and A. S. Verkman, Annu. Rev. Biophys. 37, 247 (2008).

[1]Work supported by NSF-CHE- #1004987.

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Date submitted: 18 Nov 2012 Electronic form version 1.4