Hard Spheres with Tails

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Molecular dynamics is typically formulated in terms of a classical potential energy function with various macroscopic quantities recovered from the resulting (Hamiltonian) dynamics by averaging. One component of the potential energy is a Lennard-Jones term for each pair of atoms presenting a hard soft wall r^{-12} repulsion and an attractive tail. This term is not particularly physical, and qualitatively similar results are obtained if it is replaced by a steeper potential wall or even a hard wall, which sometimes simplifies comparison analytical results. Moreover, some fluid models use this type of "billiard ball" formulation, together with soft potential energy terms (due to charge, for example) acting at longer distances. In polymer models, the hard spheres are further connected by rigid rods, leading to billiard models on manifolds.

In this talk, various algorithms issues related to hard sphere and hard soft-sphere molecular simulation will be discussed, and a new method which appears to have improved the state of the art for this type of simulation will be presented.

This work is joint with Yao Houndougbo and Brian Laird (Kansas).