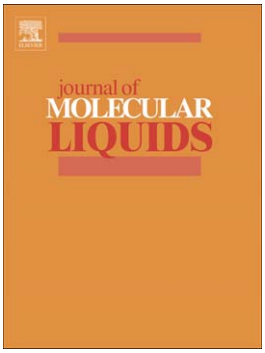

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Two-dimensional molecular simulations using rose potentials

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Abstract

Molecular simulations of two-dimensional (2D) systems can provide behavior and insight analogous to three-dimensional systems, often with reduced complexity and computational cost. We describe here an approach for molecular dynamics simulation of single point particles using rose potentials for orientation dependent pairwise interactions. Modifying both the shape and range of a 3-petal rose function, we construct an efficient and dynamical mimic of the 2D Mercedes Benz (MB) water model. This *rose water* model is structurally similar to MB water and demonstrates the same water-like anomalous properties. When given a mass distribution similar to real water, we observe rose water to diffuse at a faster rate, only with longer lived "hydrogen-bonds". This is likely due to the use of the significantly expanded acceptable hydrogen-bond length relative to the particle size parameter, resulting in more free volume for translation coupled with relatively strong hydrogen-bonds. We also show how one can extend the rose potential to generate alternate models with varying numbers of interacting arms.

Keywords: molecular dynamics, Mercedes-Benz water, orientational potential, liquid simulation

1. Introduction

Investigation of systems at reduced dimensionality can provide a degree of clarity and insight not immediately obvious from higher dimensional systems. From Onsager's seminal work on the linear and two-dimensional (2D) Ising model [1] to Ben-Naim's one-dimensional and 2D water-like models [2], [3], [4], [5], [6] and [7], reduced dimensionality modeling provides a simpler but more complete picture of collective behavior of microscopic particles. For example, Ben-Naim's three-armed 2D water-like model was popularized as the Mercedes Benz (MB) water model by Dill *et al.* and used to explain the anomalous properties of water and the subtleties of aqueous solvation [8], [9], [10], [11], [12], [13], [14] and [15]. This 2D modeling work has since extended into a variety of analytical models and related toy models that capture similar physical properties and features [16], [17], [18], [19], [20], [21], [22], [23], [24], [25], [26], [27] and [28]. Most of these investigations are rooted in Monte Carlo style sampling or integral equation theories rather than with molecular dynamics. While this can have benefits, such as for instruction in the technique of Monte Carlo [29], this does restrict dynamical studies. In the cases where dynamics has been implemented [15] and [30], the use is specialized, likely due to the unique makeup of a given model.

We discuss here an alternate strategy for orientational potentials to describe 2D water-like models. By using polar coordinate potential functions of the form $\sin(n\theta)$, or *rose potentials*, a rigid multi-site model can be represented as a pairwise interacting point particle with a single angular degree of freedom. The benefits of this single-point trigonometric form include flexible construction, clear and simple evaluation of derivatives for forces and torques, and an increase in computational efficiency due to the resulting decrease in neighboring pairwise interaction sites [31]. As an example application, we map a single-point rose function to the MB water model, which is a four-site model consisting of a single central Lennard-Jones (LJ) potential with three fixed Gaussian potential "hydrogen-bonding" arms [8], to craft a single-point *rose water* model that exhibits the same water-like behaviors. While this