

Conservative Potentials for Lattice-Like Coarse-Grained Schemes

Siwei Luo and Mark Thachuk

Department of Chemistry, University of British Columbia, BC, Email: siweiluo@chem.ubc.ca

Coarse-grained (CG) models reduce the number of degrees of freedom in a system, allowing the dynamics of large systems to be studied for longer times. Many CG models have been developed since the way of generating a CG system highly depends on the question one interests in. It is common to treat one or multiple molecules as one CG bead by their center of mass. However, this way fails to study non-bonded particles since the motion of free particles disperses them and disintegrates the cluster.

The conservative potentials, arising from CG mapping schemes for non-bonded atomistic particles, are studied. These schemes map atomistic particles to fluid element-like cells whose centers lie on a regular, cubic lattice. Equilibrium atomistic molecular dynamics trajectories for a liquid and gaseous Lennard-Jones fluid are converted to CG ones, from which CG probability distribution functions are calculated. Correlation studies show that position and mass CG variables are uncoupled, as are different vector components of position. Furthermore, the strongest coupling occurs with neighbouring cells in specific directions, and the resulting distribution is well described by a multivariate Gaussian. This implies the potential has a generalized quadratic form, whose derivative can be derived analytically. A microscopic rationalization is provided for the signs and relative magnitudes of different correlation coefficients, and in some cases a connection is made with bulk properties of the fluid. We argue that the generalized quadratic form should be robust to changes in the particulars of the CG scheme, as well as the nature of the atomistic intermolecular potential. Only a few potential parameters need to be calculated from the underlying atomistic system. This is significant because it indicates the transferability of this form to other, more complex systems. This transferability is tested by exploring the connection between several mapping schemes. Our theory and data suggest that the parameters for the conservative potential of different schemes converge to the same limiting scheme.