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Adaptive Resolution Molecular Dynamics Scheme LUIGI DELLE SITE, MATEJ PRAPROTNIK, KURT PRAPROTNIK, Max Planck Institute for Polym.Res. — A new adaptive resolution scheme for efficient particle-based multiscale molecular dynamics (MD) simulations is presented. The key feature of the method is that it allows for a dynamical change of the number of molecular degrees of freedom during the course of the MD simulation by an on-the-fly switching between the atomistic and coarse-grained levels of detail. The new approach is tested on a model system of a liquid of tetrahedral molecules. The simulation box is divided into two regions: one containing only atomistically resolved tetrahedral molecules, and the other containing only one particle coarse-grained spherical molecules. The molecules can freely move between the two regions while changing their level of resolution accordingly. The hybrid and the corresponding all-atom systems have the same statistical properties.

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