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Adaptive Resolution in Molecular Dynamics Simulations MATEJ PRAPROTNIK, LUIGI DELLE SITE, KURT KREMER, Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany, SILVINA MATYSIAK, CECILIA CLEMENTI, Department of Chemistry, Rice University, 6100 Main Street, Houston, Texas 77005 — For the study of complex synthetic and biological molecular systems by computer simulations one is still restricted to simple model systems or to by far too small time scales. To overcome this problem multiscale techniques are being developed. However in almost all cases, the regions treated at different level of resolution are kept fixed and do not allow for a free exchange. We here give a basic theoretical framework for an efficient and flexible coupling of the different regimes. The approach leads to a concept, which can be seen as a geometry induced phase transition and to a counterpart of the equipartition theorem for fractional degrees of freedom. The efficiency of the presented approach is illustrated on two numerical examples, i.e., the molecular dynamics simulations of bulk water and a generic polymer in a solvent.

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