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Scalable and fast concurrent multiscale molecular simulation with predictive parallelization scheme HORACIO V. GUZMAN, Max Planck Institute for Polymer Research, CHRISTOPH JUNGHANS, Computer, Computational, and Statistical Sciences Division, Los Alamos National Laboratory, KARSTEN KREIS, AOIFE FOGARTY, KURT KREMER, TORSTEN STUEHN, Max Planck Institute for Polymer Research — Concurrent multiscale simulation enables the study of molecular systems with different resolutions in specific subdomains of a simulation box. Modeling soft-matter and biological systems in the context of multiscale simulations are challenging research avenues which drive the permanent development of new simulation methods and algorithms. In computational terms, those methods require parallelization schemes that make productive use of computational resources for each simulation and from its genesis. Here, we introduce the dual resolution domain decomposition algorithm that is a combination of a resolution sensitive spatial domain decomposition with an initial sliding subdomain-walls procedure. The algorithm modeling is presented for dual resolution systems in terms of scaling properties as a function of the size of the low-resolution region and the high to low resolutions ratio. The algorithm competences are validated within adaptive resolution simulations, by comparing its scalability and speedup to a spatial domain decomposition. Two representative adaptive resolution simulations have been employed in this work, namely, a biomolecule solvated in water and water in an ideal gas reservoir.

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