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Adaptive Resolution Simulations: Applications and New Developments towards Open Systems MD

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The relation between atomistic structure, architecture, molecular weight and material properties is a basic concern of modern soft matter science. A typical additional focus is on surface interface aspects or the relation between structure and function in nanoscopic molecular assemblies. Here computer simulations on different levels of resolution play an increasingly important role. To progress further adaptive schemes are being developed, which allow for a free exchange of particles (atoms, molecules) between the different levels of resolution. The lecture will concentrate on these methods, however will also include first approaches to connect particle based simulations to continuum as well as to include quantum effects. Furthermore the extension to open systems MD as well as new recent methodology advances will be explained. A general review on the first part can be found in M. Praprotnik et al. Ann. Rev. Phys. Chem. 59, 2008 and recent advances in S. Fritsch et al. PRL 108, 170602 (2012)