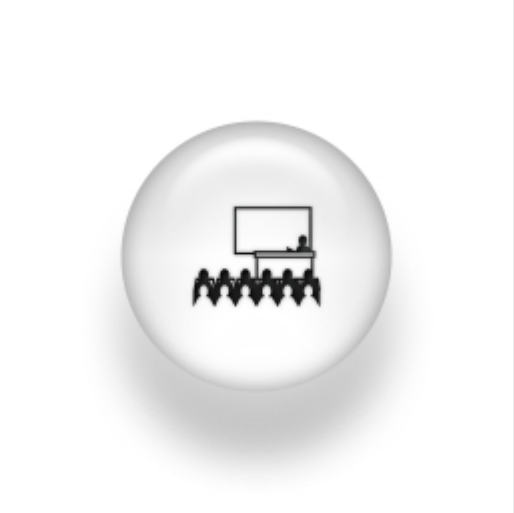
Adaptive Resolution Molecular Dynamics Scheme

Wednesday, 23 May 2007, 12.00-13.00



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We have been developing a novel adaptive resolution technique for efficient multiscale molecular dynamics (MD) simulations. The new approach is tailor-made for studying molecular systems that require in some regions an atomistic resolution but otherwise involve length and time scales that are difficult to capture by the conventional atomistic MD simulation. Our method allows an on-the-fly interchange between a given molecule's atomic and coarse-grained level of description, enabling to reach large length and time scales while spatially retaining atomistic details of the system. The new approach is tested on the model system of a liquid of tetrahedral molecules. The simulation box is divided into two regions: one containing only atomistically resolved tetrahedral molecules, the other containing only one particle coarse-grained molecules. Molecules can freely move between regions while changing their level of resolution accordingly. It is shown that this system has the same statistical properties as the corresponding fully atomistically resolved system at the same physical conditions.