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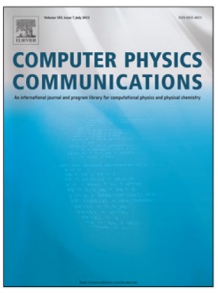

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Computational Efficiency and Amdahl's law for the Adaptive Resolution Simulation Technique

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Abstract

We discuss the computational performance of the adaptive resolution technique in molecular simulation when it is compared with equivalent full coarse-grained and full atomistic simulations. We show that an estimate of its efficiency, within $10-15\%$ accuracy, is given by the Amdahl's Law adapted to the specific quantities involved in the problem. The derivation of the predictive formula is general enough that it may be applied to the general case of molecular dynamics approaches where a reduction of degrees of freedom in a multiscale fashion occurs.

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