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Title (English)

Parallelisation of a Molecular Dynamics Program using MPI

Title (Swedish)

Abstract

A parallel algorithm was implemented in a molecular dynamics program. The communication is handled with the standardised library 'Message Passing Interface'. The parallel version of the program was tested on a system with an aspartate molecule solvated in a 20 Å sphere of water. The efficiency obtained with ten nodes was 75%, i.e. the parallel computation was 7.5 times faster than the sequential. Maximum efficiency, 78%, was obtained with 8 nodes.

Keywords

Molecular dynamics, parallel, MPI, speedup

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