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Computational Chemistry - requirements and experiences with use of MPI in EGEE

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Abstract

The increasing availability of computer power on Grid platforms is a strong incentive to implement complex suites of codes on distributed systems.
As an active Computational Chemistry Community, this has urged us to implement on the EGEE Grid environment some suites of programs devoted to the calculation of the properties of molecular systems and able to explore the parallel performance of the mentioned infrastructure.
To this end, to evaluate the performance of the used platform the parallel version of the DL_POLY suite of codes, based on the Replicated Data parallelization strategy, was submitted in all the EGEE-Grid computer clusters supporting MPI-START and MPICH requirements and the corresponding results have been analyzed.

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