

A Hierarchical MPI Communication Model for the Parallelized Solution of Multiple Integrals

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Abstract

For the modeling of polymer meso-structures, the spinodal points can be obtained by random phase approximations. The necessary number of these spinodal points to describe a phase diagram can significantly be reduced, if the usual sampling-point method is replaced by a Newton iteration, utilizing all the transiently computed data. This has the consequence that the simple inner parallelism of the problem gets lost, i.e. the possibility to compute a high number of independent sampling-points in parallel. On the other hand, the overall CPU time requirement is rather drastic and parallelism seems to be the only way to achieve acceptable turn-around times. Hence, there is no other way than to parallelize the objective functions of the Newton iteration, mainly consisting of a handy set of multiple integrals, which have to be numerically solved using step-width adaption.

Computing multiple integrals with step-width adaption in parallel results in nested parallelism, which is difficult to implement. A lot of applications need the concept of nested parallelism. In many implementations, OpenMP does not support nested parallelism at the moment, and for MPI, the granularity has to be sufficient. As a case study, the present paper describes the parallelization and the communication model for the solution of multiple integrals. The results show adequate parallel efficiency values for executions up to 256 processes. The parallel integral solver code is modularized in the sense that it can easily be applied to any other integrands. Keywords: Parallel numerical solution, multiple integrals, step-width adaption, army communication model.