John von Neumann Institute for Computing

Parallelization of the Dirac-Fock Package MOLFDIR: A Pathway for the Treatment of Large Relativistic Systems

M. Pernpointner, W.A. de Jong, L. Visscher, R. Broer

published in

Modern Methods and Algorithms of Quantum Chemistry,
J. Grotendorst (Ed.), John von Neumann Institute for Computing, Jülich, NIC Series, Vol. **2**, ISBN 3-00-005746-3, p. 50, 2000.

http://www.fz-juelich.de/nic-series/

Parallelization of the Dirac-Fock package MOLFDIR: A pathway for the treatment of large relativistic systems

M.Pernpointner, W. A. de Jong, L. Visscher, R. Broer

Department of Theoretical Chemistry, Vrije Universiteit, 1081 HV Amsterdam, The Netherlands
Theoretical Chemistry, Rijksuniversiteit Groningen, 9747 AG Groningen, The Netherlands

The treatment of relativity and electron correlation on an equal footing is essential for the computation of systems containing heavy elements. Even if there are several reliable approximations to the Dirac-Fock equation mostly based on reduction to fewer components of the wave function full Dirac-Fock calculations will provide the most accurate way for taking relativity into account. Since the treatment of electron correlation is already a very demanding task in nonrelativistic calculations the memory and disk space requirements grow much bigger when the wave function has four components. Especially the integral generation and the corresponding transformation from the AO to the MO basis need a lot of computer resources. For larger systems the enormous memory and disk space requirements can only be handled by a parallel approach to the problem. Here we present the parallelization of the program package MOLFDIR up to the four-index transformation step. A parallelization of the CCSD(T) code is necessary when the active space becomes very large but in the case of large basis sets and moderately large active spaces the parallelization of the CCSD(T) code is not urgent and will be done later on. The integral calculation, the SCF part and four-index transformation are fully parallelized whereas the one-electron integrals and their transformation can be performed on each node separately or on one node with a subsequent distribution of the corresponding files depending on the computer architecture. The current implementation is based on a distributed memory system since these architectures can be easily enlarged and are cheaper than shared memory machines. Since communication is a bottleneck on these systems large data transfer has to be avoided. We therefore generate the two-electron integrals in a way that makes it possible to keep the four-index transformation independent from the other nodes up to the very last step where the MO contributions are added up. Calculations on a test system show the scaling properties of the code up to the transformation step.