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POSTER ABSTRACT FOR ISTCP-VIII CONFERENCE

The Divide-Expand-Consolidate MP2 scheme goes massively parallel

Kasper Kristensen[a]*, Thomas Kjærgaard[a], Ida-Marie Høyvik[a], Patrick Ettenhuber[a], Poul Jørgensen[a], Branislav Jansik[b], Simen Reine[c], and Jacek Jakowski[d]

[a] *qLEAP – Center for Theoretical Chemistry, Department of Chemistry, Aarhus University, Langelandsgade 140, 8000 Aarhus C, Denmark*; [b] *IT4Innovations, VSB – Technical University of Ostrava,17. listopadu 15/2172, Ostrava, Czech Republic*; [c] *Centre for Theoretical and Computational Chemistry, Department of Chemistry, Oslo University, Postbox 1033, Blindern, 0315 Oslo, Norway;* [d] *National Institute for Computational Sciences, JICS-ORNL, One Bethel Valley Road, Bldg 5100 ms 6173, Oak Ridge, Tennessee 37831, USA*

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For large molecular systems conventional implementations of second order Møller-Plesset (MP2) theory encounter a scaling wall, both memory- and time-wise. We describe how this scaling wall can be removed. We present a massively parallel algorithm for calculating MP2 energies and densities using the Divide-Expand-Consolidate scheme [1–6] where a calculation on a large system is divided into many small fragment calculations employing local orbital spaces. The resulting algorithm is linear-scaling with system size, exhibits near perfect parallel scalability, removes memory bottlenecks, and does not involve any I/O. The algorithm employs three levels of parallelization combined via a dynamic job distribution scheme [6]. Results for two molecular systems containing 528 and 1056 atoms (4278 and 8556 basis functions) using 47120 and 94240 cores are presented. The results demonstrate the scalability of the algorithm both with respect to the number of cores and with respect to system size. The presented algorithm is thus highly suited for large super computer architectures and allows MP2 calculations on large molecular systems to be carried out within a few hours – for example, the correlated calculation on the molecular system containing 1056 atoms took 2.37 hours using 94240 cores.

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*Corresponding author. Email: kasperk@chem.au.dk

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