MRChem, a quantum chemistry code with unlimited basis sets. Parallelization and scaling

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MRChem completely avoids the use of traditional Gaussian type basis sets. Instead the real space is subdivided into smaller regions according to the shape of the functions, based on multiresolution analysis. The division of space is done dynamically, to guarantee a predefined precision, without predefined limited basis set. For small systems with low accuracy, this is not a very efficient approach. But for larger systems or if high accuracy is required, the method is expected to be competitive with other methods. In our present implementation, systems with hundreds of electrons can be described. The problems of truncations and near linear-dependencies of the basis set are avoided naturally. The intrinsic adaptation of the grid to the actual functions, leads directly to a decrease of computation time for long range interactions. We present the parallelization strategy adopted, and examples of scalability for large molecules.

References

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