MOLMPS: the massively parallel quantum chemical density matrix renormalization group program

Jiří Brabec[1], Jan Brandejs[1], Örs Legeza[2], Karol Kowalski[3], Sotiris Xantheas[3], Libor Veis[1]

[1]*J. Heyrovský Institute of Physical Chemistry, ASCR, 18223 Prague, Czech Republic*
[2]*Strongly Correlated Systems "Lendület" Research group, Wigner Research Centre for Physics, H-1525 Budapest, Hungary*
[3]*Pacific Northwest National Laboratory, Richland, WA 99352, USA*

In the past decade, the quantum chemical version of the density matrix renormalization group method (QC-DMRG) [1, 2] has established itself as the method of choice for accurate calculations of strongly correlated molecular systems requiring large active spaces. Several groups have presented their own QC-DMRG implementations, but to the best of our knowledge, none of them has been presented as trully massively parallel.
We present MOLMPS, the new C++ QC-DMRG implementation with the emphasis on scalability and high flexibility [3]. Our parallel approach employs MPI and is based on low level lightweight tensor library allowing global memory storage. By combining operator and symmetry sector parallelisms, sufficient number of tasks to achieve massive parallelization is generated. We will present the scaling tests on typical candidates for DMRG calculations, namely Fe(II)-porphyrine model, extended π-conjugated system, and FeMoCo cofactor with the active spaces containing up to 76 orbitals.
Due to its capabilities, our implementation is e.g. an ideal tool for machine learning. We believe that it has a potential to open the way for computations of challenging problems requiring very large active spaces not only in non-relativistic quantum chemistry, but due to its flexibility also for example in fully relativistic setting.

[1] G. Chan, S. Sharma, *Annu. Rev. Phys. Chem.* **62**, 465 (2011).

[2] Sz. Szalay, et al., *Int. J. Quant. Chem.* **115**, 1342 (2015).

[3] J. Brabec, J. Brandejs, Ö. Legeza, K. Kowalski, S. Xanteas, L. Veis, "Massively parallel quantum chemical density matrix renormalization group method", *in preparation*.