Advancements for the three-legged tree tensor network

Klaas Gunst[a], Frank Verstraete[a] and Dimitri Van Neck[a]

[a] *University of Ghent*
Klaas.Gunst@UGent.be

Recently, we introduced the three-legged tree tensor network state (T3NS) [1,2]. It is a variational state and a natural extension of the matrix product state (MPS) used in density matrix renormalization group theory (DMRG). Its structure allows an efficient optimization of the wave function while enjoying more flexibility in representing the entanglement of the system than the linear MPS.

In this poster, we demonstrate the spin-adapted T3NS [2]. The implementation is freely available on github [3]. Just as for DMRG, exploiting the spin and molecular point group symmetries of the quantum chemical hamiltonian provide considerable speed-ups.
Not only conserved quantum numbers such as the total spin can be easily used in the T3NS but also non-conserved quantum numbers. We demonstrate this by executing seniority-restricted calculations. In these type of calculations only Slater determinants with a certain maximal amount of unpaired electrons contribute to the optimized wave function.
When optimizing the T3NS, the convergence is dependent on the used orbitals, the ordering of the orbitals on the network and the geometry of the network. We briefly touch on this and have an outlook on future research for the optimization of the geometry and orbital ordering itself.

References

1. K. Gunst, F. Verstraete, S. Wouters, Ö. Legeza and D. Van Neck *J. Chem. Theory Comput.* **14**, 2026-2033 (2018).
2. K. Gunst, F. Verstraete and D. Van Neck, *J. Chem. Theory Comput.* **15**, 2996-3007 (2019).
3. K. Gunst, T3NS: An implementation of the three-legged tree tensor network algorithm `https://github.com/klgunst/T3NS`, 2018.