QC calculations with machine-learning assisted scheduling optimization & DMRG-SCF approach and its usage in the bio-luminescence molecules with parallel acceleration

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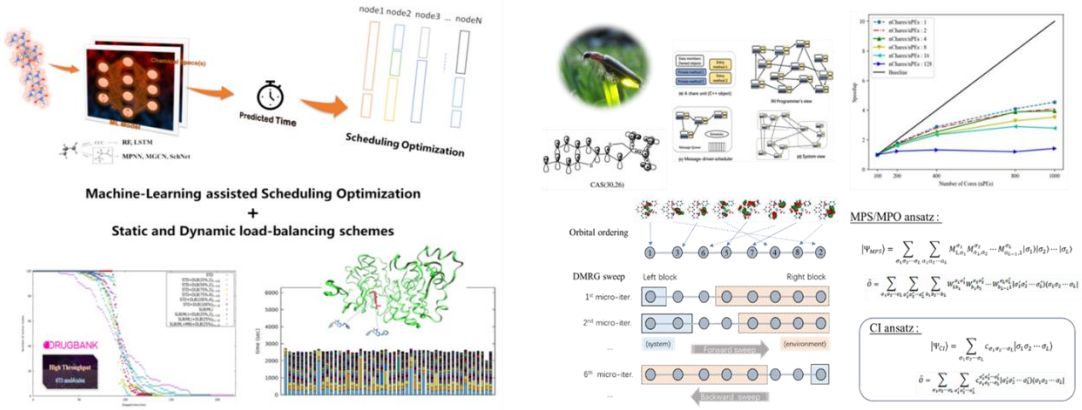
In the first part, we would like to present a procedure for easy and effective implementations of quantum-chemical (QC) calculations benefited from machine-learning assisted scheduling optimization and different load-balancing algorithms.[1,2] Employing this procedure, we showed that the high throughput and large-scale fragmentation QC calculations can primarily profit, and faster accomplishing computational tasks can be expected when employing HPC clusters.

In the second part, we would like to talk about DMRG-SCF and its gradient [3,4], and use this approach in the description of bio-luminescence molecules together with the quantum information theory and multi-reference approach [5]. The importance of utilizing full valence active spaces by means of DMRG-SCF calculations was described. Our results revealed that the neglect of some valence orbitals can affect the quantitative accuracy in later multi-reference calculations or the qualitative conclusion when optimizing conical intersections. Beyond these, different massively parallel implementations, e.g., re-constructing the CI wave function from DMRG state via *Charm++*[6] and heterogeneous refactoring post-DMRG approaches via GPU/DCU,[7] can be achieved for the study of these near-degeneracy systems.



Reference

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