General low-order scaling multiconfiguration SCF

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The complete active space MCSCF approach has been extraordinarily successful in providing a robust zero-order formulation for ground-state and low-lying excited-state electronic structure problems. Its principal defect is that its demand on computational resources grows in principle exponentially with system size; for practical applications this usually means that a difficult choice of a reduced set of active orbitals has to be made.

This poster presents a comparative analysis of some possible schemes for black-box MCSCF-like methods where the number of parameters describing the wavefunction scales algebraically with system size ($\mathcal{O}(N^4)$ or $\mathcal{O}(N^2)$). The prospects of combining such approaches with local truncation thresholds, in order to further reduce computational effort, is also discussed.