Tensor numerical methods in computational quantum chemistry

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Novel grid-based tensor numerical methods providing accuracy at the level of analytical computations are now used in grid-based solution of many problems in natural sciences. They are based on representation of d-variate functions and operators on large $n^{\otimes d}$ grids in the rank-structured tensor formats in view of results from nonlinear approximation theory and provide $O(dn)$ complexity of numerical calculations instead of $O(n^d)$ by conventional methods [5].

A starting point was the tensor-based solution of the three-dimensional integro-differential Hartree-Fock equation, which is a classical model for ab-initio calculation of the ground state energy of molecules [3]. When using tensor approach for calculation of all involved operators, the 3D analytical integration is completely avoided, and substituted by the grid-based tensor algorithms in 1D complexity [1,3]. The low-rank tensor numerical approach enables calculation of the 3D convolution integral operators in $O(n \log n)$ complexity [1]. Moreover, the low-rank two-electron integrals tensor [2] calculated in this Hartree-Fock solver enables economical computational scheme of the excitation energies and optical spectra of molecules.

Another challenge in scientific computing is the numerical modeling of the collective electrostatics for large many particle systems. Our tensor method for summation of the long-range potentials on $L \times L \times L$ 3D lattices [5] provides computational complexity of the order of $O(L)$ which is much less as compared with $O(L^3)$ in traditional approaches, like Ewald-type summation. Recent range-separated (RS) tensor format [4] is an efficient tool for computation of the collective electrostatics for multiparticle systems of general type.

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