3D lattice summation of long range potentials by assembled tensor method

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Novel tensor numerical methods are based on representation of d-variate functions and operators on large $n \times n \times \ldots \times n$ grids in rank-structured tensor formats which provide $O(dn)$ complexity of numerical calculations instead of $O(n^d)$ by conventional methods in numerical analysis. The starting point in this direction was the tensor-structured Hartree-Fock eigenvalue solver which realises a 3D grid-based calculation of all parts of the integro-differential Fock operator by tensor operations in 1D complexity [1,2,3]. The performance of the tensor-based solver in time and accuracy (for molecules) is close to standard quantum chemistry programs based on analytical evaluation of the 3D convolution integrals. Now this solver is being developed further for electronic structure calculations of large crystalline clusters, where the summation of the electrostatic potentials on large $L \times L \times L$ 3D lattices in the non-periodic case is one of the challenging problems. We invented an efficient method for summation of the long-range potentials, using the assembled vectors of the canonical tensor representation of a single Newton kernel [4], which provides the computational complexity of the order of $O(L)$ instead of $O(L^3)$ in the traditional approaches, like Ewald-type summation. For cubic 3D lattices the canonical tensor rank of the resulting sum is the same as for tensor representation of a single Newton kernel. For other shapes of potentials distributions, like L-shape, O-shape or hexagonal lattices the rank is increased by a small factor. For the case of multiple defects and vacancies in the crystalline molecular structures the Tucker rank truncation is efficiently employed [5]. Matlab simulations on a laptop will be demonstrated during the presentation for the tensor-based summation of millions of electrostatic potentials on finite 3D lattices.

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