Tensor numerical modeling of the collective electrostatic potentials of many-particle systems

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Abstract

The novel tensor-structured numerical methods appeared as bridging of the algebraic tensor decompositions and the nonlinear approximation theory on separable low-rank representation of multivariate functions and operators [1, 2]. Nowadays the rank-structured tensor approach facilitates new means for numerical modeling of long-range potentials in many-particle systems. The method of grid-based assembled tensor summation of the electrostatic potentials on $(L \times L \times L)$ 3D finite lattices [4] exhibits the computational complexity of the order of $O(L)$ which is much less than $O(L^3)$ in traditional Ewald-type summation. The canonical tensor rank of the collective potential of a finite 3D rectangular lattice system (containing millions of particles) is proven to be as low as a rank for a single reference tensor for a Newton kernel. For lattices with multiple impurities the tensor rank is increased by a small factor [2].

Recent range-separated (RS) tensor format [3] applies to many-particle systems of general type. These can be the free space electrostatic potentials of large bio-molecules or the multidimensional scattered data modeled by radial basis functions. The main advantage of the RS tensor format is that the rank of the canonical/Tucker tensor representing the sum of long range contributions from all particles in the collective potential depends only logarithmically on the number of particles N. Partitioning of long and short range parts of the potentials is performed simply by sorting vectors of the generating Newton kernel. The interaction energies and forces of the many-particle system are computed by using only the long-range part of the collective potential, with representation complexity $O(n \log N)$, where n is the univariate grid size. The basic tool for calculation of the RS tensor representation is the reduced higher order SVD (RHOSVD) introduced in [5]. The representation complexity of the short range part is $O(N)$ with a small prefactor independent on the number of particles. The numerical examples are presented.

References

[1] B.N. Khoromskij: *Tensor Numerical Methods in Scientific Computing*, De Gruyter, Berlin, 2018.

[2] V. Khoromskaia and B.N. Khoromskij: *Tensor Numerical Methods in Quantum Chemistry*, De Gruyter, Berlin, 2018.

[3] P. Benner, V. Khoromskaia and B.N. Khoromskij: *Range-Separated Tensor Format for Many-particle Modeling*, SIAM J Sci. Comput., 40(2):A1034-A1062, 2018.

[4] V. Khoromskaia, B.N. Khoromskij: *Grid-based Lattice Summation of Electrostatic Potentials by Assembled Rank-structured Tensor Approximation*, Comput. Phys. Comm., 185:3162-3174, 2014.

[5] B.N. Khoromskij and V. Khoromskaia: *Multigrid Tensor Approximation of Function Related Arrays*, SIAM J Sci. Comput., 31(4):3002-3026, 2009.