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

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We consider the rank-structured tensor approach for numerical modeling of long-range potentials in many-particle systems. The method of grid-based assembled tensor summation of the electrostatic potentials on 3D finite lattices [3] exhibits the computational complexity of the order of $O(L)$ which is much less than $O(L^3)$ in traditional Ewald-type summation.

Novel range-separated (RS) tensor format [4] applies to many-particle systems of general type. These can be the free space electrostatic potentials of large biomolecules 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. 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 interaction energies and forces of the many-particle system can be 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 new regularization scheme for the Poisson-Boltzmann equation (PBE) describing the electrostatic potential in biomolecules is based on the RS tensor representation to the discretized Dirac delta [2]. It leads to solving a single system of FDM/FEM equations only for the smooth long-range part of the initially singular right-hand side of the PBE [1]. The resulting solution of PBE is the sum of the long- and short-range parts, where the latter is precomputed by the direct tensor summations, without solving the PBE. The numerical examples are presented.

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[2] Boris N. Khoromskij. Tensor Numerical Methods in Scientific Computing. De Gruyter, Berlin, 2018.
[3] Venera Khoromskaia and Boris N. Khoromskij. Tensor Numerical Methods in Quantum Chemistry. De Gruyter, Berlin, 2018.
[4] 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.
[5] B. N. Khoromskij and V. Khoromskaia. Multigrid Tensor Approximation of Function Related Arrays. SIAM J Sci. Comput., 31(4), 3002-3026, 2009.

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