Range-separated tensor format for computation of electrostatics in large multi-particle systems

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Tensor numerical methods allow to construct computational schemes for solving d-dimensional PDEs with the linear complexity scaling in dimension, [1], [2]. We discuss how the tensor numerical methods apply to calculation of electrostatic potential of many-particle systems by using the novel Range-Separated (RS) tensor format [3]. The particular application of the RS tensor representation for numerical solution of the Poisson-Boltzmann equation modeling electrostatics in bio-molecular systems will be discussed [5]. The approach is based on application of the RS tensor decomposition for the discretized Dirac delta [4]. Numerics illustrates the efficiency of the new tensor techniques.

This talk is mainly based on the joint works with P. Benner and V. Khoromskaia.

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

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

[3] P. Benner, V. Khoromskaia and B.N. Khoromskij. *Range-separated tensor formats for many-particle modeling*. SIAM J. Sci. Comp., (2): A1034-A1062, 2018.

[4] Boris N. Khoromskij. *Range-separated tensor representation of the discretized multidimensional Dirac delta and elliptic operator inverse.* E-Preprint arXiv:1812.02684v1, 2018.

[5] P. Benner, V. Khoromskaia, B.N. Khoromskij, C. Kweyu, and M. Stein. *Computing electrostatic potentials using regularization based on the range-separated tensor format*. E-Preprint arXiv:1901.09864, 2019.