The prospects of tensor numerical methods in large-scale scientific computing

Boris N. Khoromskij

Max-Planck-Institute for Mathematics in the Sciences,
Inselstr. 22-26, D-04103 Leipzig, Germany
bokh@mis.mpg.de; *http://personal-homepages.mis.mpg.de/bokh*

Rank-structured tensor representation (approximation) of functions and operators by using the traditional canonical (CP), Tucker and tensor train (TT) formats allows the linear complexity scaling in dimension. Further data-compression to the logarithmic scale in the data size can be achieved by using the method of quantized-TT (QTT) approximation. The novel range-separated (RS) tensor format allows the efficient low-rank representation of highly non-regular functions in $\mathbb{R}^d$.

We discuss how the tensor numerical methods based on modern rank structured approximation techniques apply to the solution of complicated multi-dimensional problems in the PDE driven modeling, and for the efficient representation and analysis of large multi-dimensional data arising, for example, in machine learning. In particular, we

– demonstrate the various aspects of tensor numerical methods applied in computational quantum chemistry beginning from the Hartree-Fock model, up to calculation of excitation energies and optical spectra of molecules.

– sketch the application of RS tensor format for calculation of many-particle electrostatic potentials of bio-molecules (the Poisson-Boltzmann equation).

– show an example on how the RS tensor format can be gainfully applied in modeling and analysis of scattered data in $\mathbb{R}^d$.

– overview how the tensor numerical methods apply in stochastic homogenization of the elliptic PDEs in random composites (highly varying unstructured coefficients), and in the control problems constrained by multi-dimensional PDEs.

Talk is mainly based on the results presented in the research monographs [1,2].

[1] Boris N. Khoromskij. Tensor Numerical Methods in Scientific Computing. De Gruyter Verlag, Berlin, 2018.

[2] Venera Khoromskaia, Boris N. Khoromskij. Tensor Numerical Methods in Quantum Chemistry. De Gruyter Verlag, Berlin, 2018.