Tensor numerical methods in grid-based electronic structure calculations

Venera Khoromskaia

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

Novel tensor numerical methods are based on representation of d-variate functions and operators on large $n^{\otimes d}$ grids in the rank-structured tensor formats which provide $O(dn)$ complexity of numerical calculations instead of $O(n^d)$ by conventional methods. A starting point was the Hartree-Fock solver based on the tensor-structured calculation of the two-electron integrals, the Laplace and nuclear potential operators using a Gausssian-type basis, discretized on $n \times n \times n$ 3D Cartesian grids [1-4]. The low-rank tensor numerical approach enables calculation of the 3D convolution integral operators in $O(n \log n)$ complexity [1].

The main contribution to tensor-based electronic structure calculations is the efficient computation of the two-electron integrals tensor in a form of Cholesky factorization [3]. For all 3D operators in the Hartree-Fock equation the 3D analytical integration is completely avoided, since it is substituted by the grid-based tensor algorithms of 1D complexity. The reduced $O(\log n)$ complexity is provided by calculation of the 3D operators in the QTT tensor format [4]. Tensor methods are now developed towards calculation of excitation energies for molecules by iterative solution of the Bethe-Salpeter eigenvalue problem [6,7].

Other important direction concerns crystalline systems, where one of the challenges is the summation of electrostatic potentials on large 3D lattices in a non-periodic case [5]. Recent tensor method for summation of the long-range potentials on $L \times L \times L$ 3D finite lattices with defects provides computational complexity of the order of $O(L)$ outperforming traditional approaches like the $O(L^3)$ Ewald-type summation.

References

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

[2] B. N. Khoromskij, V. Khoromskaia and H.-J. Flad. *Numerical Solution of the Hartree-Fock Equation in Multilevel Tensor-structured Format.* SIAM J. Sci. Comp., **33**(1), 45-65 (2011).

[3] V. Khoromskaia, B.N. Khoromskij and R. Schneider. *Tensor-structured Calculation of the Two-electron Integrals in a General Basis.* SIAM J. Sci. Comp., **35** (2), A987-A1010, 2013.

[4] V. Khoromskaia, B. N. Khoromskij and R. Schneider. *QTT Representation of the Hartree and Exchange Operators in Electronic Structure Calculations.* CMAM, v.11, No.3, pp. 327-41, 2011.

[5] V. Khoromskaia and B. N. Khoromskij. *Fast tensor method for grid-based summation of long-range potentials on 3D lattices with defects.* Numer. Lin. Algebra Appl., 23, 2016, pp. 249-271.

[6] P. Benner, V. Khoromskaia and B. N. Khoromskij. *A Reduced Basis Approach for Calculation of the Bethe-Salpeter Excitation Energies using Low-Rank Tensor Factorizations.* Molecular Physics, 114 (7-8) 2016.

[7] P. Benner, S. Dolgov, V. Khoromskaia and B.N. Khoromskij. *Fast iterative solution of the Bethe-Salpeter eigenvalue problem using low-rank and QTT tensor approximation.* J. Comp. Phys., 334, 2017, 221 - 239.