

Tensor approximation in quantum chemistry

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The talk will present recent developments in tensor product approximations with a particular focus on problems in electronic structure calculations. Tensor product approximation is a tool for the treatment of high-dimensional problems. Low rank approximations of matrices, like SVD, partial Cholesky decomposition, RI techniques and pair natural orbitals have been proved to be powerful instruments in quantum chemistry. However the generalization to higher order tensors is not straightforward. We will demonstrate some examples with the so-called canonical format. Recently, new tensor formats have been introduced by several groups which allow a stable approximation of any order d tensor into order three tensors! We will discuss perspectives of these new formats for wave function methods.

Literature: