Wavelet Tensor Product Approximation in Electronic Structure Calculations

Dissertation, Universität Leipzig, June 2008

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Abstract

The most challenging problems of numerical computation are integral and differential equations in high dimensions. The tensor product approximation provides an efficient tool to represent integral operators and the inverse of elliptic operators in high dimensions. The basic idea for the representation of certain quantities in terms of tensor products is to factorize the expensive parts of the calculation in order to reduce the dimensionality and thereby the computational complexity. An efficient numerical representation of operators in high dimensions is required in a wide range of applications.

In this dissertation, we study the tensor product approximation in electronic structure calculations in particular for the Hartree-Fock method by using wavelets and a new compression algorithm based on the Newton method. Our main objective is to obtain an efficient and optimal tensor product approximation for the Fock operator and its Galerkin discretization, i.e., the Fock matrix. The optimal tensor product approximation is performed in the sense that for a given accuracy an approximate tensor with minimal rank is determined. The optimal tensor product approximation provides an interesting alternative to the traditional Gaussian-type basis functions in electronic structure calculations. In combination with stable quadrature schemes for the Coulomb potential, tensor product formats enable an efficient evaluation of complicated two-electron integrals which appear in the Fock matrix. This is demonstrated by means of best separable approximations for the electron density and Hartree potential of some molecules, where univariate components of the tensor products can be efficiently represented in wavelet bases. We then study the accuracy of Hartree-Fock energy which includes complicated two-electron integrals. We also study the sparse wavelet representation of univariate components which paves the way for the fast computation of various integrals involving the orbitals, orbital products and electron density. We present a fairly detailed error analysis, which provides the basis for further improvements of this novel approach. Our results suggest a broad range of applications within density fitting schemes, which have been recently successfully applied in quantum chemistry. Furthermore, this approach can be merged with methods from multiresolution analysis.