

Accepted Manuscript

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PII: S0045-7825(18)30106-3
DOI: <https://doi.org/10.1016/j.cma.2018.02.026>
Reference: CMA 11801

To appear in: *Comput. Methods Appl. Mech. Engrg.*

Received date : 18 August 2017
Revised date : 8 February 2018
Accepted date : 26 February 2018

Please cite this article as: P. Rai, K. Sargsyan, H. Najm, Compressed sparse tensor based quadrature for vibrational quantum mechanics integrals, *Comput. Methods Appl. Mech. Engrg.* (2018), <https://doi.org/10.1016/j.cma.2018.02.026>

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Compressed sparse tensor based quadrature for vibrational quantum mechanics integrals

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Abstract

A new method for fast evaluation of high dimensional integrals arising in quantum mechanics is proposed. The method is based on sparse approximation of a high dimensional function followed by a low-rank compression. In the first step, we interpret the high dimensional integrand as a tensor in a suitable tensor product space and determine its entries by a compressed sensing based algorithm using only a few function evaluations. Secondly, we implement a rank reduction strategy to compress this tensor in a suitable low-rank tensor format using standard tensor compression tools. This allows representing a high dimensional integrand function as a *small* sum of products of low dimensional functions. Finally, a low dimensional Gauss-Hermite quadrature rule is used to integrate this low-rank representation, thus alleviating the curse of dimensionality. Numerical tests on synthetic functions, as well as on energy correction integrals for water and formaldehyde molecules demonstrate the efficiency of this method using very few function evaluations as compared to other integration strategies.

Keywords: Low rank, High dimensional, Tensor approximation, Quantum chemistry, Sparse approximation, Quadrature

1. Introduction

Electronic structure calculations have been developed as a powerful tool that is used in several fields including chemical sciences and biochemistry, as well as material and energy sciences. In *ab initio* electronic structure calculations, for instance, computation

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