The SHARK Integral Generation and Digestion System

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The generation of integrals over basis functions (usually contracted Gaussian functions) is one of the central parts of any electronic structure package. While the principles of integral generation are well understood and have been studied for decades, there are still rather dramatic differences in the user friendliness and performance of different integral packages. In this work, a completely new integral package (named SHARK, no acronym implied) has been developed from the ground up.[1]

The SHARK algorithm essentially consists of a reformulation of the well-known and elegant McMurchie Davidson approach.[2] It leads to a very convenient factorization of the two-electron integrals that allows for the use of BLAS level 3 operations in the time critical steps. This is a major advantage since such operations are known to drive the computer hardware at peak performance. The factorization can also be exploited to fold integral generation into a specific task, such as the generation of Coulomb matrices. It is demonstrated that the performance of the algorithm is state of the art, in particular for higher angular momenta.

Perhaps even more importantly, SHARK has been designed with a new design philosophy that relieves the developer of the electronic structure program largely from having to take care of any technical aspect of integral generation other than writing a short routine that specifies how the integrals are being used in the desired context. The latter feature allowed us to delete several hundred thousand lines of legacy code and replace it with highly code.

SHARK is very flexible in being able to handle segmented-, generally contracted and partially generally contracted basis sets efficiently. SHARK is able to handle a wide variety of one- and two-electron integral kernels as well as integral derivatives.

SHARK also provides a new interface to the powerful Libint integral engine [3] that has been - and continues to be - an important library that drives the ORCA package[4]. By default, the new algorithm decides on the fly whether the SHARK or Libint algorithms are being used for a given integral batch in the interest of optimal performance.

[1] Neese, F. “The SHARK integral generation and digestion system” *J. Comp. Chem.*, **2022**, 1-16

[2] (a) McMurchie, L.; Davidson, E.R. “One and Two Electron. Integrals over Gaussian Functions” *J. Comp. Phys.*, **1978**, 26,218-231 (b) Helgaker, T.; Taylor P.R. “Gaussian Basis Sets and Molecular Integrals” In: Yarkony, D.R: (Ed) Modern Electronic Structure Theory, Part II. World Scientific, Singapore, **1995**, pp 725-856

[3] Valeev, E. **2021**, http://libint.valeyev.net/

[4] Neese, F. “The ORCA Program System - Version 5.0” *WIRES Comput. Mol. Sci.*, **2022**, e1606