Automated approach to molecular integrals for many-body electronic structure.

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Current state-of-the-art molecular electronic structure computations depend on evaluation of numerous two-electron integrals over nuclei-centered Gaussian functions. Evaluation of such integrals using recursive techniques is general and efficient. However, high performance requires complex graph-search and complicated (hand-optimized) implementation. Here we present an automated approach to implementation of recursive integrals algorithms. The advantages of our approach: 1) highly optimized solutions to the graph-search can be obtained; 2) high performance (up to 603) the approach can be applied to recursive computation of many new molecular integrals. Lastly we demonstrate how the automated approach was useful in rapid implementation of an explicitly-correlated MP2 method with linear Gaussian geminal factors.

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