ACES III: Efficient Electronic Integrals and their open-ended Derivatives for Parallel Implementations of Electronic Structure Calculations

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For the new parallel implementation of electronic structure methods in the ACES III suite of programs the present state-of-the-art algorithms for the evaluation of electronic integrals and their open-ended derivatives were implemented in new codes with attention paid to efficient execution on modern processors with a deep hierarchy of data storage including multiple caches and memory banks. Particular attention has been paid to generate efficient electronic integral block evaluation units which can be called at any time and in any sequence from the main parallel ACES III program. The coded integral modules ERD (*E*lectronic *R*epulsion *D*irect) and OED (*O*ne-*E*lectron *D*irect) have been thoroughly tested and are currently being used by several groups running ACES III on molecular calculations involving energy, gradient and Hessian evaluations at Hartree-Fock, MP2 and CC level.

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