Title:	PAREMD: A parallel program for the evaluation of momentum space properties of atoms and molecules
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Abstract:	The present work describes a code for evaluating the electron momentum density (EMD), its moments and the associated Shannon information entropy for a multi-electron molecular system. The code works specifically for electronic wave functions obtained from traditional electronic structure packages such as GAMESS and GAUSSIAN. For the momentum space orbitals, the general expression for Gaussian basis sets in position space is analytically Fourier transformed to momentum space Gaussian basis functions. The molecular orbital coefficients of the wave function are taken as an input from the output file of the electronic structure calculation. The analytic expressions of EMD are evaluated over a fine grid and the accuracy of the code is verified by a normalization check and a numerical kinetic energy evaluation which is compared with the analytic kinetic energy given by the electronic structure package. Apart from electron momentum density, electron density in position space has also been integrated into this package. The program is written in C++ and is executed through a Shell script. It is also tuned for multicore machines with shared memory through OpenMP. The program has been tested for a variety of molecules and correlated methods such as CISD, Møller–Plesset second order (MP2) theory and density functional methods. For correlated methods, the PAREMD program uses natural spin orbitals as an input. The program has been benchmarked for a variety of Gaussian basis sets for different molecules showing a linear speedup on a parallel architecture.
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