Calculating high precision, two-electron correlation data

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The aim of our work is to calculate high-accuracy two-electron correlation data using fully correlated and Hartree Fock methodologies implemented using in-house code[1], where higher than hardware double precision is essential. Although it is possible to calculate high precision data using computer algebra software, such as Maple, this comes with a substantial computational overhead. Numerically demanding linear algebra is preferred in C or C++, which requires libraries such as MPFR for arbitrary precision.

Recently, we have implemented ball arithmetic[2] for calculating two-electron integrals and Hartree Fock energies; which shows promising potential for quantum chemistry. It is shown that ball arithmetic provides rigorous error bounds for two-electron integrals and Hartree Fock energies where arbitrary precision data types suffer substantial and unpredictable error accumulation. Additionally DoubleDouble and QuadDouble data types[3] are employed within the fully correlated method to solve both sparse and dense linear systems providing high accuracy whilst minimising computational overhead. The fully correlated and Hartree Fock data provided using these in-house codes are used to calculate high accuracy correlation energies and Coulomb holes for heliogenic systems[4].

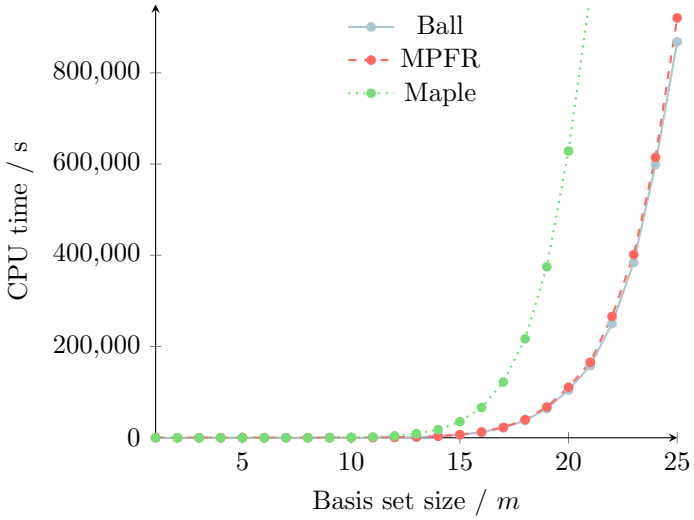

Figure 1: CPU time to calculate two-electron integrals at 200-digit precision using Ball arithmetic, MPFR and Maple.

References

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3. D. H. Bailey, et al., *qd - High-Precision Software Directory.* `www.davidhbailey.com/dhbsoftware/`.
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