Recently we developed a RAM-based I/O layer in MOLCAS called Files In Memory (FiM). In framework of FiM scratch data generated and processed by MOLCAS module reside entirely in RAM throughout the computation. Unlike to the memory-resident I/O layer of CRAY FFIO [1], FiM is a general framework and can be used on any POSIX compliant operation system such as Linux, AIX, Windows, Solaris.

The beauty of FiM that it is easy to use for both MOLCAS end user and developer: there is no need to change source code, one just needs to edit an external resource file! In addition, FiM provides environment variables that control the execution of MOLCAS and automatic (dynamical) switching between I/O layers at runtime.

By design, FiM provides precise control over data needed for solving a problem and provides functionality for: efficient debugging, analysis of intermediate data and verifying the numerical stability of quantum chemistry algorithms implemented.

In particular, test for numerical stability is accomplished by adding artificial numerical noise to requested/used data at every ‘read/write’ I/O operation. The numerical noise is constructed as random floating point number from a user-specified interval $[\delta_{\min}, \delta_{\max}]$.

![IEEE Standard 754 Floating-point](image)

For instance, for single precision the corresponding numerical noise will be in the range $[-2^{-24}, 2^{-24}]$.

Our approach does not introduce substantial computational overhead and thus can be applied for large systems!

- Halves memory demands;
- On modern processing units single precision arithmetic at least 2x times faster than double precision arithmetic;
- High Throughput 64-c<=32 conversion: 3.5 Gb/s;
- CASPT2 code spends up to 80% of the computational time in DGEMM.

By using FiM with perturbing the CD-CASPT2 data used and the benchmarks suite for the electronically excited states (196 valence excitations in 26 organic molecules) [2], we found that single precision can be sufficient for the CD-CASPT2 method. Specifically, the error introduced in CD-CASPT2 total and excitations energies are typically on the order of $10^{-6}$ hartree or even less.

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References


http://www.molcas.org