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Performance/Scaling of the UKRMol Code

The UKRmol+ code is parallelized using a combination of OpenMP and MPI. Table I shows the scaling of the UKRmol+ code on ARCHER for the diagonalization of the Hamiltonian matrix in an electron-uracil calculation. The "Expected" scaling is given approximately by (Configurations)3/(tasks).

MPI tasks	Configurations	Time	Expected
32	19668	10m 48s	-
121	39725	19m 41s	23m 32s
2025	135835	37m 39s	56m 13s

TABLE I. UKRmol+ Hamiltonian diagonalization for electron-uracil calculation for the number of configurations indicated run on ARCHER. The 'Expected' scaling is given approximately by $(\text{Configurations})^3/(\text{tasks})$

Figure 1 shows the scaling of the construction of the Hamiltonian matrix by MPI-SCATCI for phosphoric acid. The linear scaling begins to deteriorate at about 32 cores.

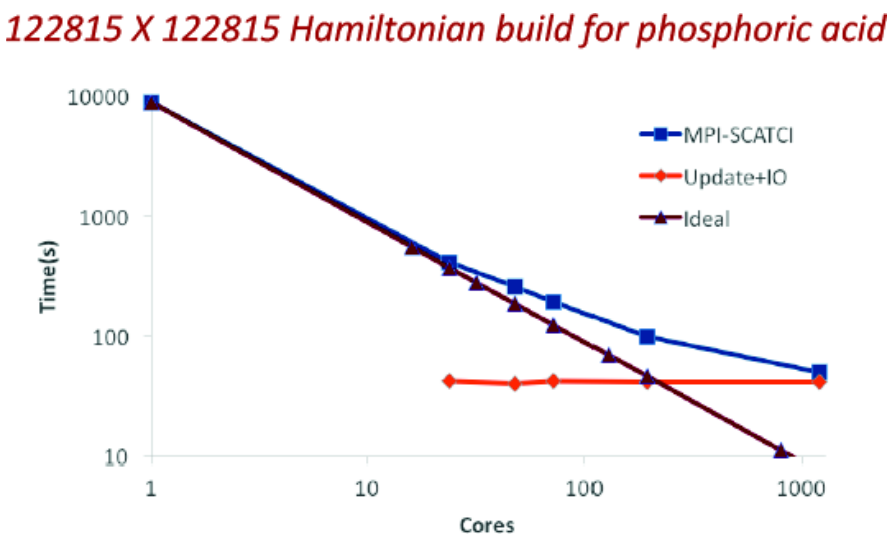

FIG. 1. UKRmol+ Hamiltonian construction for electron-scattering from phosphoric acid using the program MPI-SCATCI. The update+IO time is the time taken for MPI synchronization steps that include disk writes. The time taken by MPI-SCATCI includes the update+IO time.