



TREX QMC Code: NECI

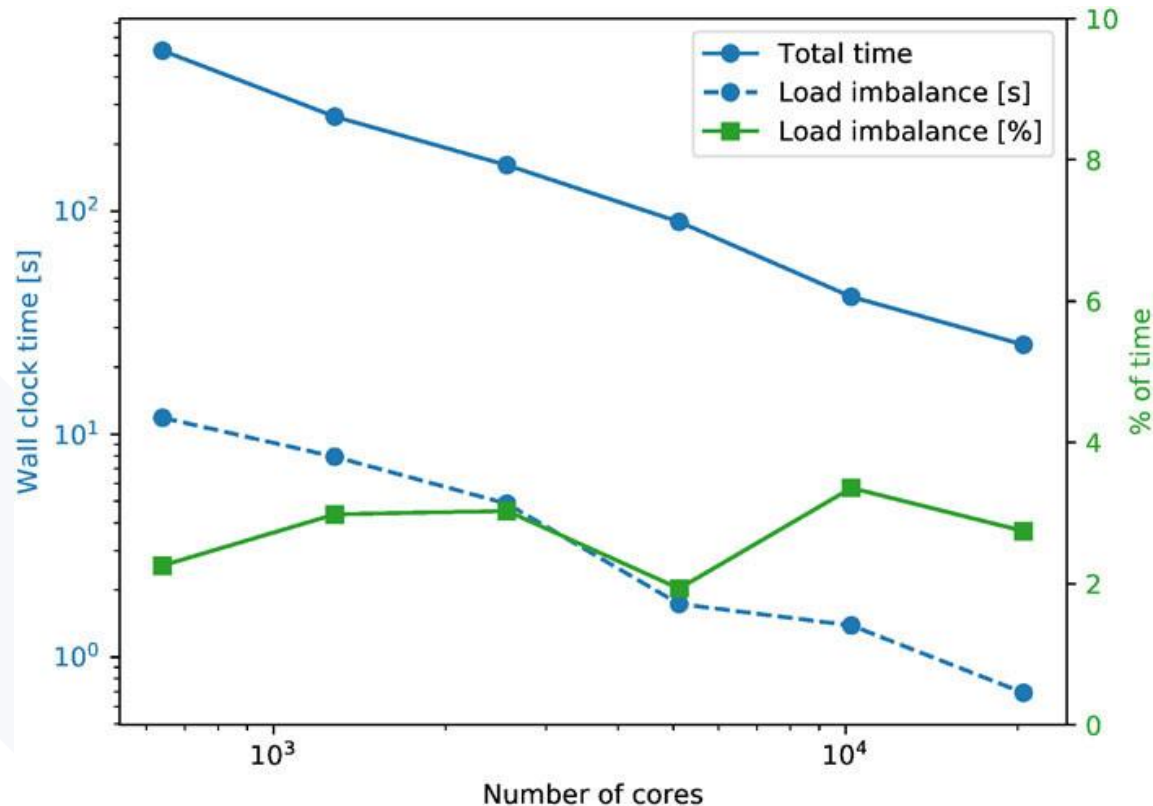


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NECI: Stochastic Full Configuration Interaction Solver (FCIQMC)

- Second-quantized Schrodinger and **Transcorrelated** (similarity-transformed) Hamiltonians based on Jastrow-factorized wavefunctions
- TC method: Non-Hermitian Hamiltonians and **3-body** interactions
- Annihilating random walkers in Slater determinant and **Spin-adapted** Hilbert spaces
- Particular emphasis on strongly **open-shell** chemistry problems (FeS complexes WP5)
- Strong scaling parallalisability demonstrated up to **20480** processes (MPI)
- TRESIO compatible **TCHint** library for calculation of 2-body and 3-body interactions (WP2).



Total time and time lost due to load imbalance for running 100 iterations with 1.6×10^9 walkers for the $Cr_2/cc\text{-}pVDZ$ (28e in 76o) on 640–20 480 cores (not counting initialization). The calculations were run on Intel Xeon Gold 6148 Skylake processors with a 100 Gb/s OmniPath node interconnect.

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