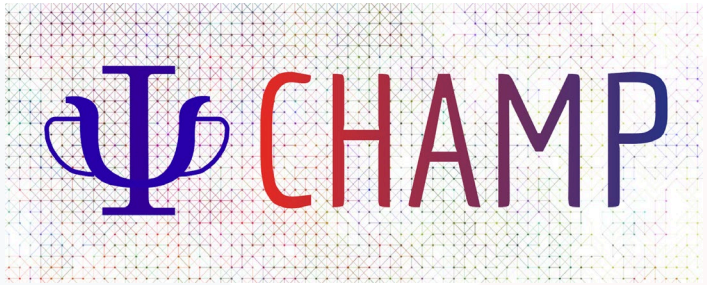
CHAMP : Cornell-Holland Ab-initio Materials Package

QMC suite of programs for accurate electronic structure calculations of molecular systems



Dr. Ravindra Shinde
University of Twente, Netherlands

CHAMP : Cornell-Holland Ab-initio Materials Package

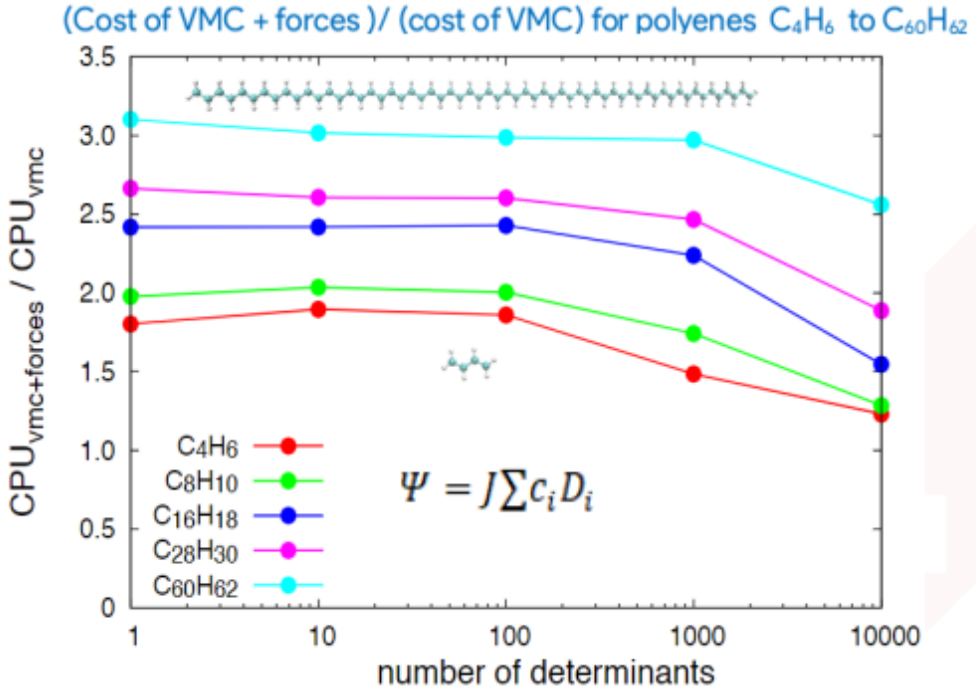
QMC suite of programs for accurate electronic structure calculations of molecular and periodic systems

Noteworthy functionalities

- Efficient optimization schemes for ground and excited states in VMC
  - ⟹ State-specific energy minimization implemented
- Efficient analytical interatomic forces in VMC
- Fast evaluation of multi-determinants and their derivatives
- Multiscale hybrid QMC calculations (QMC/PCM, QMC/MM, and QMC/MMpol)

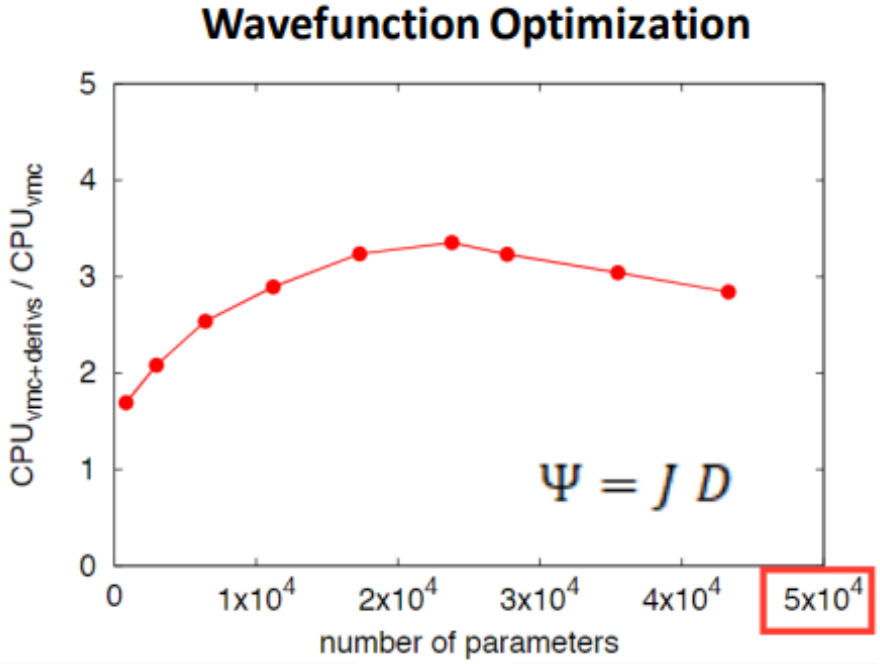
Noteworthy functionalities

Geometry Optimization



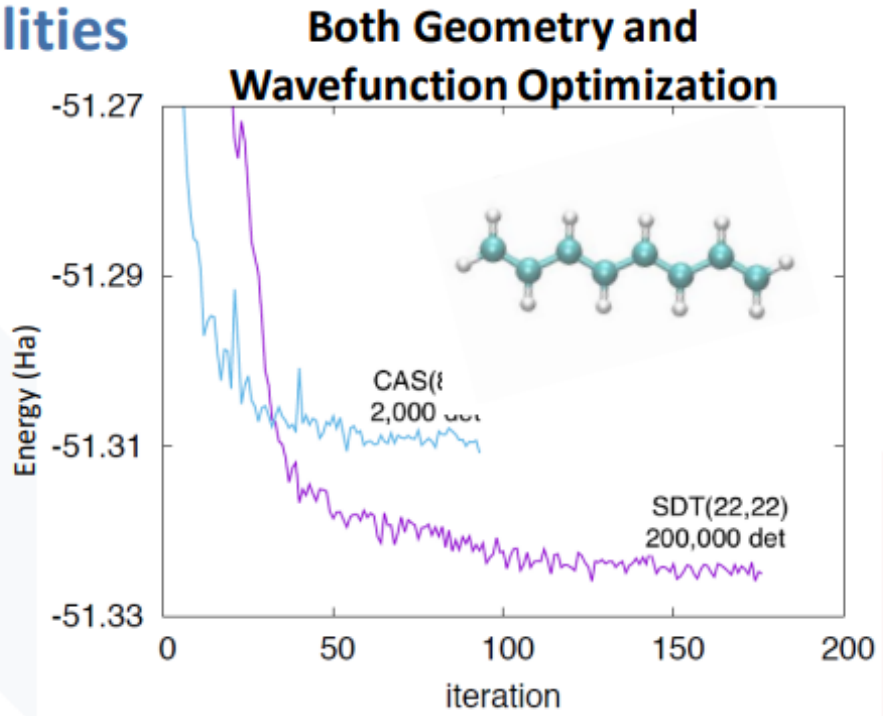
Efficient analytical interatomic forces in VMC

Noteworthy functionalities



Fast evaluation of multideterminants and their derivs

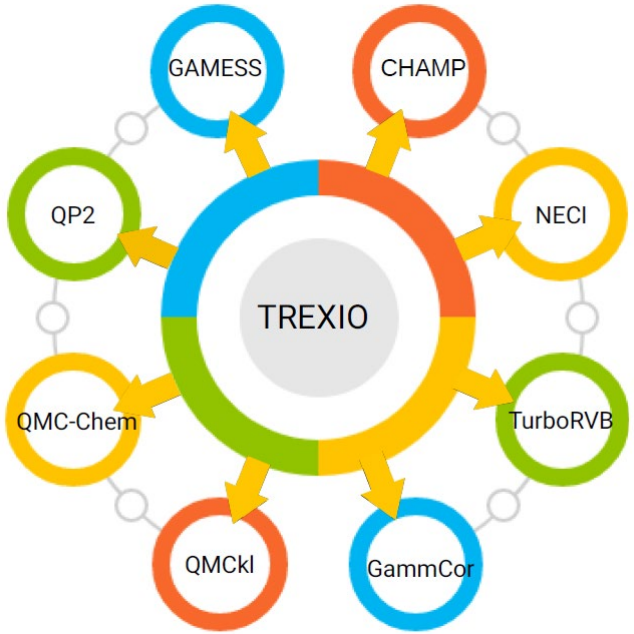
Noteworthy functionalities



65000 wave function parameter optimization of C_8H_{10}

Efficient optimization schemes for ground and excited states in VMC

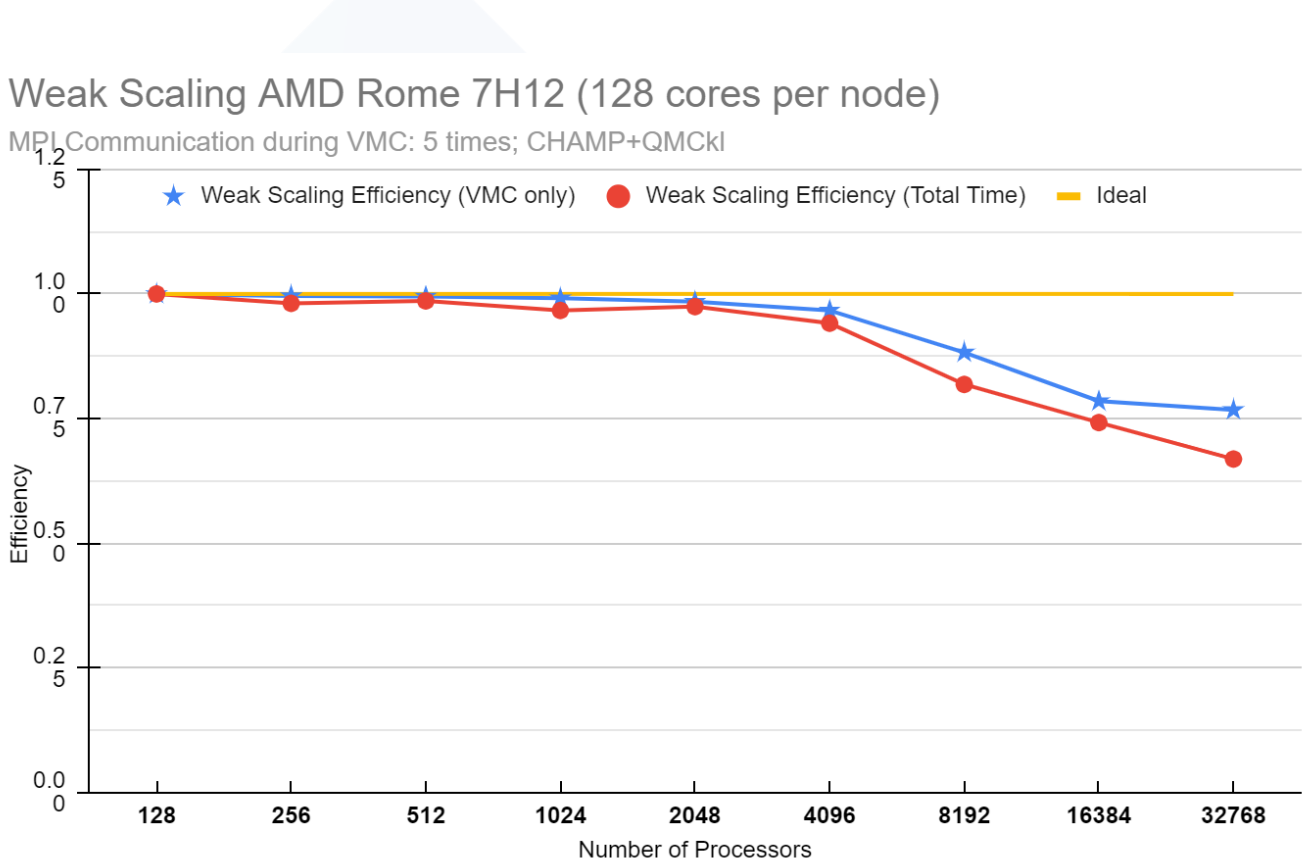
Interoperability with codes within and outside TREX using trexio

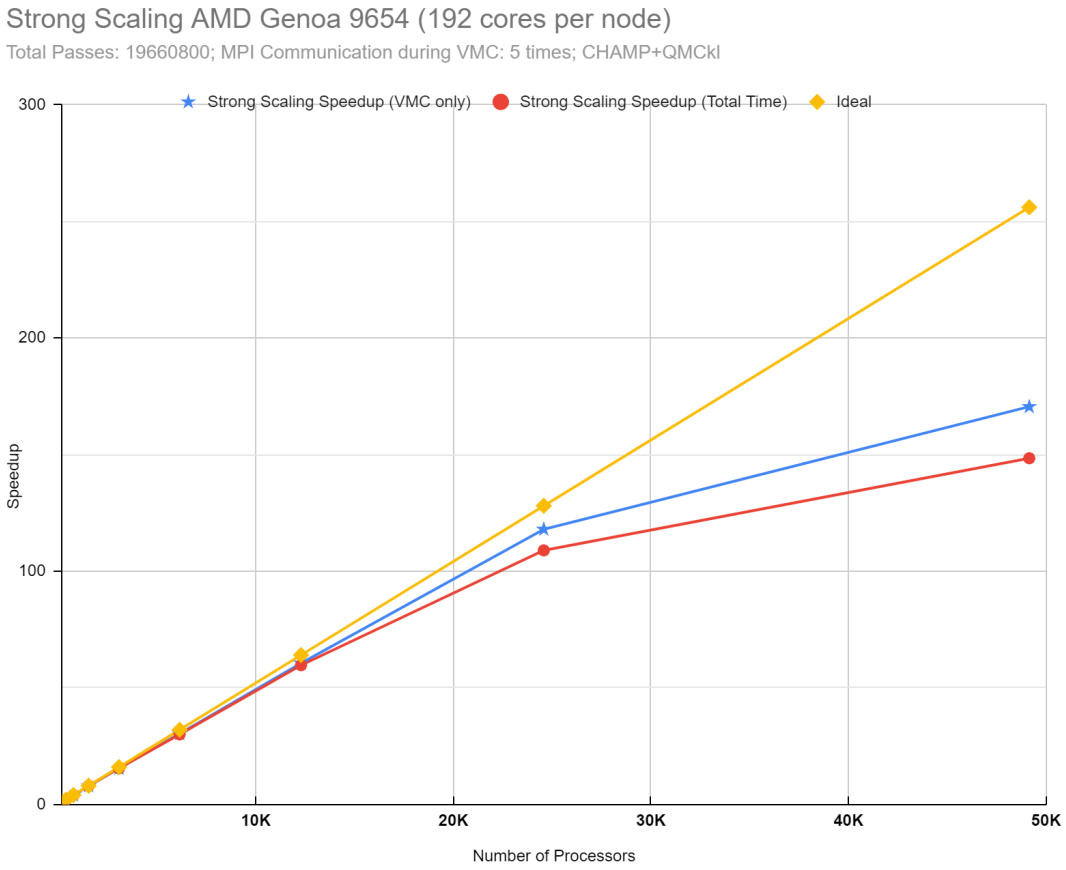


Massive parallelization and efficient scaling

- Improved vectorization
- Improved I/O
- Highly scalable
- QMCkl library for highly-efficient, optimized, scalable, common QMC tasks
- Code ported on Lumi, Fugaku, Snellius, Juwels

Massive parallelization and efficient scaling





Codes available on GitHub

Acknowledgements