



CHAMP : Cornell-Holland Ab-initio Materials Package

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

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

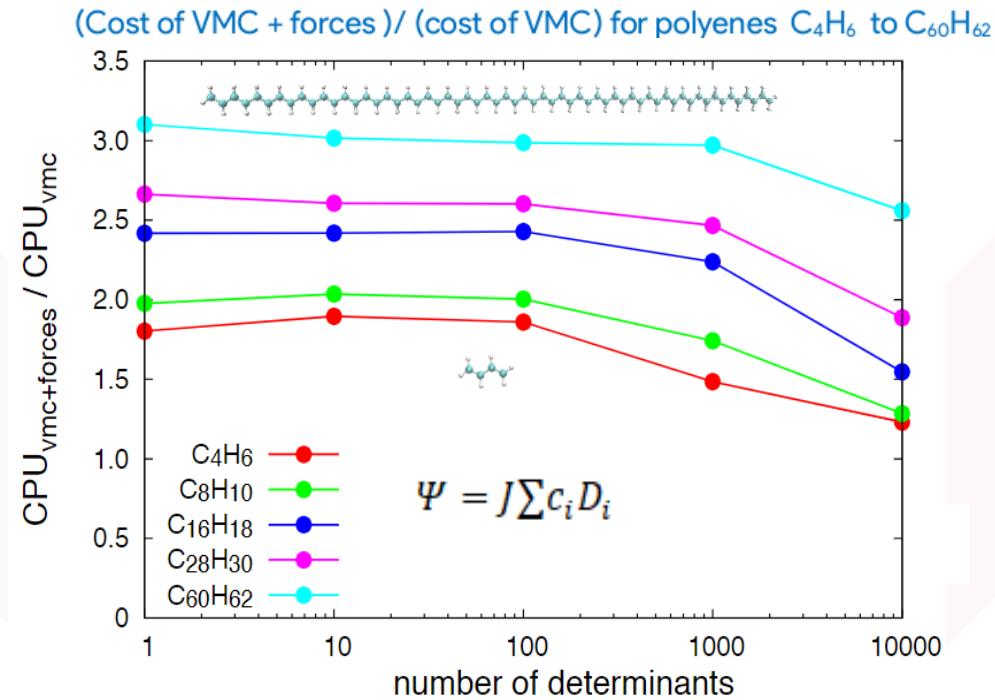
Noteworthy functionalities

- 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

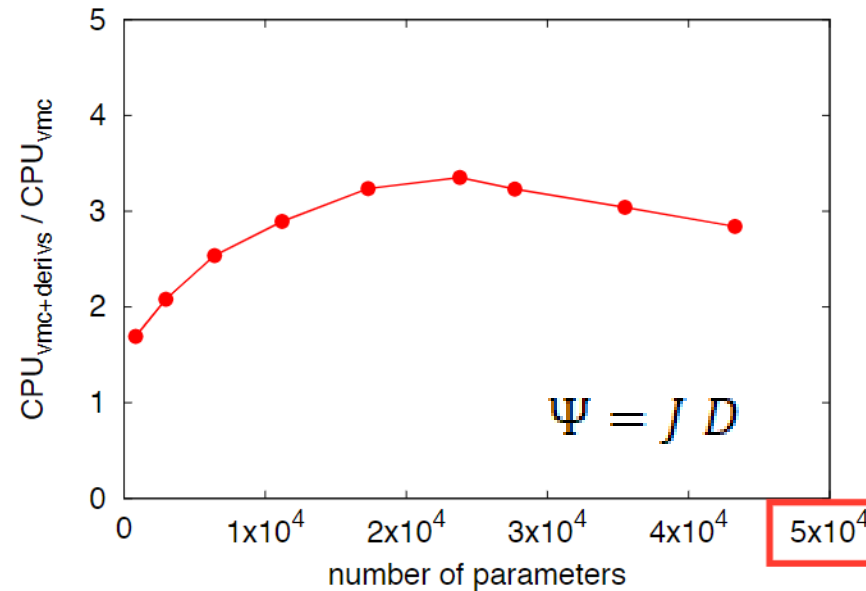


Efficient analytical interatomic forces in VMC



Noteworthy functionalities

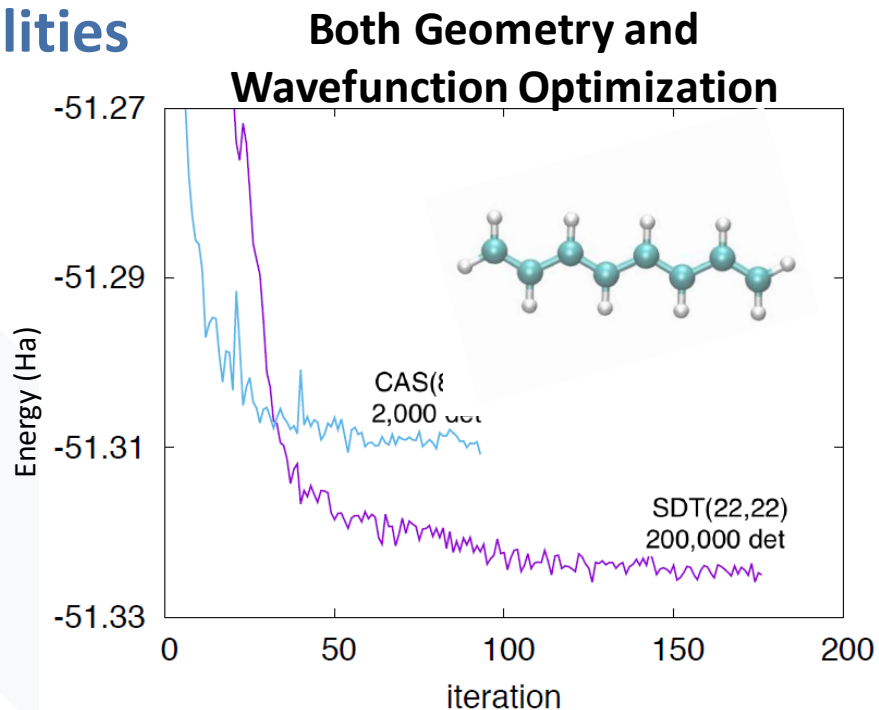
Wavefunction Optimization



Fast evaluation of multideterminants and their derivs



Noteworthy functionalities



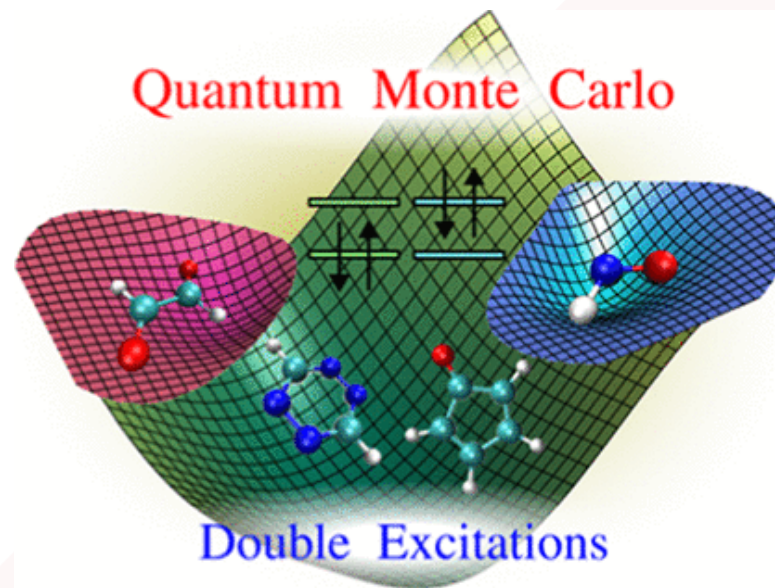
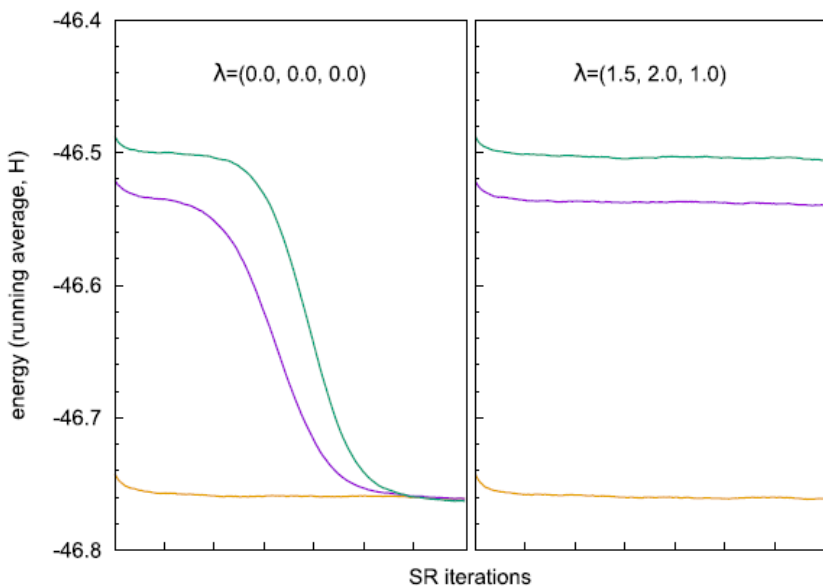
65000 wave function parameter optimization of C_8H_{10}

Efficient optimization schemes for ground and excited states in VMC

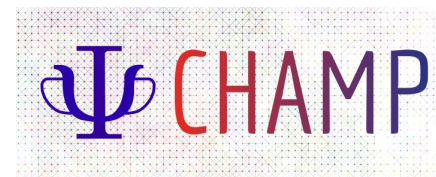


Noteworthy functionalities

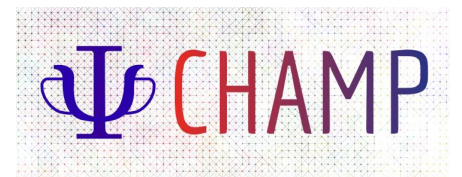
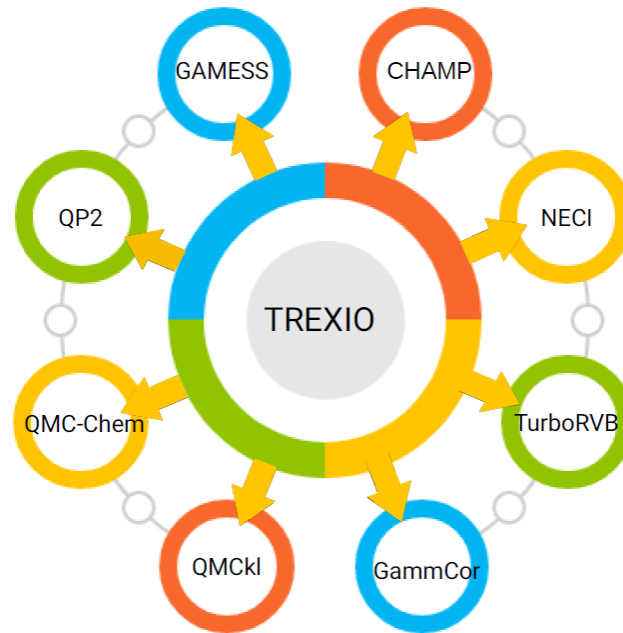
With constraints



State-specific energy optimization

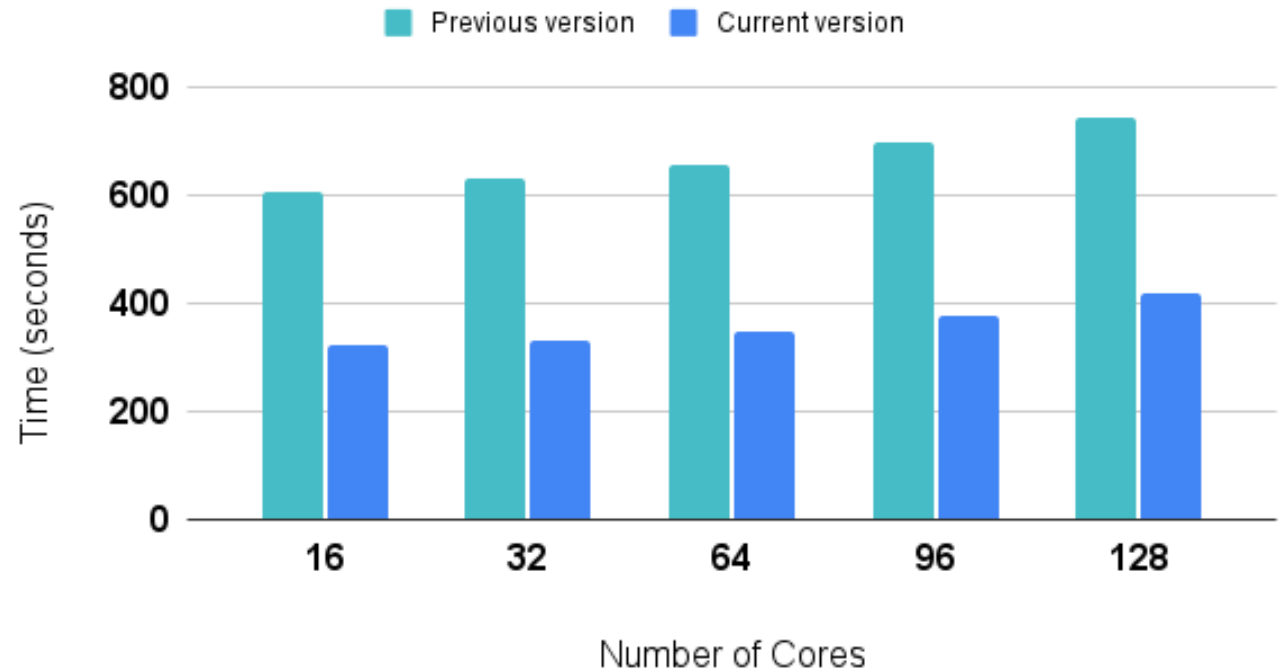


Interoperability with codes within and outside TREX



Massive parallelization and efficient scaling

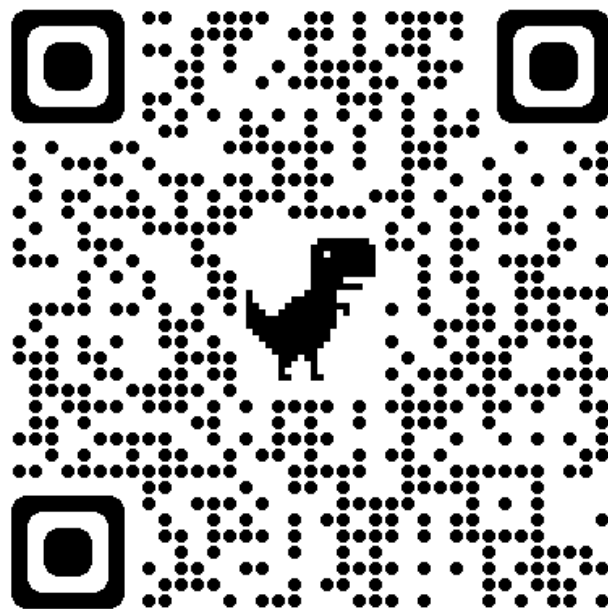
- Improved vectorization
- QMCKI library for highly-efficient, optimized, scalable, common QMC tasks



Run on Snellius/SURFsara AMD Epyc 128 cores/node

Total energy calculation

Codes available on GitHub



Thank you!

