Targeting Real chemical accuracy at the EXascale

TREX High Performance Software Solutions for Quantum Mechanical Simulations at the Exascale

Webinar, 8 February 2023

Sara Pittonet, Trust-IT

Targeting Real Chemical Accuracy at the Exascale project has received funding from the European Union Horizoon 2020 research and innovation programme under Grant Agreement **No. 952165.**

About this Webinar

This webinar will guide participants through the six different quantum chemistry codes, and the open-source libraries developed in the framework of the TREX Centre of Excellence, optimised for upcoming Exascale systems and ready to be integrated into quantum chemical codes which thus could benefit from the Exascale transition.

trex-coe.eu

About you!


Universitat de Barcelona
CNRS
University of Twente
Institute of Nano Science and Technology Mohali, India
Chalmers university
Forschungszentrum Juelich
BWI
University of Iceland
JNCASR
Université de Bejaia
E4 Computer Engineeering SpA
University of South Florida
UCLA
SVNIT
IFM, Linkoping University
Barcelona Supercomputing Center
STFC Daresbury Laboratory
Institute of Electrophysics UB RAS
University of Nairobi
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University of the Witwatersrand, Johannesburg, South Africa
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Weizmann Institute of Science
GSFC University, Vadodara, Gujarat, India
Nilamber-Pitamber University
University of South Carolina
Faculty of Sciences and Technologies Sultan Moulay Slimane U
University of Bologna, Italy
National Research and Innovation Agency (BRIN)
Indian Institute of Technology Indore India

Agenda/ part 1
TREX inter-operable QMC codes for exascale application

Time	Title	Speaker
15:00-15:10	TREX Quantum MonteCarlo Methods and benefits from the Exascale transition. Welcome overview	**Claudia Filippi**, TREX project Coordinator
15:10-15:15	NECI	**Ali Alavi**, Director of the Max Planck Institute for Solid State Research
15:15-15:20	GAMMCOR	**Kasia Pernal**, Professor at the Institute of Physics at the Lodz University of Technology (TUL) and a leader of the Quantum Chemistry Group
15:20-15:25	TurboRVB	**Kosuke Nakano**, Research Associate, SISSA
15:25-15:30	CHAMP	**Ravindra Shinde**, Research Scientist, University of Twente
15:30-15:35	QMC=Chem	**Anthony Scemama**, Senior Research Engineer, CNRS
15:35-15:40	Quantum Package	**Emmanuel Giner**, CNRS, Paris
15:40-15:50	TREX I/O library	**Evgeny Posenitskiy**, a former member of TREX, Qubit Pharmaceuticals

Agenda/ part 2
Case of use of TREX codes

Time	Title	Speaker
16:00 – 16:25	Experience in using TREX codes	**Anthony Ferté** (University of Nantes) - using Quantum Package **Pablo Lopez Rios** - using NECI **Giacomo Tenti and Andrea Zen**, Sissa **Stuart Shepard** (University of Twente) - using CHAMP

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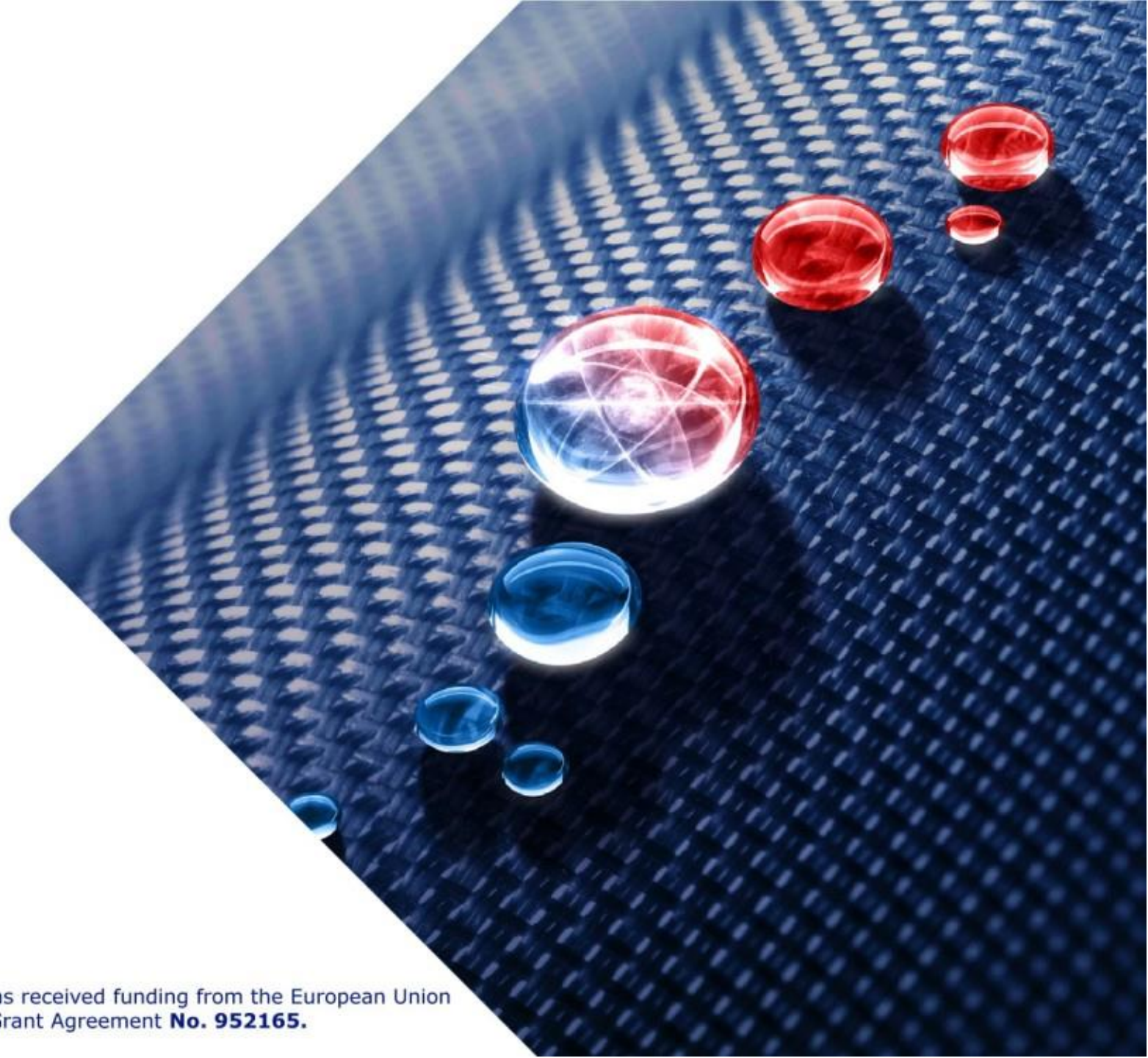
Introduction TREX Center of Excellence

Claudia Filippi

University of Twente, NL



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TREX - Center of Excellence in Exascale Computing

European Commission | CORDIS EU research results

English EN

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HORIZON 2020

Targeting Real chemical accuracy at the EXascale

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Project description

DE EN ES FR IT PL

Complex quantum molecular simulations of unprecedented speed and accuracy

Computers and the rapid mathematical calculations they are able to perform, which would take human beings years to accomplish, have provided the fuel to power innovation. High-performance computing (HPC) and high-throughput computing (HTC) have enabled us to simulate large-scale complex processes and analyse tremendous amounts of data, benefitting applications ranging from climate research and drug discovery to material design. Emerging exascale computers will make the best even better, 50 times faster than today's most powerful supercomputers. The EU-funded TREX project is developing a platform that combines the upcoming exascale HPC and HTC architectures for stochastic quantum chemical simulations of unprecedented accuracy. The software and services will be designed for ease of use to ensure widespread utilisation, spurring a new age of discovery in molecular simulations.

Hide the project objective

Project Information

TREX

Grant agreement ID: 952165

Status
Ongoing project

Start date 1 October 2020

End date 30 September 2023

Funded under
H2020-EU.1.4.1.3.

Overall budget
€ 4 998 847,50

EU contribution
€ 4 998 847,50

Coordinated by
UNIVERSITEIT TWENTE
Netherlands

TREX - Targeting Real chemical accuracy at the EXascale

— Started in October 2020

– Focus → High-accuracy quantum chemical approaches

  -
  -

– Objective → make codes ready for exascale systems

– How → provide libraries instead of monolithic codes

  - In particular, stochastic Monte Carlo (QMC) methods Massively parallelisable n
  - One library for high-performance QMC (QMC=Chem)
  - One library for exchanging info between codes (TREXIO)

high-performance QMC (QMC=Chem)

Scientists in quantum chemistry, physics, and machine learning

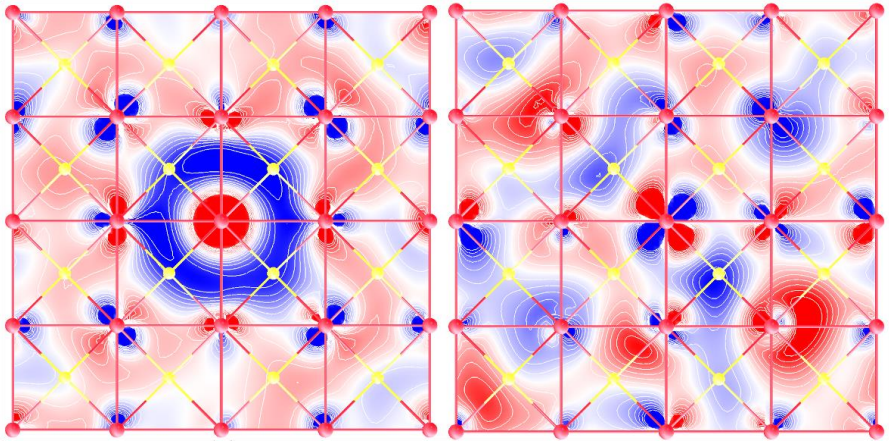
+ Software and HPC experts + Tech and communication SMEs

+ Representative of user communities

Quantum Monte Carlo

→ Stochastic simulation of the quantum interacting problem

Very accurate calculations for medium-large molecules and periodic systems!



Casula and Sorella (2013)

CPU intensive but can scale to massive parallelism

Quantum Monte Carlo and exascale: why now?

Ease in parallelization of QMC is not sufficient for accurate results

Recent methodological advances → new prospects

— Efficient computation of analytical energy derivatives + optimization tools

→ QMC "internally consistent" method

with geometries and wave functions determined in QMC

— Truly exploit freedom of choice of wave function $\Psi(r_1, \ldots, r_N)$

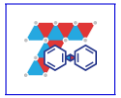
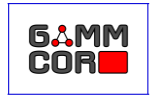
→ development of new functional forms (geminals, FermiNet ..)

Software model → HPC platform of interoperable codes/libraries

- QMCkl high-performance (CPU and GPU) library of QMC kernels
- TREXIO library to exchange wave function data

  → Easy use of TREX + other codes (GAMESS, PySCF, Gaussian …) in a pipeline
- TREX codes refactored and modularized to use these libraries
- Machine learning tools integrated in our workflows

  → AiiDA Informatics Framework adopted for workflow managment/HTC

- Real-space QMC:  CHAMP,  QMC=Chem,  TurboRVB
- Full configuration interaction QMC:  NECI
- Deterministic quantum chemical codes:  Quantum Package,  GammCor

- Real-space QMC: CHAMP, QMC=Chem, TurboRVB
- Full configuration interaction QMC: NECI
- Deterministic quantum chemical codes: Quantum Package, GammCor
- Machine learning: QMMLPACK
- Performance and optimization tools: MAQAO, Verificarlo
- Software for cloud-style access to HPC resources: MEGWARE

- TREX website : https://trex-coe.eu
- Training :

  https://trex-coe.eu/trex-training-and-educational-programme
- TREX repository : https://github.com/TREX-CoE

- Presentation of codes and TREXIO library
- Presentation of examples of use of codes

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TREX QMC Code: NECI

Ali Alavi,

Director of the Max Planck Institute for Solid State Research

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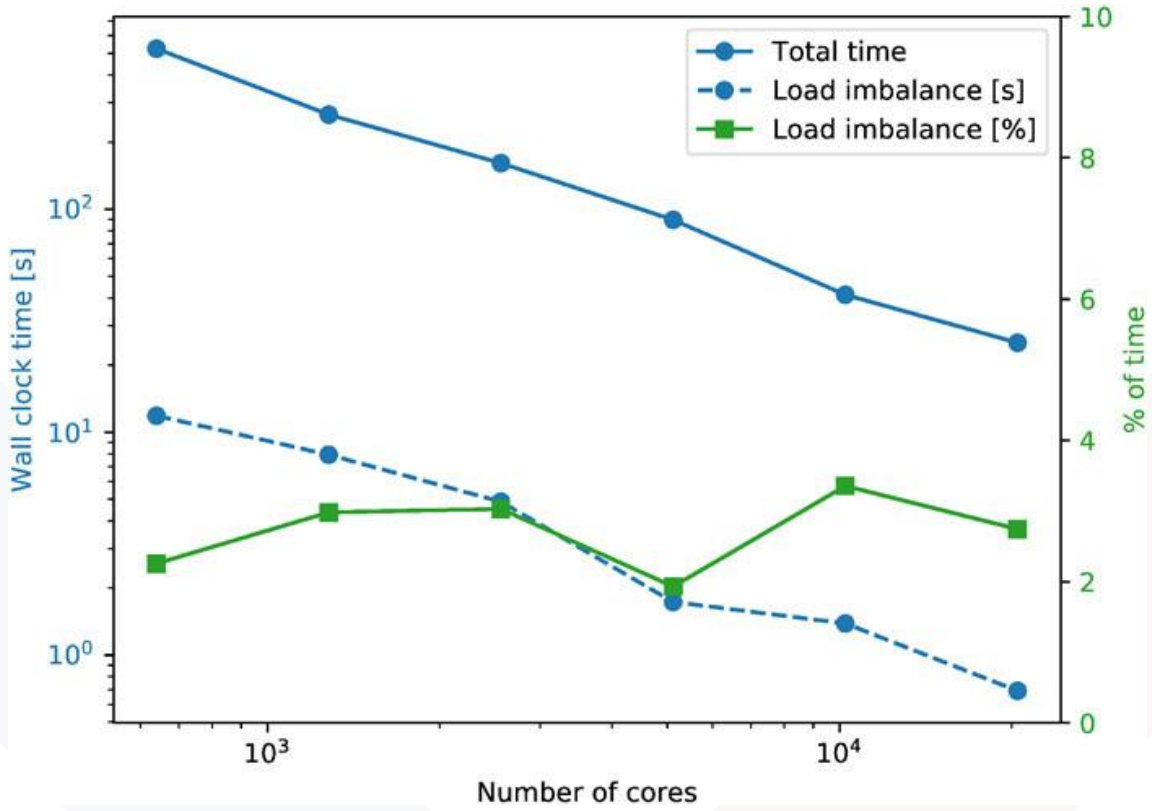
8 February 2023

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)
- TREXIO 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-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.

Guther et al ; *J. Chem. Phys.* **153,** 034107 (2020) DOI: 10.1063/5.0005754

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TREX QMC Code:

GAMMCOR

Kasia Pernal,
Professor at the Institute of Physics at the Lodz University of Technology (TUL) and a leader of the Quantum Chemistry Group

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GammCor: electron correlation and molecular interaction calculations

Authors: K. Pernal, M. Hapka, M. Modrzejewski, M. Przybytek

- Electron correlation energy for strongly correlated molecules
  unique feature: capable of treating ~10^2 strongly correlated electrons
- Molecular interaction energy decomposed into physically meaningful components
  unique features: applicable to electronically excited systems (local excitons), open-shell molecules, and molecules out of equilibrium geometries; visualization of dispersion energy density in real space.

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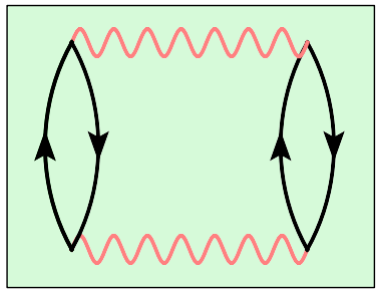
  unique feature: capable of treating ~10^2 strongly correlated electrons
- Molecular interaction energy decomposed into physically meaningful components
  unique features: applicable to electronically excited systems (local excitons), open-shell molecules, and molecules out of equilibrium geometries; visualization of dispersion energy density in real space.

Interoperability with other codes:

- Requires 1- and particle reduced density matrices
- Compatible with **TREXIO** library
- Interfaced with: Molpro, Dalton, Quantum Package, Orca

Interaction energy in molecular complexes with localized excitons

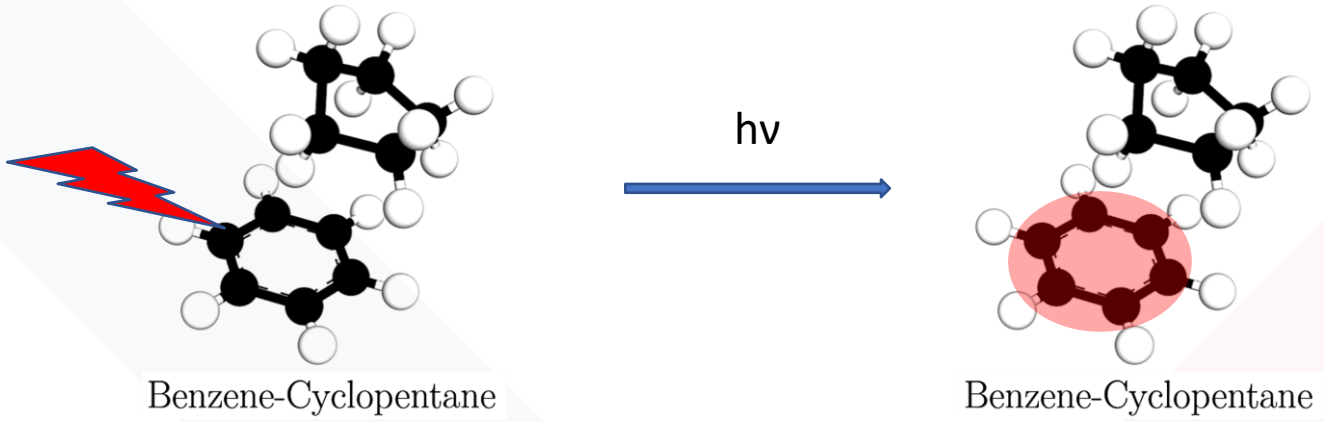
$\{\gamma,\ \Gamma\}$ →  →

$$E_{\text{int}}^{\text{SAPT(MC)}} = E_{\text{elst}}^{(1)} + E_{\text{exch}}^{(1)} + E_{\text{ind}}^{(2)} + E_{\text{exch-ind}}^{(2)} + E_{\text{disp}}^{(2)} + E_{\text{exch-disp}}^{(2)}$$

MC-WF ERPA multiconfigurational SAPT

M. Hapka et al., J. Chem. Theory Comput., 17, 5538 (2021)

Interaction energy in molecular complexes with localized excitons



E_{int} changes by 0.15 kcal/mol. Mainly electrostatic and dispersion interaction effects.

SAPT(MC) in GammCor: up to 10^2 electrons in 10^3 basis set functions.

Wavefunctions for monomers: CASSCF, CI.

M.R. Jangrouei et al., J. Chem. Theory Comput., 18, 3497 (2022)

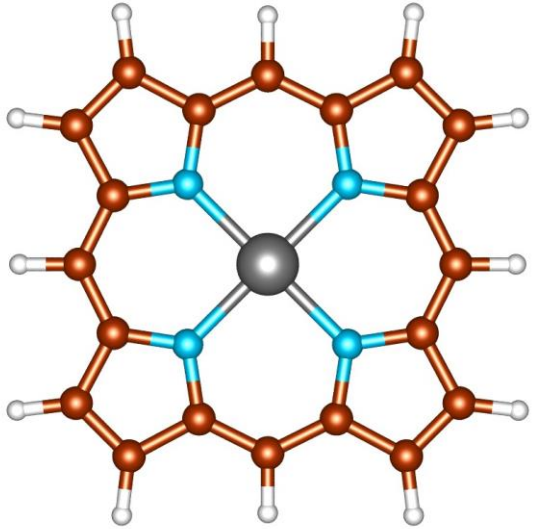
Density Matrix Renormalization Group with **Dynamical Correlation via Adiabatic Connection**

$$E = E^{\mathrm{DMRG}} + E^{\mathrm{AC}}_{\mathrm{corr}}$$

MOLMPS

GAMMCOR

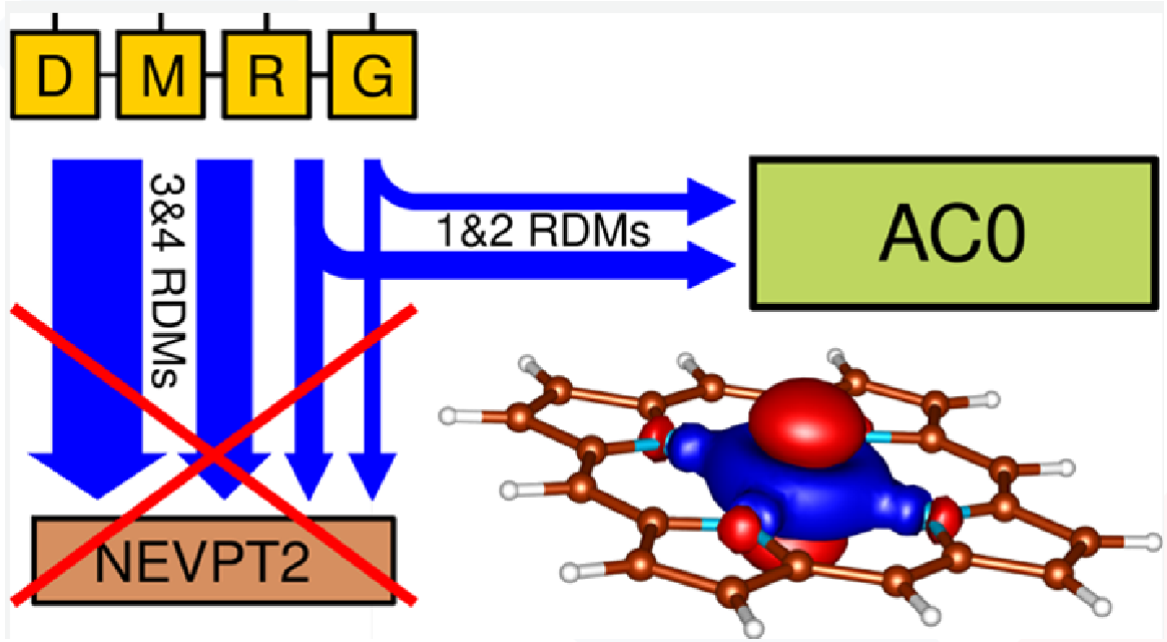
1,2-RDMs



P. Beran et al., J. Chem. Theory Comput., 17, 7575 (2021)

GAMMCOR

Density Matrix Renormalization Group with **Dynamical Correlation via Adiabatic Connection**



Fe(II)-porphyrin

Quintet-Triplet energy gap

40 active electrons in 42 orbitals

Wall Time of AC0 calc.: ~10^3 sec.

P. Beran et al., J. Chem. Theory Comput., 17, 7575 (2021)

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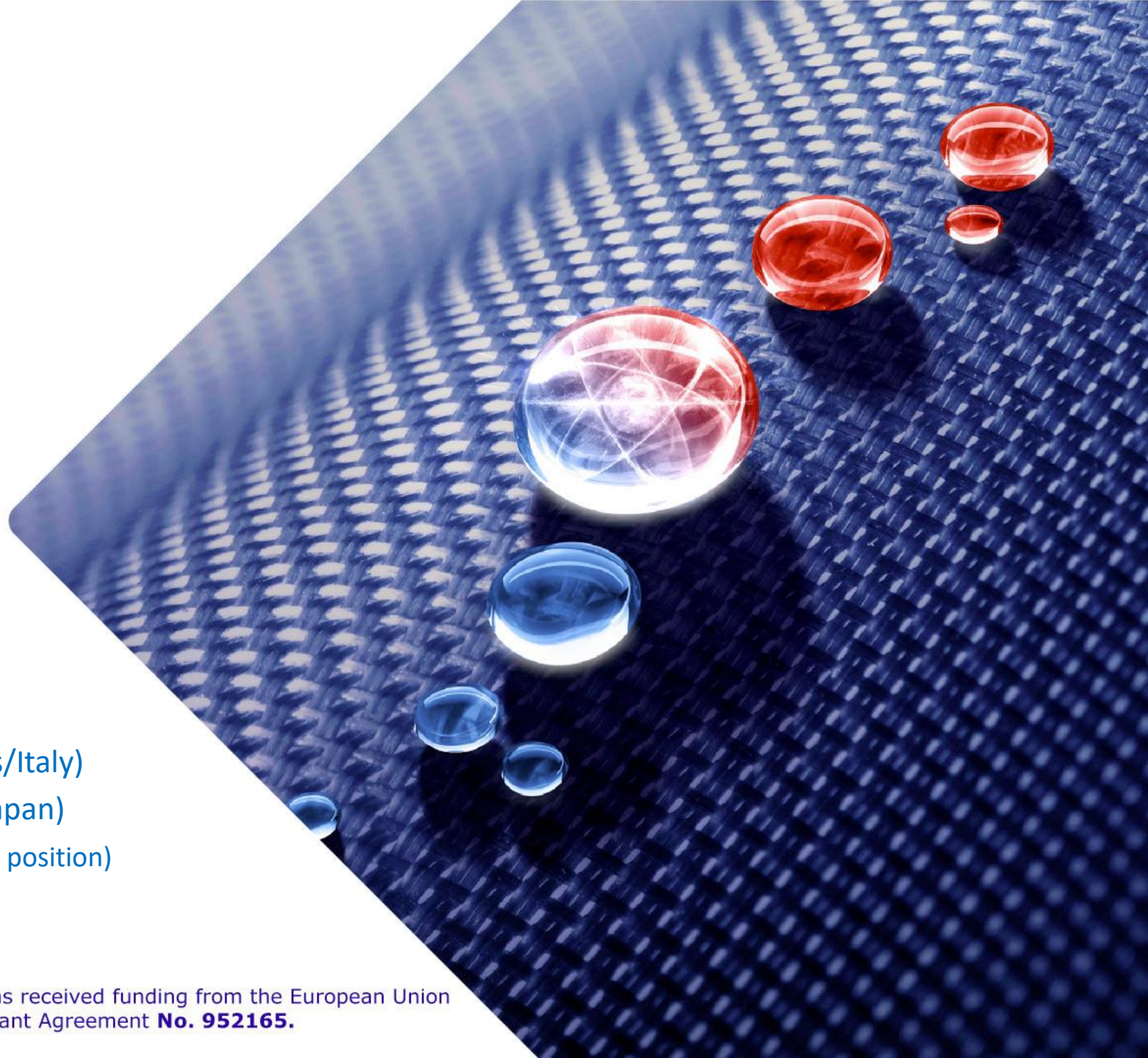
TurboRVB and TurboWorkflows



Kosuke Nakano

- SISSA (International School for Advanced Studies/Italy)
- NIMS (National Institute for Materials Science/Japan)

(Current position)

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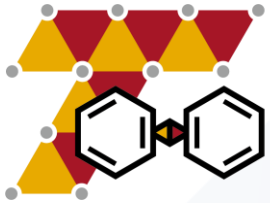
Packages: TurboRVB and TurboWorkflows



TurboRVB
Quantum Monte Carlo Package SISSA

QMC engines (DFT, VMC, and DMC).

K. Nakano, C. Attaccalite, M. Barborini, L. Capriotti, M. Casula, E. Coccia, M. Dagrada, Y. Luo, G. Mazzola, A. Zen, and S. Sorella, ***J. Chem. Phys.*** 152, 204121 (2020)

TurboGenius

Command line tools (python).

Turbo Workflows

Workflow systems (python).

K. Nakano et al., ***in preparation*** (2023)

TurboRVB Quantum Monte Carlo Package SISSA

The main developer was Prof. Sandro Sorella.

The project PIs are M. Casula and K. Nakano.

open-source by July 2023!!

- Variational Monte Carlo (VMC) and Lattice regularized Diffusion Monte Carlo (LRDMC).

M. Casula et al., ***Phys. Rev. Lett*** 95, 100201 (2005)

- Atomic Forces by exploiting the algorithmic differentiation (AD).

S. Sorella et al., ***J. Chem. Phys.*** 133, 234111 (2010)

- Flexible ansatz such as Antisymmetrized Geminal Power (AGP) and Pfaffian (Pf).

M. Casula et al., ***J. Chem. Phys. 119***, 6500 (2003)

C. Genovese et al., ***J. Chem. Theory Comput.*** 16, 6114 (2020)

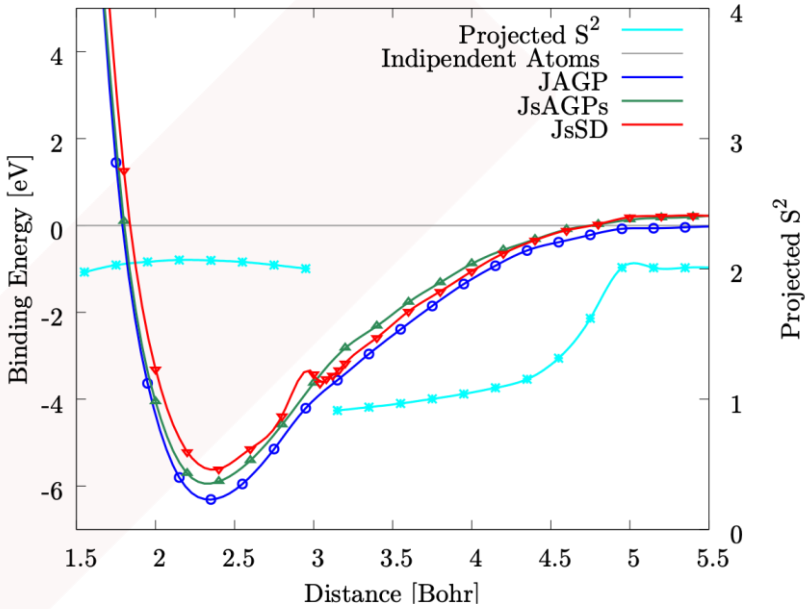
- Parallelized by MPI/OpenMP (hybrid) and GPU.

O. Kohulak et al., in prerаration (2023)

Example: Potential Energy Surface: C_2-dimer

Binding energies of the C_2 dimer obtained by LRDMC

Wavefunction	C atom (Ha)	C_2 molecule (Ha)	Binding (eV)
Jastrow Slater	−37.82966(4)	−75.8672(1)	5.656(3)
Jastrow Geminal (Singlet)	−37.8364(1)	−75.8938(2)	6.01(1)
Jastrow Geminal (Singlet + broken sym.)	−37.8364(1)	−75.8935(2)	6.00(1)
Jastrow Geminal (All-pairing, Pfaffian)	− 37.8363(1)	−75.9045(2)	**6.31(1)**
Estimated exact	-37.8450	−75.9045(2)	6.44(2) (Exp.)



More complex ansatz.

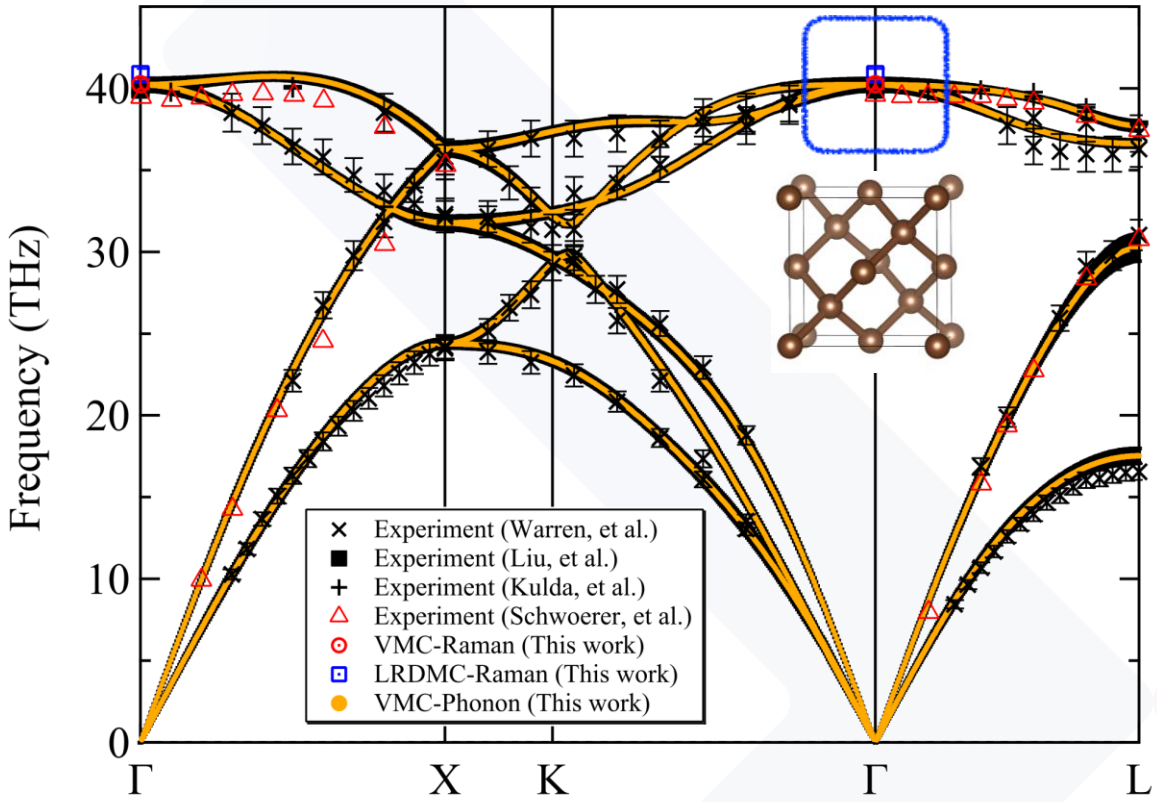
C. Genovese et al., ***J. Chem. Theory Comput.*** 16, 6114 (2020)

DMC gives a more accurate result than CCSD(T) does for the challenging molecule.

Example: Phonon dispersion of Diamond

- Diamond: the conventional 2x2x2 supercell with the experimental lattice parameter
- Employed the frozen phonon method implemented in Phonopy package.

A. Togo and I. Tanaka, *Scr. Mater.* 108, 1 (2015).



* including anharmonic corrections.

Raman Freq. (optical phonon at Γ)

DFT-LDA	38.55 THz
VMC	40.65(38) THz
Exp.	40.35 THz

** These are harmonic frequencies

K. Nakano *et al.*, ***Phys. Rev. B*** 103, L121110 (2021)

TurboWorkflows Features

- Controlling QMC jobs on a python script

```
vmcopt_workflow = eWorkflow(
    label=f'vmcopt-workflow',
    dirname=f'vmcopt-workflow',
    input_files=[Variable(label=f'trexio-workflow', vtype='file', name='fort.10'),
                 Variable(label=f'trexio-workflow', vtype='file', name='pseudo.dat')],
    workflow=VMCopt_workflow(
        ## job
        server_machine_name="fugaku",
        cores=48,
        openmp=1,
        queue="small",
        version="stable",
        sleep_time=180,
        ## vmcopt
        vmcopt_max_continuation=2,
        vmcopt_target_error_bar=1.0e-3, # Ha
        vmcopt_trial_optsteps=50,
        vmcopt_trial_steps=50,
        vmcopt_production_optsteps=20,
        vmcopt_optwarmupsteps_ratio=0.8,
        vmcopt_bin_block=1,
        vmcopt_warmupblocks=0,
        vmcopt_optimizer="lr",
        vmcopt_learning_rate=0.35,
        vmcopt_regularization=0.001,
        vmcopt_onebody=True,
        vmcopt_twobody=True,
        vmcopt_det_mat=False,
        vmcopt_jas_mat=True,
        vmcopt_det_basis_exp=False,
        vmcopt_jas_basis_exp=False,
```

https://github.com/kousuke-nakano/turboworkflows

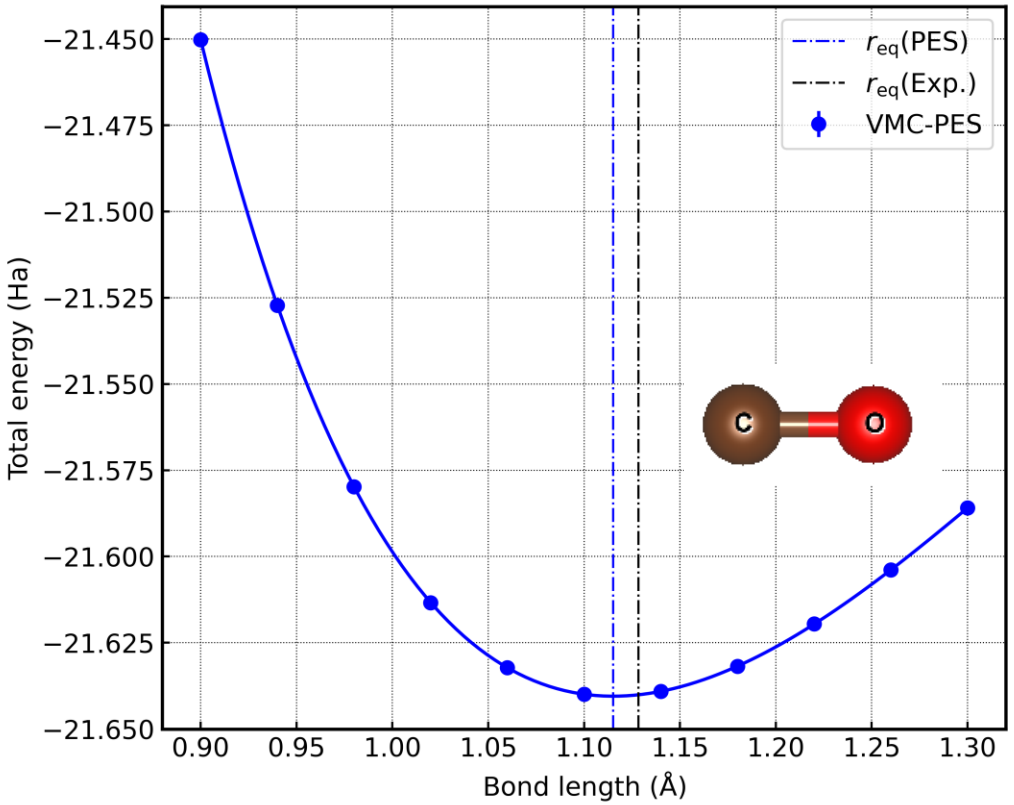
Turbo Workflows

In production from 2022 -

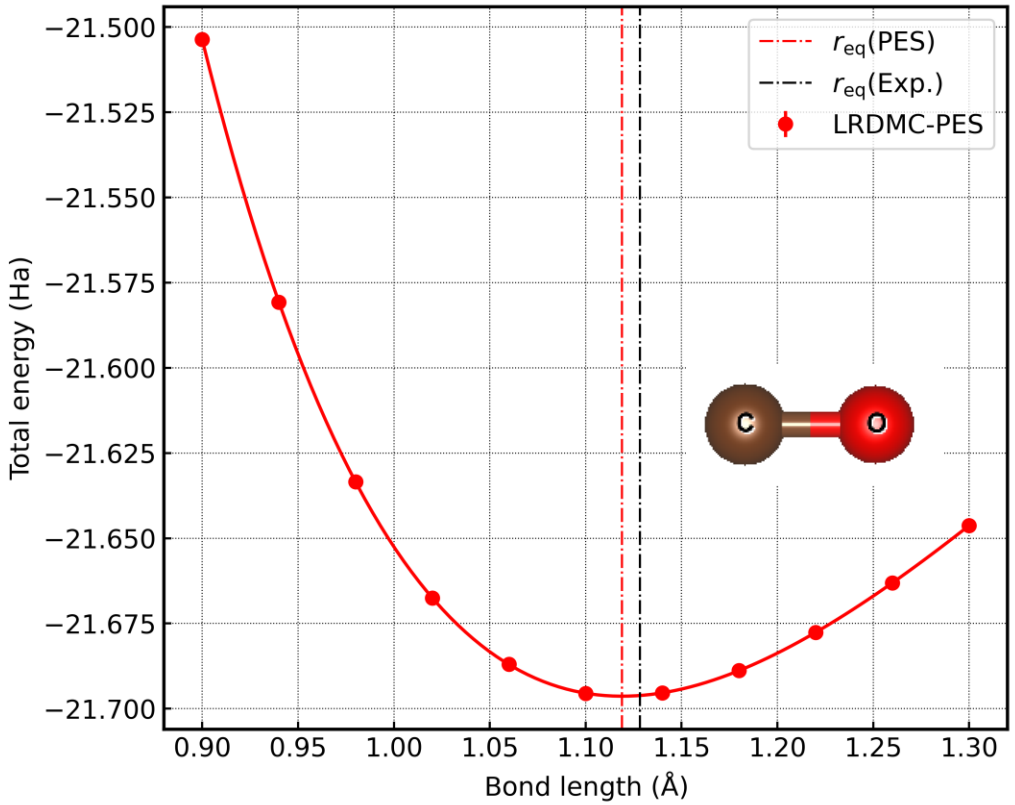
- Implemented in object-oriented fashion by Python3
- Solving dependencies and monitoring jobs
- Allowed to define user's own workflows
- Open source under the BSD3 license (Jul. 2023-)

K. Nakano *et al*., in preparation (2023)

TurboWorkflows Example: Pontential Energy Surface of CO



PES at the VMC level.



PES at the LRDMC level.

TurboWorkflows Example: Pontential Energy Surface of CO

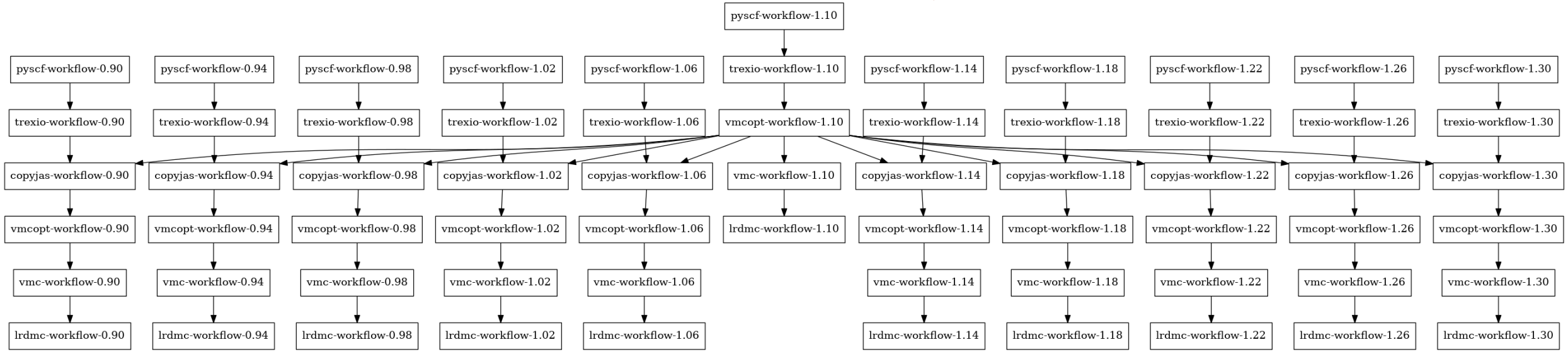
```
vmcopt_workflow = eWorkflow(
    label=f'vmcopt-workflow',
    dirname=f'vmcopt-workflow',
    input_files=[Variable(label=f'trexio-workflow', vtype='file', name='fort.10'),
                 Variable(label=f'trexio-workflow', vtype='file', name='pseudo.dat')],
    workflow=VMCopt_workflow(
        ## job
        server_machine_name="fugaku",
        cores=48,
        openmp=1,
        queue="small",
        version="stable",
```

A python script defining the QMC workflows.

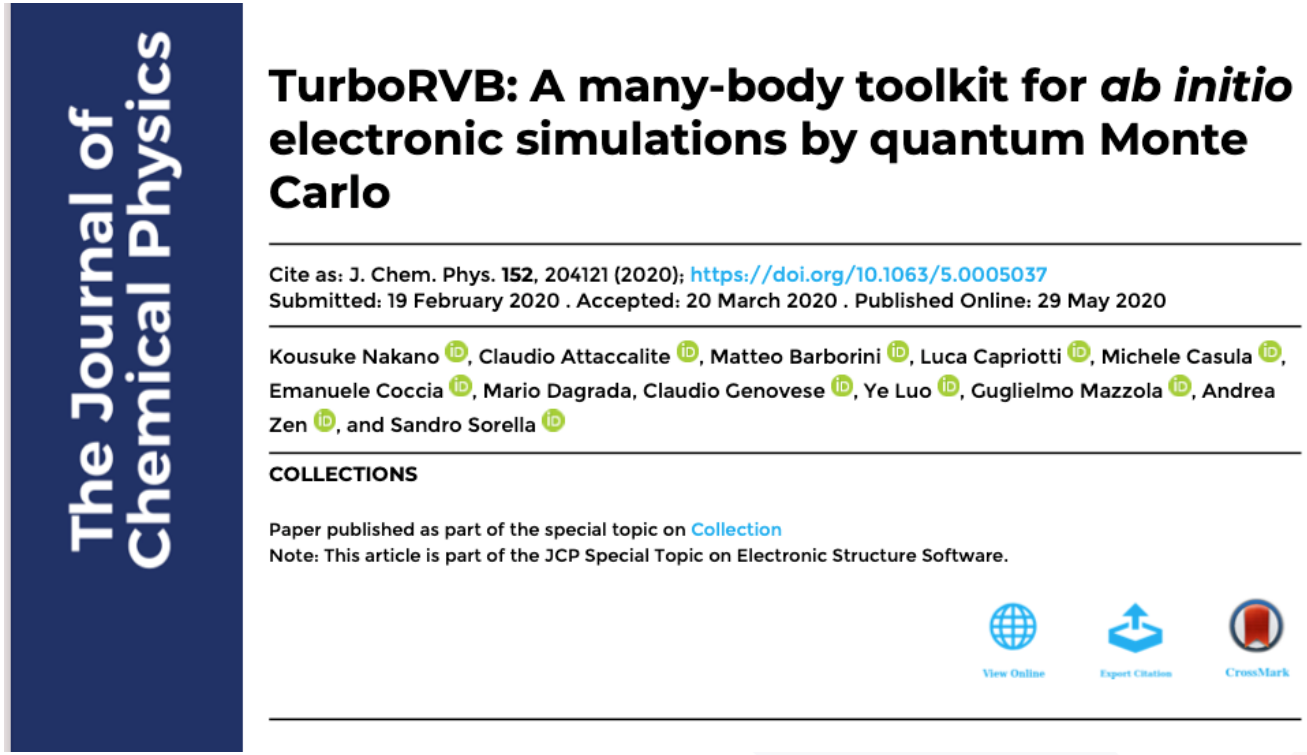
with TREXIO

Turbo Workflows

It automatically solves the dependencies of the calculations.



Review and Website


The Journal of Chemical Physics

TurboRVB: A many-body toolkit for *ab initio* electronic simulations by quantum Monte Carlo

Cite as: J. Chem. Phys. **152**, 204121 (2020); https://doi.org/10.1063/5.0005037
Submitted: 19 February 2020 . Accepted: 20 March 2020 . Published Online: 29 May 2020

Kousuke Nakano, Claudio Attaccalite, Matteo Barborini, Luca Capriotti, Michele Casula, Emanuele Coccia, Mario Dagrada, Claudio Genovese, Ye Luo, Guglielmo Mazzola, Andrea Zen, and Sandro Sorella

COLLECTIONS

Paper published as part of the special topic on Collection
Note: This article is part of the JCP Special Topic on Electronic Structure Software.

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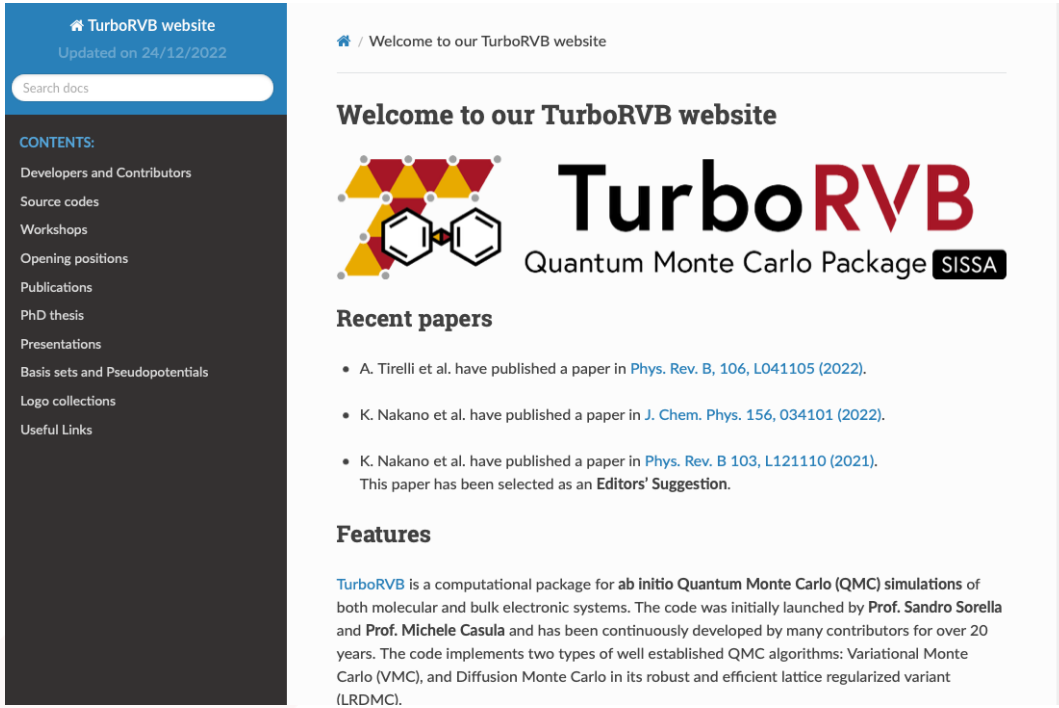
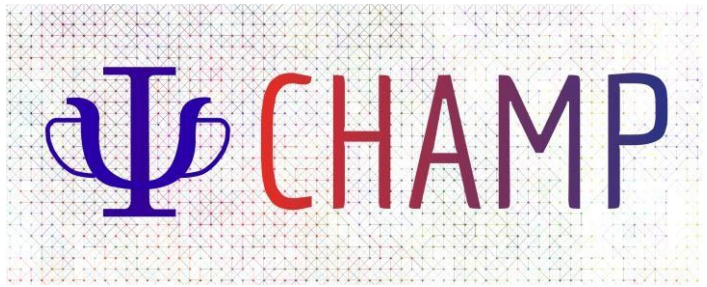


https://turborvb.sissa.it

K. Nakano, C. Attaccalite, M. Barborini, L. Capriotti, M. Casula, E. Coccia, M. Dagrada, Y. Luo, G. Mazzola, A. Zen, and S. Sorella, ***J. Chem. Phys.*** 152, 204121 (2020)



CHAMP : Cornell-Holland Ab-initio Materials Package

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

Ravindra Shinde
University of Twente, The Netherlands

CHAMP : Cornell-Holland Ab-initio Materials Package

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

Noteworthy functionalities

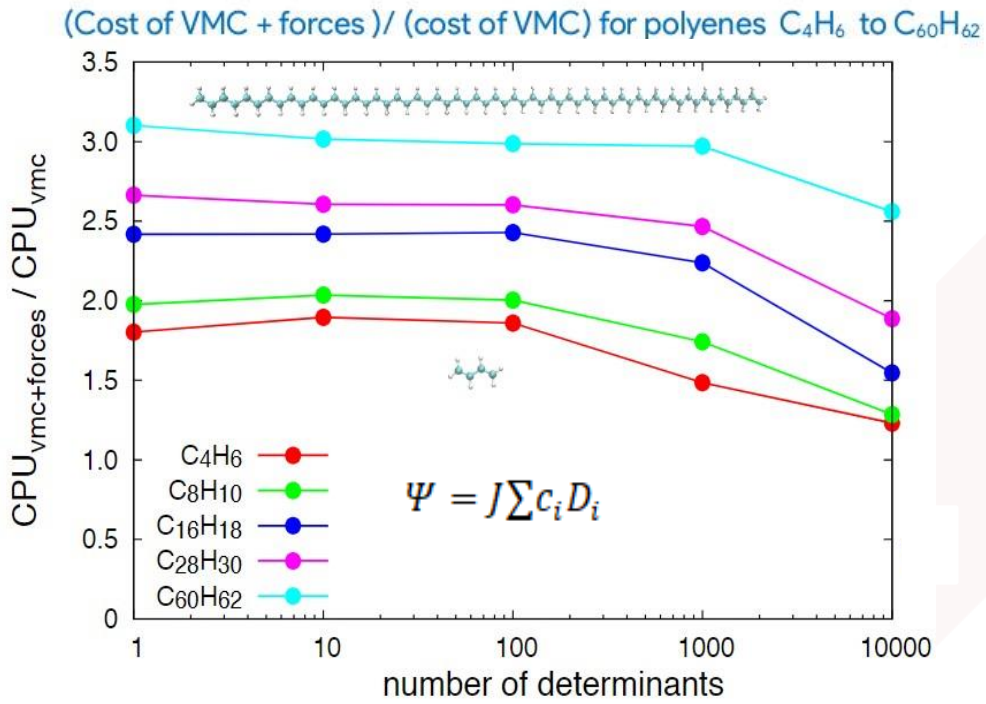
- Efficient optimization schemes for ground and excited states in VMC

  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

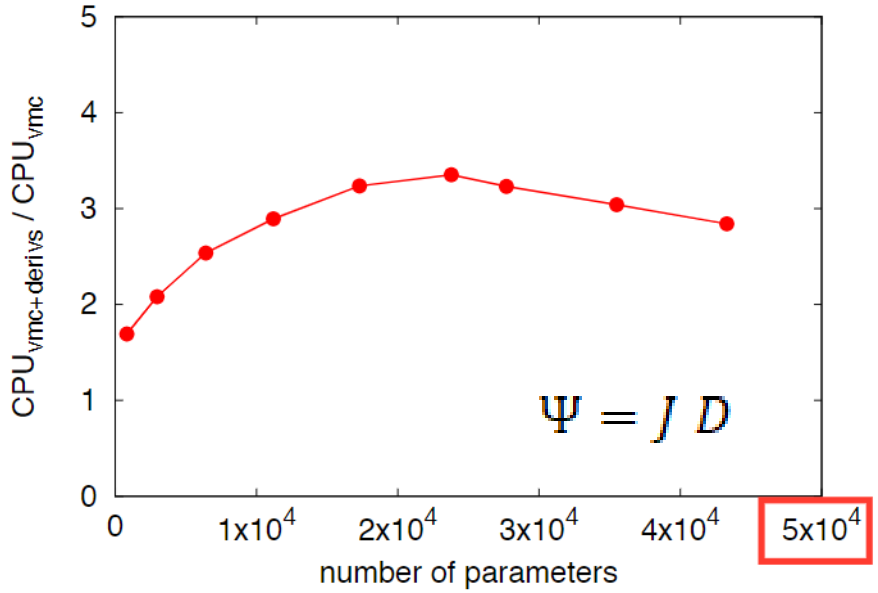
Geometry Optimization



Efficient analytical interatomic forces in VMC

Noteworthy functionalities

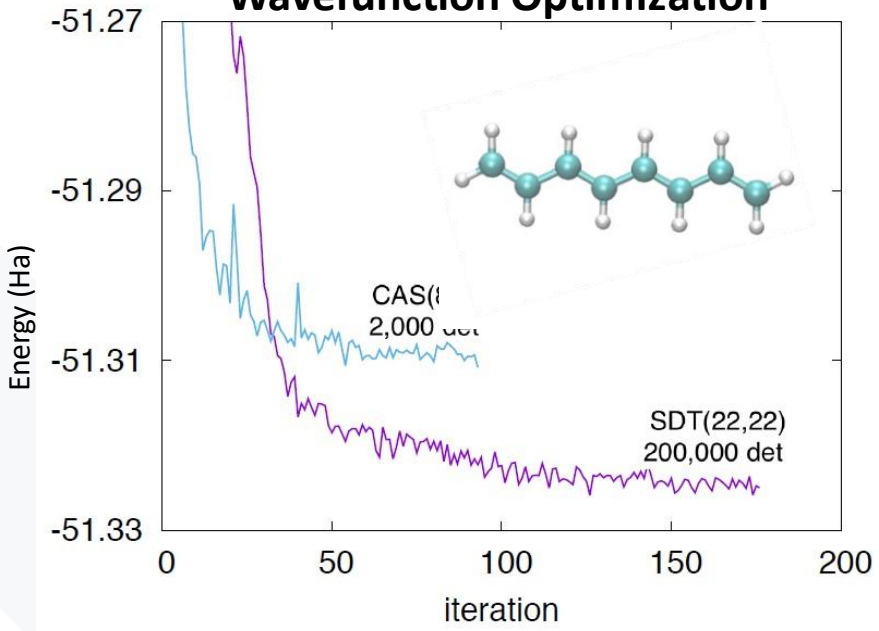
Wavefunction Optimization



Fast evaluation of multideterminants and their derivs

Noteworthy functionalities

Both Geometry and Wavefunction Optimization

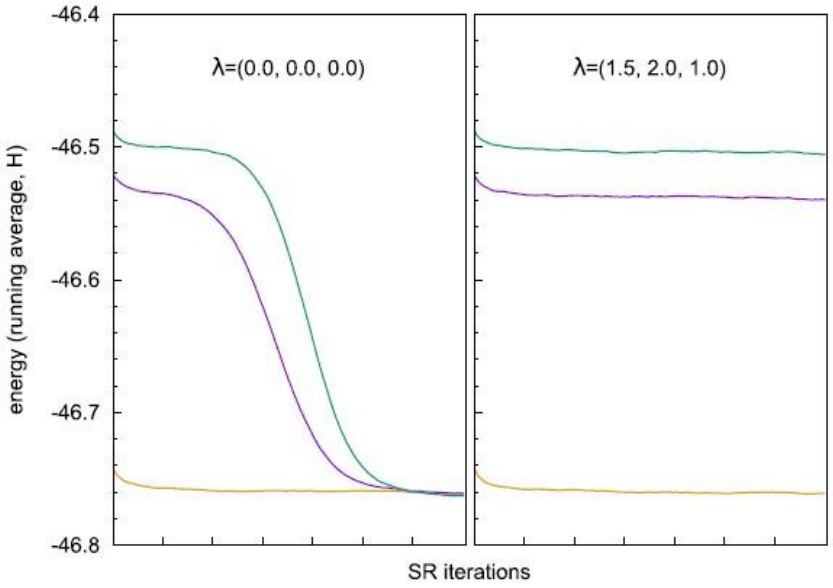


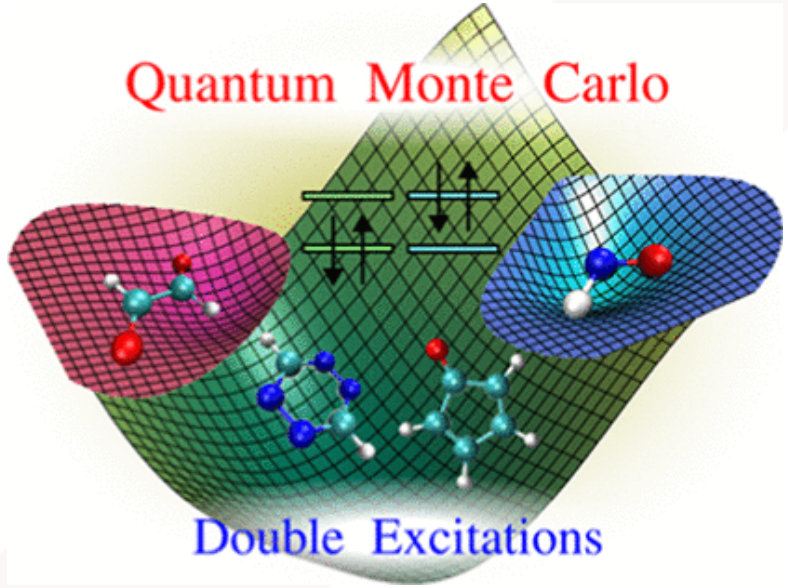
65000 wave function parameter optimization of C_8H_{10}

Efficient optimization schemes for ground and excited states in VMC

Noteworthy functionalities

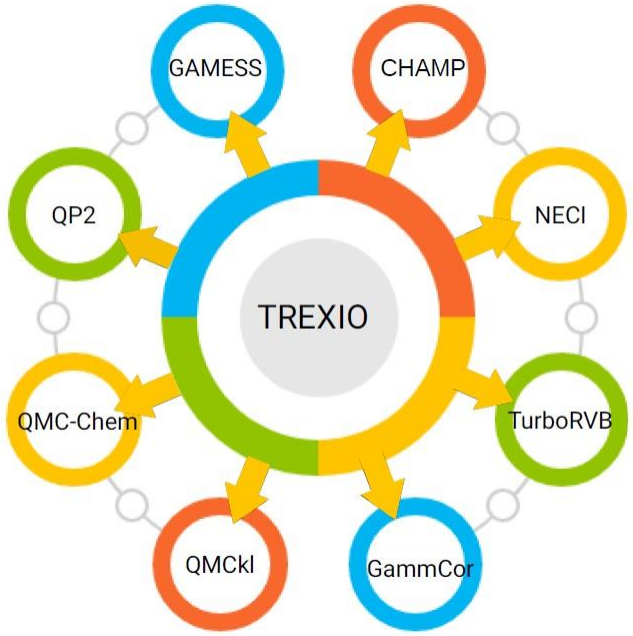
With constraints





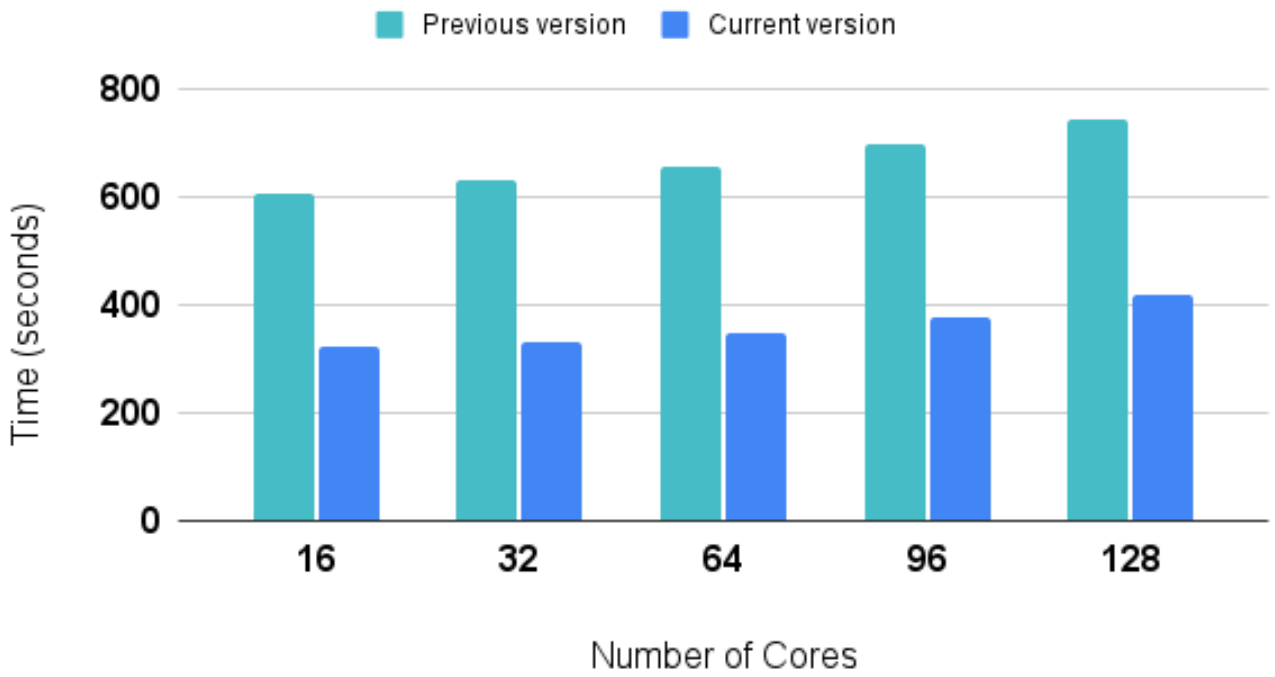
State-specific energy optimization

Interoperability with codes within and outside TREX



Massive parallelization and efficient scaling

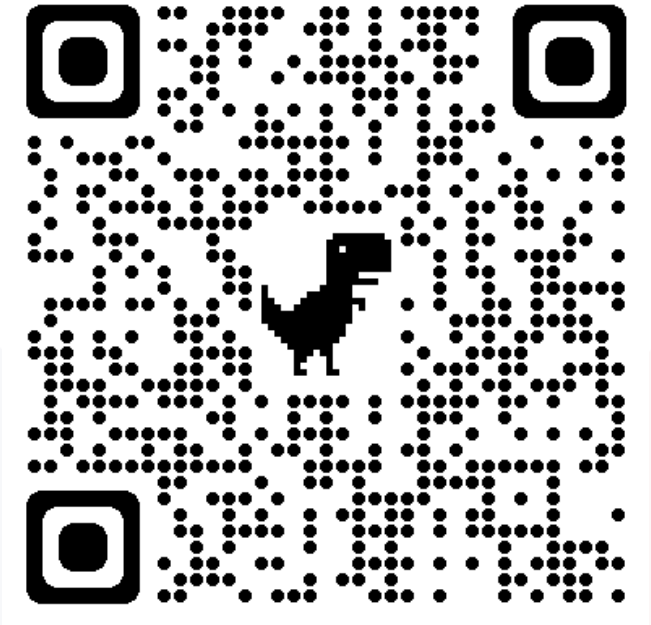
- **Improved vectorization**
- **QMCkl library for highly-efficient, optimized, scalable, common QMC tasks**



Run on Snellius/SURFsara AMD Epyc 128 cores/node

Total energy calculation

Codes available on GitHub



Acknowledgements

Thank you!

Targeting Real chemical accuracy at the EXascale

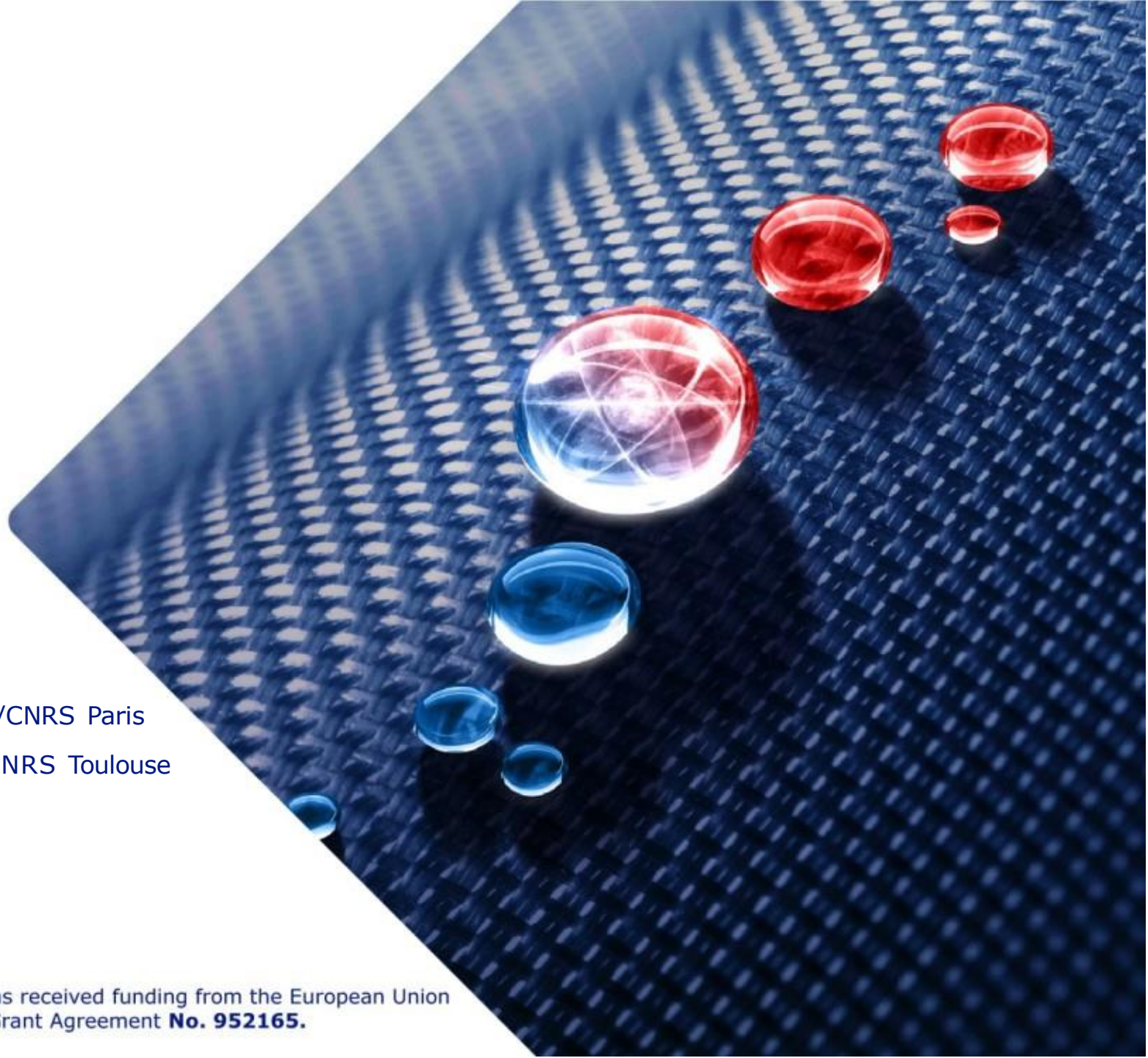
Quantum Package

Emmanuel Giner[1], Anthony Scemama[2]

08/02/2023

[1] Laboratoire de Chimie Théorique, Sorbonne Université/CNRS Paris

[2] Laboratoire de Chimie et Physique Quantiques, UPS/CNRS Toulouse



Targeting Real Chemical Accuracy at the Exascale project has received funding from the European Union Horizoon 2020 research and innovation programme under Grant Agreement **No. 952165.**

Full Configuration Interaction (FCI)

- Exact solution of $\hat{H}\Psi = E\Psi$ in a complete basis of Slater determinants
- The determinant basis is derived from the one-electron basis set
- Only approximation : one-electron basis-set incompleteness
- Intractable : $O(N!)$ scaling
- All the post-Hartree-Fock methods are approximations of the FCI within the same basis set

THE JOURNAL OF CHEMICAL PHYSICS **147**, 184111 (2017)

Pushing configuration-interaction to the limit: Towards massively parallel MCSCF calculations

Konstantinos D. Vogiatzis,[1,a),b)] Dongxia Ma,[1,c)] Jeppe Olsen,[2] Laura Gagliardi,[1,a)] and Wibe A. de Jong[3,a)]

[1]*Department of Chemistry, Minnesota Supercomputing Institute, and Chemical Theory Center, University of Minnesota, 207 Pleasant Street Southeast, Minneapolis, Minnesota 55455-0431, USA*
[2]*Department of Chemistry, Aarhus University, Langelandsgade 140, 8000 Aarhus C, Denmark*
[3]*Computational Research Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*

(Received 12 June 2017; accepted 20 October 2017; published online 14 November 2017)

A new large-scale parallel multiconfigurational self-consistent field (MCSCF) implementation in the open-source NWChem computational chemistry code is presented. The generalized active space approach is used to partition large configuration interaction (CI) vectors and generate a sufficient number of batches that can be distributed to the available cores. Massively parallel CI calculations with large active spaces can be performed. The new parallel MCSCF implementation is tested for the chromium trimer and for an active space of 20 electrons in 20 orbitals, which can now routinely be performed. Unprecedented CI calculations with an active space of 22 electrons in 22 orbitals for the pentacene systems were performed and a single CI iteration calculation with an active space of 24 electrons in 24 orbitals for the chromium tetramer was possible. The chromium tetramer corresponds to a CI expansion of one trillion Slater determinants (914 058 513 424) and is the largest conventional CI calculation attempted up to date. *Published by AIP Publishing.*
https://doi.org/10.1063/1.4989858

JCTC Journal of Chemical Theory and Computation

Article

Cite This: J. Chem. Theory Comput. 2017, 13, 5468-5478

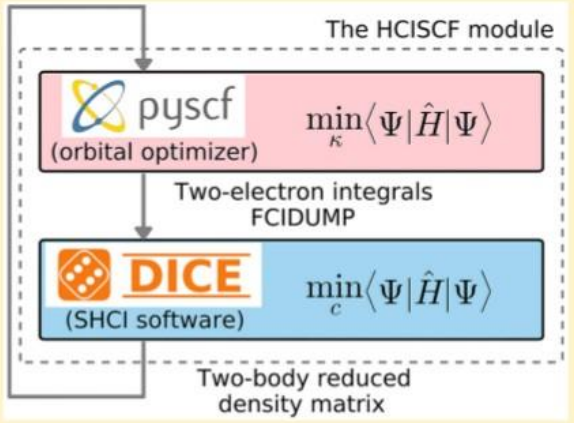
pubs.acs.org/JCTC

Cheap and Near Exact CASSCF with Large Active Spaces

James E. T. Smith,* Bastien Mussard, Adam A. Holmes, and Sandeep Sharma*

Department of Chemistry and Biochemistry, University of Colorado Boulder, Boulder, Colorado 80309, United States

ABSTRACT: We use the recently developed Heat-bath Configuration Interaction (HCI) algorithm as an efficient active space solver to perform multiconfiguration self-consistent field calculations (HCISCF) with large active spaces. We give a detailed derivation of the theory and show that difficulties associated with non-variationality of the HCI procedure can be overcome by making use of the Lagrangian formulation to calculate the HCI relaxed two-body reduced density matrix. HCISCF is then used to study the electronic structure of butadiene, pentacene, and Fe−porphyrin. One of the most striking results of our work is that the converged active space orbitals obtained from HCISCF are relatively insensitive to the accuracy of the HCI calculation. This allows us to obtain nearly converged CASSCF energies with an estimated error of less than 1 mHa using the orbitals obtained from the HCISCF procedure in which the integral transformation is the dominant cost. For example, an HCISCF calculation on the Fe−porphyrin model complex with an active space of (44e, 44o) took only 412 s per iteration on a single node containing 28 cores, out of which 185 s was spent in the HCI calculation and the remaining 227 s was used mainly for integral transformation. Finally, we also show that active space orbitals can be optimized using HCISCF to substantially speed up the convergence of the HCI energy to the Full CI limit because HCI is not invariant to unitary transformations within the active space.

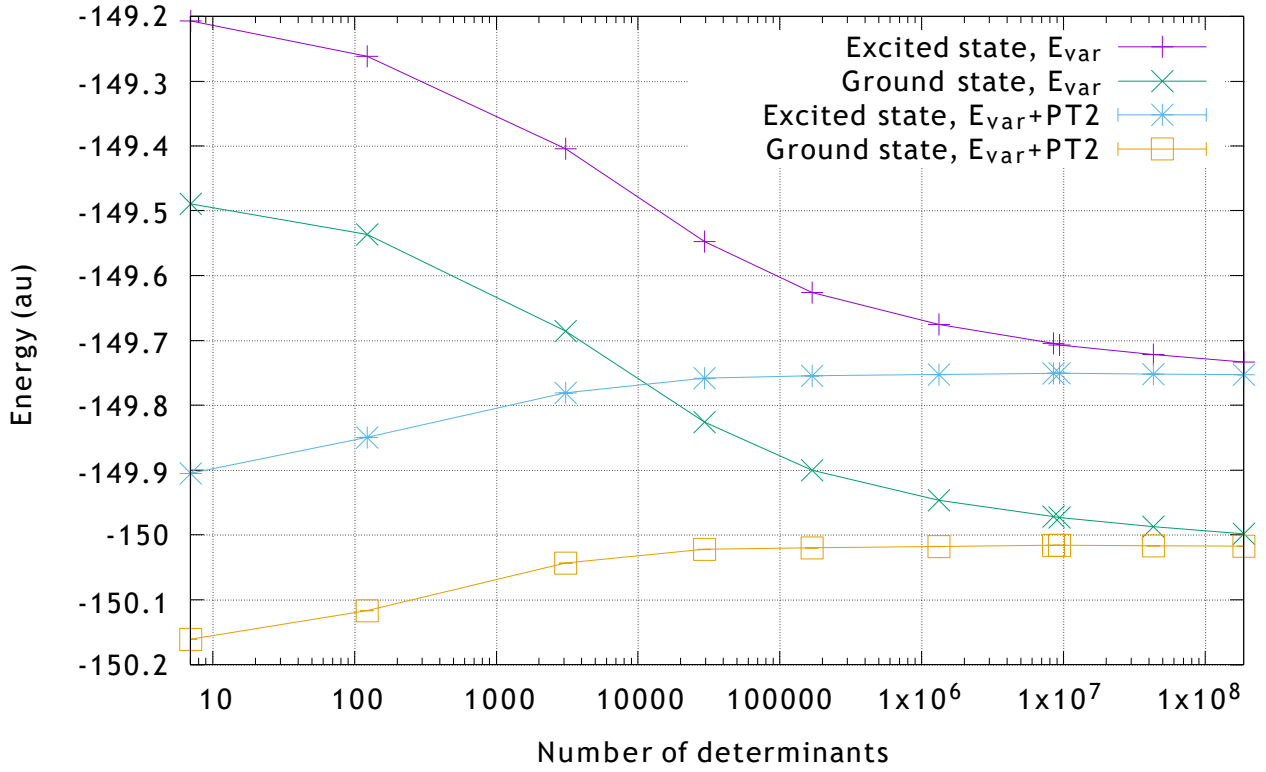


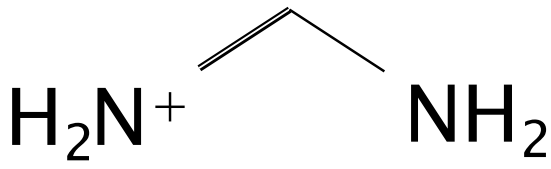
CIPSI Algorithm[1]

Start with $\mathrm{D}_0 = \{|\mathrm{HF}\rangle\}$ and $|\Psi_0\rangle = |\mathrm{HF}\rangle$.

1. $\forall |i\rangle \in \{\hat{T}_{\mathrm{SD}}|\Psi_n\rangle\} \setminus \{\mathrm{D}_n\}$, compute $e_i = \frac{\langle i|\mathrm{H}|\Psi_n\rangle^2}{E(\Psi_n) - \langle i|\mathrm{H}|i\rangle}$
2. if $|e_i| > \epsilon_n$, select $|i\rangle$
3. Estimated energy : $E(\Psi_n) + E_{\mathrm{PT2}}(\Psi_n) = E(\Psi_n) + \sum_i e_i$
4. $\mathrm{D}_{n+1} = \mathrm{D}_n \cup \{\cup_{i(\mathrm{selected})}|i\rangle\}$
5. Minimize $E(\Psi_{n+1})$ (Davidson),
   $\Psi_{n+1} = \Psi_n + \sum_{i(\mathrm{selected})} c_i|i\rangle$
6. Choose $\epsilon_{n+1} < \epsilon_n$
7. Iterate

[1] B. Huron, J.P. Malrieu, and P. Rancurel, *J. Chem. Phys.* **58**, 5745 (1973).



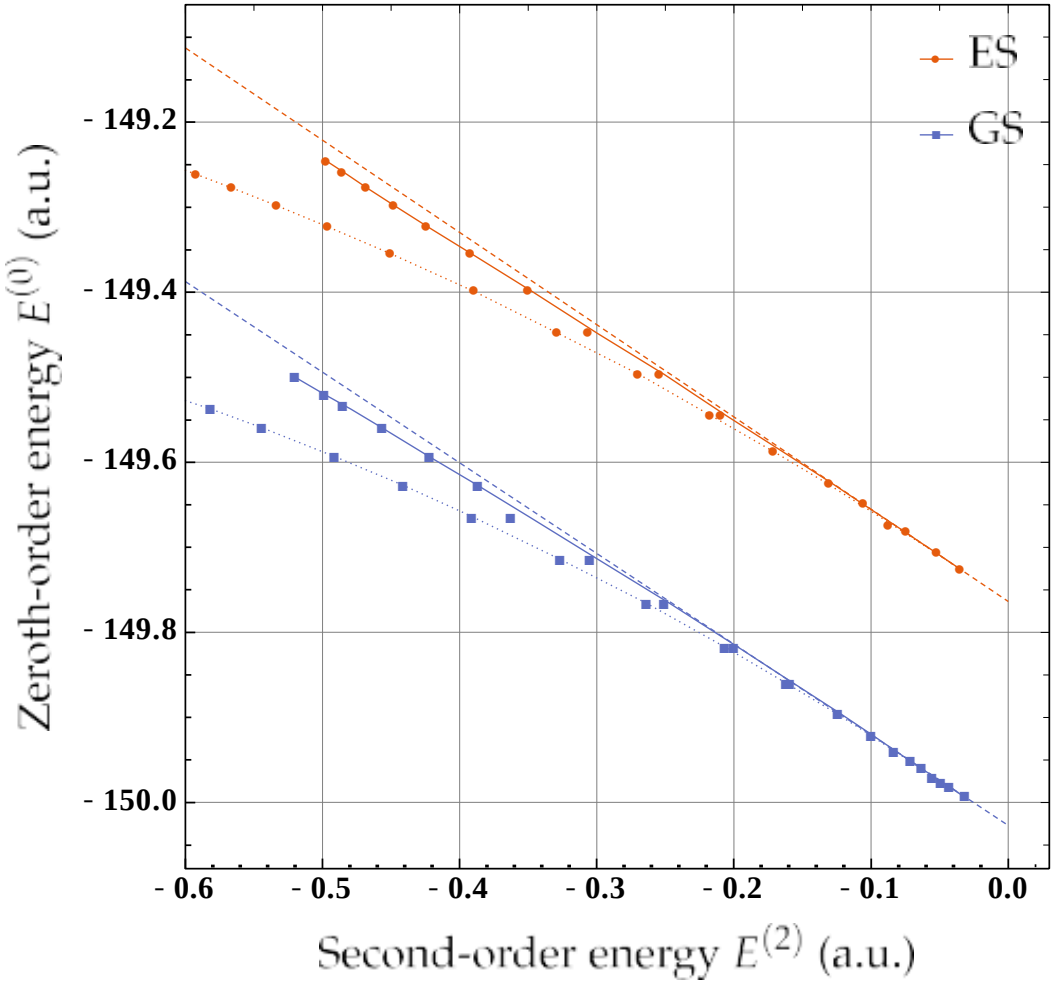


aug-cc-pVDZ

- When $N_{det} = N_{FCI}$, $E_{PT2} = 0$, CI is solved *exactly*.
- Every CI problem can be solved by iterative perturbative selection

Extrapolated FCI energy

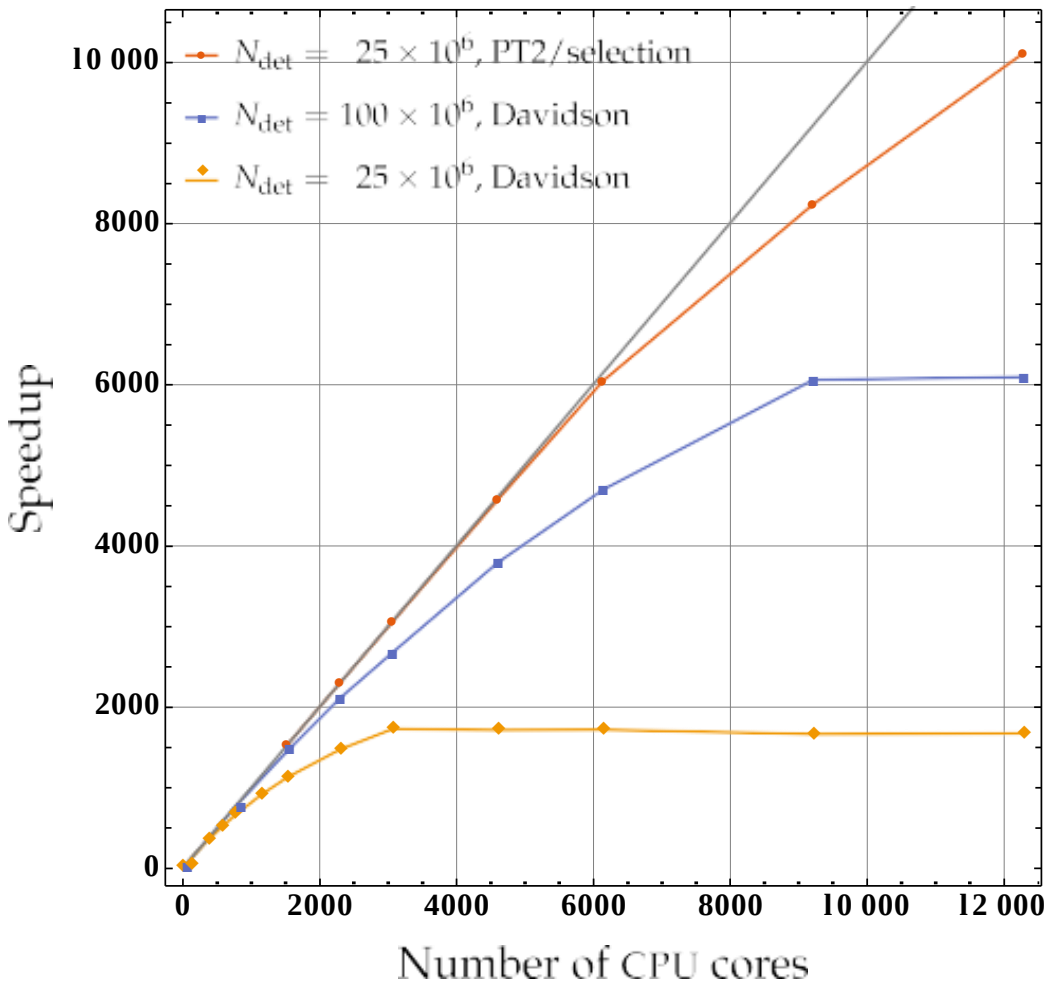
- exFCI : Extrapolate $E = f(E_{PT2})$ at $E_{PT2} = 0$, estimates the complete CI solution.



FCI wave function can't be computed or even stored:

$$N_{FCI} = 2.5 \times 10^{25}$$
$$= 42.4 \text{ moles}$$

- OpenMP / MPI / ZeroMQ
- HPC environments
- Cloud environments
- Resources can be increased dynamically



THE JOURNAL OF PHYSICAL CHEMISTRY Letters

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Perspective

The Quest for Highly Accurate Excitation Energies: A Computational Perspective

Pierre-François Loos,* Anthony Scemama, and Denis Jacquemin*

Cite This: *J. Phys. Chem. Lett.* 2020, 11, 2374–2383

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ABSTRACT: We provide an overview of the successive steps that made it possible to obtain increasingly accurate excitation energies with computational chemistry tools, eventually leading to chemically accurate vertical transition energies for small- and medium-size molecules. First, we describe the evolution of *ab initio* methods employed to define benchmark values, with the original Roos CASPT2 method, then the CC3 method as in the renowned Thiel set, and more recently the resurgence of selected configuration interaction methods. The latter method has been able to deliver consistently, for both single and double excitations, highly accurate excitation energies for small molecules, as well as medium-size molecules with compact basis sets. Second, we describe how these high-level methods and the creation of representative benchmark sets of excitation energies have allowed the fair and accurate assessment of the performance of computationally lighter methods. We conclude by discussing possible future theoretical and technological developments in the field.

Applications

Received: 2 December 2020 | Revised: 5 January 2021 | Accepted: 7 January 2021
DOI: 10.1002/wcms.1517

FOCUS ARTICLE

WIREs COMPUTATIONAL MOLECULAR SCIENCE WILEY

QUESTDB: A database of highly accurate excitation energies for the electronic structure community

Mickaël Véril[1] | Anthony Scemama[1] | Michel Caffarel[1] | Filippo Lipparini[2] | Martial Boggio-Pasqua[1] | Denis Jacquemin[3] | Pierre-François Loos[1]

[1]Laboratoire de Chimie et Physique Quantiques, Université de Toulouse, CNRS, UPS, Toulouse, France
[2]Dipartimento di Chimica e Chimica Industriale, University of Pisa, Pisa, Italy
[3]Université de Nantes, CNRS, CEISAM UMR 6230, Nantes, France

Correspondence
Denis Jacquemin, Université de Nantes, CNRS, CEISAM UMR 6230, F-44000 Nantes, France.
Email: denis.jacquemin@univ-nantes.fr
Pierre-François Loos, Laboratoire de Chimie et Physique Quantiques, Université de Toulouse, CNRS, UPS, France.
Email: loos@irsamc-ups-tlse.fr

Funding information
Agence Nationale de la Recherche, Grant/Award Number: ANR-18-EURE-0012; H2020 European Research Council, Grant/Award Number: 863481

Edited by: Peter R. Schreiner, Editor-in-Chief

Abstract

We describe our efforts of the past few years to create a large set of more than 500 highly accurate vertical excitation energies of various natures ($\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$, double excitation, Rydberg, singlet, doublet, triplet, etc.) in small- and medium-sized molecules. These values have been obtained using an incremental strategy which consists in combining high-order coupled cluster and selected configuration interaction calculations using increasingly large diffuse basis sets in order to reach high accuracy. One of the key aspects of the so-called QUEST database of vertical excitations is that it does not rely on any experimental values, avoiding potential biases inherently linked to experiments and facilitating theoretical cross comparisons. Following this composite protocol, we have been able to produce theoretical best estimates (TBEs) with the aug-cc-pVTZ basis set for each of these transitions, as well as basis set corrected TBEs (i.e., near the complete basis set limit) for some of them. The TBEs/aug-cc-pVTZ have been employed to benchmark a large number of (lower-order) wave function methods such as CIS(D), ADC(2), CC2, STEOM-CCSD, CCSD, CCSDR(3), CCSDT-3, ADC(3), CC3, NEVPT2, and so on (including spin-scaled variants). In order to gather the huge amount of data produced during the QUEST project, we have created a website (https://lcpq.github.io/QUESTDB_website) where one can easily test and compare the accuracy of a given method with respect to various variables such as the molecule size or its family, the nature of the excited states, the type of basis set, and so on. We hope that the present review will provide a useful summary of our effort so far and foster new developments around excited-state methods.

This article is categorized under:
Electronic Structure Theory > Ab Initio Electronic Structure Methods

KEYWORDS
benchmark, coupled cluster theory, database, excitation energies, excited states, full configuration interaction

The Journal of Chemical Physics ARTICLE scitation.org/journal/jcp

Accurate full configuration interaction correlation energy estimates for five- and six-membered rings

Cite as: J. Chem. Phys. **155**, 134104 (2021); doi: 10.1063/5.0065314
Submitted: 31 July 2021 • Accepted: 9 September 2021 •
Published Online: 1 October 2021

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Yann Damour,[1] Mickaël Véril,[1] Fábris Kossoski,[1] Michel Caffarel,[1] Denis Jacquemin,[2,a)] Anthony Scemama,[1,b)] and Pierre-François Loos[1,c)]

AFFILIATIONS

[1] Laboratoire de Chimie et Physique Quantiques (UMR 5626), Université de Toulouse, CNRS, UPS, Toulouse, France
[2] Université de Nantes, CNRS, CEISAM UMR 6230, F-44000 Nantes, France

[a)]**Electronic mail:** Denis.Jacquemin@univ-nantes.fr
[b)]**Electronic mail:** scemama@irsamc.ups-tlse.fr
[c)]**Author to whom correspondence should be addressed:** loos@irsamc.ups-tlse.fr

ABSTRACT

Following our recent work on the benzene molecule [P.-F. Loos, Y. Damour, and A. Scemama, J. Chem. Phys. **153**, 176101 (2020)], motivated by the blind challenge of Eriksen *et al.* [J. Phys. Chem. Lett. **11**, 8922 (2020)] on the same system, we report accurate full configuration interaction (FCI) frozen-core correlation energy estimates for 12 five- and six-membered ring molecules (cyclopentadiene, furan, imidazole, pyrrole, thiophene, benzene, pyrazine, pyridazine, pyridine, pyrimidine, s-tetrazine, and s-triazine) in the standard correlation-consistent double-ζ Dunning basis set (cc-pVDZ). Our FCI correlation energy estimates, with an estimated error smaller than 1 millihartree, are based on energetically optimized-orbital selected configuration interaction calculations performed with the *configuration interaction using a perturbative selection made iteratively* algorithm. Having at our disposal these accurate reference energies, the respective performance and convergence properties of several popular and widely used families of single-reference quantum chemistry methods are investigated. In particular, we study the convergence properties of (i) the Møller–Plesset perturbation series up to fifth-order (MP2, MP3, MP4, and MP5), (ii) the iterative approximate coupled-cluster series CC2, CC3, and CC4, and (iii) the coupled-cluster series CCSD, CCSDT, and CCSDTQ. The performance of the ground-state gold standard CCSD(T) as well as the completely renormalized CC model, CR-CC(2,3), is also investigated. We show that MP4 provides an interesting accuracy/cost ratio, while MP5 systematically worsens the correlation energy estimates. In addition, CC3 outperforms CCSD(T) and CR-CC(2,3), as well as its more expensive parent CCSDT. A similar trend is observed for the methods including quadruple excitations, where the CC4 model is shown to be slightly more accurate than CCSDTQ, both methods providing correlation energies within 2 millihartree of the FCI limit.

JCTC Journal of Chemical Theory and Computation

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Ground- and Excited-State Dipole Moments and Oscillator Strengths of Full Configuration Interaction Quality

Yann Damour,* Raúl Quintero-Monsebaiz, Michel Caffarel, Denis Jacquemin, Fábris Kossoski, Anthony Scemama, and Pierre-François Loos*

Cite This: *J. Chem. Theory Comput.* 2023, 19, 221–234 Read Online

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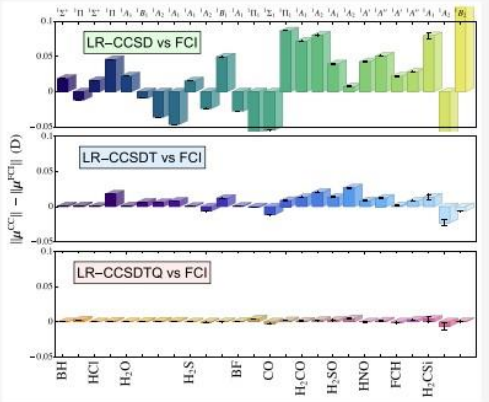
ABSTRACT: We report ground- and excited-state dipole moments and oscillator strengths (computed in different "gauges" or representations) of full configuration interaction (FCI) quality using the selected configuration interaction method known as *Configuration Interaction using a Perturbative Selection made Iteratively* (CIPSI). Thanks to a set encompassing 35 ground- and excited-state properties computed in 11 small molecules, the present near-FCI estimates allow us to assess the accuracy of high-order coupled-cluster (CC) calculations including up to quadruple excitations. In particular, we show that incrementing the excitation degree of the CC expansion (from CC with singles and doubles (CCSD) to CC with singles, doubles, and triples (CCSDT) or from CCSDT to CC with singles, doubles, triples, and quadruples (CCSDTQ)) reduces the average error with respect to the near-FCI reference values by approximately 1 order of magnitude.

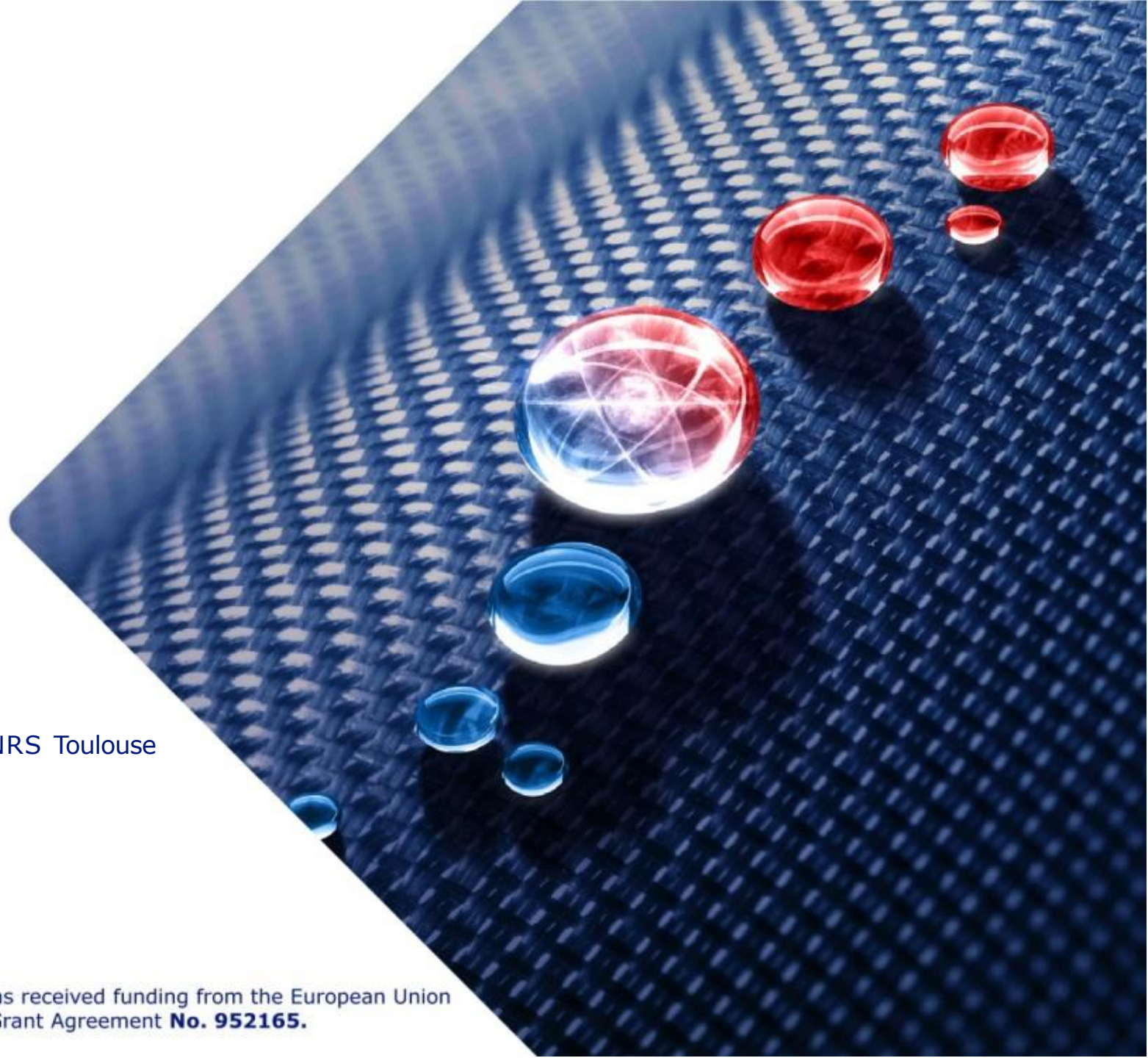


Quantum Package

https://quantumpackage.github.io/qp2

- Open-source programming environment for quantum chemistry
- Uses determinant-driven algorithms : can solve CI problems with arbitrary CI spaces
- Efficient CIPSI and stochastic PT2 computational kernels
- Designed first for for programmers, but easy to use
- Users are encouraged to develop their own plugins, which they can redistribute autonomously

Targeting Real chemical accuracy at the EXascale



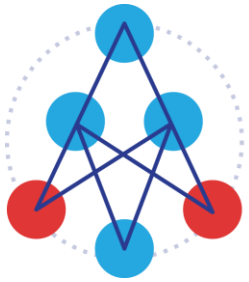
QMC=Chem

Anthony Scemama

08/02/2023

Laboratoire de Chimie et Physique Quantiques, UPS/CNRS Toulouse

Targeting Real Chemical Accuracy at the Exascale project has received funding from the European Union Horizoon 2020 research and innovation programme under Grant Agreement **No. 952165.**



QMC=Chem

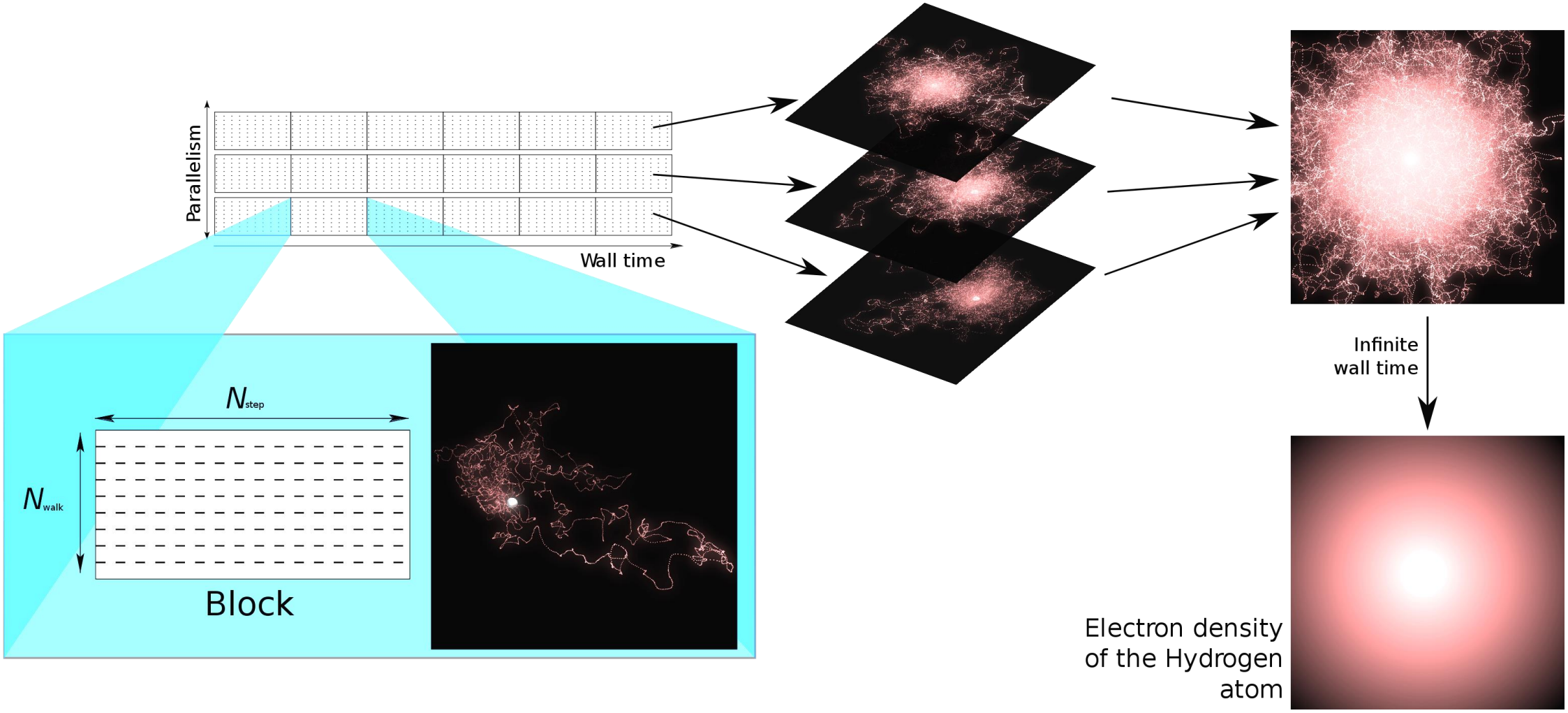
What it can do

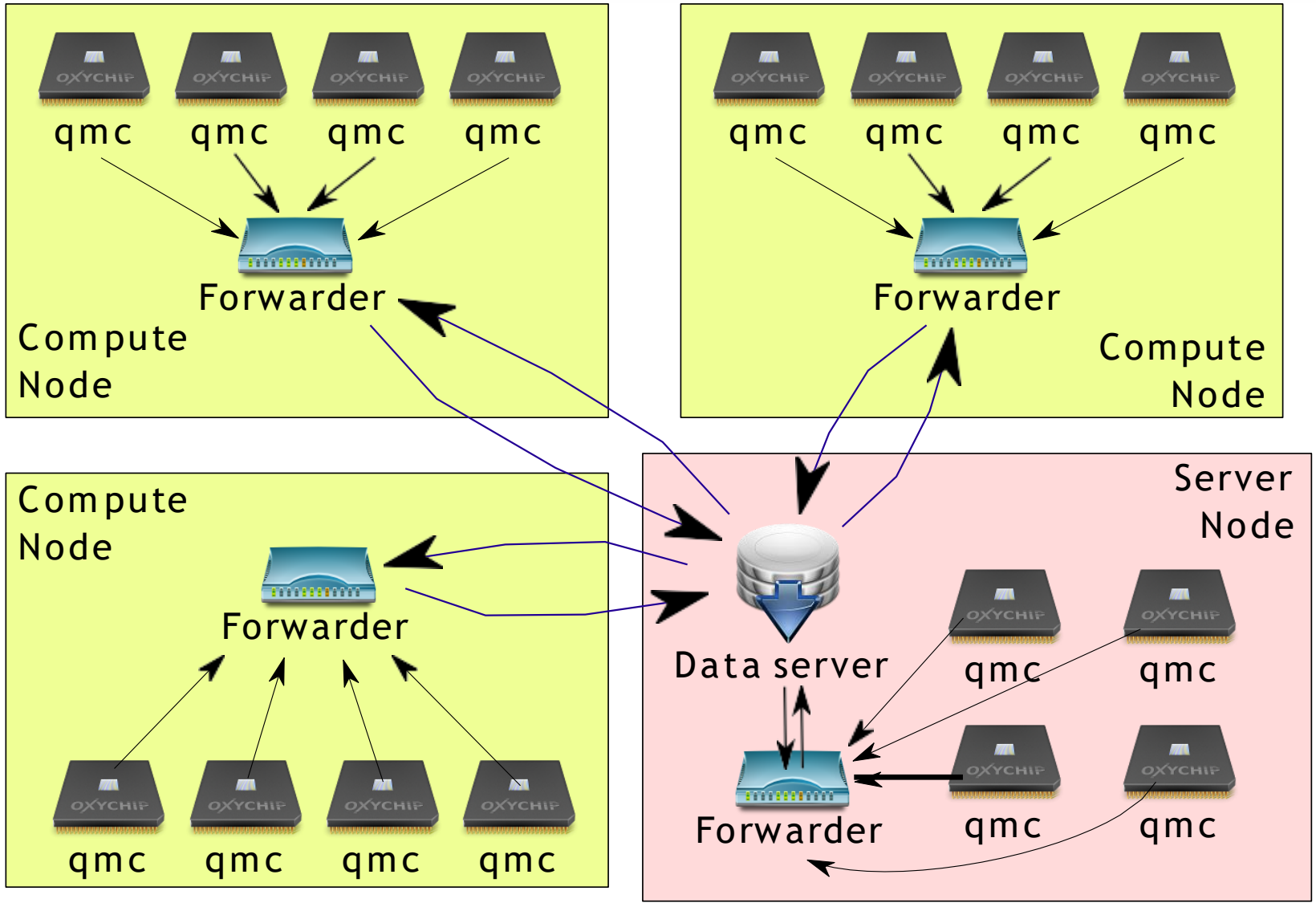
- VMC and DMC of large CI expansions
- Ground and excited states
- All-electron / Pseudo-potentials (DLA)
- Optimization of very large CI expansions
- Massively parallel calculations

What it cannot do

- Periodic systems
- T-moves
- Sophisticated Jastrow factors
- Backflow
- JAGP
- Nuclear forces

Algorithm


Parallelism
Wall time
N_{step}
N_{walk}
Block
Infinite
wall time
Electron density
of the Hydrogen
atom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Server Node
Data server
qmc
qmc
Forwarder
qmc
qmc

Programming

- Wave function preparation: Quantum Package
- Computation: Fortran
- Communication + post-processing: OCaml
- ZeroMQ for communication $\Longrightarrow$ HPC systems + Cloud infrastructures
- Fault tolerance + dynamical resource management

Large scale applications

- 0.96 PFlops/s in 2011 on Curie (TGCC/CEA), 76 800 cores
- Distributed HPC+Cloud calculations in 2015 (France Grilles)

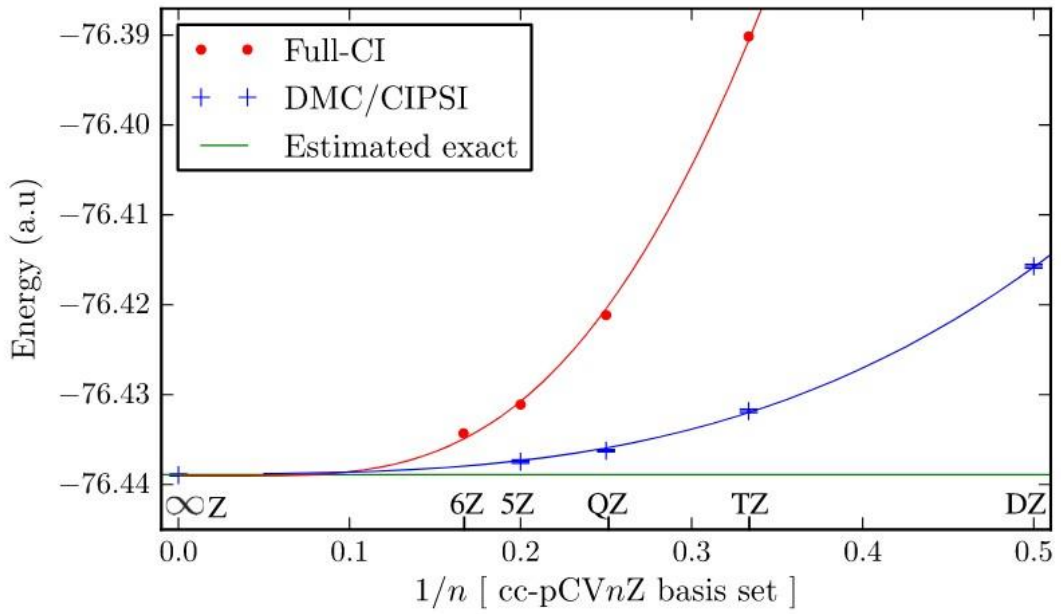

FIG. 1. CBS extrapolation of FCI and DMC/CIPSI energies. Error bars on DMC data are plotted but almost imperceptible.

TABLE III. Comparison of nonrelativistic ground-state total energies of water obtained with the most accurate theoretical methods. Energies in a.u.

Clark *et al.*,[20] DMC (upper bound)	−76.436 8(4)
This work, DMC (upper bound)	−76.437 44(18)
Almora-Dìaz,[27] CISDTQQnSx (upper bound)	−76.434 3
Helgaker *et al.*,[29] R12-CCSD(T)	−76.439(2)
Muller and Kutzelnigg,[30] R12-CCSD(T)	−76.437 3
Almora-Dìaz,[27] FCI + CBS	−76.438 6(9)
Halkier *et al.*,[31] CCSD(T) + CBS	−76.438 6
Bytautas and Ruedenberg,[32] FCI + CBS	−76.439 0(4)
This work, DMC + CBS	−76.438 94(12)
Experimentally derived estimate[25]	−76.438 9

Toward an improved control of the fixed-node error in quantum Monte Carlo: The case of the water molecule M. Caffarel, T. Applencourt, E. Giner, A. Scemama, *J. Chem. Phys.*, 2016, **144**, pp.151103.

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- QMC=Chem: A Quantum Monte Carlo Program for Large-Scale Simulations in Chemistry at the Petascale Level and beyond
- Quantum Monte Carlo for large chemical systems: Implementing efficient strategies for petascale platforms and beyond
- Quantum Monte Carlo with very large multideterminant wavefunctions
- Optimization of large determinant expansions in quantum Monte Carlo
- Toward an improved control of the fixed-node error in quantum Monte Carlo: The case of the water molecule
- Deterministic construction of nodal surfaces within quantum Monte Carlo: the case of FeS
- Excitation energies from diffusion Monte Carlo using selected configuration interaction nodes
- Taming the fixed-node error in diffusion Monte Carlo via range separation

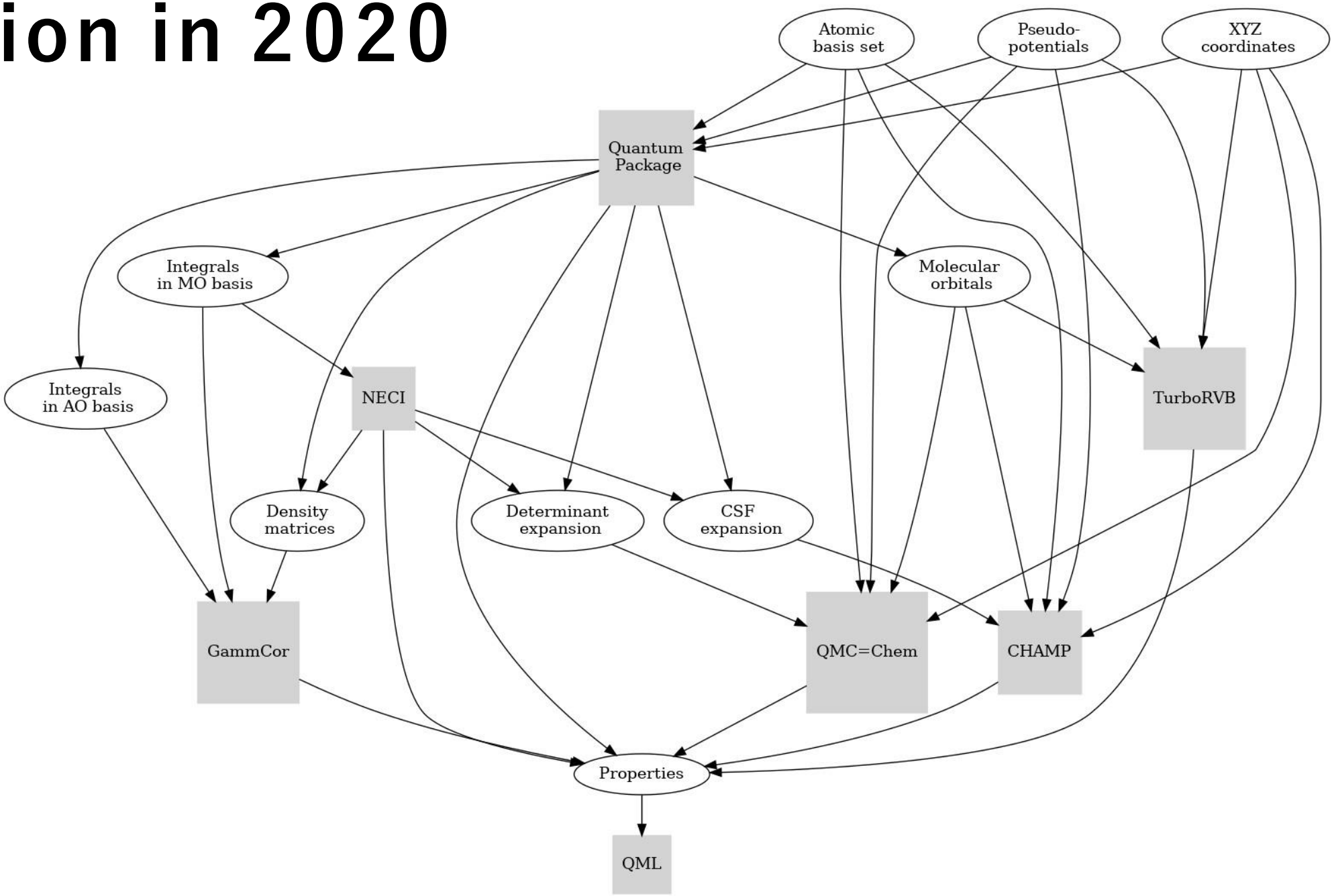
TREX libraries:

TREXIO & QMCkl

Evgeny Posenitskiy,* Anthony Scemama
Laboratoire de Chimie et Physique Quantiques (LCPQ)
@ CNRS and University of Toulouse, France
***currently @ Qubit Pharmaceuticals, France**
08/02/2023

TREXIO as I/O format

Situation in 2020



TREXIO configuration file (trex.json)

group:

data : [data type , [list of dimensions]]

```
"nucleus": {
    "num"         : [ "dim"    , []                      ],
    "charge"      : [ "float"  , ["nucleus.num"]         ],
    "coord"       : [ "float"  , ["nucleus.num", "3" ] ],
    "label"       : [ "str"    , ["nucleus.num"]         ],
    "point_group" : [ "str"    , []                      ],
    "repulsion"   : [ "float"  , []                      ]
    }
```

More details in the TREXIO documentation*

* *https://trex-coe.github.io/trexio/trex.html*

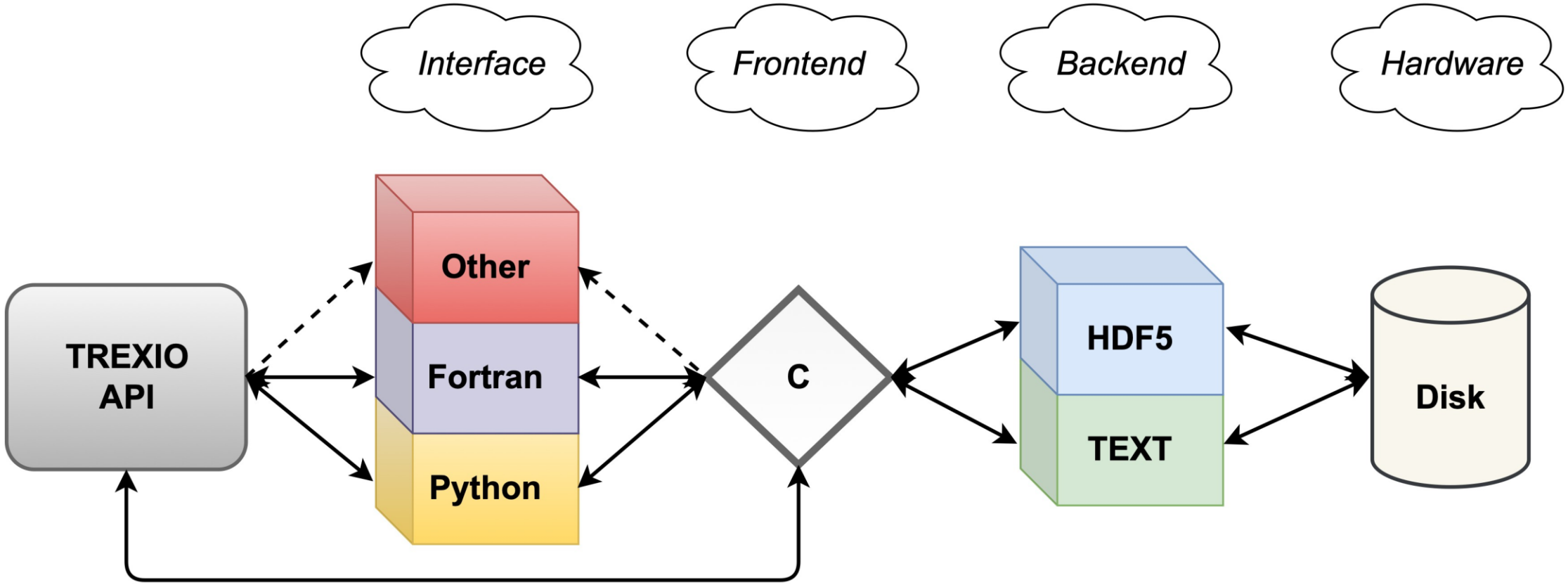
Enhancements compared to other wave function formats

- Fully self-consistent: no code-specific knowledge is required
- Normalization parameters cover all existing ambiguities
- Compact storage of sparse quantities like 2-electron integrals

- **No custom text-based formatting**, forget about typos!

* *https://trex-coe.github.io/trexio/trex.html*

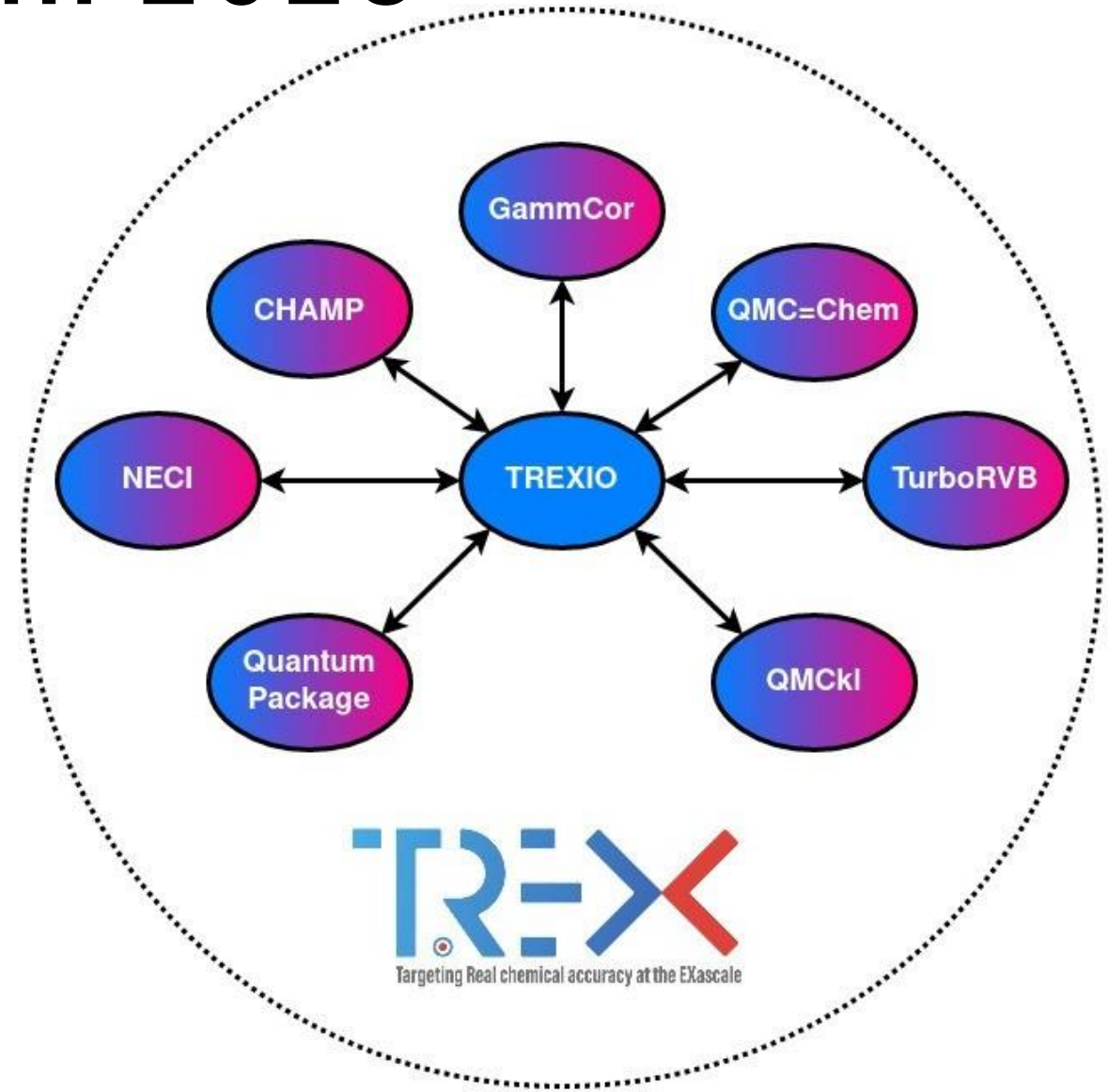
TREXIO as I/O library



- Source code in pure **C** for the best **performance and portability**
- High-performance I/O backend based on the HDF5 library
- Bindings in **Fortran**, **Python**, **OCaml**
- Very **easy to install**: Autotools/CMake, conda, Spack, Guix, pip, apt, opam, you name it :-)

https://github.com/TREX-CoE/trexio

Situation in 2023



Adoption of TREXIO enabled

- Enhanced data exchange and I/O performance in TREX codes
- **QP ⇨ TREXIO ⇨ GammCor** : SAPT with CIPSI density matrices
- **QP ⇨ TREXIO ⇨ CHAMP** : QMC with CIPSI wave functions

·trexio_tools ⇨ TREXIO ⇨ all TREXIO users are interfaced with external programs like GAMESS, Gaussian, PySCF

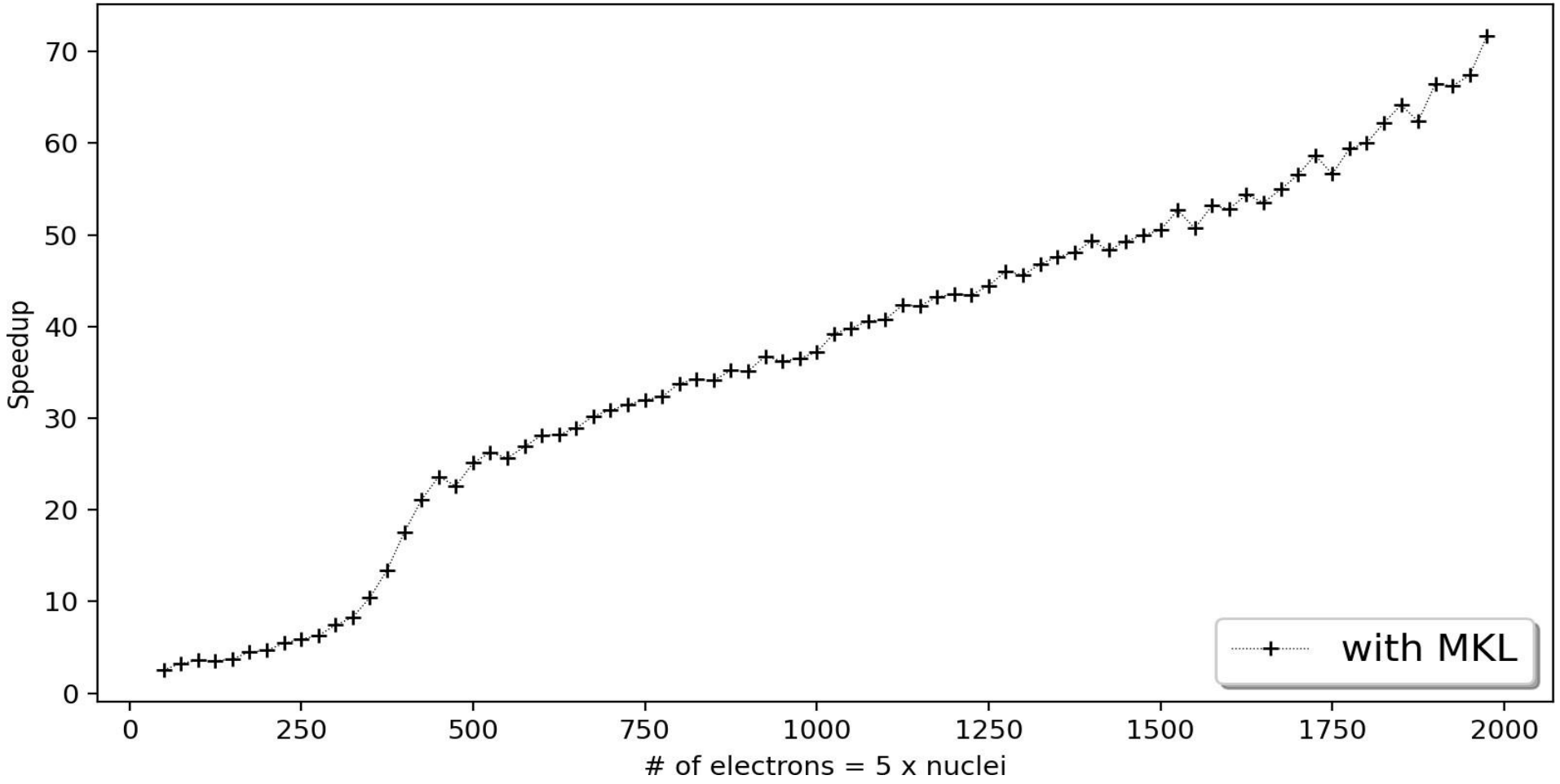
- **QP ⇨ TREXIO ⇨ QMCkl** : user-friendly QMC tutorials in pure Python

QMC Kernel Library: QMCkl

- API for main algorithms of Quantum Monte Carlo
- **Pedagogical** and **high-performance** implementations
- Low-level functions: linear algebra
- High-level functions: domain-specific
- Bindings in **C**, **Fortran**, **Python**

https://github.com/TREX-CoE/qmckl

QMCkl use case: Jastrow factor*



work of Vijay Gopal Chilkuri @ Aix-Marseille University

- TREXIO repository: https://github.com/TREX-CoE/trexio
- QMCkl repository: https://github.com/TREX-CoE/qmckl

Thank you for your at ention!

The TREX: Targeting Real Chemical Accuracy at the Exascale project has received funding from the European Union's Horizon 2020 - Research and Innovation program - under grant agreement no. 952165.

TREX WEBINAR
Quantum Package - User Feedback

Anthony Ferté

Laboratoire de Chimie Et Interdisciplinarité, Synthèse, Analyse, Modélisation

8th February 2023

Quantum Package user since 2018

Master 2 Internship, LCT, Sorbonne Université :

- With Emmanuel Giner and Julien Toulouse
- Multideterminant range separated DFT
- Development and implementation in QP

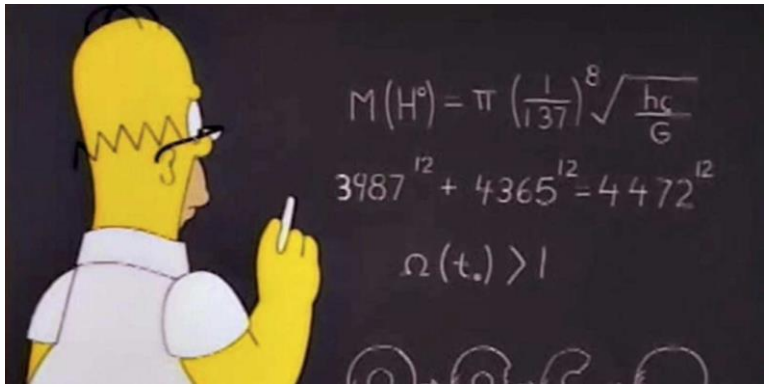
PhD, LCPMR, Sorbonne Université :

- With Stéphane Carniato and Richard Taïeb
- Description of double core hole spectroscopies
- Development and implementation in QP

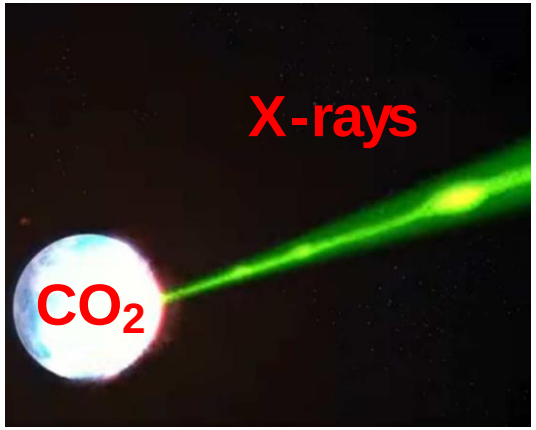
My PhD in a nutshell

Theoretical study of double ionisation/excitation in core shell

Quantum Chemistry

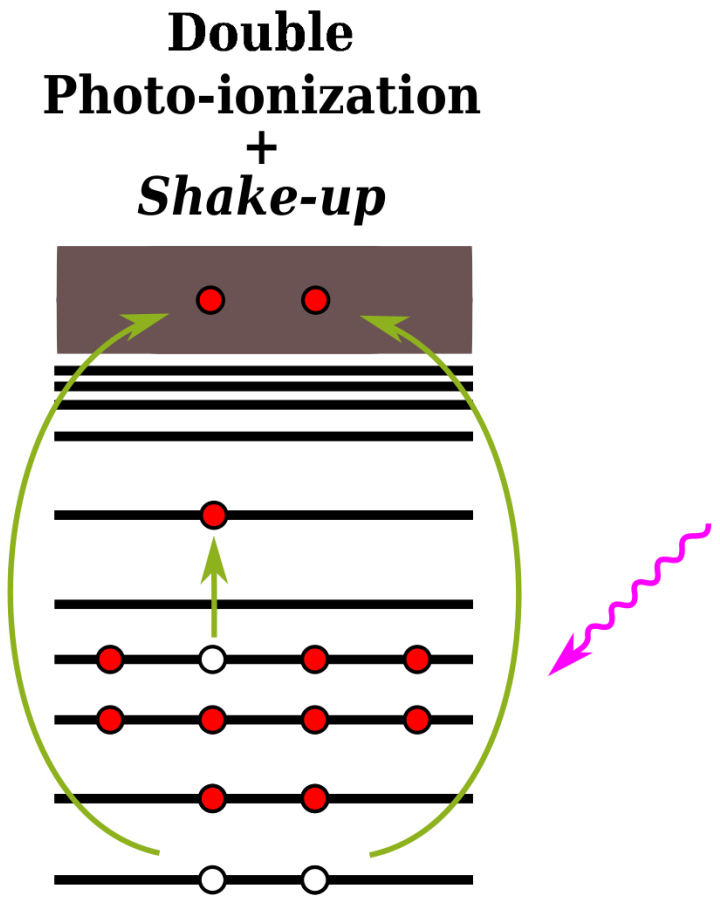


Computational Chemistry

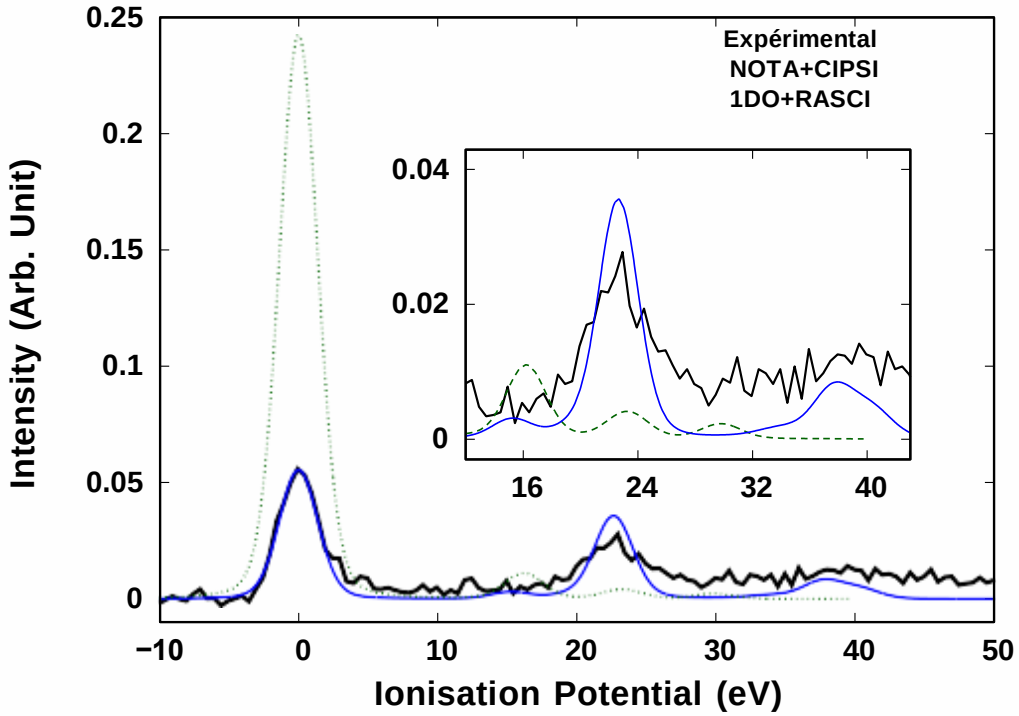


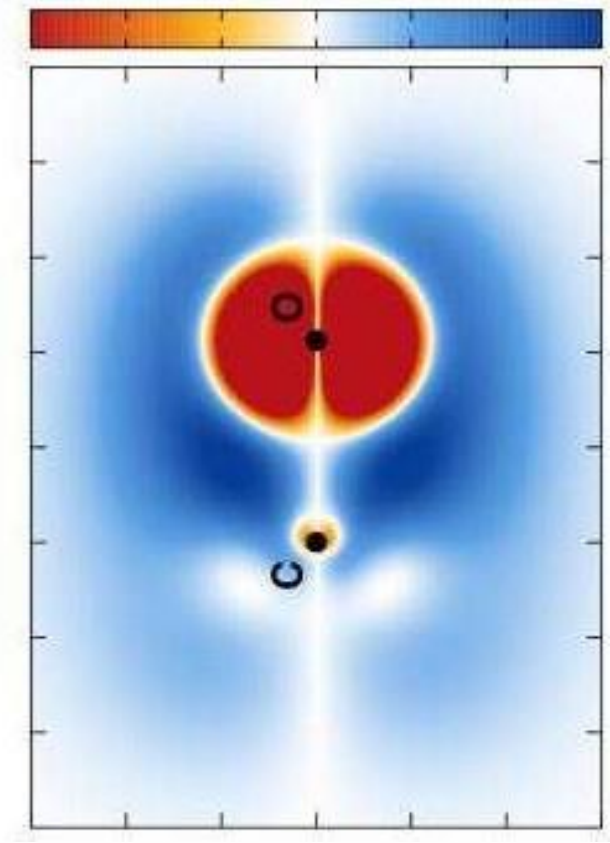
Spectroscopy - XPS

Why did we need new methodological developments ?



Why did we need new methodological developments?





Due to relaxation a given one electron MO basis can not properly describe both initial and final systems

A. Ferté *et al.*, J. Phys. Chem. Lett., 11, 4359-4366, 2020

Why did I use Quantum Package?

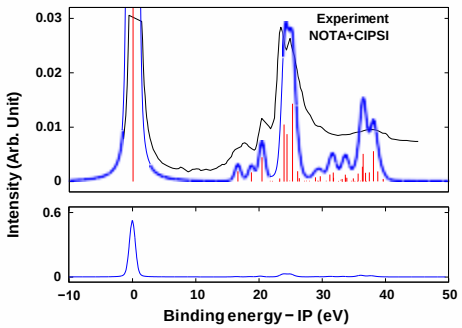
- QP do not fight back (Flexible ; IRPF90 ; EZFIO ; Plugin system)
- Easy to find pertinent documentation for developer
- QP do not fight back (Flexible ; IRPF90 ; EZFIO ; Plugin system)
- Easy to find pertinent documentation for developer Especially made to handle Slater determinants Produces high quality wave functions
- Helpful and Friendly team Free and Open source

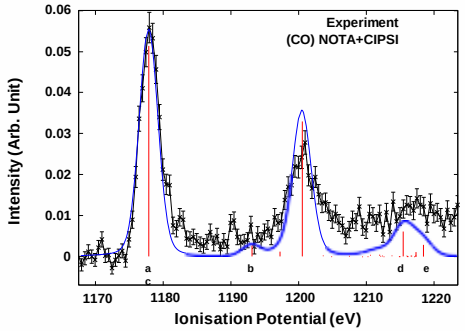
What did I use Quantum Package for ?

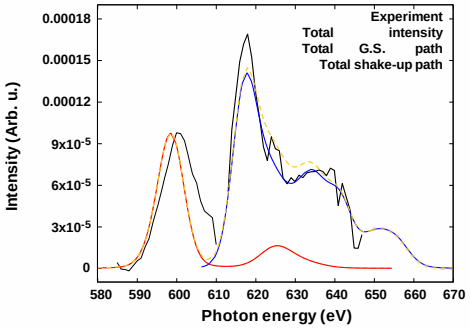
Methodological aspects

- How to use the native programs of QP for core hole state calculation
- Development of a large plugin series fully interfaced with QP

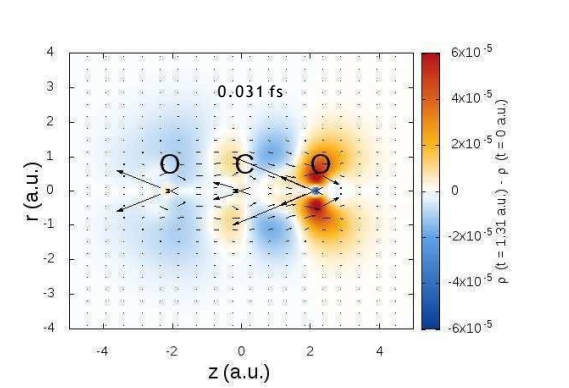
Simulation / Production

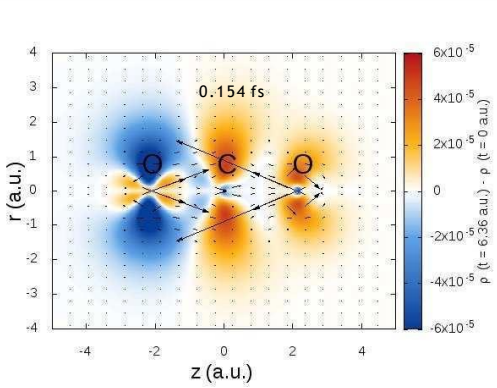


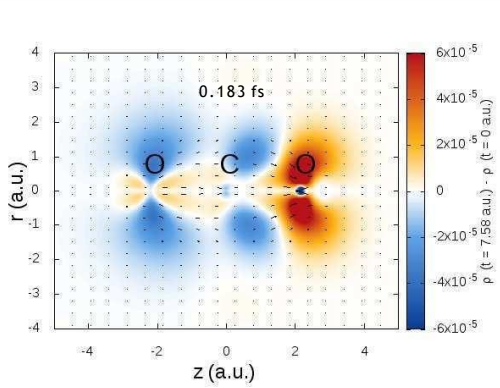




Physics Interpretation







&

Team ModES (CEISAM)

Experimentalist collaborators :
Jérôme Palaudoux, Francis Penent,
Pascal Lablanquie, Iyas Ismail,
Marc Simon *et al.*

Emmanuel Giner
Anthony Scemama

&
Team ModES (CEISAM)

LabEx MiChem

TREX
Targeting Real chemical accuracy at the EXascale

Thank you for your attention.

Experimentalist collaborators :
Jérôme Palaudoux, Francis Penent,
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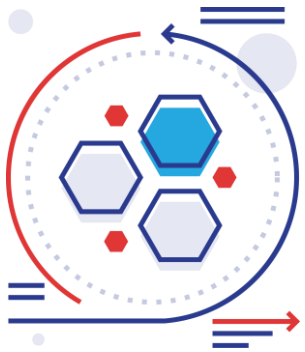
Emmanuel Giner
Anthony Scemama

Targeting Real chemical accuracy at the EXascale

User Experience with NECI



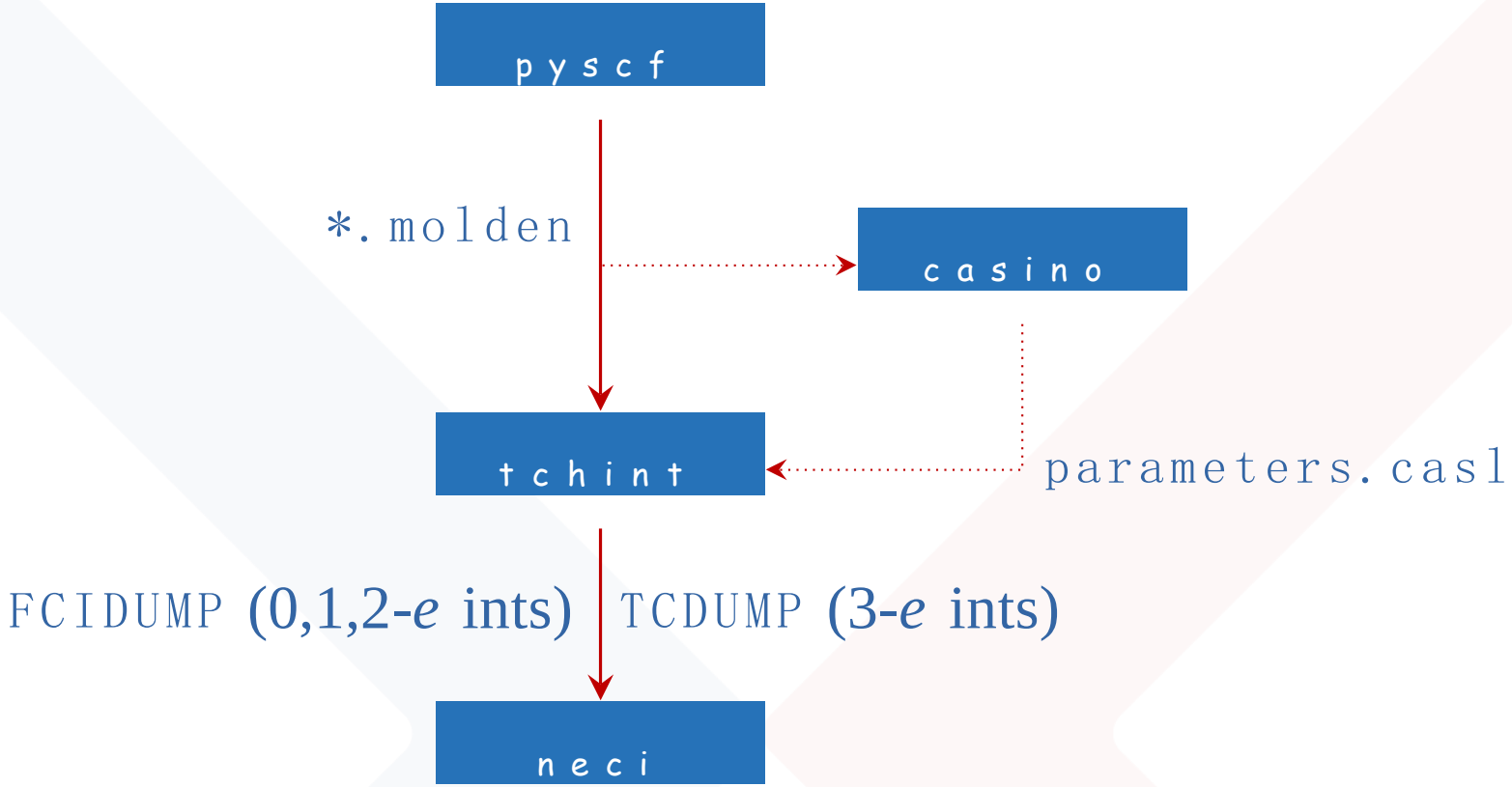
Pablo Lopez Rios,
Max Planck Gesellschaft

Targeting Real Chemical Accuracy at the Exascale project has received funding from the European Union Horizoon 2020 research and innovation programme under Grant Agreement **No. 952165.**

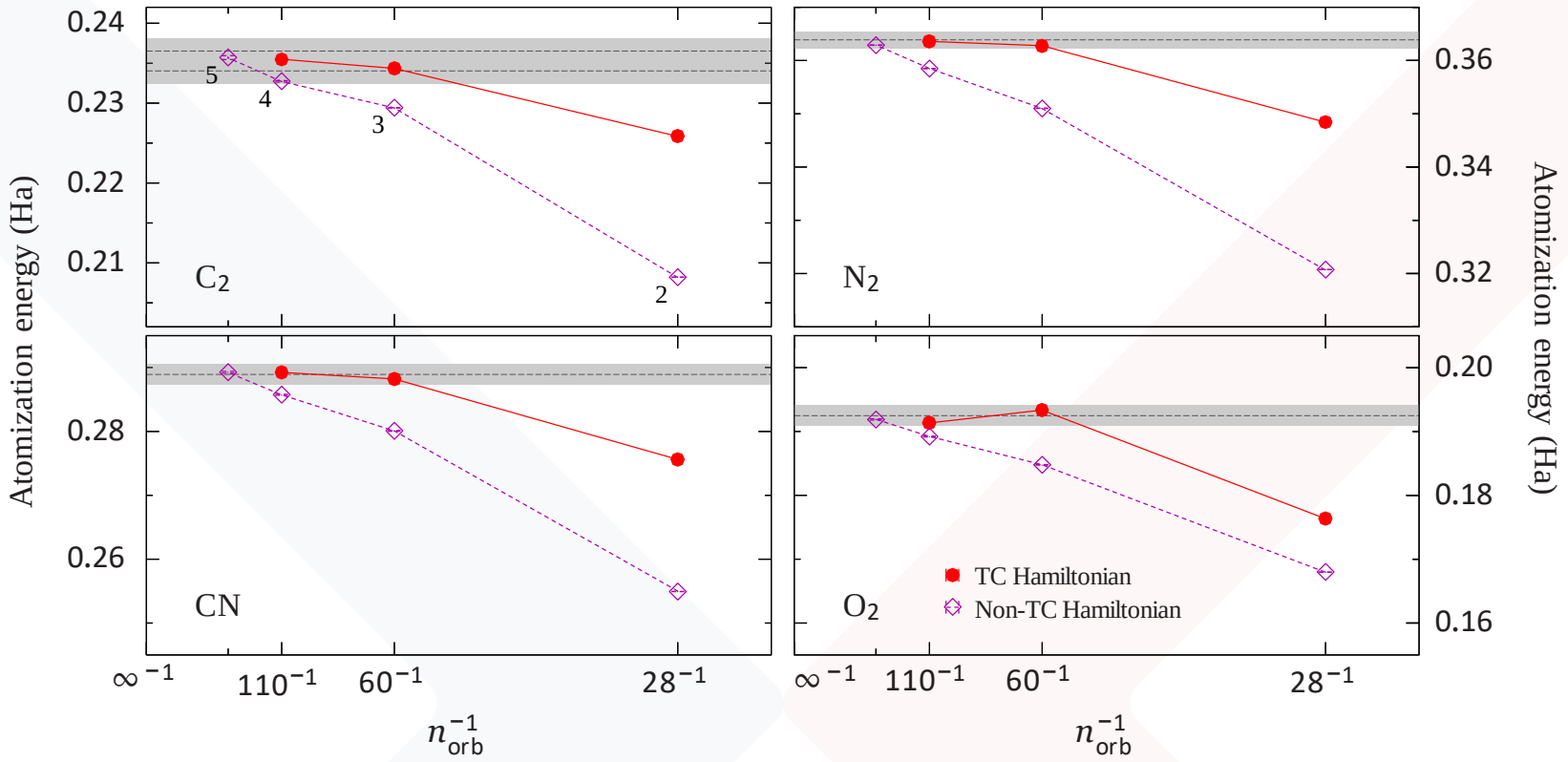
8 February 2023

neci + tchint workflow

- TC-FCIQMC with `neci` and `tchint`:



- TC method provides ~ 2 cardinal-number advantage:



Targeting Real chemical accuracy at the EXascale

User experience with TurboRVB

Webinar, 8 February 2023

Giacomo Tenti, - SISSA

Targeting Real Chemical Accuracy at the Exascale project has received funding from the European Union Horizoon 2020 research and innovation programme under Grant Agreement **No. 952165.**

My experience with TurboRVB

First contact with TurboRVB:

Study of the hydrogen chain with a Pfaffian wave function (Master's thesis with prof. Sandro Sorella)

Learning Turbo **the hard way** (complex workflow, lots of parameters to control…)

The **easy way**:

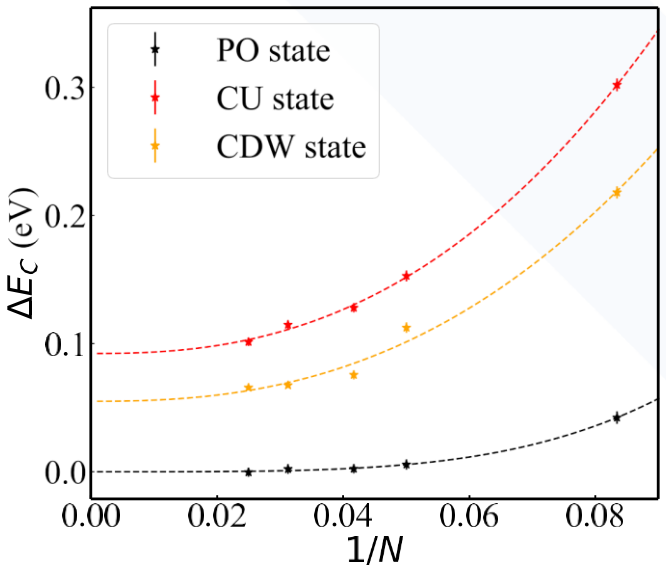
Using TurboGenius, the workflow of a typical calculation becomes much simpler!

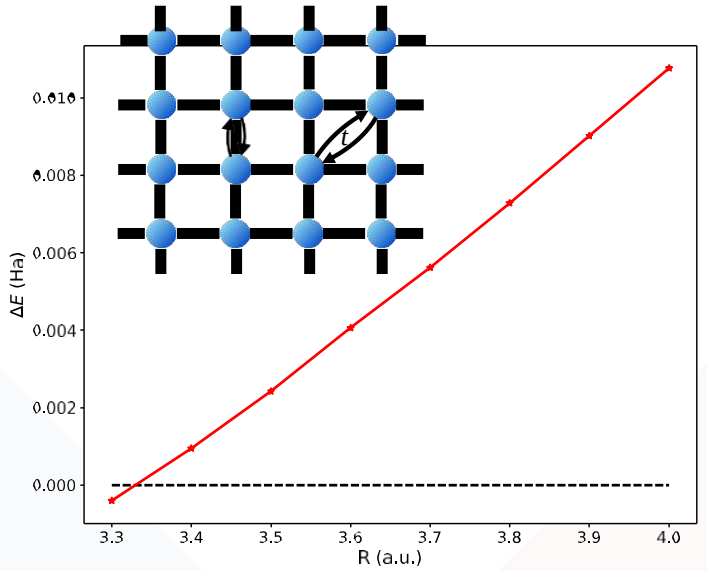
(Best way to learn how to use TurboRVB)

Moreover, advanced users still have complete control of the calculation

Projects with TurboRVB Quantum Monte Carlo Package SISSA:

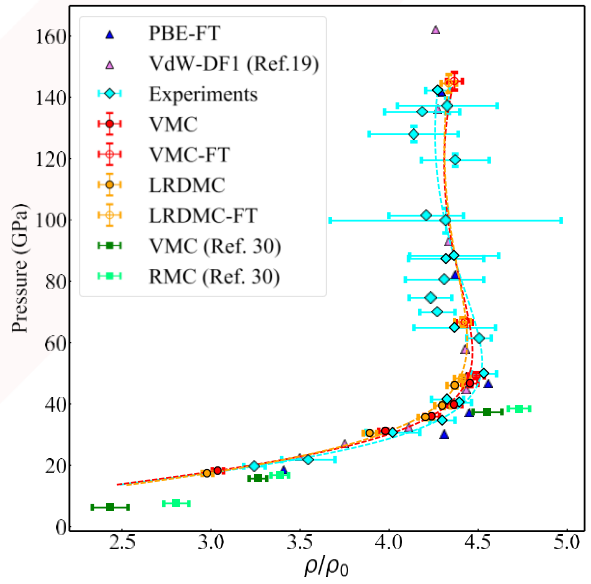
Structure optimization and CDW states





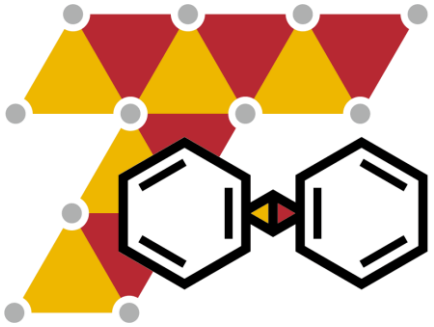
Phase diagram of hydrogen model systems

Generation of training sets for QMC - Machine Learning potentials



https://arxiv.org/abs/2301.03570

Modelling molecules and materials using TurboRVB



Andrea Zen
Università di Napoli Federico II

TREX webinar

February 8th , 2023

Implicitly multideterminat ansatz

TurboRVB: A many-body toolkit for *ab initio* electronic simulations by quantum Monte Carlo

Cite as: J. Chem. Phys. **152**, 204121 (2020); https://doi.org/10.1063/5.0005037
Submitted: 19 February 2020 . Accepted: 20 March 2020 . Published Online: 29 May 2020

Kousuke Nakano, Claudio Attaccalite, Matteo Barborini, Luca Capriotti, Michele Casula, Emanuele Coccia, Mario Dagrada, Claudio Genovese, Ye Luo, Guglielmo Mazzola, Andrea Zen, and Sandro Sorella

COLLECTIONS

Paper published as part of the special topic on Electronic Structure Software

Implicitly multideterminat ansatz

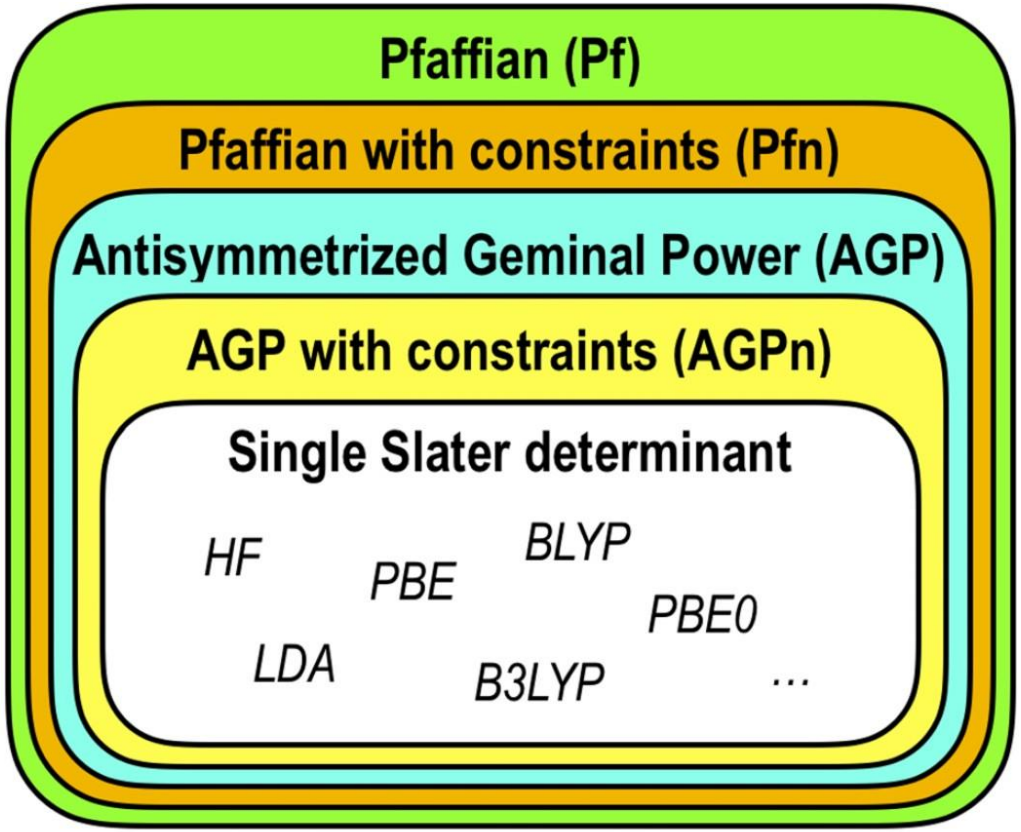


FIG. 3. *Ansatz* hierarchy. The output of Hartree–Fock (HF) or DFT simulations with different exchange-correlation functionals are special instances of the SD *Ansatz*.

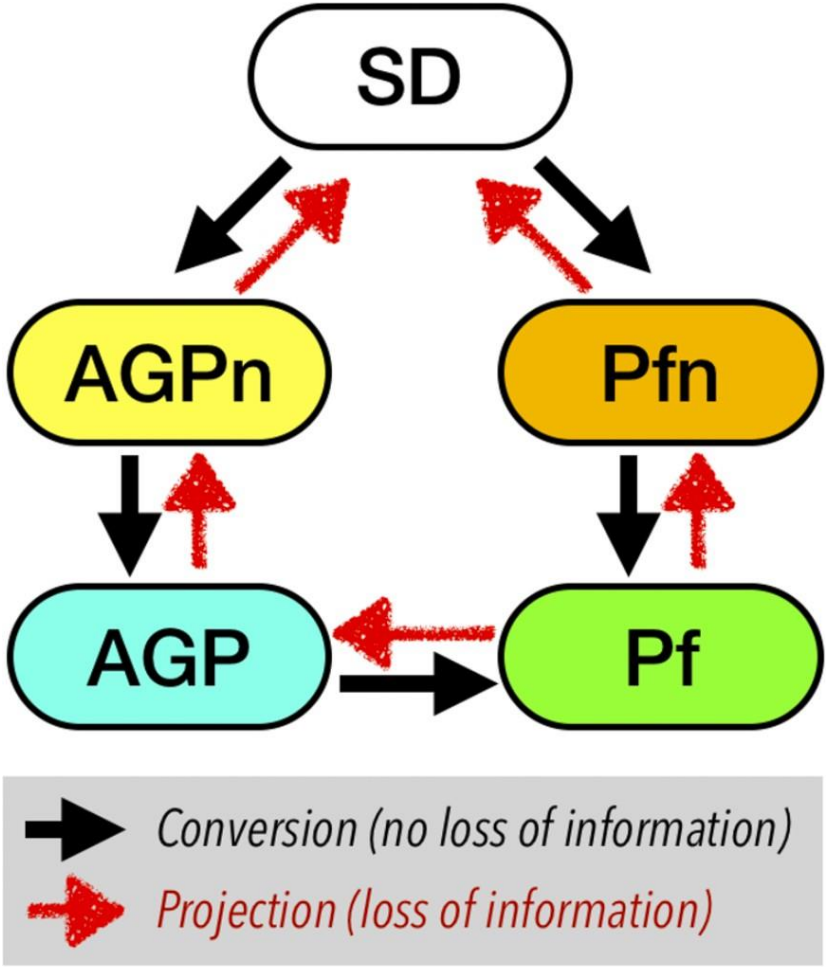
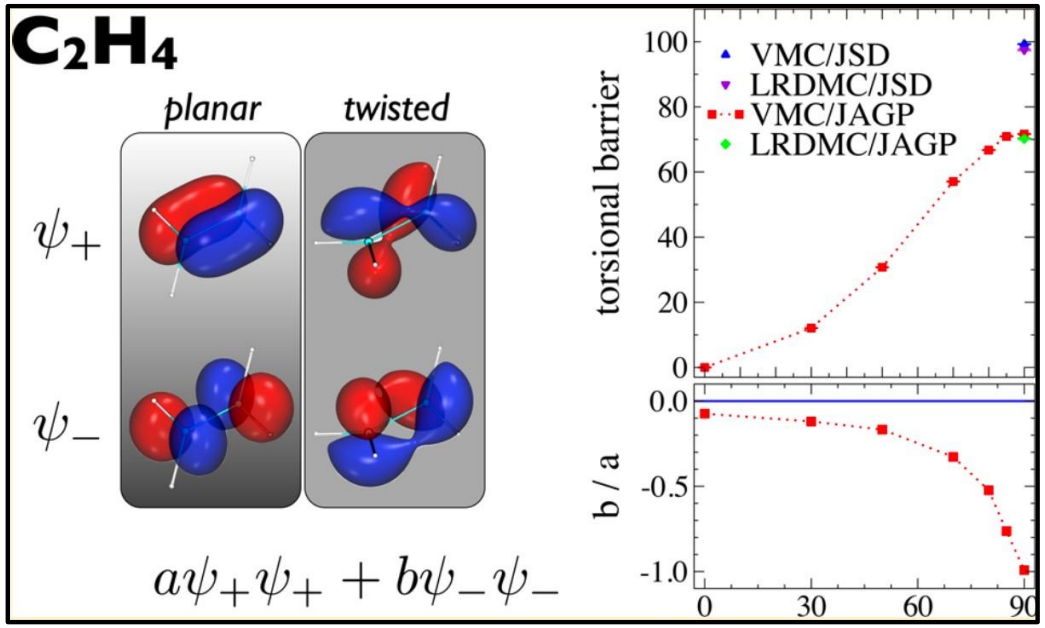


FIG. 4. *Ansatz* conversion.

J. Chem. Phys. 152, 204121 (2020)
TurboRVB: A many-body toolkit for ab initio electronic simulations by quantum Monte Carlo

When do we need a multideterminat ansatz?

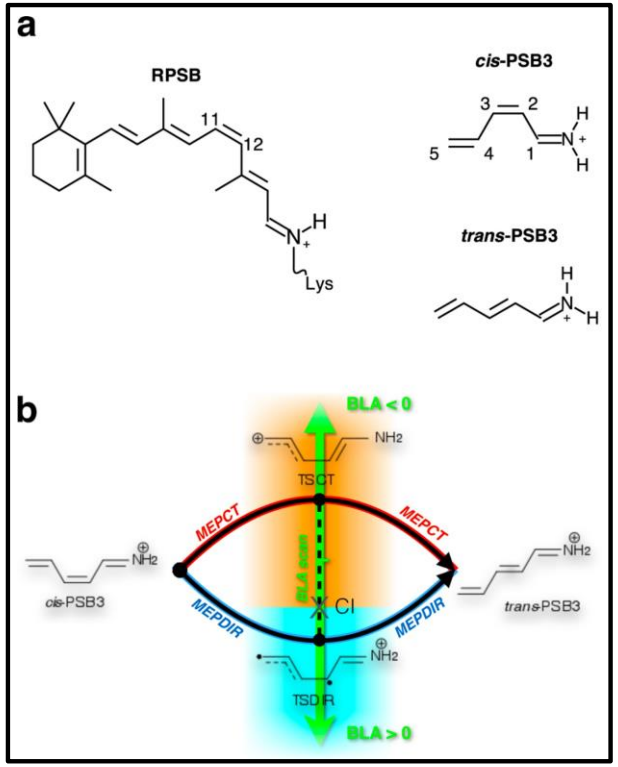
Breaking bonds



J. Chem. Theory Comput. 2014, 10, 1048−1061

Static and Dynamical Correlation in Diradical Molecules by Quantum Monte Carlo Using the Jastrow Antisymmetrized Geminal Power Ansatz

Transition states

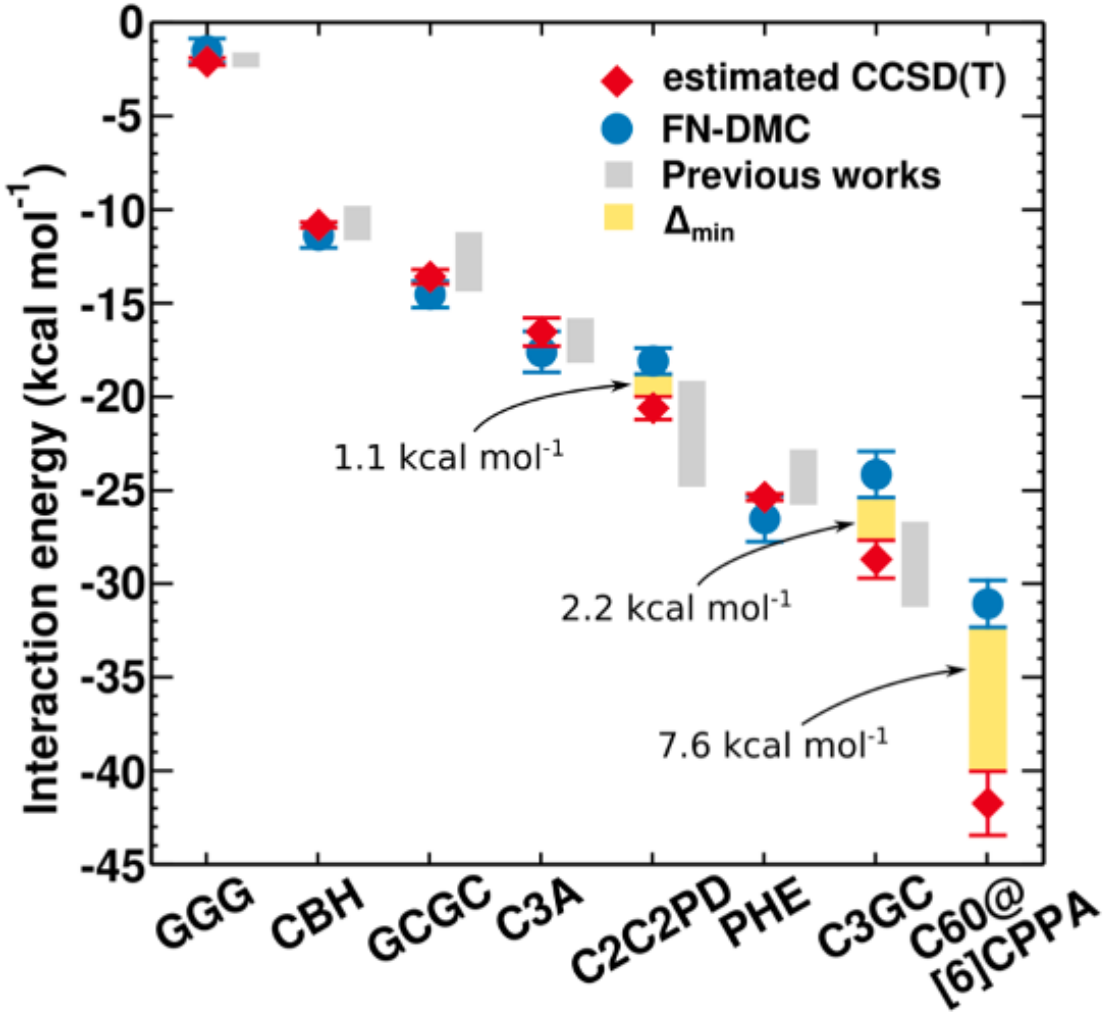


J. Chem. Theory Comput. 2015, 11, 992−1005

Quantum Monte Carlo Treatment of the Charge Transfer and Diradical Electronic Character in a Retinal Chromophore Minimal Model

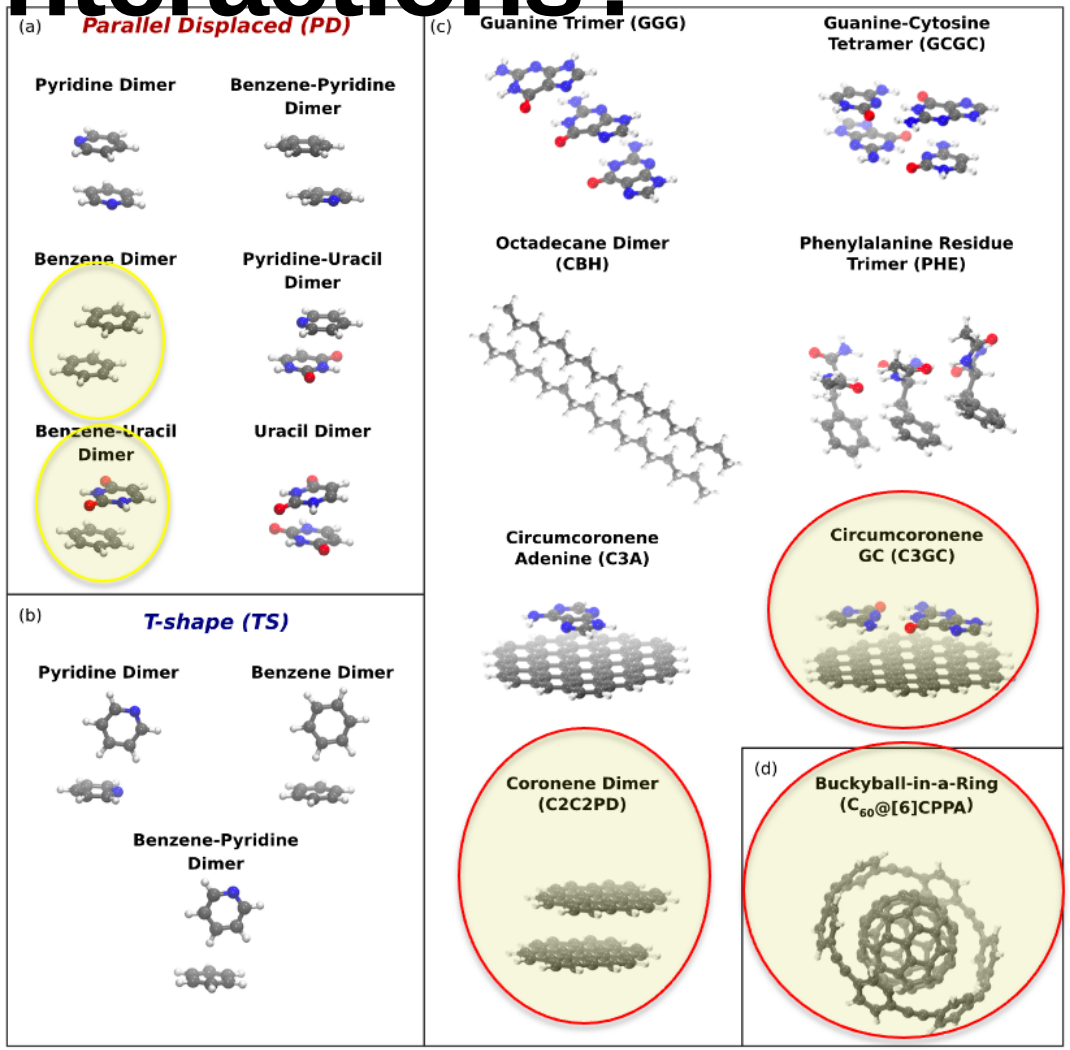
Reference methods: FN-DMC & CCSD(T)

- Generally observed a **good agreement between the CCSD(T) and the FNDMC** (with a Slater-Jastrow guide function) evaluation of **non-covalent interactions**.
- Recently observed a **disagreement in large complexes** not coming from the known issues (small basis set, timestep bias, etc.)

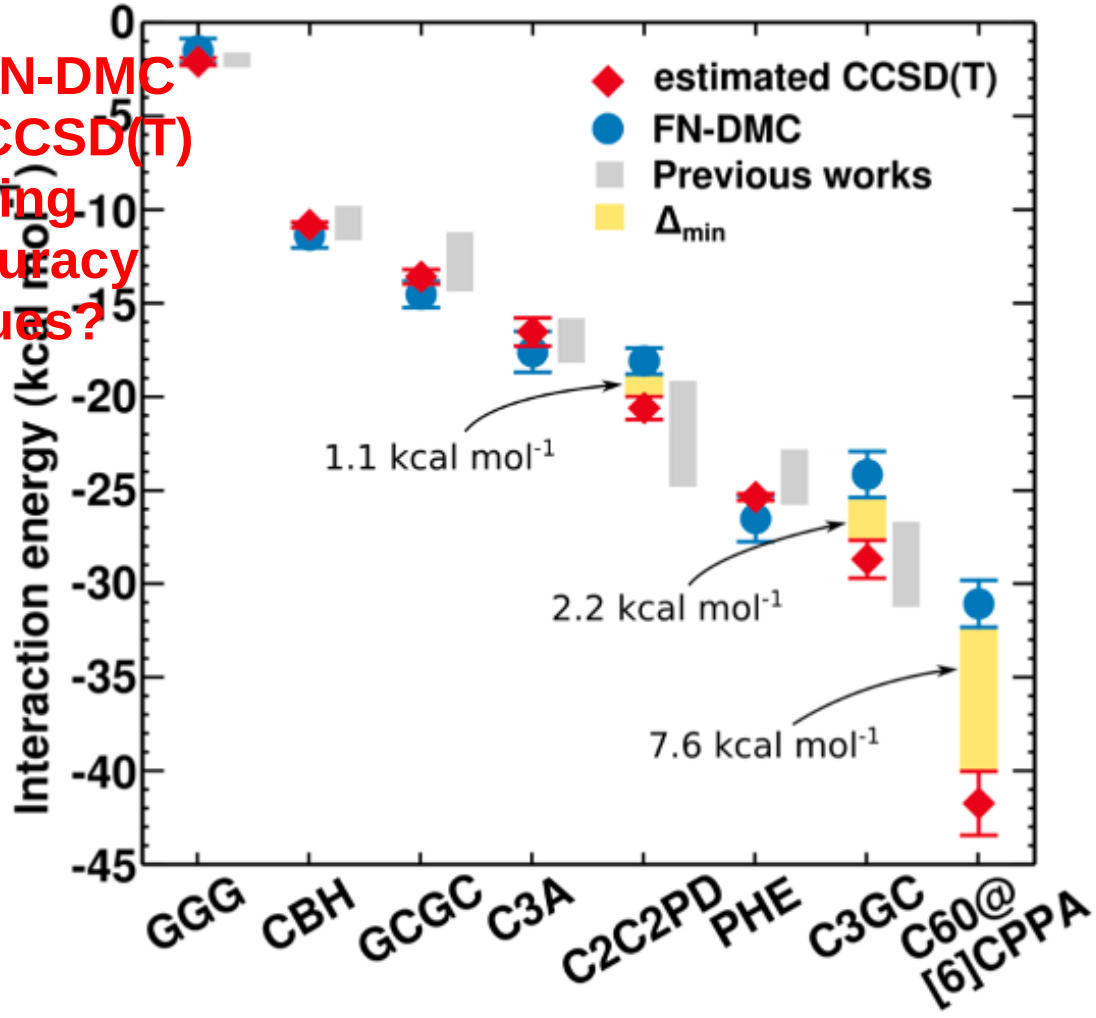


Nature Communications 12, 3927 (2021)
Interactions between Large Molecules: Puzzle for Reference Quantum-Mechanical Methods

Issue with pi-pi interactions?



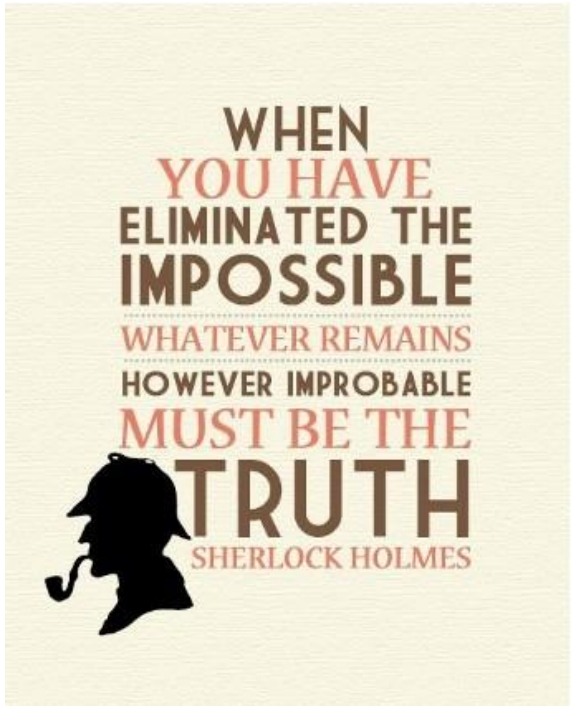
Is FN-DMC or CCSD(T) having accuracy issues?



Nature Communications 12, 3927 (2021)

Interactions between Large Molecules: Puzzle for Reference Quantum-Mechanical Methods

Inspecting FN-DMC weaknesses



Weeknesses in FN-DMC:

- ~~Bugs in the code~~ *No, 2 codes agree* [1,2]
- ~~Pseudopotentials~~ *No, AE and PP agree* [1,2]
- ~~Optimization of Jastrow~~ *No: tested LA, TM & DLA* [1]
- ~~Determinant initialization~~ *No: tested LDA, PBE, PBE0* [1]
- FN beyond single Slater (**?**) *Work in progress*

1Y.S. Al-Hamdani, P.R. Nagy, A. Zen, D. Barton, M. Kállay, J.G. Brandenburg, A. Tkatchenko, *Interactions between Large Molecules: Puzzle for Reference Quantum-Mechanical Methods*, Nature Communications 12, 3927 (2021).
Uses CASINO, DMC with pseudopotentials testing LA/TM/DLA.

2] A. Benali, H. Shin and O. Heinonen, Quantum Monte Carlo benchmarking of large noncovalent complexes in the L7 benchmark set, JCP 153, 194113 (2020).
Uses QMCPACK, DMC with all-electrons.

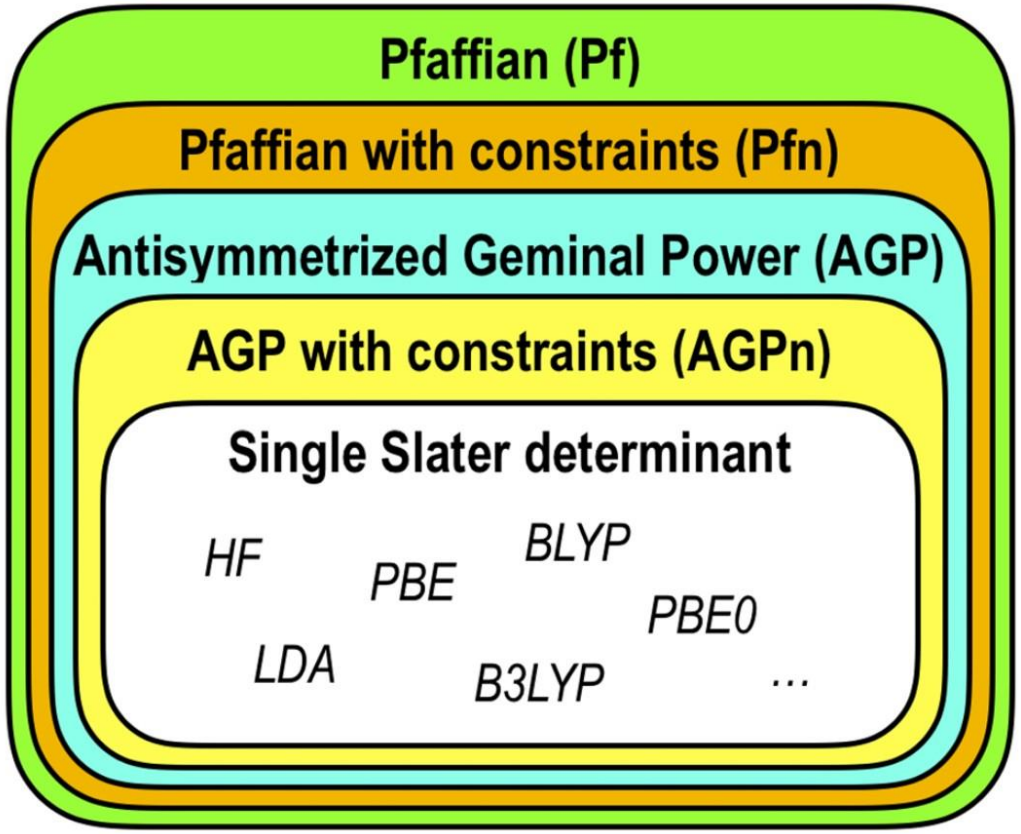
FN beyond single Slater

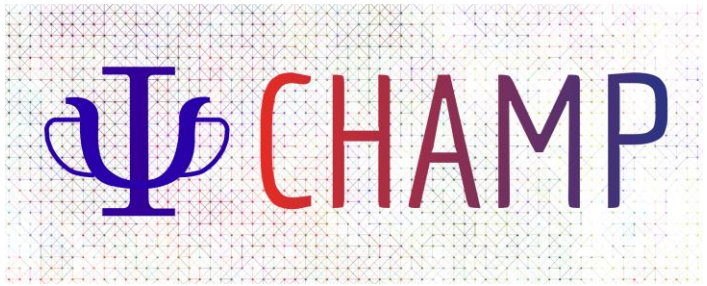
Interaction energy is the energy difference between two or more systems. It's a small fraction of the total energy of a system.
Difficulty: keeping the quality of the wave function (optimisation) consistently good in two or more systems.

pyscf

Kosuke Nakano

TREX-I/O

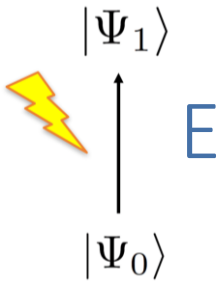




CHAMP : Cornell-Holland Ab-initio Materials Package

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

Stuart Shepard
University of Twente, The Netherlands

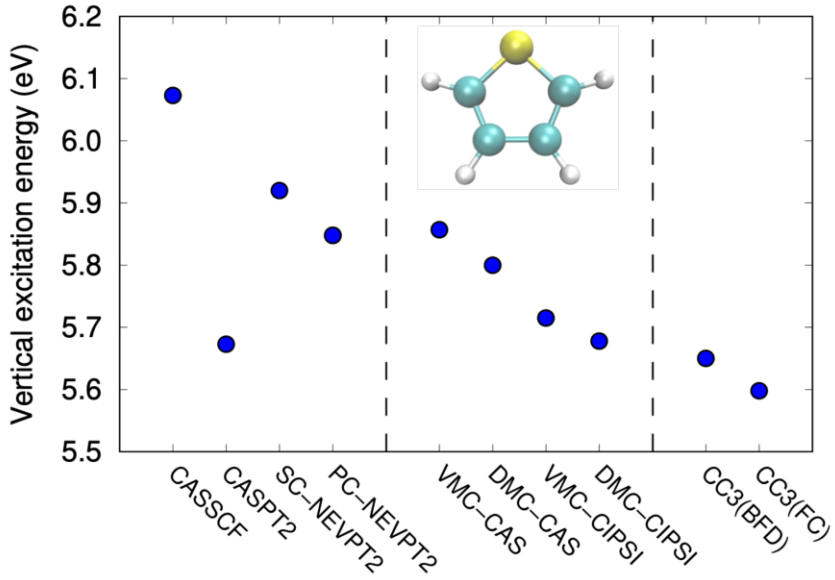


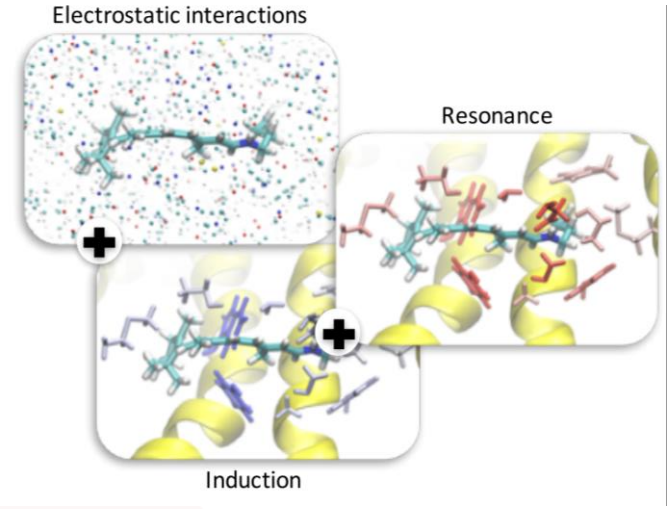
Excited States using CHAMP

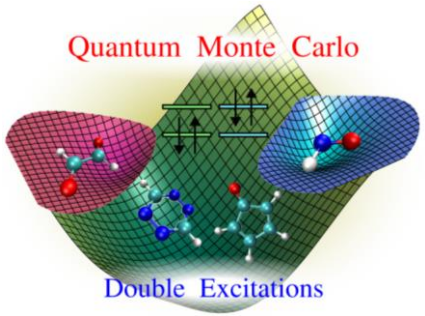
- VMC wave function optimization + DMC
  - Jastrow-Slater multi-determinant

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \mathcal{J}(\mathbf{r}_1, \ldots, \mathbf{r}_N) \times \sum_i c_i \, D_i(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

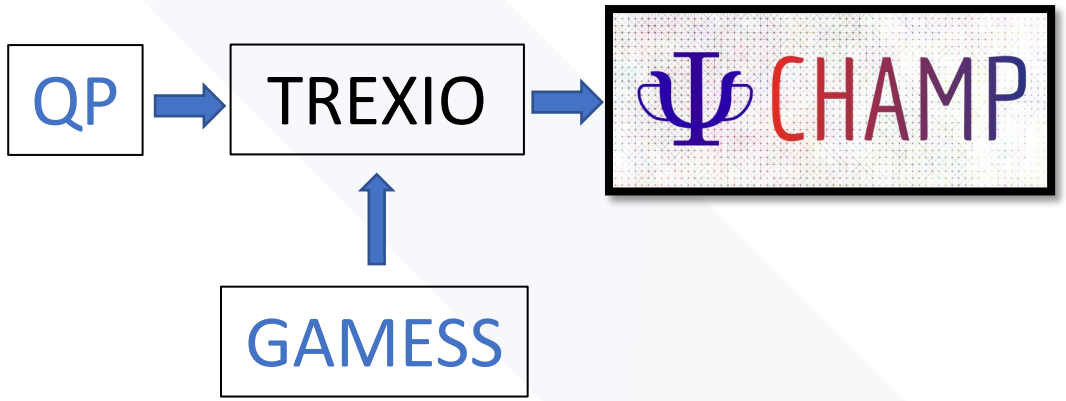
  - Any symmetry
  - Embedding



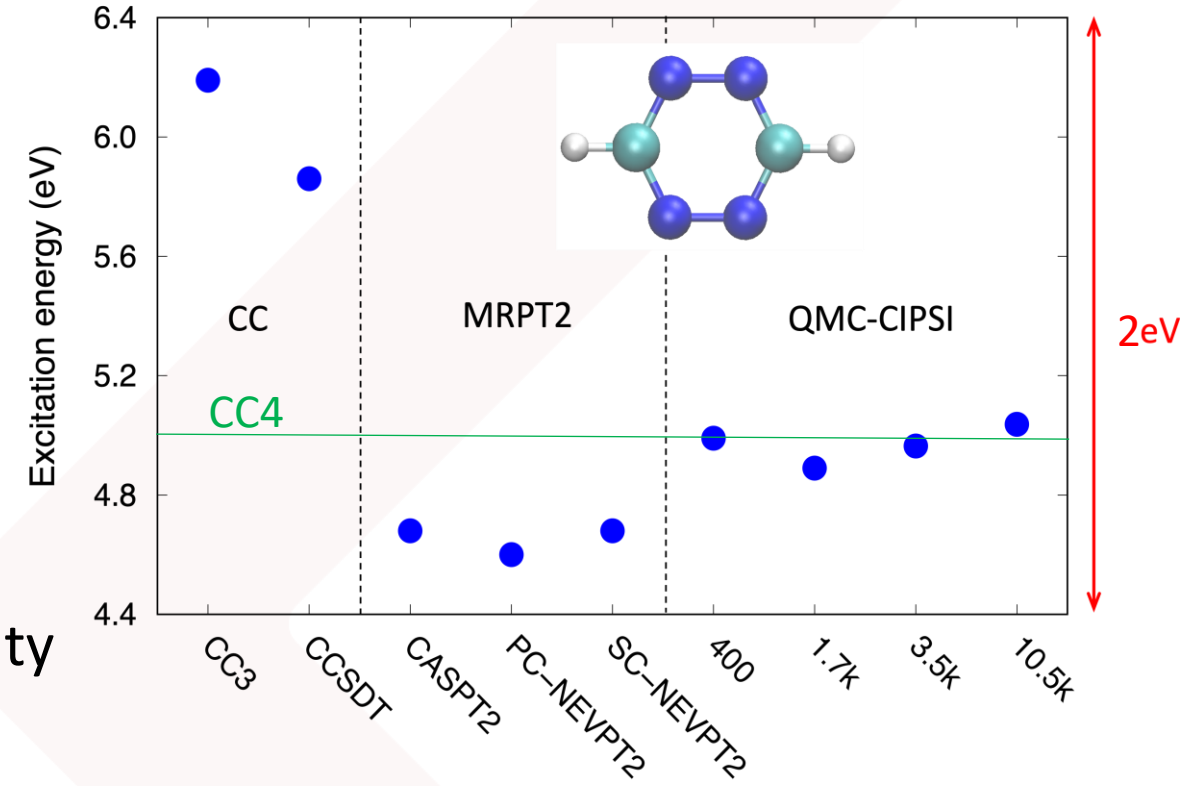




Accurate Double Excitations ➡ QP + CHAMP in action



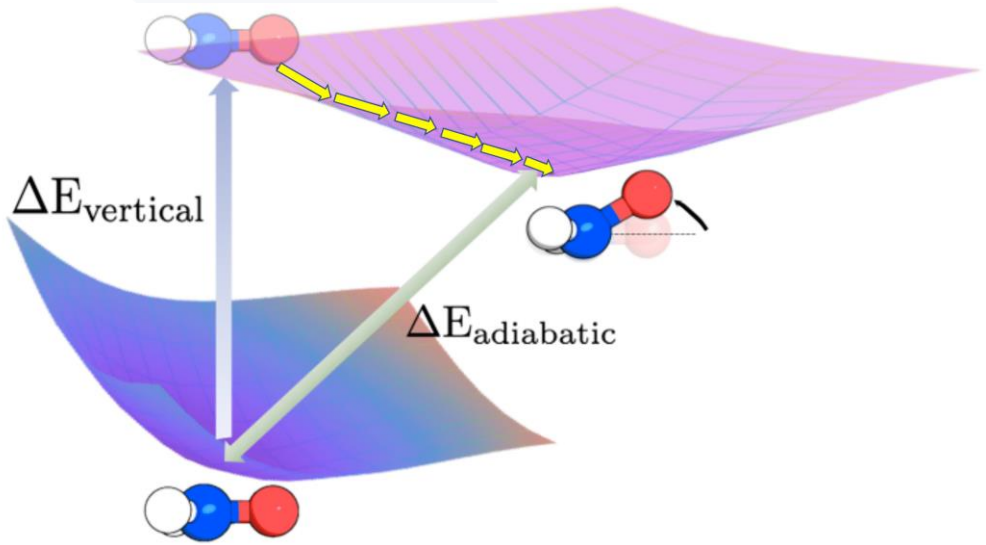
- States of same symmetry
- State-specific optimization with overlap penalty

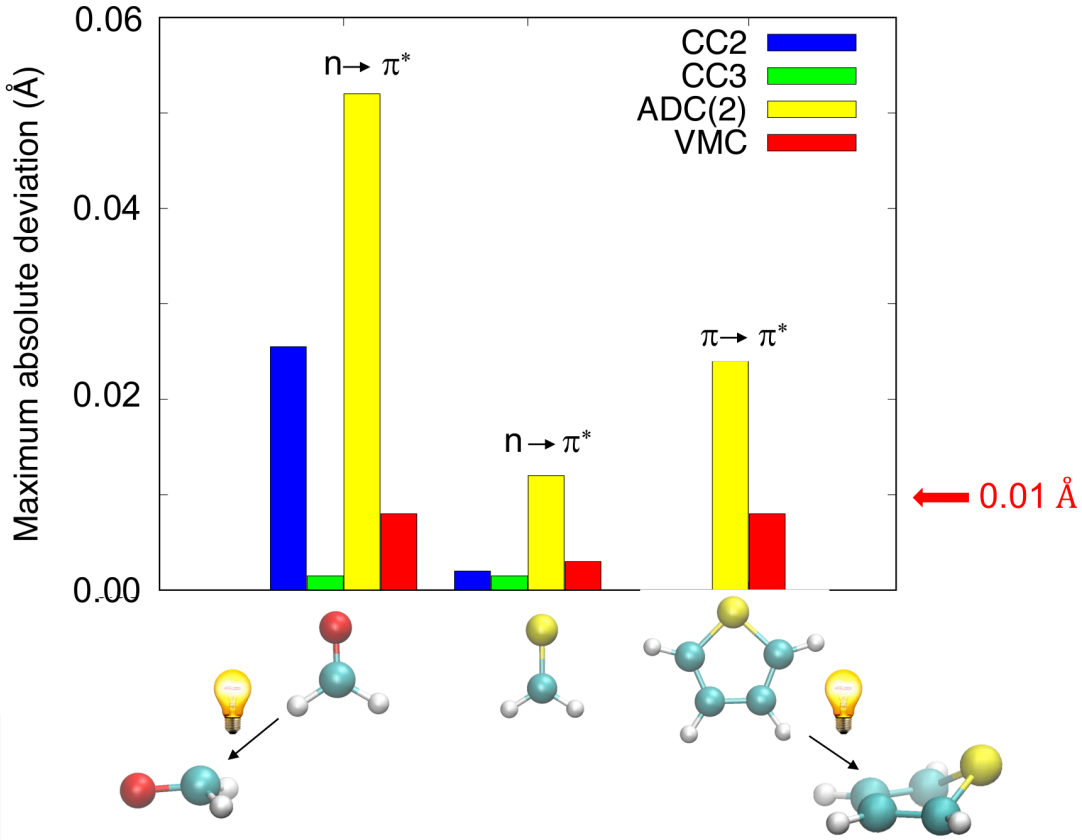


$|\Psi_1\rangle$

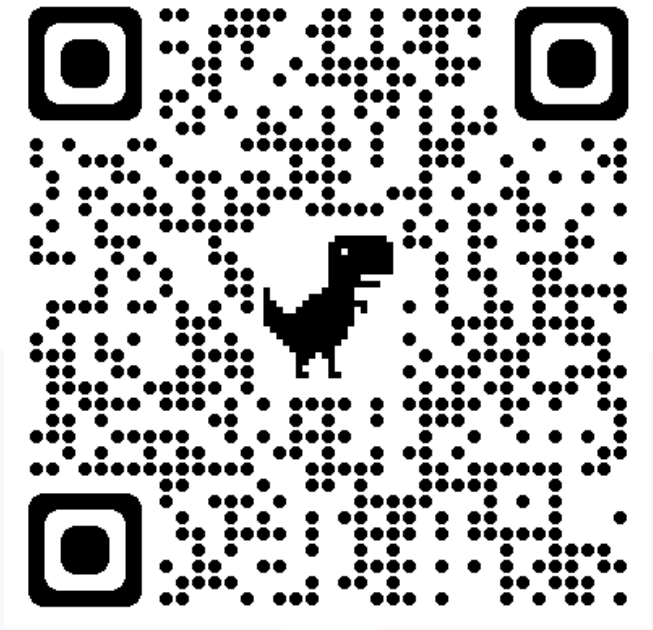
$|\Psi_0\rangle$

Example: Geometry Optimization in Excited State





Codes available on GitHub



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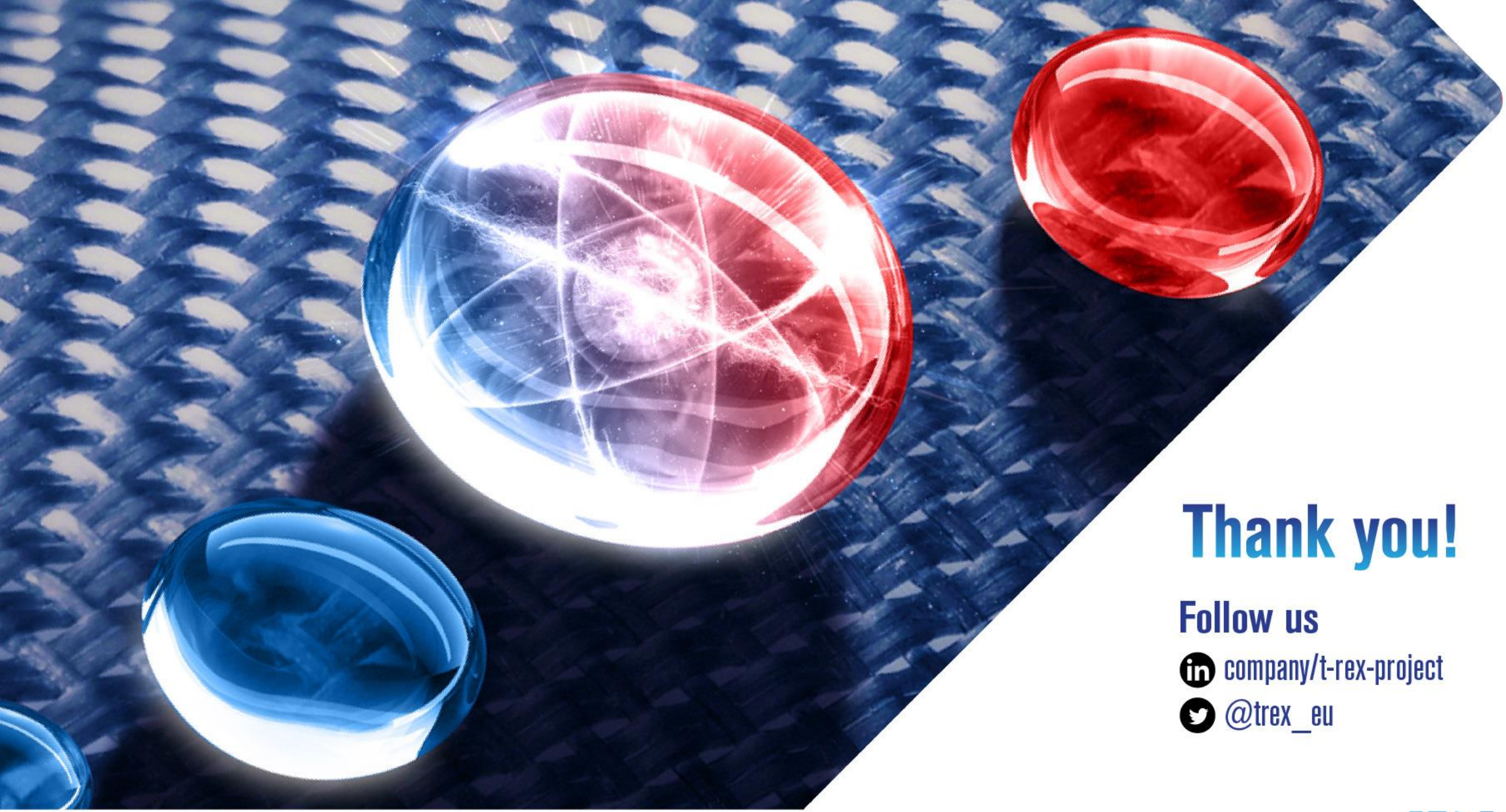
TREX Workshop - 18-20 April 2023, Lodz, Poland

Code Tuning for the Exascale - 12-14 June 2023, Bratislava (SK)

TREX School on QMC with TurboRVB - 3-7 July, 2023, Trieste (IT)



Thank you!

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