The Quantum Package: developer friendly electronic structure

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Tuesday, 20 February 2024

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    - ★ Mutual benefits of collaboration

How the Quantum Package was thought

- Typical available codes: "Old but efficient"
  - Rather ancient but efficient languages (C, Fortran 77/90)
  - Not necessarily open-source ...
  - Outsider's point of view: a nightmare !
- How we designed the QP: (short version)
  - Highly optimized fundamental building blocks
  - Modular structure: Just pick what you aim for !
  - Do not need to understand "all the code"
  - Plugin system: easy to create your own code
- Documentation material
  - Github webpage (https://quantumpackage.github.io/qp2/)
  - Read-the-Doc documentation
  - Tutorials (available on Youtube)
  - Try in your browser interface !

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A few examples of applications with the QP

- Used/developed in
  - Europe: France, Poland
  - North America: U.S.A, Canada
- Ground state and excited states with SCI
  - State-of-the art calculations
  - Benchmark done by Loos *et. al.*
  - Typical system size: Benzene
- Multi-reference range-separated DFT (Julien Toulouse, E. G.)
- Positron-binding calculations (E. G.)
- Transcorrelated/QMC calculations (Ammar, Scemama, E. G.)
- Complex Gaussian basis (Ammar)
- Application to core-excitations/ionizations (Ferté *et. al.*)
- Multi-reference adiabatic connection (Pernal *et. al.*, Poland)
- SCI for QMC (Benali *et. al.*, U.S.A)
- Extension to solid-state of SCI (Caffarel *et. al.*, U.S.A.)
- High-level Coupled Cluster calculations (Piecuch *et. al.*, U.S.A.)
- Pair-natural orbitals functionals (Hollet, Canada)

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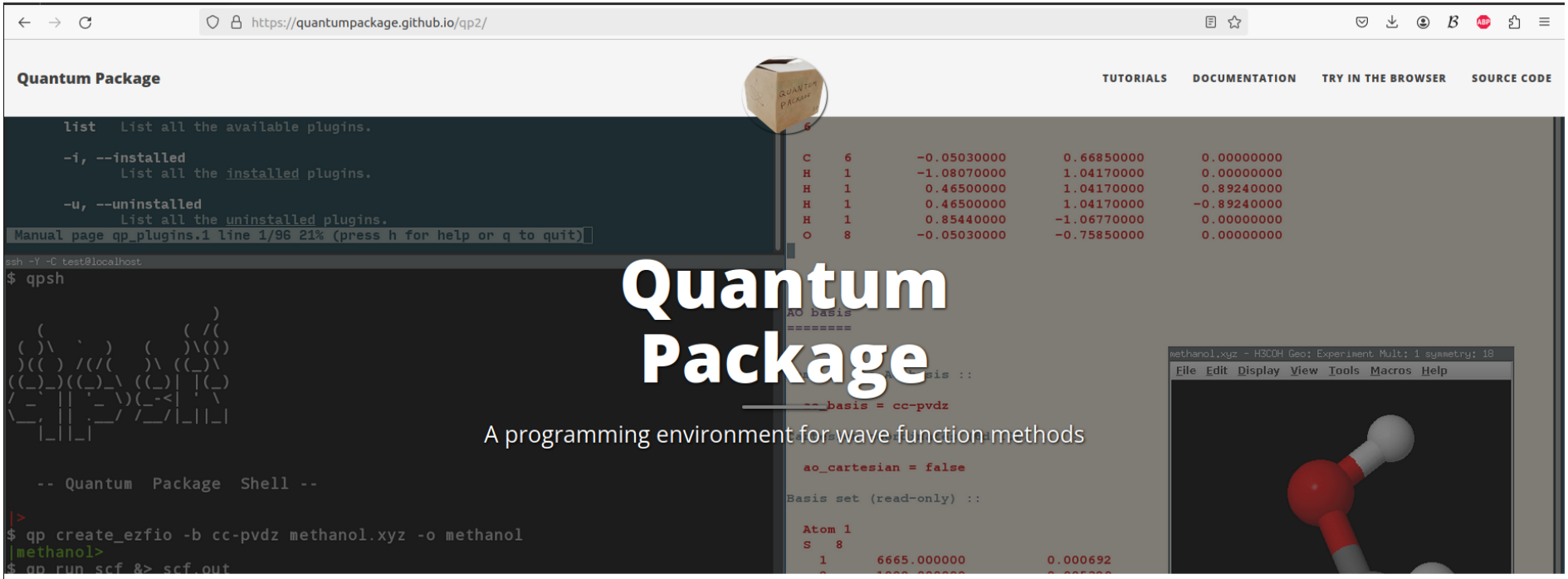

Quantum Package is an open-source programming environment for quantum chemistry specially designed for wave function methods. Its main goal is the development of determinant-driven selected configuration interaction (sCI) methods and multi-reference second-order perturbation theory (PT2).

The determinant-driven framework allows the programmer to include any arbitrary set of determinants in the reference space, hence providing greater methodological freedoms. The sCI method implemented in *Quantum Package* is based on the CIPSI (Configuration Interaction using a Perturbative Selection made Iteratively) algorithm