Quantum Package in a web browser

A quick interactive demo on the Web

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Quantum Package 2.0: An Open-Source Determinant-Driven Suite of Programs

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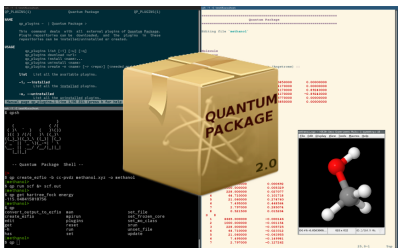
Quantum chemistry is a discipline which relies heavily on very expensive numerical computations. The scaling of correlated wave function methods lies, in their standard implementation, between $\mathcal{O}(N^5)$ and $\mathcal{O}(e^N)$, where N is the number of one-electron basis functions. Therefore, performing accurate calculations on chemically meaningful systems requires i) approximations that can lower the computational scaling, and ii) efficient implementations that take advantage of modern massively parallel architectures. 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 which complements the variational sCI energy with a PT2 correction. Additional external plugins have been recently added to perform calculations with multireference coupled cluster theory and range-separated density-functional theory. All the programs are developed with the IRPF90 code generator, which simplifies collaborative work and the development of new features. Quantum Package strives to allow easy implementation and experimentation of new methods, while making parallel computation as simple and efficient as possible on modern supercomputer architectures. Currently, the code enables, routinely, to realize runs on roughly 2 000 CPU cores, with tens of millions of determinants in the reference space. Moreover, we have been able to push up to 12 288 cores in order to test its parallel efficiency. In the present manuscript, we also introduce some key new developments: i) a renormalized second-order perturbative correction for efficient extrapolation to the full CI limit, and ii) a stochastic version of the CIPSI selection performed simultaneously to the PT2 calculation at no extra cost.



TOC graphical abstract

https://arxiv.org/abs/1902.08154

What is Quantum Package

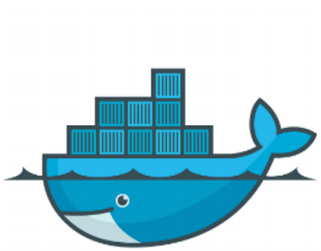
- Easy-to-use quantum chemistry software
- Come out of the box with common wave function methods (Hartree-Fock, Full CI . . .)
- In V2
  - `qpsh`: `bash` + `Quantum Package` (manpage autocomplete and $PATH. . .)
  - `qp plugins`: Plugins can be downloaded independently from internet

How to work with it

- Install it
- Run `qpsh`
- Create `ezfio` database or load an old `ezfio`
- Run some calculations with `qp run`

A demo on the web

How does it work

Terminal	Isolation	Environment
Shellinabox	Docker 	Ubuntu  + Quantum Package 

Live demo

Let's Go

https://quantumpackage.github.io/qp2