How good is Quantum Package?

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Quantum Package demo specifications

- An interactive terminal with all standard `Unix` and `Quantum Package` commands
- A non-persistent and isolated environment for each user

How does it work

- **shellinabox:** a web-based terminal
- **Docker:** isolate each user
- **Linux environment:** Ubuntu
- **Electronic structure software:** Quantum Package

Conclusion

This demo follow the `Quantum Package` philosophy — easy-to-use and easy-to-develop — by allowing future users to test it directly from a web page without the painful installation process

Quantum Package is an **easy to use and easy to develop** quantum chemistry software developed at the LCPQ (Toulouse) and LCT (Paris)

Flash this QR code to go to the **Quantum Package** website `https://quantumpackage.github.io/qp2`

The CIPSI algorithm [1]:

1. Variational wave function and energy

$$\Psi^{(0)} = \sum_I c_I |I\rangle$$

$$E^{(0)} = \frac{\langle \Psi^{(0)} | \hat{H} | \Psi^{(0)} \rangle}{\langle \Psi^{(0)} | \Psi^{(0)} \rangle} \geq E_{\text{FCI}}$$

2. Second-order perturbative contribution

$$e_\alpha = \frac{\langle \Psi^{(0)} | \hat{H} | \alpha \rangle^2}{E^{(0)} - \langle \alpha | \hat{H} | \alpha \rangle}$$

3. Missing correlation energy estimation

$$E^{(2)} = \sum_\alpha e_\alpha$$

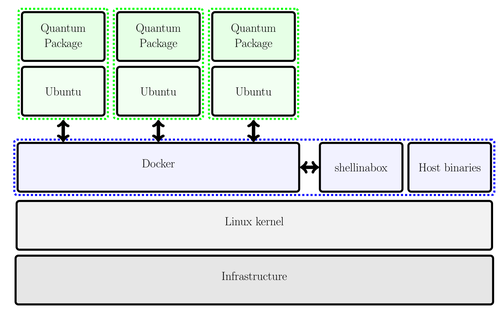
$$E_{\text{FCI}} \approx E^{(0)} + E^{(2)}$$

4. We select $|\alpha\rangle^{(n)}$ the subset of external determinants with the largest contribution

$$|I\rangle^{(n+1)} = |I\rangle^{(n)} \cup |\alpha\rangle^{(n)}$$

5. If convergence has not reached, go back to 1

Demo architecture



Useful resources

[1] Yann Garniron et al. "Quantum Package 2.0: An Open-Source Determinant-Driven Suite of Programs". In: *Journal of Chemical Theory and Computation* 15 (2019), pp. 3591–3609. DOI: 10.1021/acs.jctc.9b00176. URL: http://dx.doi.org/10.1021/acs.jctc.9b00176.
[2] Luka Krajger and Thomas Spalinger. *Shellinabox*. Version 2.20. Nov. 10, 2016. URL: https://github.com/shellinabox/shellinabox.
[3] Docker, Inc. *Docker*. Version 18.09.2. Feb. 11, 2018. URL: https://www.docker.com/.
[4] Docker, Inc. *Docker Documentation*. URL: https://docs.docker.com.
[5] Canonical Ltd. *Ubuntu*. Version 18.04. Apr. 26, 2018.