Psi4NumPy: An Interactive Quantum Chemistry Programming Environment for Reference Implementation, Rapid Development, and Education

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Abstract: A cornerstone of the development of novel quantum chemistry methods is the translation of paper-and-pencil theory into an efficient computer program. To do this, low-level programming languages are typically employed; however, such implementations tend to be convoluted, as raw speed is the focus rather than either readability or reproducibility. Any attempt at re-implementation must then proceed with the originally published equations as the only reference, whereby critical programming details must be re-discovered through a similarly heroic effort to the original implementation. To address these issues, the Psi4NumPy project [1] leverages the Psi4 quantum chemistry package and the Numerical Python (NumPy) library to create an interactive quantum chemistry programming environment for reference implementations, rapid development, and education. This environment allows for quantum chemistry-specific quantities computed with Psi4 and strided tensor manipulations performed with NumPy to be called directly from within the high-level Python programming language. Therefore, implementations of novel methods may be developed quickly and programmed concisely, while maintaining a relatively low execution time. Provided as a series of short Python scripts, reference implementations for a variety of popular quantum chemistry methods (including Hartree–Fock, Møller–Plesset, coupled cluster, electron propagator, and symmetry-adapted perturbation theories) address the community need for clear, readable programs which disseminate the details of such methods' implementation. Additionally, interactive tutorials discussing both the theory and implementation of these methods and others offer a unique educational framework for novice and experienced quantum chemists alike.

References

[1] Daniel Smith, Dominic A. Sirianni, Lori A. Burns, Konrad Patkowski, & David Sherrill. (2017). psi4/psi4numpy: v0.2-beta [Data set]. Zenodo. http://doi.org/10.5281/zenodo.438691