
mwfn-fu Documentation

Release 0.0

Brian Skinn

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`mwfn-fu` is intended to provide two-fold assistance when working with `Multiwfn`, “A Multifunctional Wavefunction Analyzer.” Interaction with `Multiwfn` is primarily conducted through a command-line interface, and many of the generated results are reported only as text printed to `stdout`. The goals of this package are

1. Enabling automatic execution and operation of `Multiwfn`, as in a scripting context.
2. Implementing a command-line ‘wrapper’ around `Multiwfn` that permits more convenient extraction of its computational outputs into a numerically manipulable form.

`mwfn-fu` is in a preliminary stage of development, and so far only a basic driver class for `Multiwfn` has been implemented, which provides an initial implementation of #1 above.

mwfn-fu Usage Instructions

Guide to usage of `mwfn-fu`.

RESUME

mwfn-fu API

Just one API page at this early stage.

CHAPTER 2

Indices and tables

- `genindex`
- `modindex`
- `search`