VCHKPlotter Manual

VCHKPlotter version 0.314159. Author: Ben-Lukas Thornton (Ben.Thornton955@cranfield.ac.uk), s405955

Requirements

- Python >= 3.10
- · A suitable install of pip
- Windows requires you to install dependencies manually. (Install all the packages in DEPENDENCIES.txt to a VENV) These
 are suitably referenced and cited in the report, where necessary.

Installation

Linux:

Inside the folder that contains setup.py, execute:

```
pip install .
```

Windows:

No install available. See usage instructions for Windows below.

Usage

For all specified output types, the program will create a subfolder in ./output_location with the name identical to the title of the section in the input file. E.g. "st". Lower case. The program will always print the "sn" section to *stdout*. If this option is passed as a command-line flag, then it will be saved additionally as a .txt file in the sn subfolder, but there will be no graph for this section.

Linux:

After install, to produce all plots in "verbose" mode, execute:

```
VCHKPlotter ./path to input.vchk ./output location -a -v
```

Windows:

This package provides a ./windows directory. This directory contains a windows friendly copy of the code and can be executed by running:

```
python ./__main__.py ...args...
```

Advanced Usage Instructions:

- Use the -a flag to request all output types. Note that with use of this flag, you can use the -no- variants of the file-type flags to exclude them. As opposed to typing all the outputs you do want, sometimes it's easier to just specify those you don't.
- Use the -v for verbose output. Will catch superfluous arguments and print to stderr in yellow.
- Use the following flags to select manually the types of outputs you want: -af, -dp, -hwe, -idd, -psc, -psi, -qual, -sis, -sn, -st, -tstv. You can provide these in all capitals or all lower case.
- When using the -a flag, you can switch off certain outputs by prefixing the above arguments with -no-. The on and off variant of a flag are mutually exclusive. The program will *error* if you provide -af -no-af for example.