README

1 aRMSD – minimalWindowsSupport

1.1 background

aRMSD (https://github.com/nbehrnd/aRMSD), a program to compare molecular structures with each other, works sufficiently well in an ecosystem of Debian (reference system, testing / Sid toward version 10 / Buster), or Xubuntu (test system was Xubuntu 18.04 LTS, point release 18.04.1) if the model data are provided in the *.xyz format. With the help of openbabel (version 2.4.1), it equally reads *some* model data in the *.pdb format, too.

At present (December 2018), however, the instructions provided by the original developer of the program, Arne Wagner, to render the program functional in the Windows environment *appear* to be invalidated by the continued development of the vtk-rendering engine aRMSD relies.[1]

This project aims to provide *an elementary* support for aRMSD in Windows, allowing to use the program *at all* – even if some of the functions of the program are unavailable. It is meant as a *ad hoc* and temporary fix only and assumes Windows 7 Pro (64 bit). At present, there is no similar fix addressing the 32 bit variant of this platform.

1.2 tools

The footprint of this *temporary fix* is quite large (about 2 GB permanent hard disk space is needed), but is portable (e.g., USB thumb-drive) since it does not affect the PATH variable of Windows.

On one hand, it relies on WinPython (version WinPython64-3.6.7.0Qt5)[2] providing Python 3.6. Among this compilation, some of the dependencies outlined by Arne Wagner are already included: matplotlib, uncertainties, and performance related cython. With 488 MB size (as compressed archive), it is too large to be mirrored here below, but beside on the project page itself you find it here on a dedicated page on GitHub.[3]

[1] Compare the issue deposit in the original branch of the program, https://github.com/armsd/aRMSD/issues.

[2] https://winpython.github.io/

[3] Project site's entry: https://github.com/winpython/winpython/releases/tag/1.11.20181031, download link: https://github.com/winpython/winpython/releases/download/1.11.20181031/Winpython32-3.6.7.0Qt5.exe

The other *essential* dependency of aRMSD is the vtk-rendering engine.[4] Currently, the wheel-directory maintained by Christoph Gohlke[5] provides only one vtk-wheel working smoothly with the versions of WinPython tested. It is worth about 27 MB and is mirrored in *this* repository, too.

The two are characterized by these md5sums:

```
2254b65e50a8c1834d10d253e243d23a  VTK-7.1.1-cp36-cp36m-win_amd64.whl
72b0612de9fdc341e87f01d9ca7b230f  WinPython64-3.6.7.0Qt5.exe
```

1.3 Install process

It is mandatory that the hosting Windows operating system is 64 bit. The system's PATH variable of the system is not touched, and no administrator privilege is required. However, anticipate about 2 GB disk space to be used since WinPython will provide you with many more packages than only the ones needed to run aRMSD.

Download the two files into a directory easy accessible for you. A mouse double-click on the WinPython executable will extract an archive. After about one or two minutes, the newly generated folder WPy-3670 equally contains an entry

```
WinPython Control Panel.exe
```

which basically is the package manager of WinPython.

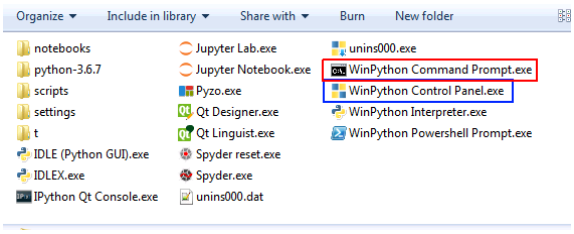

Figure 1: Automatically extracted folder by WinPython. Note the entry about the package manager (Control Panel, blue rectangle), and the CLI (red rectangle).

A double-click on this opens this. Choose now the index card Install / Upgrade Packages. In the bottom left corner of this display, you find a button to point this manager to the location of the vtk-wheel. After a few moments, this selection will show up in the main menu of the manager, too. Subsequently, push the button in the bottom right corner to add the wheel to the packages considered by WinPython eventually managed within the WPy-3670 folder. Again after a few moments (about 10 sec), the manager will install the wheel.

Once the intermediate installation notifier clears up, you may close the manager entirely.

[4] See https://www.vtk.org/ and https://en.wikipedia.org/wiki/VTK.

[5] Unofficial Windows Binaries for Python Extension Packages, https://www.lfd.uci.edu/~gohlke/pythonlibs/, accessed in December 2018.

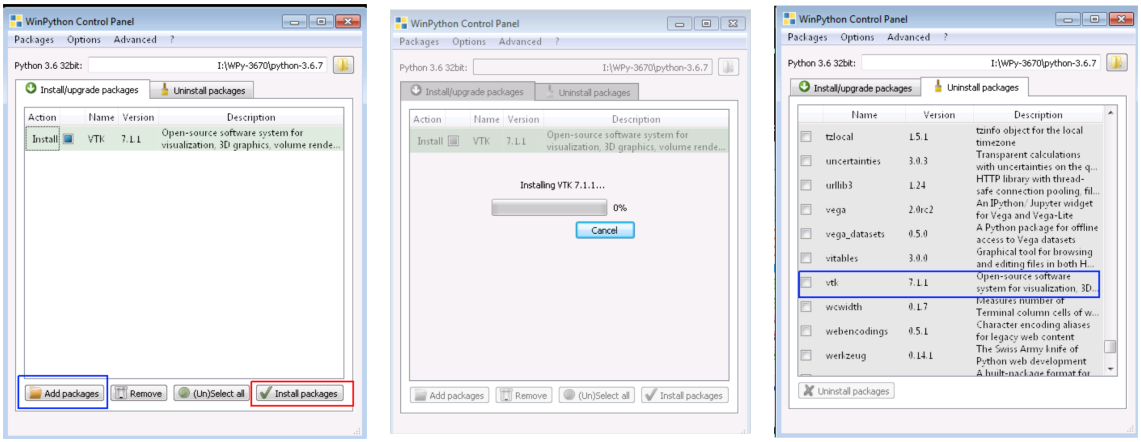

Figure 2: Stages of the installation process. Left figure: the manager with a wheel already loaded (blue rectangle) *prior* to launch the installation (red rectangle) on the index card "Install / upgrade packages". Middle figure: processing the wheel-installation. Right figure: confirmation of installation (index card "Uninstall packages")

1.4 Working with the fix

Folder `WPy-3670` contains its own CLI, `WinPython Command Prompt.exe`. A mouse double-click will open this. As with the native Windows `cmd.exe`, enter the directory of `aRMSD` housing `aRMSD.py`. You launch the program with

```
python aRMSD.py
```

1.5 Known limitations of this fix

Again, this solution is meant as *temporary fix* only. Hence, not requiring assistance by `openbabel`[6] to convert file formats, `aRMSD` reads most likely *only* model data provided in the `*.xyz` format. It actually *is expected* that `aRMSD` will inform you about the missing link to `openbabel`. (Since this fix does not accesses the `PATH` variable, it will not recognize `openbabel` even if it were installed on the hosting computer, either.)

If you need to compare models in a file format different than `*.xyz`, the freeware `openabel` may assist in the data conversion toward this format.

Equally, some of options accessible in the Linux-based use (e.g., anaglyph representation, less dominating display of the coordinate system by vtk) are skipped here. Saving the renderings by vtk as *.png (key stroke s) is supported.

However, alignment and scrutiny of the model data, including report generation in a permanent log and provision of the statistics plots are functional.

◇

[6] Open Babel: The Open Source Chemistry Toolbox, `http://openbabel.org/wiki/Main_Page`