

Best practices for how to use the MembraneAnalysisToolbox

Installation and Usage are described in the GitHub page. Here I want to collect best practices on how to work with the Toolbox and especially in the workstation environment. There are two options, either the toolbox is installed and used on its own (A) or the existing python environment and scripts are being used (B).

(A) Using existing python environment and scripts

During the development of the code, I set up a virtual python environment with the MembraneAnalysisToolbox already installed. There are also the scripts I used to create the analysis results and plots which can be used as a blueprint for own scripts or that can just be run as they are.

- Log onto the workstation using “ssh -X username@ipadress” to forward plot output to the client PC.
- Navigate to “/bigpool/users/st166545/TransitionAnalysisProject”.
- Run “source .venv/bin/activate” to activate the virtual python environment that is stored in that directory.
- Run “python interactive_analysis.py” to run the interactive analysis for example.

(B) Setting up own development environment

If you wish to run scripts outside of the workstation or wish to install it on your own, this is how:

- (optional) Install the remote ssh extension in visual studio code and set up a remote connection to the workstation using the user account and the IP address.
- Then download or clone the GitHub repository into your desired directory.
- (optional) Install the python environment extension on visual studio code.
- Create a python virtual environment using a python version ≥ 3.12 in a folder using either the vs-code extension or the python command.
- Then use pip install to install the MembraneAnalysisToolbox into that virtual environment.
- Make a script following the example.ipynb file to build the analysis class.
- Log onto the workstation using ssh -X username@ipadress to forward plot output to the client PC.
- Activate the virtual python environment.
- Then run the script in the python environment where the MembraneAnalysisToolbox is installed, and you will be able to see the plots on the screen and not only see them in the respective analysis folder as files.