
pyMODE-TASK Documentation

Release 1.0.0

Bilal Nizami

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pyMODE-TASK is a PyMOL plugin of MODE-TASK tool. MODE-TASK is a collection of open source tools to perform Principle component analysis (PCA), Kernel PCA, Incremental PCA, Multi dimensional analysis (MDS), t-distributed Stochastic Neighbor Embedding (t-SNE) on a protein MD trajectory and, Normal mode analysis (NMA) on a protein/viral capsid with a novel coarse graining algorithm.

Kindly see the detailed documentation of MODE-TASK here

<http://mode-task.readthedocs.io/en/latest/index.html>

1.1 Cite this project

A publication is currently being prepared

1.2 License

The project is licensed under GNU GPL 3.0

CHAPTER 2

Installation

MODE-TASK can be installed by following the instruction given at <http://mode-task.readthedocs.io/en/latest/installation.html>

For installing the pyMODE-TASK - a pymol plugin.

Requirements:

```
python
Tkinter
Pmw
numpy==1.13.1
cython==0.26
scikit-learn==0.19.0
scipy==0.19.1
sklearn==0.0
matplotlib==2.0.2
mdtraj==1.8.0
```

1. Download the project:

```
git clone https://github.com/RUBi-ZA/pyMODE-TASK.git
```

OR

Download zip from github page and extract to a directory.

2. Install dependencies:

Run the following command from within pyMODE-TASK directory

```
sudo pip install -r requirements.txt
```

pyMODE-TASK requires Tkinter and Pmw.1.3. Tkinter comes prepackaged with most standard python. Pmw could be installed by following the instruction from: <http://pmw.sourceforge.net/doc/starting.html>

3. Install pyMODE-TASK plugin in pymol:

3.1. Start pymol

3.2. Go to Plugin -> Plugin Manager, and click on install new plugin tab. Under install from local file click on 'choose file...' button. Browse the pyMODE-TASK.py and follow the on screen installation instructions.

3.3. If everything goes well, you can start the plugin from pymol plugin menu.

Usage

For more detailed documentation on installation and usage of the tool suite please see our [ReadTheDocs](<http://pymode-task.readthedocs.io/en/latest/index.html>) site

CHAPTER 3

Theory

Please see the following MODE-TASK documentation page for theory.

<http://mode-task.readthedocs.io/en/latest/theory.html>

pyMODE-TASK is a pymol plugin and GUI for command line based MODE-TASK tool. It include all the functionality of the MODE-TASK.

4.1 PCA of a MD trajectory

1. Preparation of trajectory

Prepare the MD trajectory as described in the tutorial section of MODE-TASK. It involves removing waters and periodicity if any.

2. PCA

1. Start the plugin from pymol, plugin → pyMODE-TASK.
2. Locate the pyMODE-TASK directory in the configuration tab by clicking on button “pyMODE-TASK directory”. Browse to the directory and click ok.
3. It should look something like this
4. Next go to the PCA tab. Read the trajectory, topology and reference PDB by clicking on the respective buttons. Next select the appropriate options and click on Run PCA. The results file will be saved in a folder within the output directory.
5. If the run is successful you will see something like following

4.2 MDS and t-SNE

1. Read the trajectory, topology files by clicking on the respective buttons. Select the appropriate options under MDS options widget and click on Run MDS.
2. Similarly, run the t-SNE.

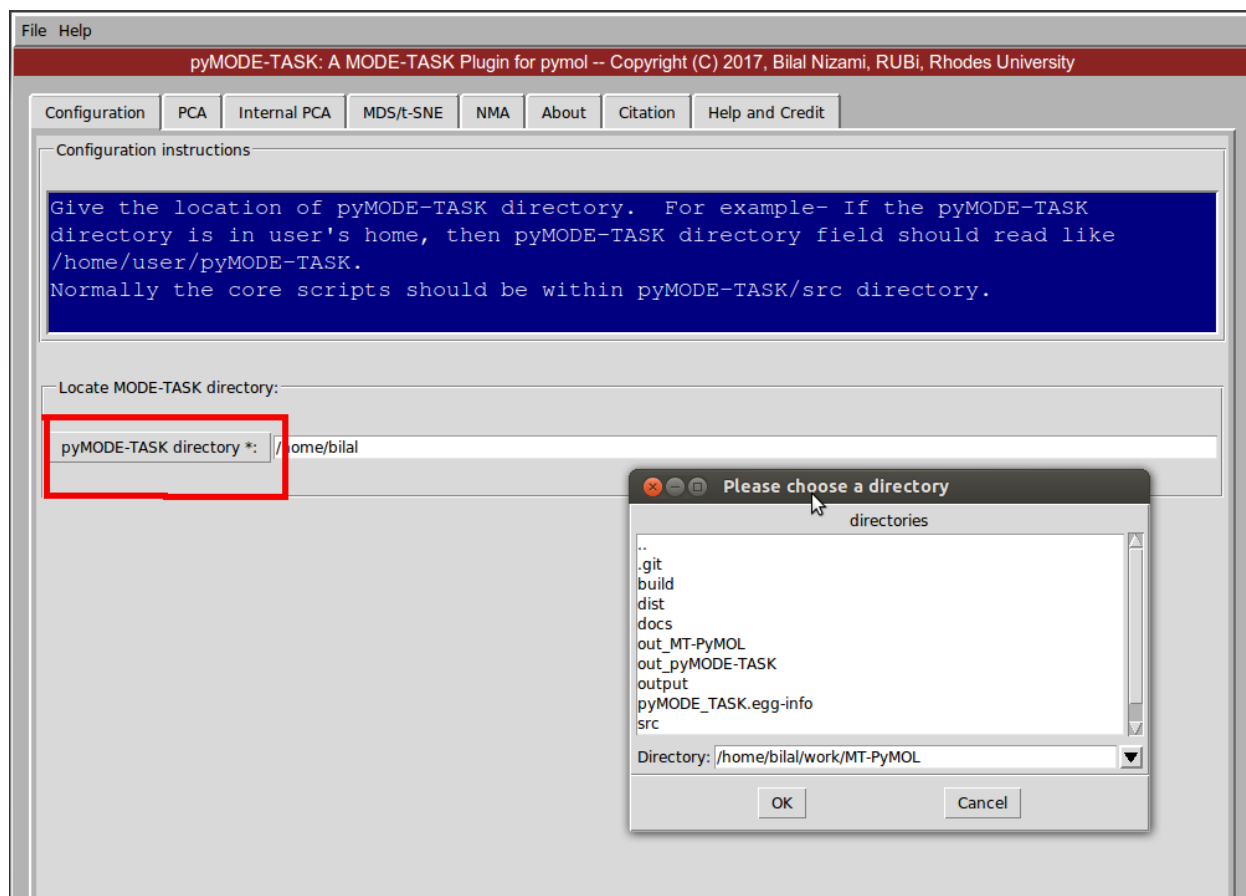


Fig. 4.1: Fig 1: Set pyMODE-TASK directory

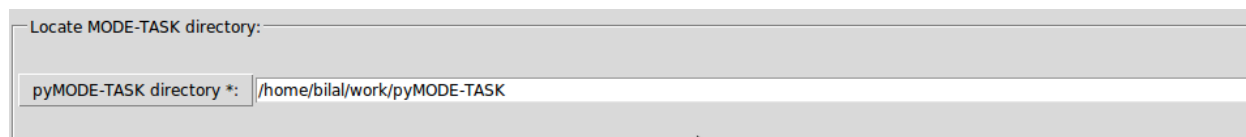


Fig. 4.2: Fig 2: Set pyMODE-TASK directory

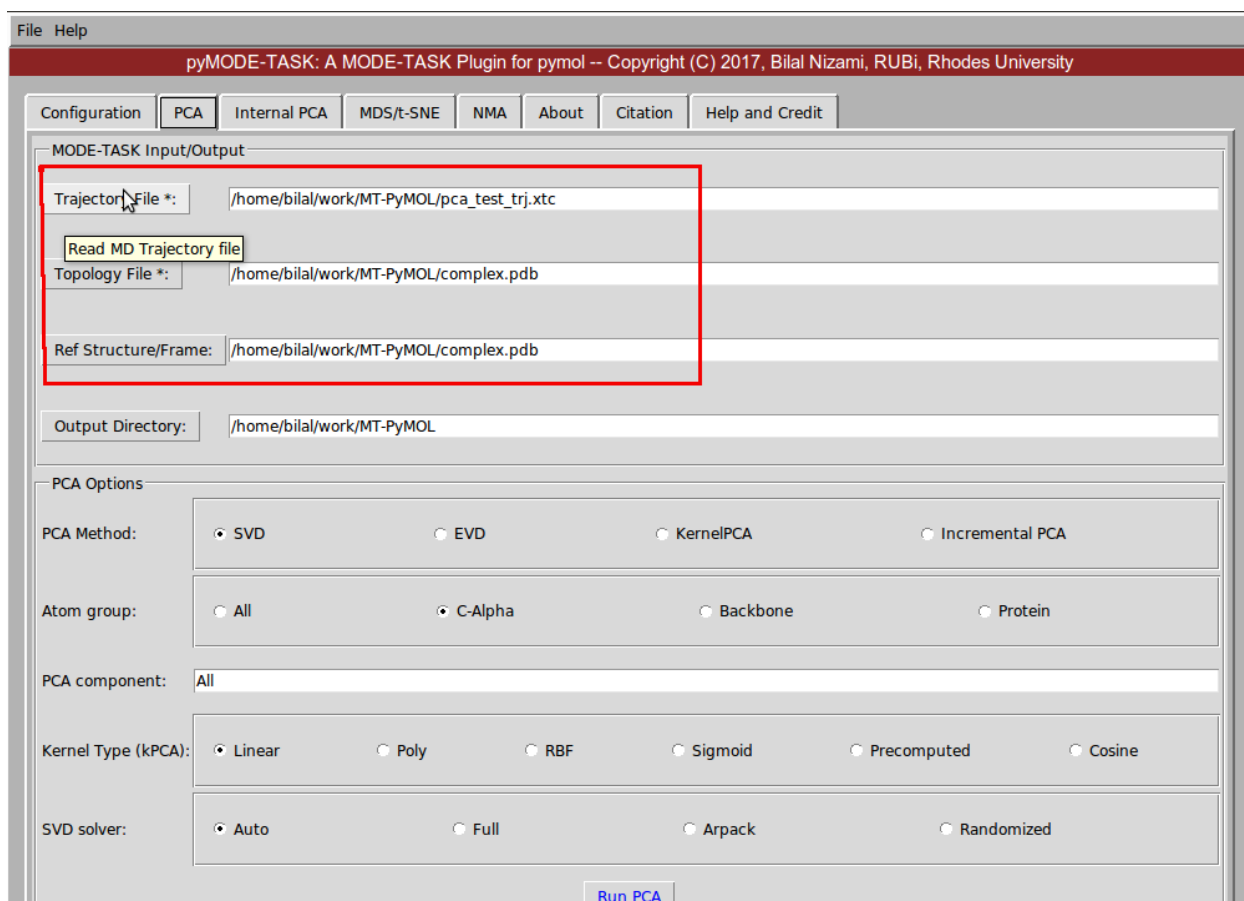


Fig. 4.3: Fig 3: PCA

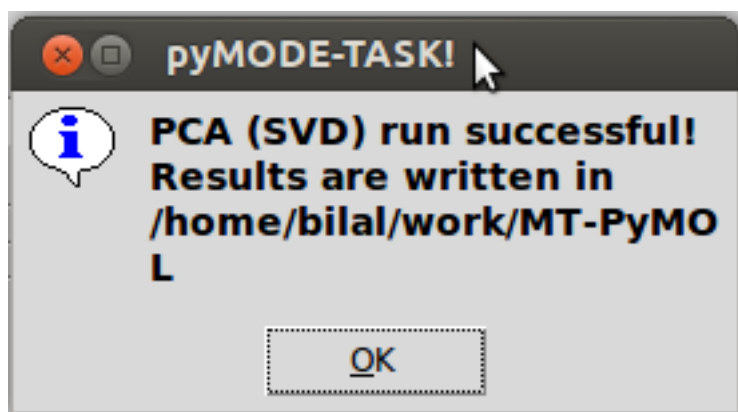


Fig. 4.4: Fig 4: PCA successful

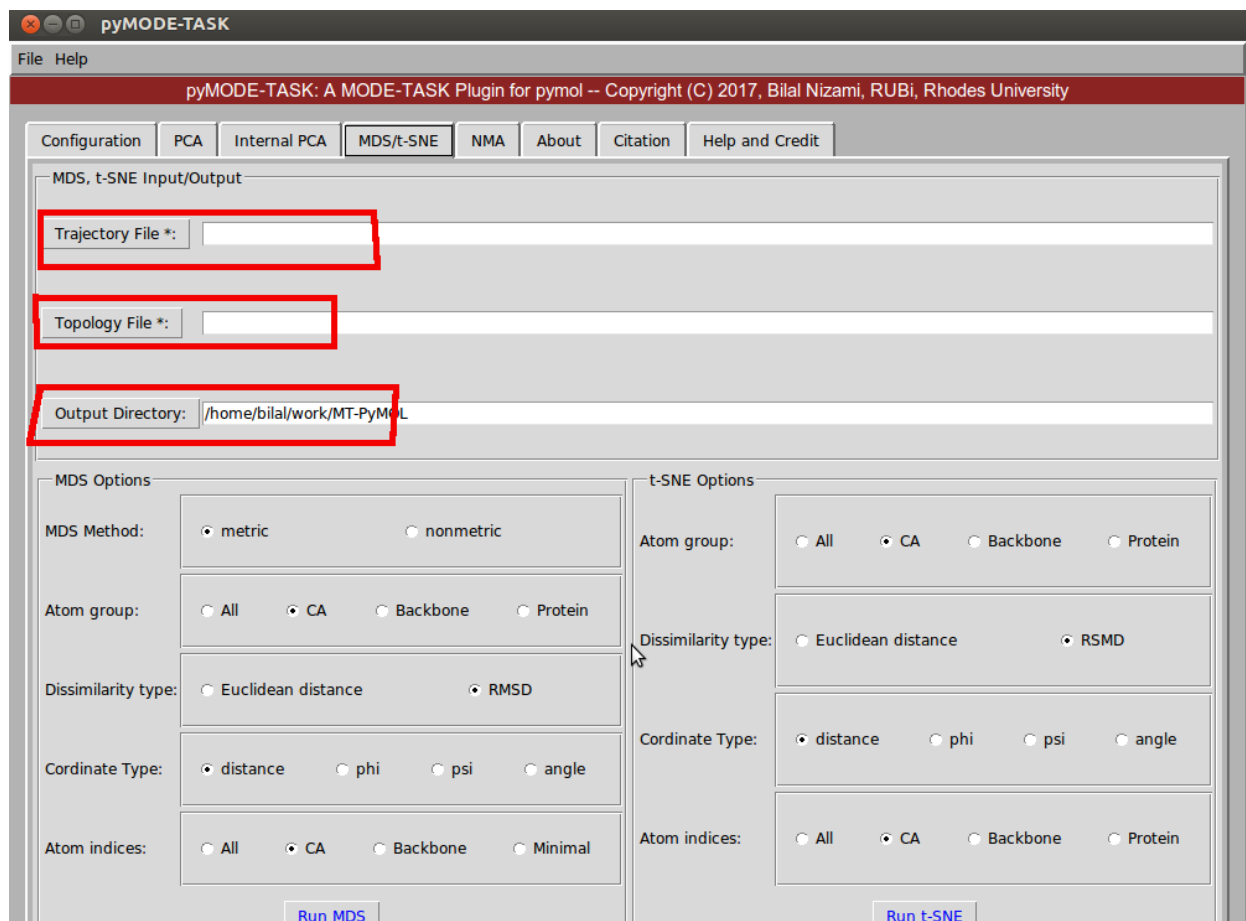


Fig. 4.5: Fig 5: MDS and t-SNE

4.3 Normal mode analysis (NMA)

1. Set the configuration page to locate the pyMODE-TASK directory.

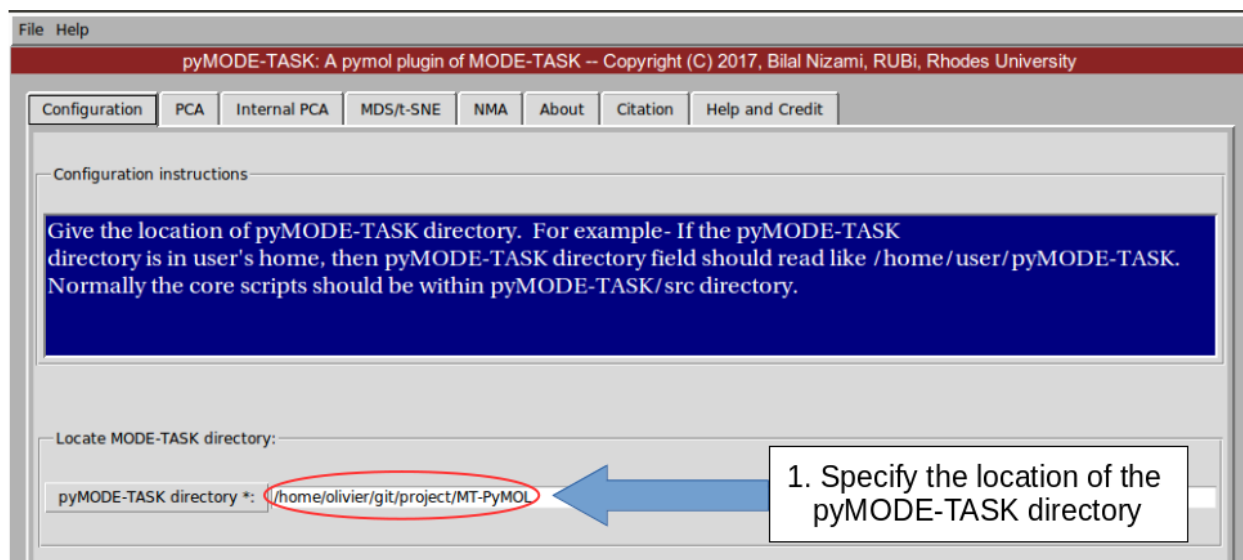


Fig. 4.6: Fig 6: NMA set configuration

2. Perform the coarse graining for large protein molecules.
3. Perform the coarse graining for second conformation of the protein. This is useful in case if you want to perform “Conformation/ Combination tool analysis” and “Mean square fluctuation”.
4. Run NMA on each coarse grained PDB using a suitable cutoff.
5. Run conformation / combination mode analysis. This require two PDB of different conformation.
6. Run MSF. This requires decomposed ANM matrices for comparing the mean square fluctuation between 2 proteins.
8. Get an assembly covariance for a specified chain of an asymmetric unit
9. Generate mode animation for visualization. Afterward use the following command in VMD for visualization

```
vmd VISUALISE/VISUAL_1.pdb -e VISUALISE/VISUAL_ARROWS_1.txt
```

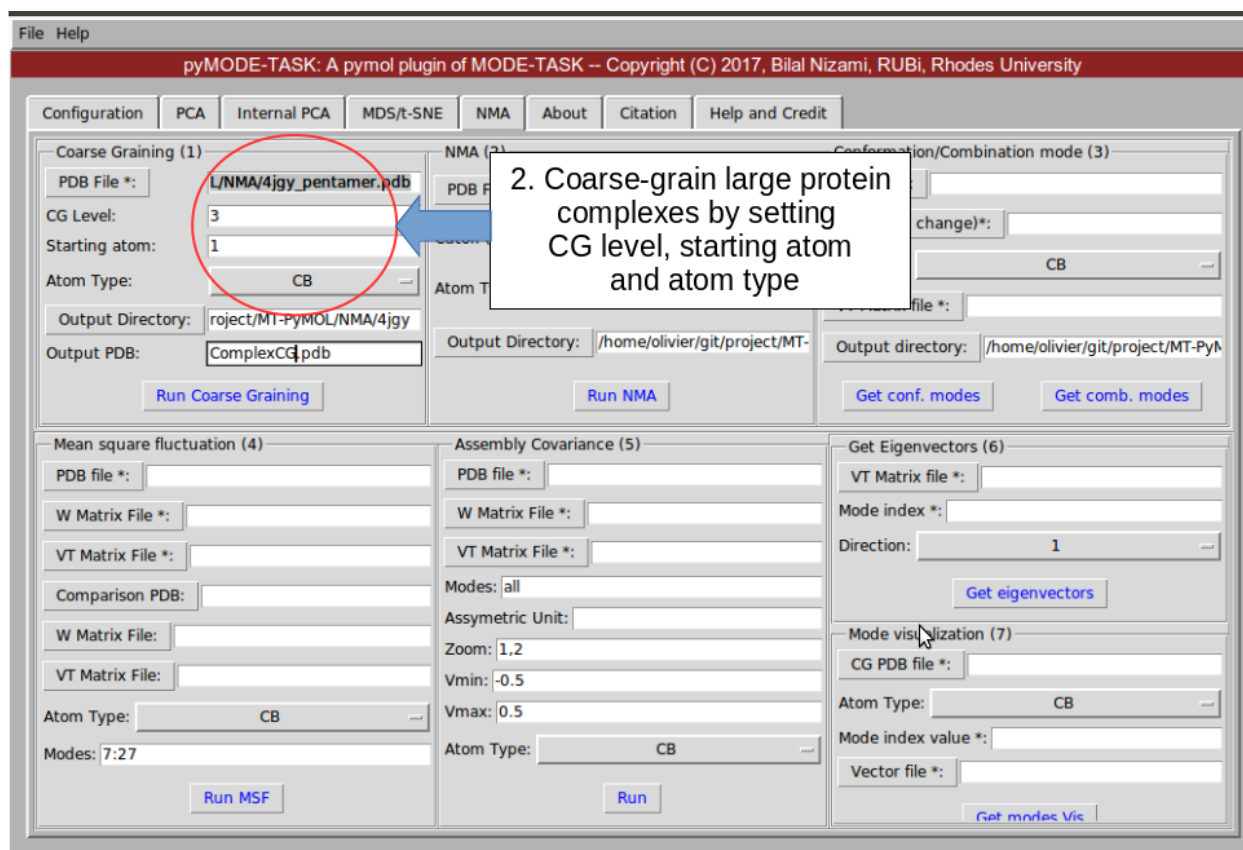


Fig. 4.7: Fig 7: Coarse graining

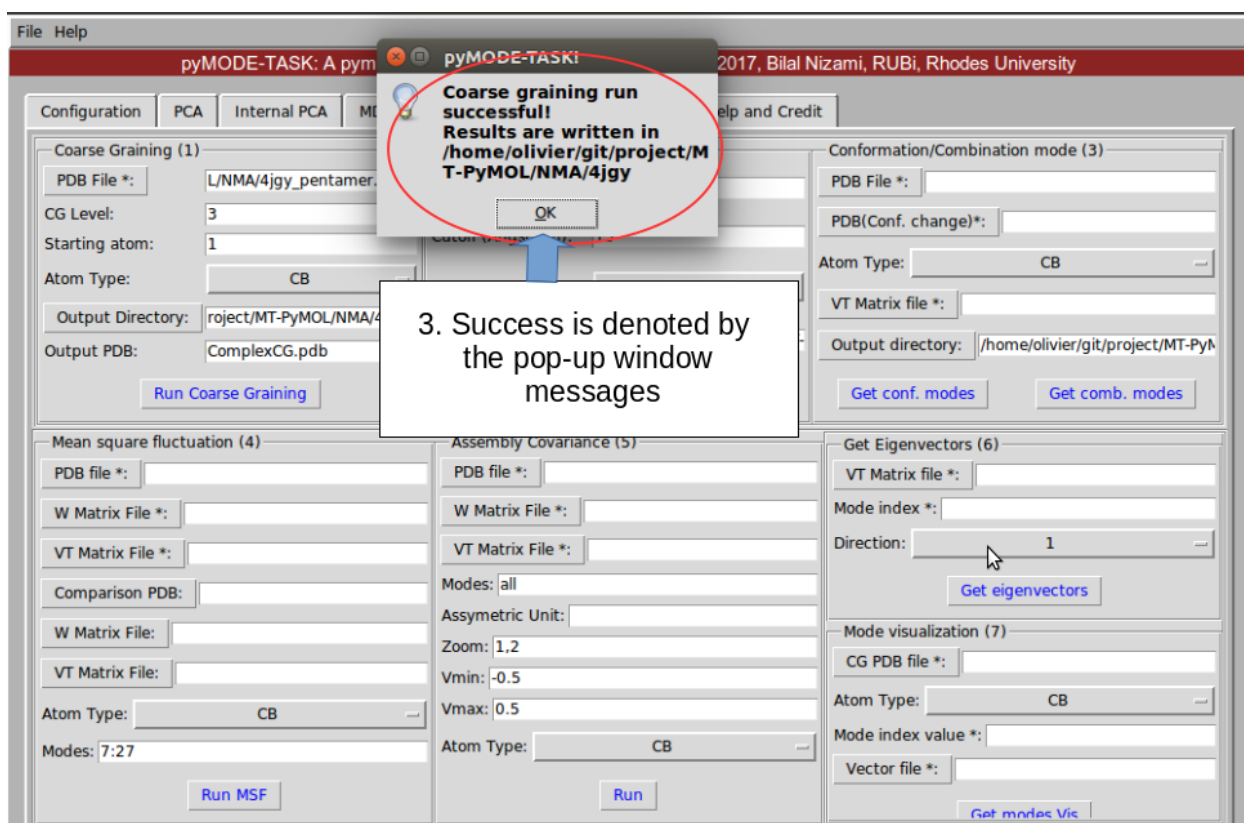


Fig. 4.8: Fig 8: Coarse graining results

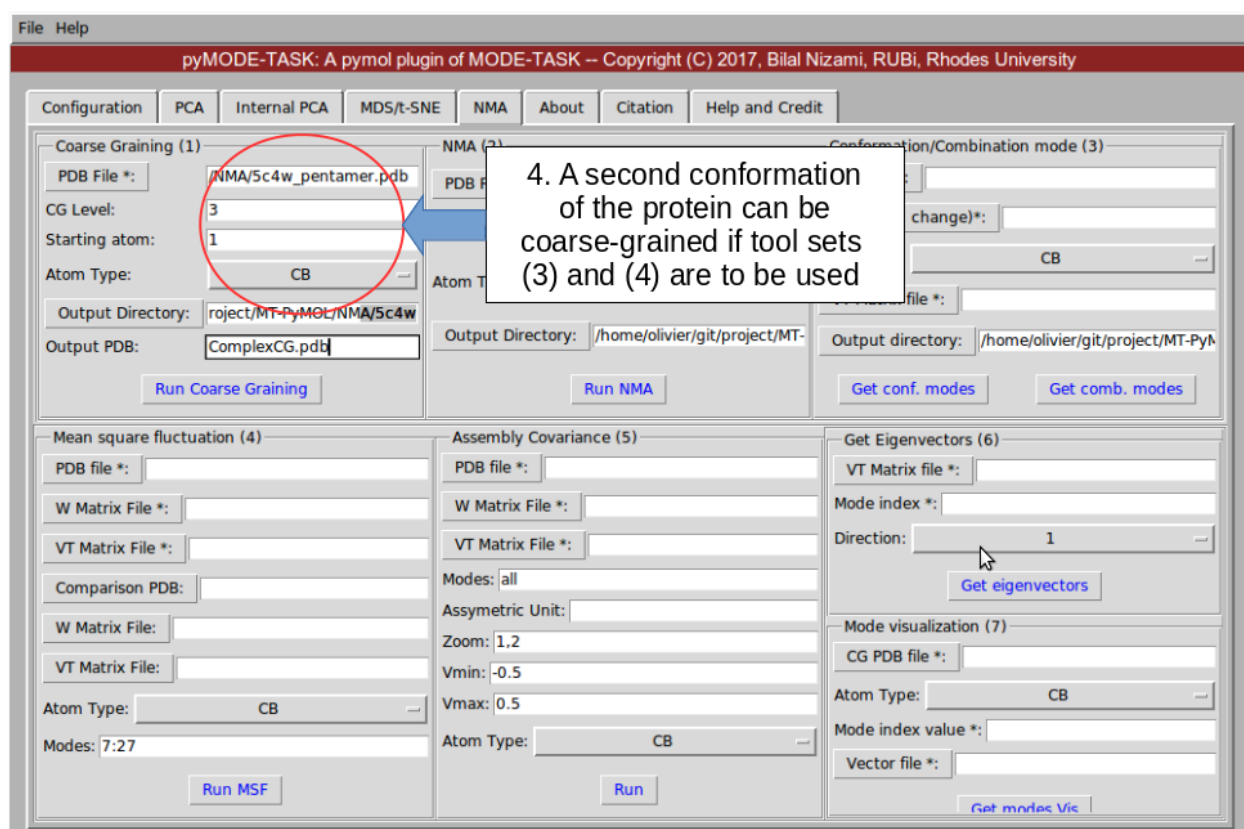


Fig. 4.9: Fig 9: Coarse graining 2

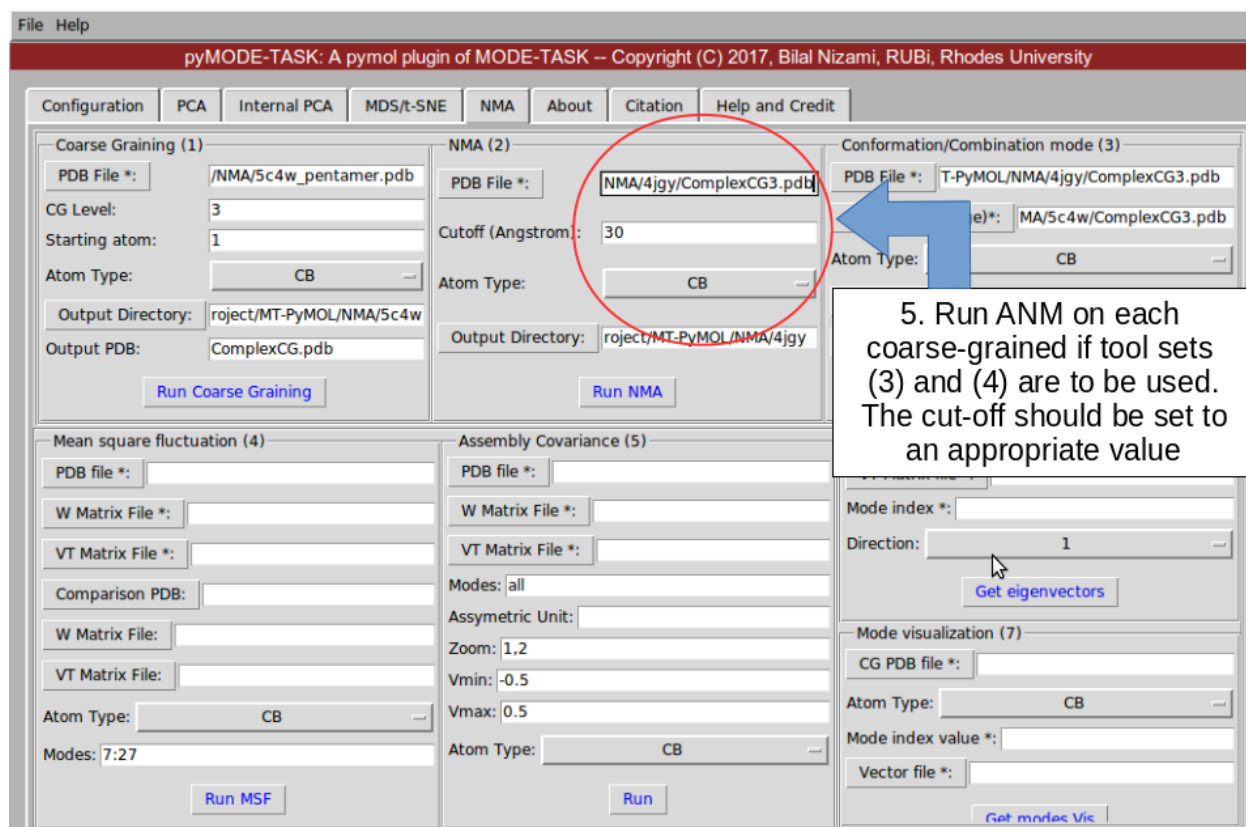


Fig. 4.10: Fig 10: NMA for first PDB

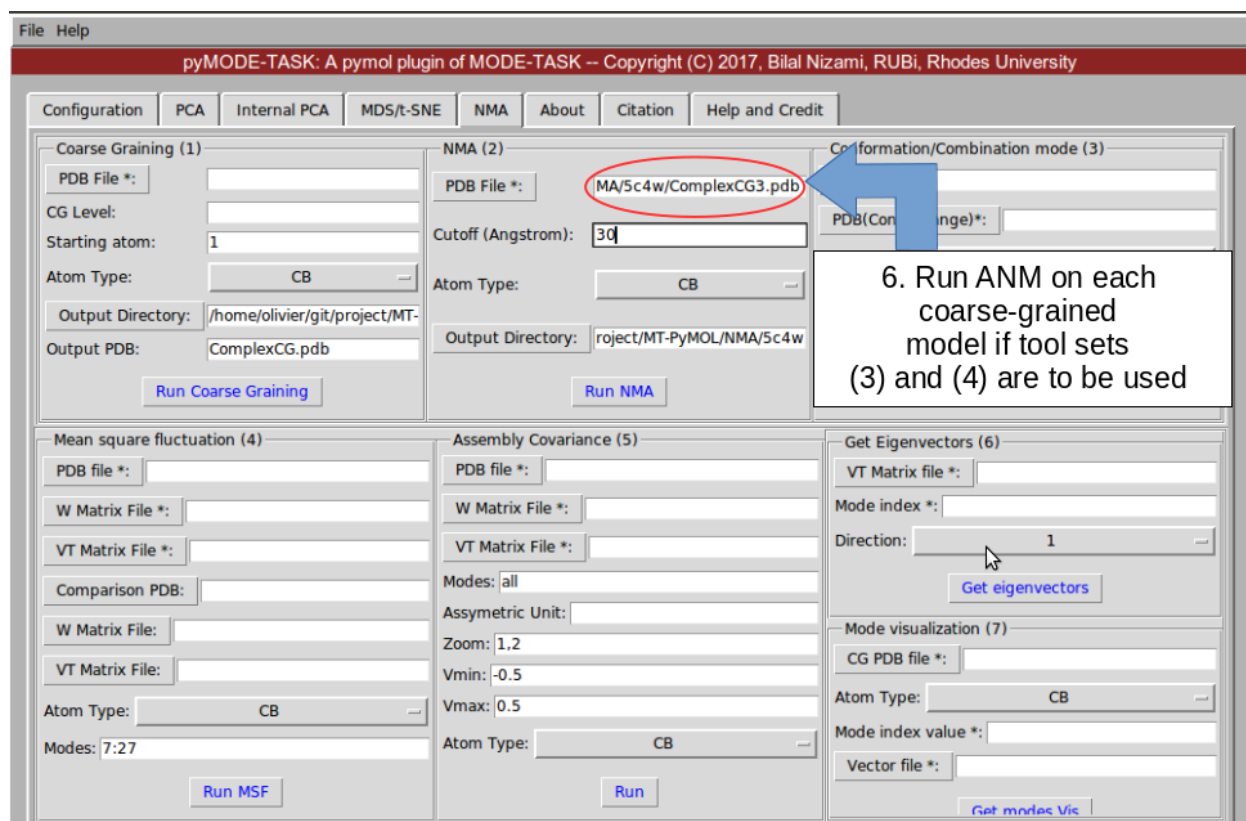


Fig. 4.11: Fig 11: NMA for second PDB

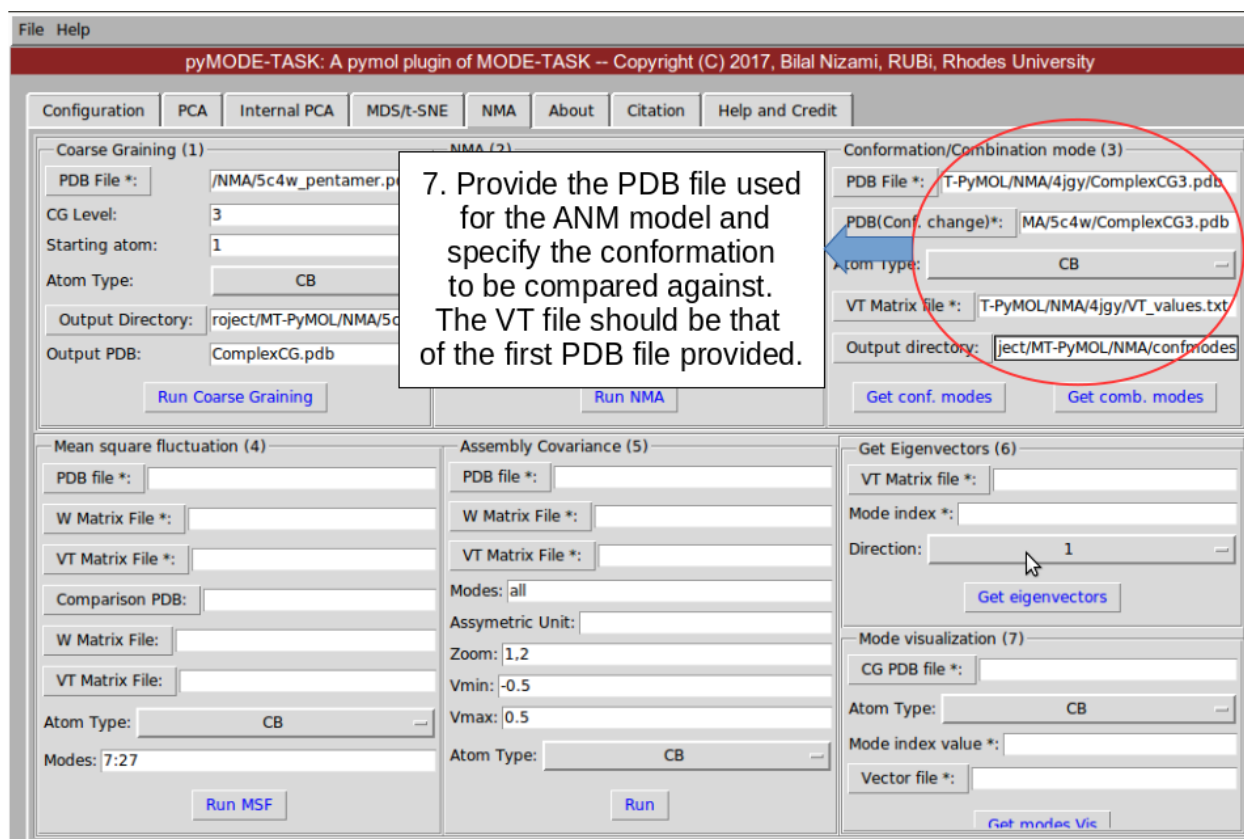


Fig. 4.12: Fig 12: conformation/combination mode analysis

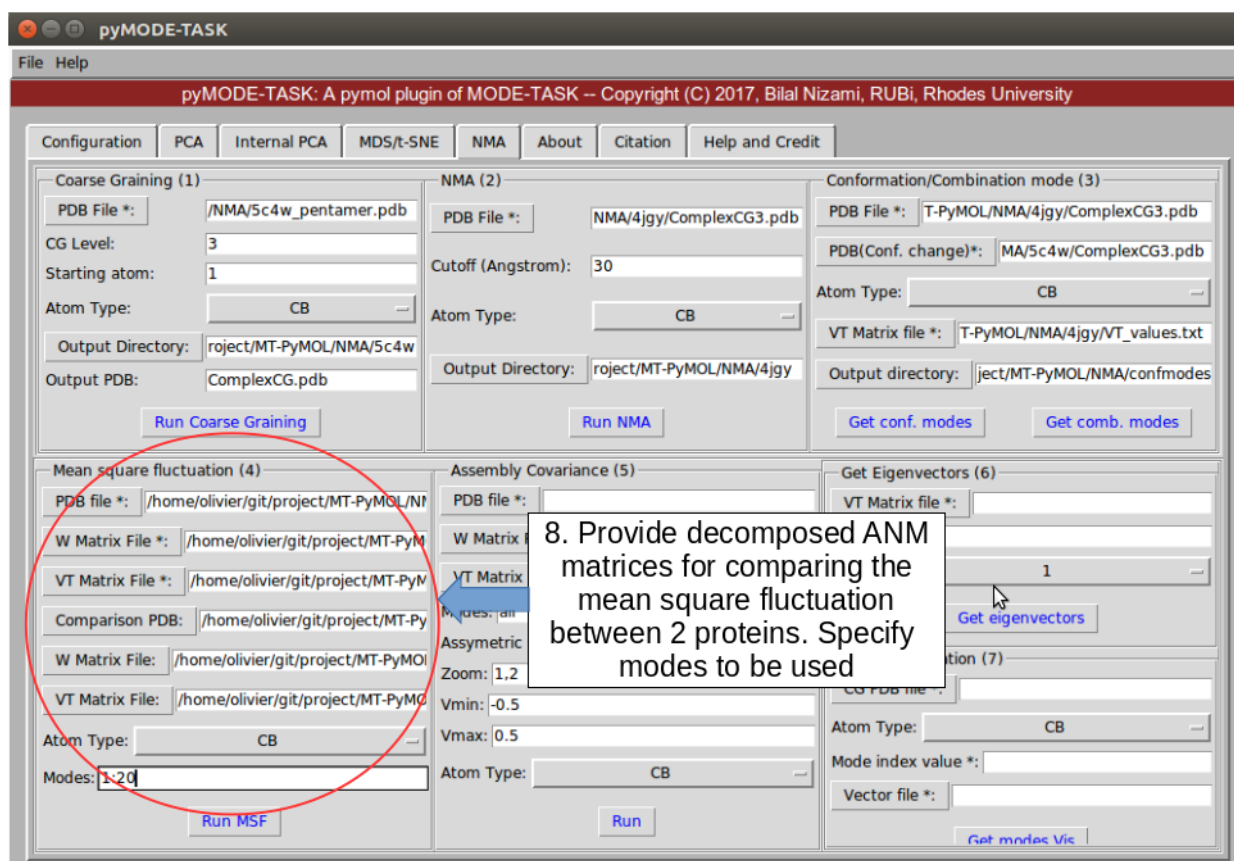


Fig. 4.13: Fig 13: MSF

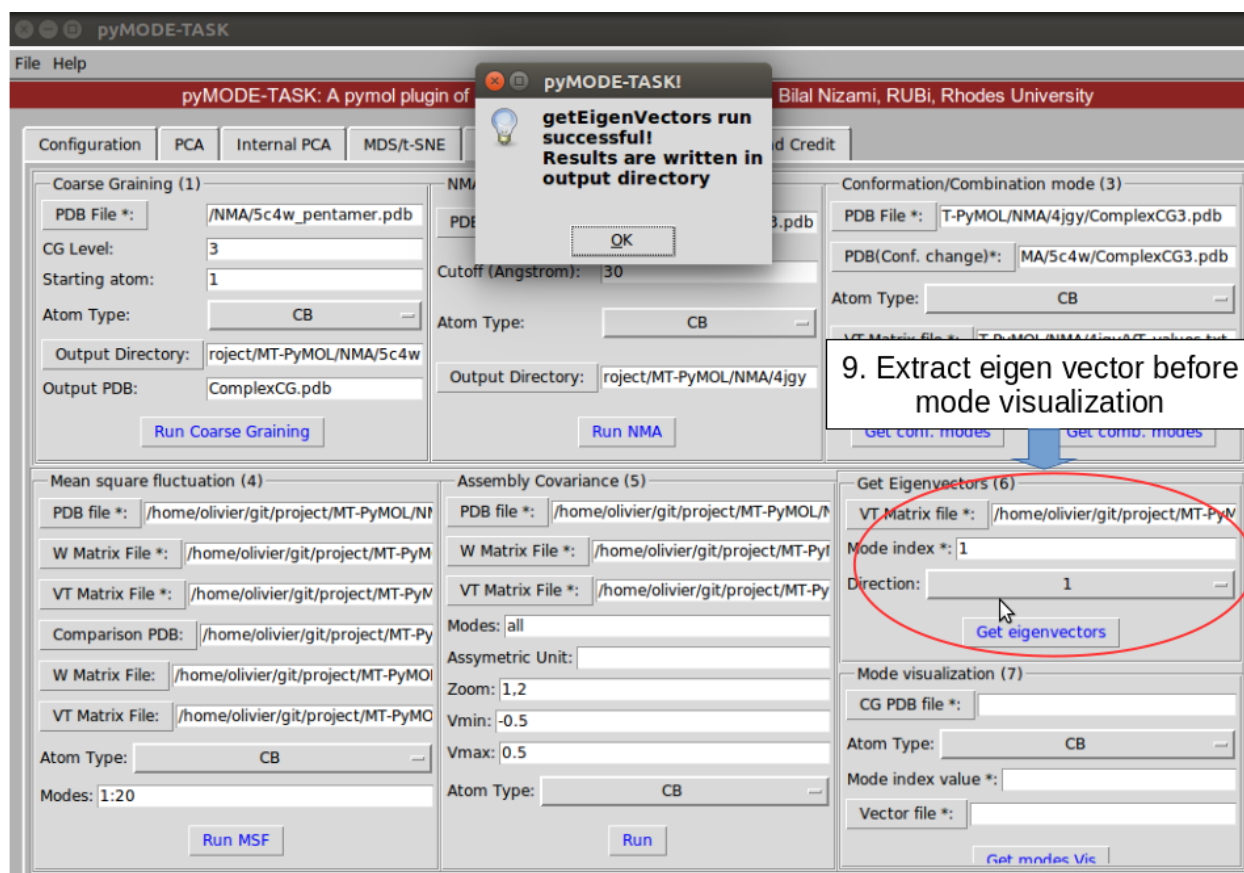


Fig. 4.14: Fig 14: Get Eigenvectors

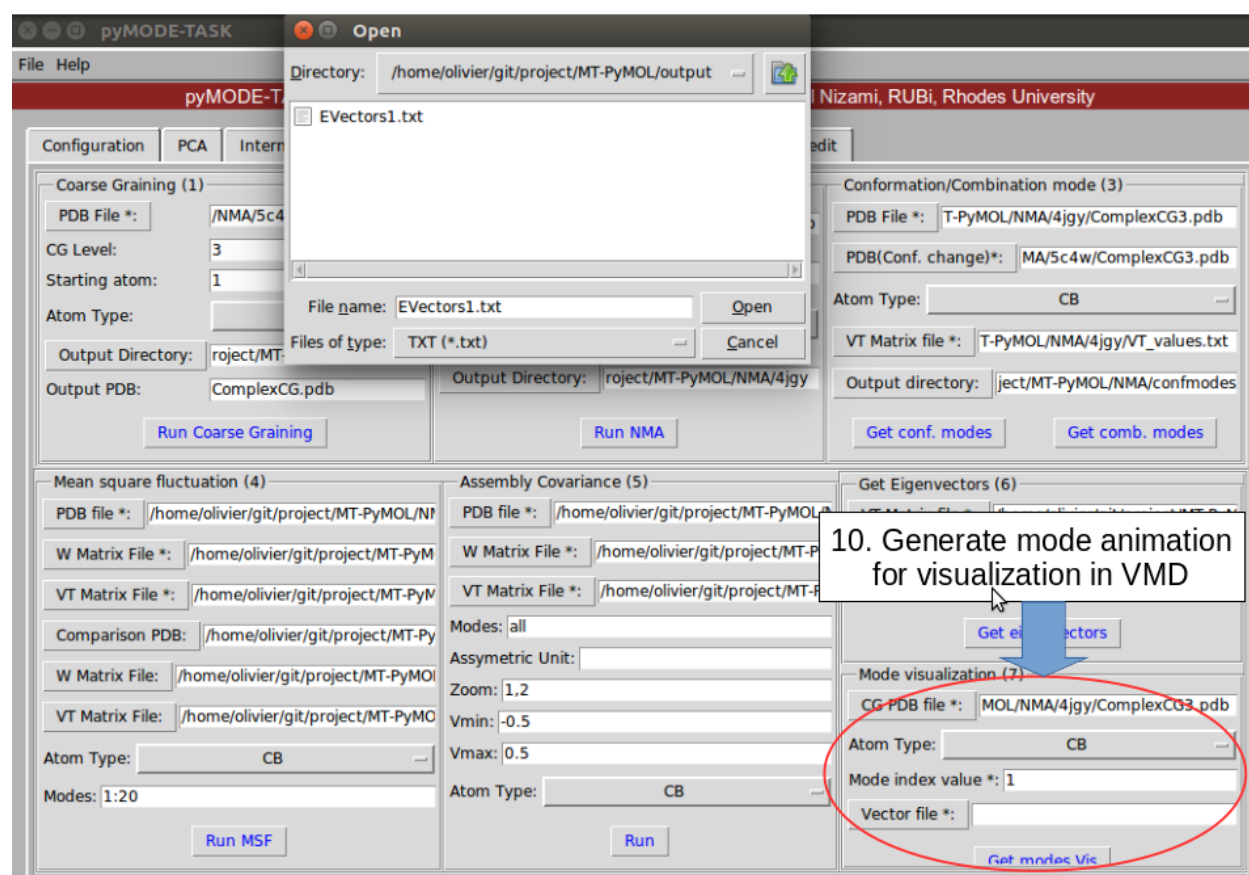


Fig. 4.15: Fig 15: Mode animation