This brief explanation will guide you to prepare your first QM/MM simulation with NAMD.

Inside the Example1 folder you will find (besides this readme file) the coordinates (PolyAla.PDB) and structure (PolyAla.PSF) files for a poly-alanine peptide in a small water box. You will also find a TCL that creates a single QM region composed of two residues (20 atoms) in the middle of an 8 residue poly-alanine helix. This script should be executed with the *latest* version of VMD, with the following command:

```
vmd -dispdev text -e prepare.qm.region.tcl
```

The "-dispdev text" option will keep VMD from opening its usual graphical interface, making it a faster execution, and will terminate VMD at the end of the script.

Three files are produced, but we will focus on "PolyAla-qm.PDB", the file that contains values in the beta and occupancy fields of atoms in the QM region and atoms participating in QM/MM bonds, respectively.

If you chose to use the configuration file as it is provided in this example, you need only change the variable that indicated the location of your MOPAC executable, and the variable indicating the folder where you wish to run the QM calculations. We advise using a folder mounted on RAM, rather than a hard disc folder. In most Linux systems, the folder "/dev/shm/" is mounted in RAM and a sub-folder can be created with the following command:

```
mkdir /dev/shm/NAMD_Example1
```

Now you can start your simulation by running the following command (and substituting the correct path to your local NAMD installation):

```
/path/to/namd2 config.namd | tee out.log
```

The "tee" command allows you to store all output in a file ("log.out", in this case) while still visualizing the progress of your simulation.
With the original parameters placed in the "config.namd" file, the simulation takes ~35 minutes to run 100 minimization steps and 20000 MD steps if MOPAC is used.

You can now visualize and analyze QM atoms positions and/or charges and how they change throughout the simulation. For this, the other two files produced by our preparation TCL script will be necessary. Using the QM-only PSF file (PolyAla-qm.Qmonly.psf), which contains the topology for the QM region only, and the indexing file (PolyAla-qm.idDict.txt), which relates atom indices between the full system and the QM-only system.
The simulation will produce two "specialized" DCD files: "PolyAla_out.QMonly.dcd", which contains only the positions of QM atoms in the system, and "PolyAla_out.qdcd", which contains the partial charge calculated for each QM atom.
The accompanying TCL script "display_charges.tcl" will load the QM region of this system and display it with atoms colored by their partial charge. It will also write a text file with all charges for all atoms as calculated in each simulation step. It should be ran with the following command:

```
vmd -e display_charges.tcl
```