Running MD Simulations on NAMD: QwikMD

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How to install NAMD

- *Nanoscale Molecular Dynamics (NAMD)* will be the main program that we are going to use to perform MD simulations

- How to install NAMD?

NAMD is a parallel molecular dynamics code designed fro high-performance simulation of large biomolecular system

NAMD is able to use GROMOS, CHARMM, AMBER, X-PLOR force field

1. Unzip the compressed file ***(NAMD_2.14_Win64-multicore.zip)***
Please put in it in a directory which has a name with no spaces in it
(like: ***C:Users/Alqaisi/Desktop/namd***)

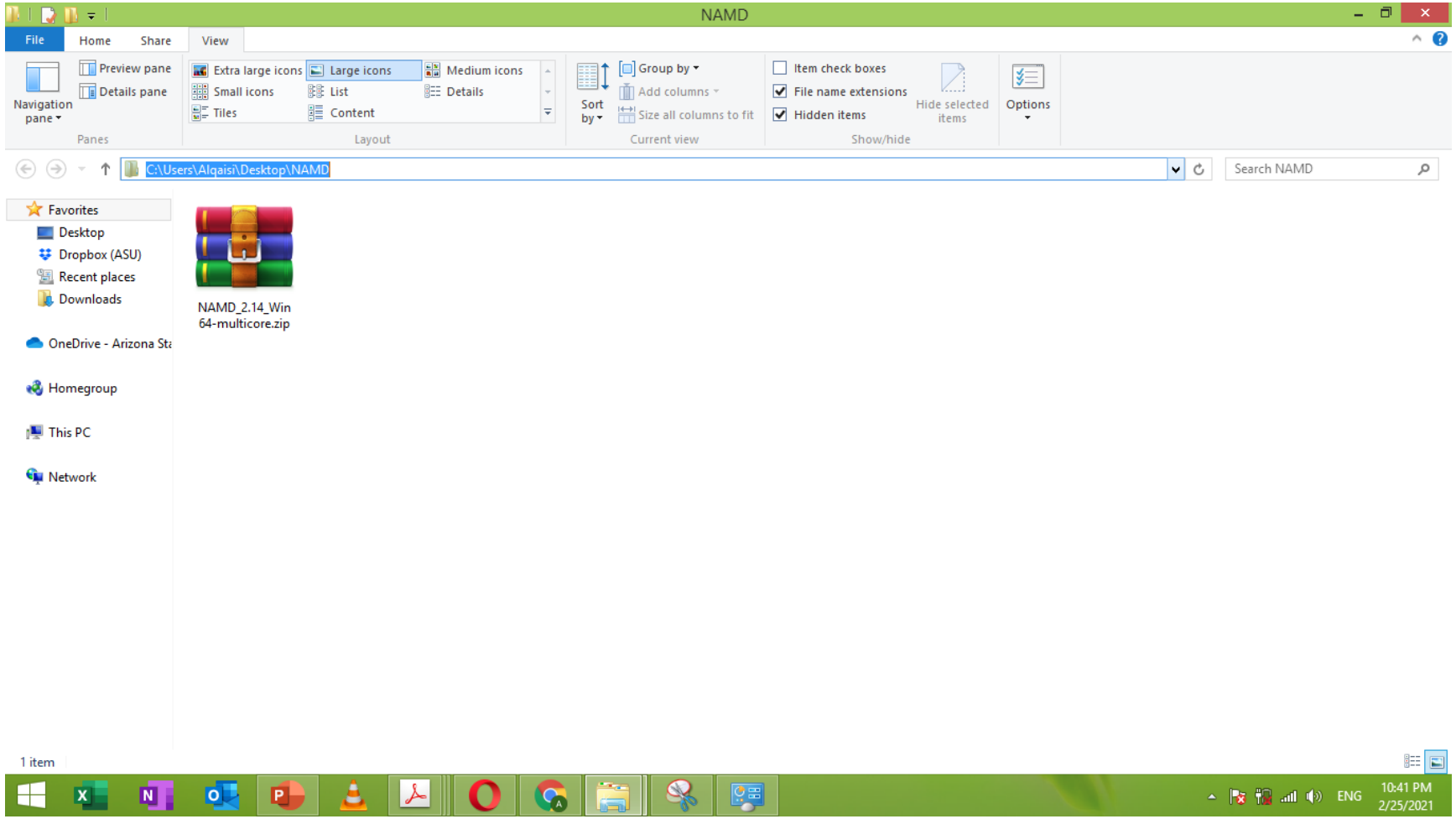
2. Copy the directory name which contains the unzipped folder

3. Go to my computer: click ***system properties*** > ***Advanced system settings*** > ***Environment variables***

4. You will see ***system variables*** window: click on ***path*** > ***edit***

5. write ***;*** then the directory of the NAMD program (:C:\Users\Alqaisi\Desktop\Theoretical and Computational Chemistry Lab\Molecular Dynamics\Nanoscale Atomistic Molecular Dynamics (NAMD)\NAMD_2.14_Win64-multicore)

How to install NAMD



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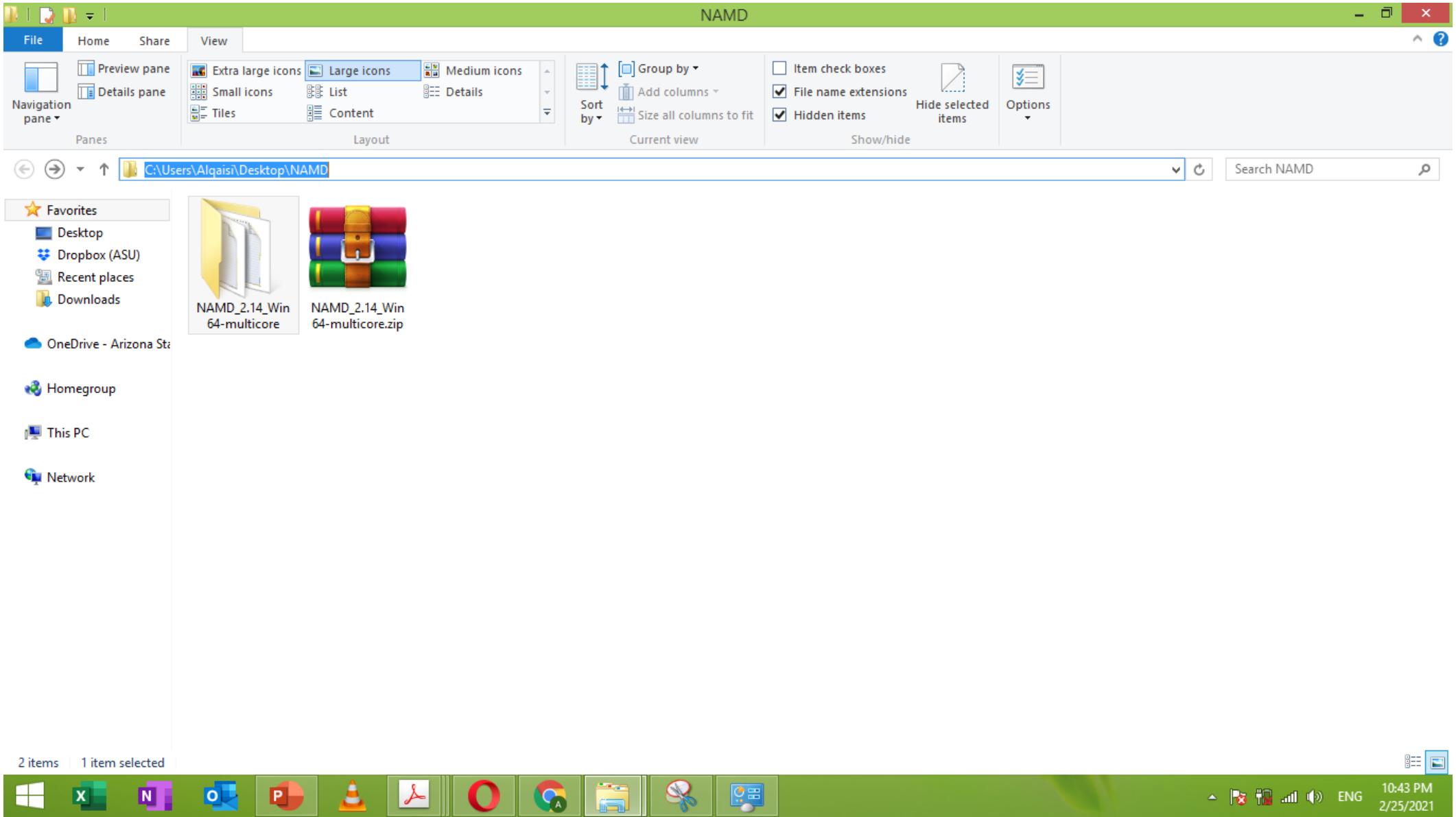

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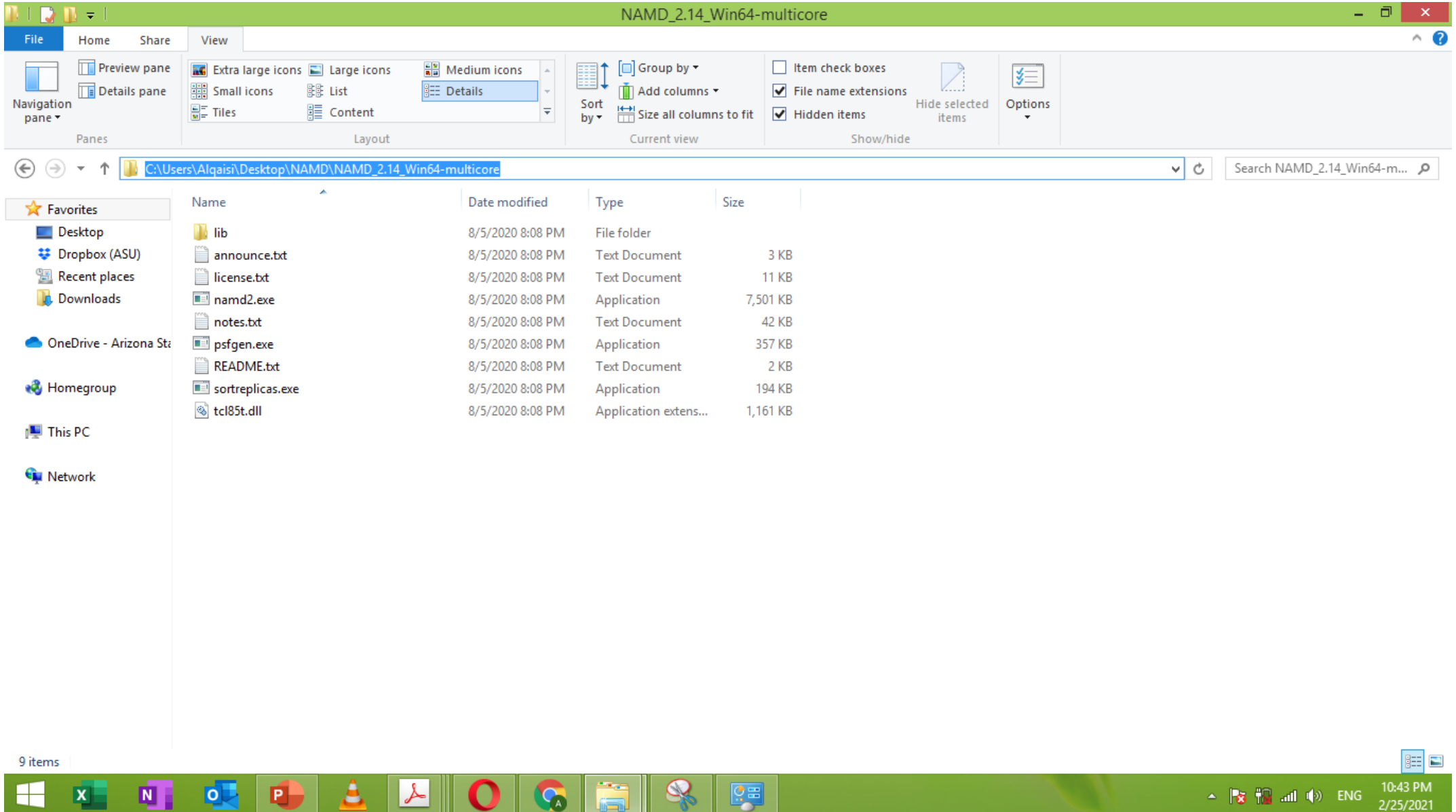

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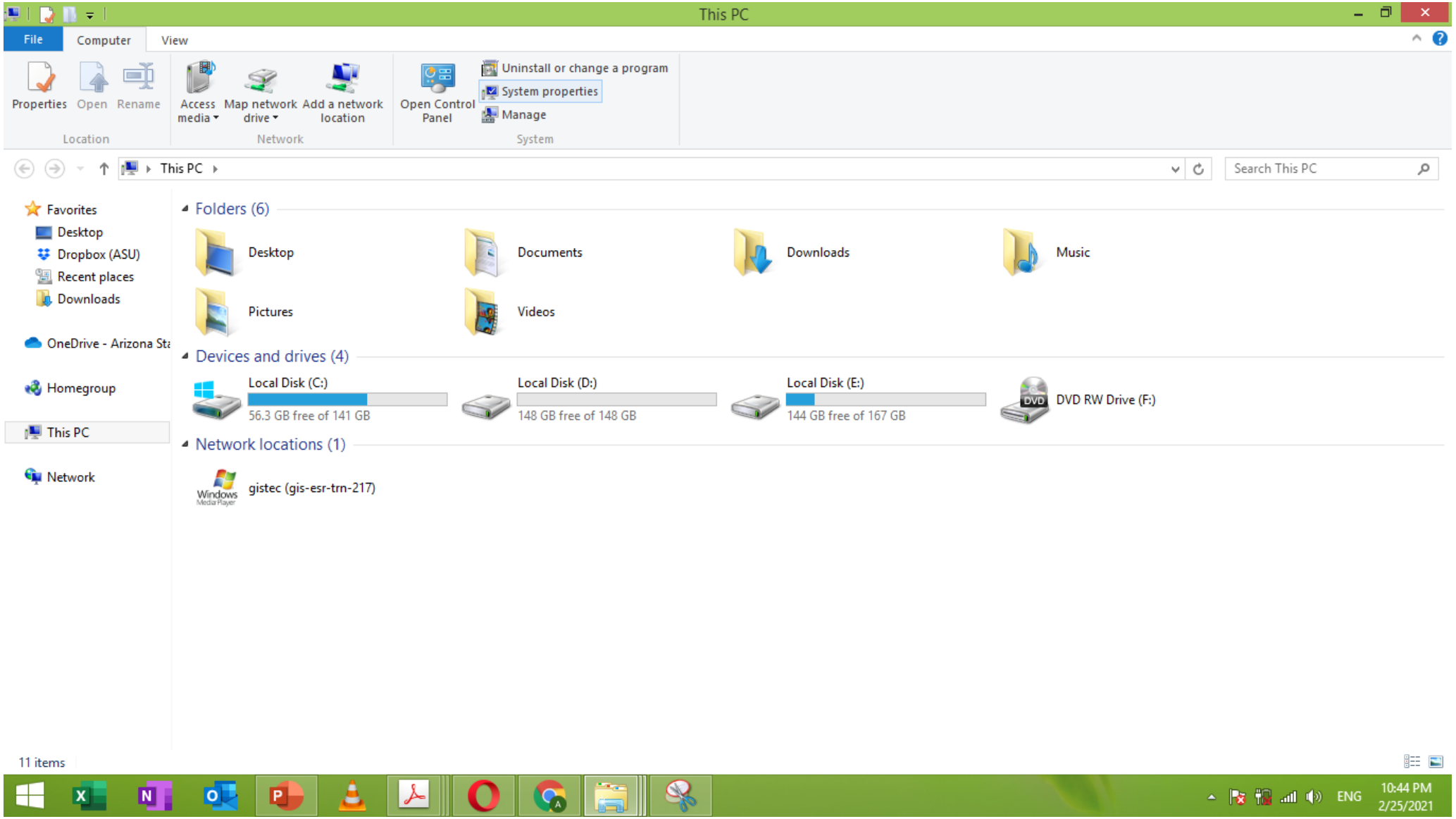

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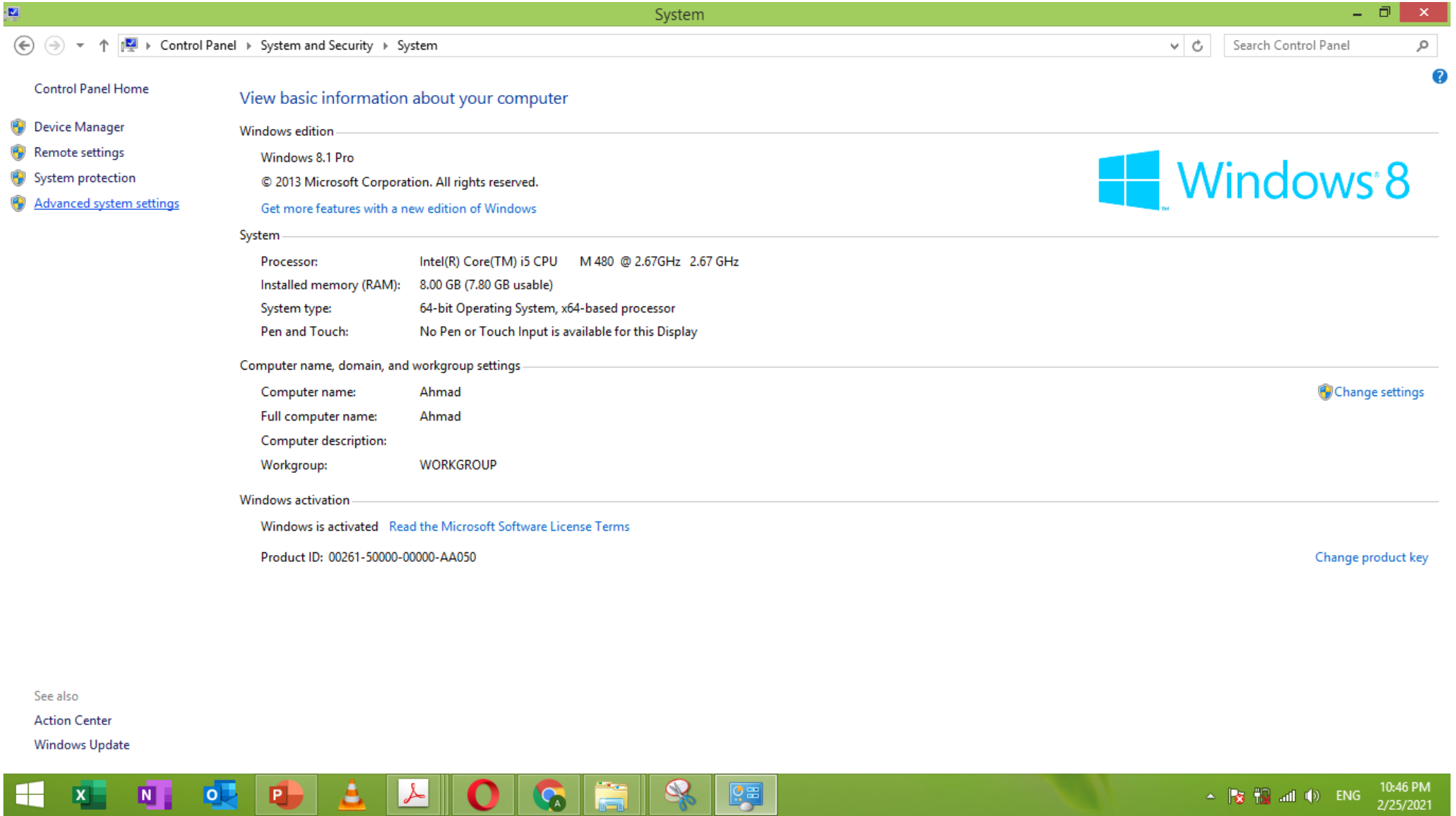

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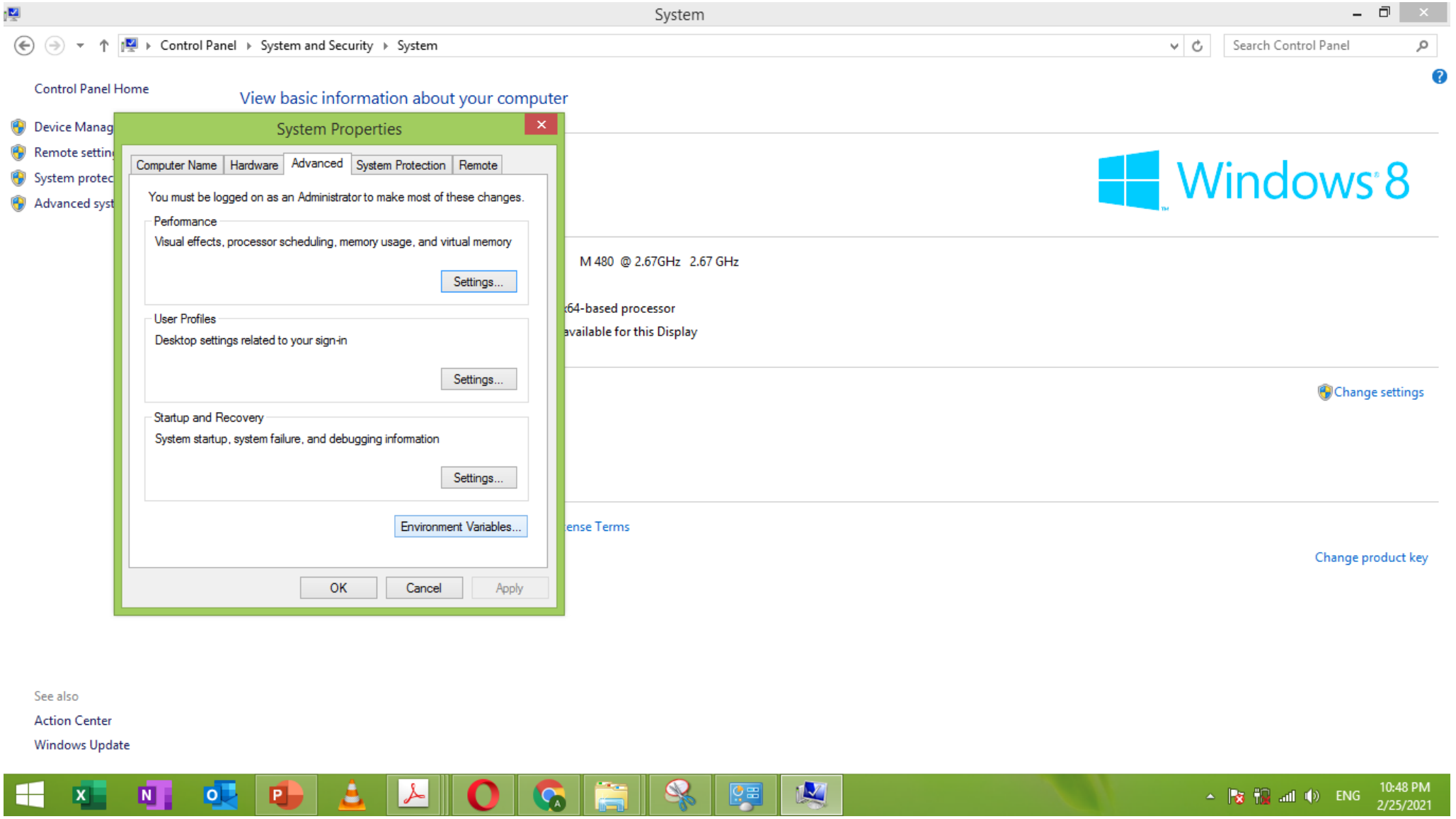

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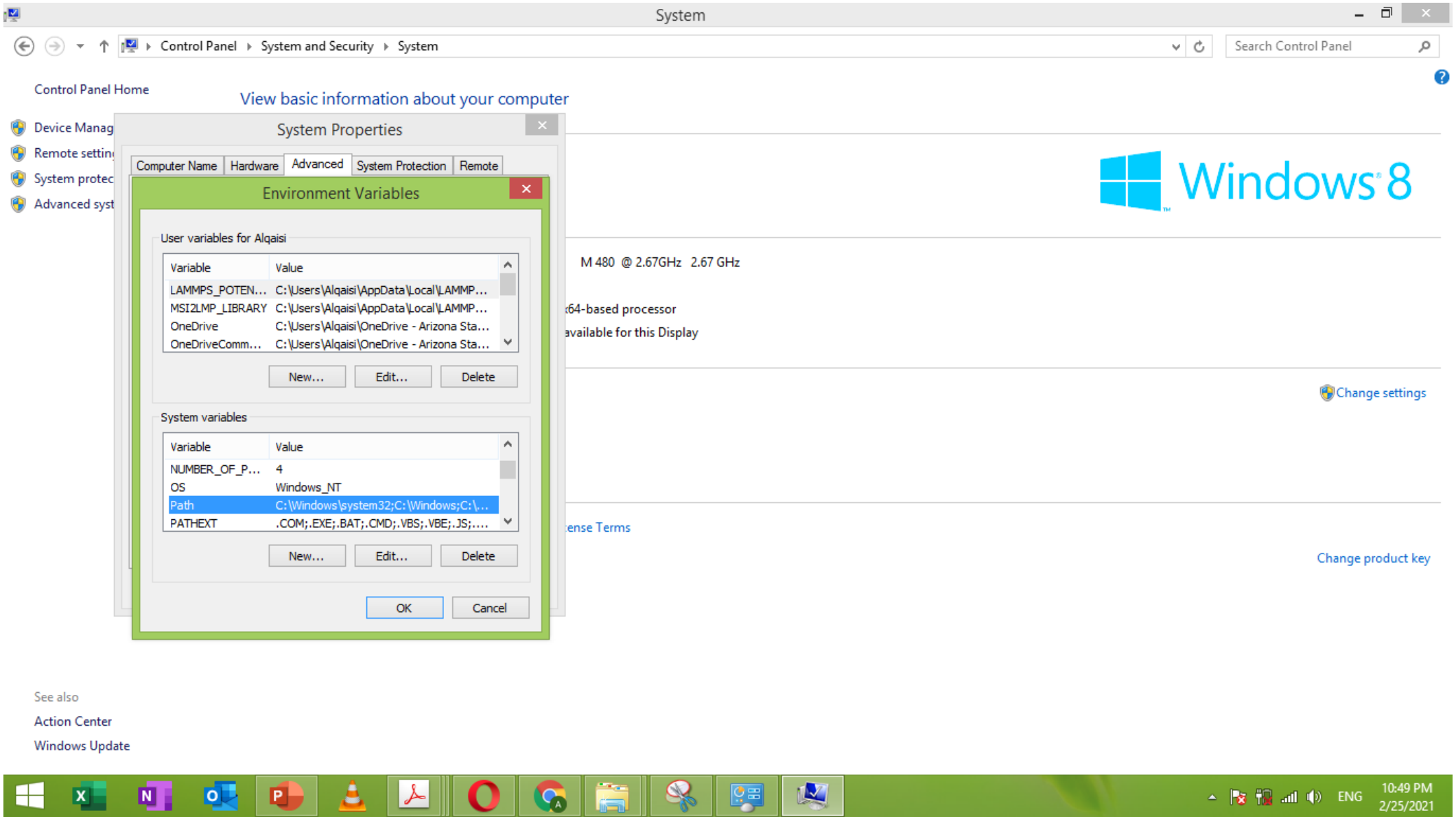

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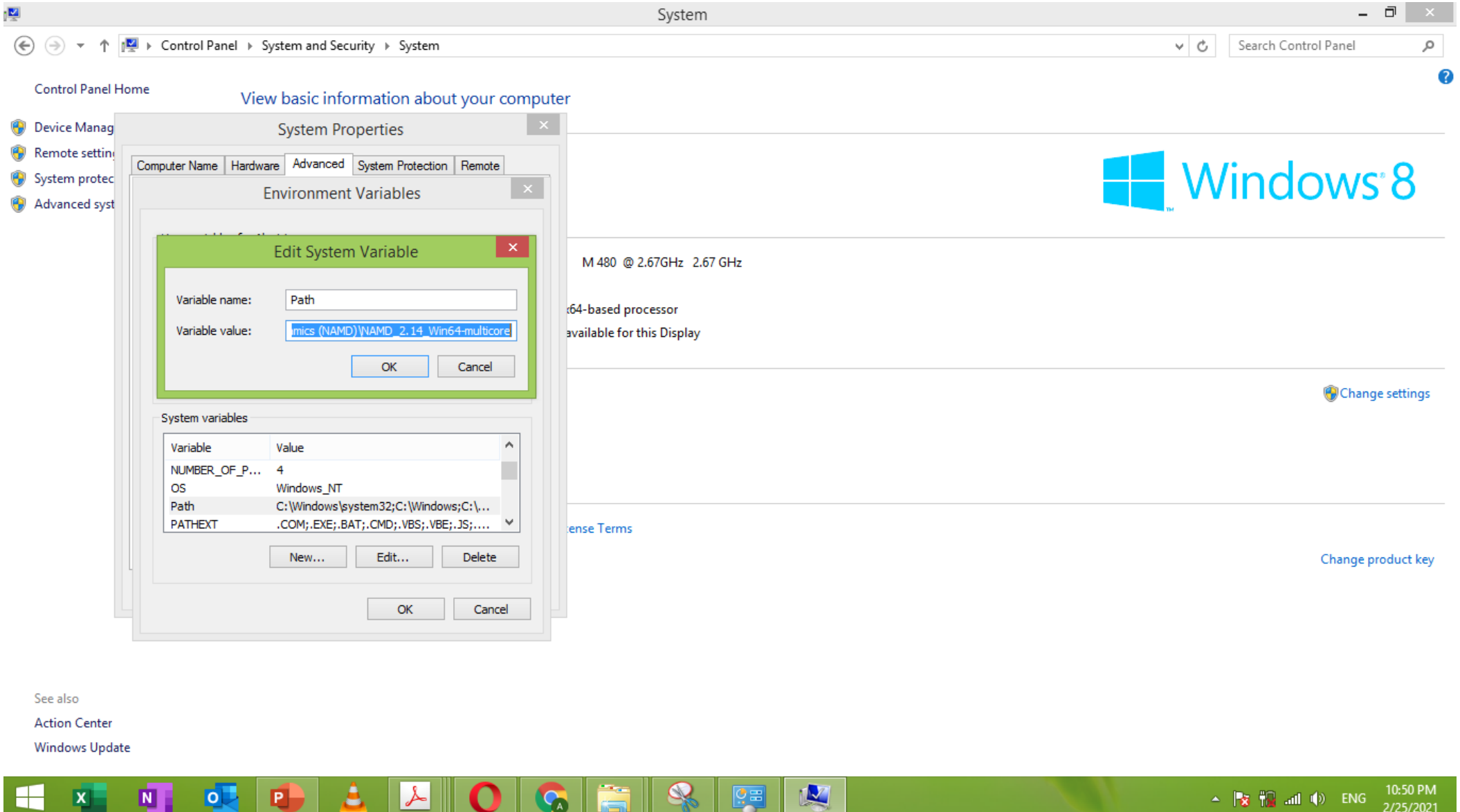
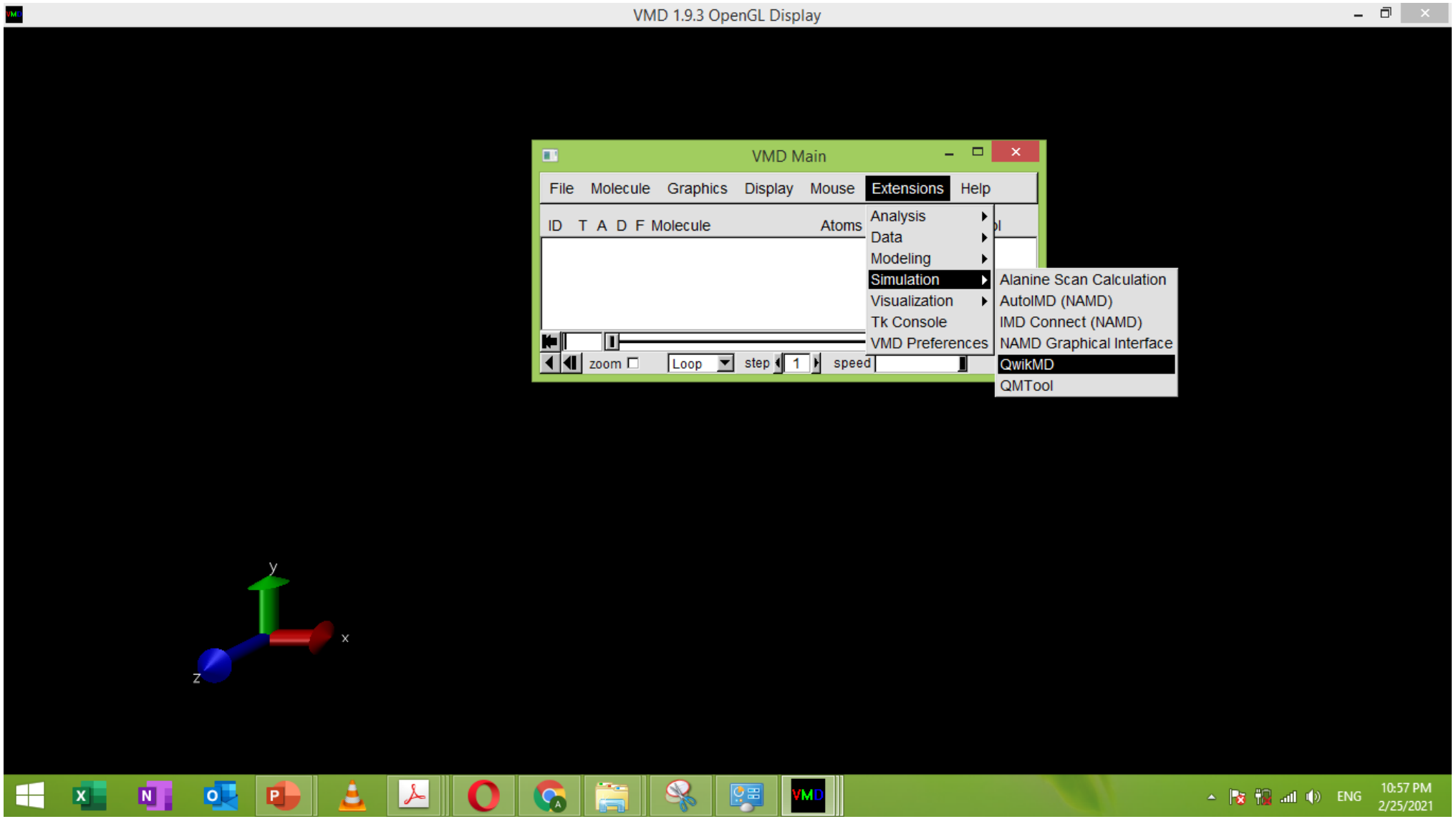


QwikMD Plugin



QwikMD: Step by Step

Select: Easy Run or Advanced Run
Analysis Tools can also be selected

Browse for a PDB file or type PDB code

In the structure manipulation window the QwikMD user can delete molecules or parts of a protein sequence; perform point mutations; change protonation states; check the structure; insert membrane model (Advanced mode only)

For structures solved by NMR, select the conformational state

Select the chains and type of molecule to be included in the simulation

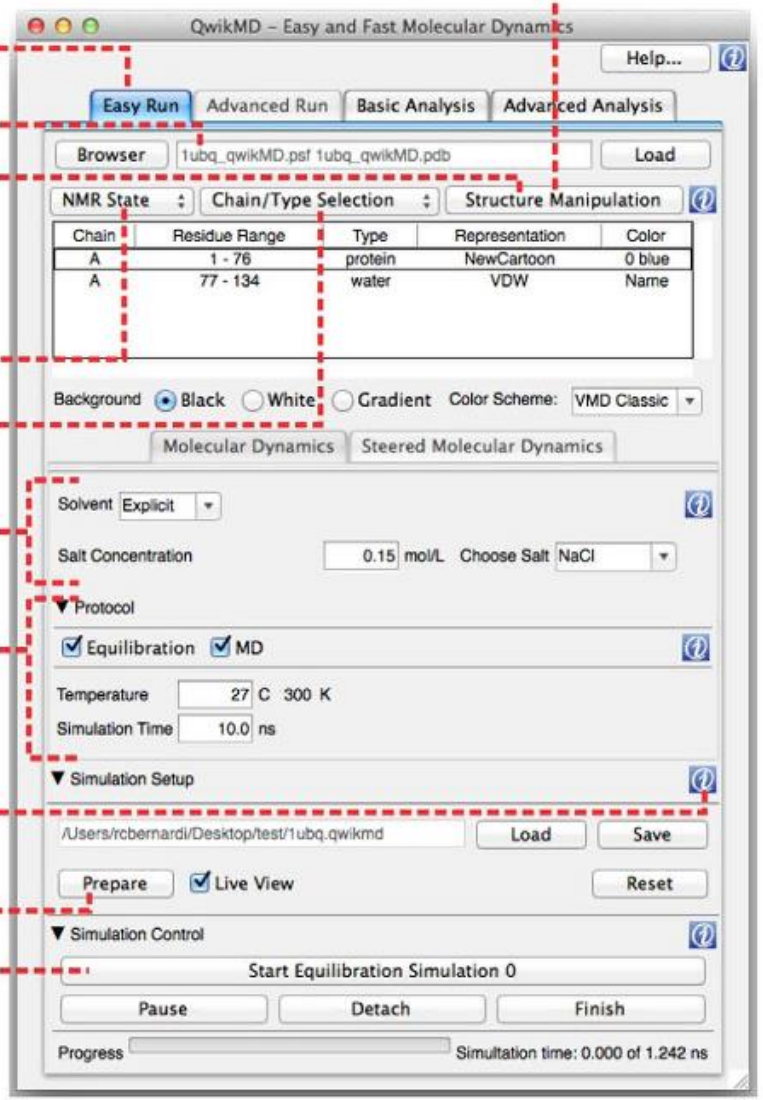
Select the environment: implicit or explicit solvent, and salt concentration

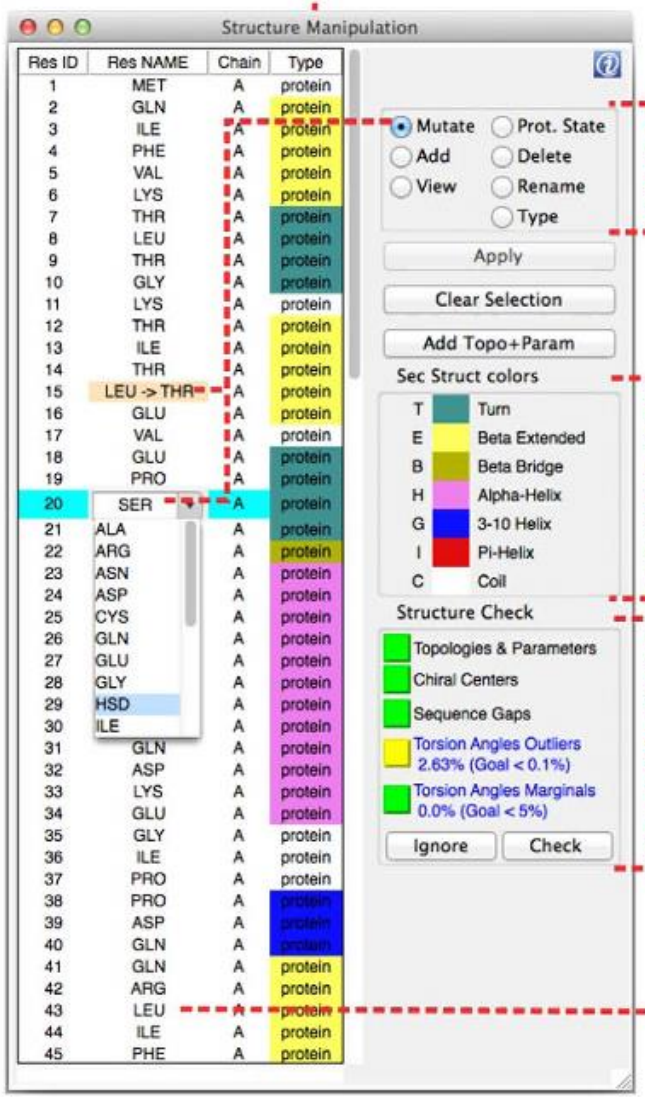
In the Protocol section the user selects temperature and duration of the simulation and also if an equilibration will be performed

"Info Buttons" provide the user with a variety of information, from protocols to a guidance on how to perform simulations and how to check results

When "Prepare" is clicked, QwikMD will invoke several scripts to perform all the operations set before, such as mutations, solvation, ...

Starts the simulation, either in "Live View" mode (if selected) or in "Background"





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The list of amino acid in the protein sequence is colored according to the secondary structure.

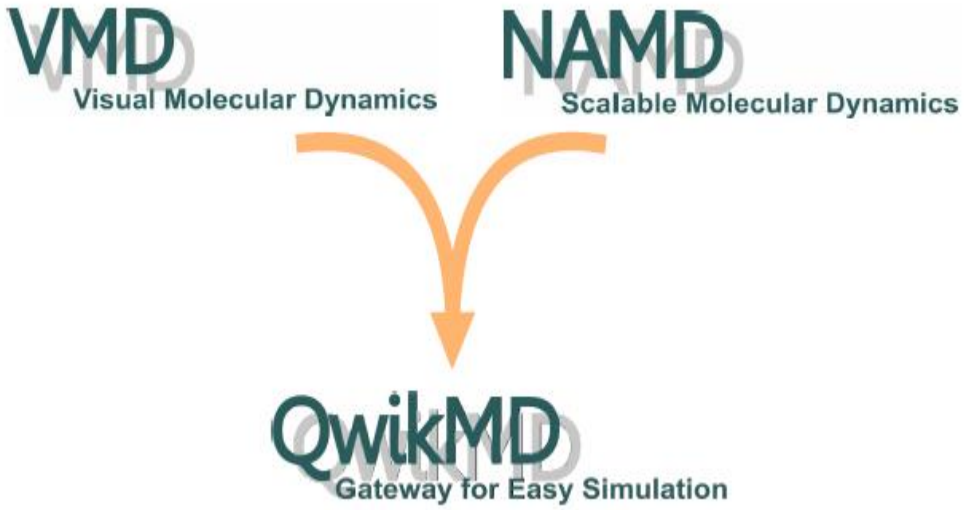
An automated check of the structure is performed when a PDB is loaded by QwikMD. If problems arise they will be marked in the "Structure Check" Tab. The user will be guided on how to fix the problems found.

All molecules of the system are presented in a list an can be separated by *type* or *chain*. The QwikMD user can easily delete parts of structure, change protonation states, perform point mutations, among other actions.

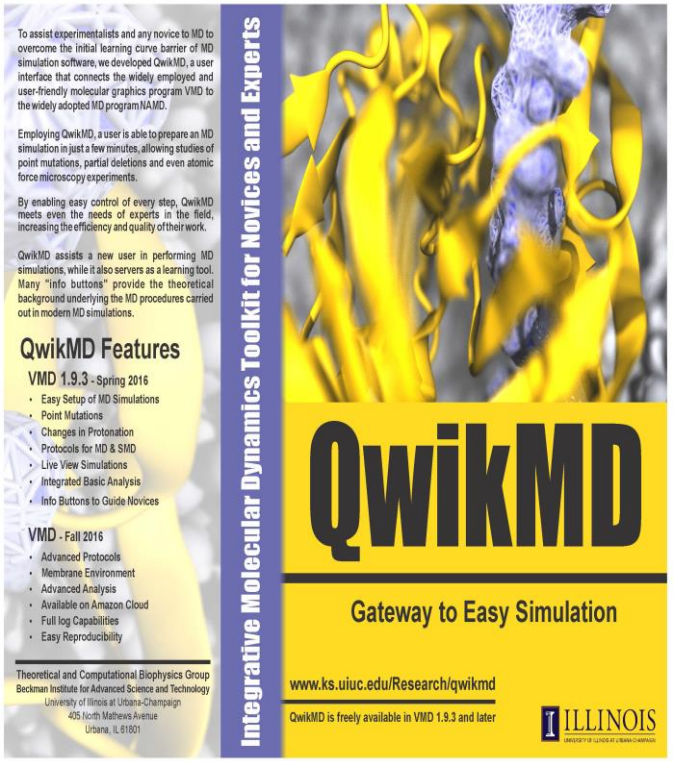
Molecular Dynamics Simulations on QwikMD

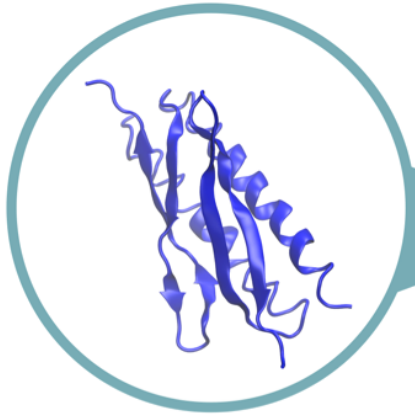
- We will do Molecular Dynamics Simulations on NAMD software
- Preparing the MD simulation will be through a VMD plugin called *QwikMD*
- *QwikMD* Features:

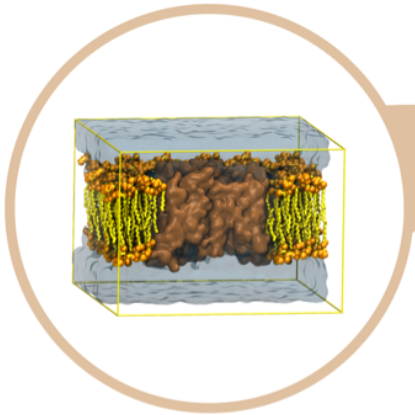
- Easy Setup of MD Simulations
- Structure Manipulation
- Basic and Advanced Protocols
- Live View Simulations
- Integrated Analysis
- Info Buttons
- Reproducibility

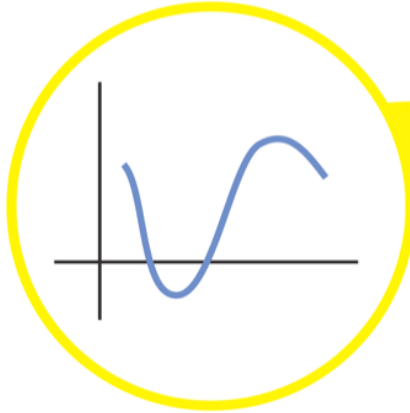


NAMD does not have graphical user interface
A graphics-based operating system interface that uses icons, menus and a mouse (to click on the icon or pull down the menus) to manage interaction with the system.









Protein Data Bank Structure

Select Chain / Molecule

Structure Check

Visualize and Check

Point Mutations

Protonation State

Solvate

Set Salt Concentration

Select Simulation Protocols

Prepare Simulation Files

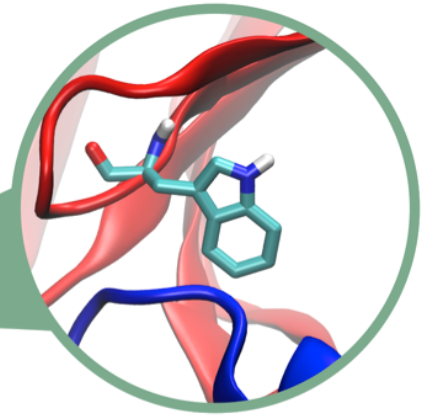
Run Simulation LIVE

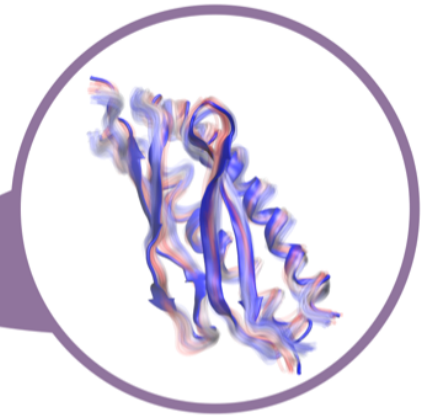
Run Simulation

Copy Files to Supercomputer

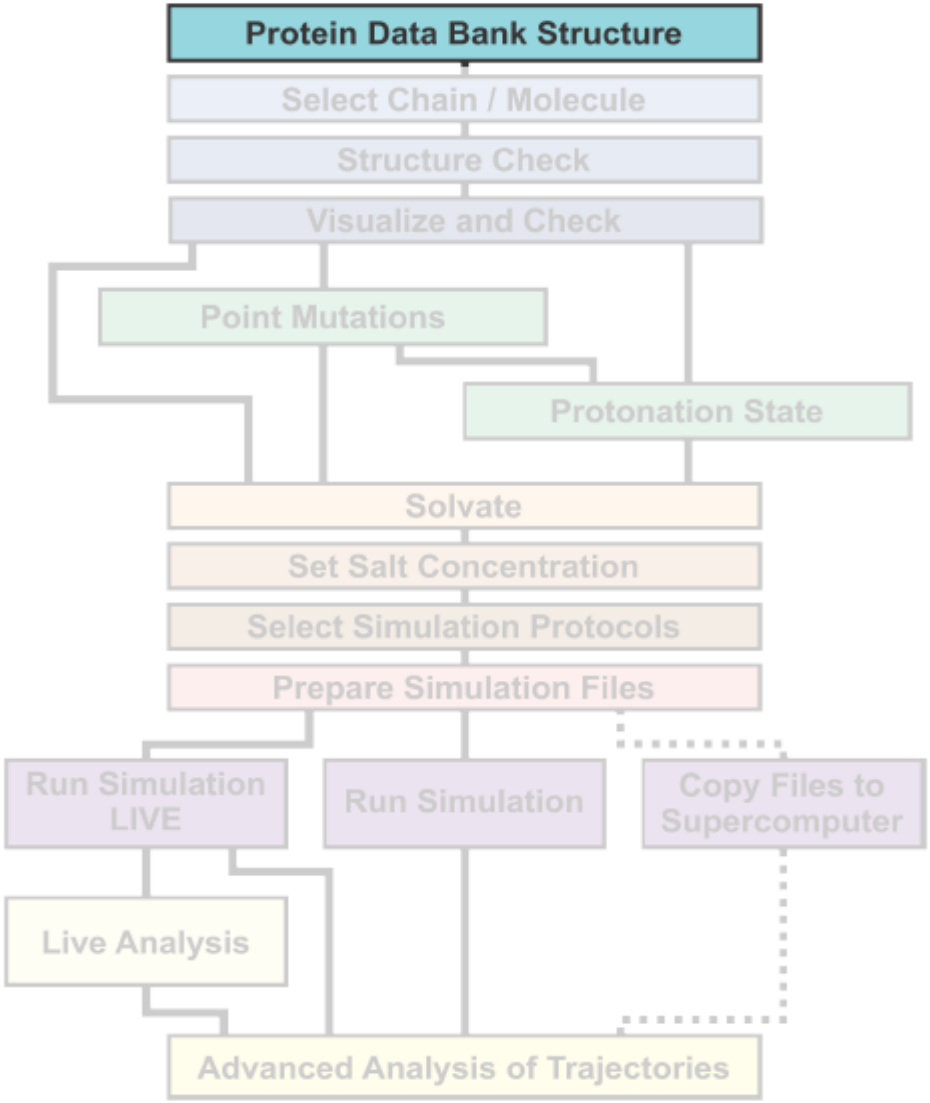
Live Analysis

Advanced Analysis of Trajectories





QwikMD: Step by Step



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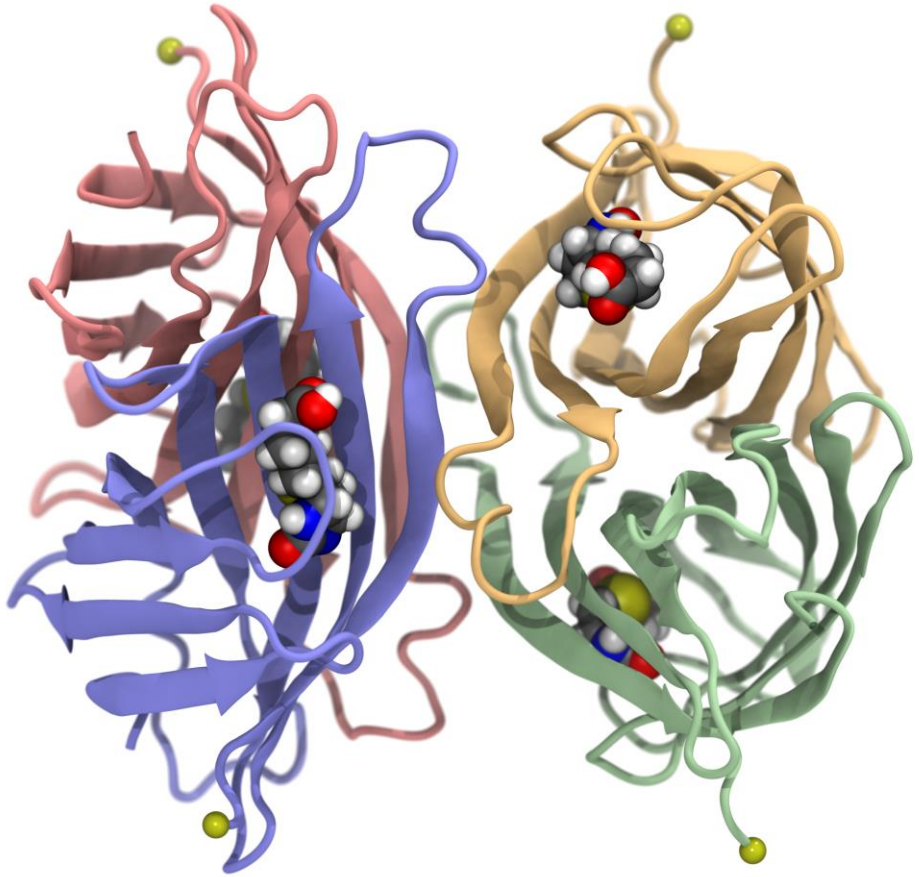

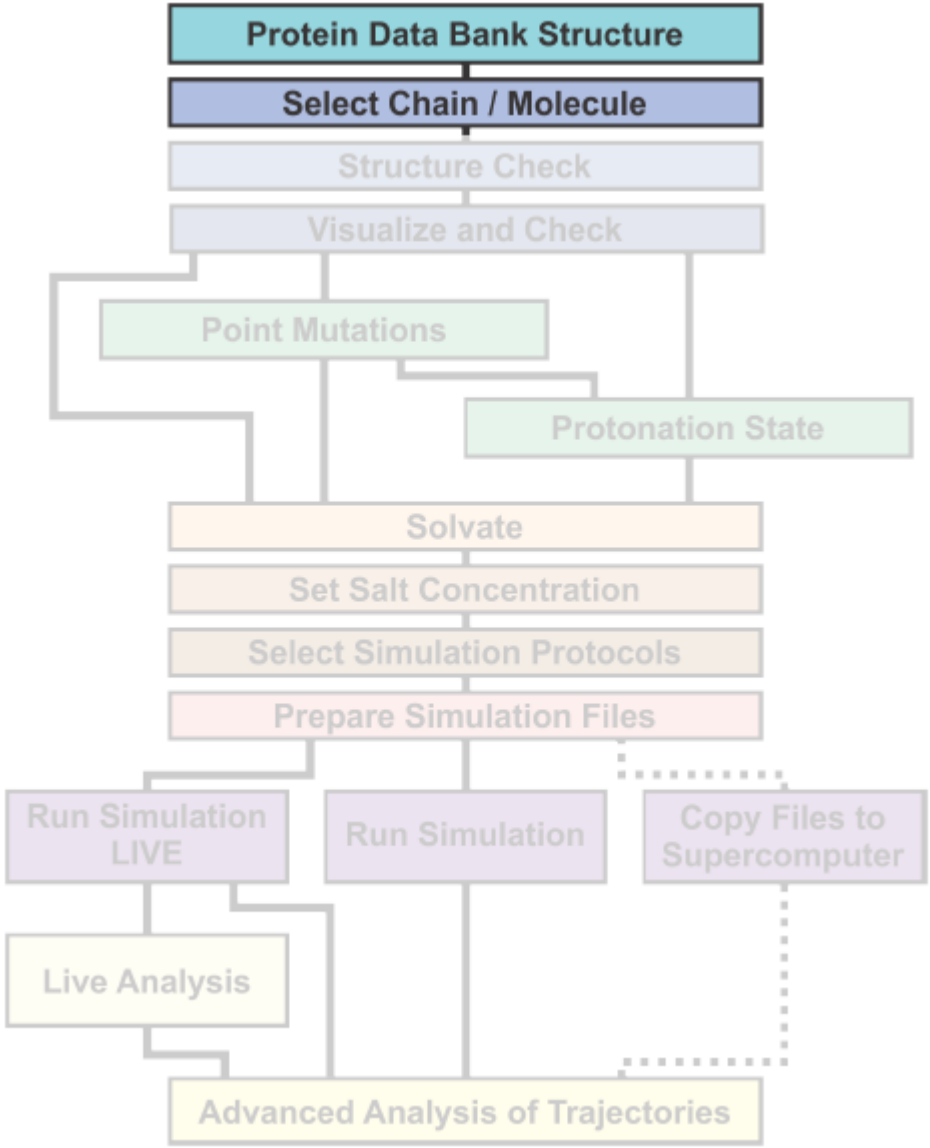

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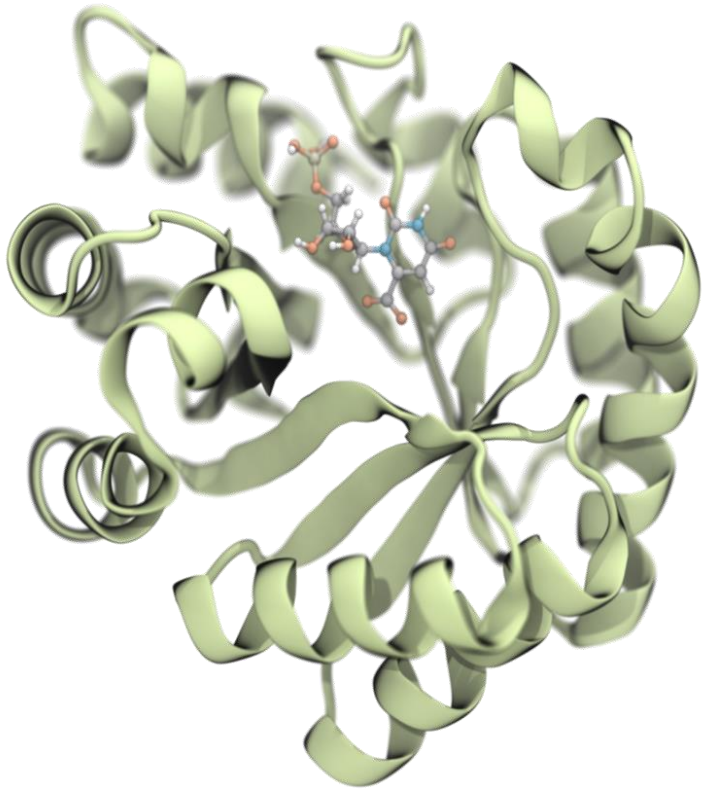

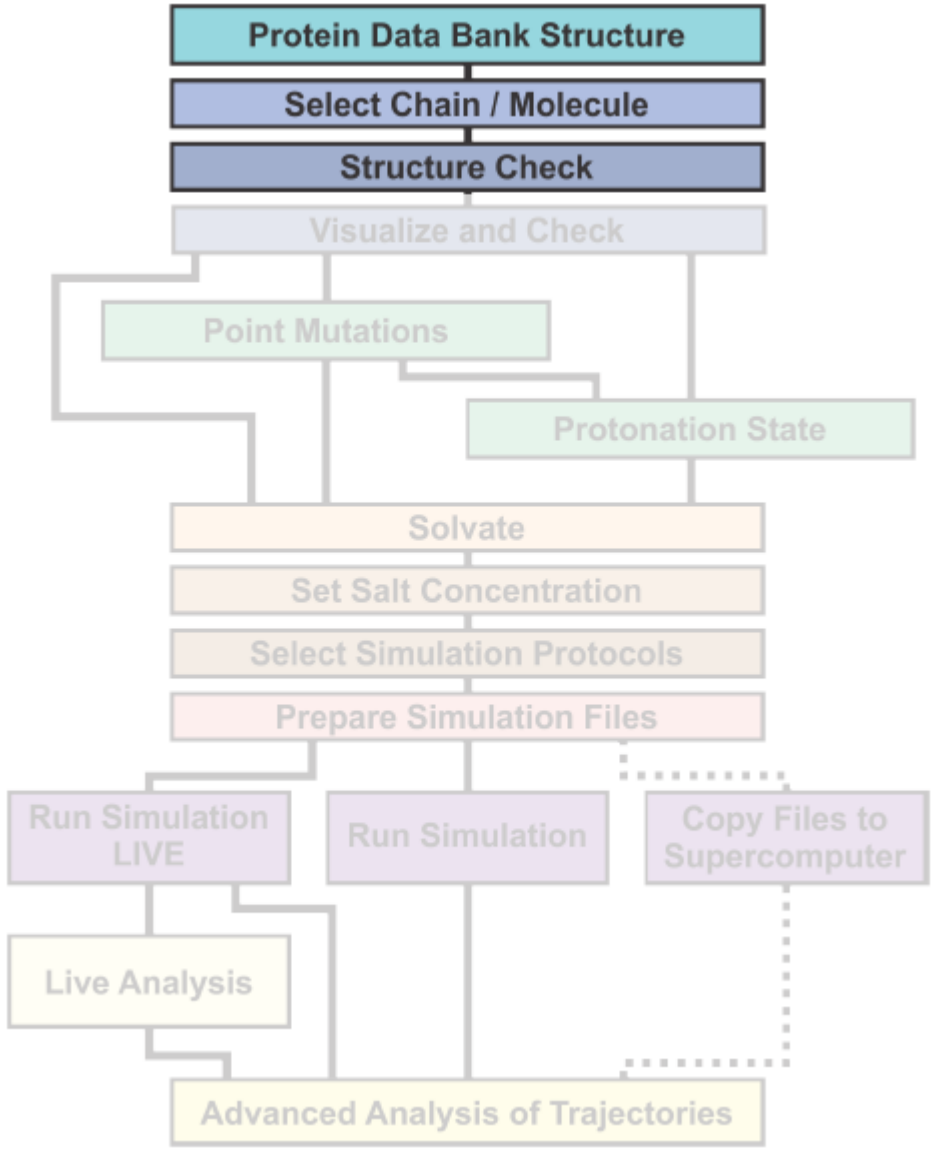

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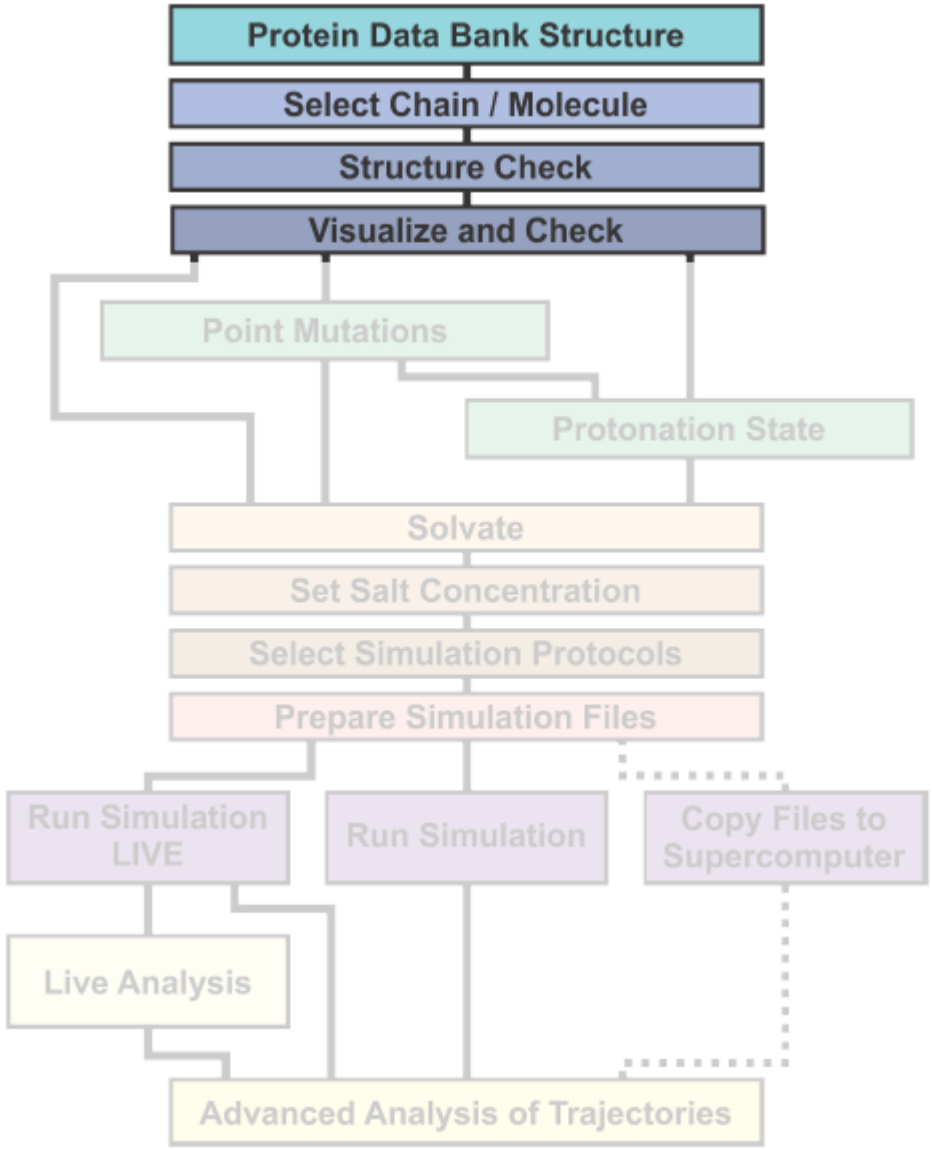
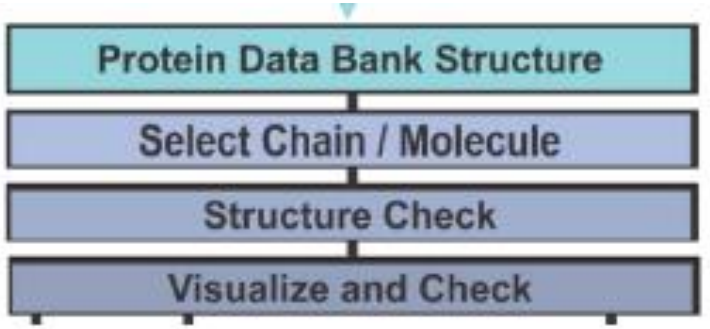


QwikMD: Step by Step

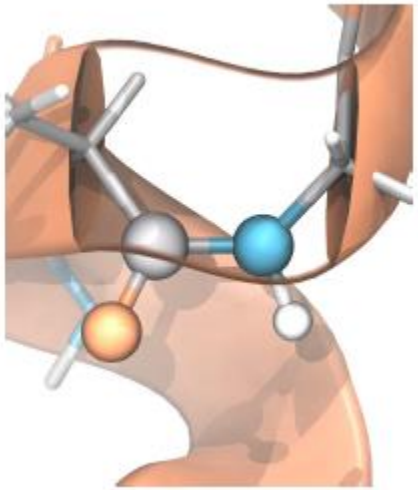
- **Structure Check:**

- Missing topologies
- Sequence Gaps
- Residues Alternative Insertions
- Chiral Centers
- Cis-peptide Bonds
- Backbone Torsion Angles

- Marginals
- Outliers

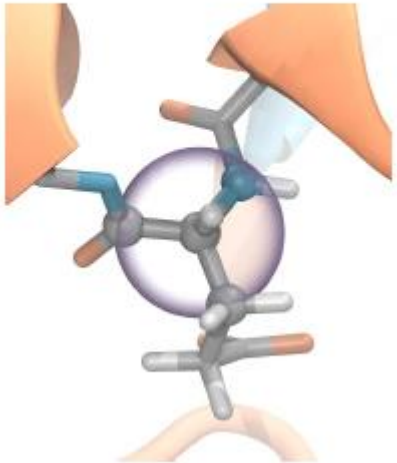


Cis-peptide

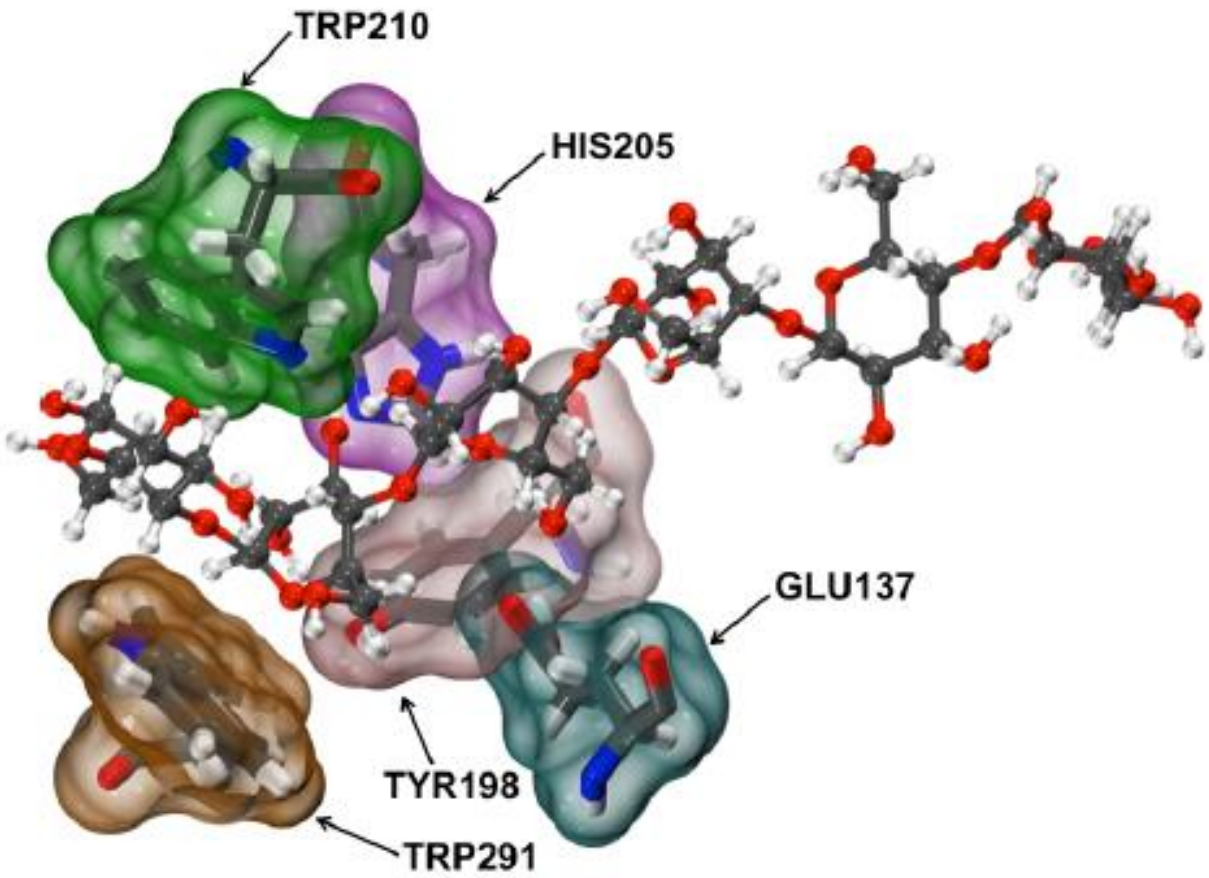


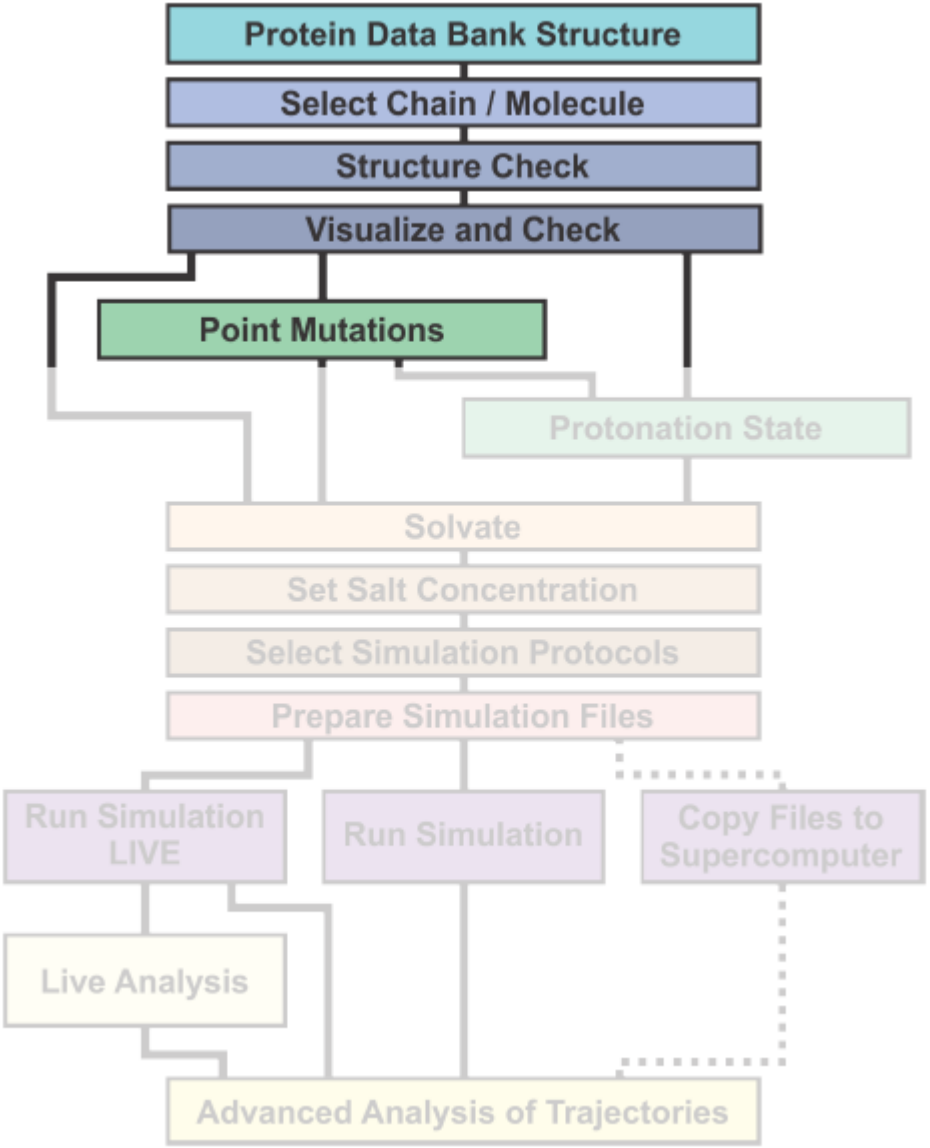
Chiral Centers

D-amino acids

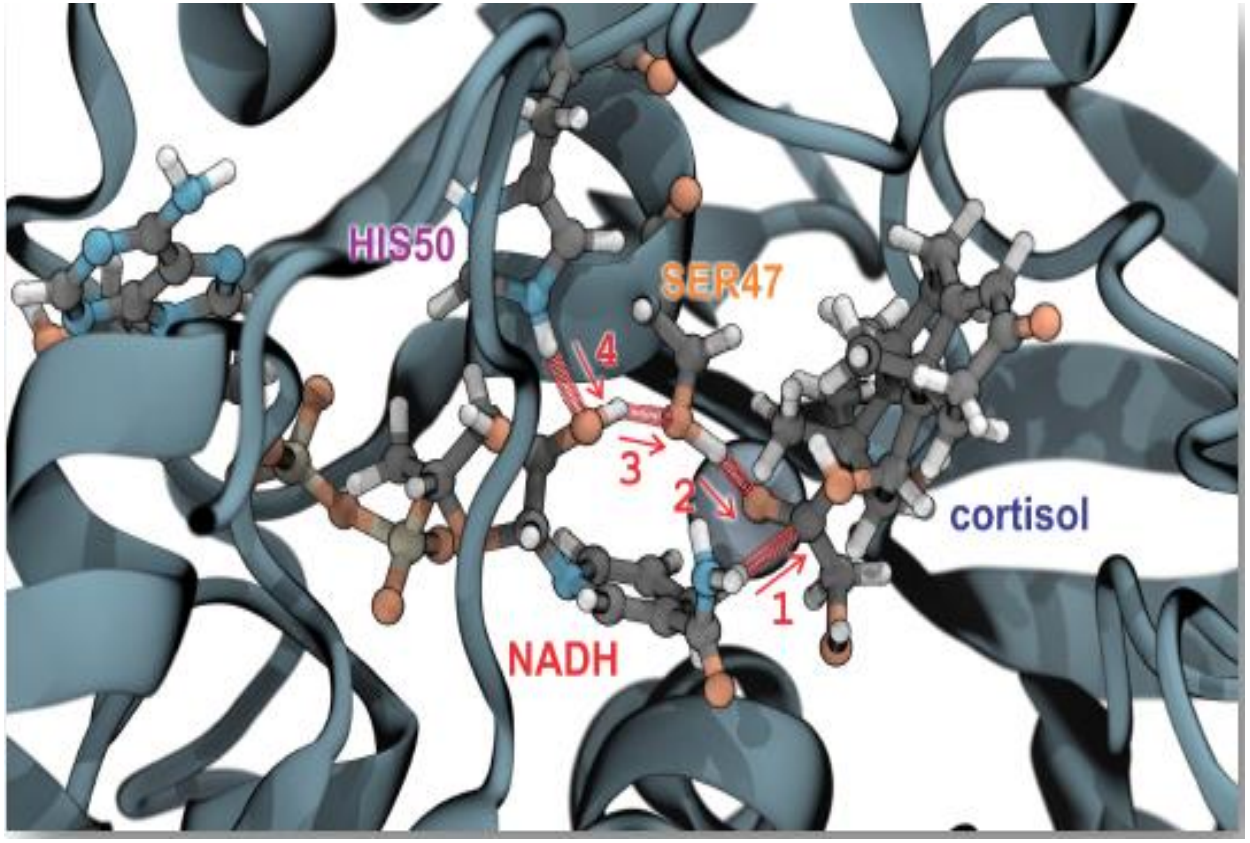


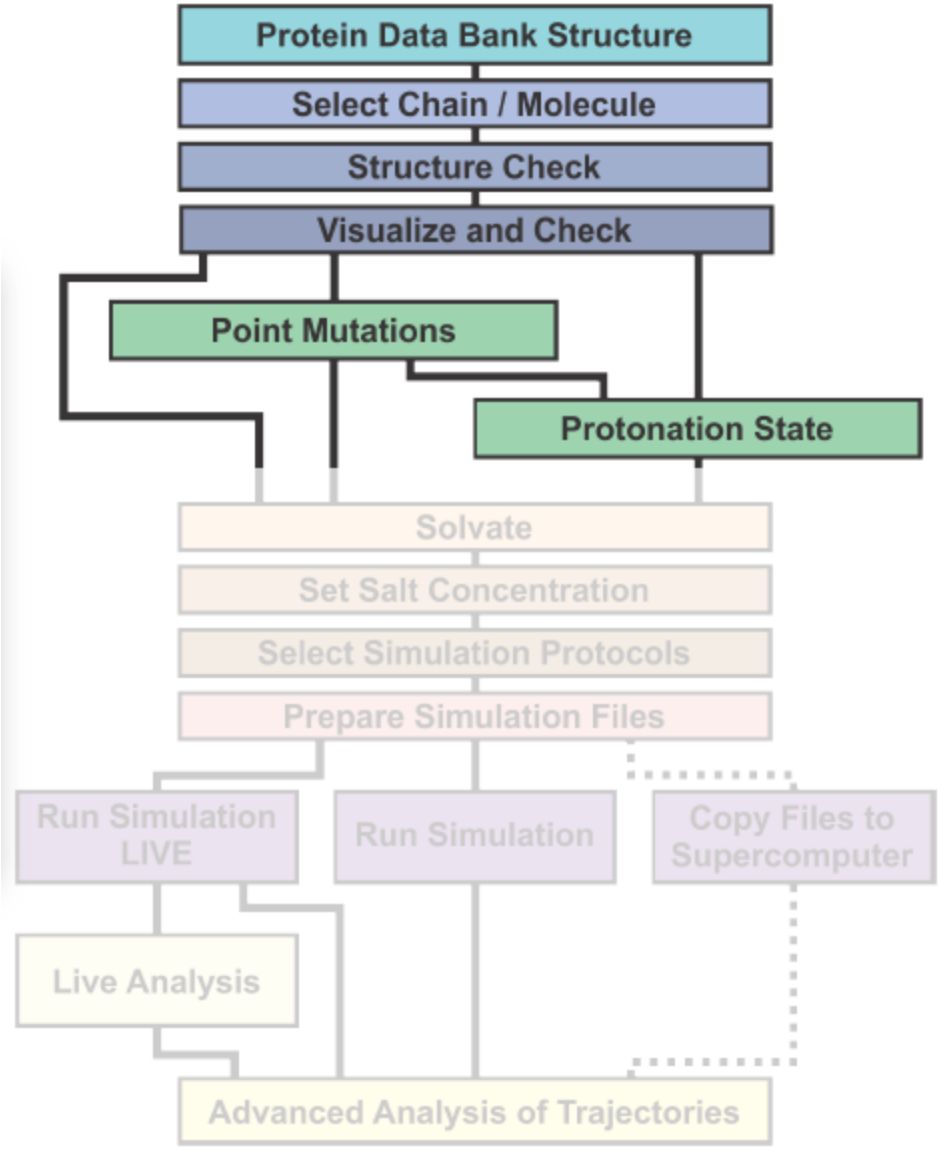
QwikMD: Step by Step





QwikMD: Step by Step

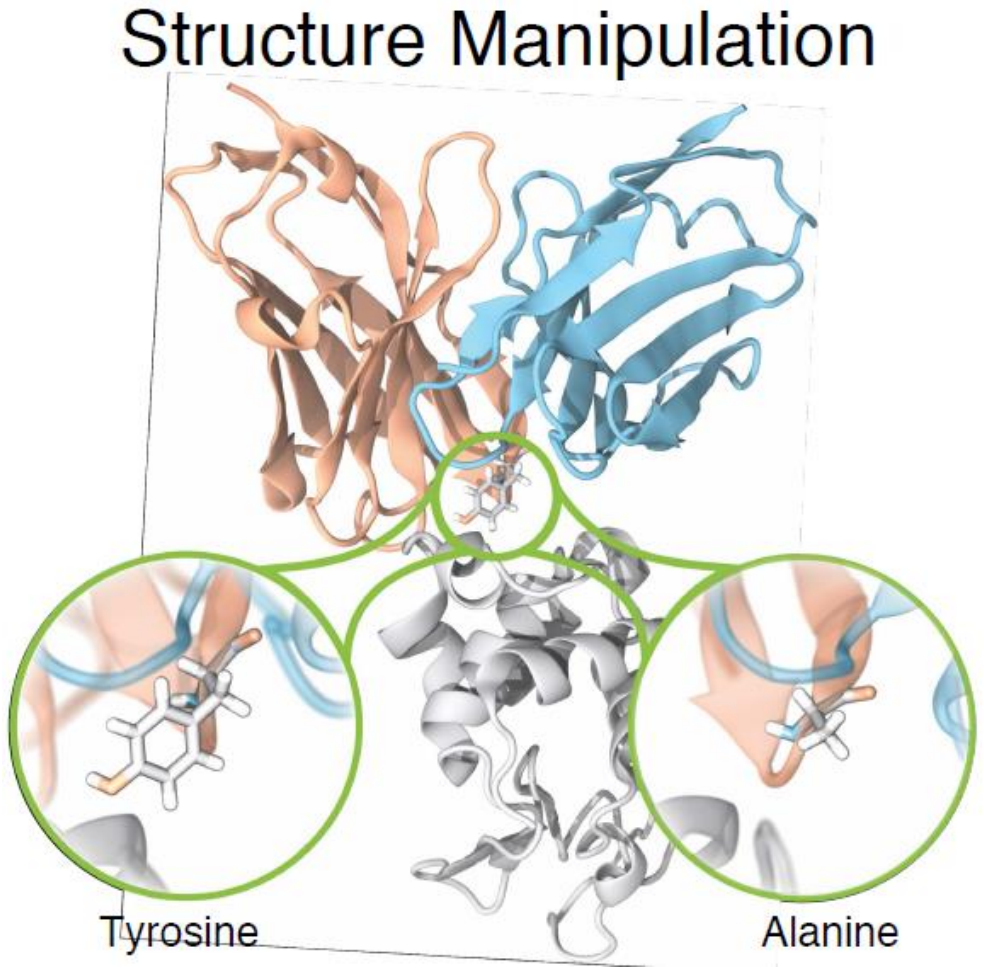




QwikMD: Step by Step

- **Structure Manipulation:**

- Point Mutations
- Protonation State Selection
- Partial Sequence Deletions
- Molecule’s Type
- Assign Topologies
- Atom Editing
- - Name
- - Indexes



QwikMD: Step by Step

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For structures solved by NMR, select the conformational state

Select the chains and type of molecule to be included in the simulation

Select the environment: implicit or explicit solvent, and salt concentration

In the Protocol section the user selects temperature and duration of the simulation and also if an equilibration will be performed

"Info Buttons" provide the user with a variety of information, from protocols to a guidance on how to perform simulations and how to check results

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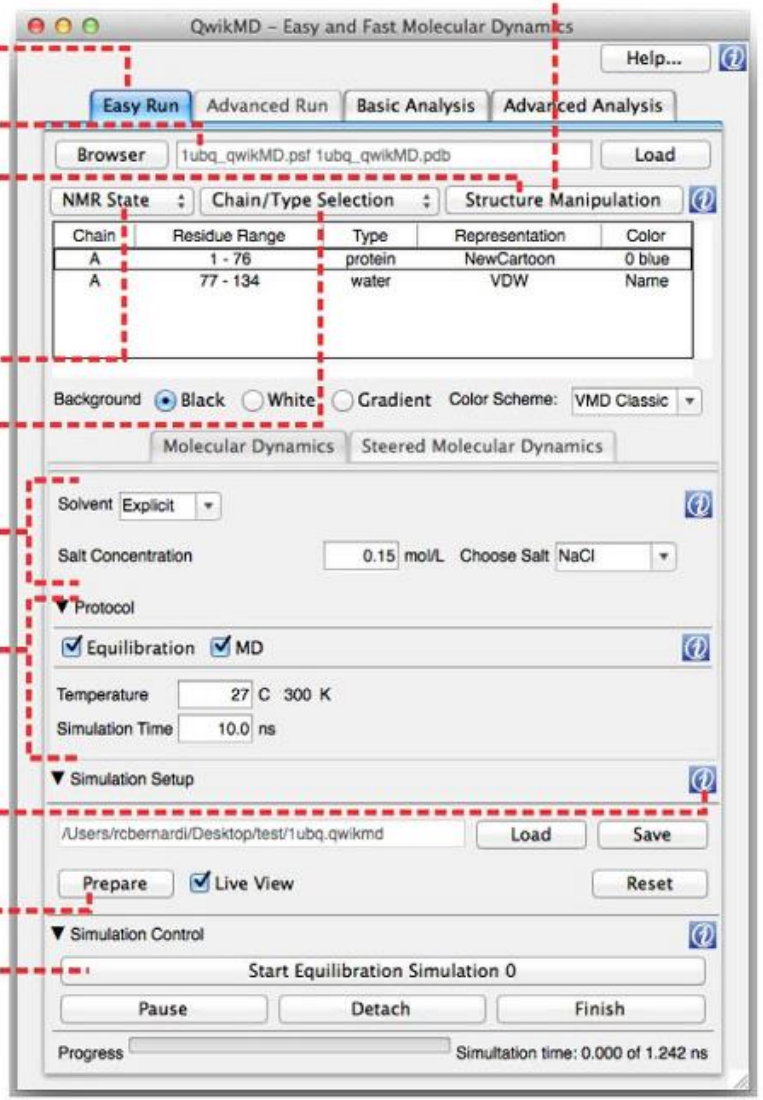

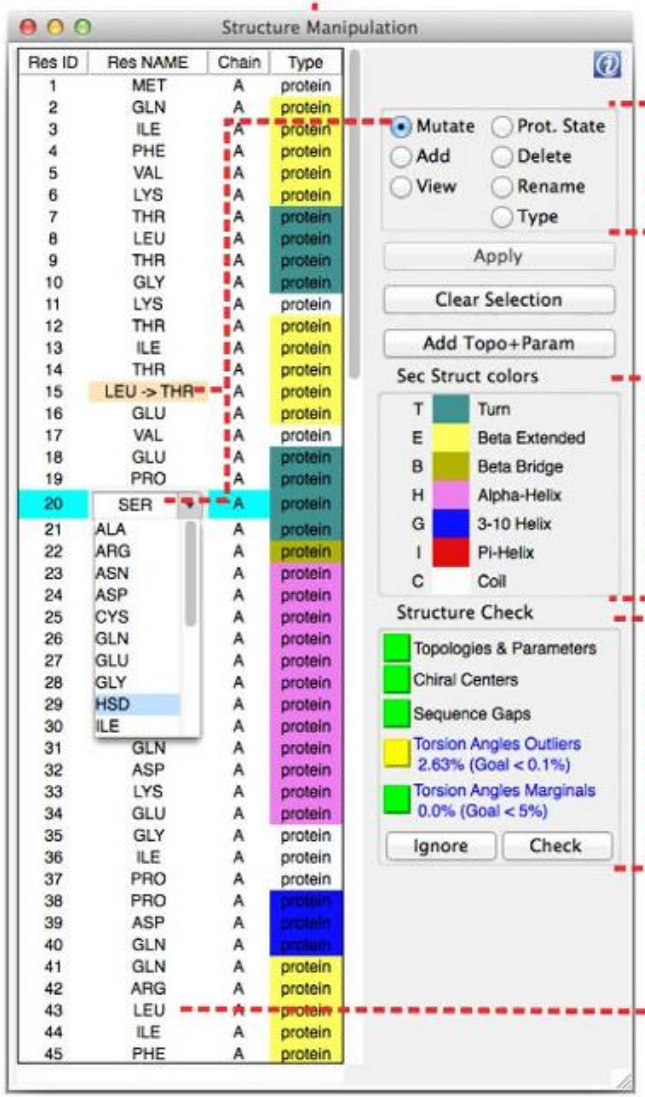

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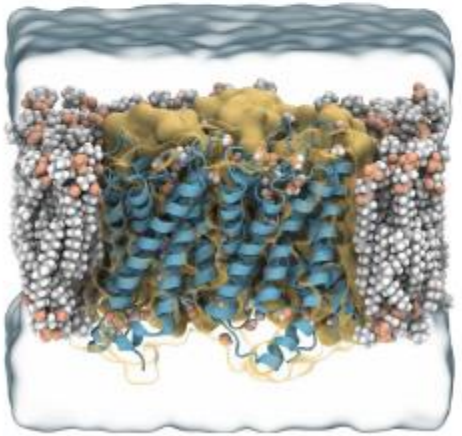
QwikMD: Step by Step

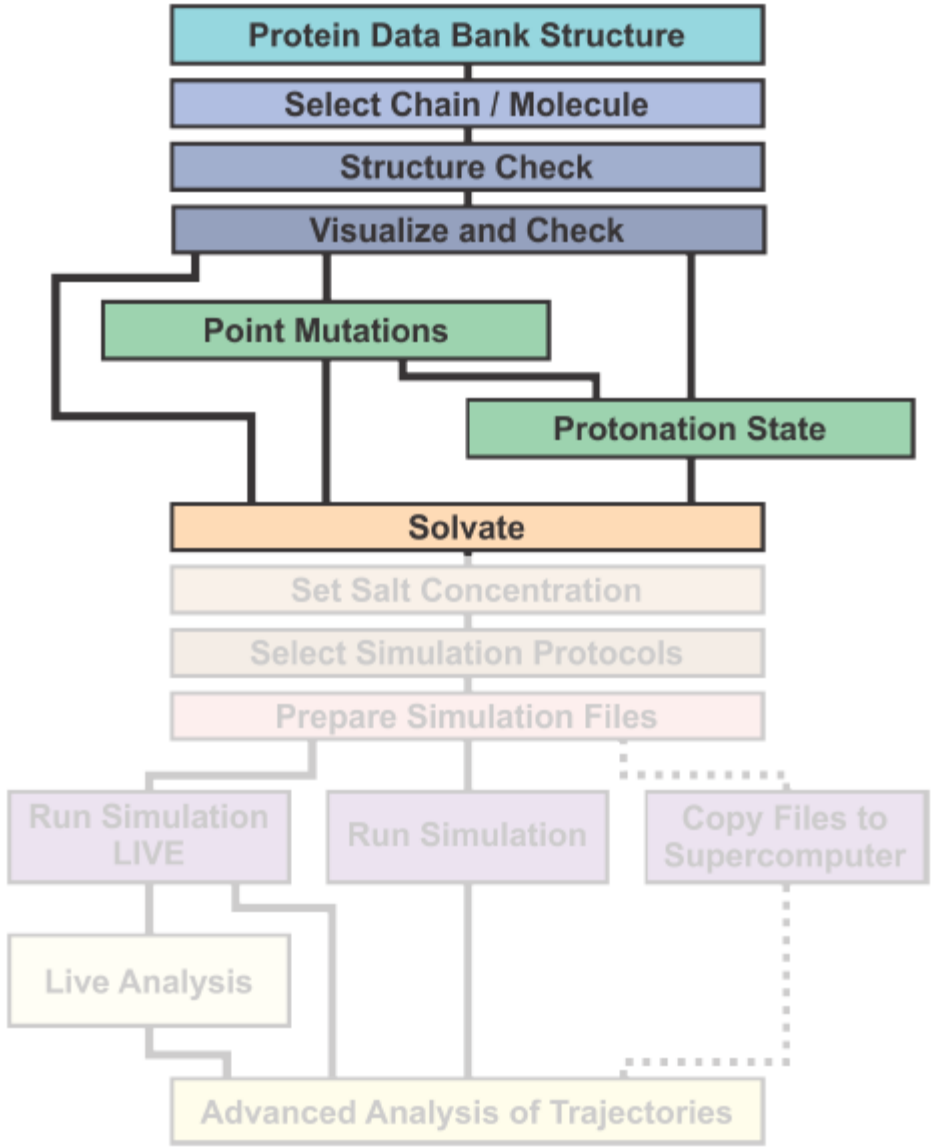
Vacuum

Implicit Solvent

Explicit Solvent

Explicit Solvent + Membrane





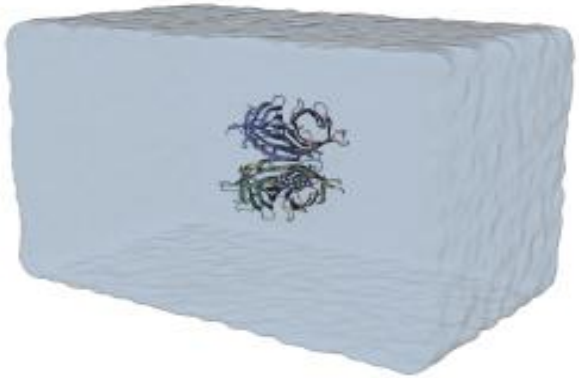
QwikMD: Step by Step

- **Simulation Environment:**

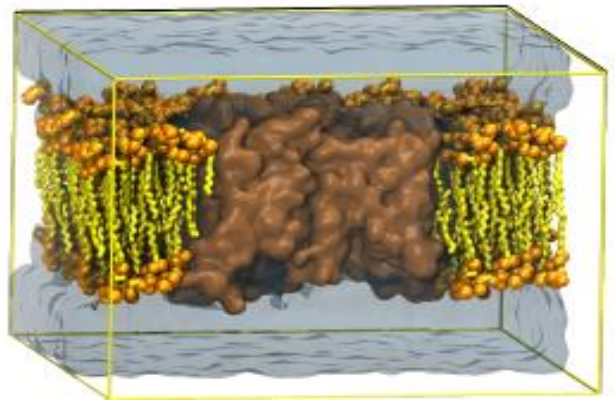
- Solvent Model
- Salt Concentration
- Water Box Size
  - Reduced Volume Available
- Membrane Protein Insertion

Vacuum / Implicit Solvent

Water Box



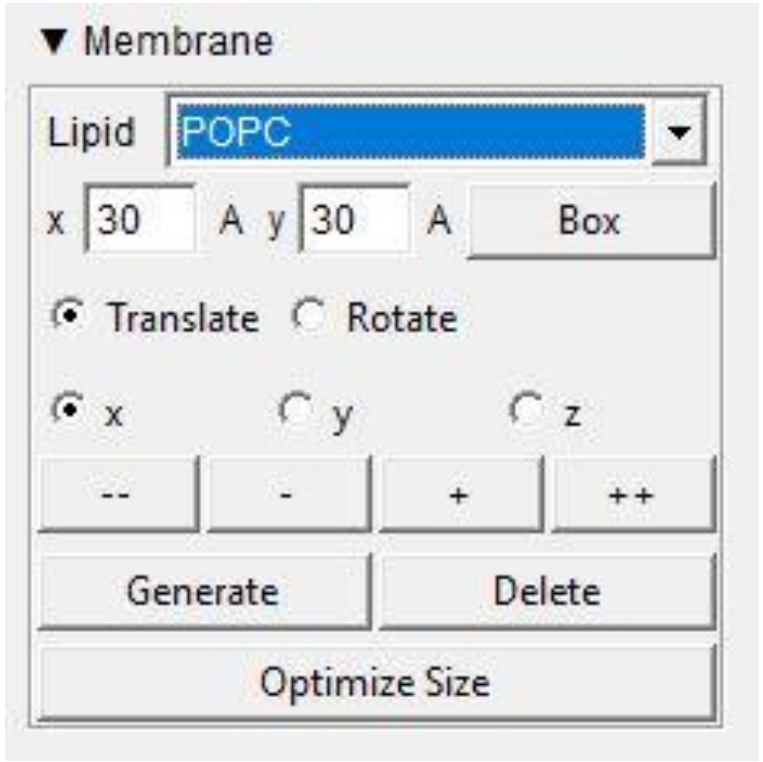
Membrane Environment

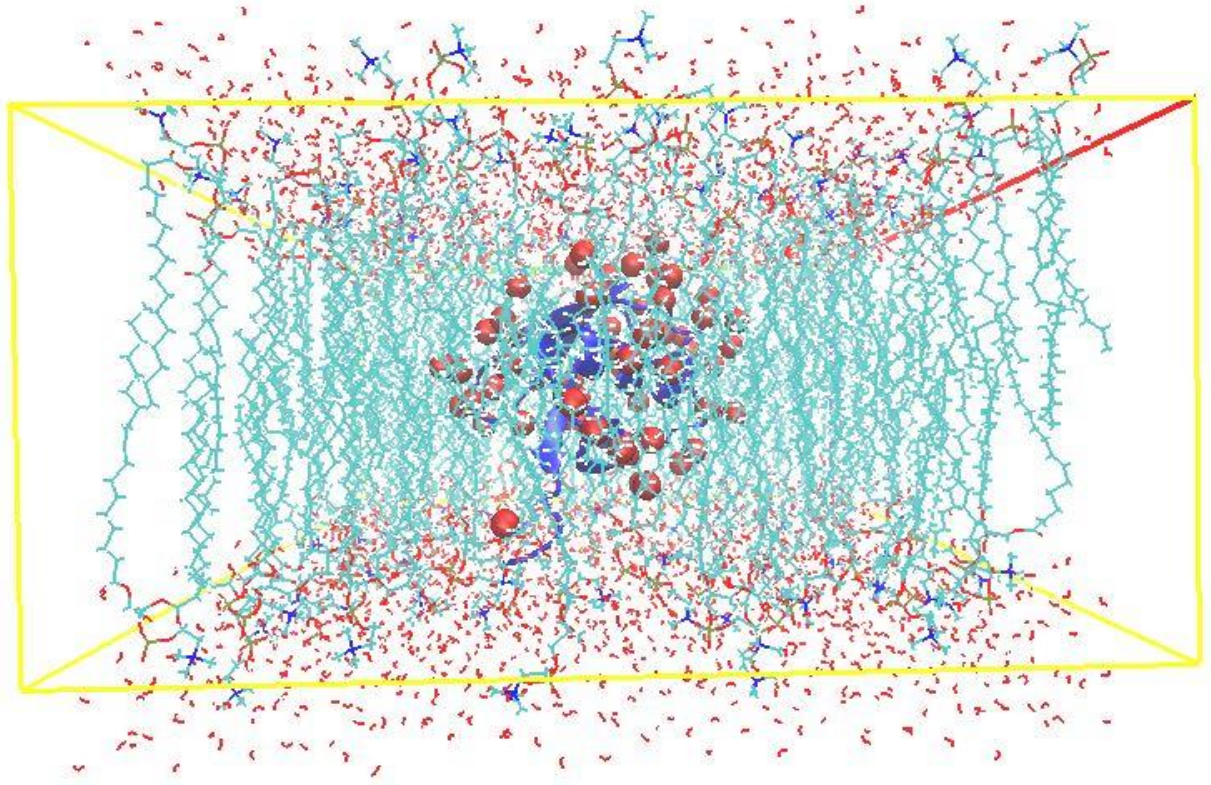


QwikMD: Step by Step

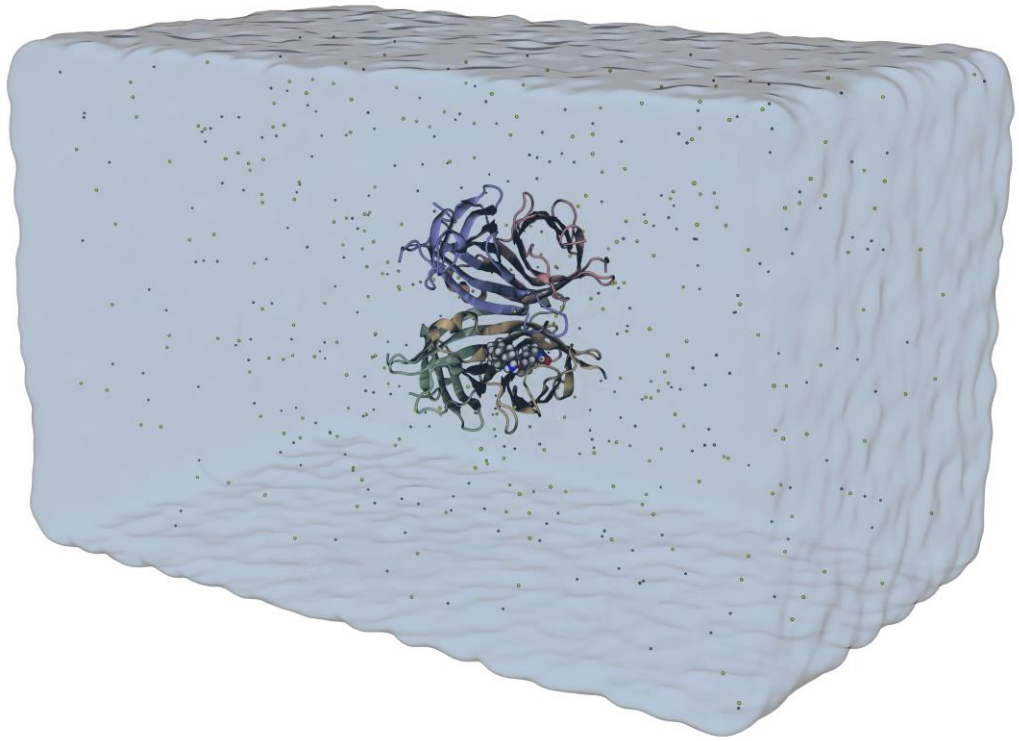
- **Simulation Environment:**

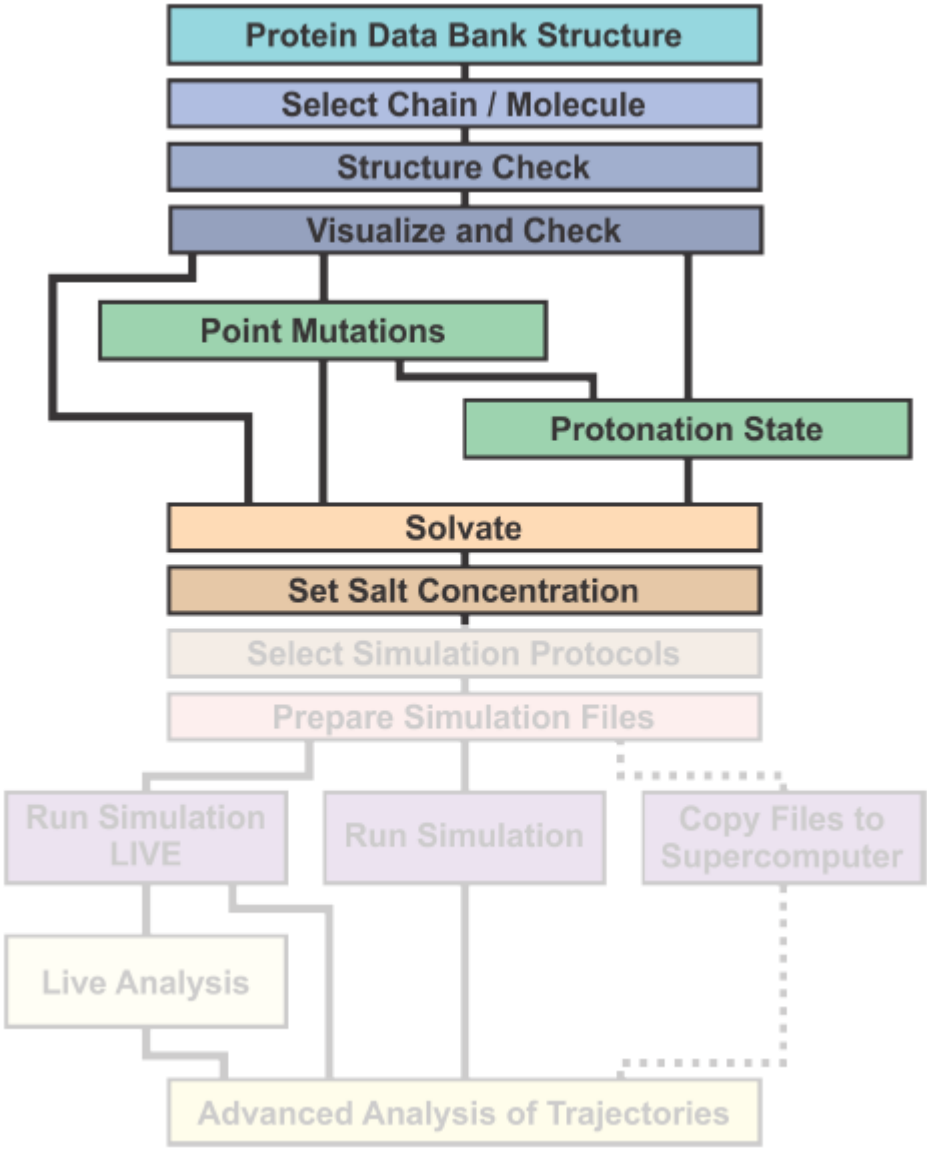
- Membrane in QwikMD



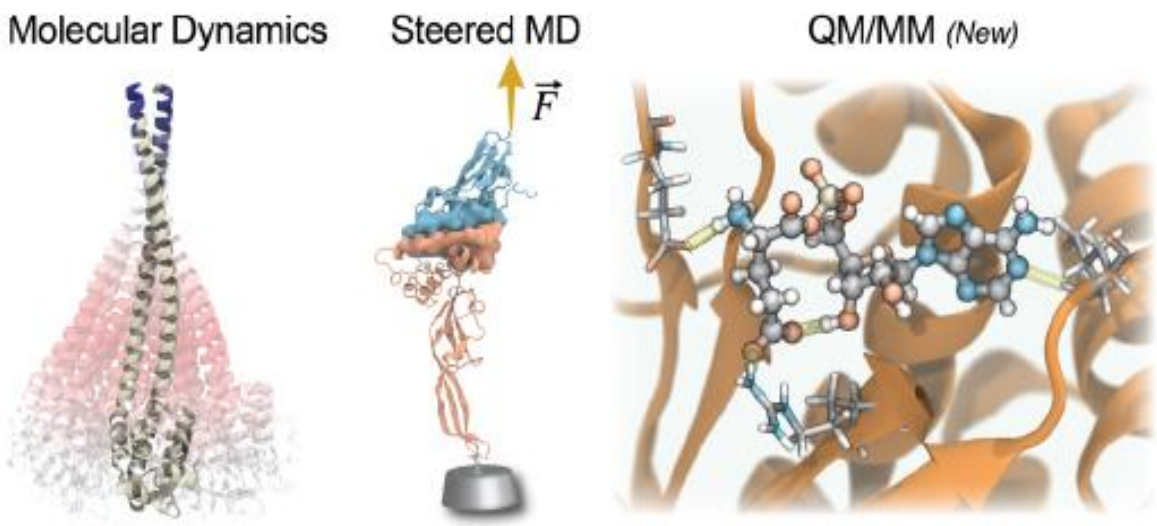


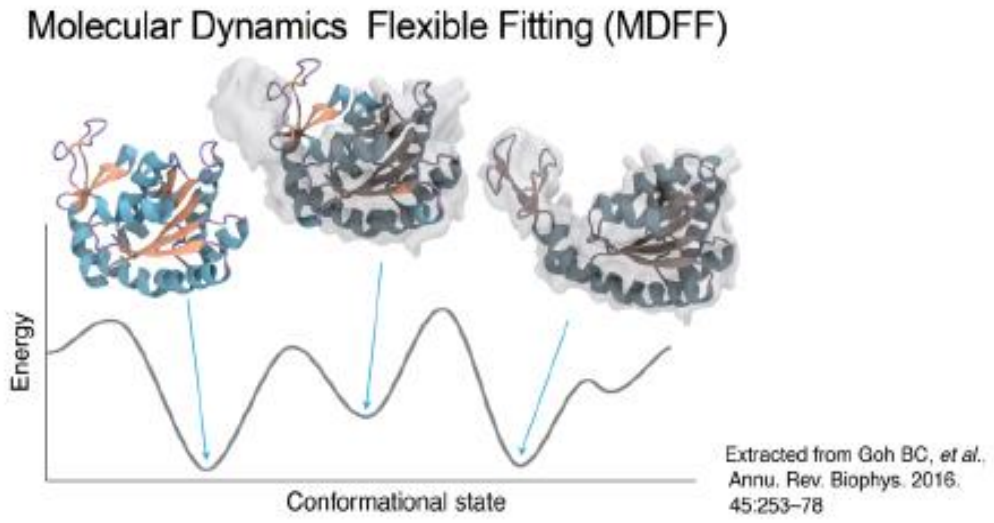
QwikMD: Step by Step

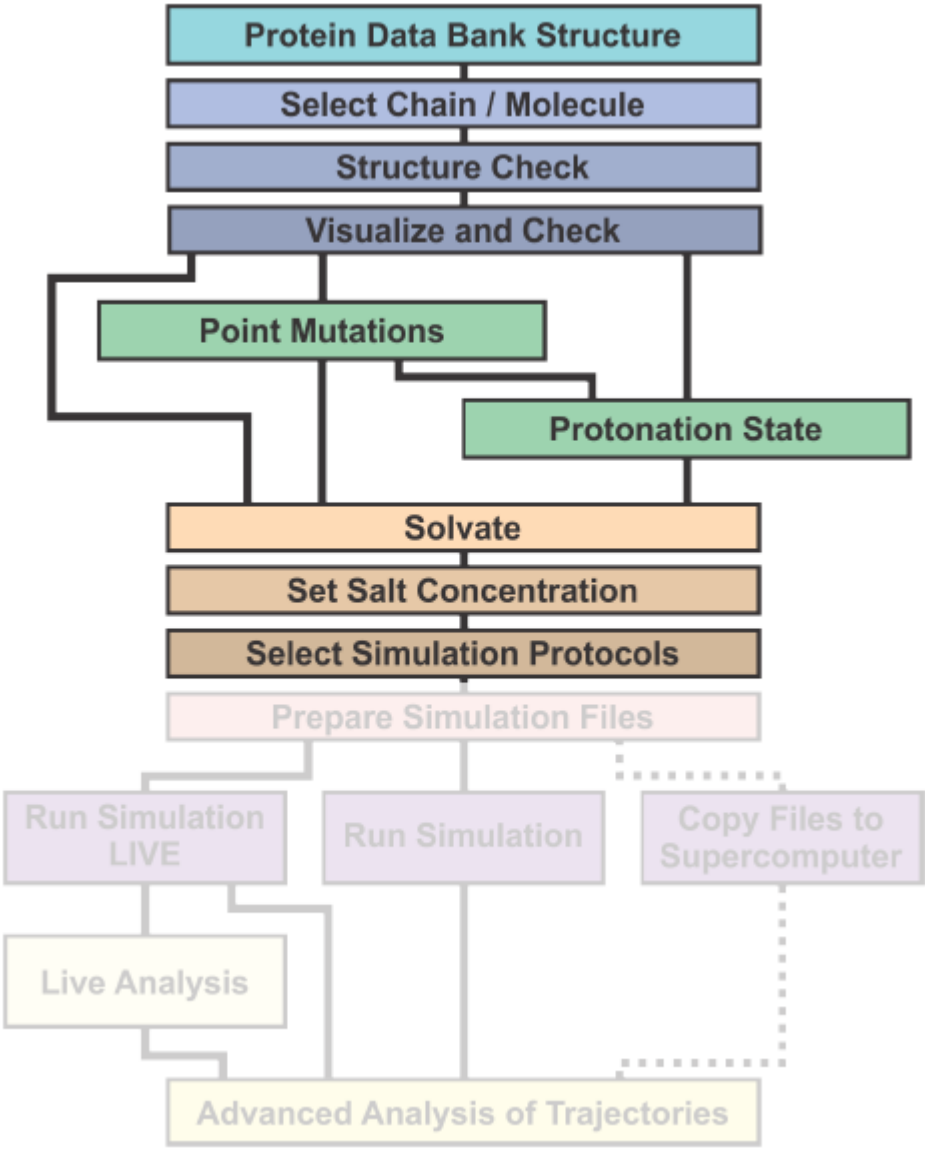




QwikMD: Step by Step





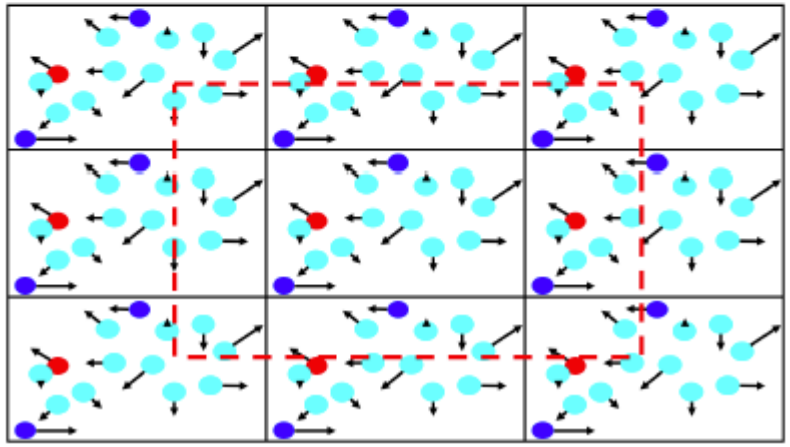


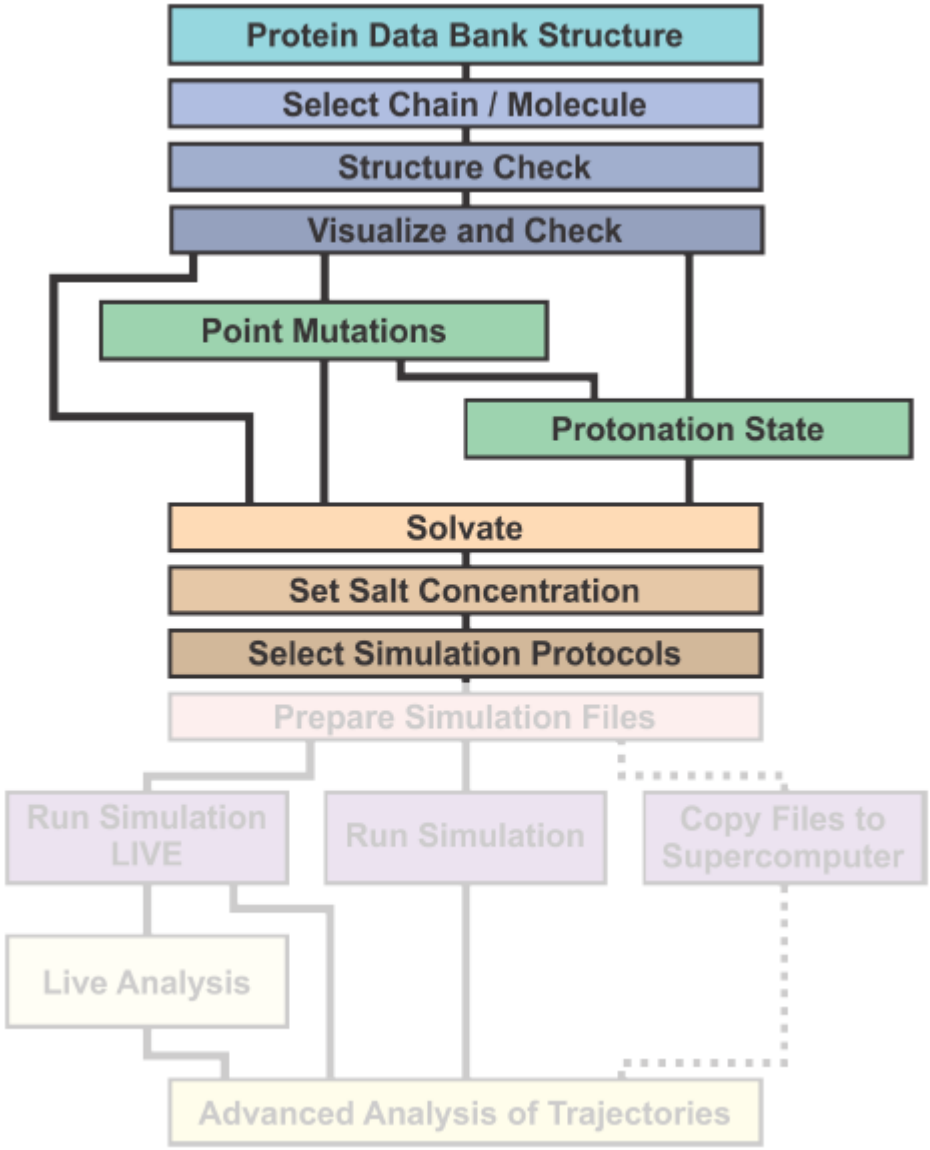
QwikMD: Step by Step

Molecular Dynamics Ensembles

- Constant energy, constant volume (NVE)
- Constant temperature, constant volume (NVT)
- Constant temperature, constant pressure (NPT)

Periodic Boundary Conditions





QwikMD: Step by Step

All files are prepared in a stand-alone folder

The NAMD Configuration File:

Files needed:

```
structure           mypsf.psf
coordinates         mypdb.pdb
```

Define temperature

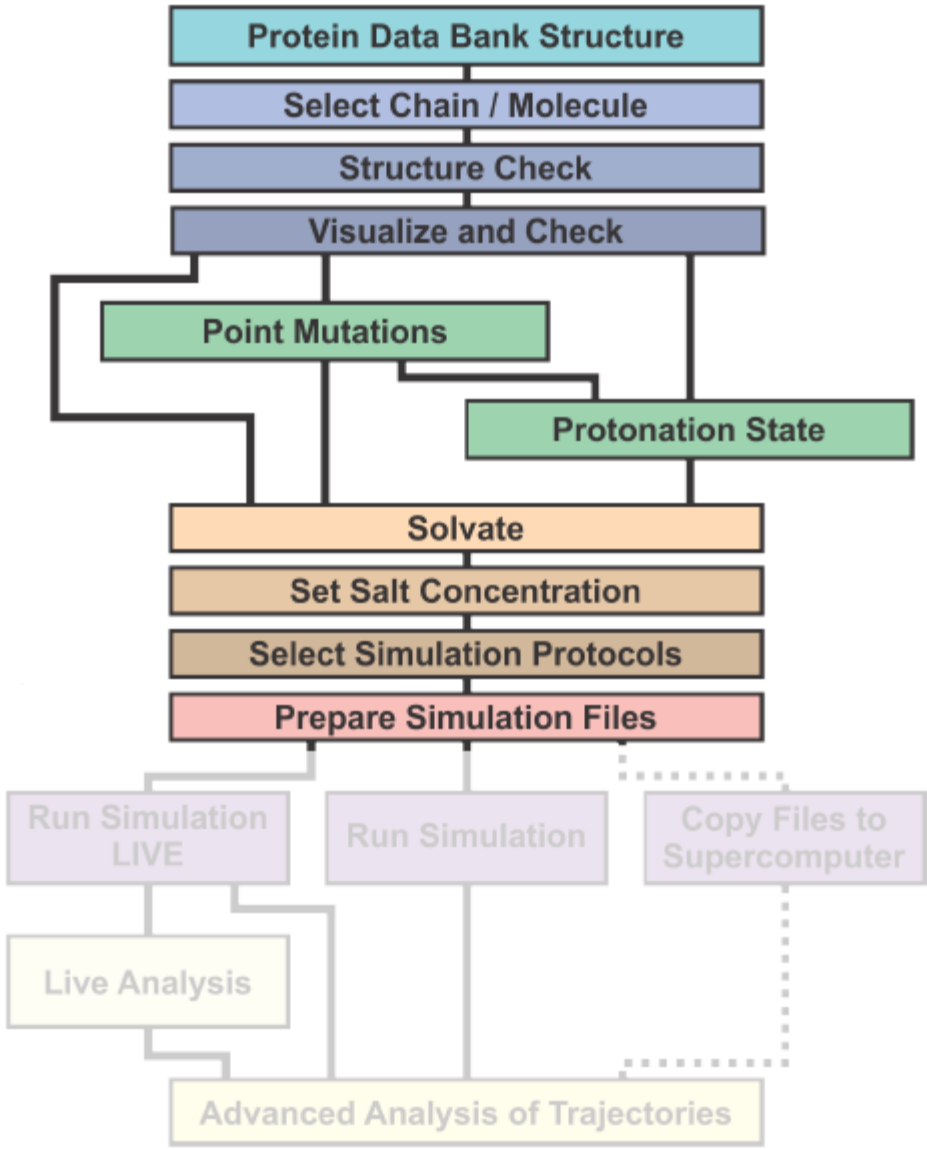
```
set temperature    310
  ;# target temperature used several times below
```

Starting simulation with random velocities

```
# starting from scratch
temperature          $temperature

        ;# initialize velocities randomly
```

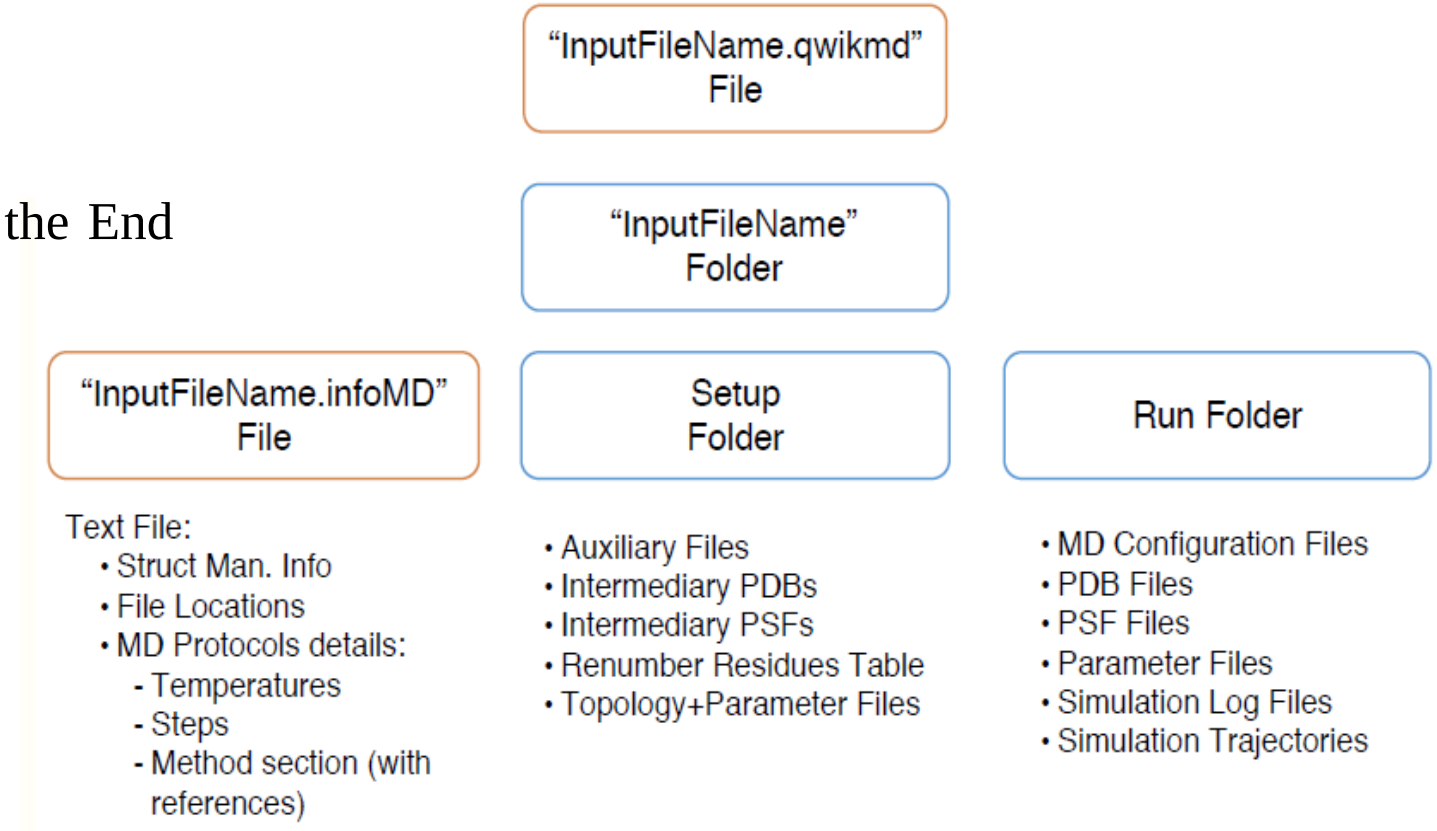
...



QwikMD: Step by Step

- **Reproducibility:**

- All Steps Logged
- Loading Script and Text Log Files
- Reproduce and/or Share the Process to the End Result



QwikMD: Step by Step

Select: Easy Run or Advanced Run
Analysis Tools can also be selected

Browse for a PDB file or type PDB code

In the structure manipulation window the QwikMD user can delete molecules or parts of a protein sequence; perform point mutations; change protonation states; check the structure; insert membrane model (Advanced mode only)

For structures solved by NMR, select the conformational state

Select the chains and type of molecule to be included in the simulation

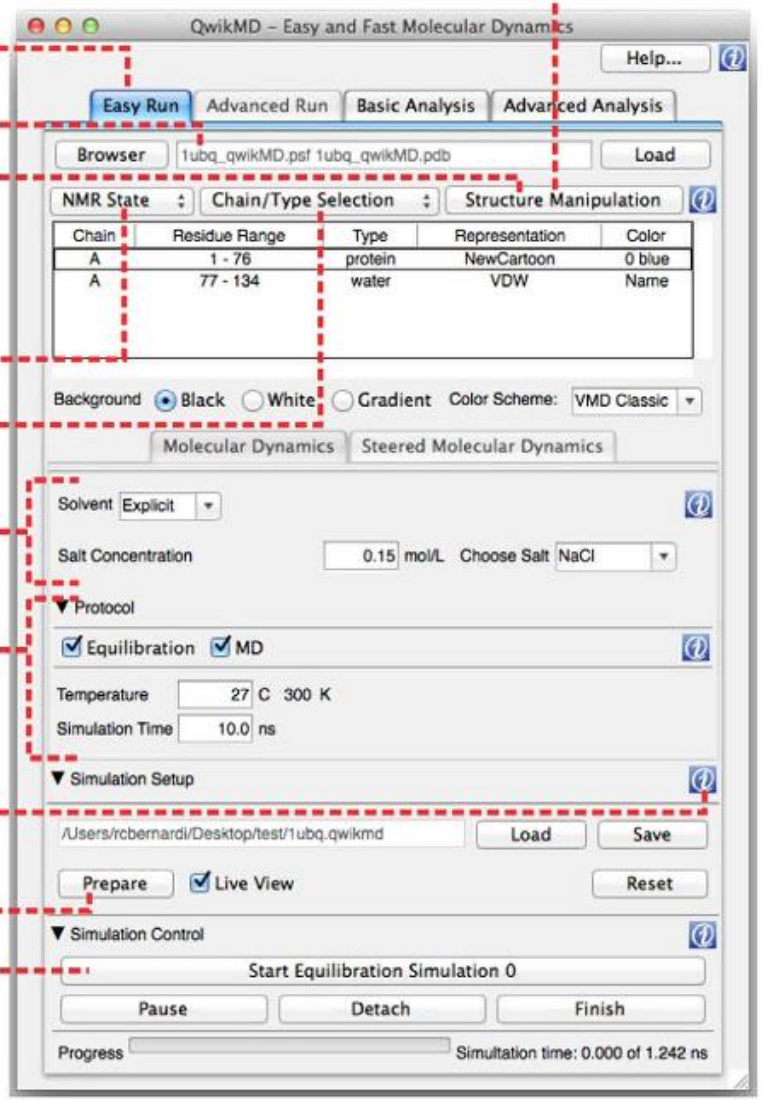
Select the environment: implicit or explicit solvent, and salt concentration

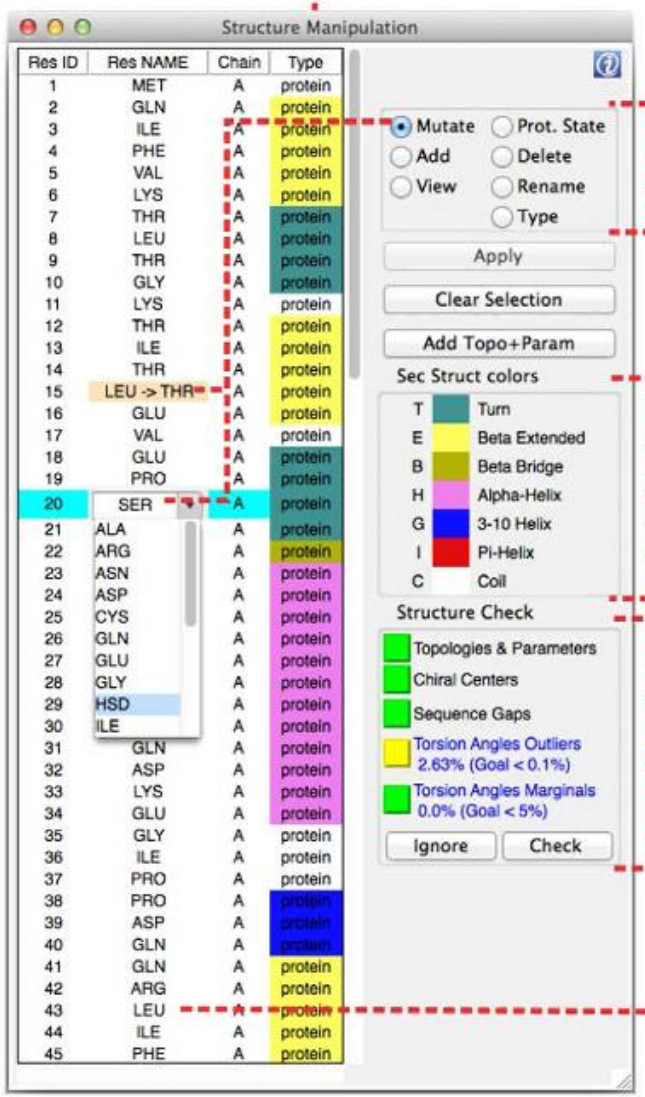
In the Protocol section the user selects temperature and duration of the simulation and also if an equilibration will be performed

"Info Buttons" provide the user with a variety of information, from protocols to a guidance on how to perform simulations and how to check results

When "Prepare" is clicked, QwikMD will invoke several scripts to perform all the operations set before, such as mutations, solvation, ...

Starts the simulation, either in "Live View" mode (if selected) or in "Background"





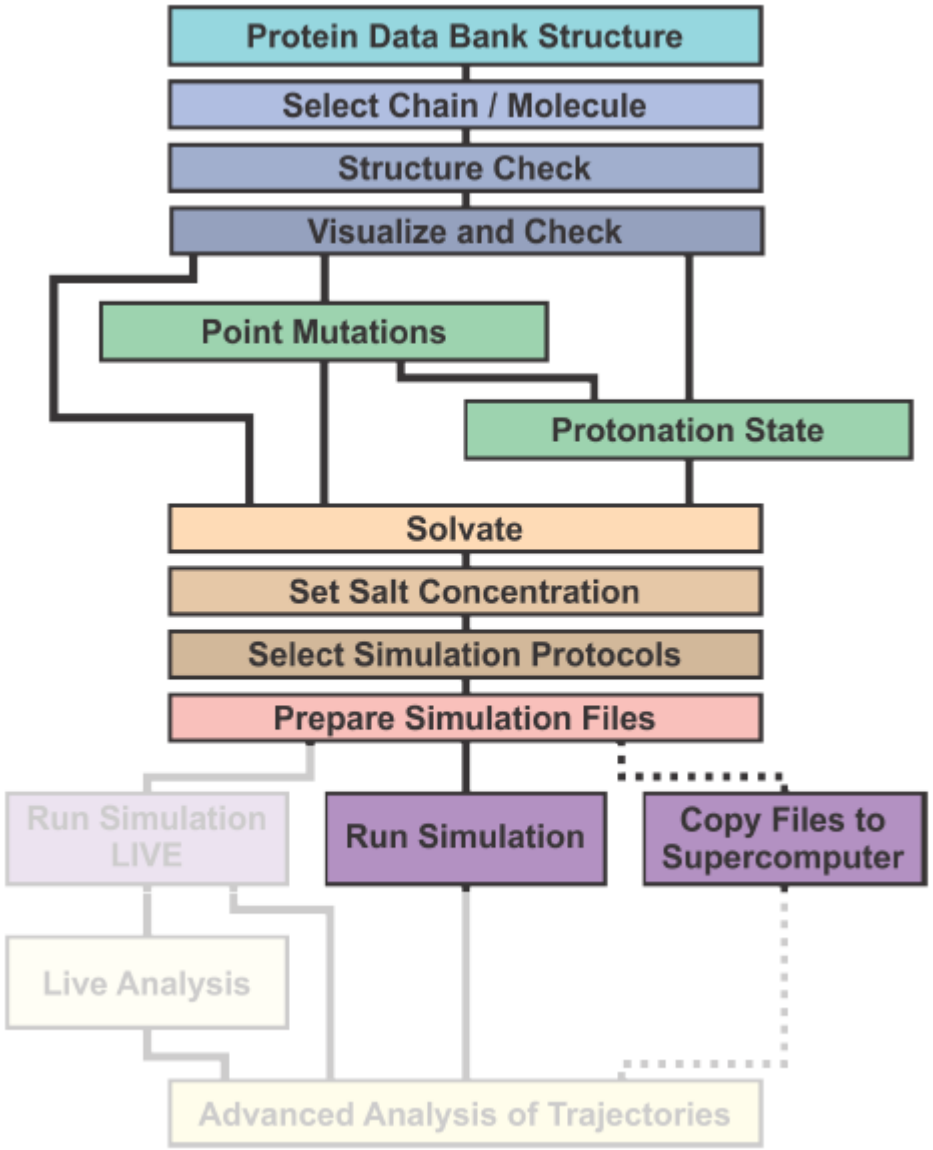
QwikMD user can easily perform point mutations. To do so, select "Mutate" and click on the amino acid from the sequence amino acid table. A list of all possible mutations will allow the user to select the desired mutation.

The list of amino acid in the protein sequence is colored according to the secondary structure.

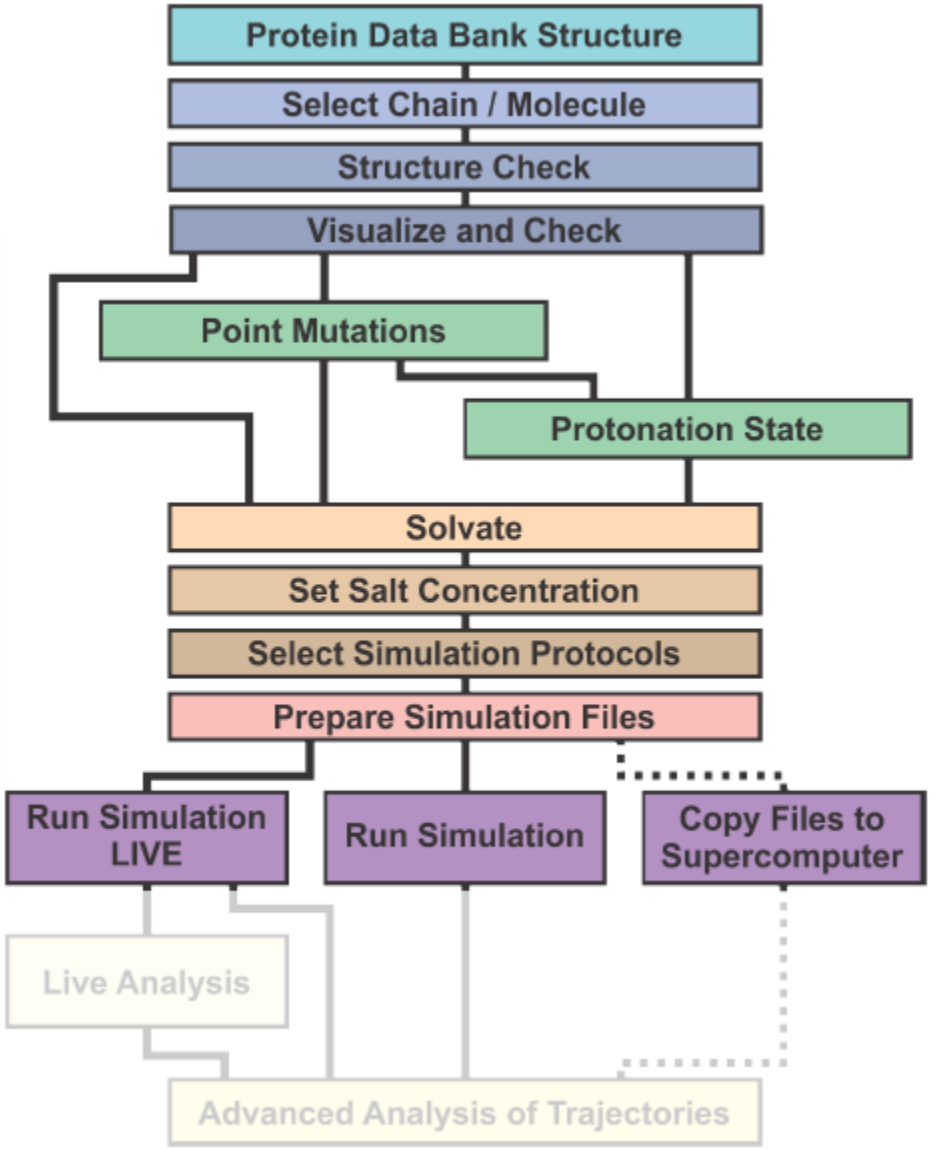
An automated check of the structure is performed when a PDB is loaded by QwikMD. If problems arise they will be marked in the "Structure Check" Tab. The user will be guided on how to fix the problems found.

All molecules of the system are presented in a list an can be separated by *type* or *chain*. The QwikMD user can easily delete parts of structure, change protonation states, perform point mutations, among other actions.

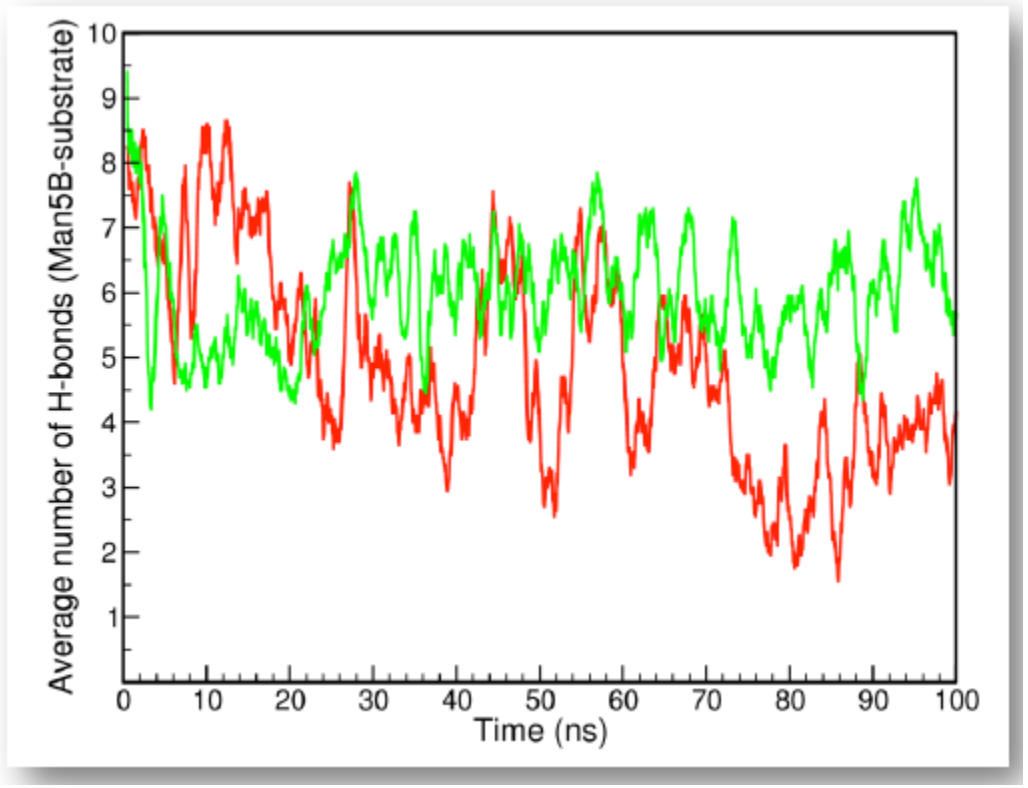
QwikMD: Step by Step

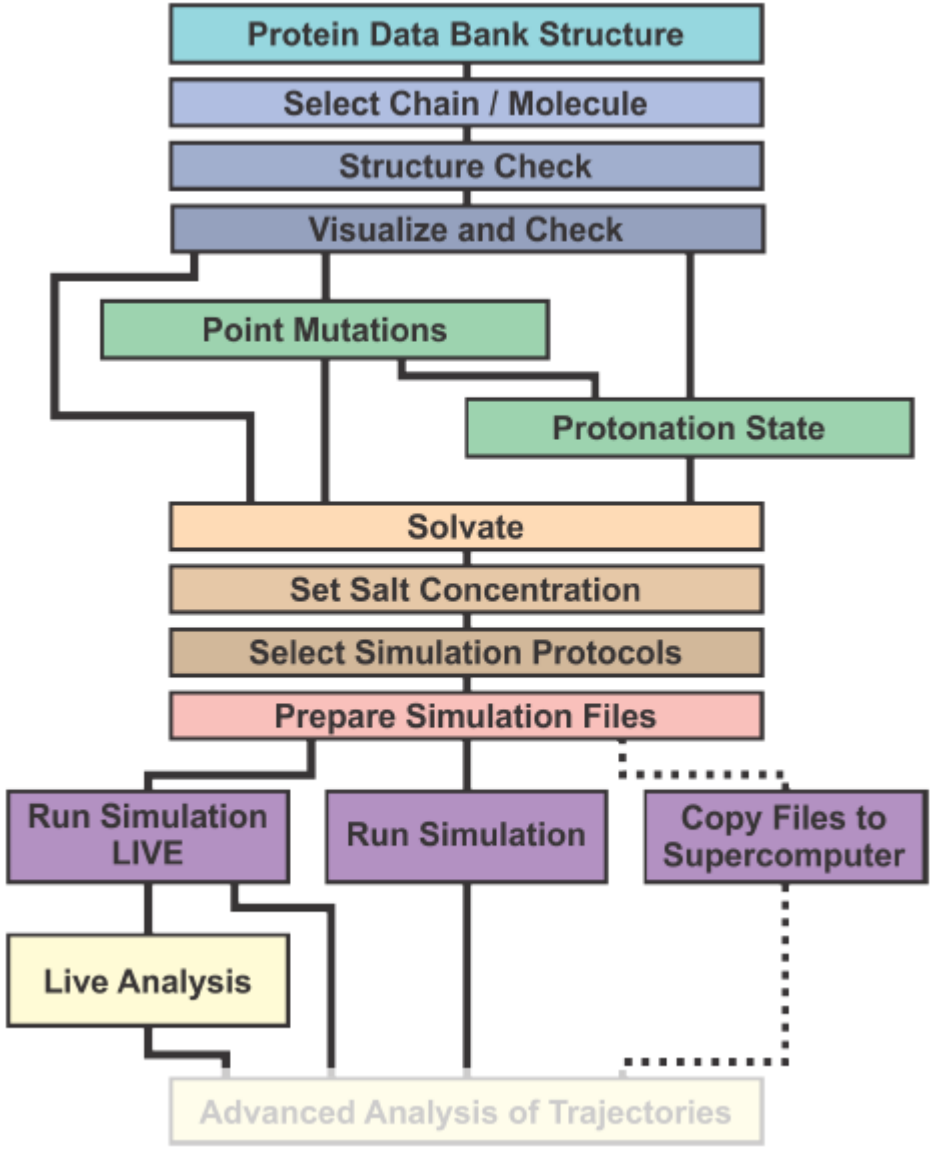


QwikMD: Step by Step



QwikMD: Step by Step





QwikMD: Step by Step