

Running MD Simulations on NAMD: QwikMD

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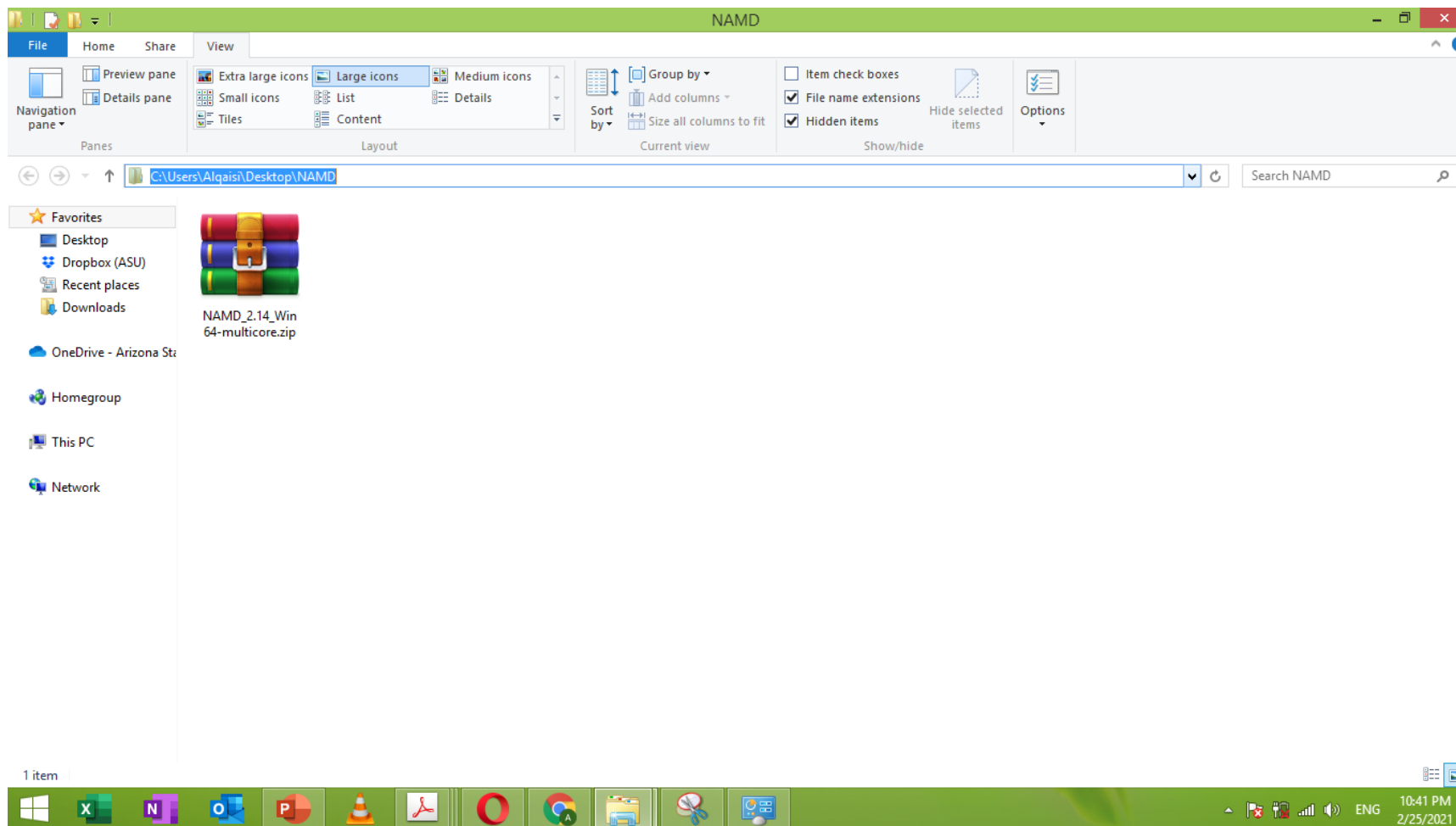
How to install NAMD

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

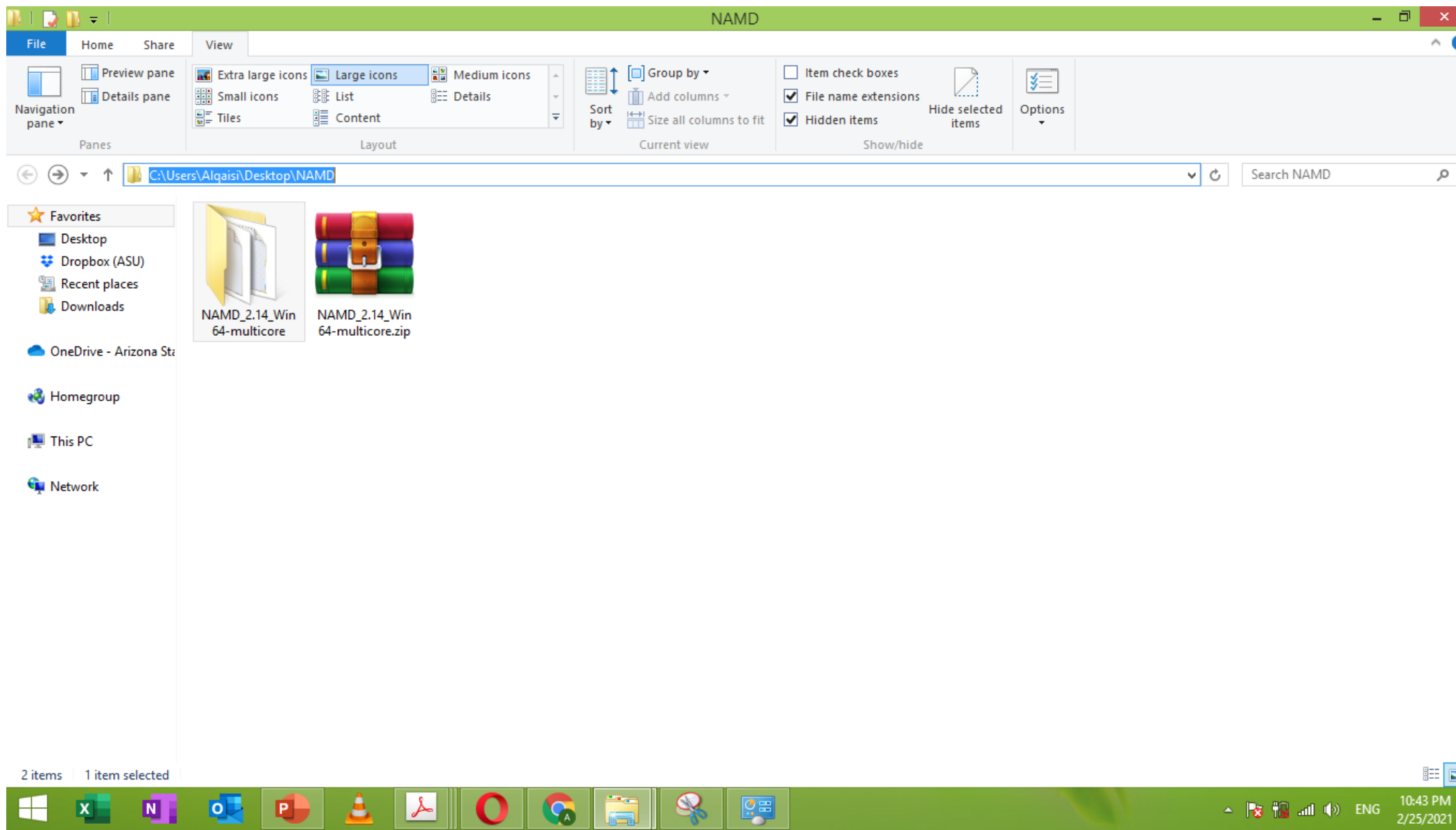
NAMD is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular system

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

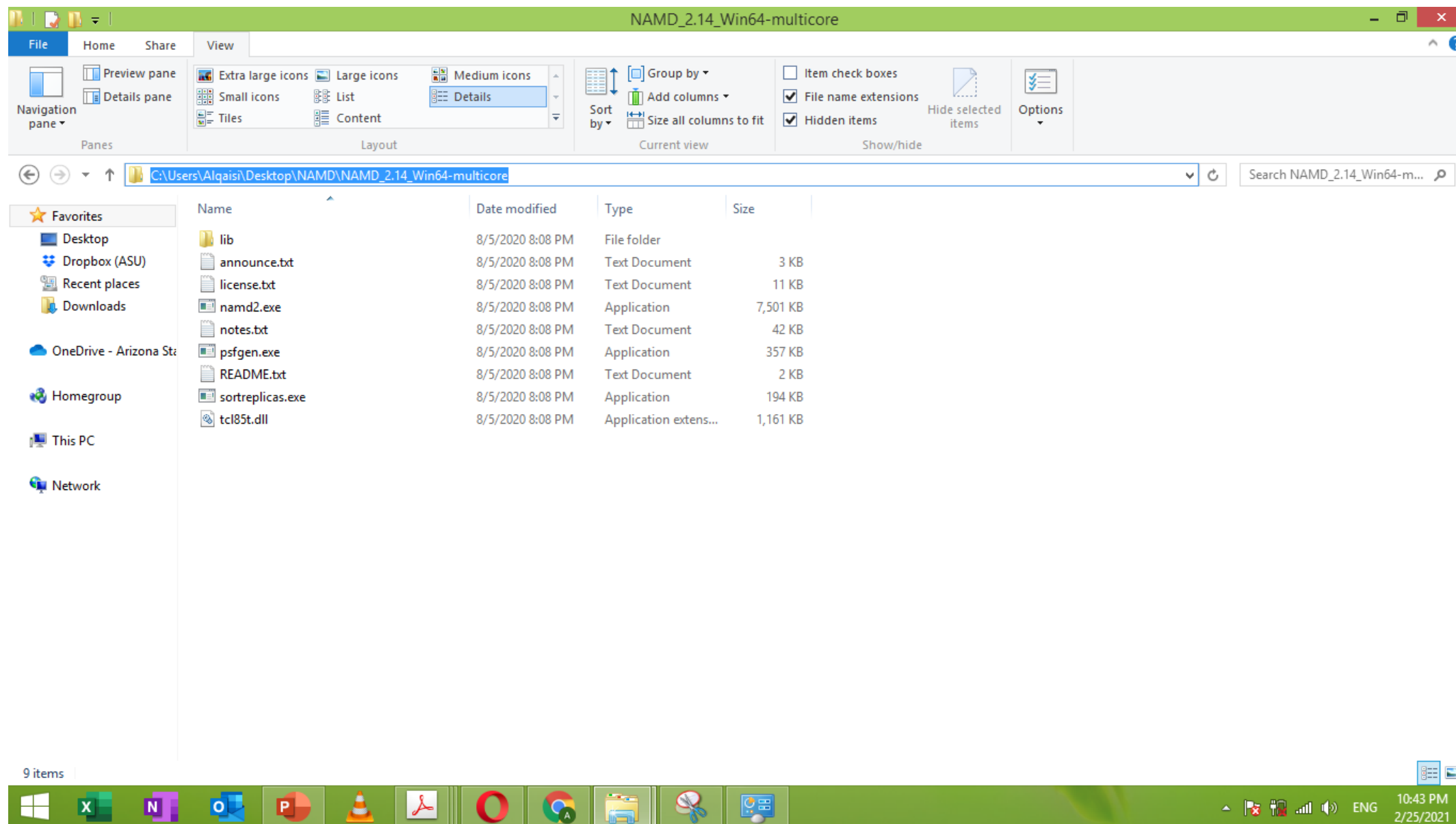
How to install NAMD



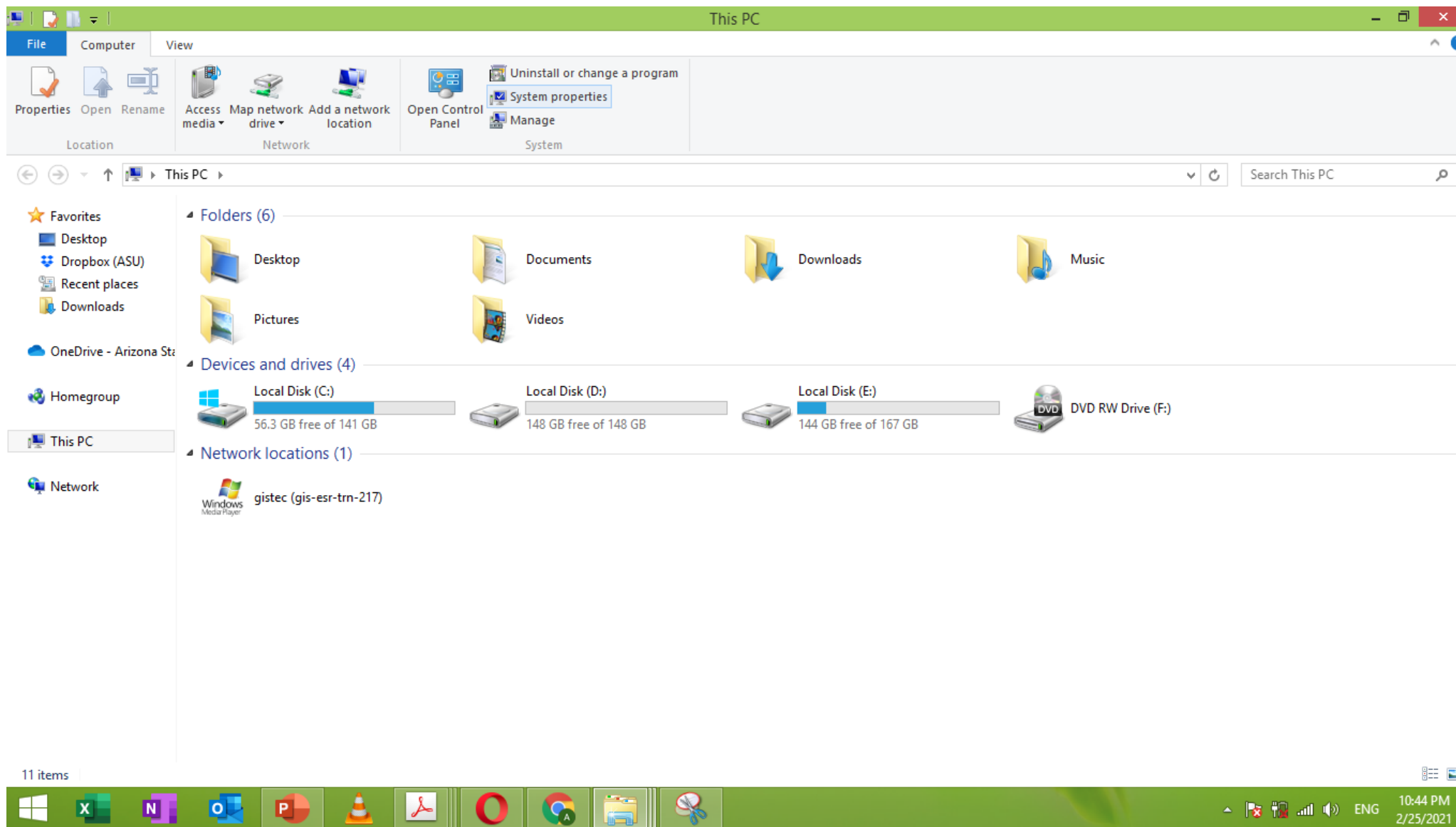
How to install NAMD



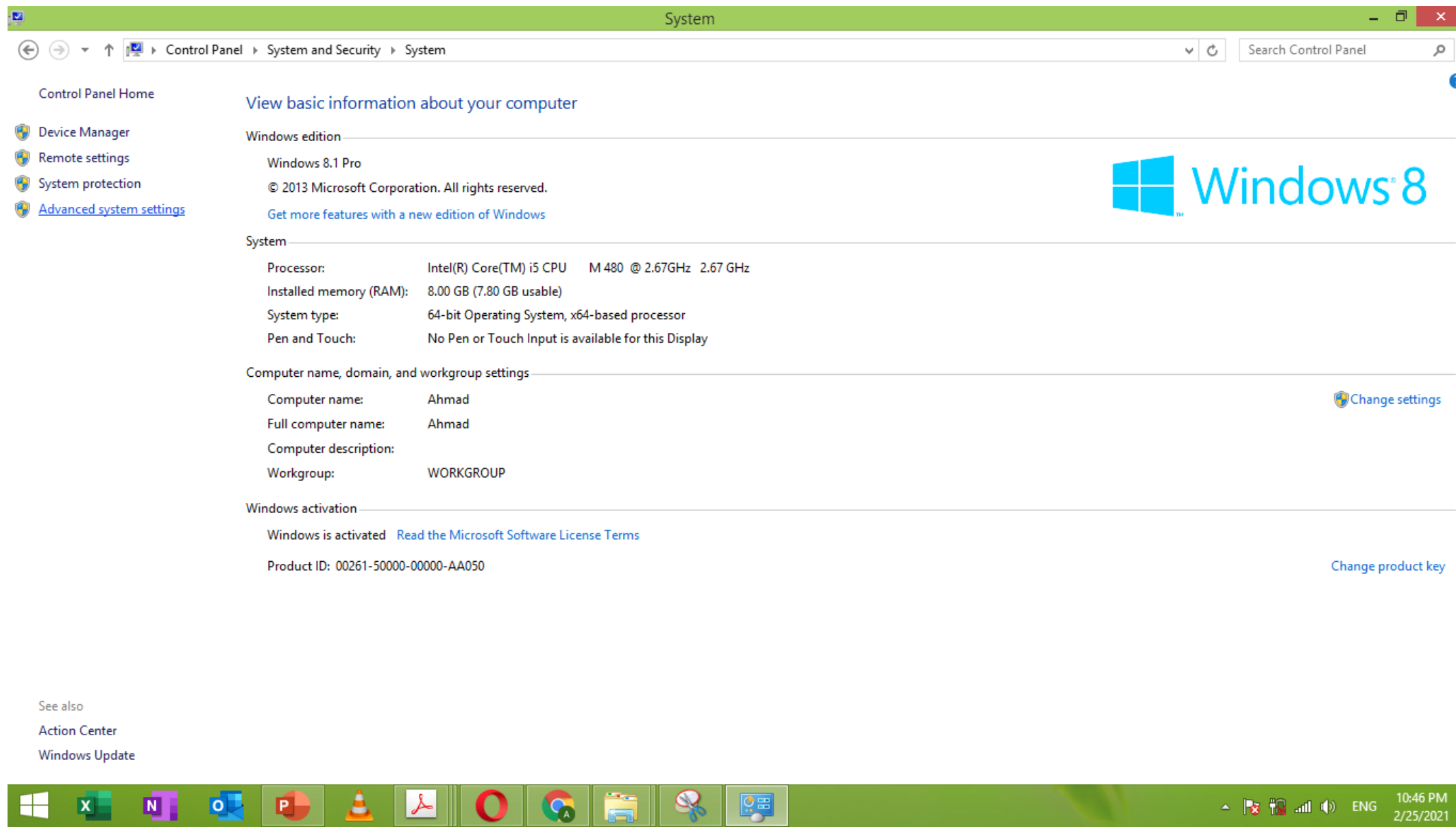
How to install NAMD



How to install NAMD



How to install NAMD



The screenshot shows the Windows 8.1 Pro 'System' settings page. The title bar is green and says 'System'. The breadcrumb path is 'Control Panel > System and Security > System'. The left sidebar has links to 'Control Panel Home', 'Device Manager', 'Remote settings', 'System protection', and 'Advanced system settings'. The main content area is titled 'View basic information about your computer' and includes sections for 'Windows edition', 'System', 'Computer name, domain, and workgroup settings', and 'Windows activation'. The 'System' section lists hardware details like the Intel Core i5 CPU and 8.00 GB RAM. The 'Computer name' section shows the name 'Ahmad' and workgroup 'WORKGROUP'. The 'Windows activation' section shows the product is activated with a Product ID. The taskbar at the bottom contains icons for Windows, Excel, PowerPoint, VLC, Firefox, Chrome, File Explorer, and NAMD. The system tray shows the time as 10:46 PM on 2/25/2021.

System

Control Panel > System and Security > System

Control Panel Home

Device Manager

Remote settings

System protection

[Advanced system settings](#)

View basic information about your computer

Windows edition

Windows 8.1 Pro

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[Get more features with a new edition of Windows](#)

System

Processor: Intel(R) Core(TM) i5 CPU M 480 @ 2.67GHz 2.67 GHz

Installed memory (RAM): 8.00 GB (7.80 GB usable)

System type: 64-bit Operating System, x64-based processor

Pen and Touch: No Pen or Touch Input is available for this Display

Computer name, domain, and workgroup settings

Computer name: Ahmad

Full computer name: Ahmad

Computer description:

Workgroup: WORKGROUP

Windows activation

Windows is activated [Read the Microsoft Software License Terms](#)

Product ID: 00261-50000-00000-AA050

[Change settings](#)

[Change product key](#)

See also

Action Center

Windows Update

Windows

X

N

O

P

VLC

Firefox

Chrome

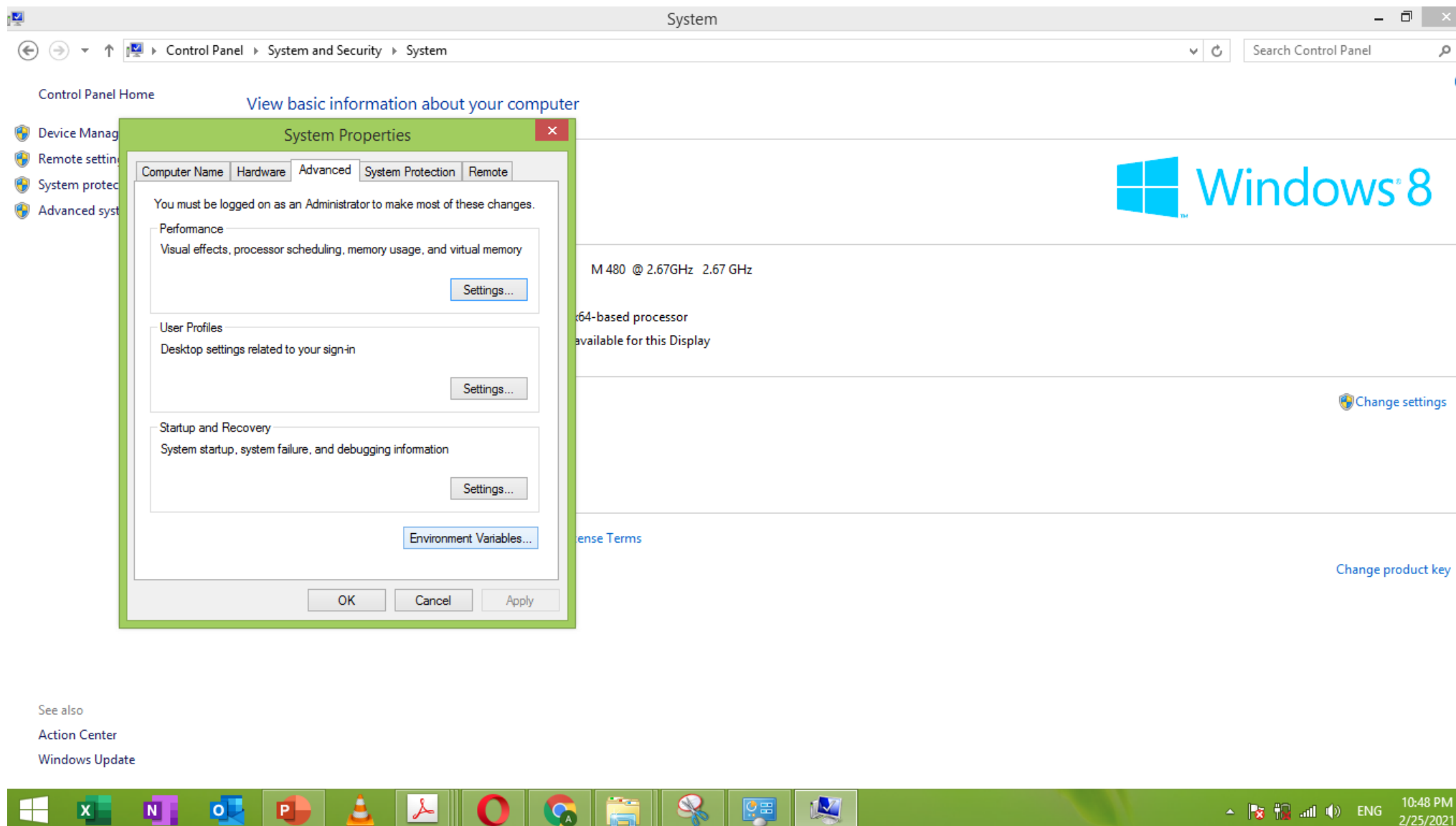
File Explorer

Scissors

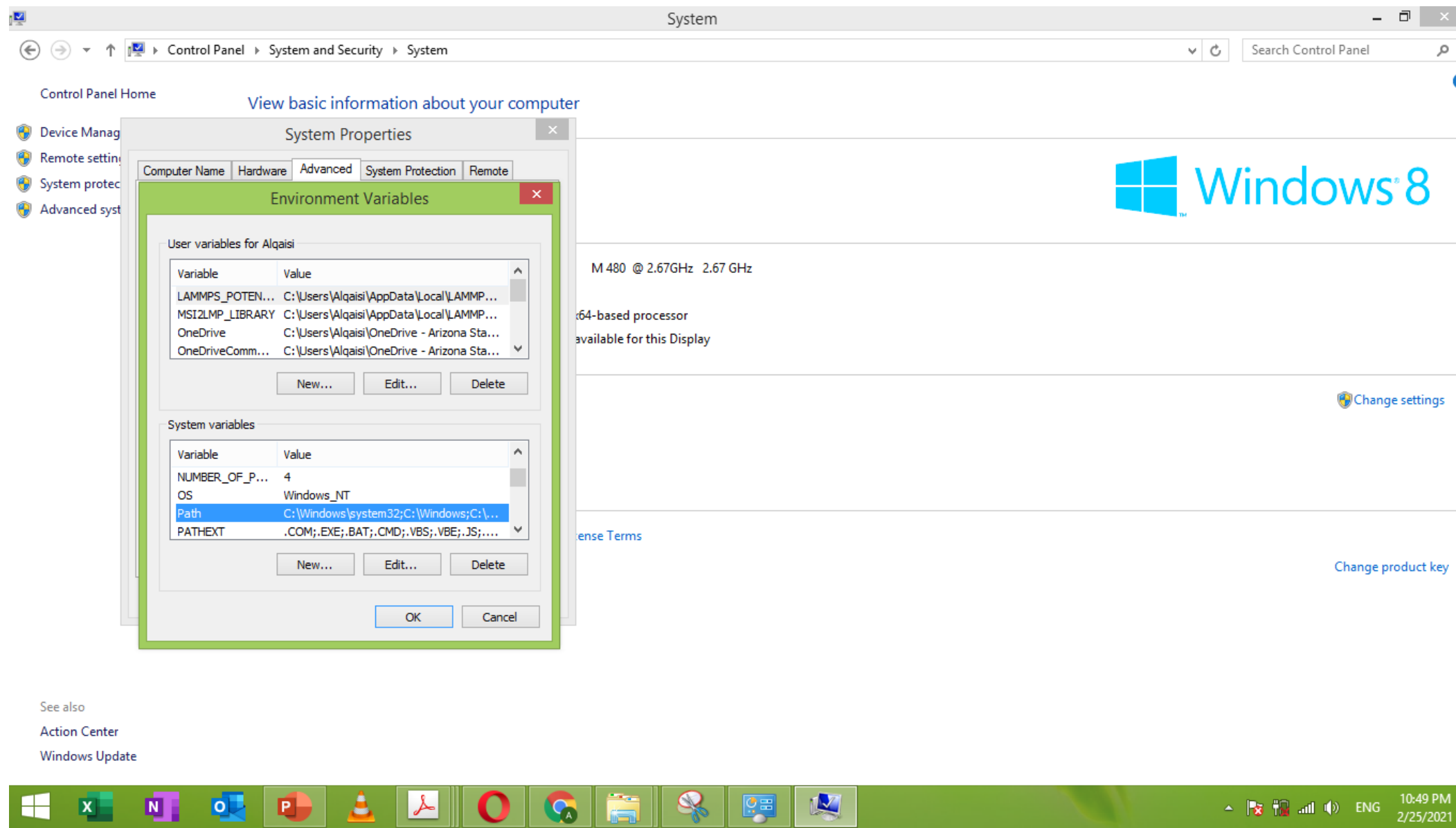
NAMD

10:46 PM 2/25/2021

How to install NAMD



How to install NAMD



The screenshot shows the Windows 8 System Properties dialog box, specifically the Environment Variables tab. The dialog box is open over the Windows 8 System page. The Environment Variables tab displays two sections: User variables for Alqaisi and System variables. The User variables section lists variables such as LAMMPS_POTEN..., MSI2LMP_LIBRARY, OneDrive, and OneDriveComm... with their respective values. The System variables section lists variables such as NUMBER_OF_P..., OS, Path, and PATHEXT. The Path variable is highlighted, showing its value as C:\Windows\system32;C:\Windows;C:\... The dialog box has OK and Cancel buttons at the bottom.

System

Control Panel > System and Security > System

View basic information about your computer

Device Manager
Remote settings
System protection
Advanced system settings

System Properties

Computer Name Hardware Advanced System Protection Remote

Environment Variables

User variables for Alqaisi

Variable	Value
LAMMPS_POTEN...	C:\Users\Alqaisi\AppData\Local\LAMMP...
MSI2LMP_LIBRARY	C:\Users\Alqaisi\AppData\Local\LAMMP...
OneDrive	C:\Users\Alqaisi\OneDrive - Arizona Sta...
OneDriveComm...	C:\Users\Alqaisi\OneDrive - Arizona Sta...

New... Edit... Delete

System variables

Variable	Value
NUMBER_OF_P...	4
OS	Windows_NT
Path	C:\Windows\system32;C:\Windows;C:\...
PATHEXT	.COM;.EXE;.BAT;.CMD;.VBS;.VBE;.JS;....

New... Edit... Delete

OK Cancel

Windows 8

M 480 @ 2.67GHz 2.67 GHz

64-based processor

available for this Display

Change settings

License Terms

Change product key

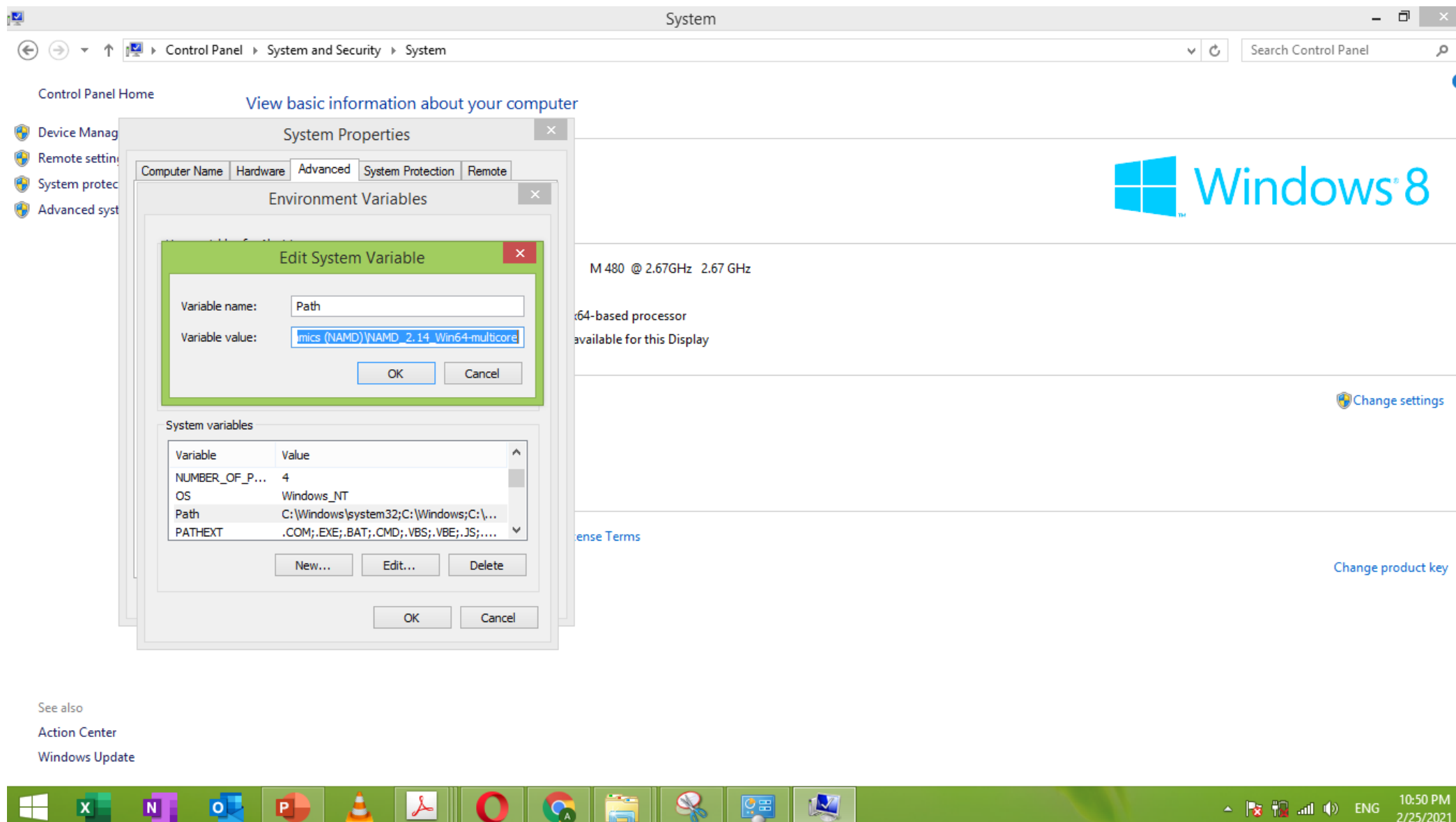
See also

Action Center

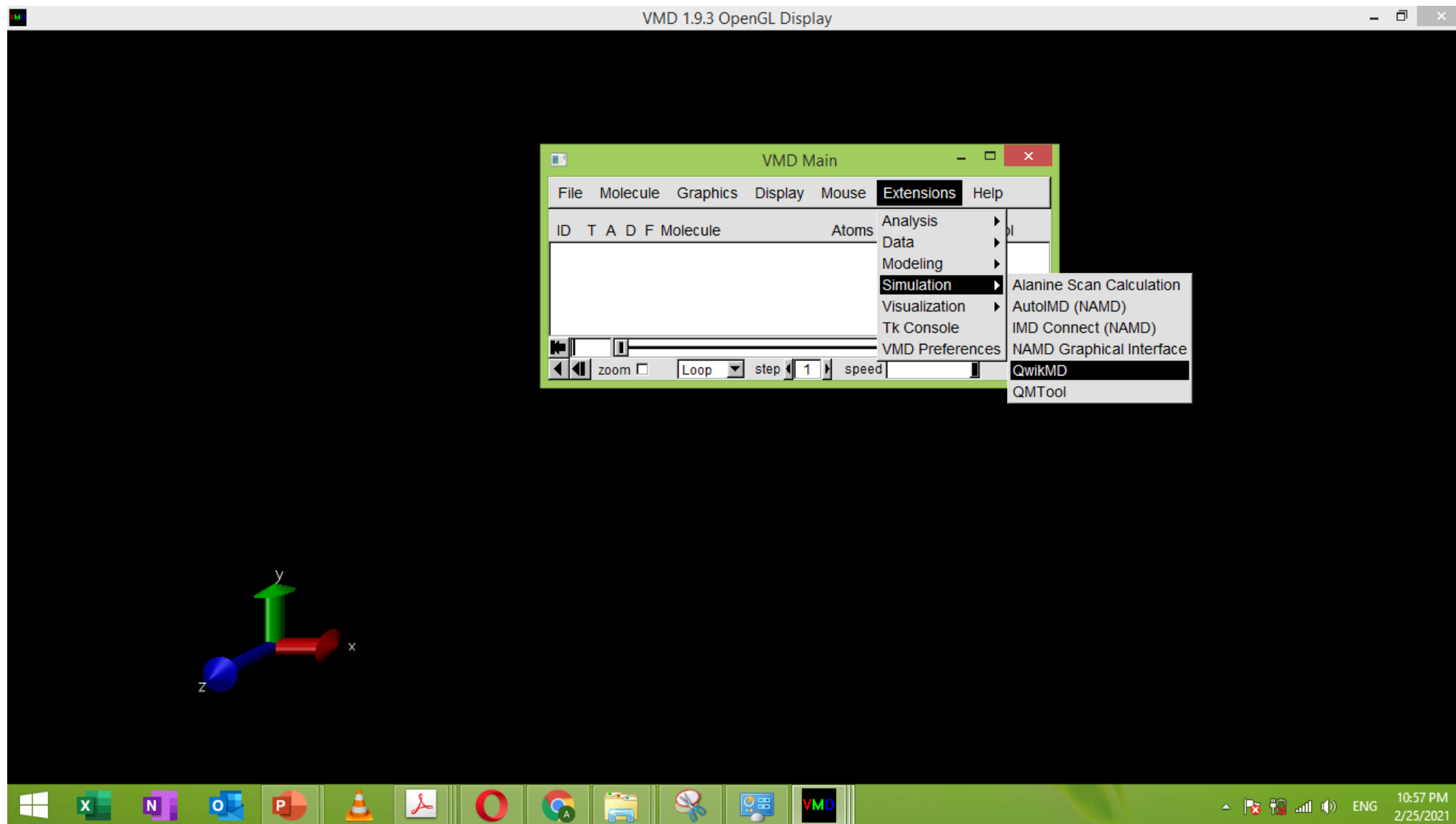
Windows Update

Taskbar icons: Windows, Excel, PowerPoint, Outlook, Word, VLC, Adobe Reader, Firefox, Chrome, File Explorer, Task Manager, System, Network, Volume, Power, ENG, 10:49 PM, 2/25/2021

How to install NAMD



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"

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.

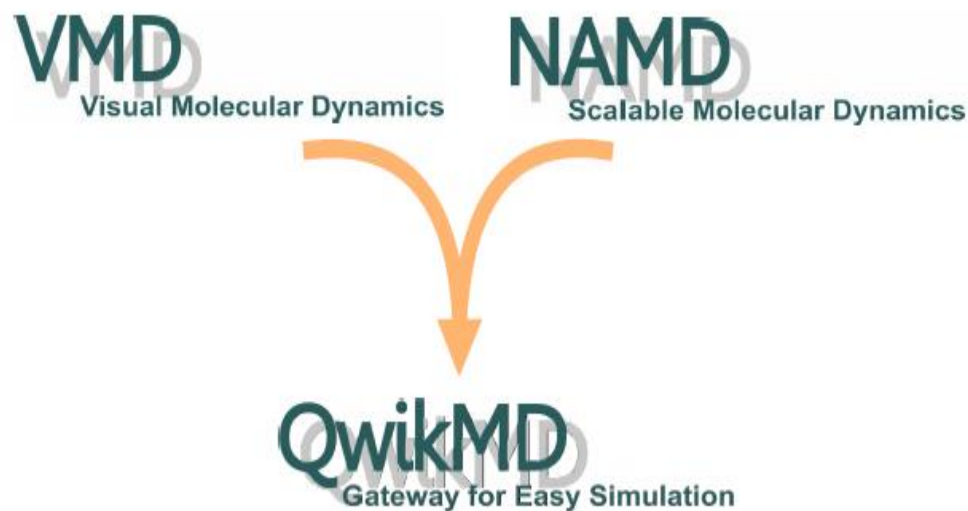
The list of amino acid in the protein sequence is colored according to the secondary structure.

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 and 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.

To assist experimentalists and any novice to MD to overcome the initial learning curve barrier of MD simulation software, we developed QwikMD, a user interface that connects the widely employed and user-friendly molecular graphics program VMD to the widely adopted MD program NAMD.

Employing QwikMD, a user is able to prepare an MD simulation in just a few minutes, allowing studies of point mutations, partial deletions and even atomic force microscopy experiments.

By enabling easy control of every step, QwikMD meets even the needs of experts in the field, increasing the efficiency and quality of their work.

QwikMD assists a new user in performing MD simulations, while it also serves as a learning tool. Many "info buttons" provide the theoretical background underlying the MD procedures carried out in modern MD simulations.

QwikMD Features

VMD 1.9.3 - Spring 2016

- Easy Setup of MD Simulations
- Point Mutations
- Changes in Protonation
- Protocols for MD & SMD
- Live View Simulations
- Integrated Basic Analysis
- Info Buttons to Guide Novices

VMD - Fall 2016

- Advanced Protocols
- Membrane Environment
- Advanced Analysis
- Available on Amazon Cloud
- Full log Capabilities
- Easy Reproducibility

Theoretical and Computational Biophysics Group
Beckman Institute for Advanced Science and Technology
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Urbana, IL 61801

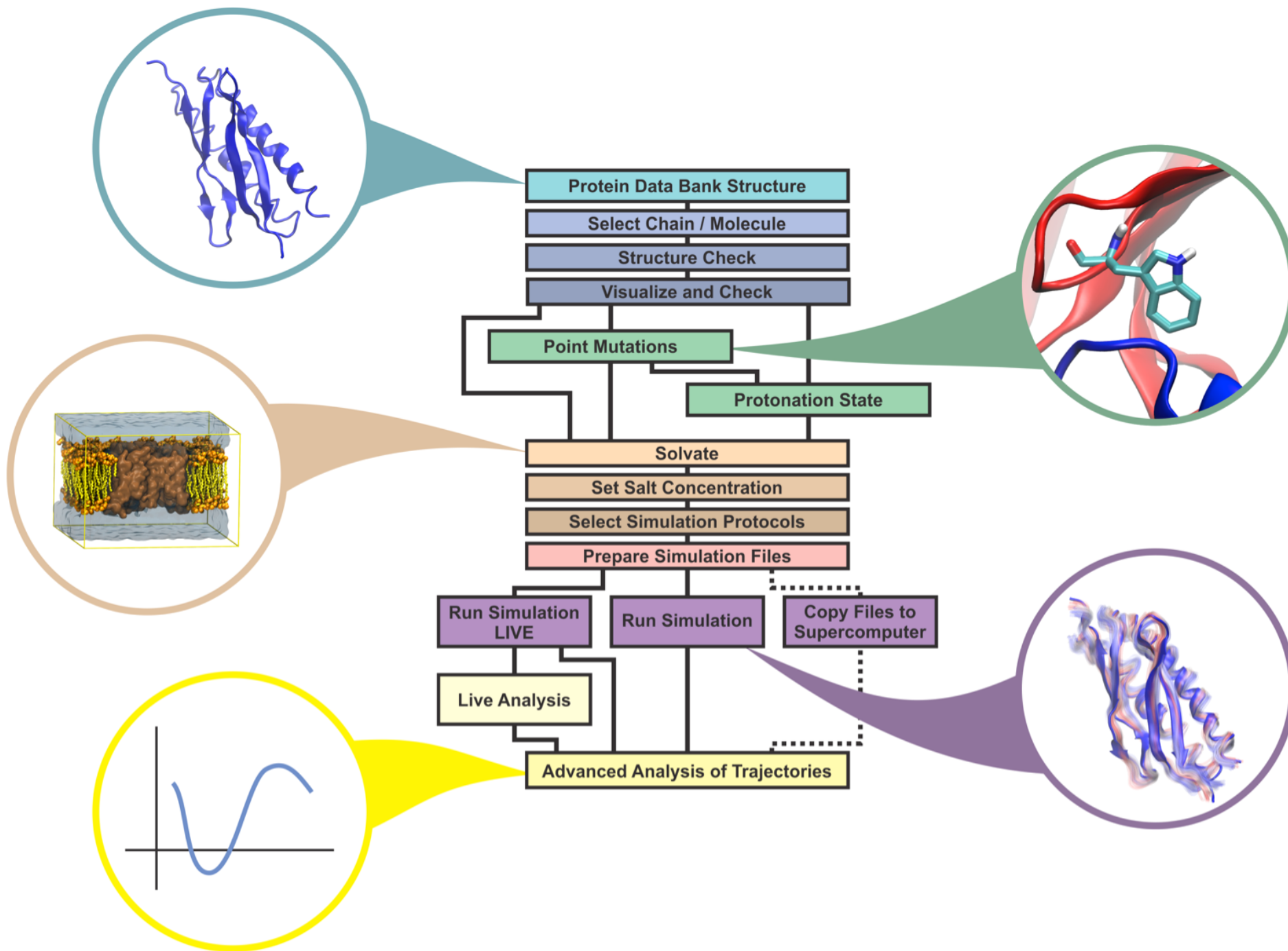
QwikMD

Gateway to Easy Simulation

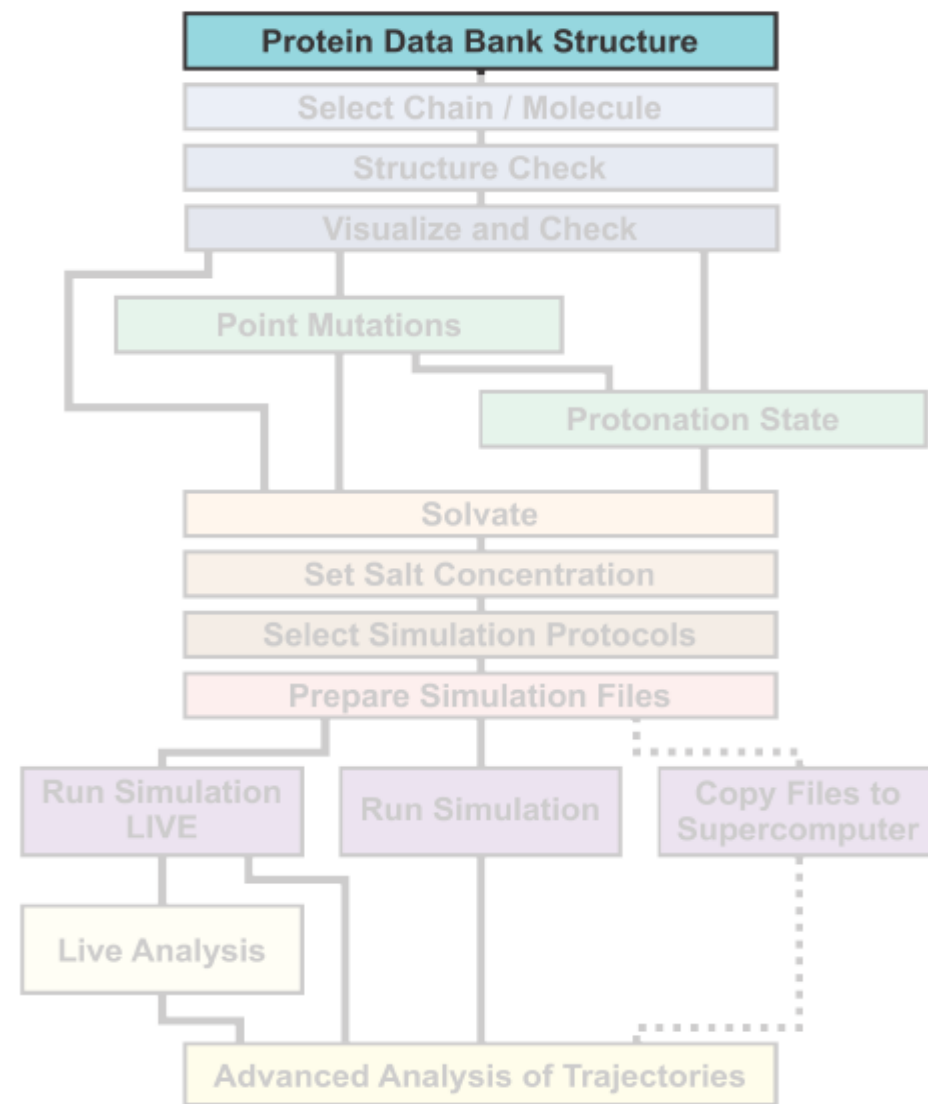
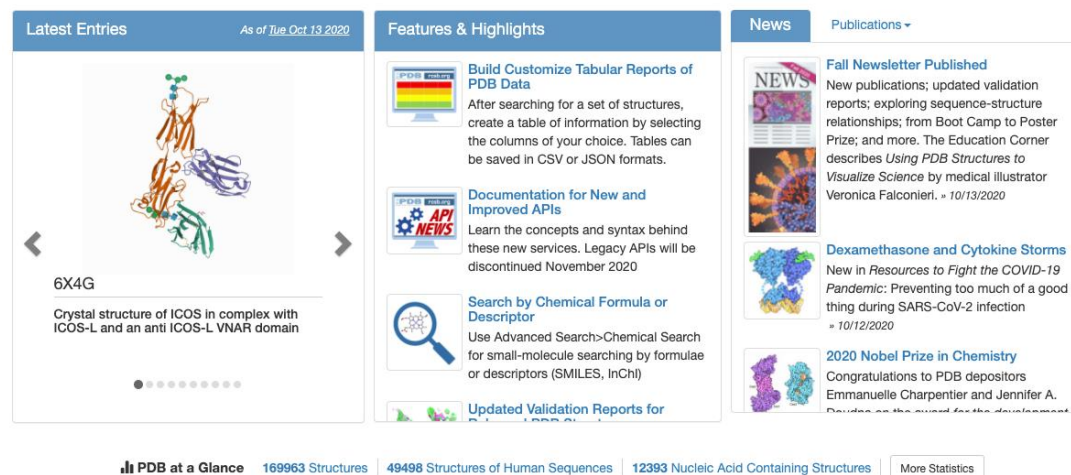
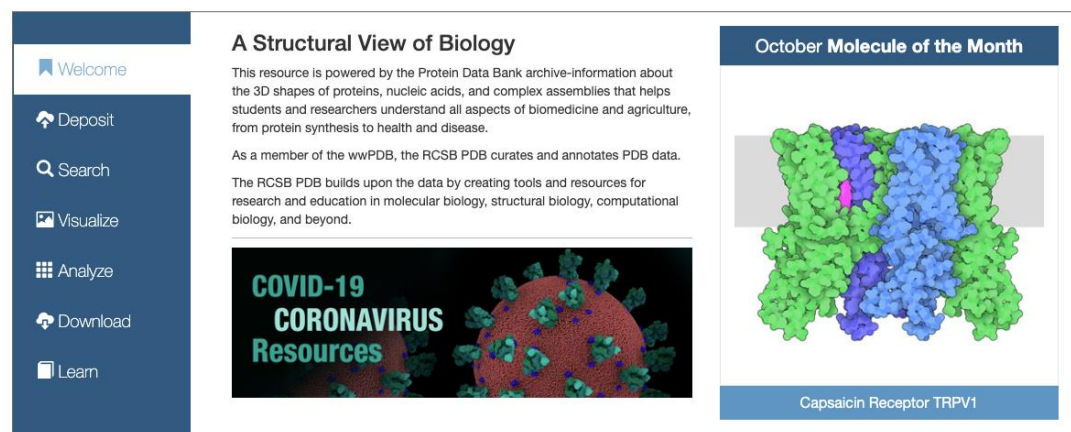
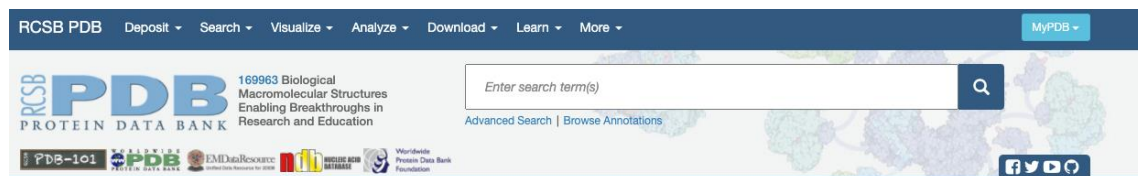
www.ks.uiuc.edu/Research/qwikmd

QwikMD is freely available in VMD 1.9.3 and later

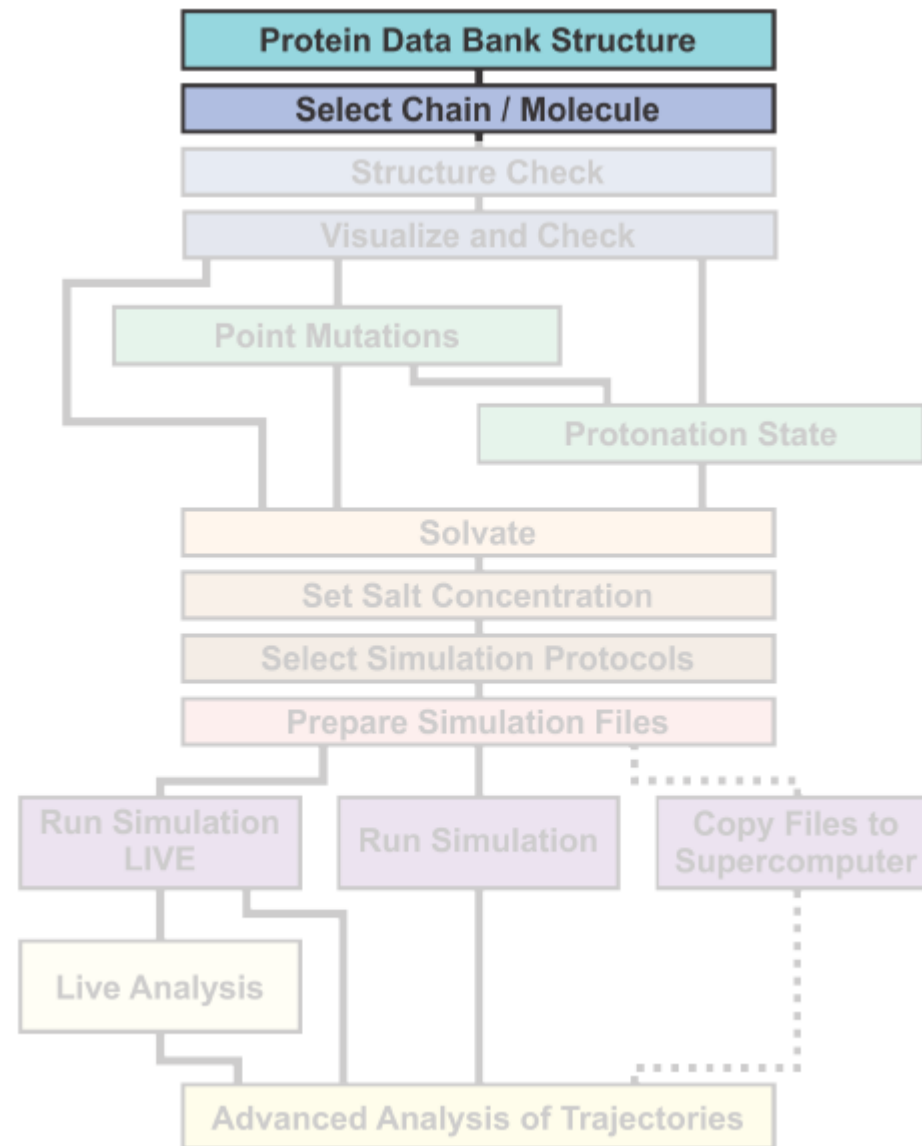
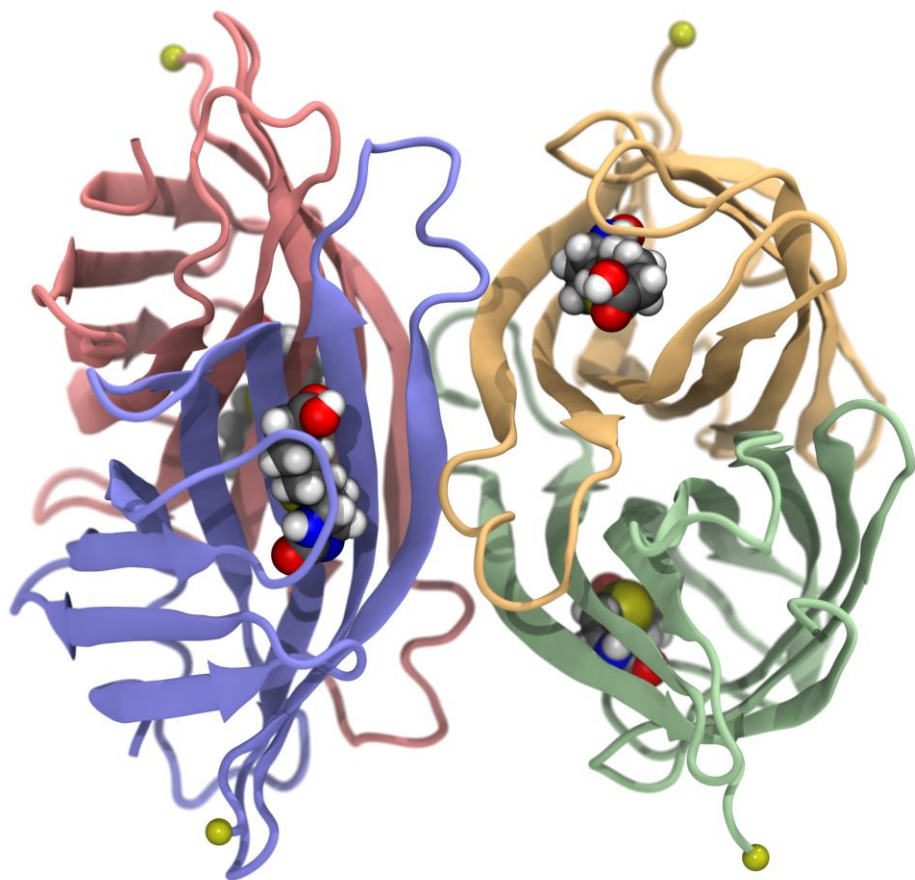
ILLINOIS
UNIVERSITY AT URBANA-CHAMPAIGN



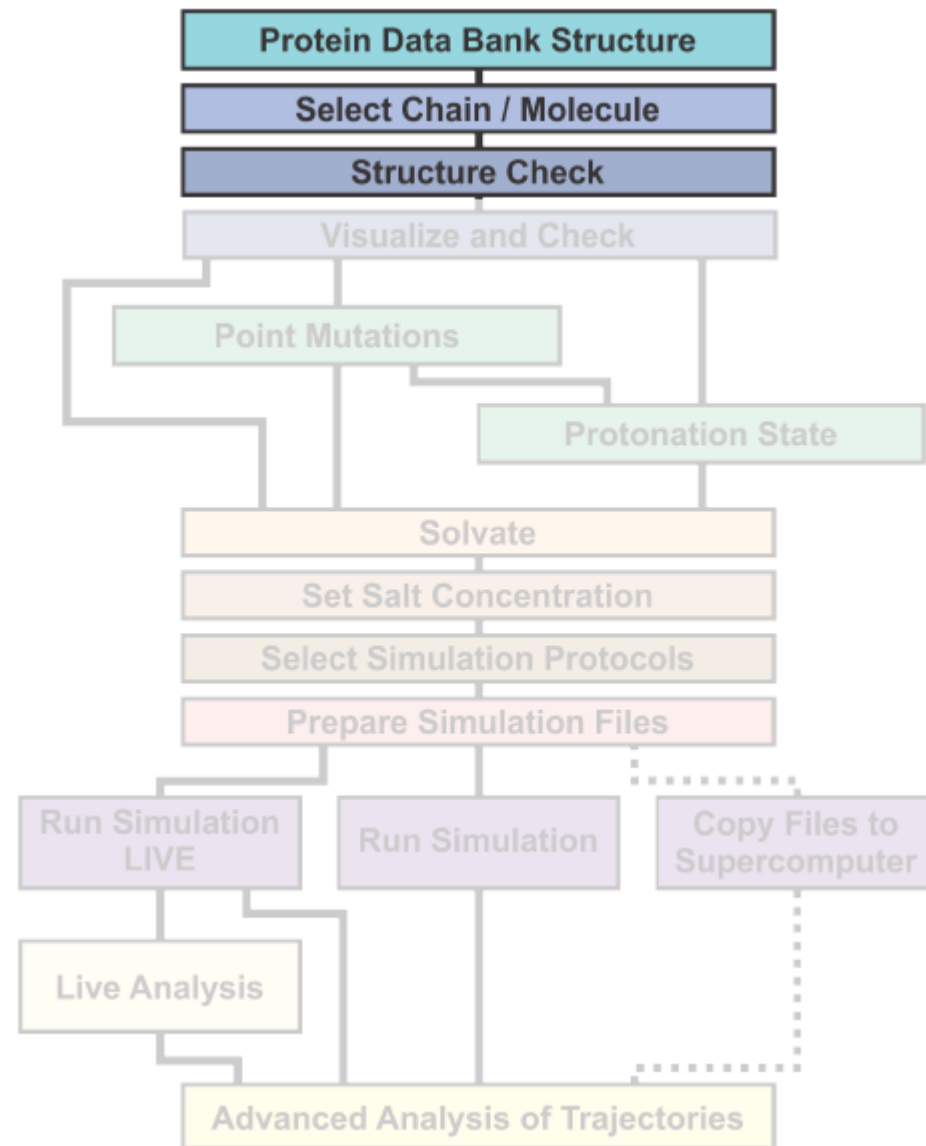
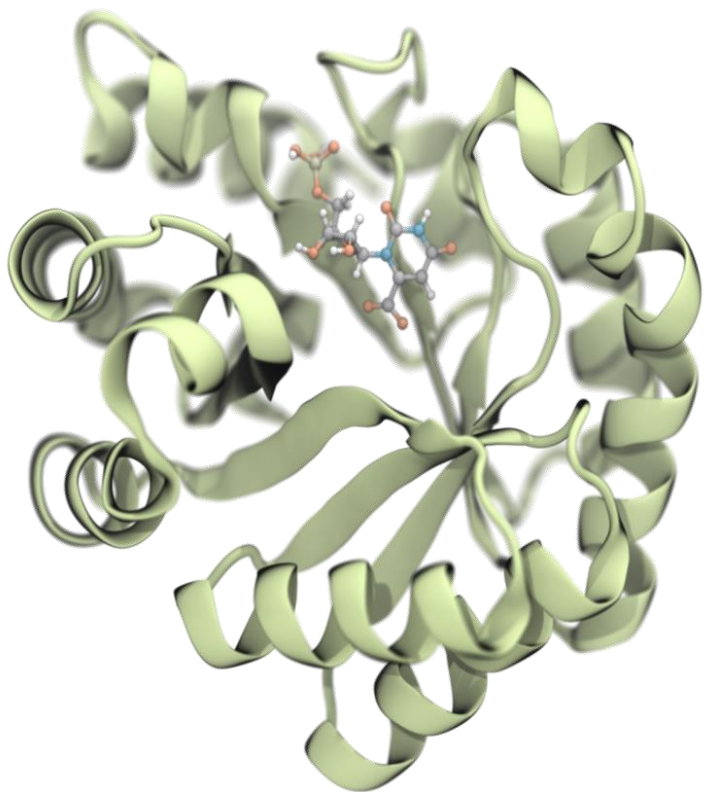
QwikMD: Step by Step



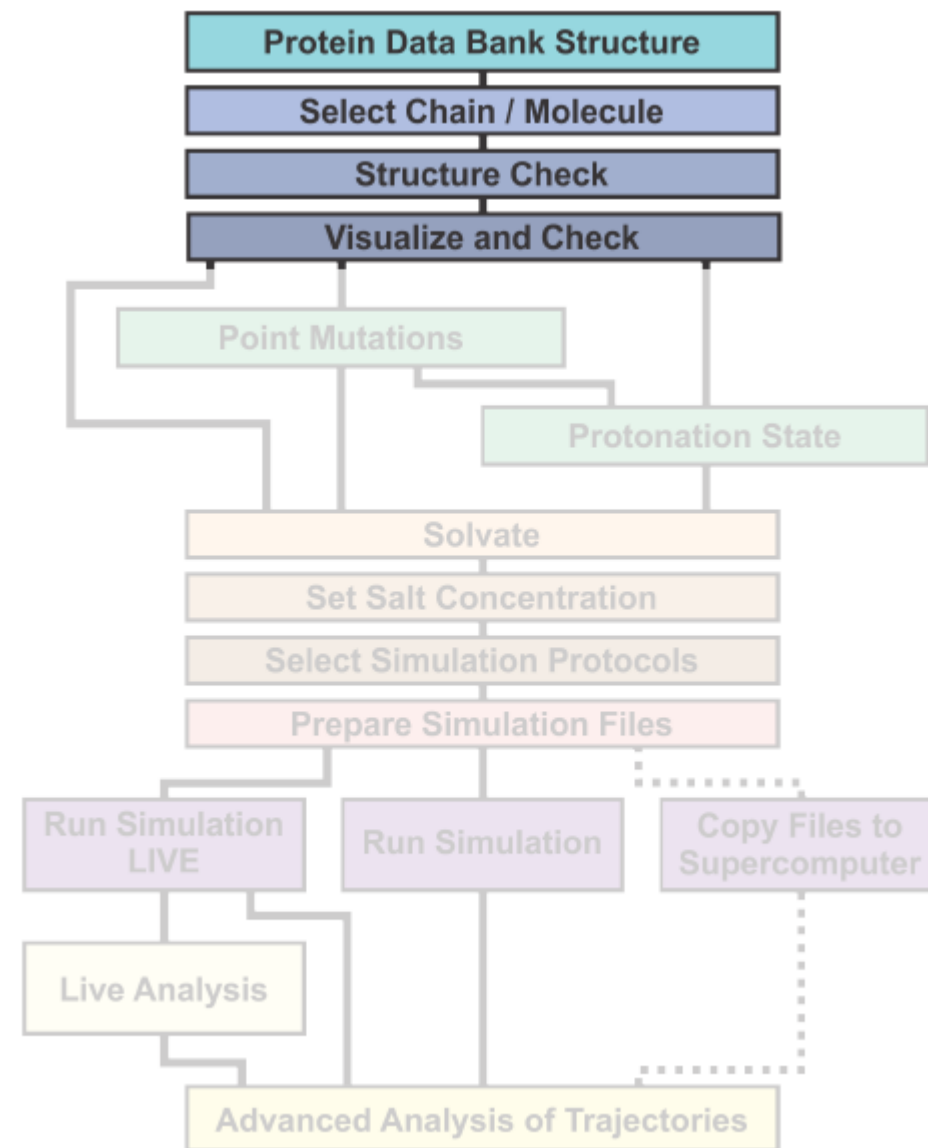
QwikMD: Step by Step



QwikMD: Step by Step



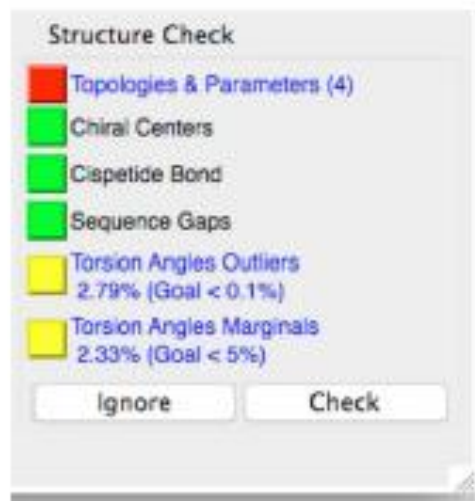
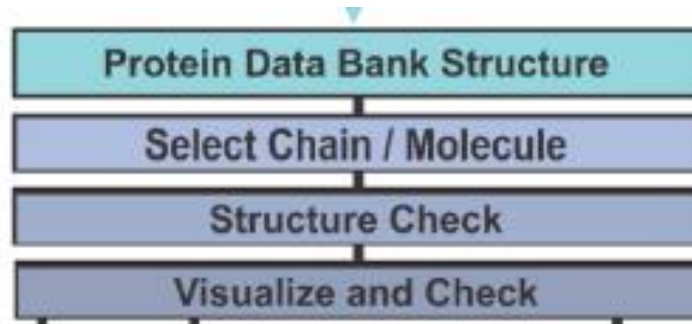
QwikMD: Step by Step



QwikMD: Step by Step

■ Structure Check:

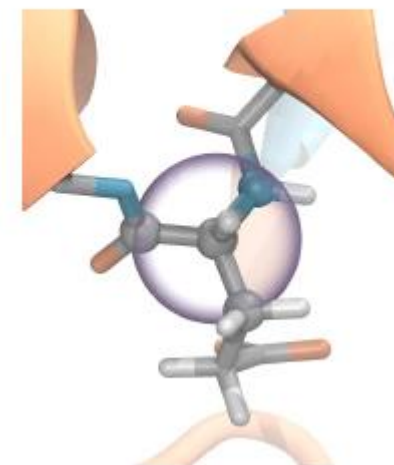
- Missing topologies
- Sequence Gaps
- Residues Alternative Insertions
- Chiral Centers
- Cis-peptide Bonds
- Backbone Torsion Angles
- Marginals
- Outliers



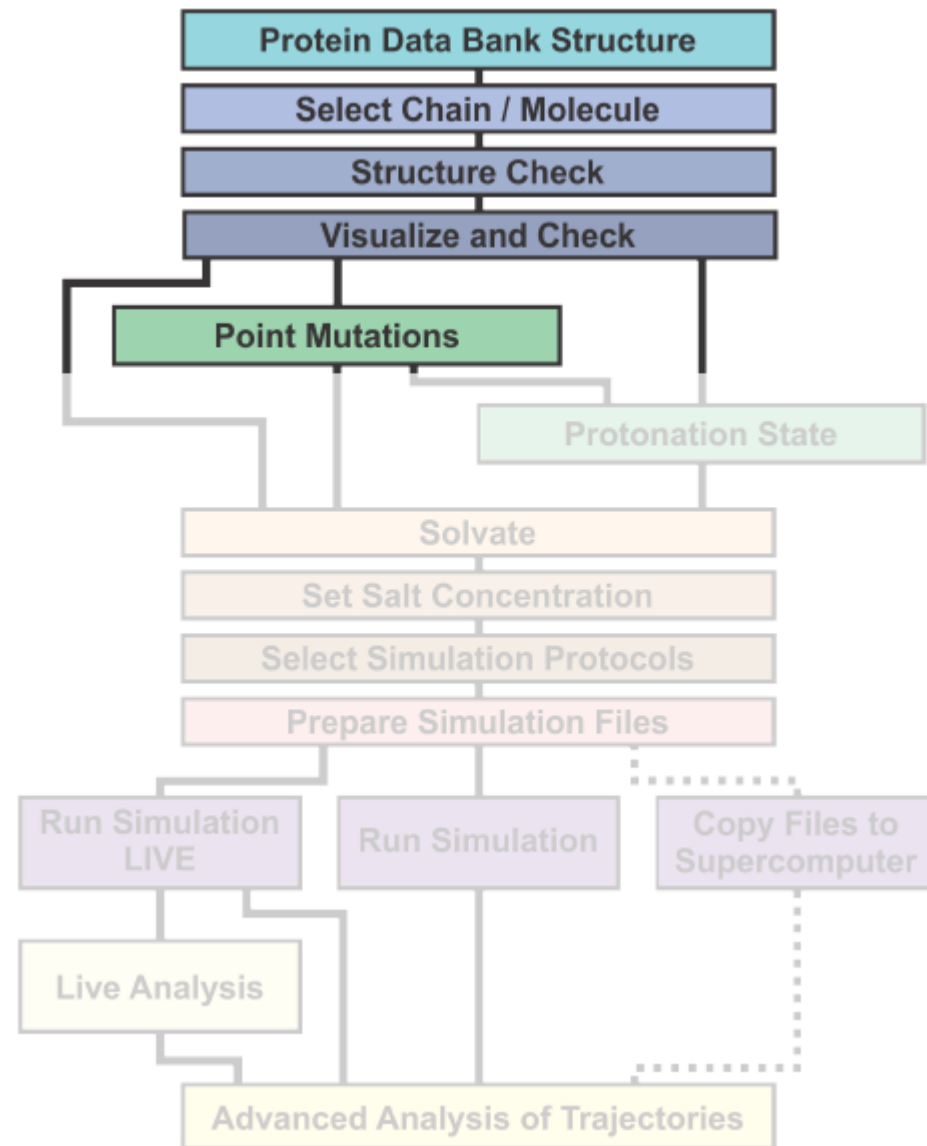
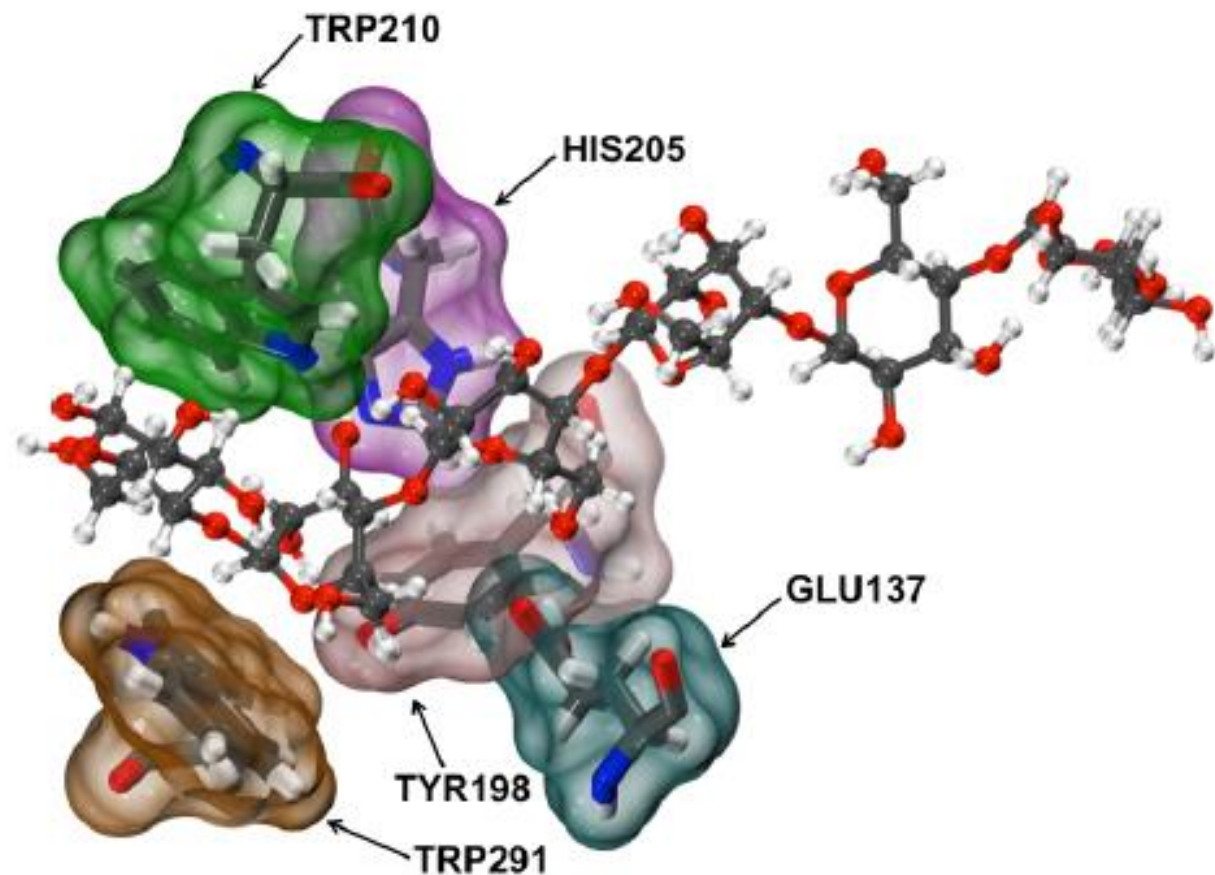
Cis-peptide



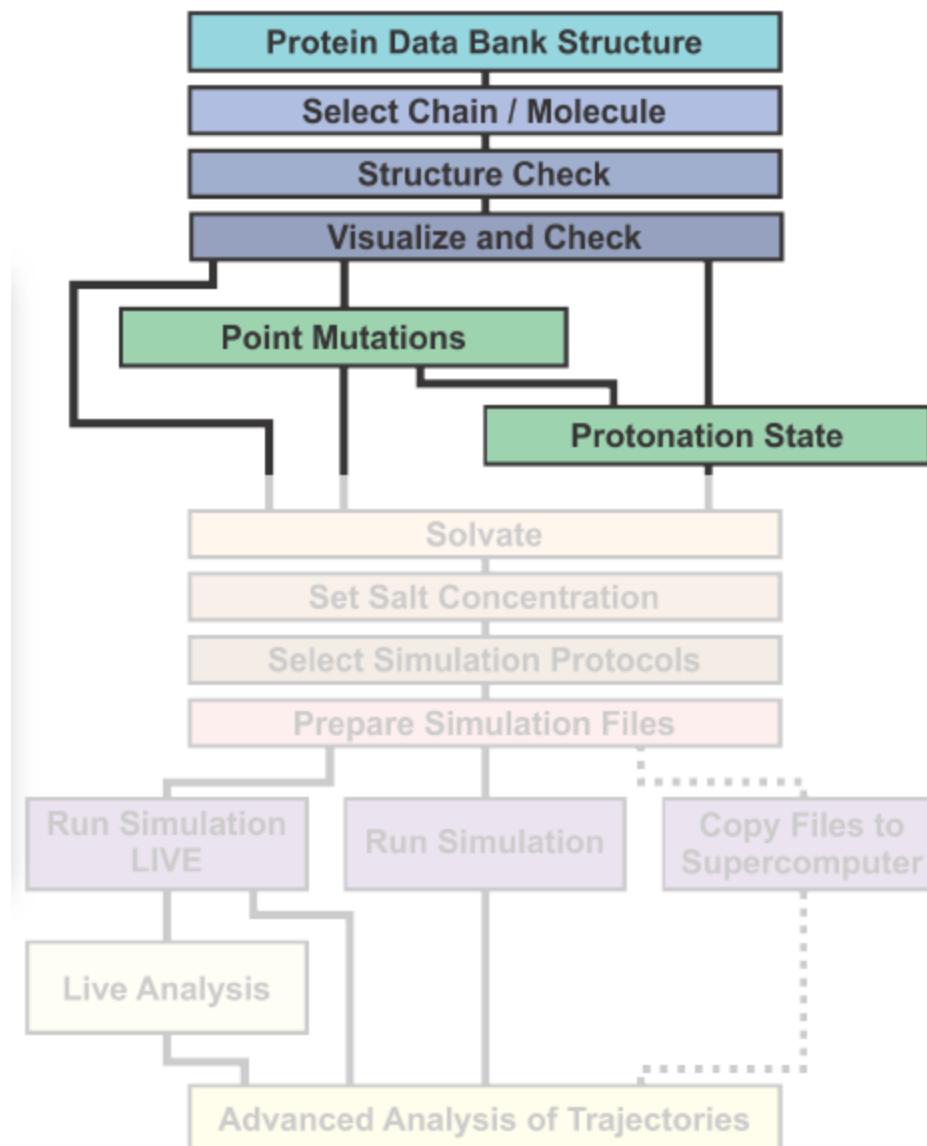
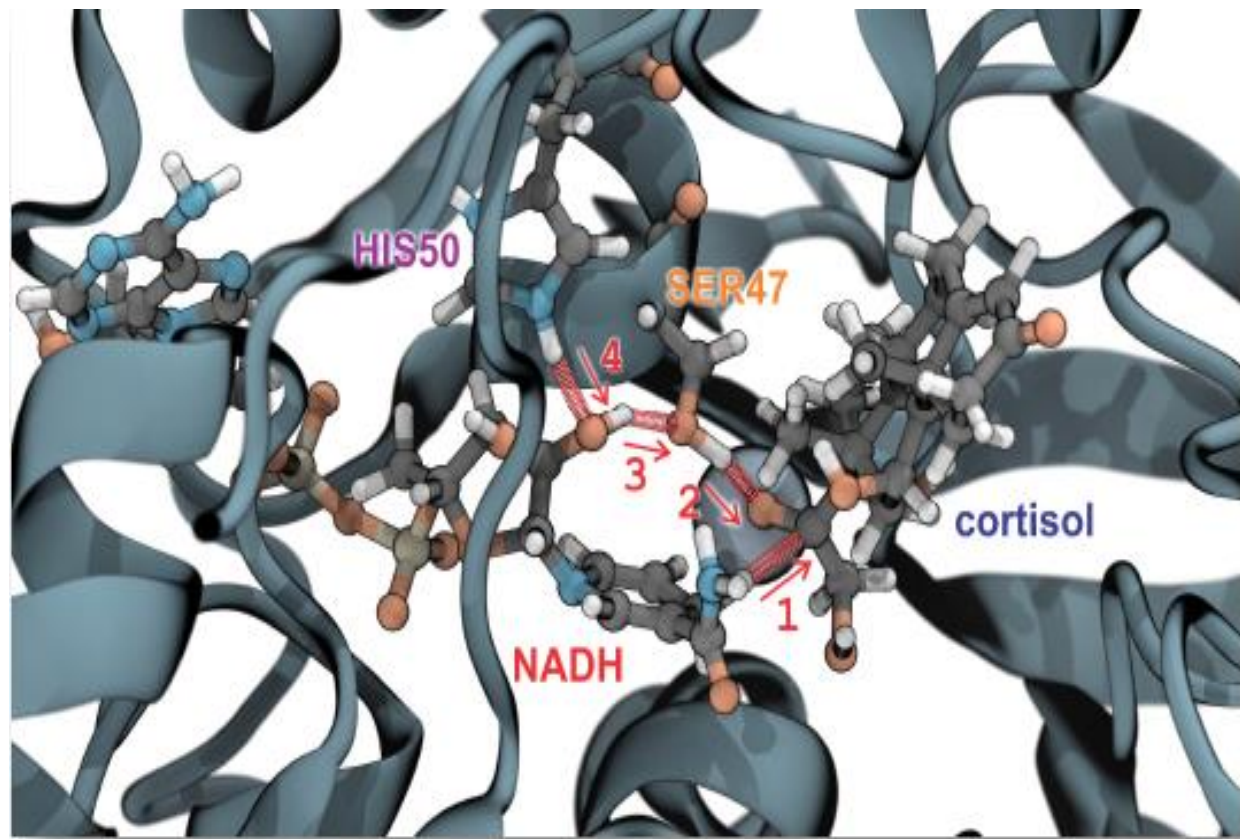
Chiral Centers
D-amino acids



QwikMD: Step by Step



QwikMD: Step by Step

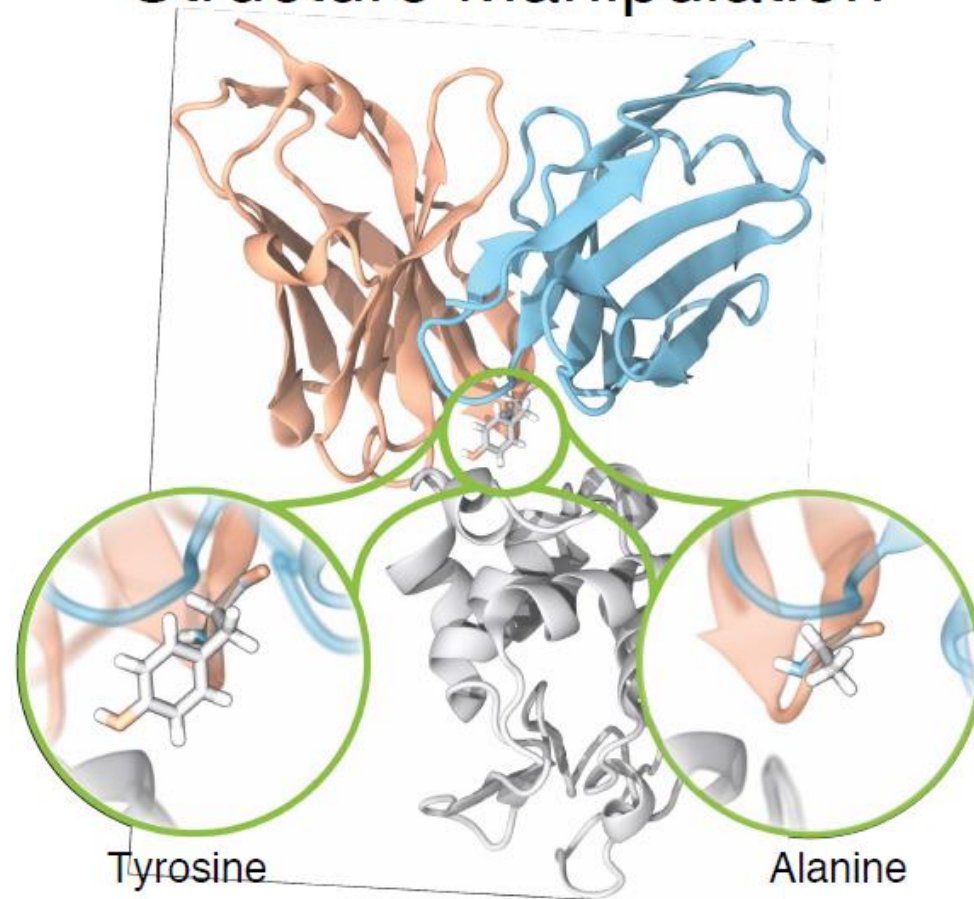


QwikMD: Step by Step

■ Structure Manipulation:

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

Structure Manipulation



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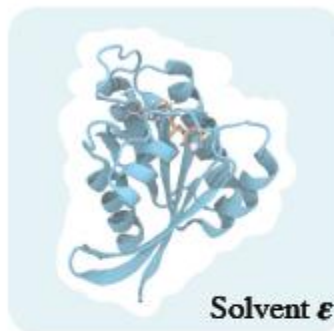
All molecules of the system are presented in a list and can be separated by type or chain. The QwikMD user can easily delete parts of structure, change protonation states, perform point mutations, among other actions.

QwikMD: Step by Step

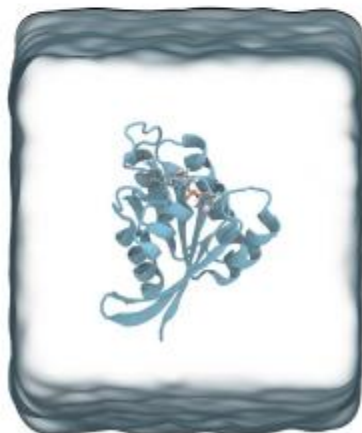
Vacuum



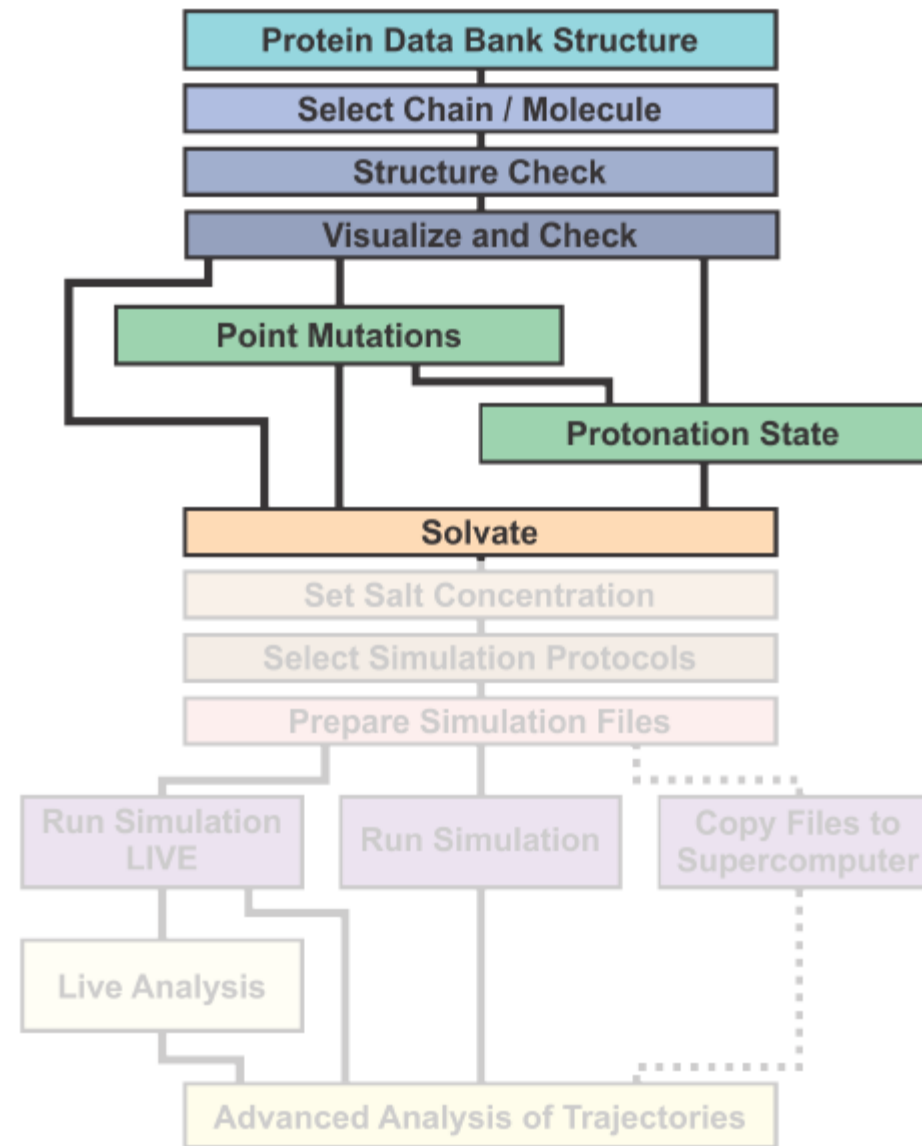
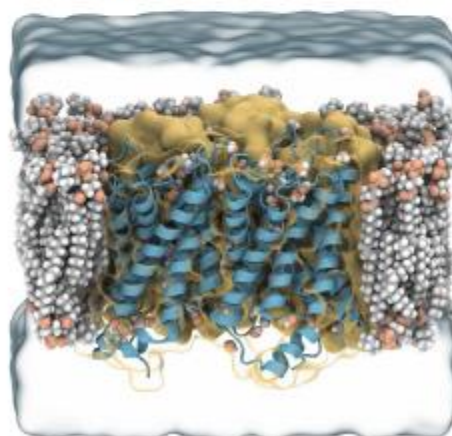
Implicit Solvent



Explicit Solvent



Explicit Solvent + Membrane



QwikMD: Step by Step

■ Simulation Environment:

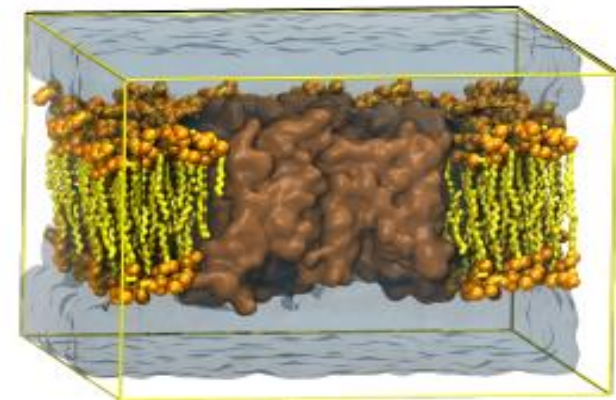
- Solvent Model
- Salt Concentration
- Water Box Size
 - Reduced Volume Available
- Membrane Protein Insertion

Vacuum / Implicit Solvent

Water Box

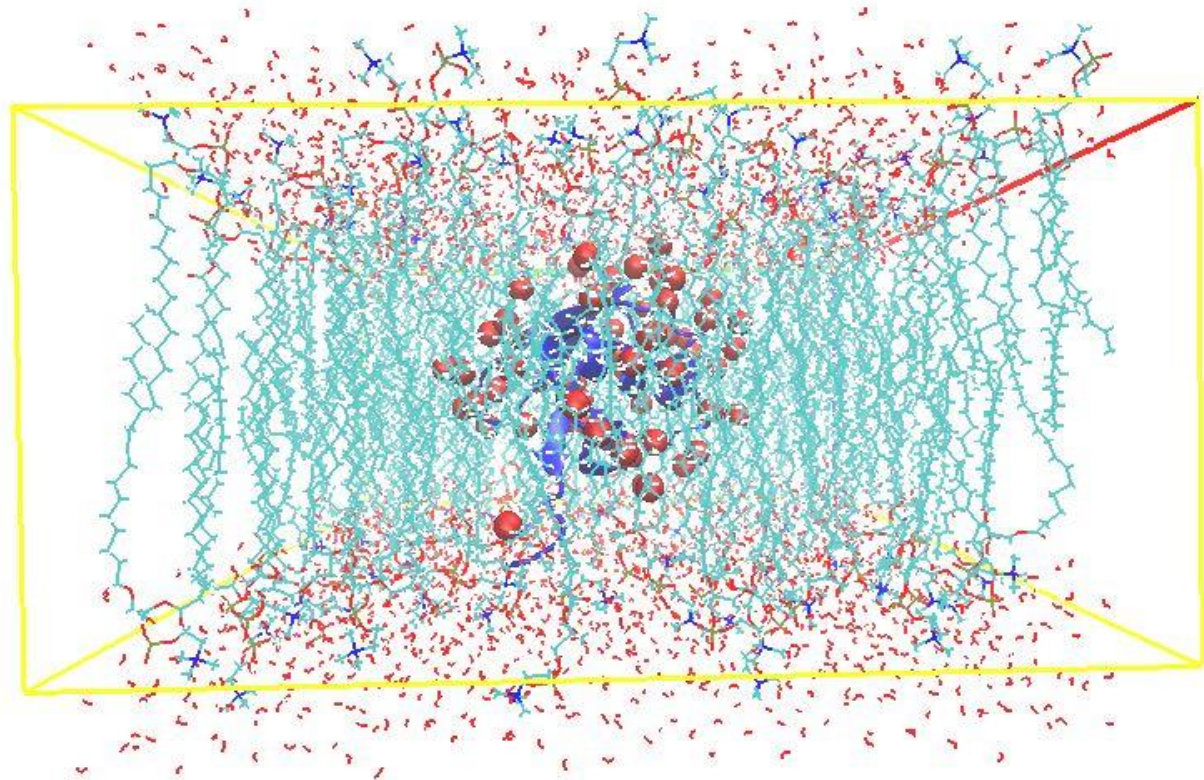
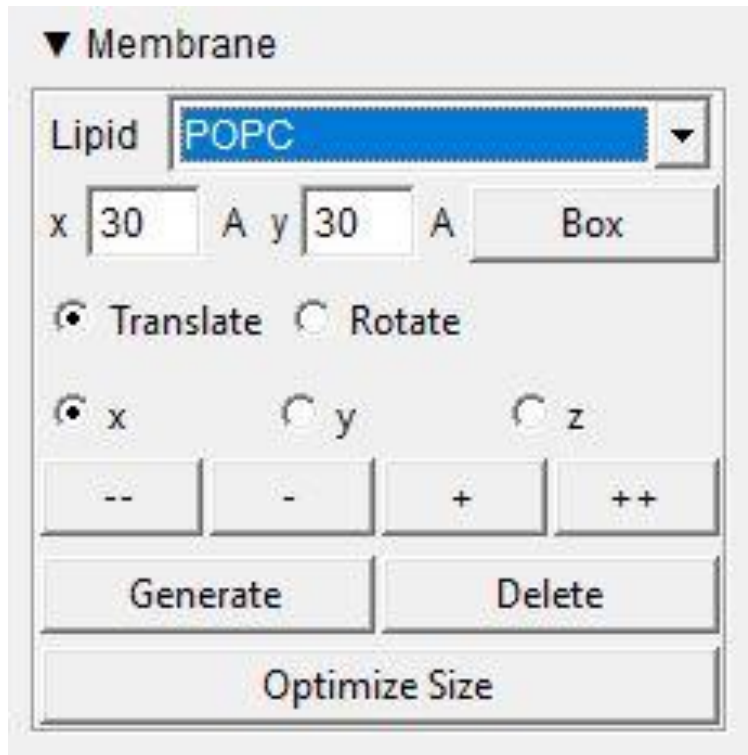


Membrane Environment

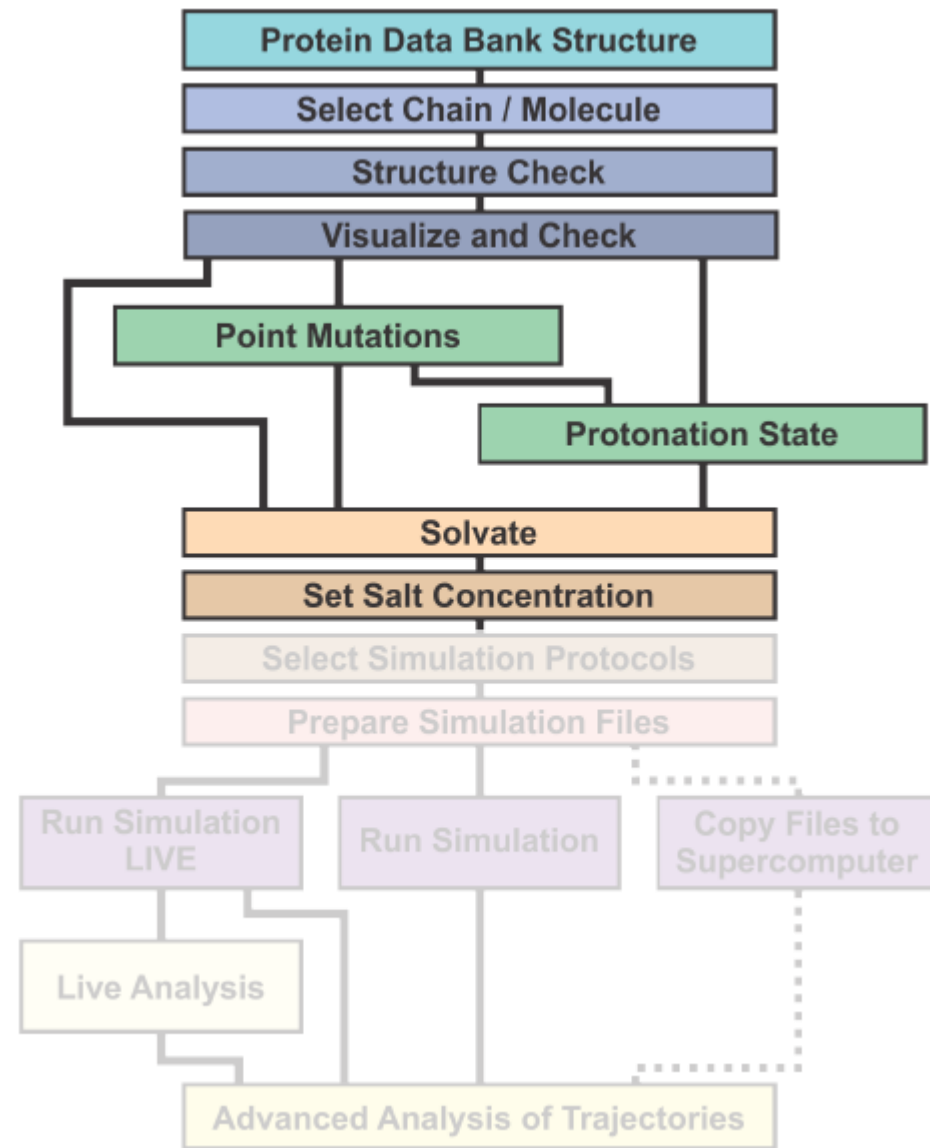
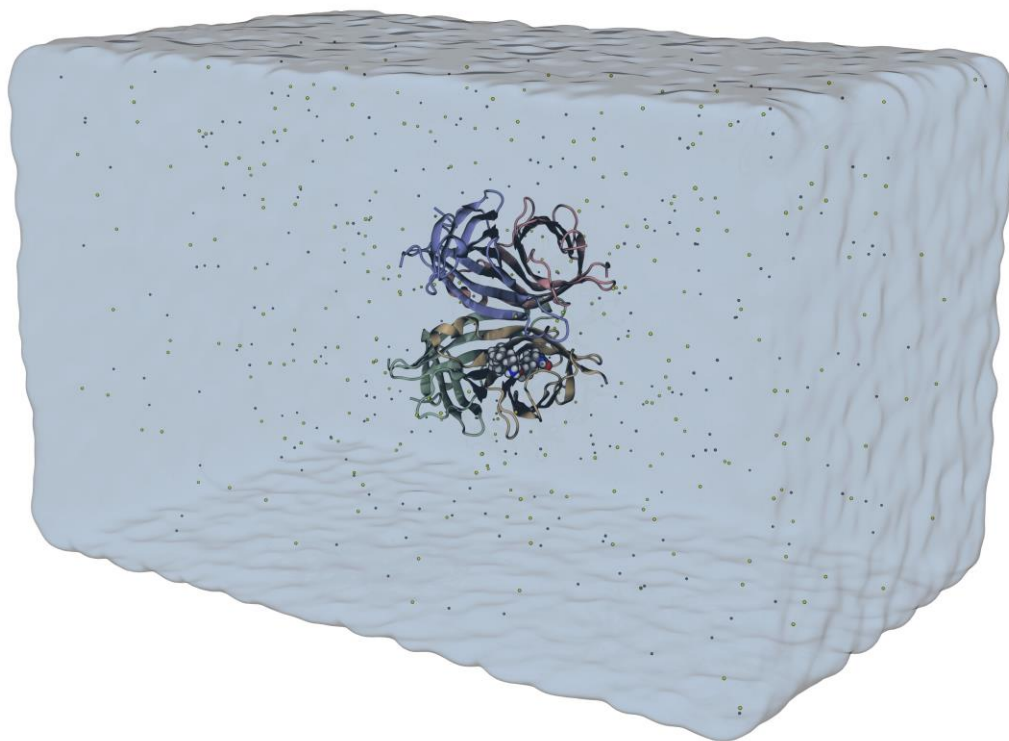


QwikMD: Step by Step

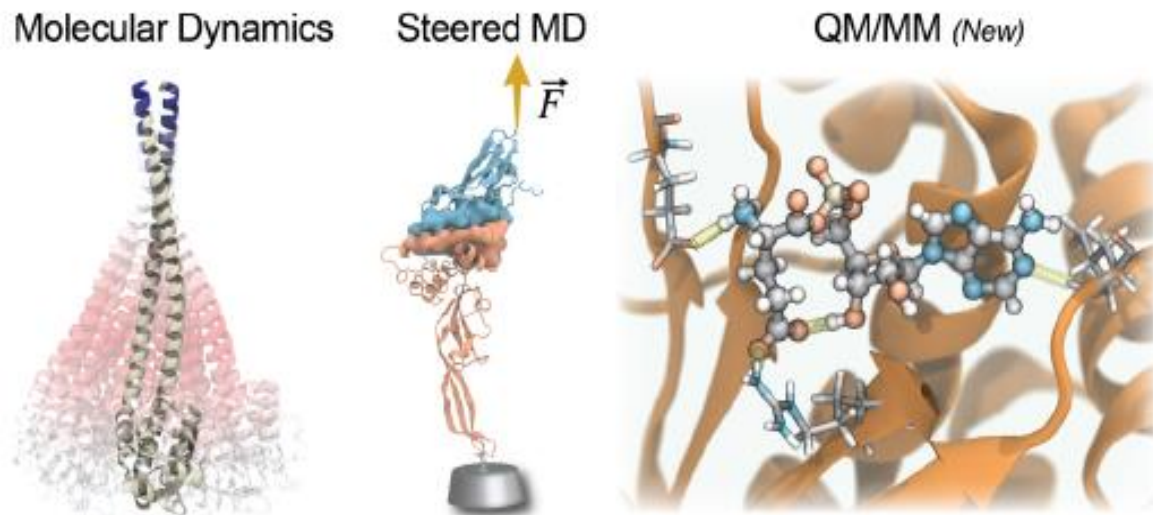
- **Simulation Environment:**
- Membrane in QwikMD



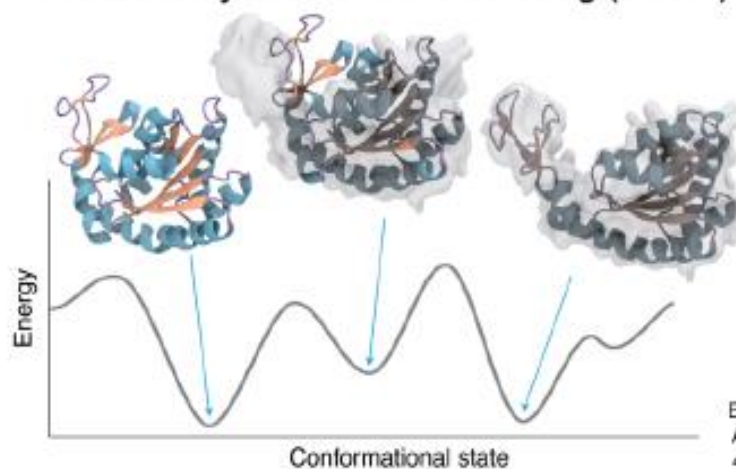
QwikMD: Step by Step



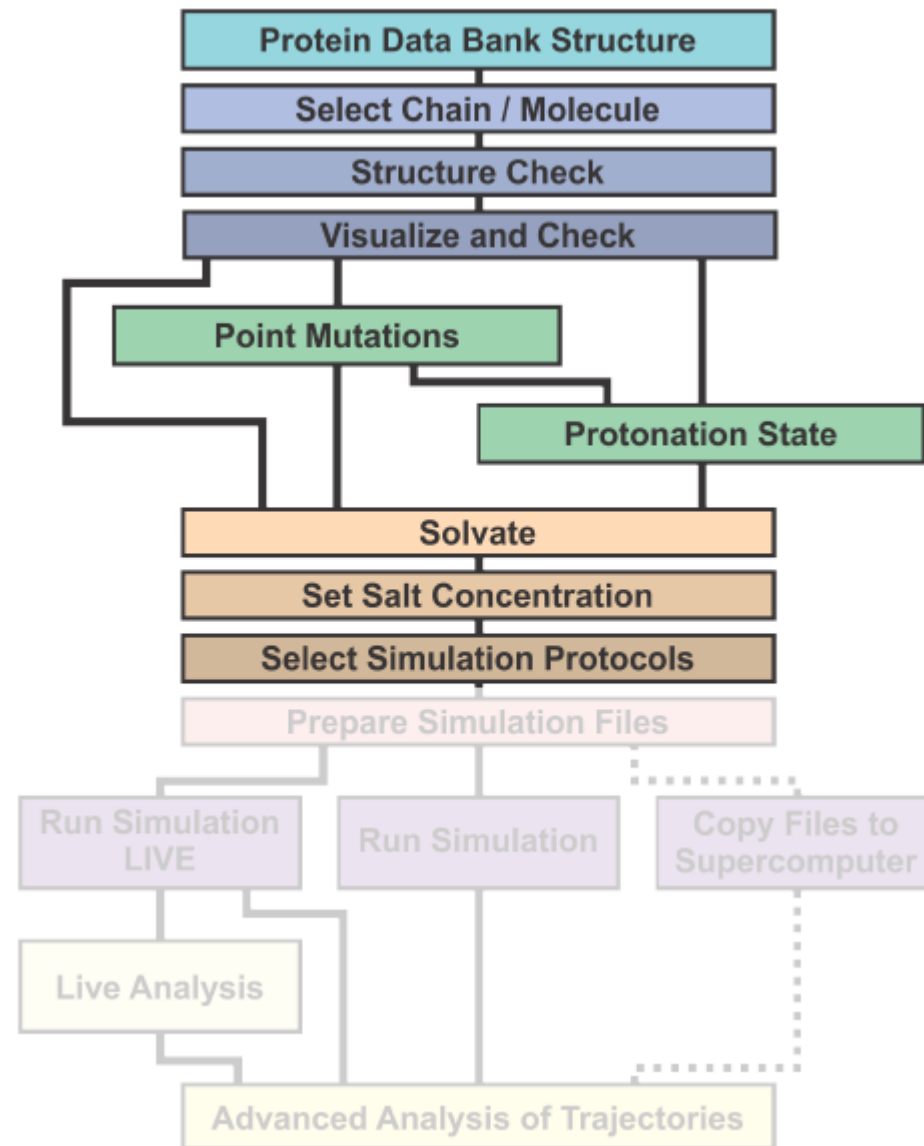
QwikMD: Step by Step



Molecular Dynamics Flexible Fitting (MDFF)



Extracted from Goh BC, *et al.*,
Annu. Rev. Biophys. 2016,
45:253–78

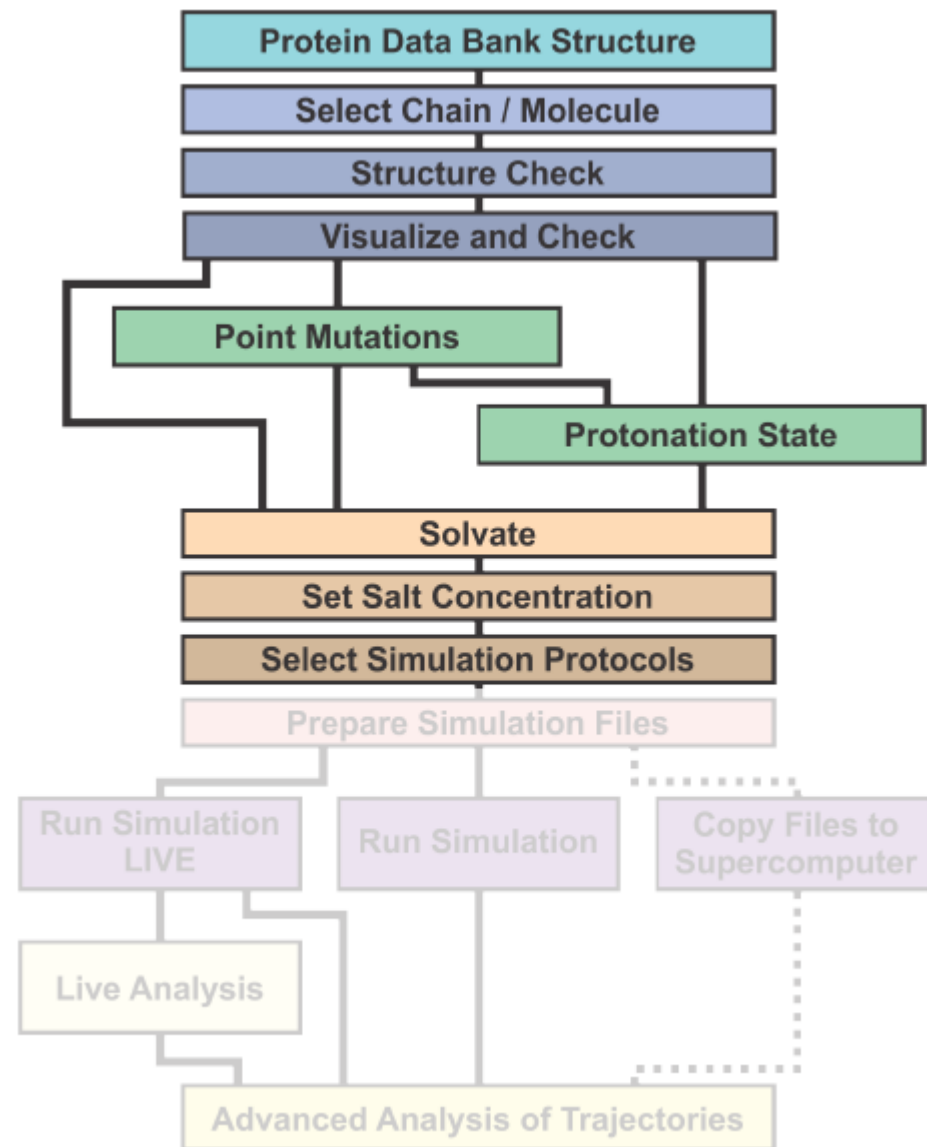
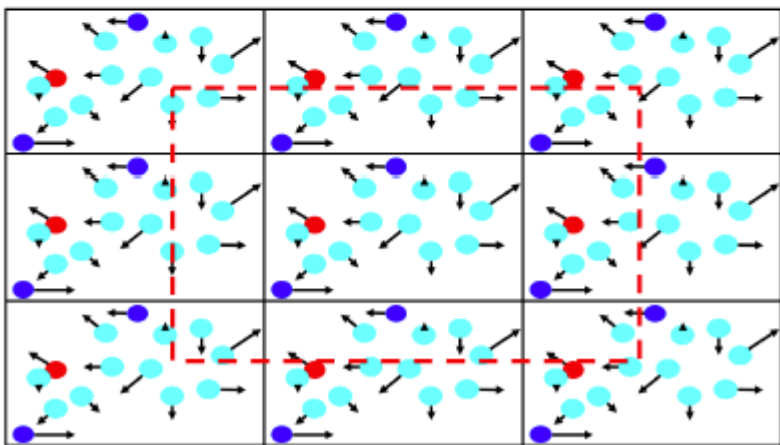


QwikMD: Step by Step

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

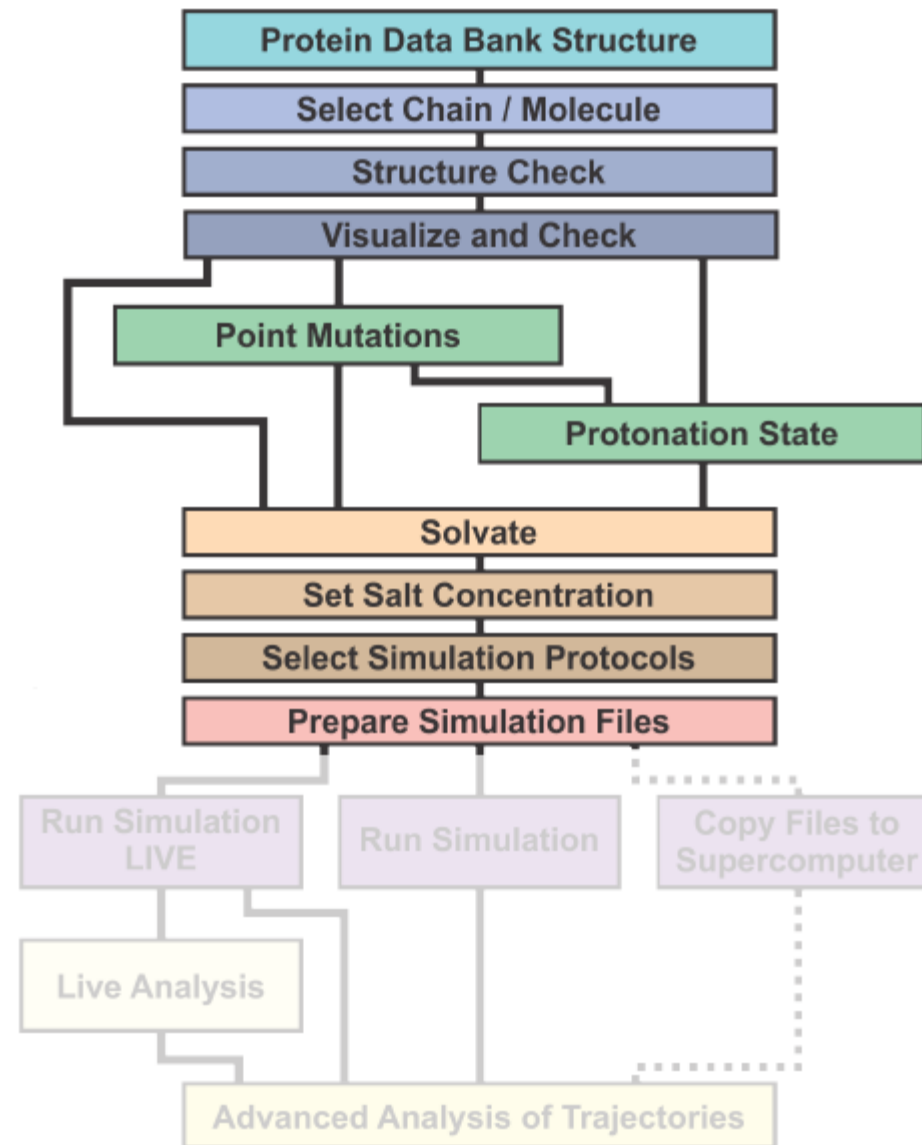
Define temperature

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

Starting simulation with random velocities

```
# starting from scratch
temperature          $temperature
    ;# initialize velocities randomly
```

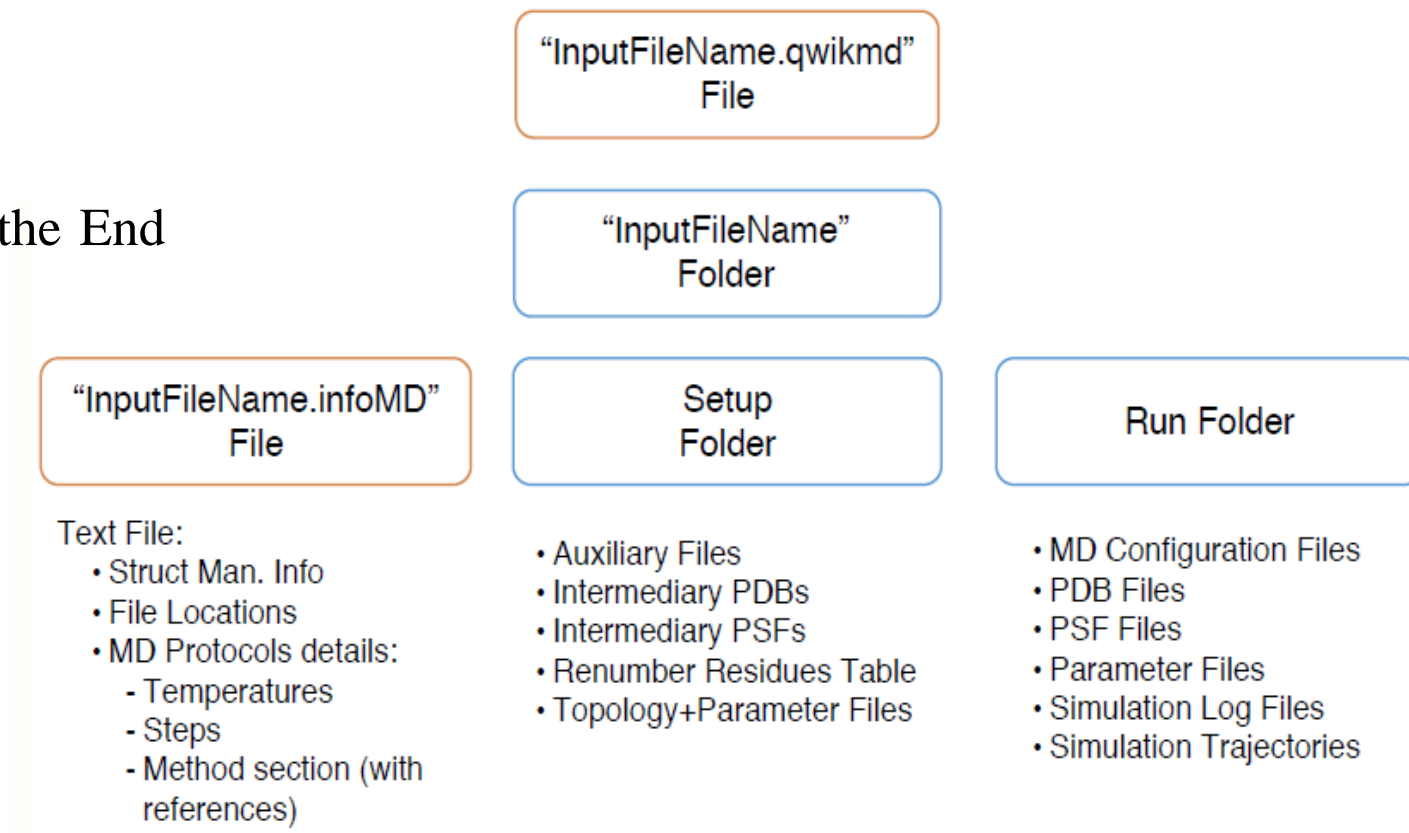
...



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

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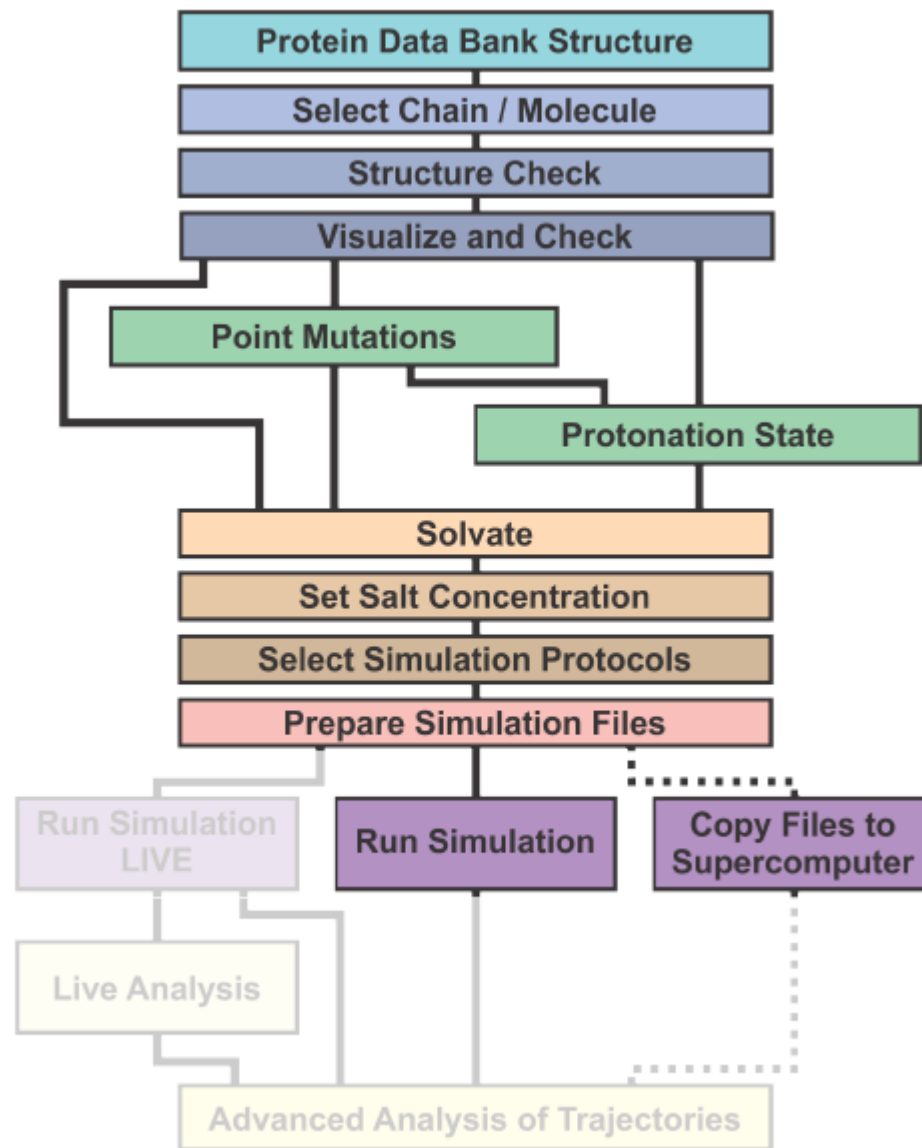
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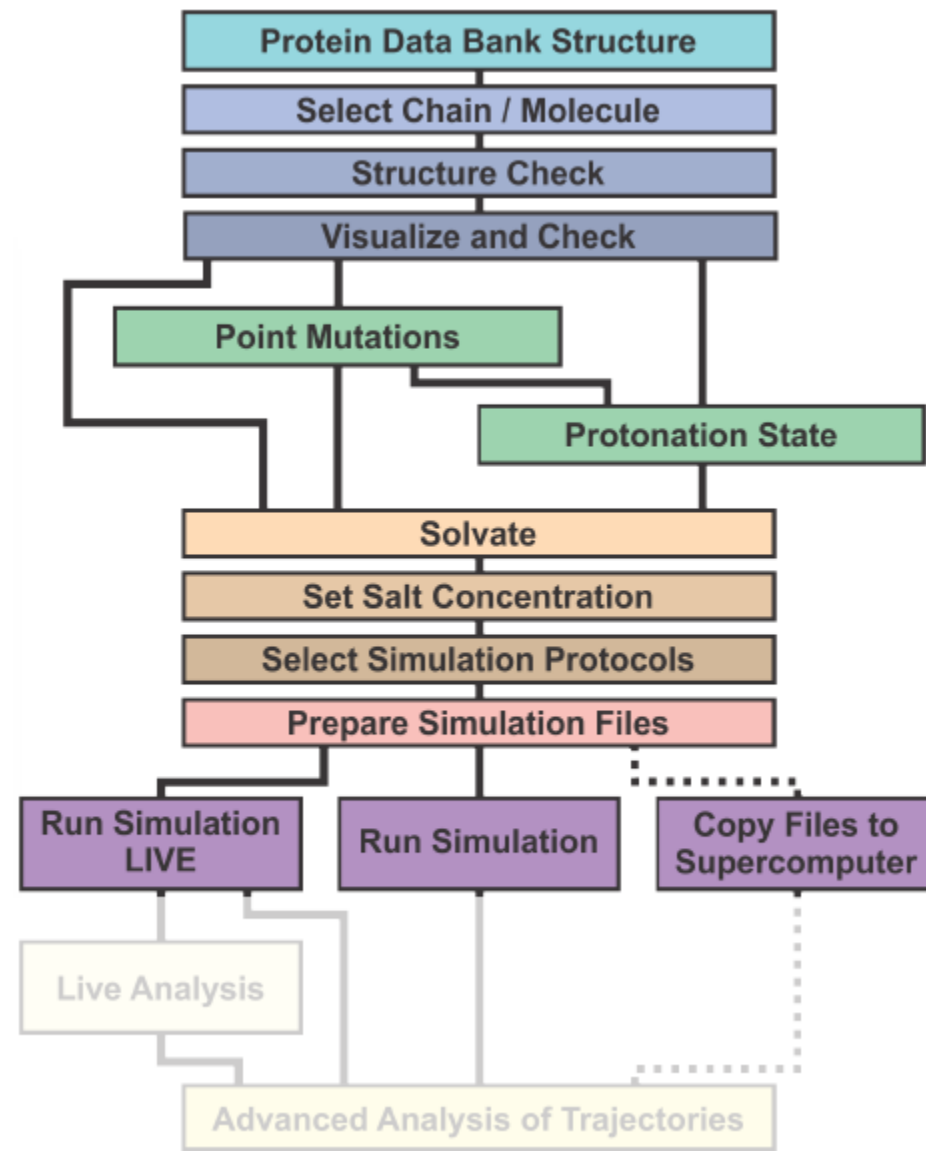
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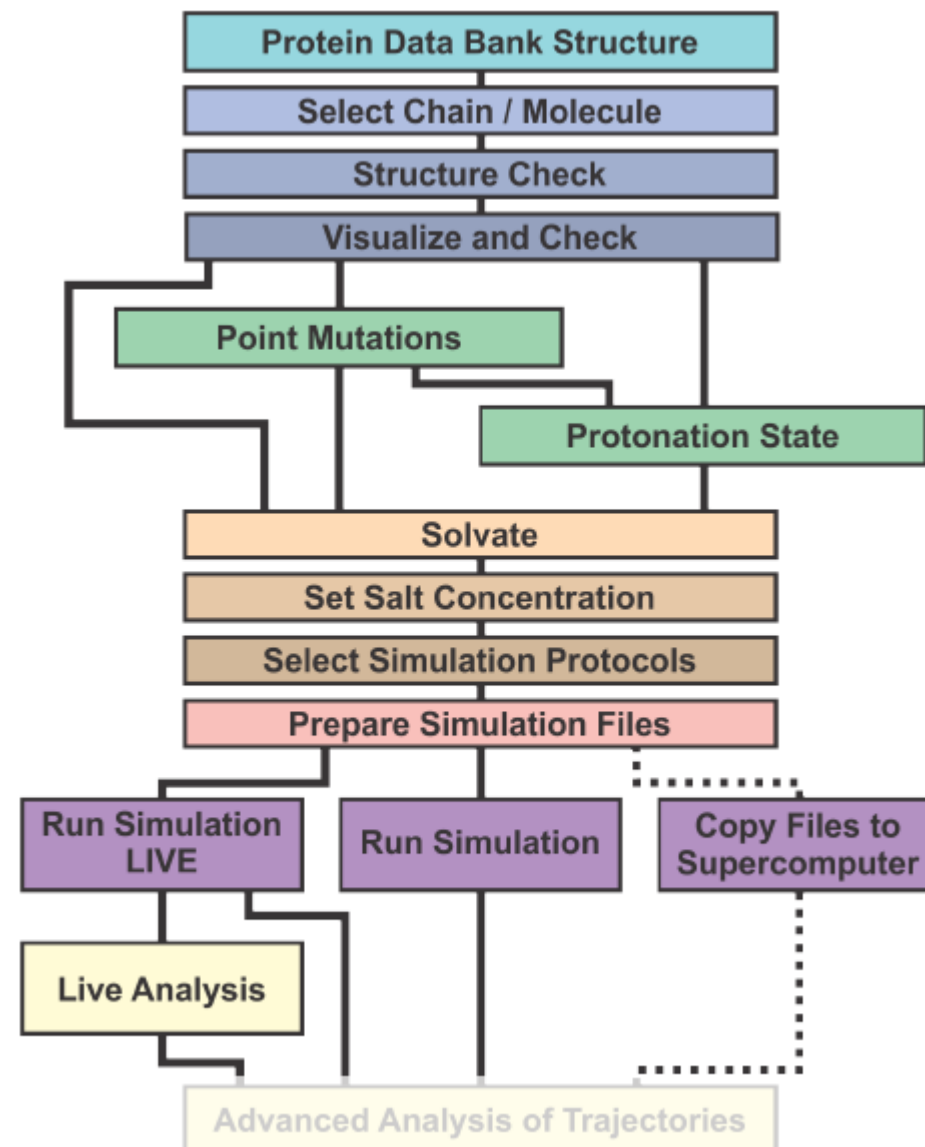
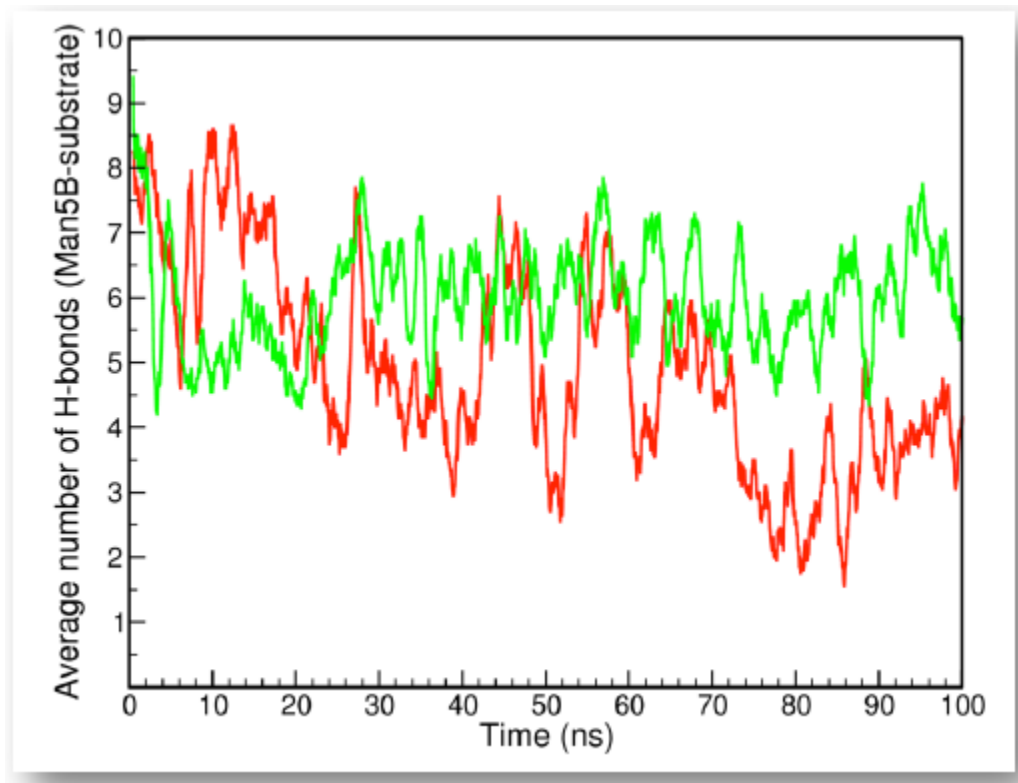
QwikMD: Step by Step



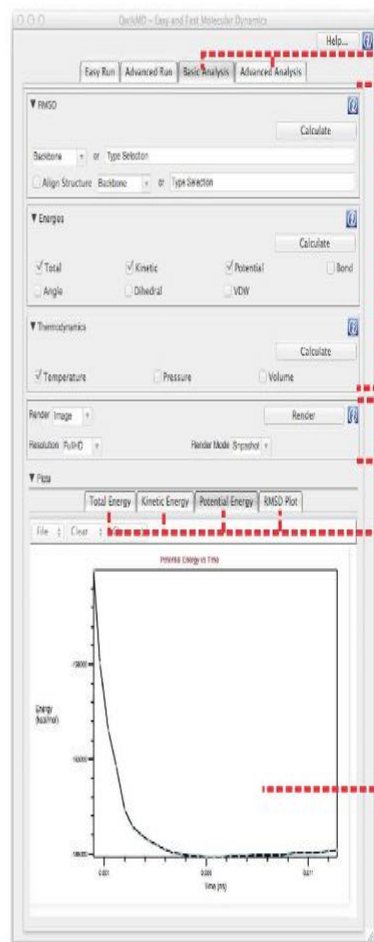
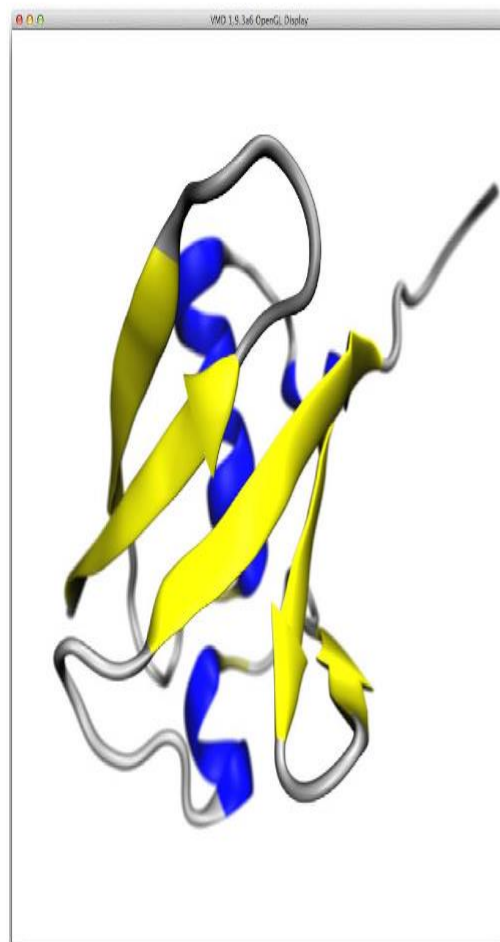
QwikMD: Step by Step



QwikMD: Step by Step



QwikMD: Step by Step



QwikMD users can select between: (1) "Basic Analysis", which include most common analysis methods used to check how stable is the structure in the simulation; or (2) "Advanced Analysis", which includes several of the most used analysis tools in VMD, i.e., Hydrogen Bond count, and Solvent Accessible Surface Area (SASA).

Here the user can select the analysis to be performed when "Calculate" is clicked.

VMD is known for its structure image rendering capabilities. In QwikMD a quick-render tab allows for a fast high-quality rendering, employing the most used settings for shadows, colors, materials, ...

Multiple analysis can be performed at the same time. The resulting plots will be presented in different tabs.

In a simulation on *live view* mode the plot will be updated while the simulation is performed

