

Introduction to Easy and Fast Simulations with QwikMD

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Pittsburgh Supercomputing Center

Pittsburgh, PA

Outline

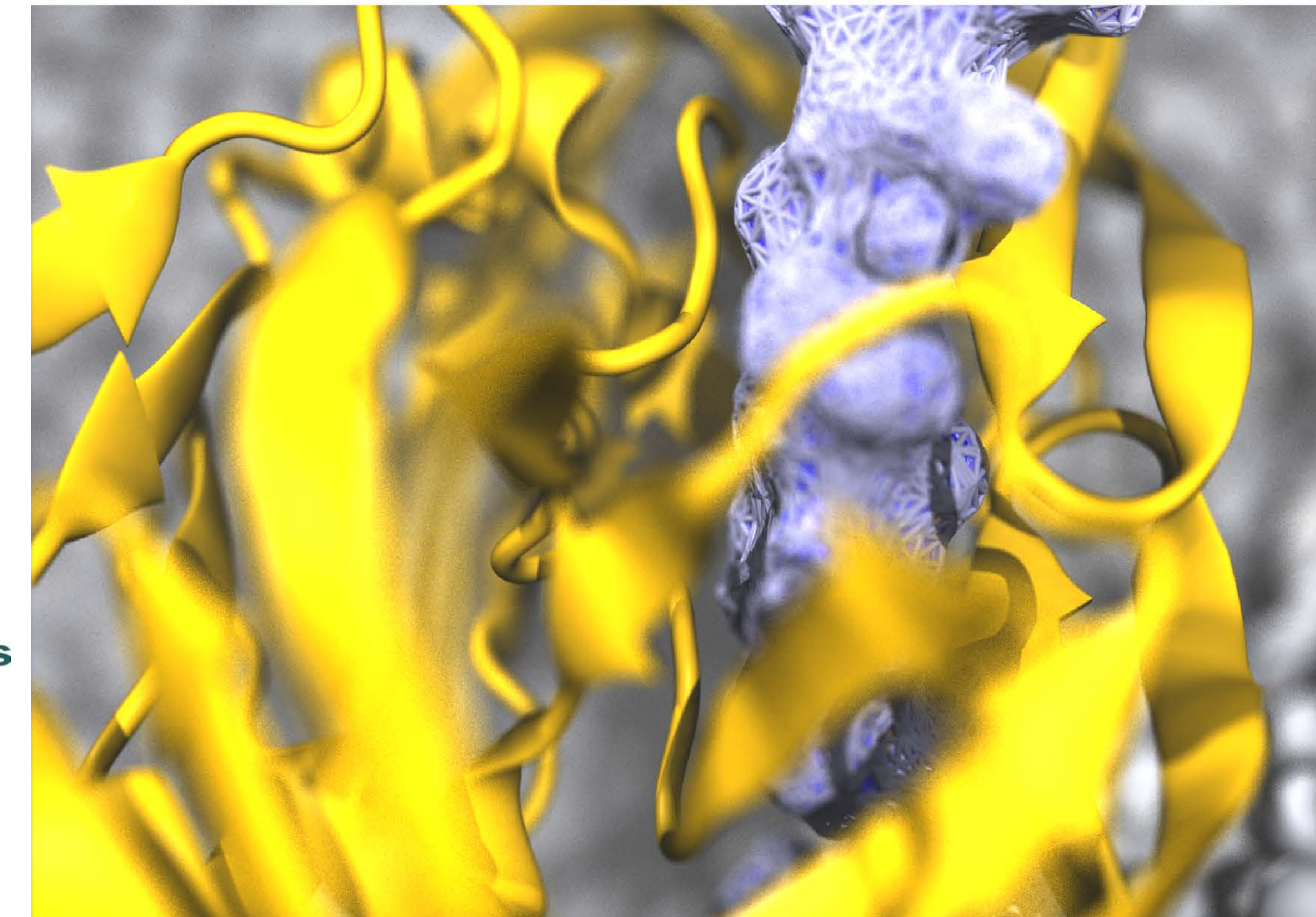
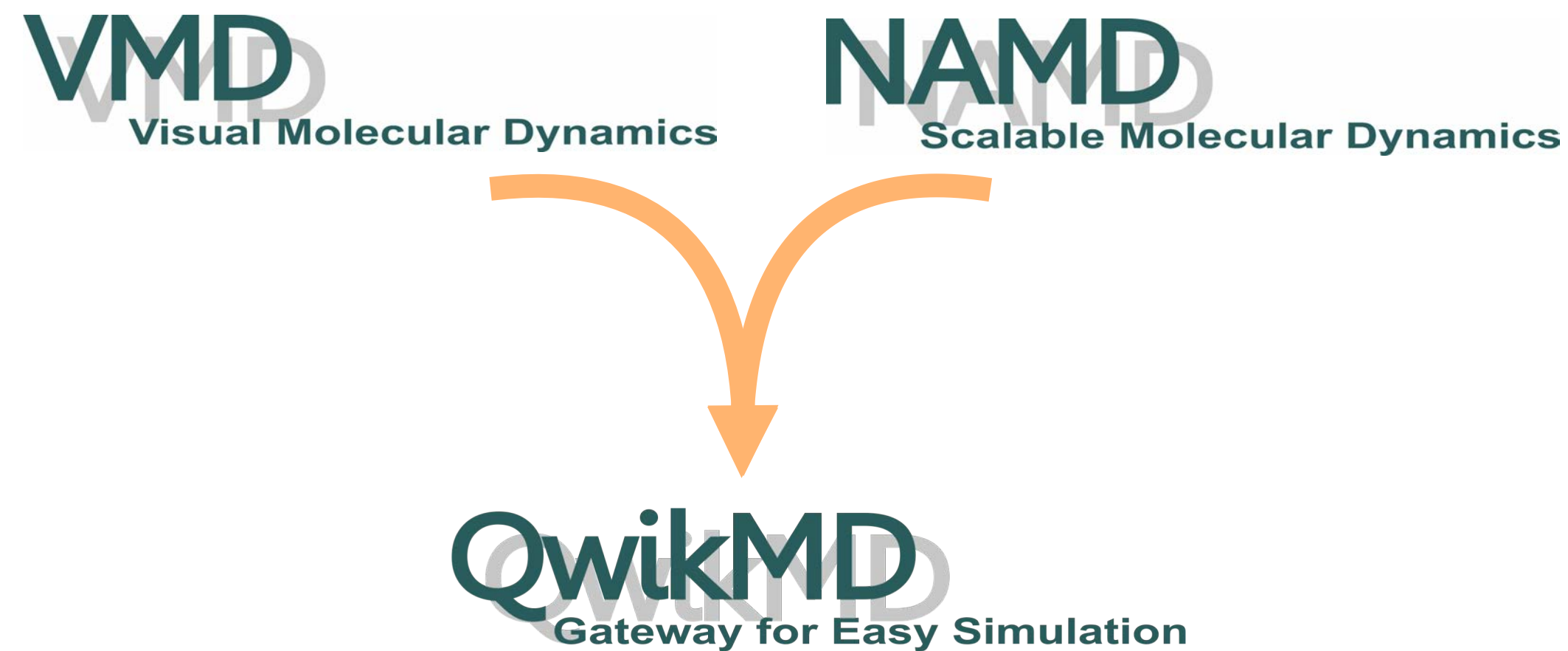
- Accessible MD Simulations
- Integrative MD Toolkit for Novices and Experts
- QwikMD Workflow
 - Initial Structure
 - Structure Manipulation
 - Simulation Environment
 - Simulation Protocols
 - QwikMD and Reproducibility
 - Load Simulation Trajectories and Analysis
 - New QM/MM Simulation and Orbitals Visualization
- QwikMD Paper - Dissemination, Documentation and User Support
- QwikMD on the Amazon Cloud
- Training others...

Integrative MD Toolkit for Novices and Experts

QwikMD is a VMD plugin to assist the user in preparing, executing and analyzing MD simulations.

QwikMD Features

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

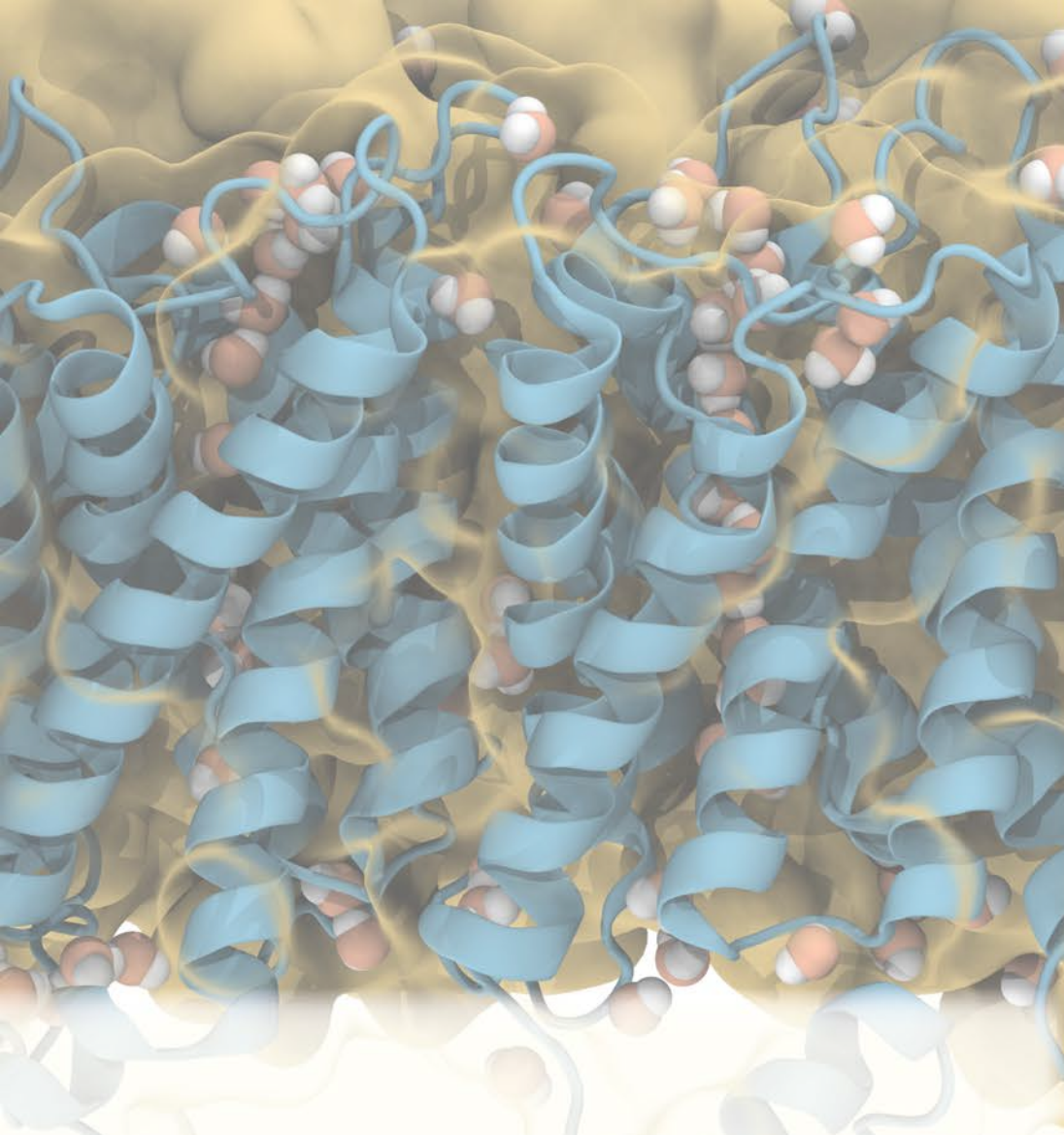


QwikMD

Gateway to Easy Simulation

www.ks.uiuc.edu/Research/qwikmd

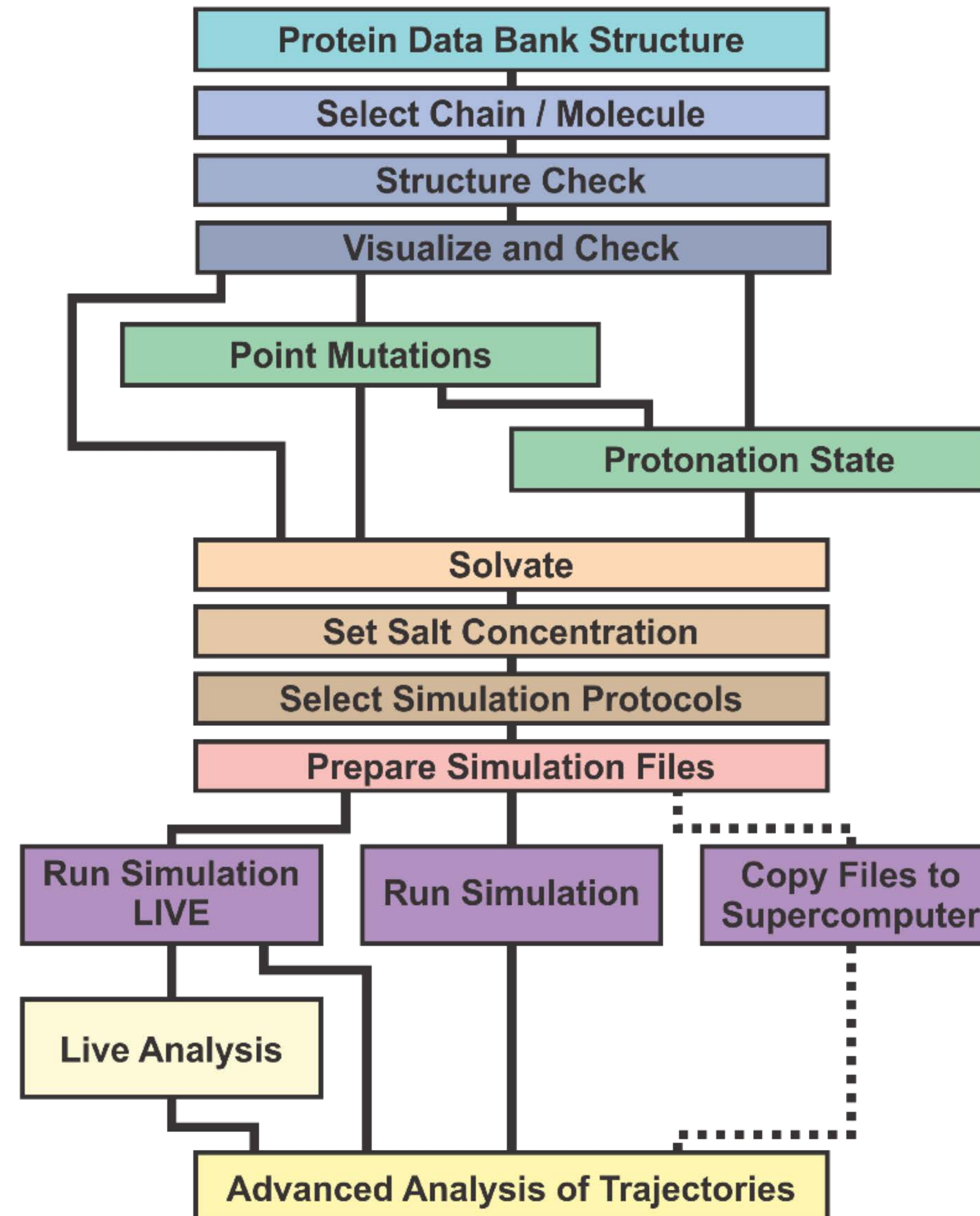
QwikMD is freely available in VMD 1.9.3 and later



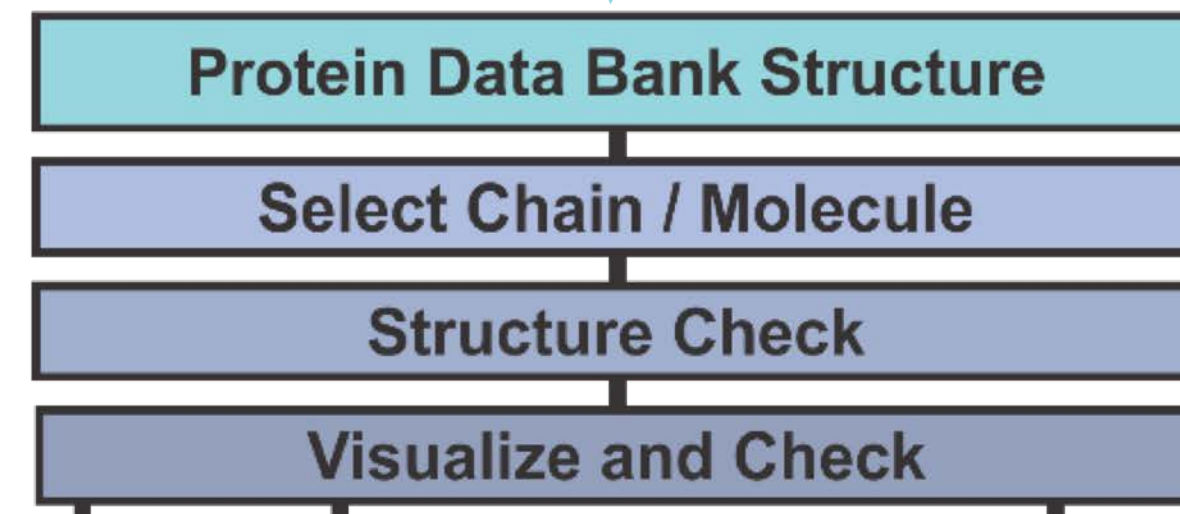
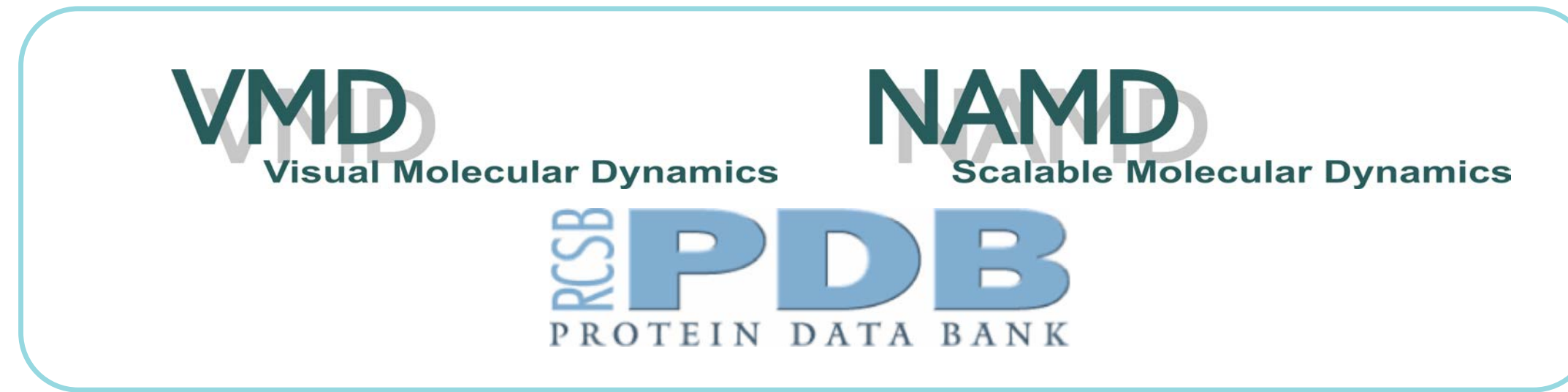
QwikMD Features

- Easy Setup of MD Simulations
- Structure Manipulation
- Basic and Advanced Protocols
- Live View Simulations
- Integrated Analysis
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- Reproducibility
- Available on Amazon Cloud

QwikMD Workflow



Initial Structure

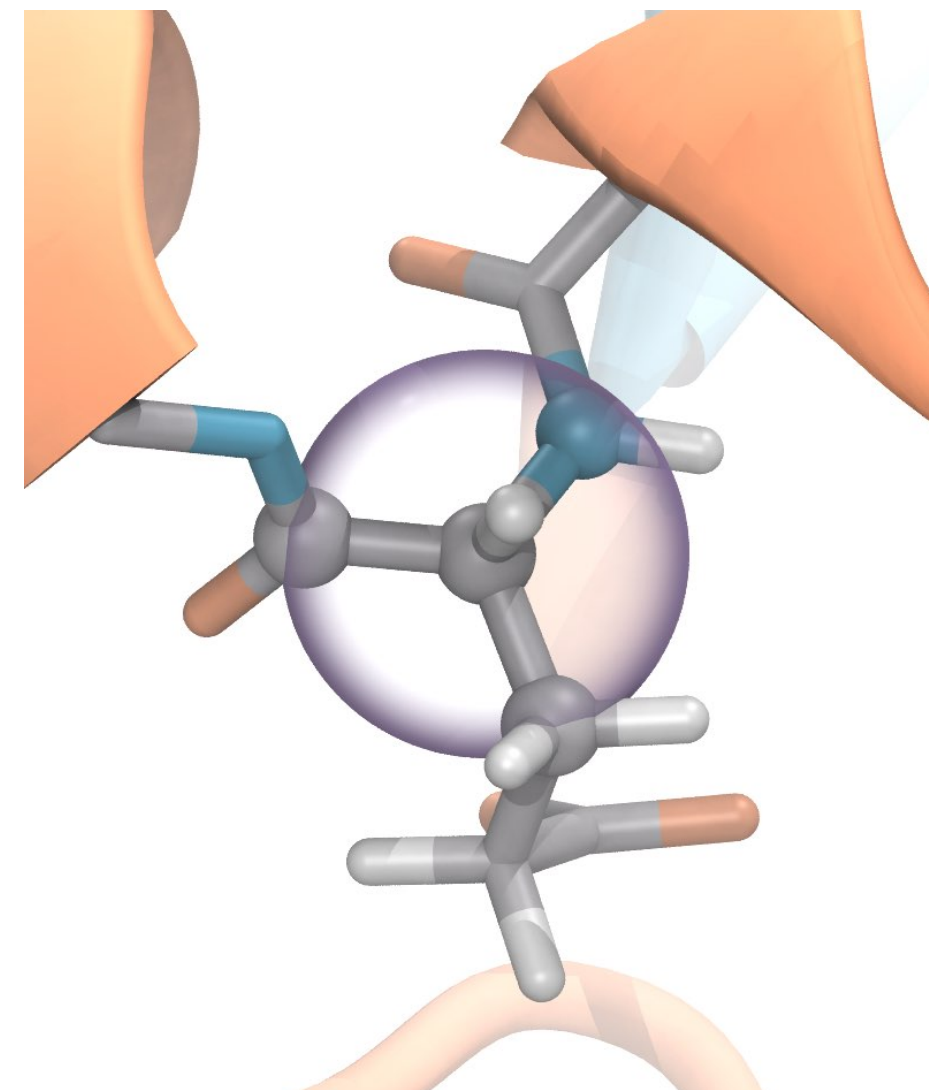


Structure Check

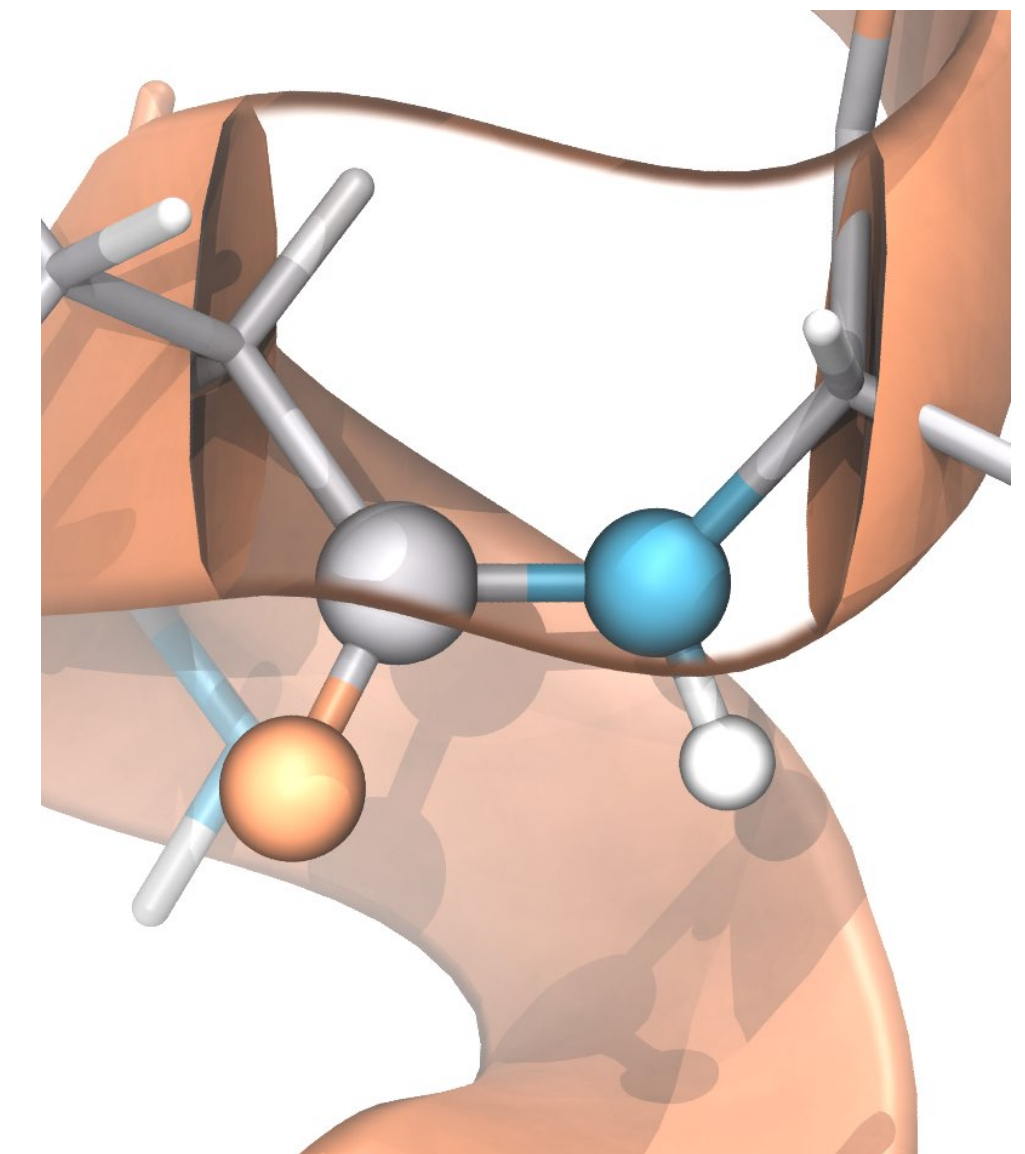
- Topologies & Parameters (4)
- Chiral Centers
- Cispetide Bond
- Sequence Gaps
- Torsion Angles Outliers
2.79% (Goal < 0.1%)
- Torsion Angles Marginals
2.33% (Goal < 5%)

Ignore Check

Chiral Centers
D-amino acids

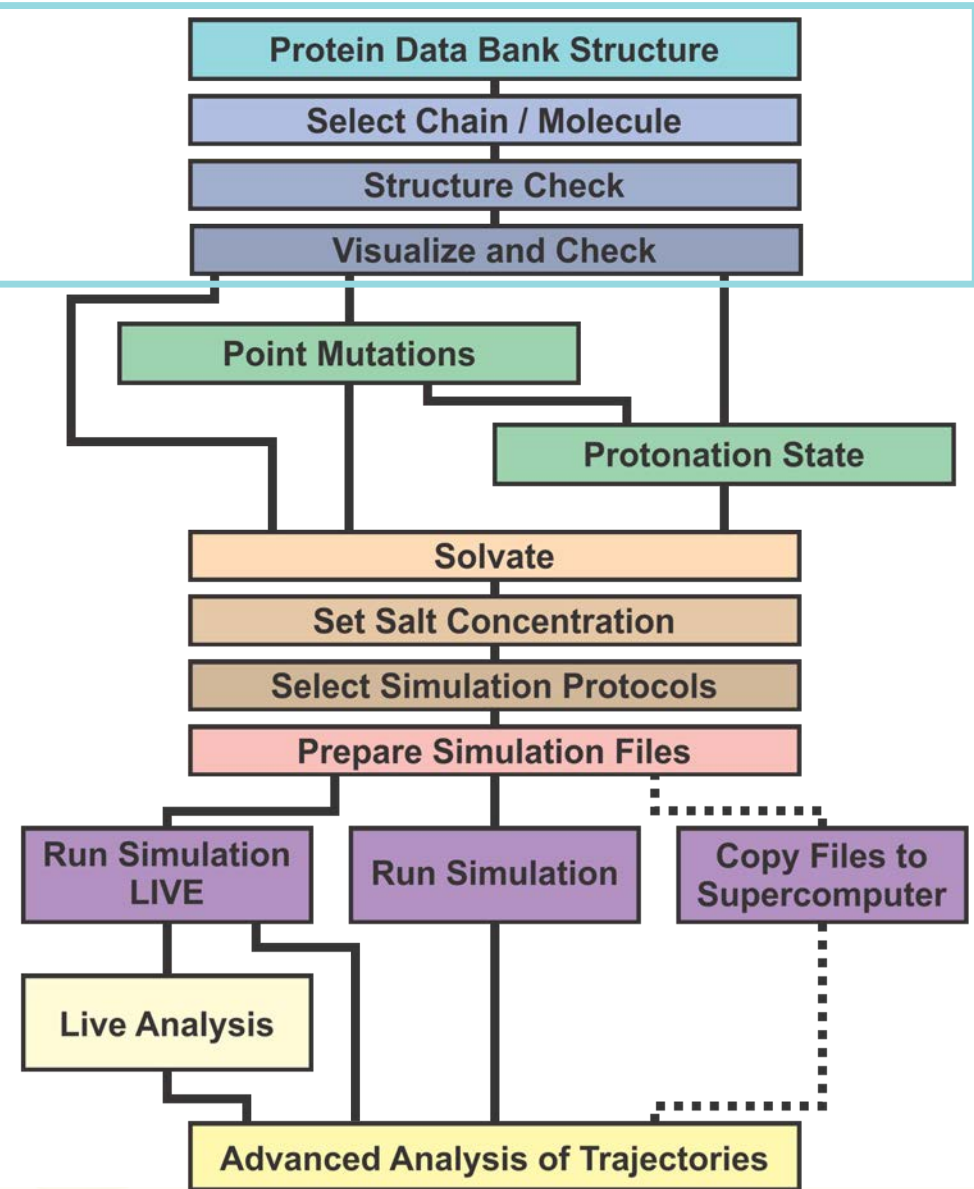


Cis-peptide

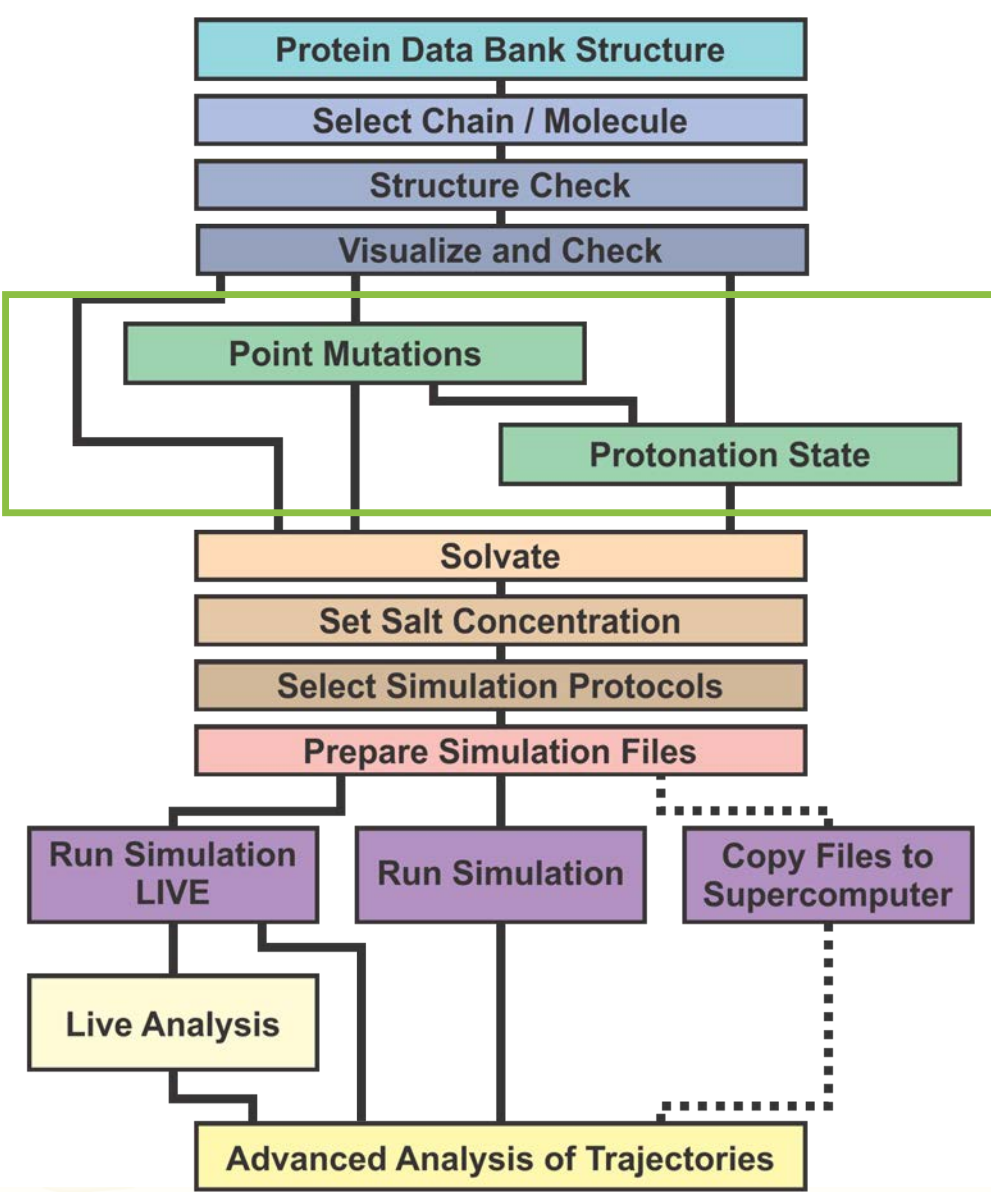


Structure Check

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

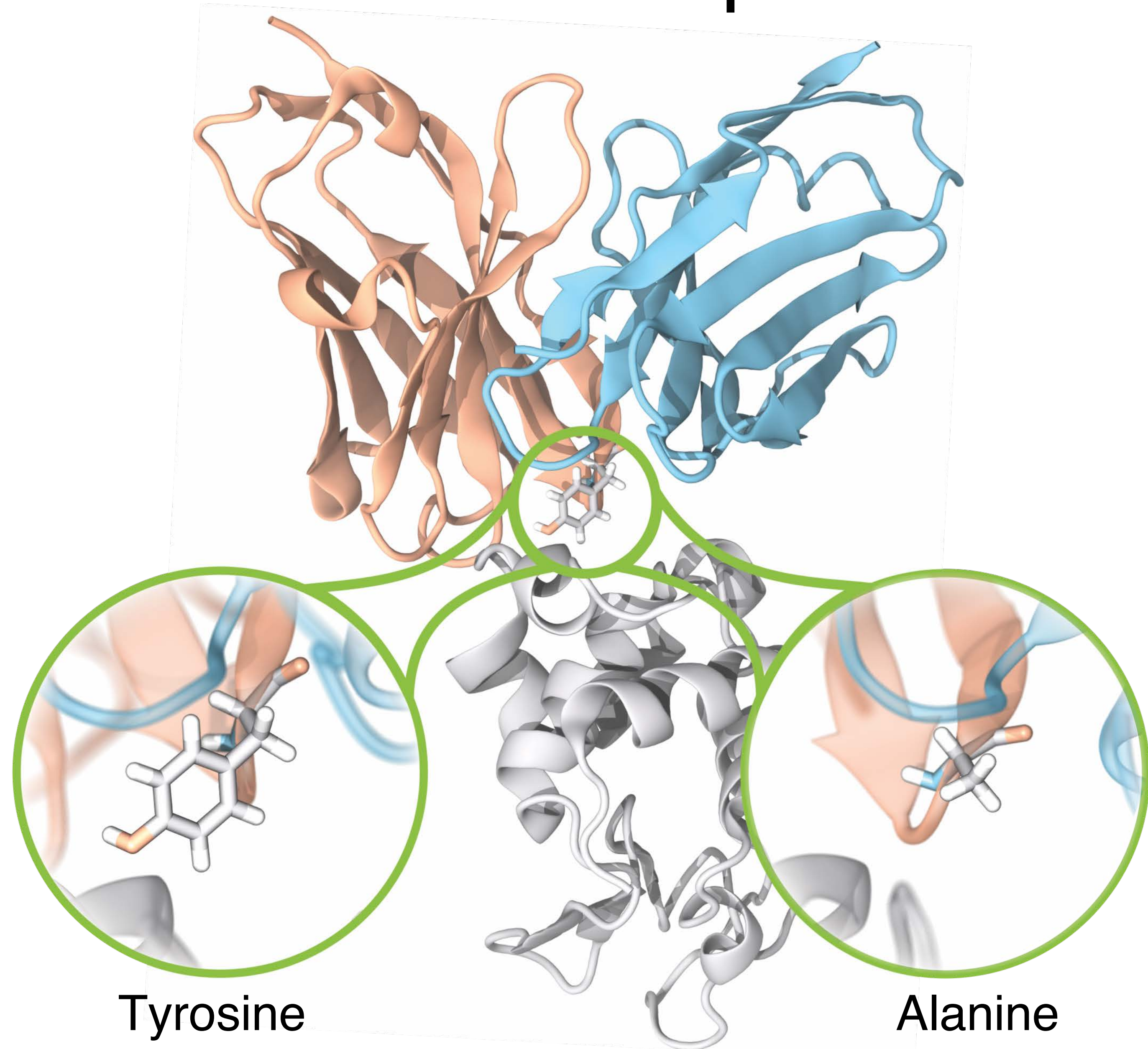


Structure Manipulation



Structure Manipulation

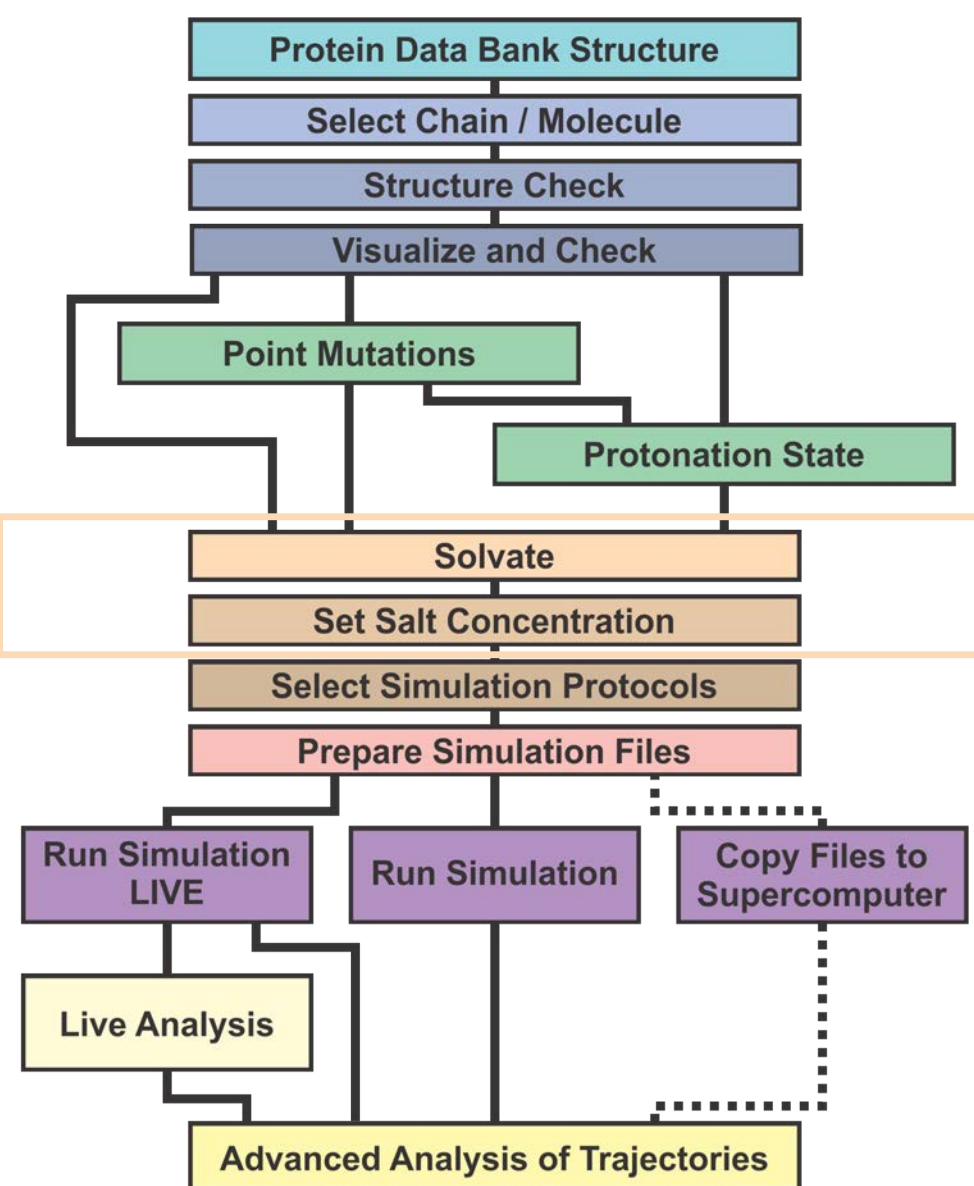
- Point Mutations
- Protonation State Selection
- Partial Sequence Deletions
- Molecule's Type
- Assign Topologies
- Atom Editing
 - Name
 - Indexes



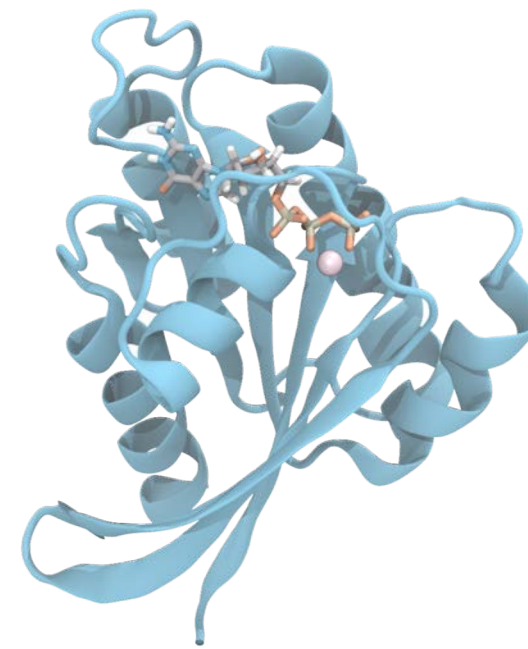
Tyrosine

Alanine

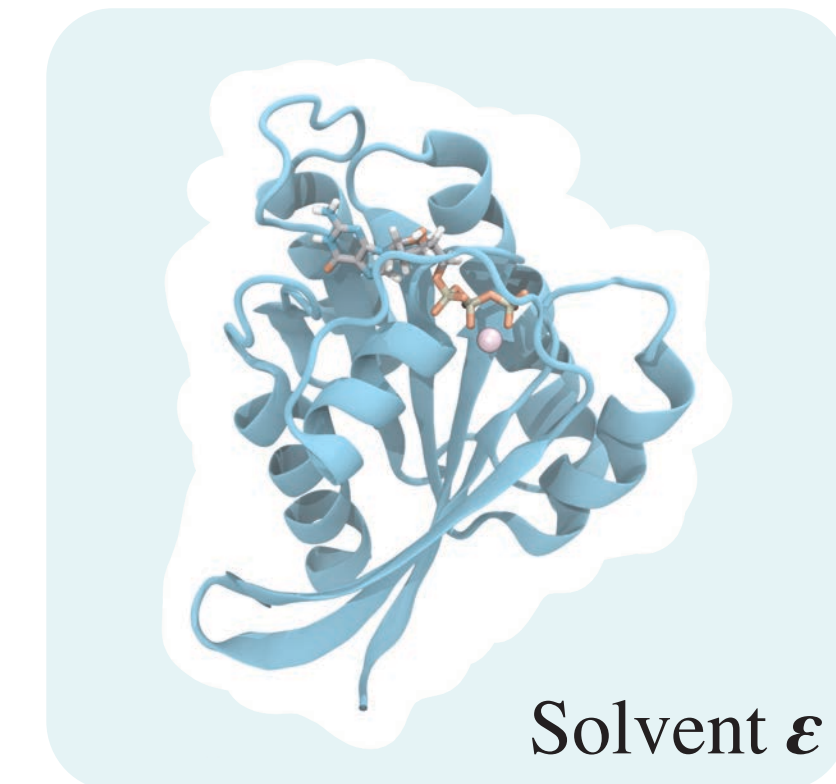
Simulation Environment



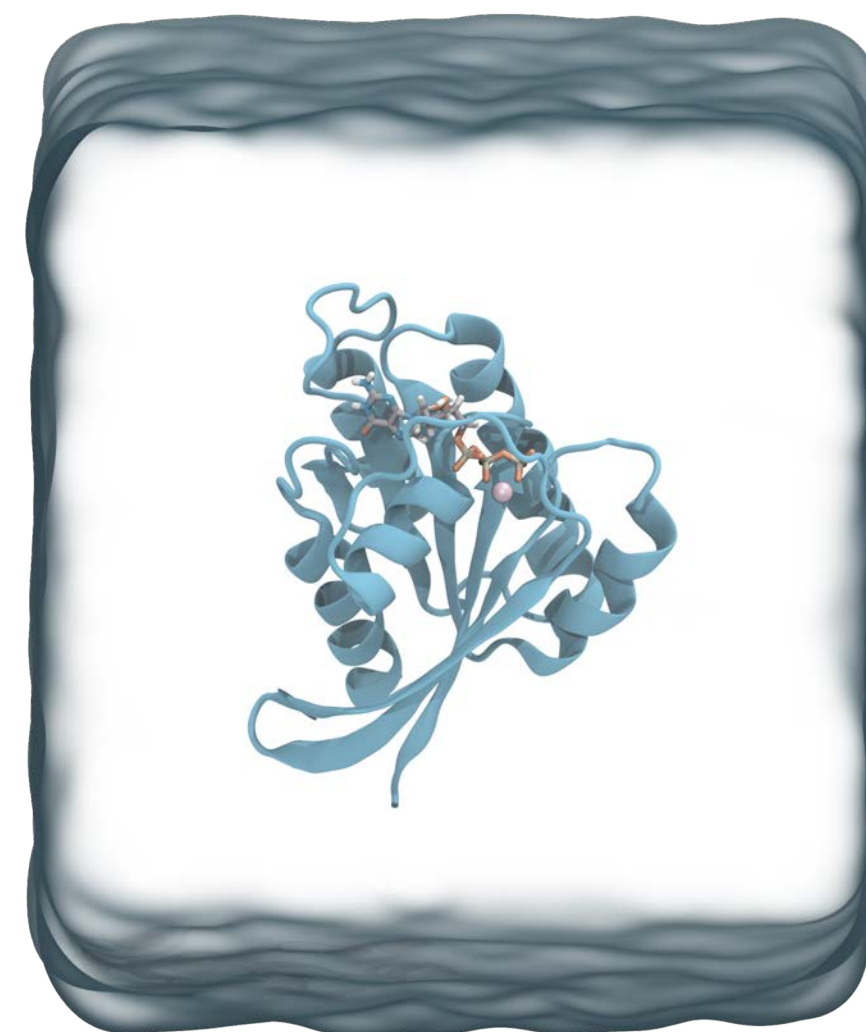
Vacuum



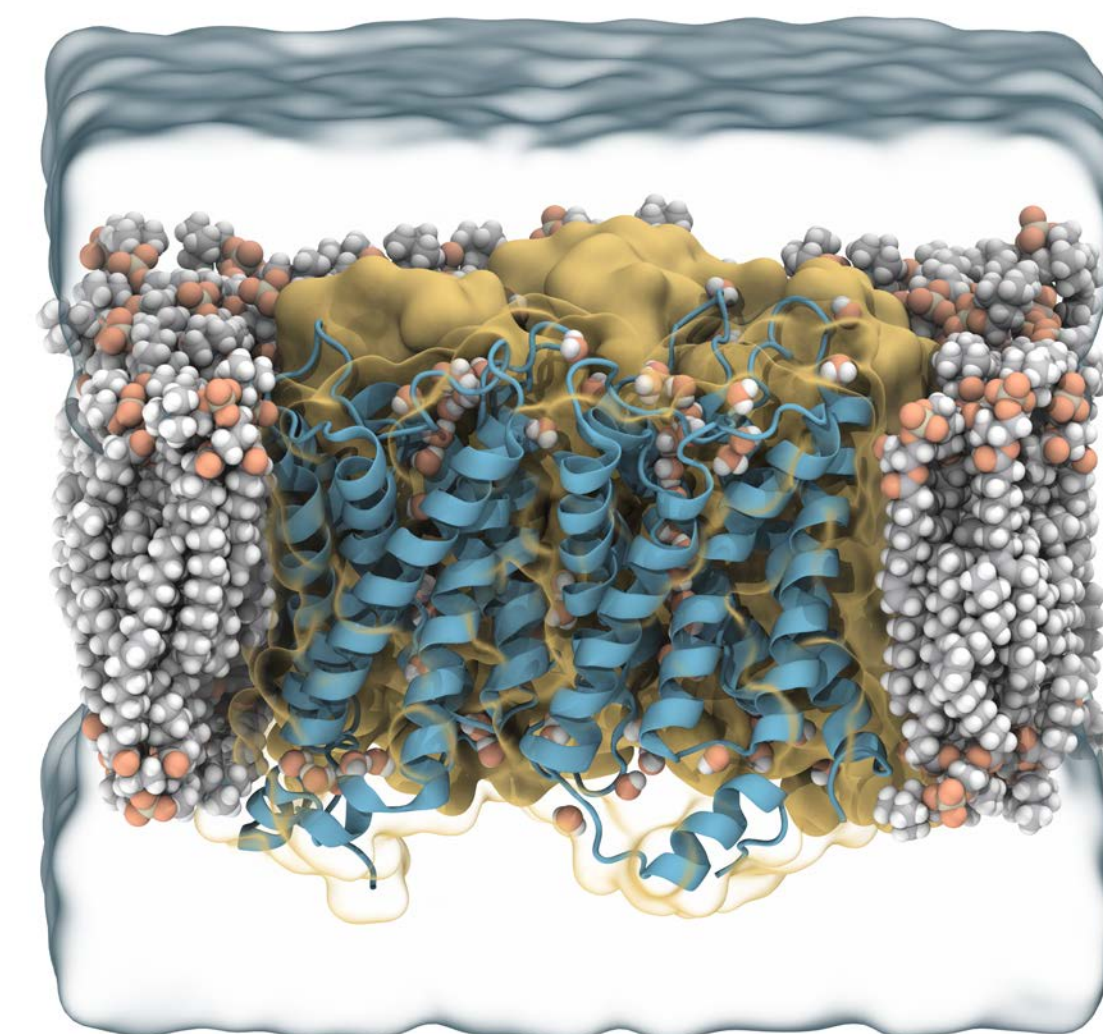
Implicit Solvent



Explicit Solvent



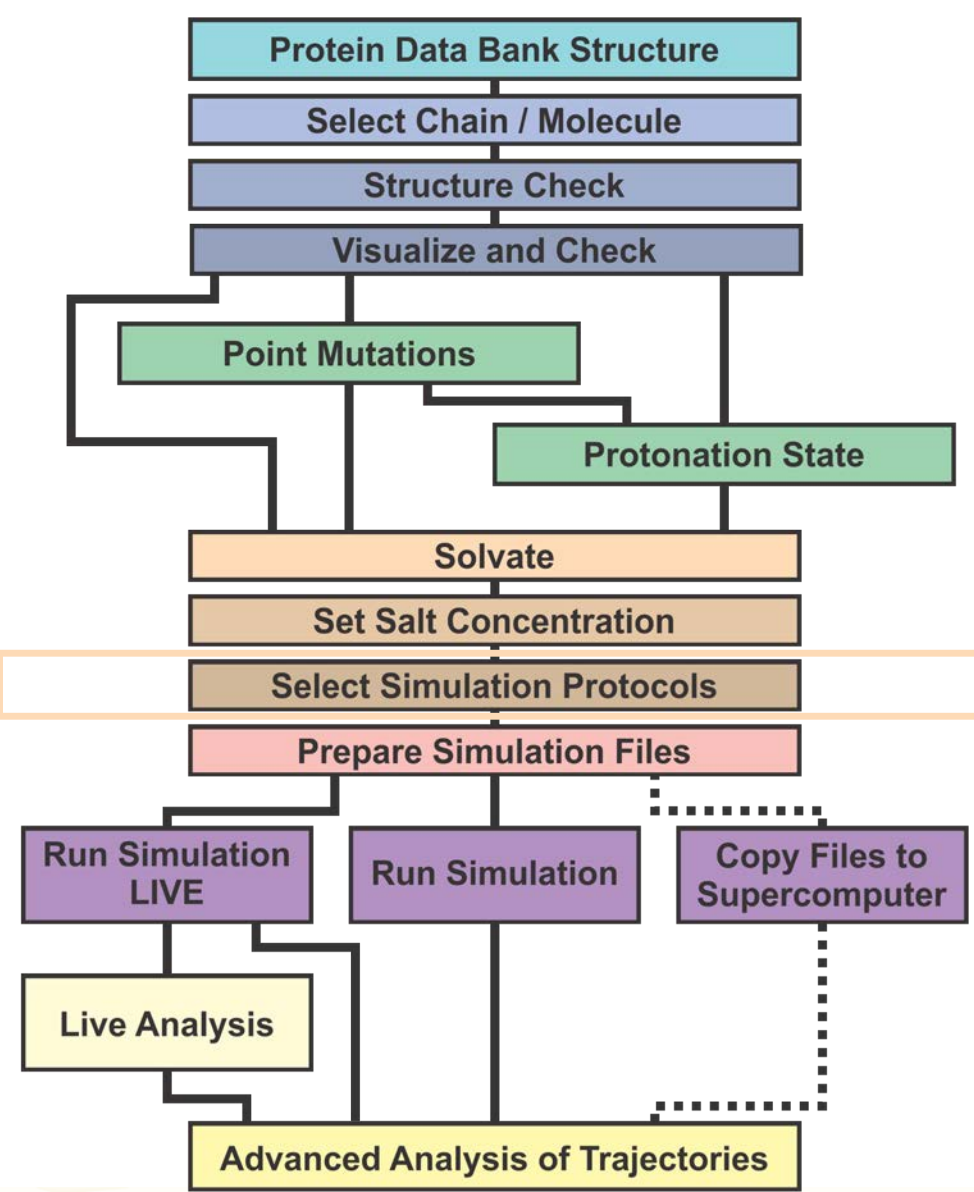
Explicit Solvent + Membrane



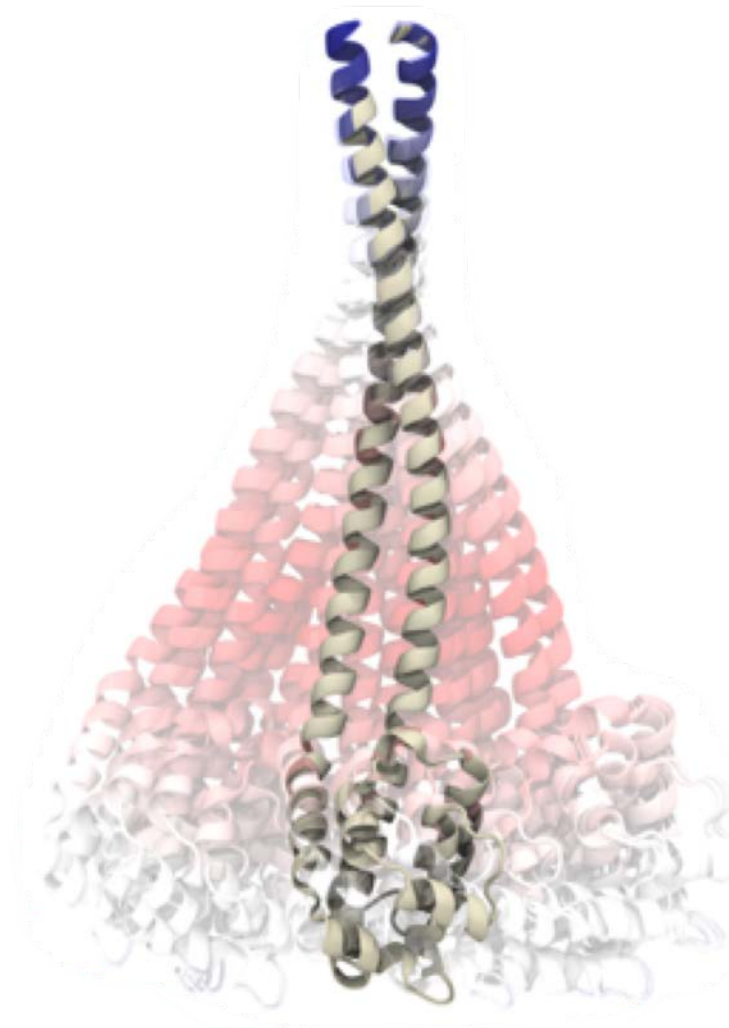
Simulation Environment

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

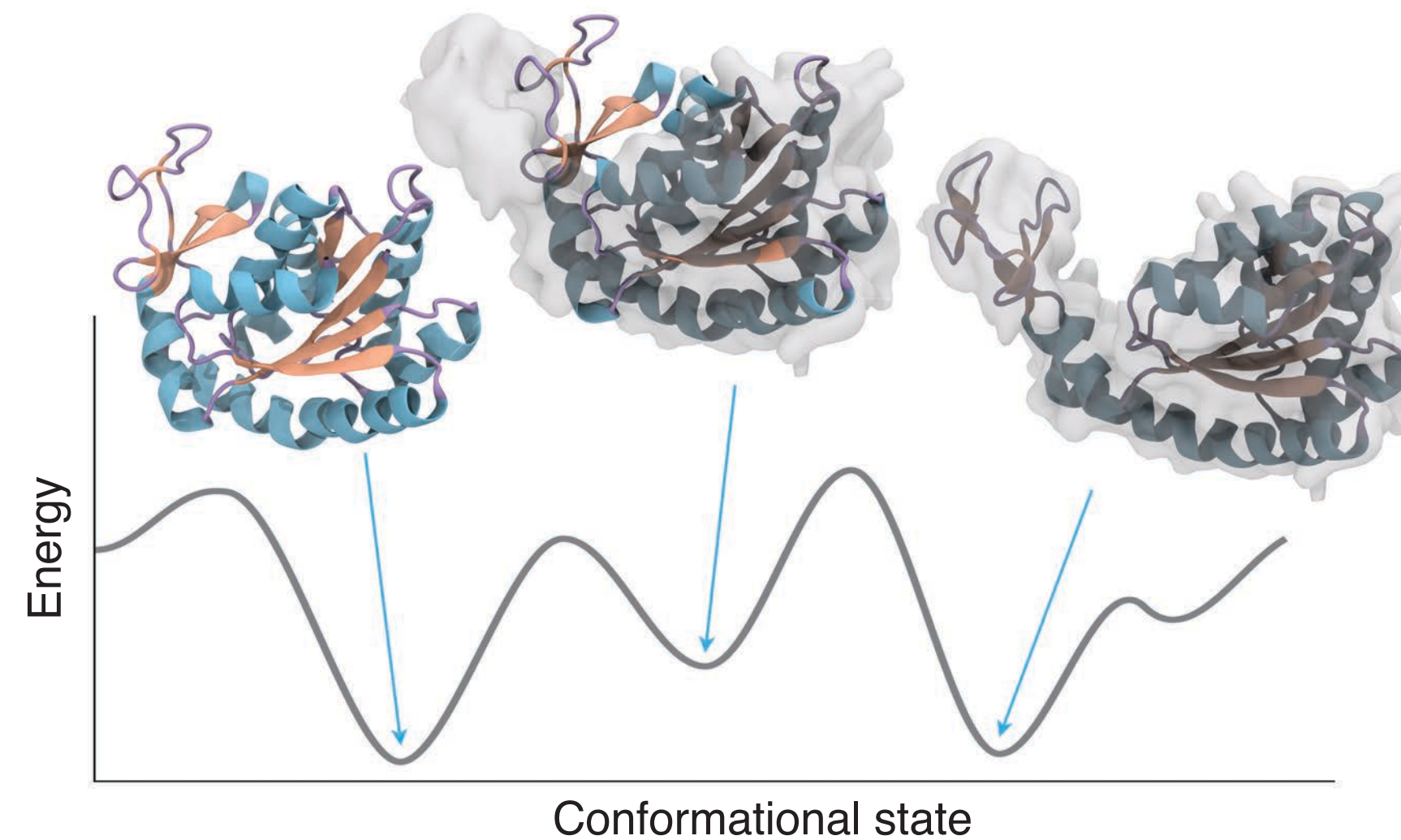
Simulation Protocols



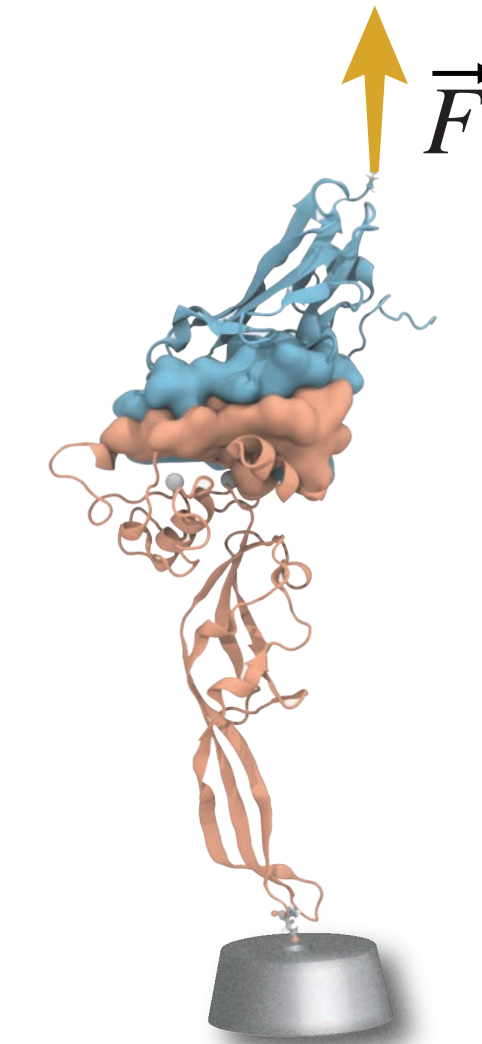
Molecular Dynamics



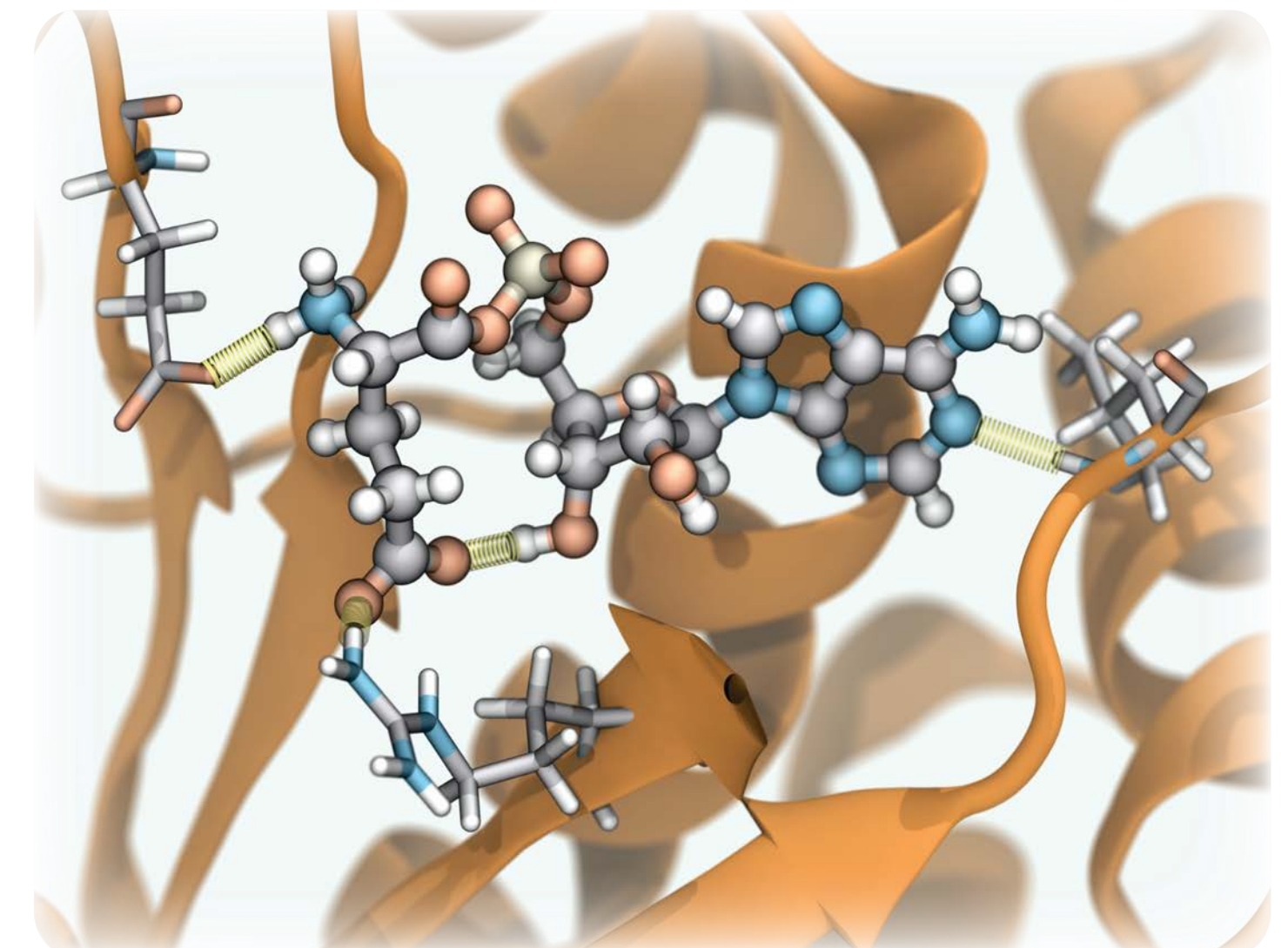
MDFF



Steered MD



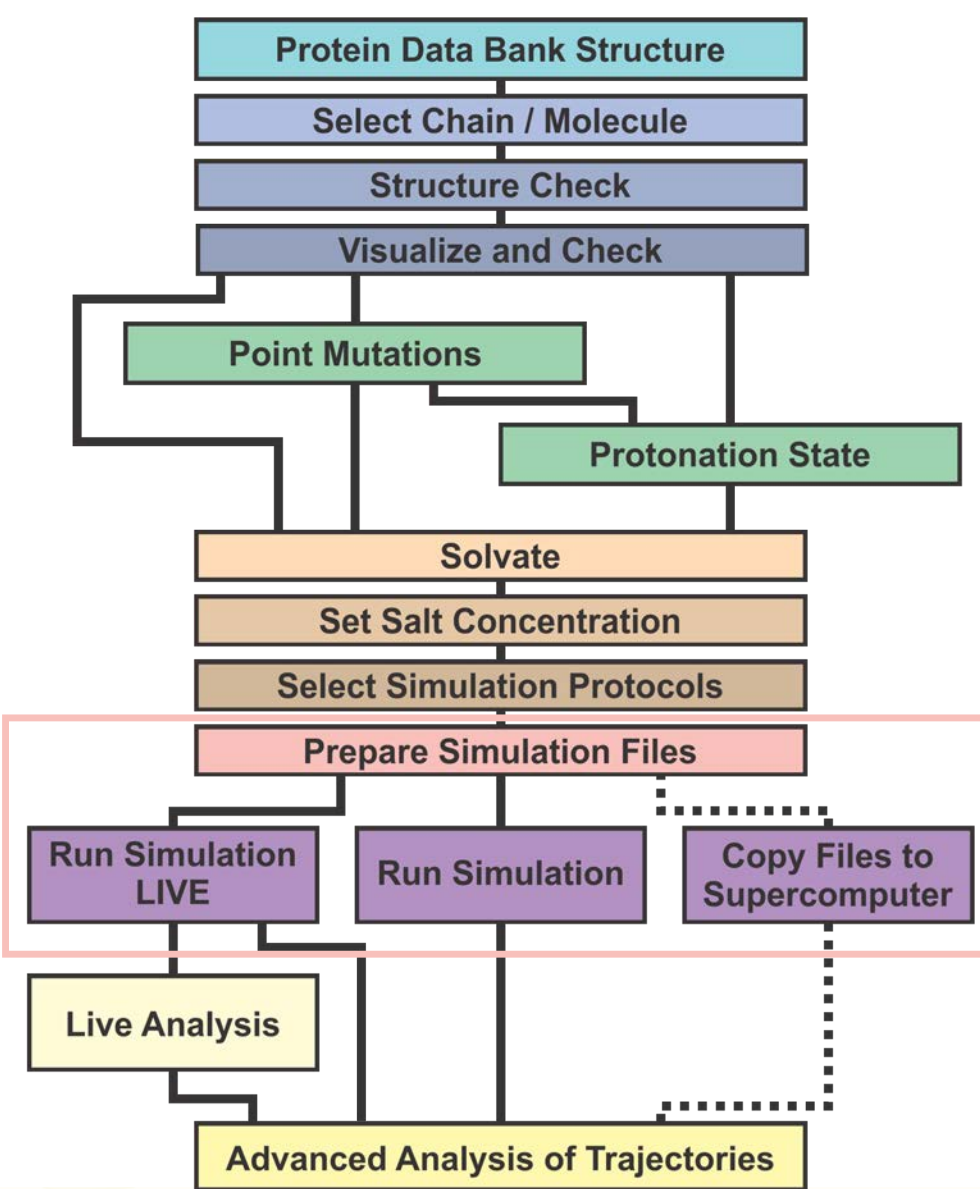
QM/MM (New)



Simulation Protocol

- Molecular Dynamics
- Steered Molecular Dynamics
 - AFM
- Molecular Dynamics Flexible Fitting (MDFF)
 - cryo-EM Densities
- Quantum Mechanics / Molecular Mechanics (QM/MM) Simulations
 - MOPAC and ORCA

QwikMD and Reproducibility



Reproducibility

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

Text File:

- Struct Man. Info
- File Locations
- MD Protocols details:
 - Temperatures
 - Steps
 - Method section (with references)

“InputFileName.qwikmd”
File

“InputFileName”
Folder

“InputFileName.infoMD”
File

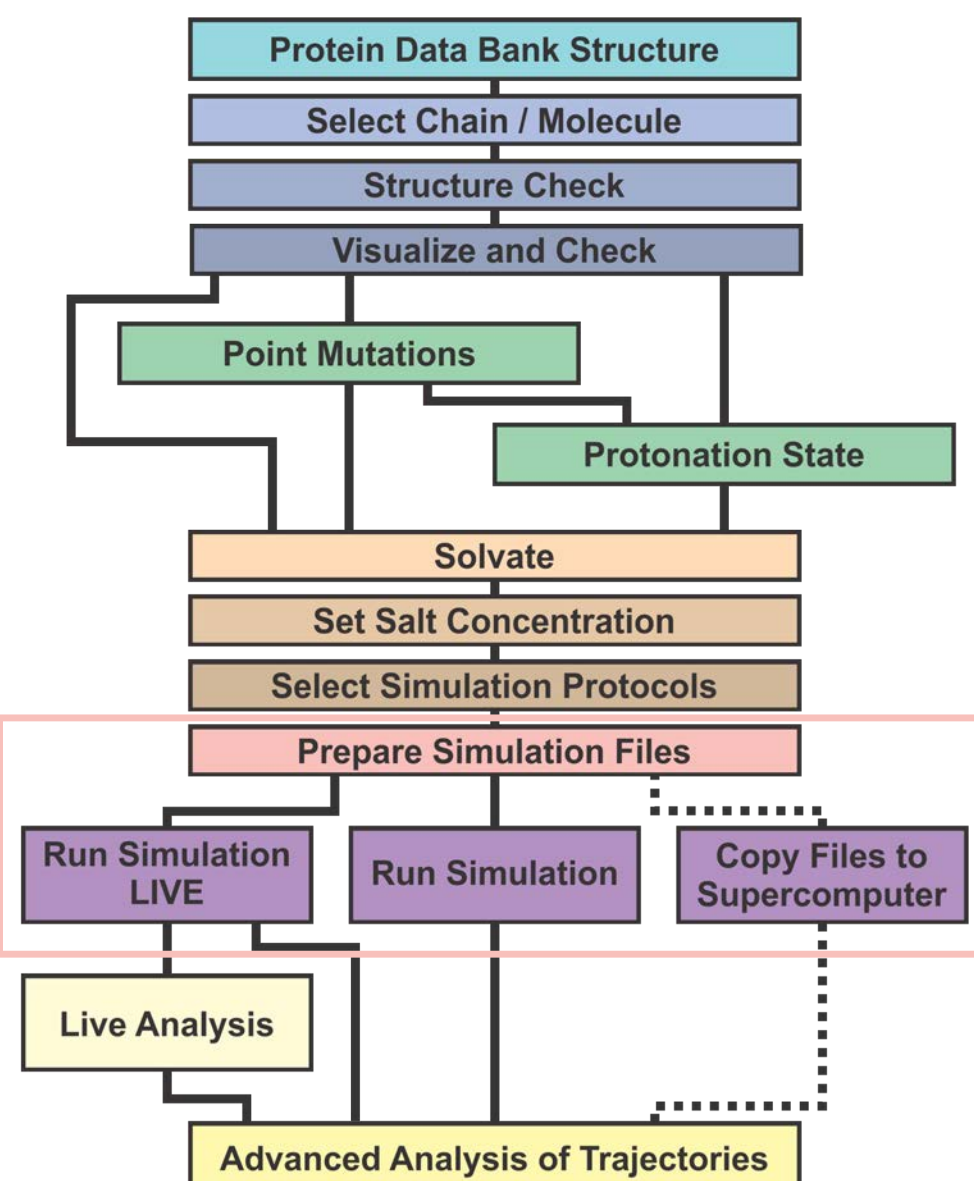
Setup
Folder

Run Folder

- Auxiliary Files
- Intermediary PDBs
- Intermediary PSFs
- Renumber Residues Table
- Topology+Parameter Files

- MD Configuration Files
- PDB Files
- PSF Files
- Parameter Files
- Simulation Log Files
- Simulation Trajectories

QwikMD and Reproducibility



“InputFileName.qwikmd”
File

QwikMD
Inputfile

```

nucleicmcr {(not name QWIKMDDELETE and nucleic)}
proteinmcr {(not name QWIKMDDELETE and protein)}
heteromcr {(not name QWIKMDDELETE and hetero and not
protein and not qwikmd_lipid and not qwikmd_nucleic and not
glycan and not water)}
set QWIKMD::glycanmcr {(not name QWIKMDDELETE and glycan)}
set QWIKMD::lipidmcr {(not name QWIKMDDELETE and lipid)}
atomselect macro qwikmd_protein $QWIKMD::proteinmcr
atomselect macro qwikmd_nucleic $QWIKMD::nucleicmcr
atomselect macro qwikmd_glycan $QWIKMD::glycanmcr
atomselect macro qwikmd_lipid $QWIKMD::lipidmcr
atomselect macro qwikmd_hetero $QWIKMD::heteromcr
$QWIKMD::topGui.nbinp select 0
set QWIKMD::prepared 1
QWIKMD::changeMainTab
$QWIKMD::topGui.nbinp.f1.nb select 0
QWIKMD::ChangeMdSmd 1
set aux "[file rootname $QWIKMD::basicGui(workdir,0)]"
set QWIKMD::outPath ${aux}
cd ${QWIKMD::outPath}/run/
set QWIKMD::inputstrct {Ubiquitin_QwikMD.psf Ubiquitin_QwikMD.pdb}
QWIKMD::LoadButt {Ubiquitin_QwikMD.psf Ubiquitin_QwikMD.pdb}
array set QWIKMD::basicGui {live 0 currenttime {Completed 0.000 of 0.000
ns} length 10.0 desktop white temperature,0 27 temperature,1 27
saltconc,0 0.15 scheme {VMD Classic} mdPrec,0 0 pspeed 2.5 saltions,0 NaCl
mdtime,0 5.0 mdtime,1 4.0 currenttime,0 {} currenttime,1 {} solvent,0
Explicit }
array set QWIKMD::advGui {live 0 currenttime {Completed 0.000 of 0.000 ns
length 10.0 desktop white temperature,0 27 temperature,1 27 saltconc,0
0.15 scheme {VMD Classic} mdPrec,0 0 pspeed 2.5 saltions,0 NaCl mdtime,0
5.0 mdtime,1 4.0 currenttime,0 {} currenttime,1 {} solvent,0 Explicit
addmol 10 protocoltb,SMD,1,restrIndex {} protocoltb,MD,0 Minimization
membrane,effect translate protocoltb,MD,1 Annealing analyze,basic,selcomb
backbone protocoltb,SMD,2,lock 0 protocoltb,MD,2 Equilibration
protocoltb,MD,3 MD scheme {VMD Classic} membrane,multi 1
protocoltb,SMD,2,restrsel {} protocoltb,MD,0,smd 0
protocoltb,MD,0,restrsel {} protocoltb,MD,2,smd 0 mdff.min 200
    
```

“InputFileName.infoMD”
File

“Methods
Section”
format

```

===== MD Protocols =====

ionized.psf was prepared using VMD[2] and the plugin QwikMD[3].
simulations in the present study were performed employing the NAMD molecular dynamics
[4]. The CHARMM36 force field[5,6] was used in all MD simulations.

The Minimization and Constrained equilibration MD Simulation was performed with explicit
solvent using the TIP3 water model[1] in the NpT ensemble.
A temperature ramp was performed consisting of 0.24 ns of simulation where the temperature was
raised from 60 K to 300.00 K The pressure was maintained at 1 atm using Nosé-Hoover Langevin
piston[7,8]. A distance cut-off of 12.0 Å was applied to short-range, non-bonded interactions,
and 10.0 Å for the smothering functions. Long-range electrostatic interactions were treated
using the particle-mesh Ewald (PME)[9] method. The equations of motion were integrated using
the r-RESPA multiple time step scheme[4] to update the short-range interactions every 1 steps
and long-range electrostatics interactions every 2 steps. The time step of integration was
chosen to be 2 fs for all simulations. Before the MD simulations all the systems were submitted
to an energy minimization protocol for 1000 steps. In this step consisted of 1.00 ns of
simulation, the atoms defined by the selection "protein and backbone" were restrained.

The MD Simulation without constrains was performed with explicit solvent using the TIP3 water
model[1] in the NpT ensemble.
The temperature was maintained at 300.00 K using Langevin dynamics. The pressure was
maintained at 1 atm using Nosé-Hoover Langevin piston[7,8]. A distance cut-off of 12.0 Å was
applied to short-range, non-bonded interactions, and 10.0 Å for the smothering functions.
Long-range electrostatic interactions were treated using the particle-mesh Ewald (PME)[9]
method. The equations of motion were integrated using the r-RESPA multiple time step scheme[4]
to update the short-range interactions every 1 steps and long-range electrostatics interactions
every 2 steps. The time step of integration was chosen to be 2 fs for all simulations. In this
step consisted of 5.0 ns of simulation, no atoms were constrained.

Bibliography:
{1} Jorgensen, W. L., Chandrasekhar, J., Madura, J. D., Impey, R. W. and Klein, M. L.,
"Comparison of simple potential functions for simulating liquid water", J. Chem. Phys., 1983,
vol 79, 6127-6129.
{2} Humphrey, W., Dalke, A. and Schulten, K., "VMD - Visual Molecular Dynamics", J. Molec.
Graphics, 1996, vol. 14, pp. 33-38.
{3} Ribeiro, J. V., Bernardi, R. C., Rudack, T., Stone, J. E., Phillips J. C., Freddolino P. L.
and Schulten, K., "QwikMD-integrative molecular dynamics toolkit for novices and experts", Sci.
Rep., 2016
{4} Phillips J. C., Braun, R., Wang, W., Gumbart, J., Tajkhorshid, E., Villa, E., Chipot,
C., Skeel, R. D., Kale, L., and Schulten, K., "Scalable molecular dynamics with NAMD", J.
Comp. Chem, 2005, vol 26, pp. 1781-1802
    
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Reproducibility

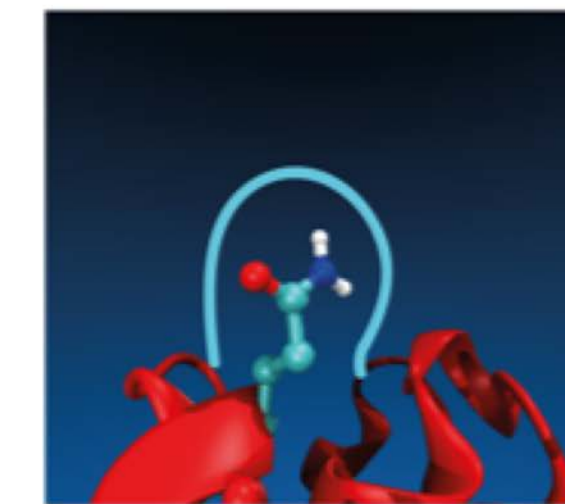
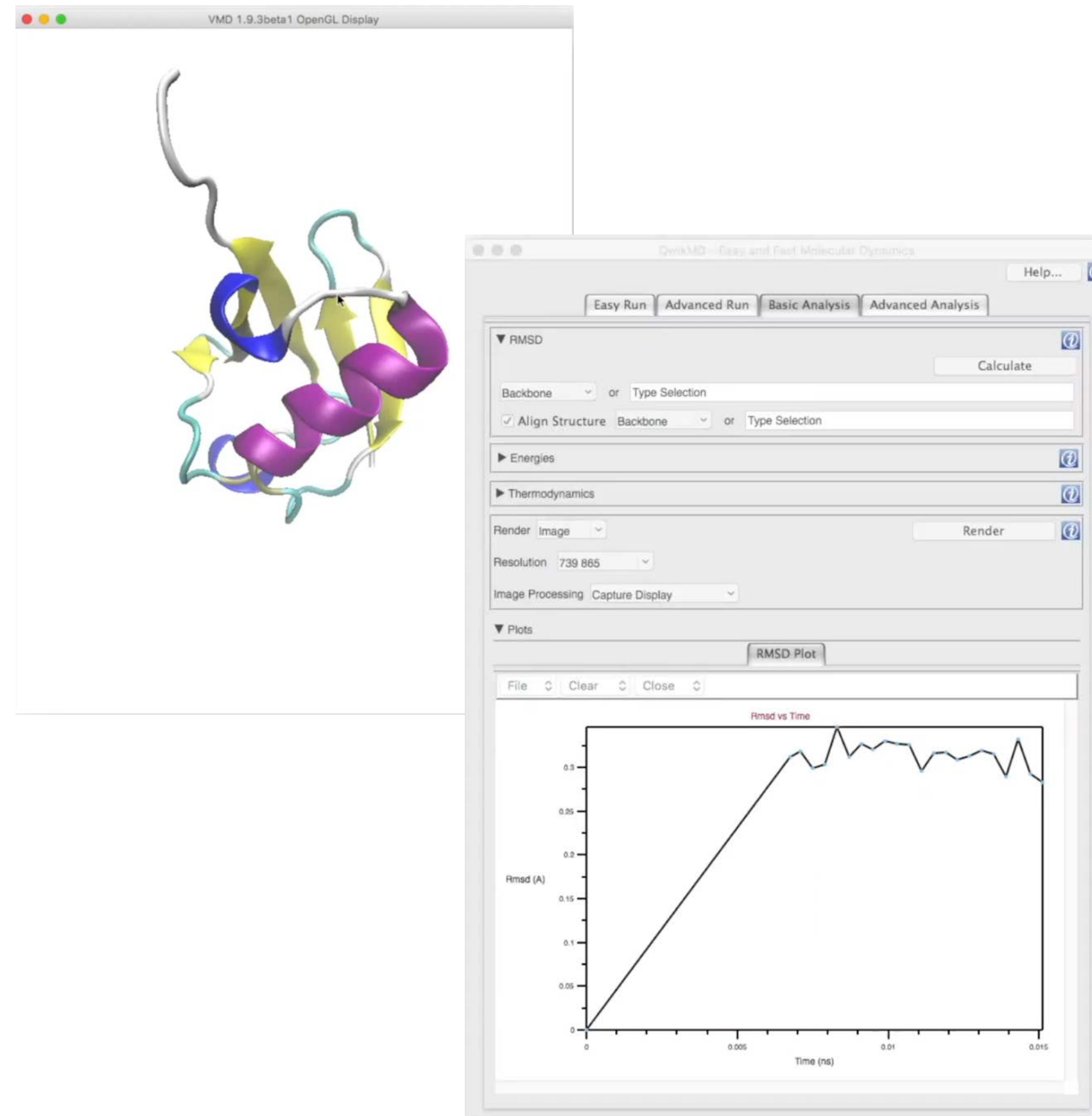
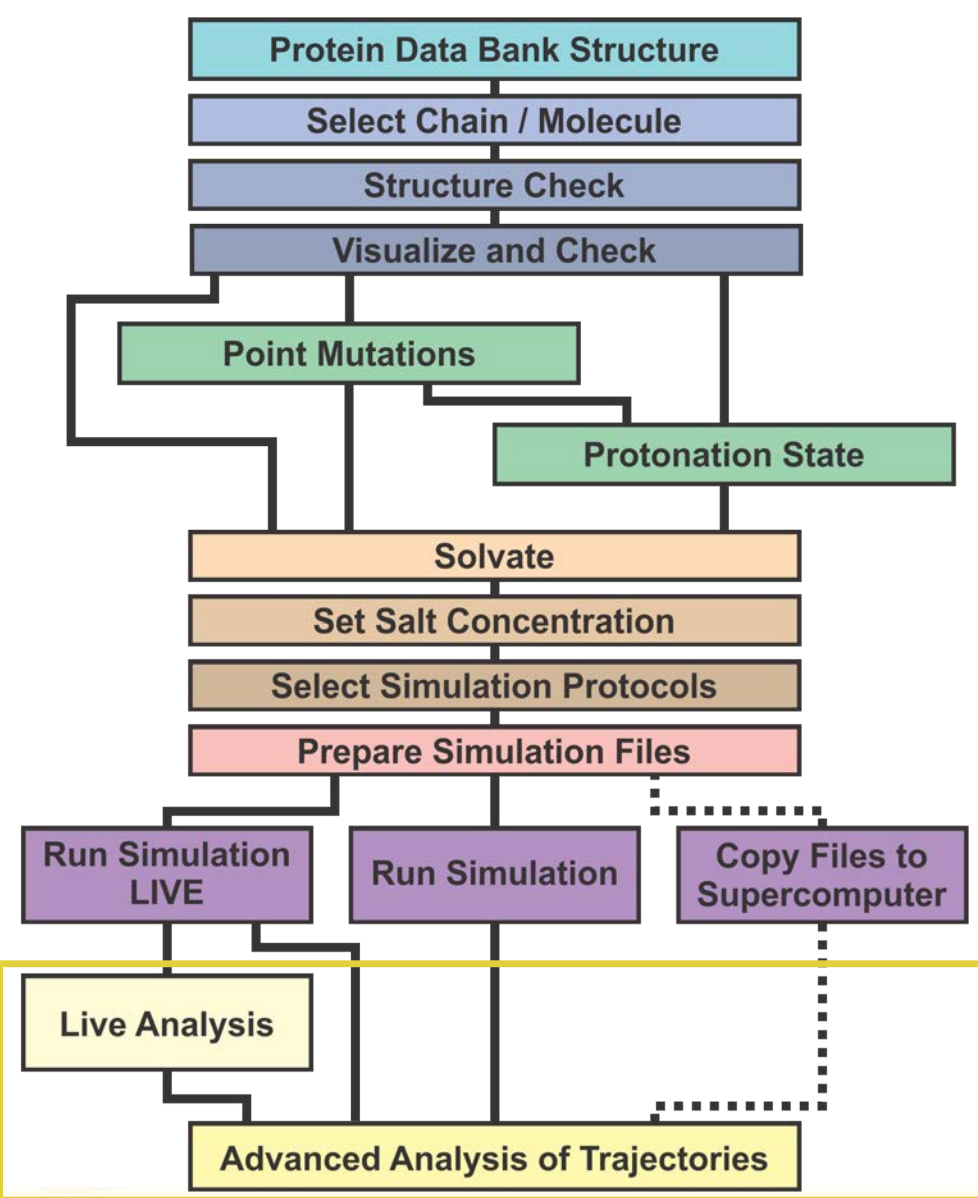
- All Steps Logged
- Loading Script and Text Log Files
- Reproduce and/or Share the Process and the End Result

Load Simulation Trajectories and Analysis

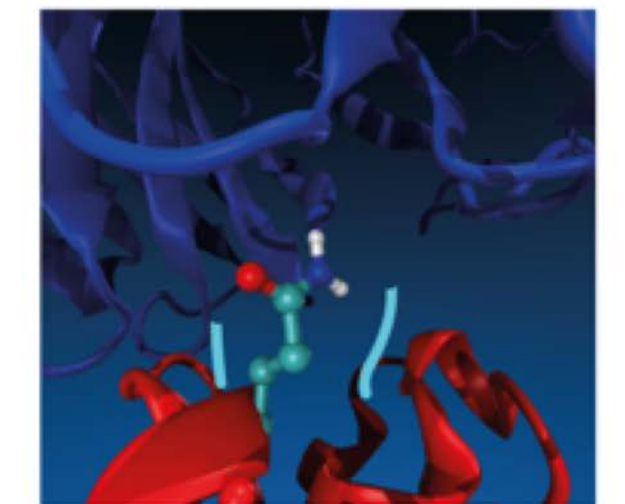
Live Simulation and After Load Analysis

Contact Area

First Implemented in CompASM as Hot Spots Filter

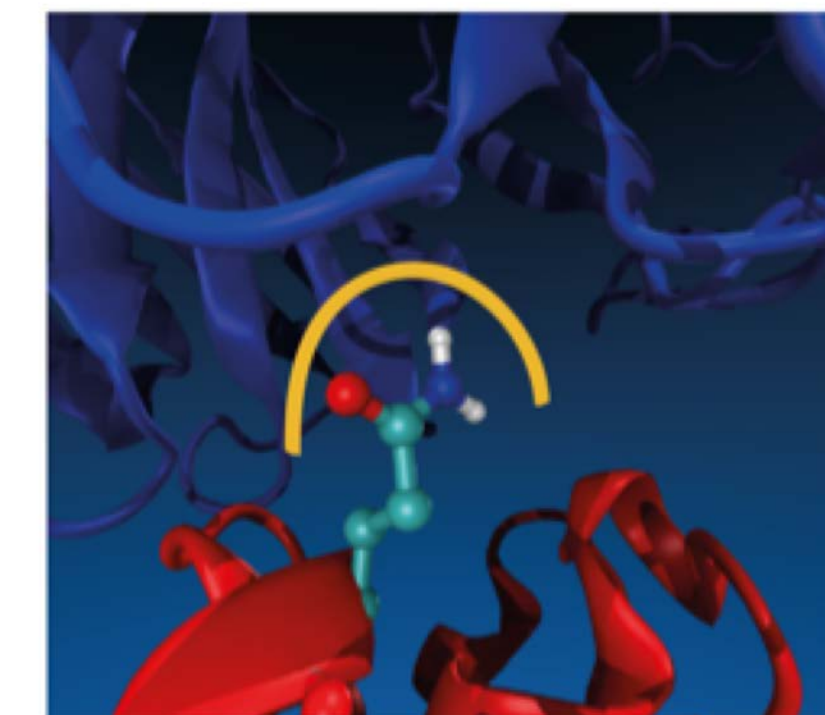


—



Ligand SASA *subtracted*

Ligand SASA in the presence of the Receptor



Ligand Exposed/Contact Surface Area

Analyses Available:

- Energies
- Temperature, Pressure and Volume
- RMSD
- Hydrogen Bonds
- SASA
- **Contact Area**
- QM Energies

Load Simulation Trajectories and Analysis

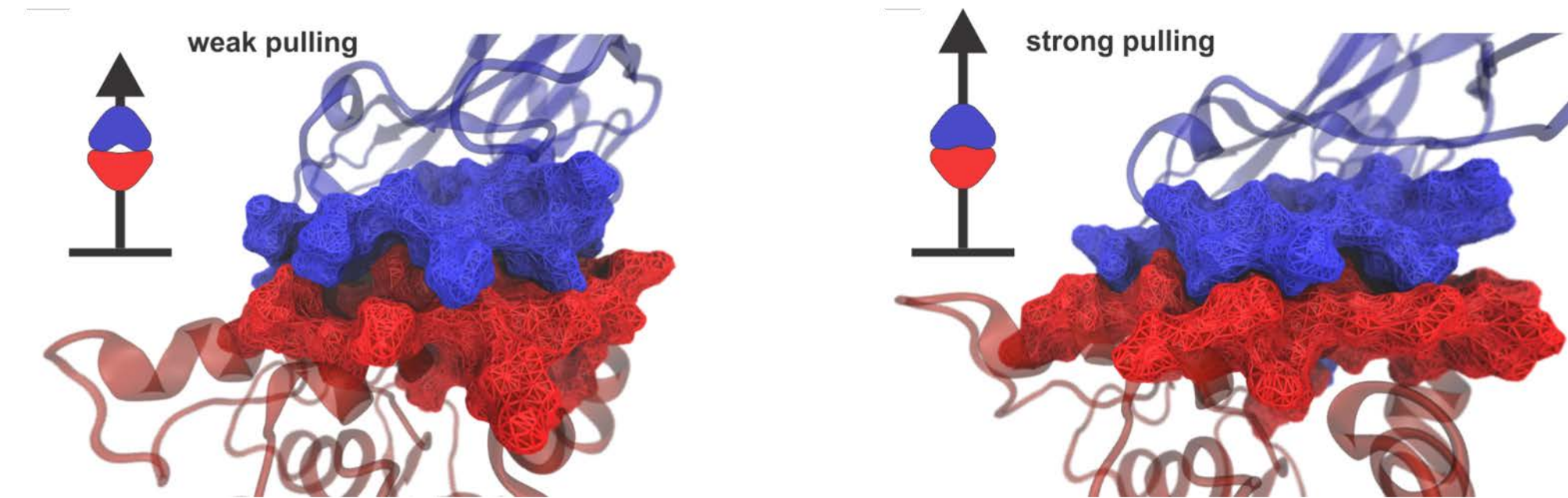
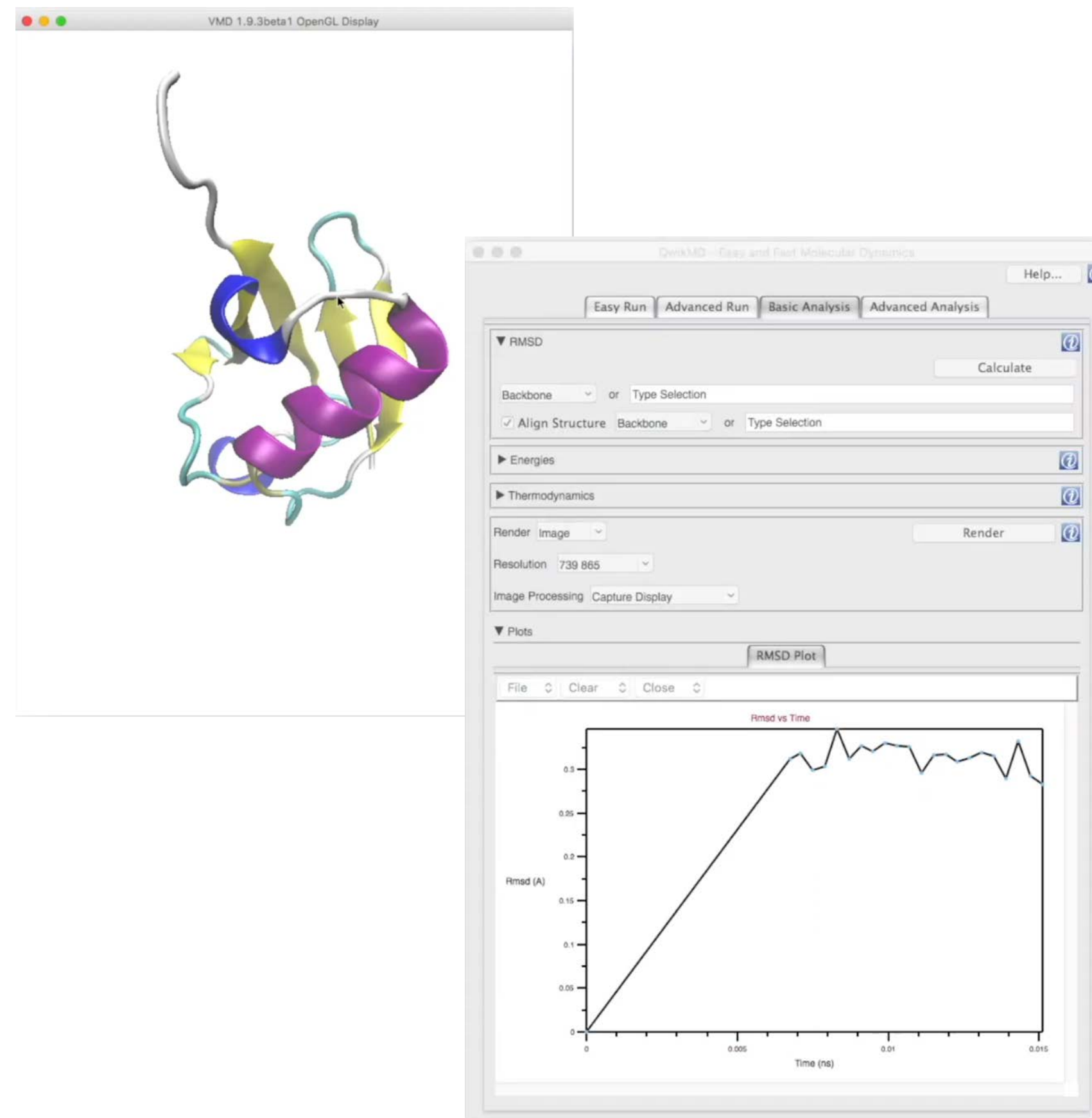
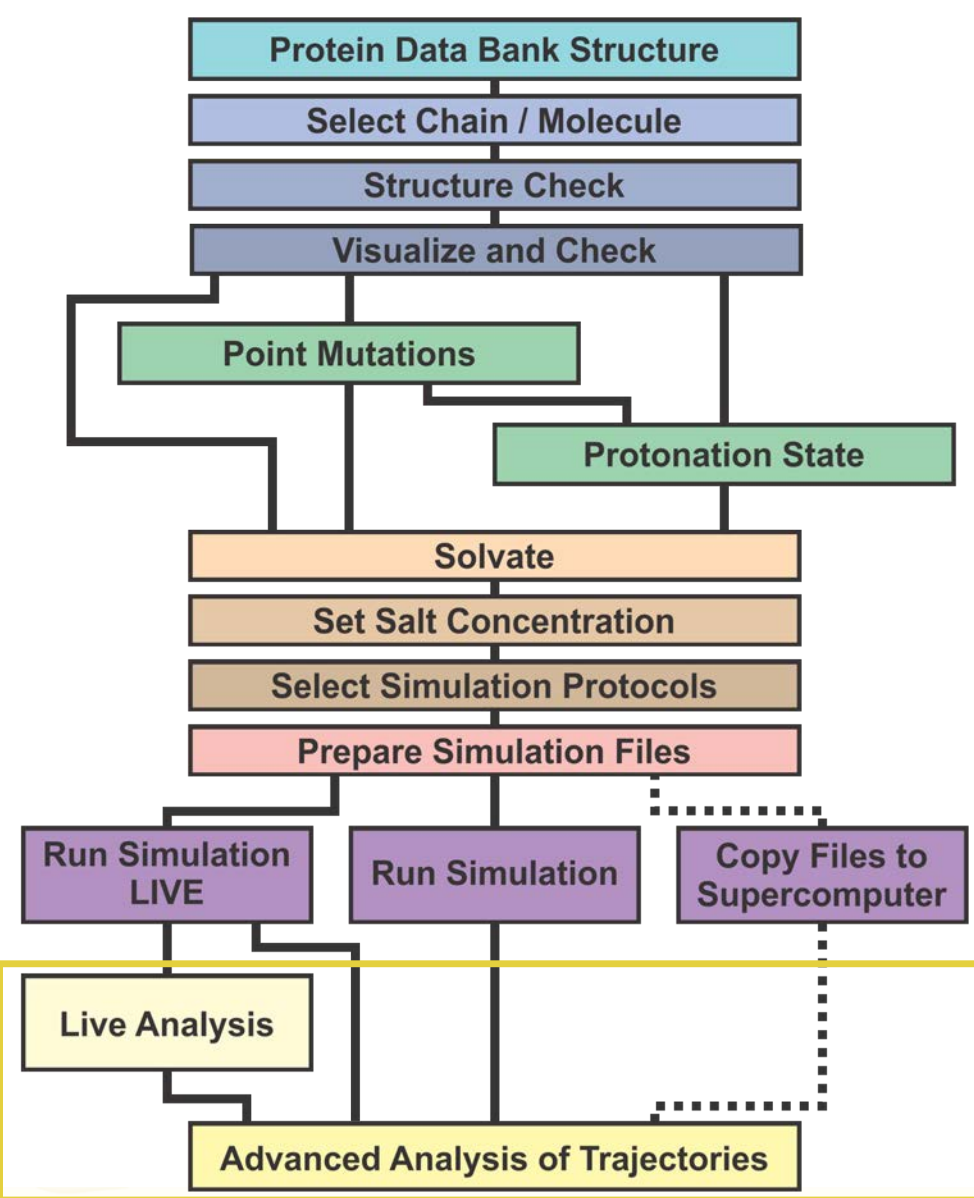


Dr. Rafael Bernardi

Live Simulation and After Load Analysis

Contact Area

First Implemented in CompASM as Hot Spots Filter

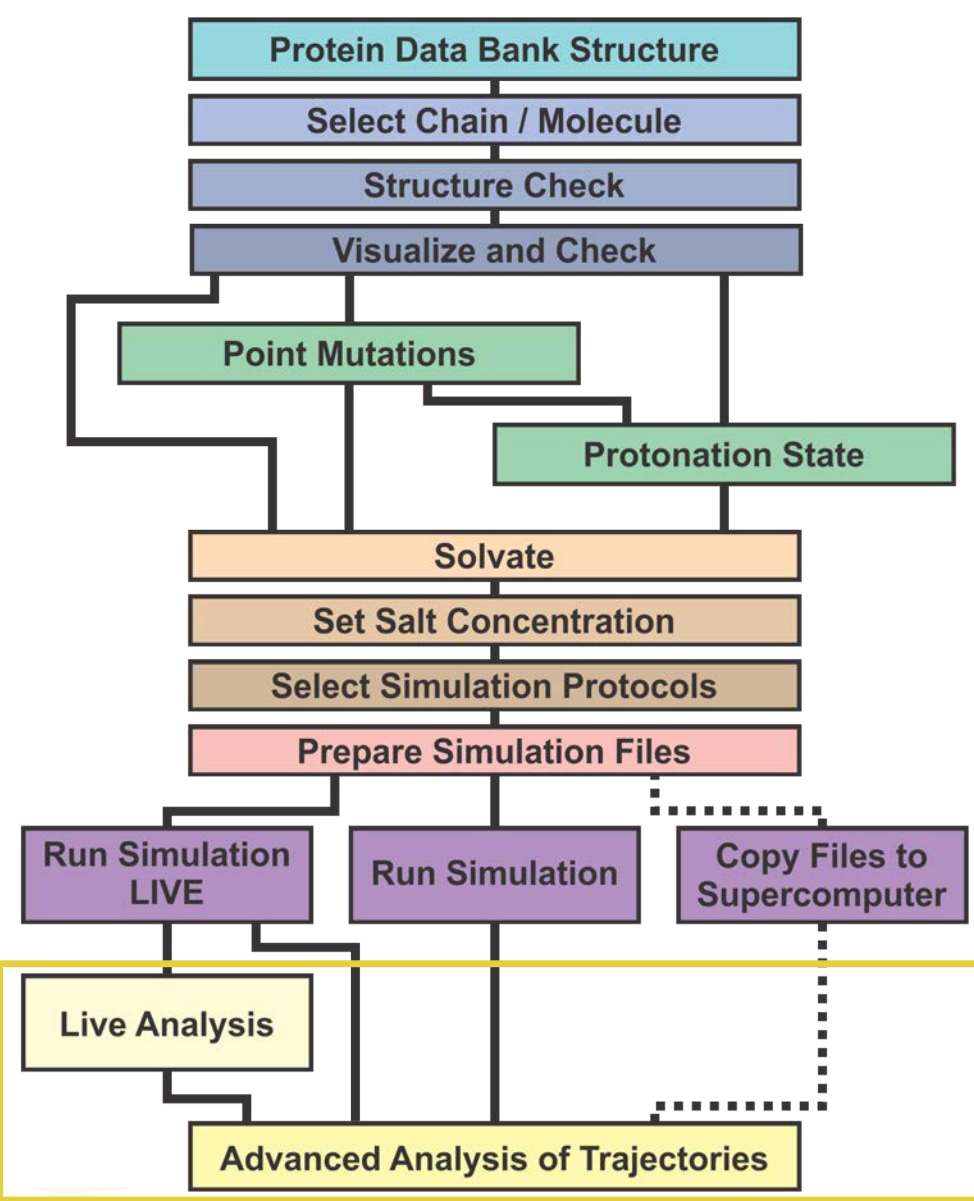


Schoeler C., et al., Ultrastable cellulosome-adhesion complex tightens under load, *Nat. Commun.*, **2014**, 6, 5635.

Analyses Available:

- Energies
- Temperature, Pressure and Volume
- RMSD
- Hydrogen Bonds
- SASA
- **Contact Area**
- QM Energies

New QM/MM Simulation and Orbitals Visualization



Analyses Available:

- Energies
- Temperature, Pressure and Volume
- RMSD
- Hydrogen Bonds
- SASA
- Contact Area
- QM Energies
- **QM Orbitals Visualization**
- **Nature Methods 2018**

QwikMD - Easy and Fast Molecular Dynamics

Browser: 4b9f_QwikMD.psf 4b9f_QwikMD.pdb

NMR State: Chain/Type Selection

Chain	Residue Range	Type	Representation	Color
A	1 - 152	protein	NewCartoon	0 blue
A	153 - 153	hetero	Licorice	Name
A	2002 - 2230	water	VDW	Name

Background: Black, White, Gradient. Color Scheme: VMD Classic

Resolution: 1080p. Quality: Max

MD: SMD, MDFF, QM/MM

Solvent: Explicit. Buffer: 12. A

Salt Concentration: 0.15 mol/L. Choose Salt: NaCl

Protocol:

Protocol	n Steps	Restrains	Ensemble	Temp (C)	Pressure (atm)
GMMM-Min	100	backbone	NpT	0	1
GMMM-Ann	720	backbone	NpT	27	1
GMMM-Equi	100	backbone	NpT	27	1
GMMM	500000	none	NpT	27	1

QM Regions:

QM ID	n Atoms	Charge	Mult	COM
1	14	1.00	1	none

QM Options:

QM Software: ORCA. Live Solv. Mode: Off

Point Charges: On. QM Switching: Switch

Custom PC: Off

QM Point Charge Scheme: Round. Print Orbitals: [checked]

QM Bond Scheme: CS. Traj. Frequency Steps: [1]

QM Command: PK3 EnGrad printbasis

```

    Line %output PrintLevel Mini Print[ P Mulliken \ 1 Print[ P_AtCharges_M \ 1 e
          %output Print[ P_Basis \ 2 Print[ P_MOs \ 1 end
  
```

Simulation Setup: /ssd2/ribeiro/GMMM/test3.qwikmd

Simulation Control: Start GMMM-Ann Simulation

Buttons: Pause, Detach, Finish

Orbitals Table:

Orb. Number	Description	Energy
12	HOMO-5	-0.481420010328
13	HOMO-4	-0.477629983386
14	HOMO-3	-0.449580013752
15	HOMO-2	-0.413480013609
16	HOMO-1	-0.360720006612
17	HOMO	-0.313400000334
18	LUMO	0.06397999231
19	LUMO+1	0.080930002034
20	LUMO+2	0.107110001147
21	LUMO+3	0.120619997382

QM Region 1 Orbitals Energy vs Time

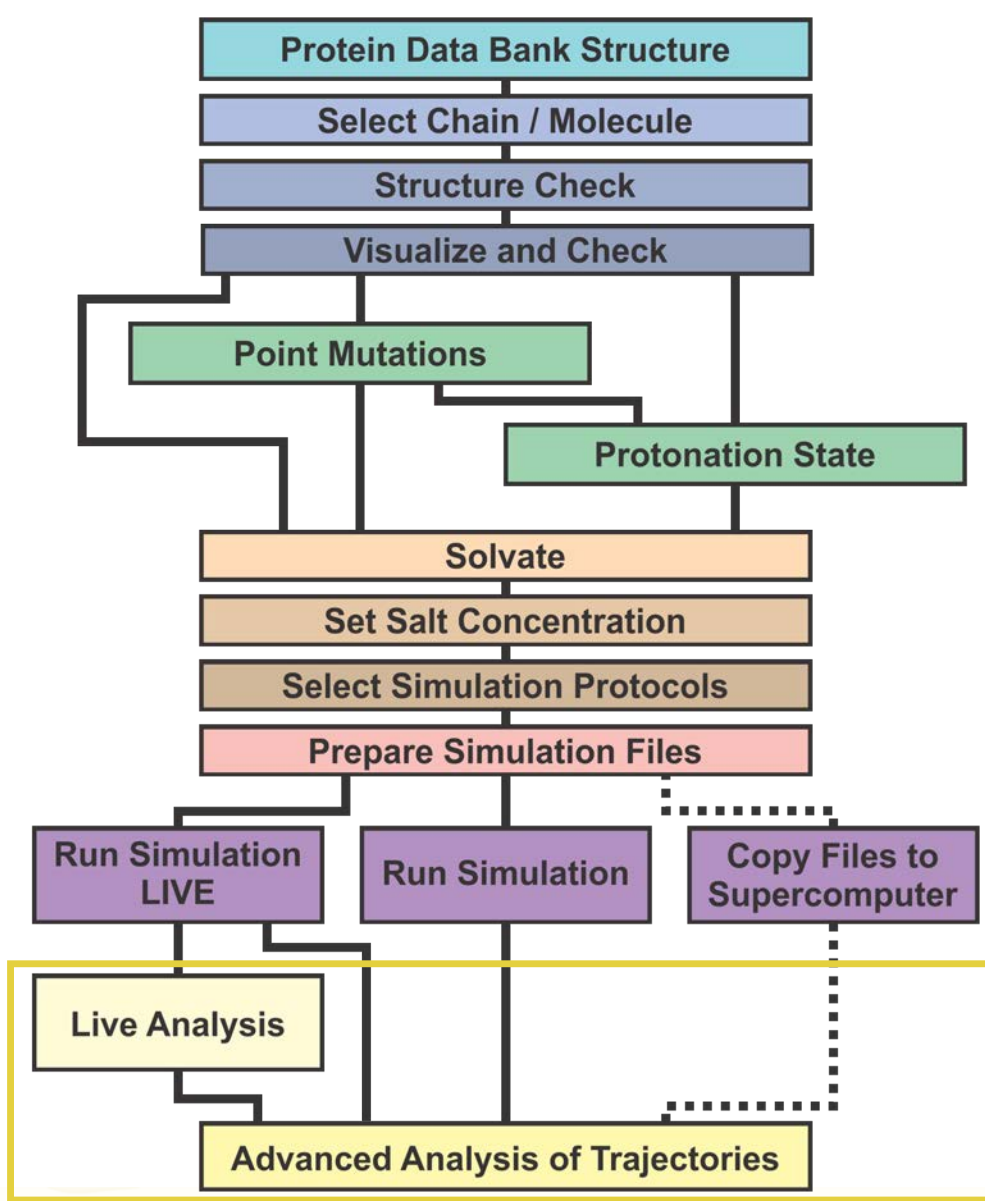
Orbital Energy vs Time (ps)

Time (ps): -0.1, 0, 0.1, 0.2, 0.3, 0.4, 0.5

Orbital Energy: -0.6, -0.55, -0.5, -0.45, -0.4, -0.35, -0.3, -0.25, -0.2, -0.15, -0.1, -0.05, 0, 0.05, 0.1, 0.15, 0.2, 0.25

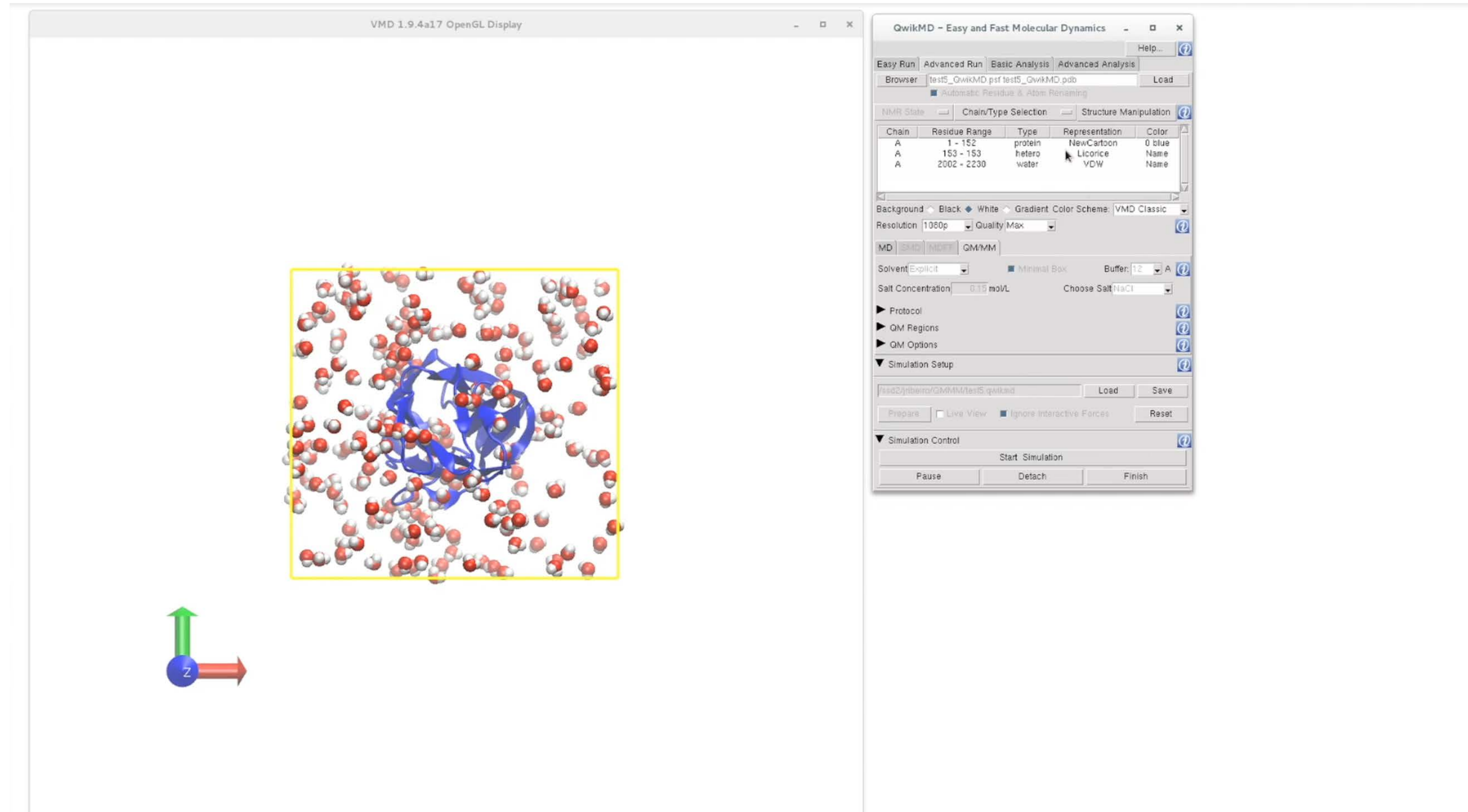
Energy values at 0, 0.2, and 0.4 ps: 0.37935, 0.37738, 0.37735

New QM/MM Simulation and Orbitals Visualization



Analyses Available:

- Energies
- Temperature, Pressure and Volume
- RMSD
- Hydrogen Bonds
- SASA
- Contact Area
- QM Energies
- **QM Orbitals Visualization**
- **Nature Methods 2018**



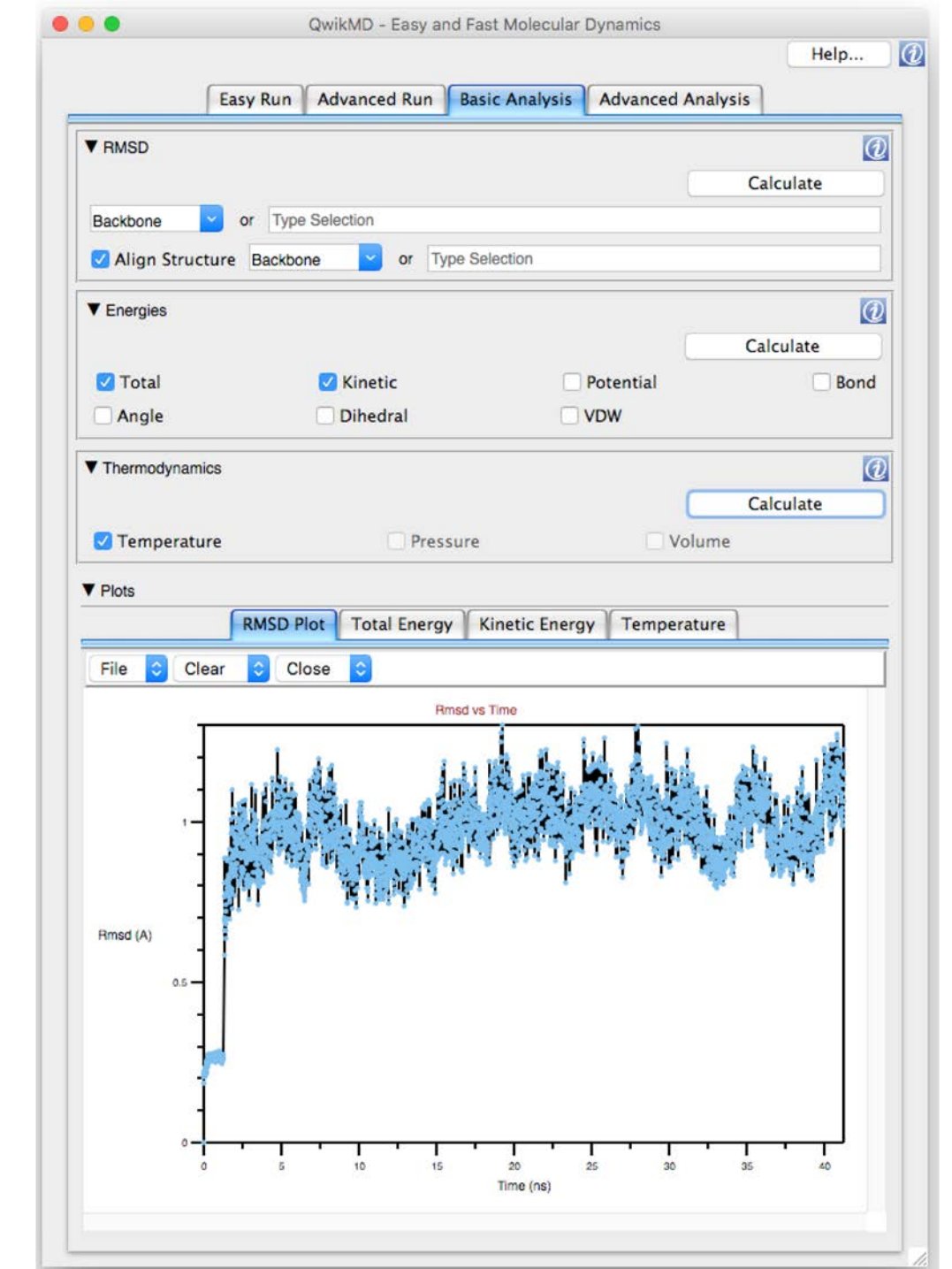
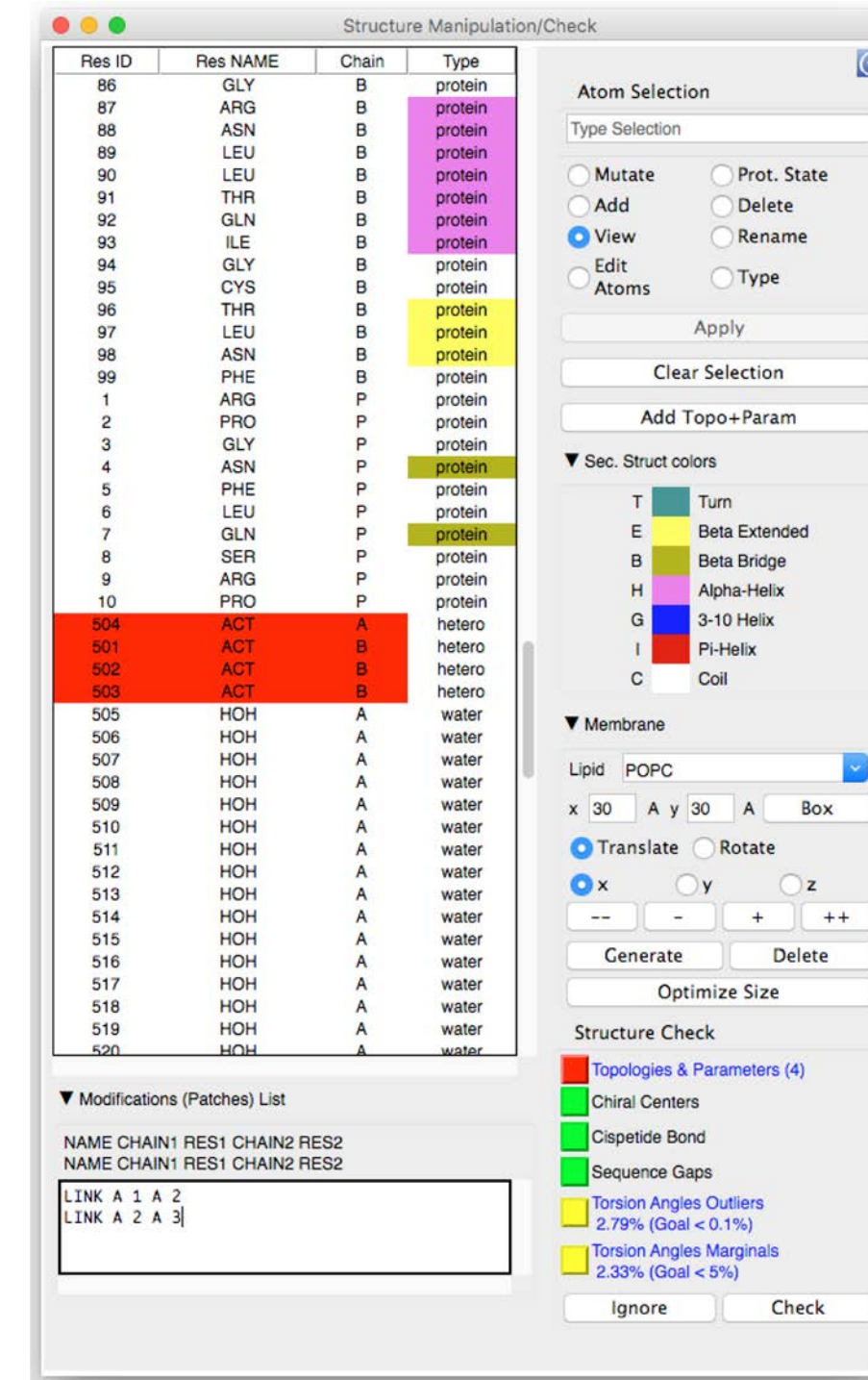
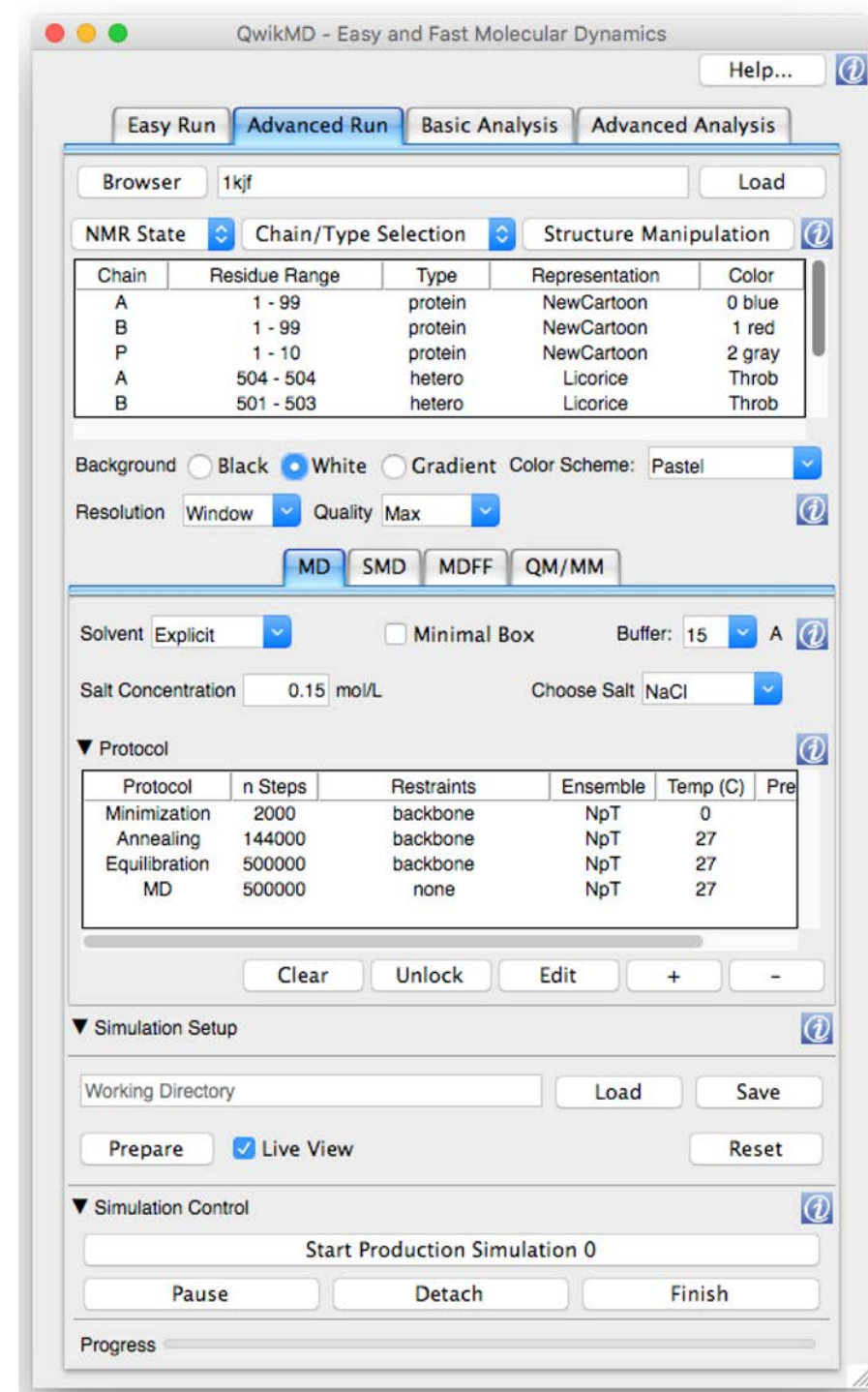
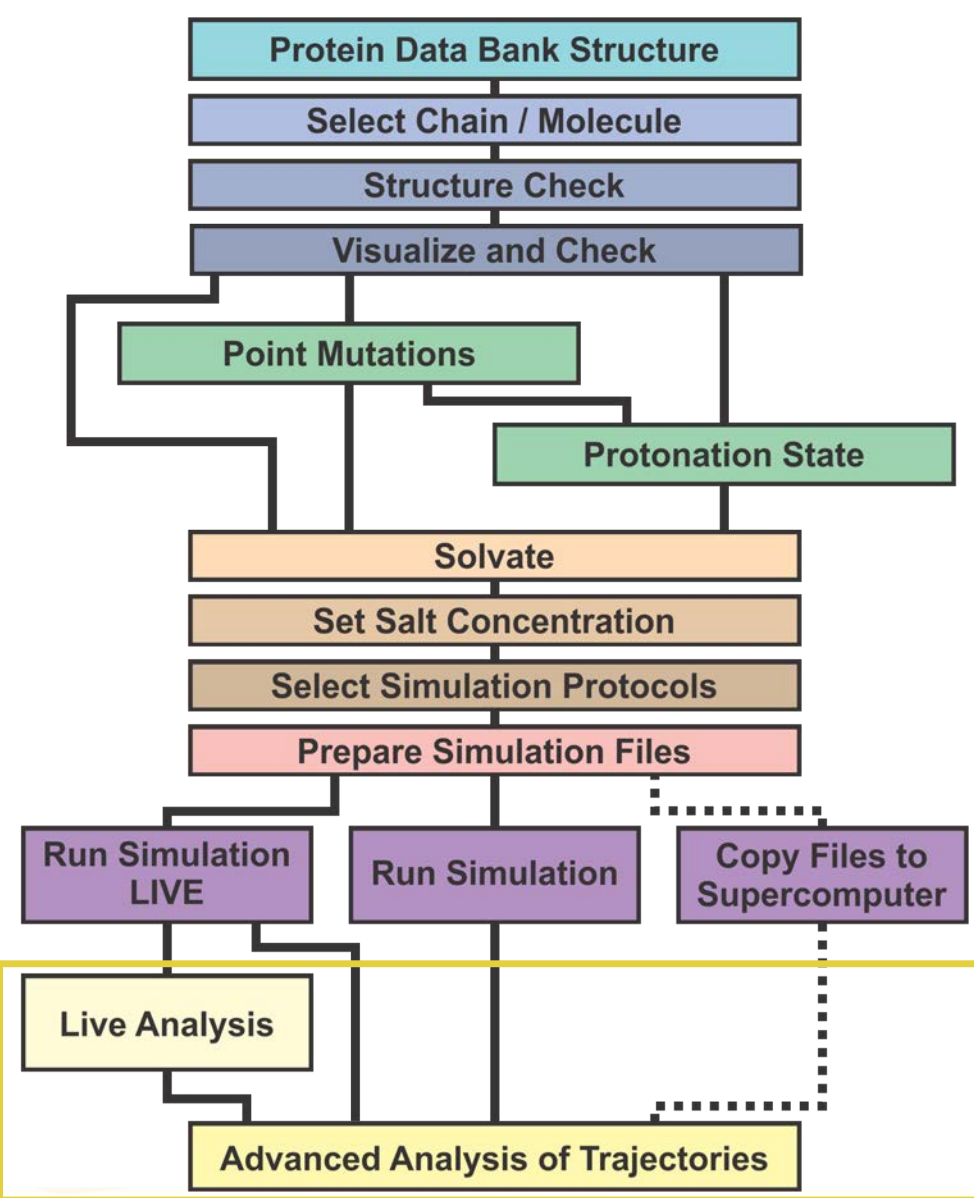
ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0	T	A	D	F	testS_QwikMD.psf	23334	924	0

QwikMD Graphical User Interface

Simulation Preparation

Struct. Manipulation

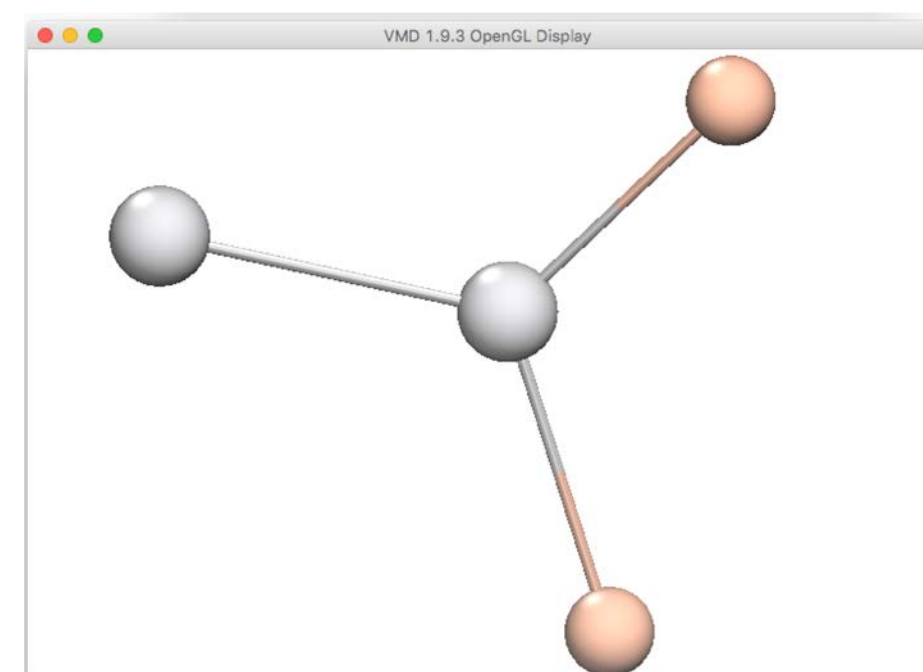
Simulation Analysis



Other Features:

- Info Buttons
- Simulation Controls

Atom Editing



Edit Atoms

Index	Resname	Res ID	Chain ID	Atom Name	Element	Type
1	ACET	504	A	C2	C	hetero
2	ACET	504	A	O1	O	hetero
3	ACET	504	A	O2	O	hetero
4	ACET	504	A	C1	C	hetero

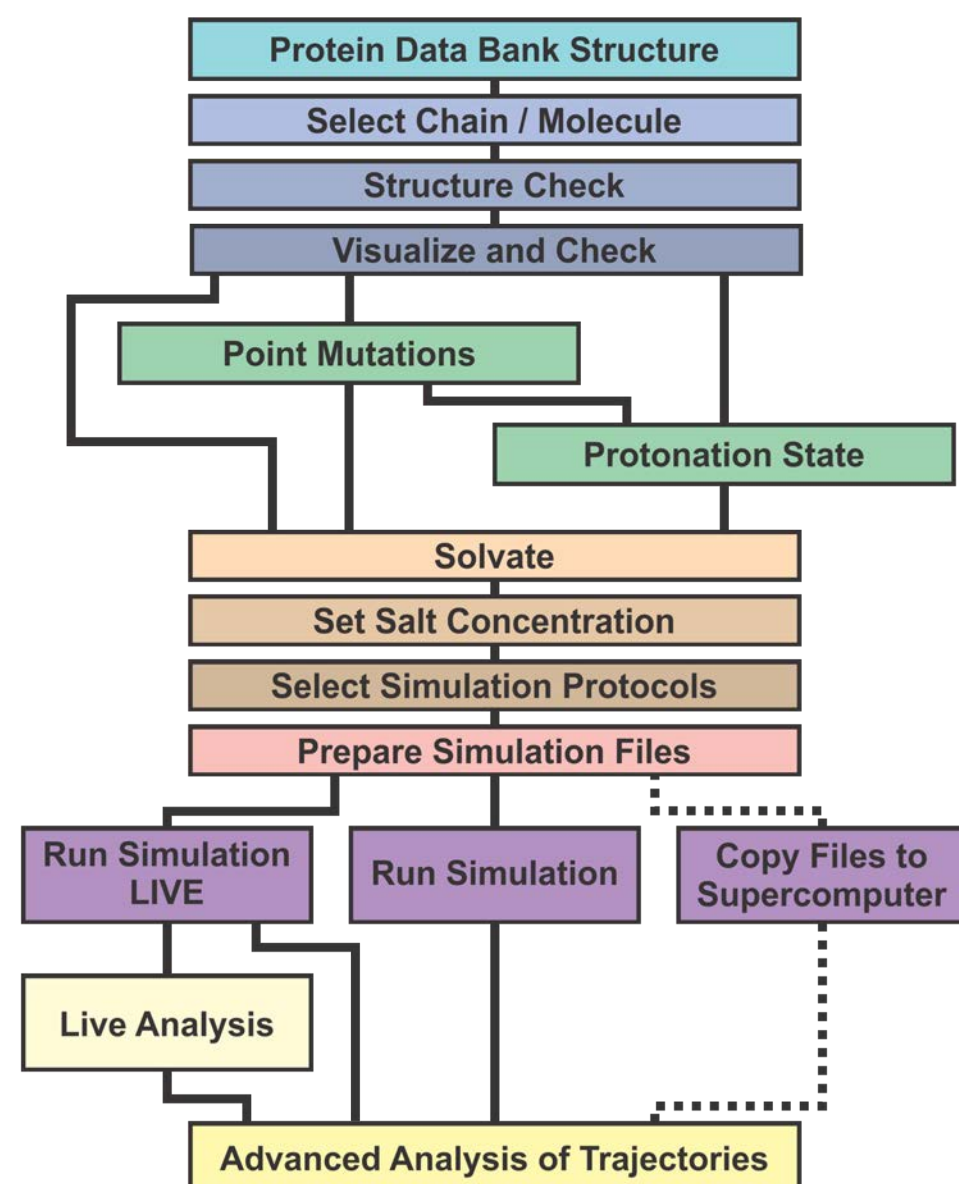
Topology File: top_all136_cgenff.rtf

```

RES1 ACET -1.00 ! C2H3O2 acetate, K. Kuczerc
GROUP
ATOM C1 CG331 -0.37 | | | |
ATOM C2 CG203 0.62 ! | H1 | O1 (-)
ATOM H1 HGA3 0.09 ! | | |
ATOM H2 HGA3 0.09 ! H2--C1--C2
ATOM H3 HGA3 0.09 ! | | \\
ATOM O1 OG2D2 -0.76 ! | H3 | O2
ATOM O2 OG2D2 -0.76
BOND C1 H1 C1 H2 C1 H3
BOND C1 C2 C2 O1
DOUBLE C2 O2
IMPR C2 O2 O1 C1
  
```

Delete Ok Cancel

QwikMD Papers



[Ribeiro, J. V, et al., QwikMD – Integrative Molecular Dynamics Toolkit for Novices and Experts. Scientific Reports, 2016, 6, 26536.](#)



[Melo, M. C. R., et al., NAMD goes quantum: an integrative suite for hybrid simulations. Nature Methods. 2018, 15:5](#)

OPEN **QwikMD—Integrative Molecular Dynamics Toolkit for Novices and Experts**









Received: 10 March 2016
Accepted: 03 May 2016
Published: 24 May 2016

João V. Ribeiro^{1,2,*}, Rafael C. Bernardi^{1,2,*}, Till Rudack^{1,*}, João V. Ribeiro^{1,2,*}, Peter L. Freddolino³ & Klaus Schulten^{1,2,4}

The proper functioning of biomolecules in living cells requires them to undergo conformational changes. Both biomolecular structure and function are highly dynamic, and a wide variety of techniques, but none offers the level of detail required for understanding the underlying mechanisms. Integrating two widely used modeling programs, we created a robust, user-friendly software, QwikMD, which enables the simulation of biomolecular systems, where often only molecular dynamics simulations are used. Performing both simple and advanced MD simulations as many steps as necessary for preparing, carrying out, and analyzing the results, QwikMD meets the needs of researchers by increasing the efficiency and quality of their work by carrying out simulations on a small laptop or performing complex and large simulations on supercomputers. QwikMD uses the same steps and user interface. QwikMD is free software and is also available on the cloud at Amazon Web Services.

BRIEF COMMUNICATIONS

NAMD goes quantum: an integrative suite for hybrid simulations

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comprehensive, customizable, easy-to-use set of features to make such tools broadly attractive to chemists, structural biologists, and material engineers.

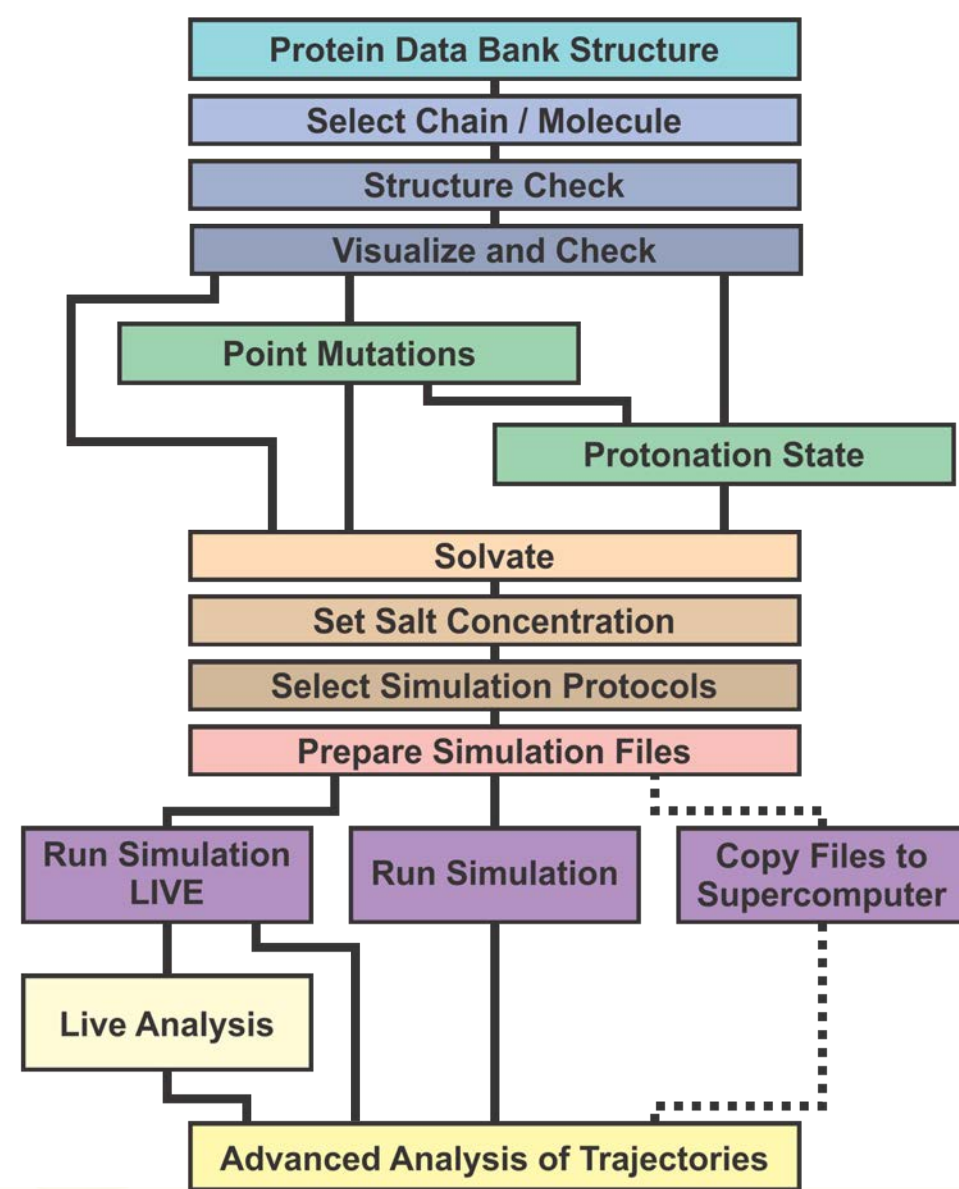
NAMD⁹ is a widely used software package for molecular dynamics (MD) simulations, particularly for large biomolecular systems, using supercomputers. NAMD's scalability and large array of enhanced sampling and free energy methods¹⁰, as well as its seamless integration with VMD¹¹, which provides extended setup, visualization, and analysis capabilities, make it an invaluable tool for exploring complex biological systems. Here we present a comprehensive QM–MM suite implemented in NAMD, to provide a broad range of QM–MM methods, and in VMD, for easy setup, visualization, and analysis through the graphical user interface QwikMD¹². In NAMD, the QM–MM interface supports the simulation of many independent QM regions and smooth integration with a collection

QwikMD:

- Scientific Reports
- BPS 2016
- BPS 2017
- **BPS 2018 (February)**

Dissemination, Documentation and User Support

www.ks.uiuc.edu/Research/qwikmd



[User's Guide](#)

The screenshot shows the QwikMD website home page. The header includes the NIH Center for Macromolecular Modeling & Bioinformatics and the University of Illinois at Urbana-Champaign. The main navigation bar lists Home, Research, Publications, Software, Instruction, News, Galleries, Facilities, and About Us. The page content includes a search bar, a description of QwikMD as a 'Gateway for Easy Simulation', and a 'Recent News and Announcements' section with a link to 'QwikMD at Urbana, IL Workshop'.

The screenshot shows the 'Table of Contents' page of the QwikMD website. It lists various sections and sub-sections, including:

- Molecular Dynamics Simulation and QwikMD
 - Molecular dynamics (MD)
 - QwikMD
 - QwikMD Library
 - NAMD (Nanoscale Molecular Dynamics)
 - For LINUX/MAC users
 - For Windows users
 - Setting up a Molecular Dynamics Simulation
 - The PDB files
 - The PSF files
 - The Parameter files
 - The NAMD Configuration file
 - How to cite
- Graphical User Interface
- Run Tabs
 - Easy Run
 - System Solvation
 - Protocols
 - Advanced Run
 - System Solvation
 - Protocols
 - Structure Manipulation/Check
 - Residues Table
 - Table Manipulation Options
 - Apply and Clear buttons
 - Topology & Parameters Selection
 - Structure Check
 - Membrane
 - Modifications (Patches) List
 - Simulation Setup & Control
 - QwikMD Output folder

System Solvation

To perform MD simulations one has to mimic the environment of the protein, or any other molecule of interest. The most common solvent is water and there are two main ways to mimic the solvent effect. Either simulating all the atoms of the solvent - explicit solvent model - or by adding dielectric constant to the electrostatic calculation - implicit solvent model.

The screenshot shows a web form for selecting simulation parameters. It includes a dropdown menu for 'Solvent' set to 'Implicit', a text input for 'Salt Concentration' set to '0.15 mol/L', and a dropdown for 'Choose Salt' set to 'NaCl'. There is also a 'Protocol' dropdown menu.

- Solvents:** Select the solvent model to employed: Implicit or Explicit
 - Implicit Solvent:** An implicit solvent model is a simulation technique that eliminates the need for explicit water atoms by including many of the effects of solvent in the inter-atomic force calculation. The elimination of explicit water accelerates conformational explorations and increases simulation speed at the cost of not modeling the solvent as accurately as explicit models. QwikMD uses the **Generalized Born Implicit Solvent** implemented in NAMD.
 - Explicit Solvent:** QwikMD uses **VMD solvate plugin** to generate a cubic box centered in the geometrical center of the system and box's edge is calculated by:
MD Protocol box: $box_{edge} = (\sqrt{x^2 + y^2 + z^2}) + 15$
SMD Protocol box: $box_x = box_y = (\sqrt{x^2 + y^2}) + 15$, $box_z = z + PullingDistance + 15$.
where x,y and z are the dimensions of structure in the three axis. Box dimensions in Å. When preparing the simulation, the simulation is translated to the origin (0,0,0).
Note: The water box created by QwikMD is somewhat big for most studies. The big water box was adopted as a safety measure. Ideally, one should work with a box, which is large enough that the protein does not interact with its image in the next cell if periodic boundary conditions are used. The use of periodic boundary conditions involves surrounding the system under study with identical virtual unit cells. The atoms in the surrounding virtual systems interact with atoms in the real system. These modeling conditions are effective in eliminating surface interaction of the water molecules. As the standard water model for CHARMM, TIP3P is the model employed in the simulations prepared with QwikMD.
- Salt Concentration:** Ions should be placed in the water to represent a more typical biological environment. They are especially necessary if the protein being studied carries an excess charge. In that case, the number of ions should be chosen to make the system neutral. One must set the desired salt concentration. The default Salt Concentration is 0.15 mol/L. QwikMD uses **VMD autoionize plugin** to place the ions and even if the Salt Concentration is set to ZERO, ions will be added to neutralize the total charge of the system. In the case of the Generalized Born implicit solvent, the salt concentration is used as ion concentration parameter value (see **Generalized Born Implicit Solvent Configuration Parameters**).
- Choose Salt:** Salt ion pairs currently available are NaCl and KCl.

Protocols

Within the "Easy Run", the user can set up two types of simulations: non-biased Molecular Dynamics (or just Molecular Dynamics - MD) and Steered Molecular Dynamics (SMD).

The screenshot compares two protocol forms. The 'MD protocol' form has fields for Temperature (27 C, 300 K), Simulation Time (10.0 ns), and checkboxes for Equilibration and MD. The 'SMD protocol' form has fields for Temperature (27 C, 300 K), Pulling Distance (10.0 Å), Pulling Speed (2.5 Å/ns), Simulation Time (4.0 ns), and checkboxes for Equilibration, MD, SMD, Pulling Residues, and Anchoring Residue.

Webpages:

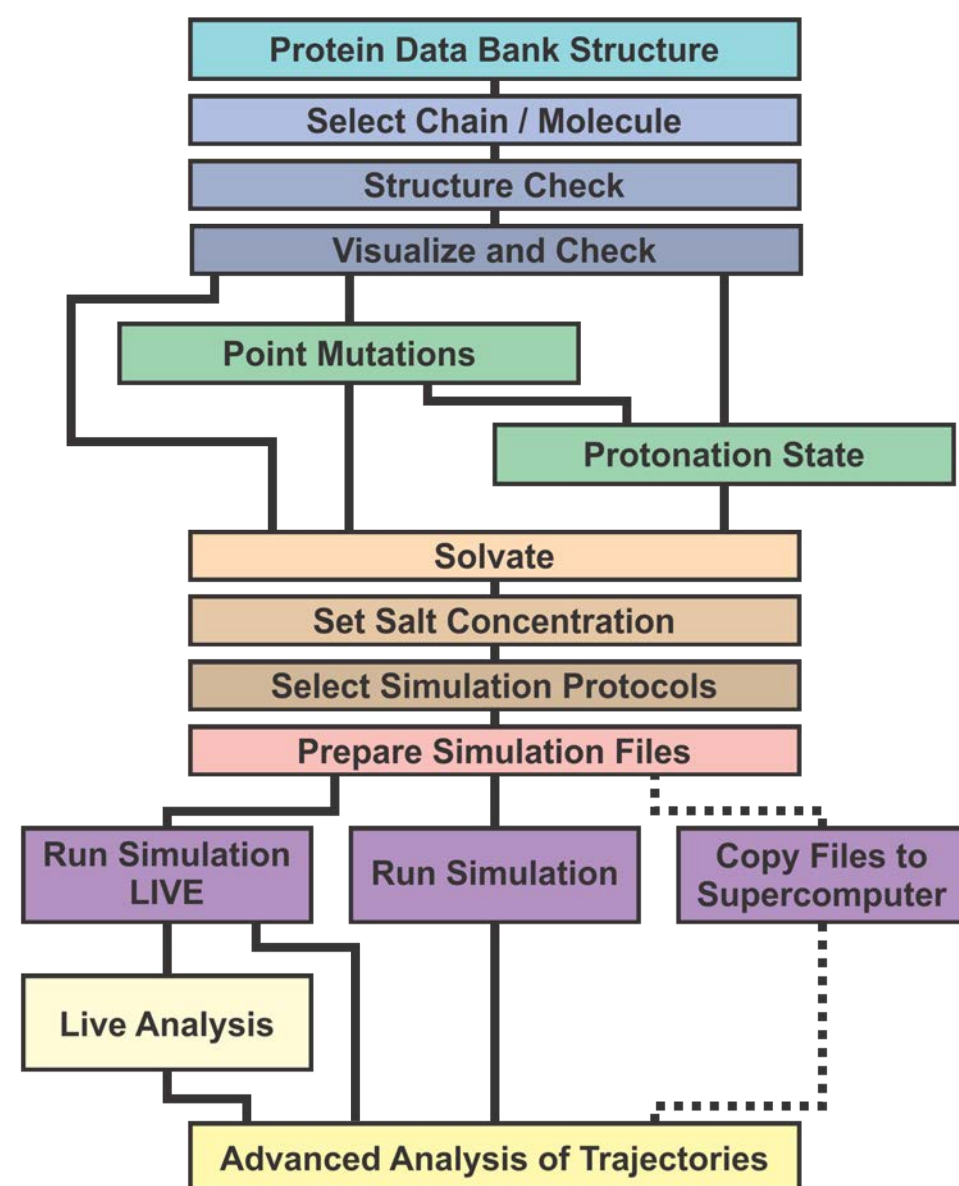
- Home page
- User's Guide Page

Dissemination, Documentation and User Support

[Bug Report Form](#)

vmd-l@ks.uiuc.edu

namd-l@ks.uiuc.edu



The screenshot displays the QwikMD website interface. On the left is a 'QwikMD Bugs Report' form with fields for Author, Email, Priority (Urgent, Not Urgent, Suggestion), General description, and Steps to reproduce Bug. On the right is a 'VMD-L Mailing List' archive page with a search bar and a list of messages. The top of the page features the 'THEORETICAL and COMPUTATIONAL BIOPHYSICS GROUP' logo and navigation links for Home, Research, Publications, Software, Instruction, News, Galleries, Facilities, and About Us. A footer contains funding information from the National Institute of General Medical Sciences.

Webpages:

- Home page
- User's Guide Page
- QwikMD Bug Report
- VMD Mailing List
- NAMD Mailing List

Automate QwikMD set up for a large number of NAMD jobs?

From: Danny Xu (quantum_mania_at_yahoo.com)
Date: Tue Dec 20 2016 - 15:24:36 CST

- Next message: [Scott Brozell: "Re: 2.11 how to remove charmrun remote-shell options"](#)
- Previous message: [zmhoseyni: "Fw \(5\): zmhoseyni"](#)
- Messages sorted by: [\[date \] \[thread \] \[subject \] \[author \] \[attachment \]](#)

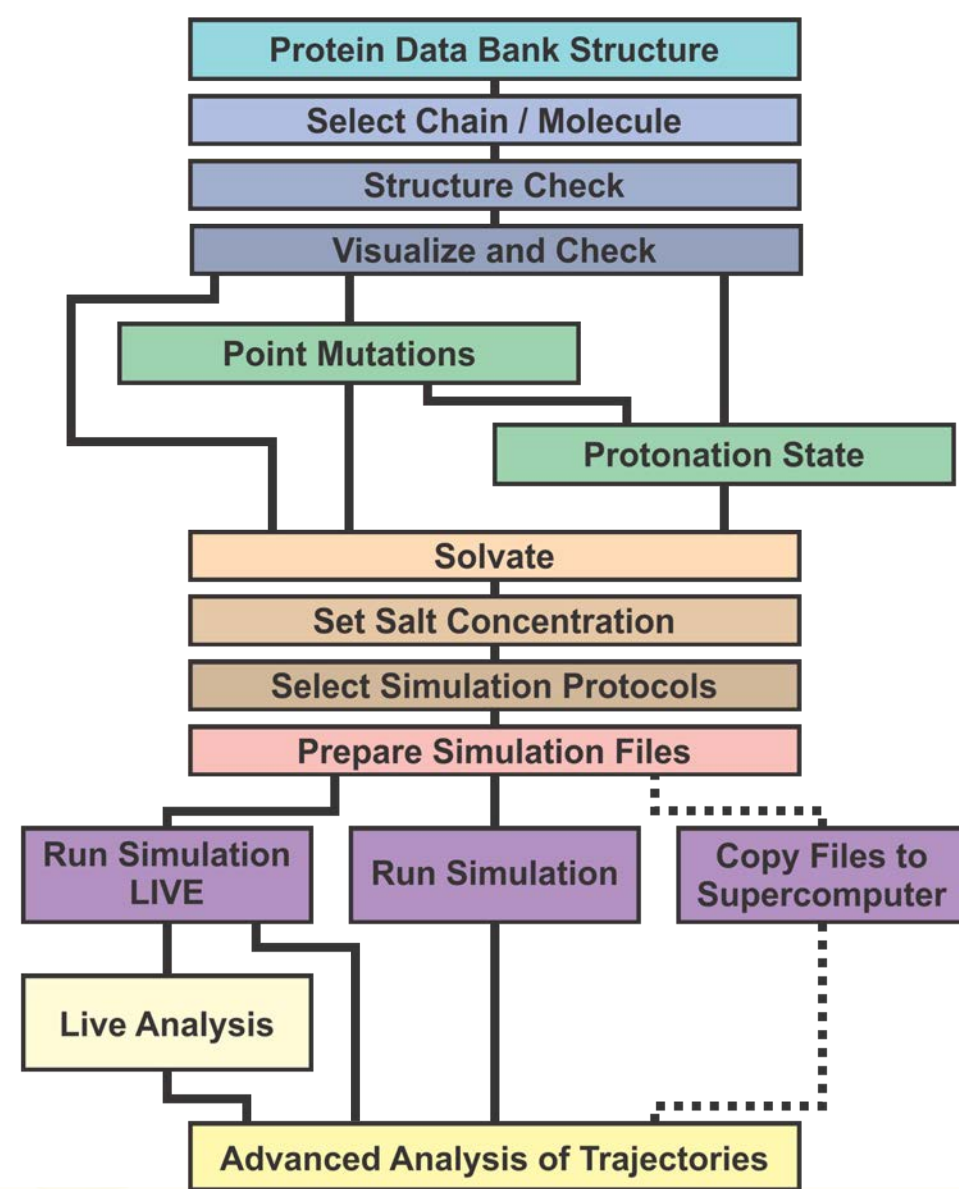
Hello,
I have hundreds of PDB files that I need to set up for explicit solvation MD simulations. Is there any way to automate QwikMD, process these PDB files and prepare NAMD input files in batch mode?
Thanks!-DX

- Next message: [Scott Brozell: "Re: 2.11 how to remove charmrun remote-shell options"](#)
- Previous message: [zmhoseyni: "Fw \(5\): zmhoseyni"](#)
- Messages sorted by: [\[date \] \[thread \] \[subject \] \[author \] \[attachment \]](#)

This archive was generated by [hypermail 2.1.6](#) : Fri Apr 14 2017 - 23:19:16 CDT

QwikMD beta Version – Latest Developments

www.ks.uiuc.edu/Research/qwikmd



Availability

QwikMD is available free of charge on VMD 1.9.3 and newer.

Download VMD for free here

To perform Molecular Dynamics simulations you will also need the widely employed **NAMD** program, which is available free of charge [here](#).

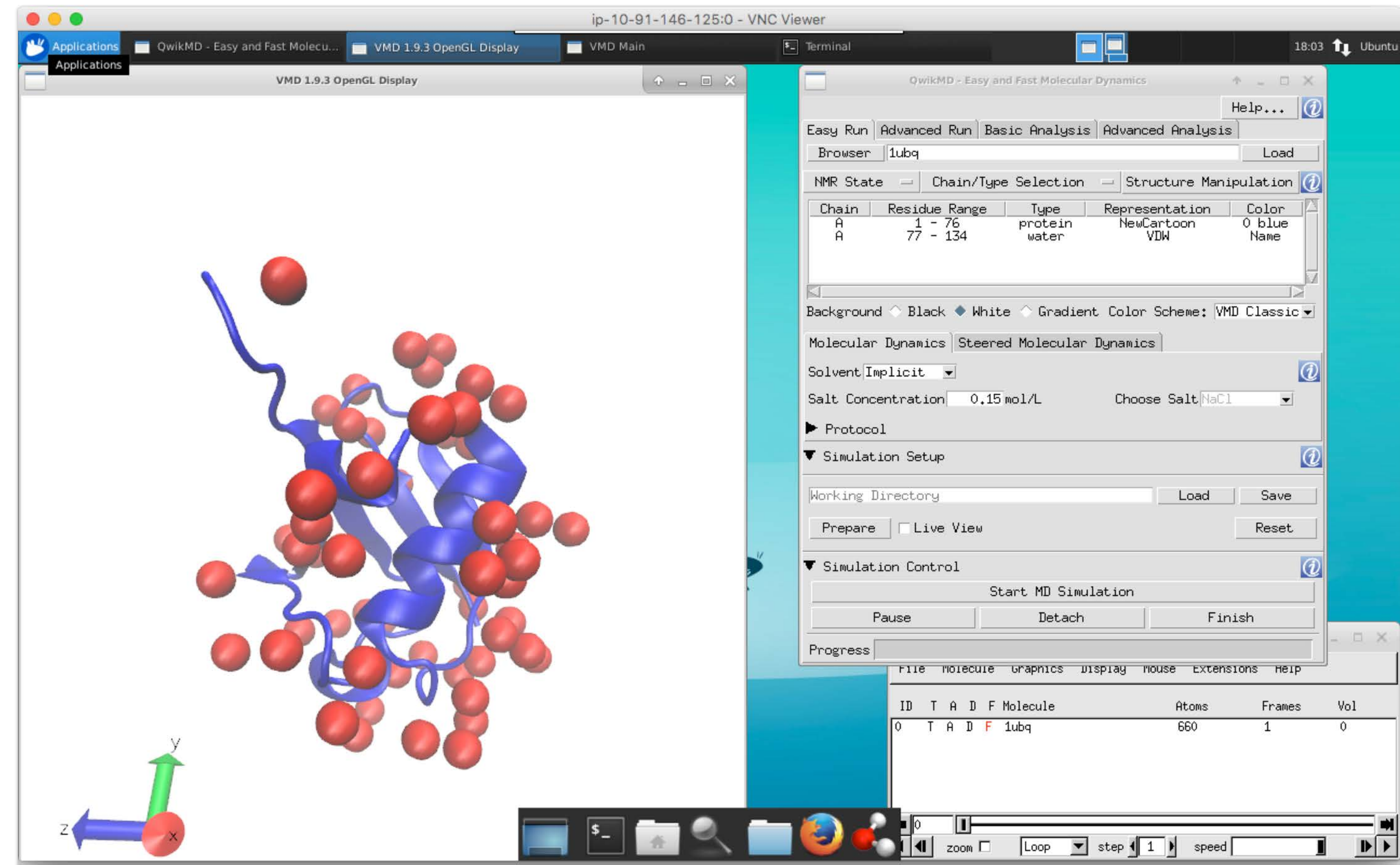
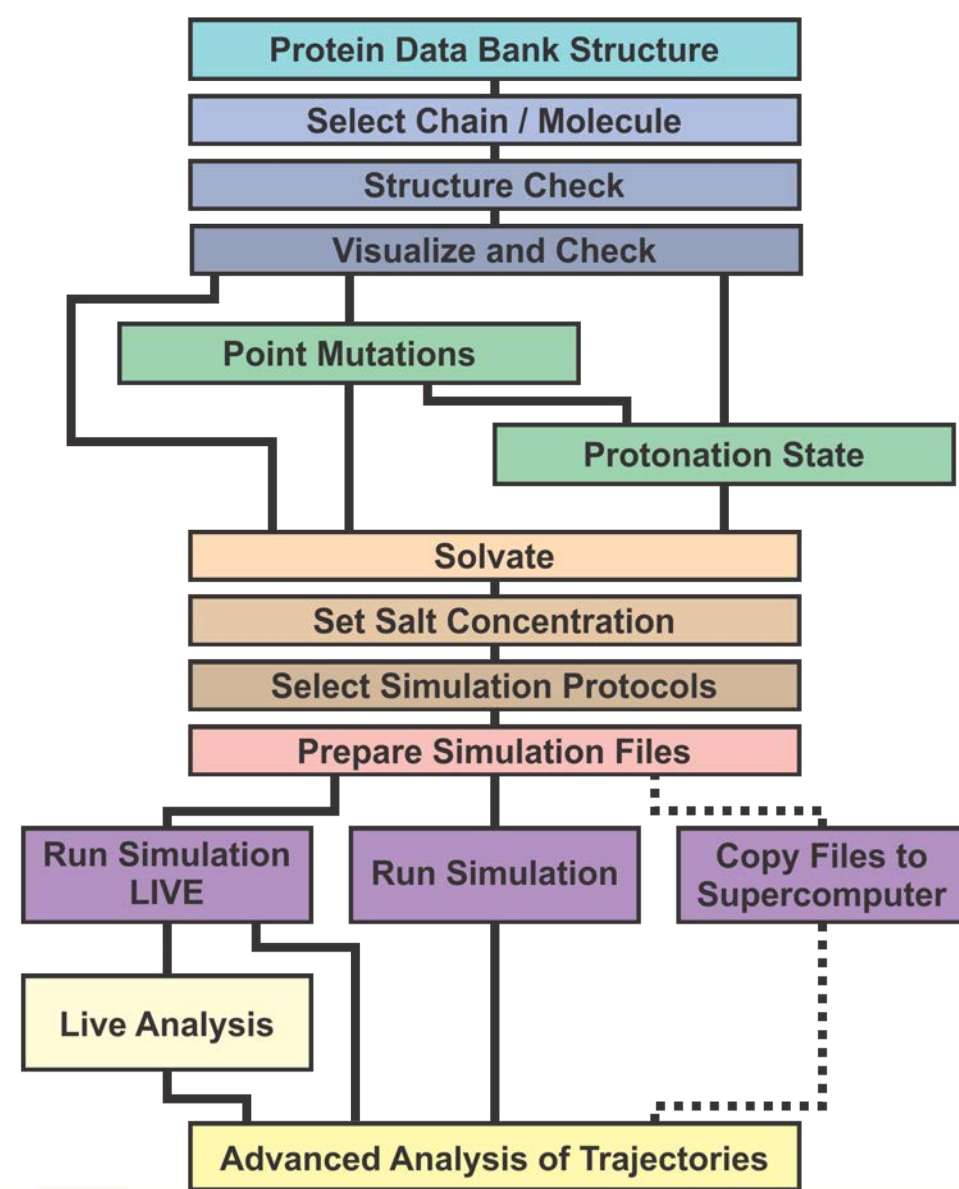
QwikMD beta. The latest version of the QwikMD including the most recent bug fixes can be downloaded [here \(last update on April 20, 2018\)](#). Please follow the instructions in the **README** file included in the qwikmd folder on how to install the beta version.

Employing QwikMD on your research? Please don't forget to cite us: *J.V. Ribeiro, R.C. Bernardi, T. Rudack, J.E. Stone, J.C. Phillips, P.L. Freddolino, K. Schulten;* **QwikMD: Integrative Molecular Dynamics Toolkit for Novices and Experts;** *Scientific Reports, 6, 26536 (2016)*

QwikMD beta:

- Latest Implementations
- Bug Fixes
- Available Before VMD Release

QwikMD on the Amazon Cloud



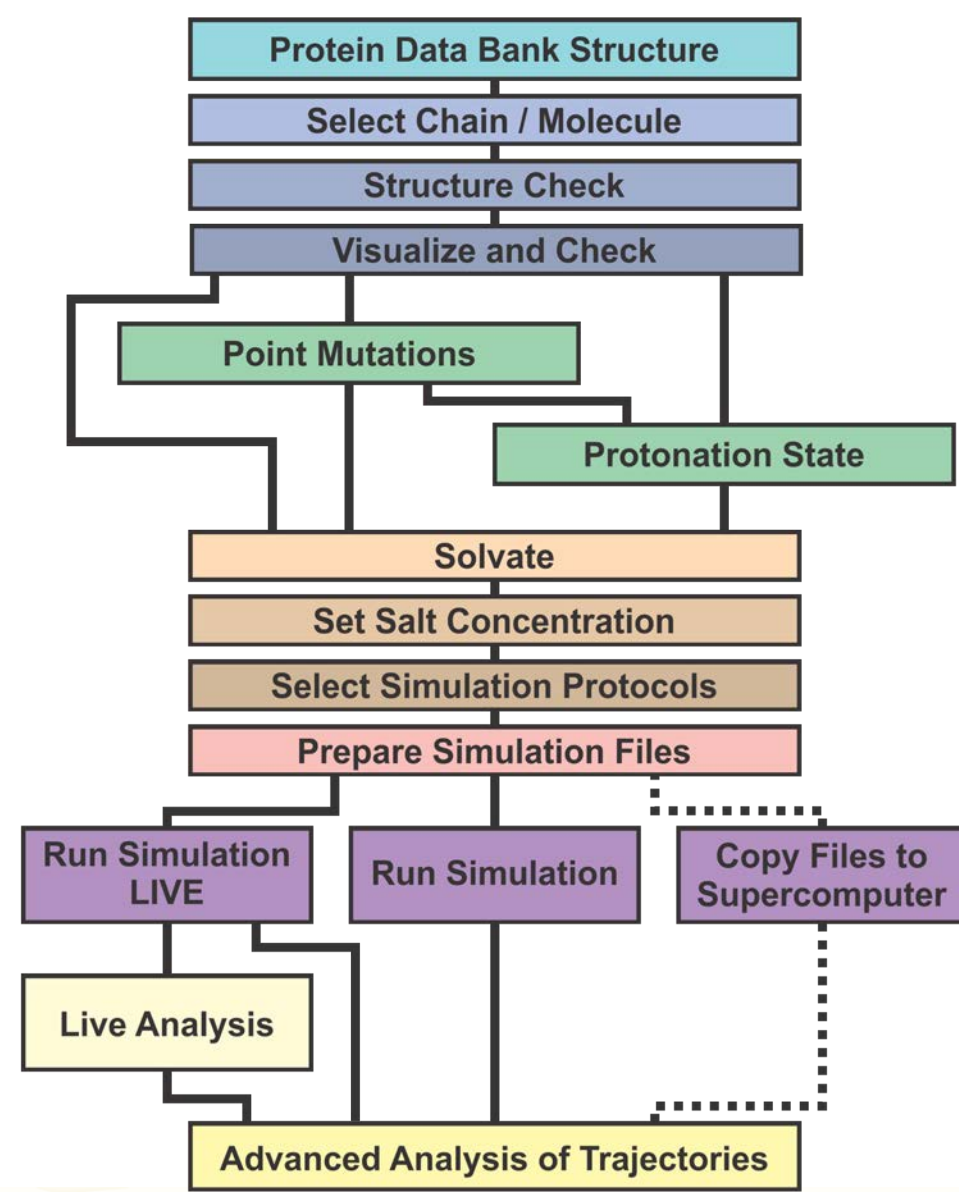
Amazon Web Services:

- Virtual Machine
- VMD & NAMD
- QwikMD and MDFF
- Used in the Center's Workshops

- <http://www.ks.uiuc.edu/Training/Workshop/Urbana2017a/>
- <http://www.ks.uiuc.edu/Training/Workshop/Urbana2018>
- <http://www.ks.uiuc.edu/Research/cloud/>



Training others...



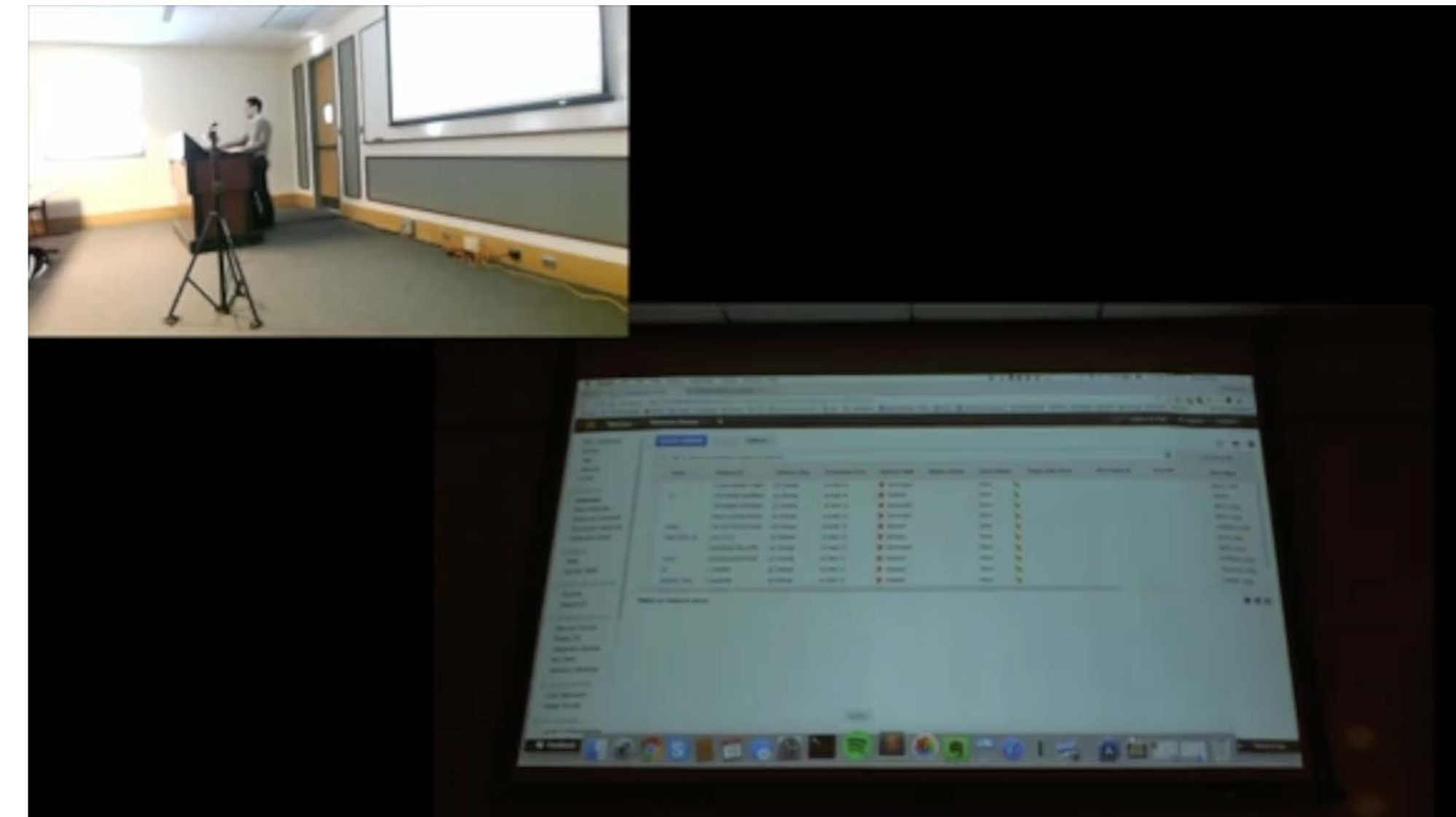
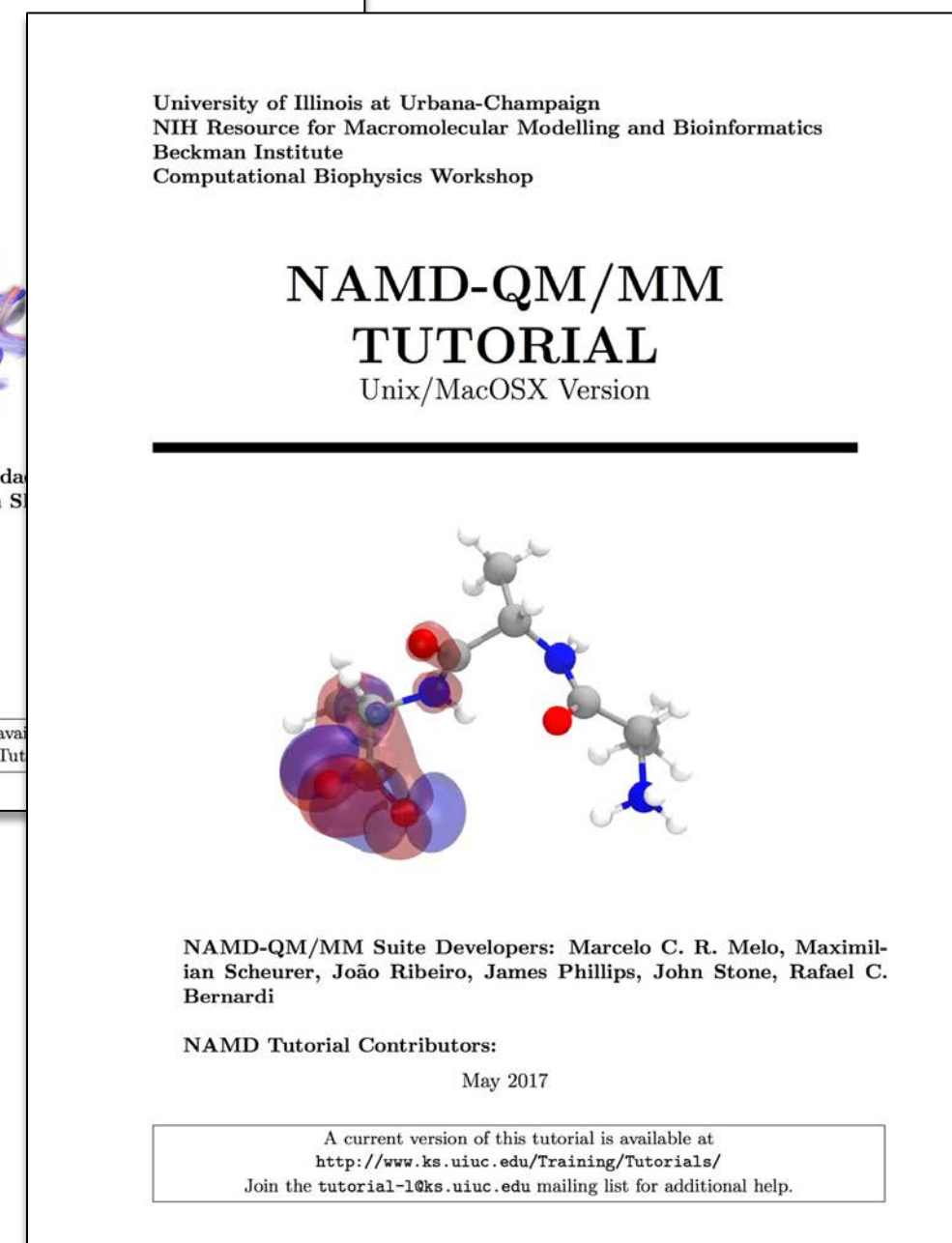
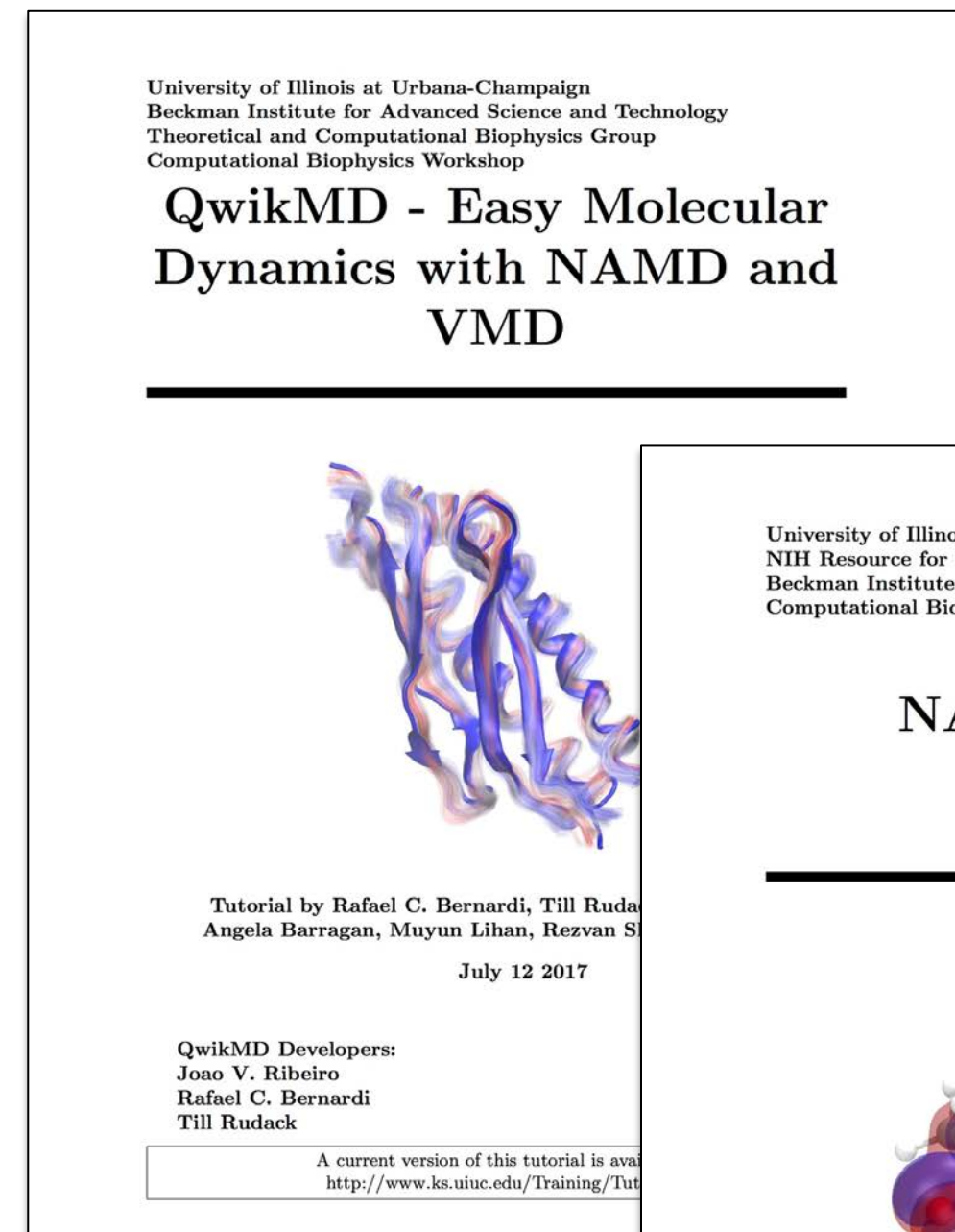
QwikMD Tutorials

QwikMD on Amazon

Workshop Live-Streamed on Facebook

Webpages:

- Home page
- User's Guide Page
- QwikMD Bug Report
- VMD Mailing List
- NAMD Mailing List



<https://www.youtube.com/user/tcbguiuc>

