

VMD Tutorial

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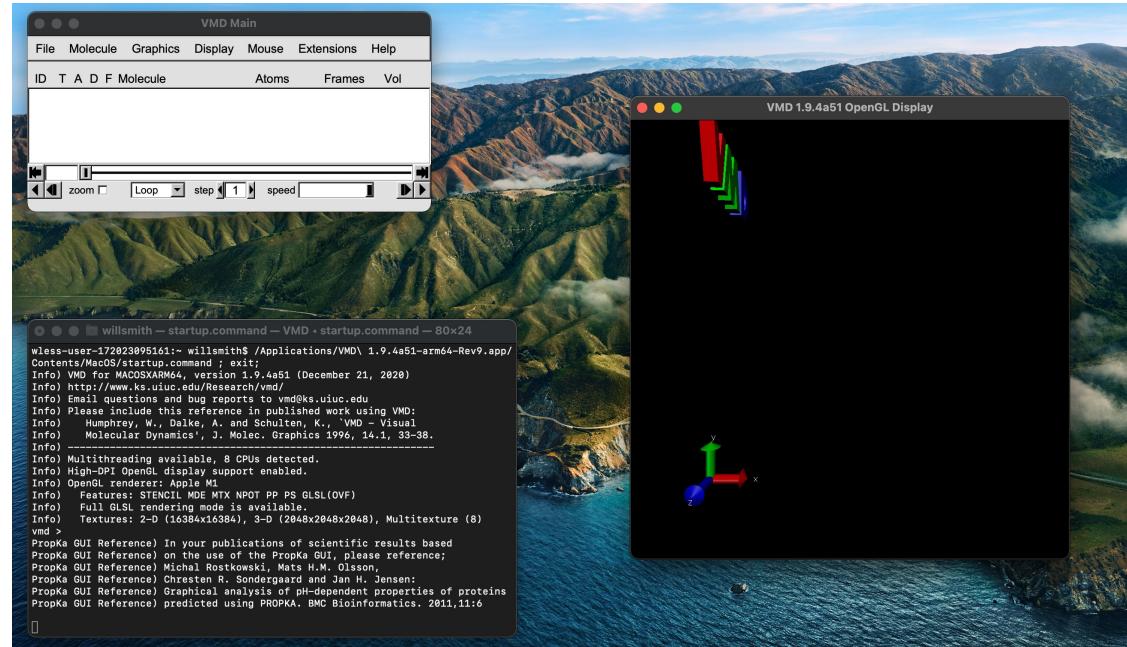
Visual Molecular Dynamics (VMD)

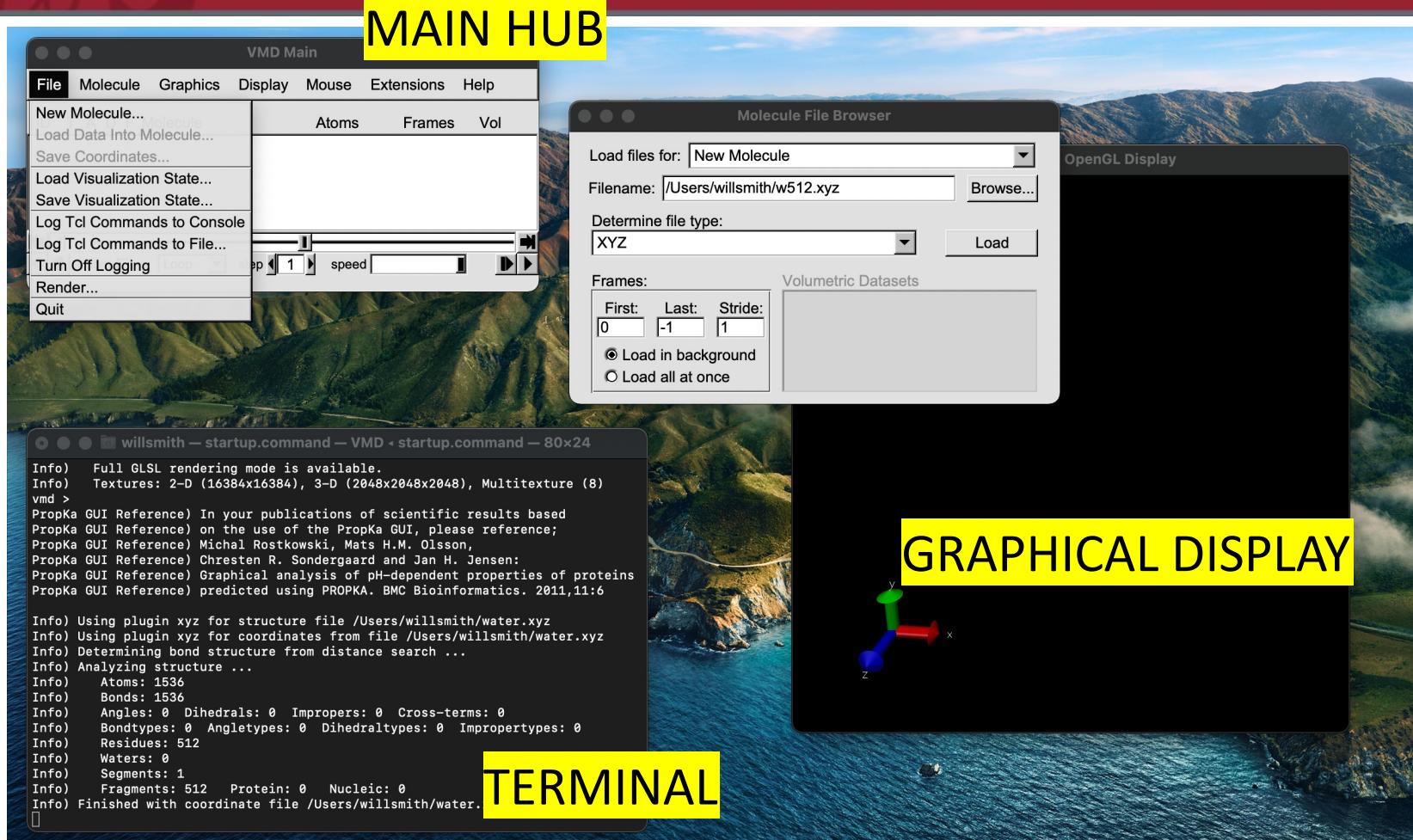
- VMD is a molecular visualization program initially used for analyzing large biomolecular systems
- Supports all major trajectory formats
 - GROMACS
 - LAMMPS
 - XYZ
 - PDB
 - CUBE



Overview of VMD

- Getting started
 - Loading trajectories
 - Molecular representation
 - Atom, bond, angle selection techniques
- Working with trajectories
 - Implementing PBC
 - Generating LAMMPS data files
- Data analysis
 - RDF and integrated RDF





Molecular Representations

MAIN HUB

↳ Display

↳ Representations

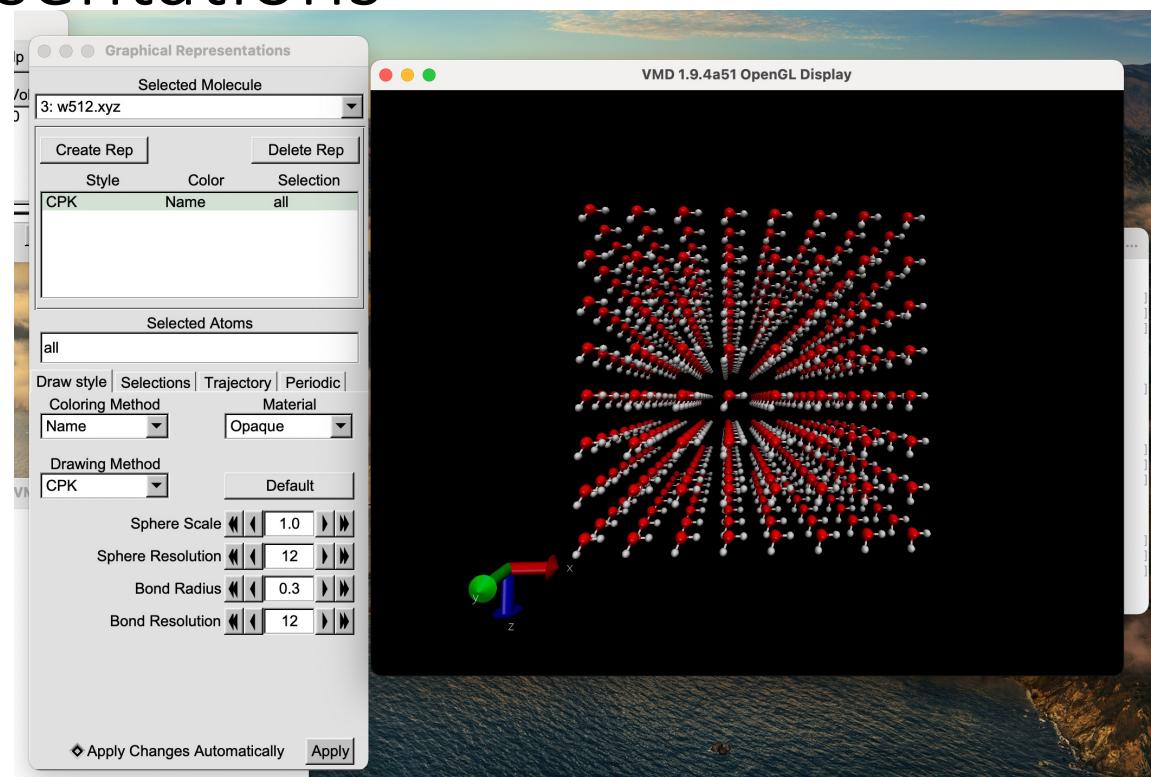
Selected atoms:

Name "H"

Index ID

Mass < x

Numbonds = x



<https://www.ks.uiuc.edu/Research/vmd/vmd-1.3/ug/node132.html>

Molecular Representations

More complex selected atoms:

Name "H" and within 5 of index 1

(name H or name O) and with 5 of index 1

Drawing Method:

Lines (default)

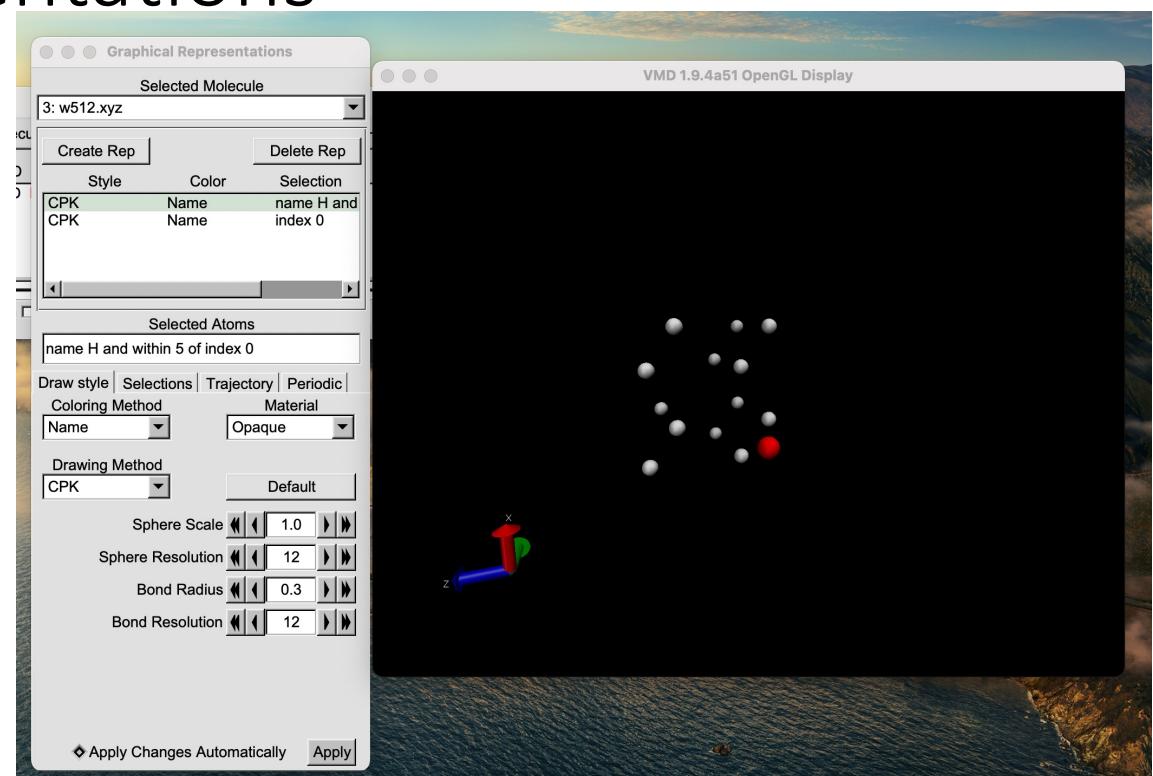
CPK (most common)

Dynamic Bonds (can visualize bonds forming/breaking)

HBONDS (Hydrogen bonds)

Polyhedra (ideal for inorganic simulations)

Isosurface/Beads/Surf (Visualize molecular orbitals or EPS)



<https://www.ks.uiuc.edu/Research/vmd/vmd-1.3/ug/node132.html>

MAIN HUB

↳ Display

↳ Orthographic/Axes

For controlling graphical display:

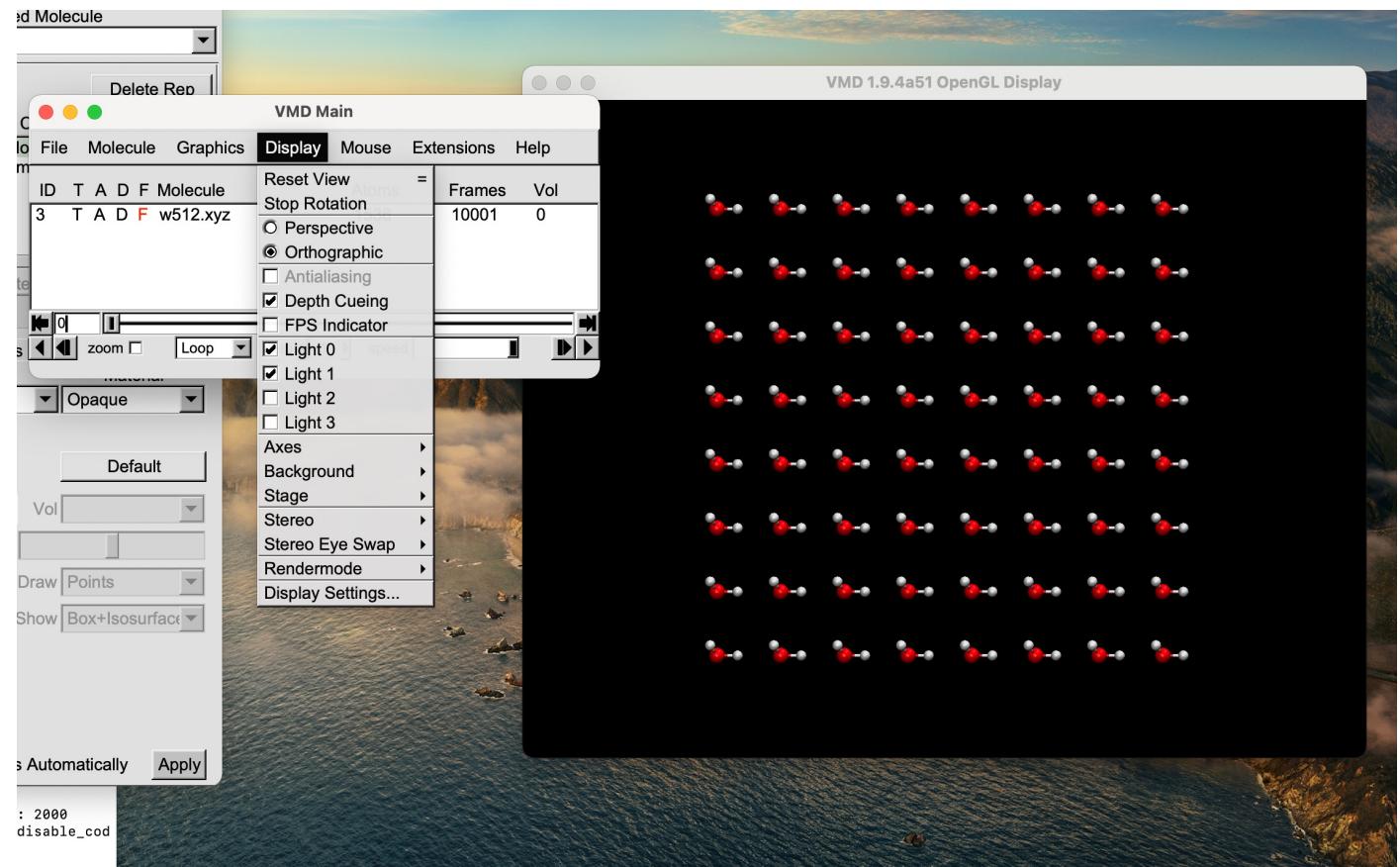
T – translate camera

R – rotate camera

1 – label atom

2 – label bond

3 - label angle



TKConsole/ Introducing PBC

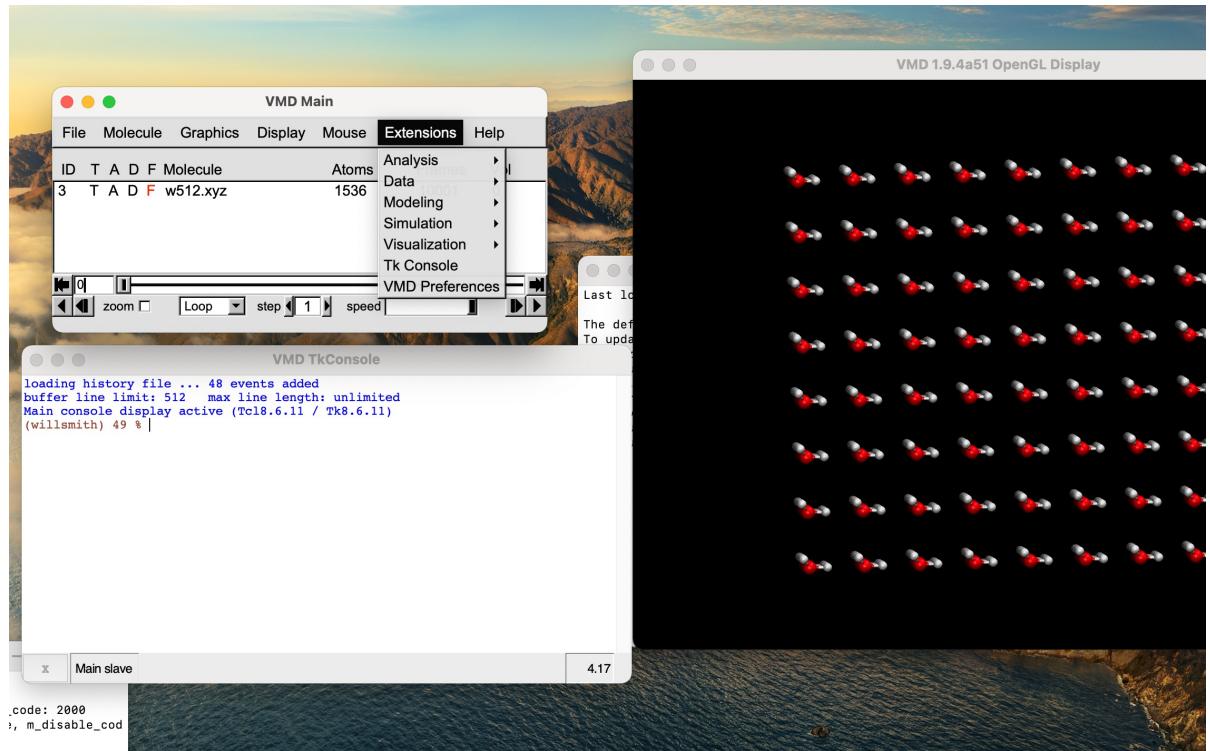
- TKConsole allows for any python scripting in VMD

PBC Tools:

pbctools set {x y z alpha beta gamma} –all

pbctools wrap

pbctools box



<https://www.ks.uiuc.edu/Research/vmd/plugins/pbctools/>

TKConsole/Topo tools

topo “command”

-numbonds

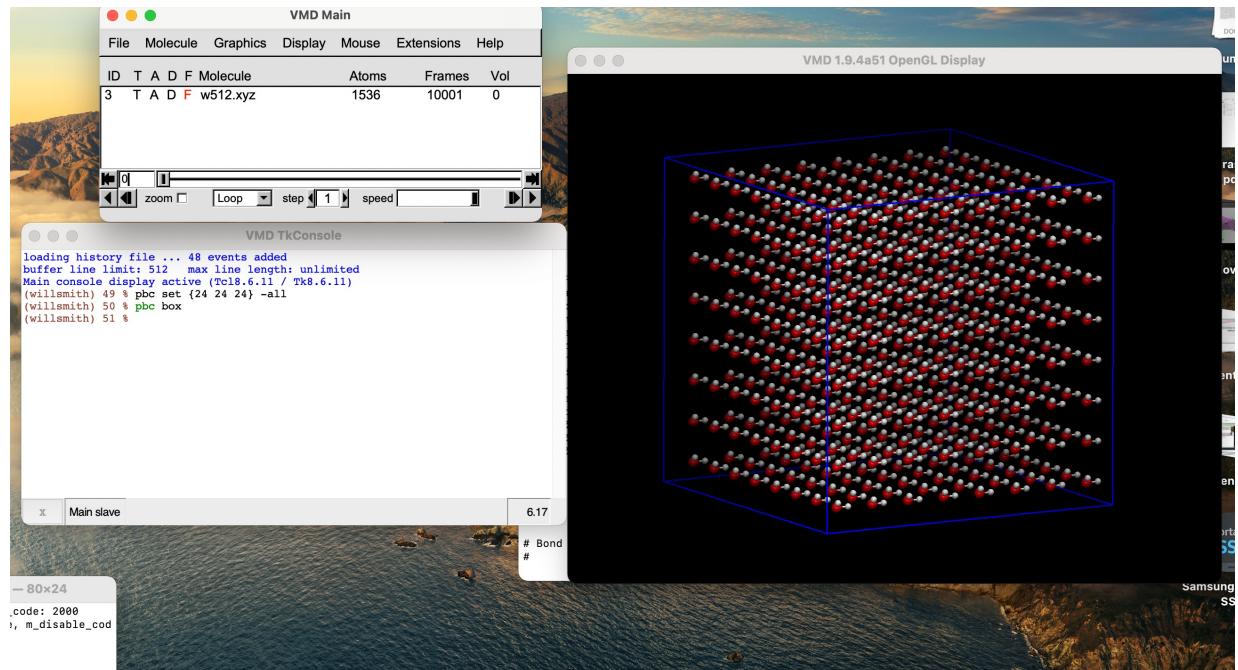
-numangles

-guessbonds

-guessangles

-clearbonds

-writelammpsdata <file name>

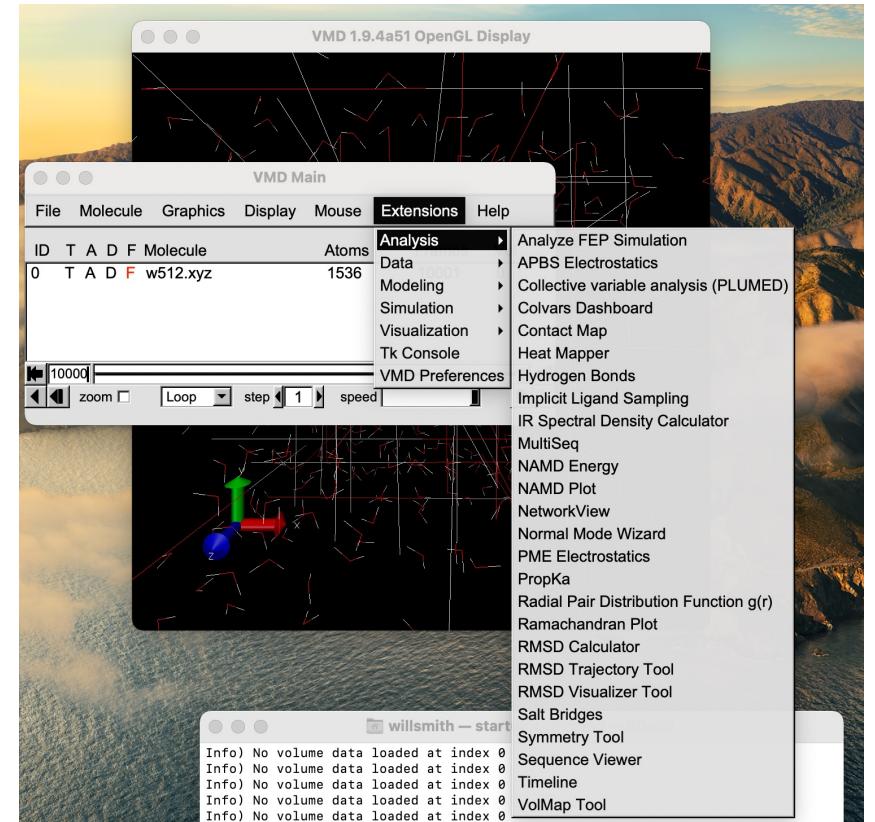


MD Analysis with VMD

MAIN HUB

↳ Analysis

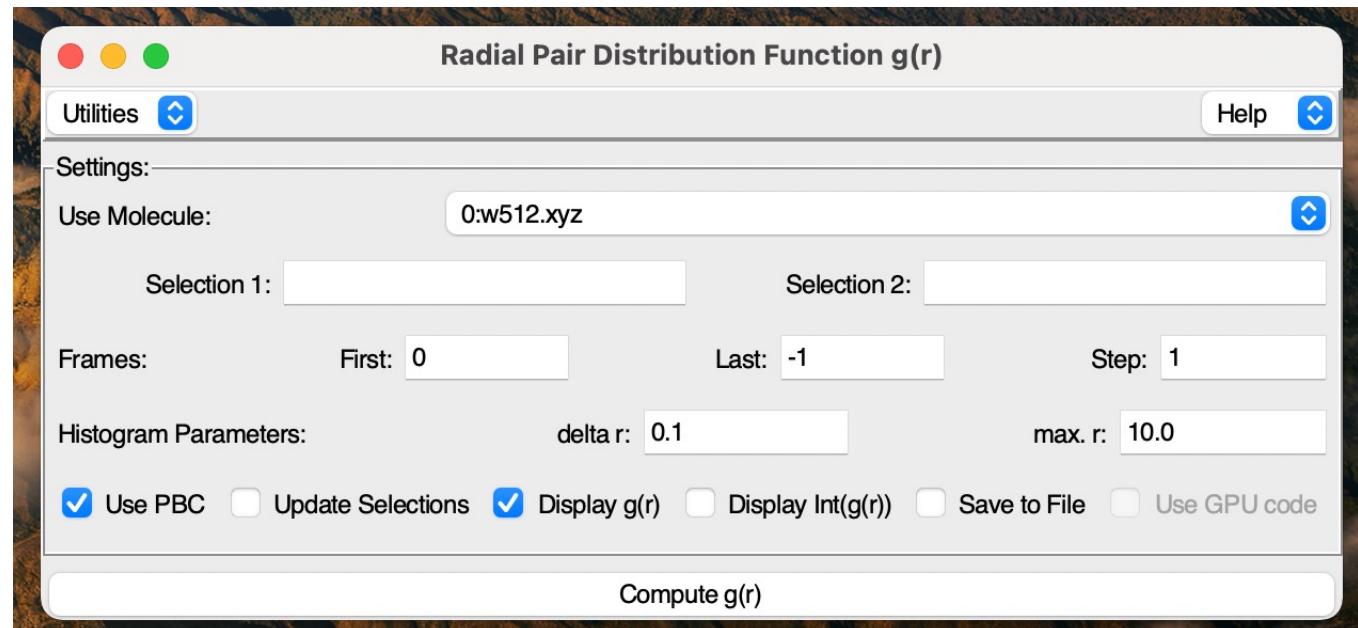
Radial Pair Distribution
Function $g(r)$



MD Analysis with VMD

- Selection uses the same input as selected atoms in graphical representation
- Frames determines which timesteps to sample
- Histogram parameters determines sampling and total length to calculate RDF

Display $\text{int}(g(r))$ gives you integrated RDF – Coordination numbers

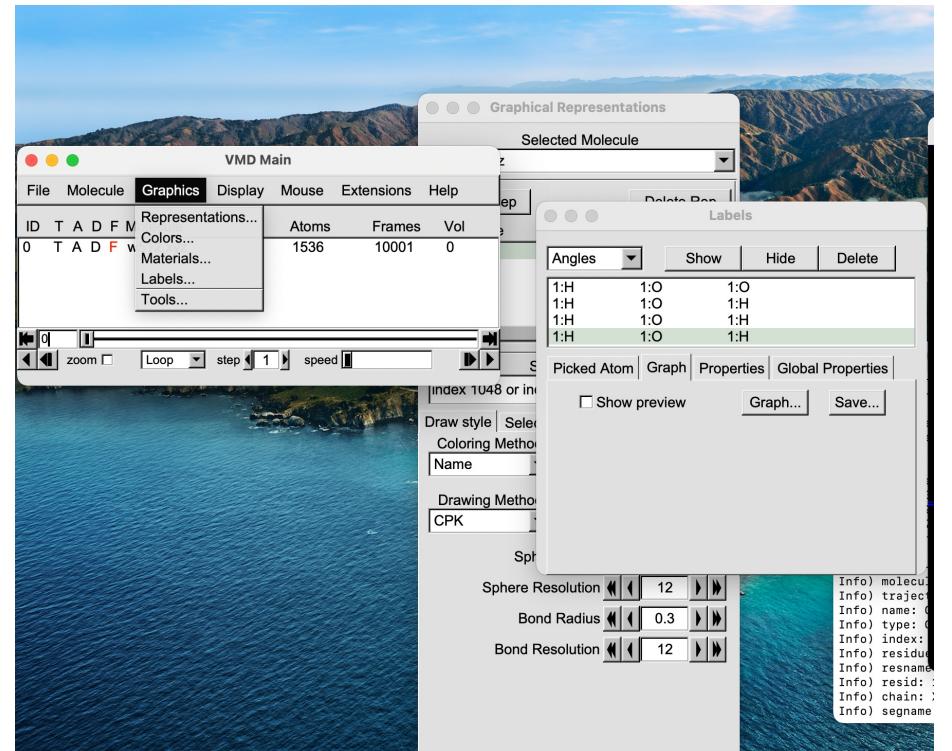


Bond length/Angle Analysis

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↳ Graphics

↳ Labels



Questions?