1.1.3 Tutorial: Visualization and Structural Alignment with VMD

- This tutorial will be about Visual Molecular Dynamics (VMD)
  - molecular graphics program developed at the University of Illinois Urbana-Champaign
  - https://www.ks.uiuc.edu/Research/vmd/
- After this tutorial, you should be able to
  - load molecules with VMD
  - create representations that involve part of a biological macromolecule
  - align different molecules with similar amino acid sequences

Why VMD?

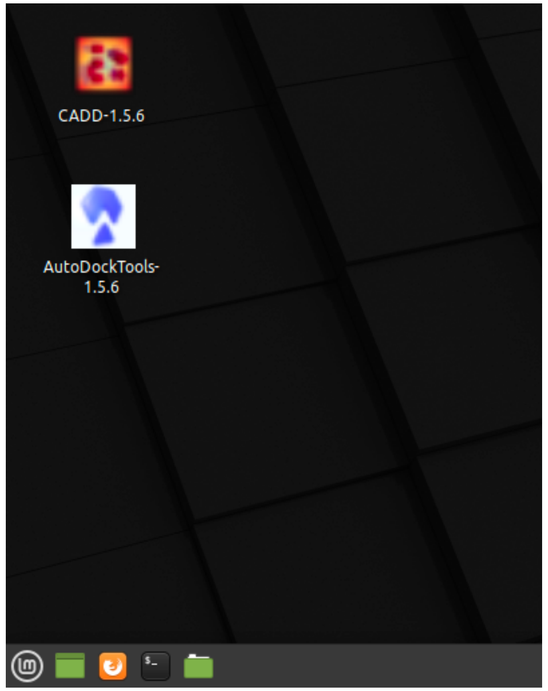
- There are many such programs, including the browser-based one on the Protein Data Bank (PDB) web site.
  - https://www.rcsb.org/pages/thirdparty/molecular_graphics
  - https://en.wikipedia.org/wiki/List_of_molecular_graphics_systems
- Why VMD?
  - Free
  - Works on multiple platforms
  - Powerful atom selection
  - Scriptable
  - Strong with molecular dynamics trajectories
  - Visualization of volumetric data, e.g. electrostatic potentials
- UCSF Chimera also satisfies most if not all of of these criteria

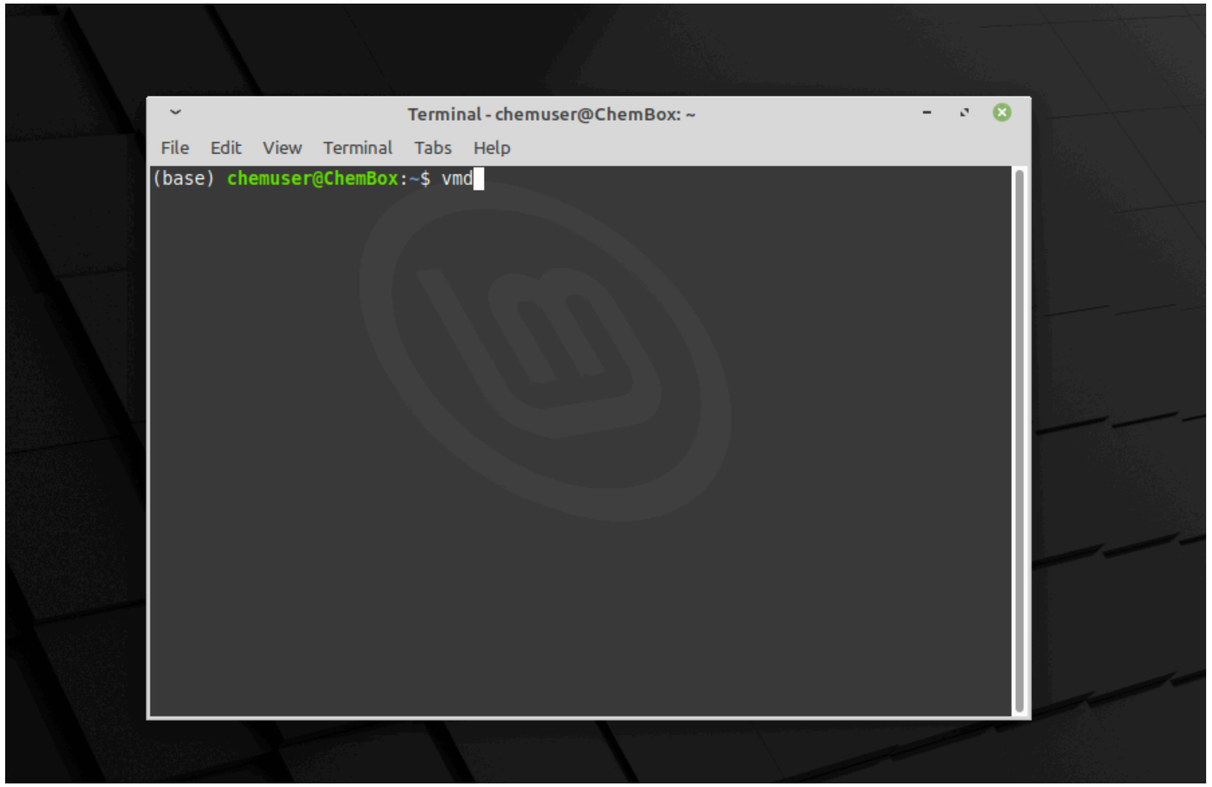
What can be done with VMD?

- Most of the “Gallery” graphics
  - the Theoretical and Computational Biophysics Group at UIUC (https://www.ks.uiuc.edu/Gallery/Science-New/)
  - on my group’s web page (http://mypages.iit.edu/~dminh)
- Scripting makes certain tasks possible

- We will go through the official VMD tutorial on
  - Working with a Single Molecule (http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/node2.html)
  - Working with Multiple Molecules (http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/node6.html)
  - Comparing Structures and Sequences with MultiSeq (http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/node7.html)
- The full tutorial
  - http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/index.html
  - http://www.ks.uiuc.edu/Training/Tutorials/vmd/vmd-tutorial.pdf

Running VMD





- Click on the black box in the lower left-hand corner. This opens up a terminal window.
- Type in ‘vmd’ and return.