C7800 Introduction to molecular modelling - seminar
TSM Modeling of molecular structures

Section Modelling
Programs for molecular modelling I

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Overview

VMD

http: //www.ks.uiuc.edu/Research/vmd/

Visualization of (bio)molecules. Available for MS Windows, macOS, and Linux for free upon registration.

Avogadro

http://avogadro.openmolecules.net/wiki/Main_Page

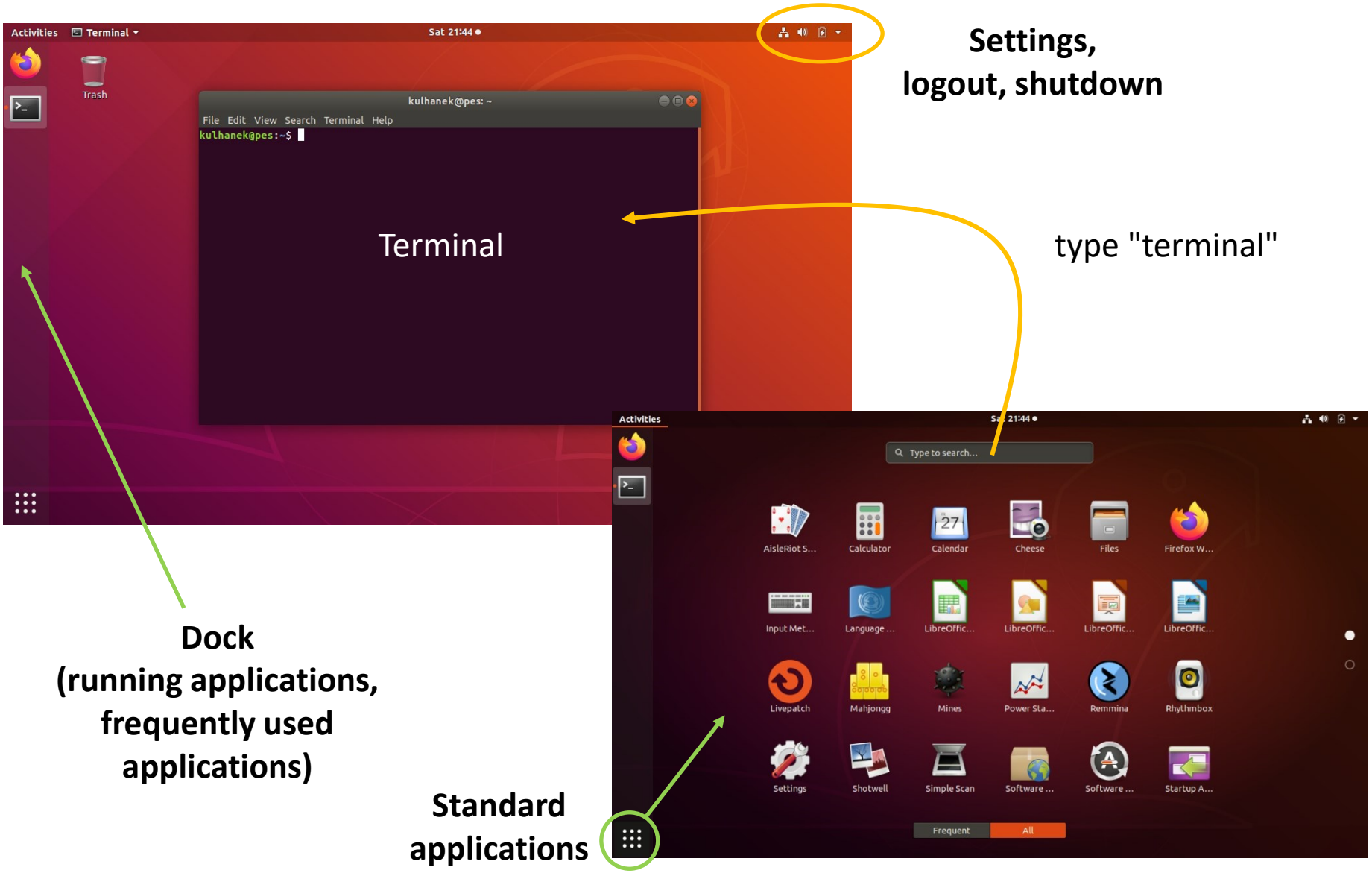
Program for molecule building and visualization. Freely available for MS Windows, macOS, and Linux.
Functionality overview: https://www.youtube.com/watch?v=xdmLoBlLmqs

Nemesis

https://nemesis.ncbr.muni.cz/

Program for molecule building and visualization. Freely available for Linux.

WOLF Cluster - GNOME Desktop



Model building

Program Avogadro

Starting Avogadro

How to start Avogadro?

- Find Avogadro in standard applications
- Or open terminal and run Avogadro as a command (all small caps!!!)

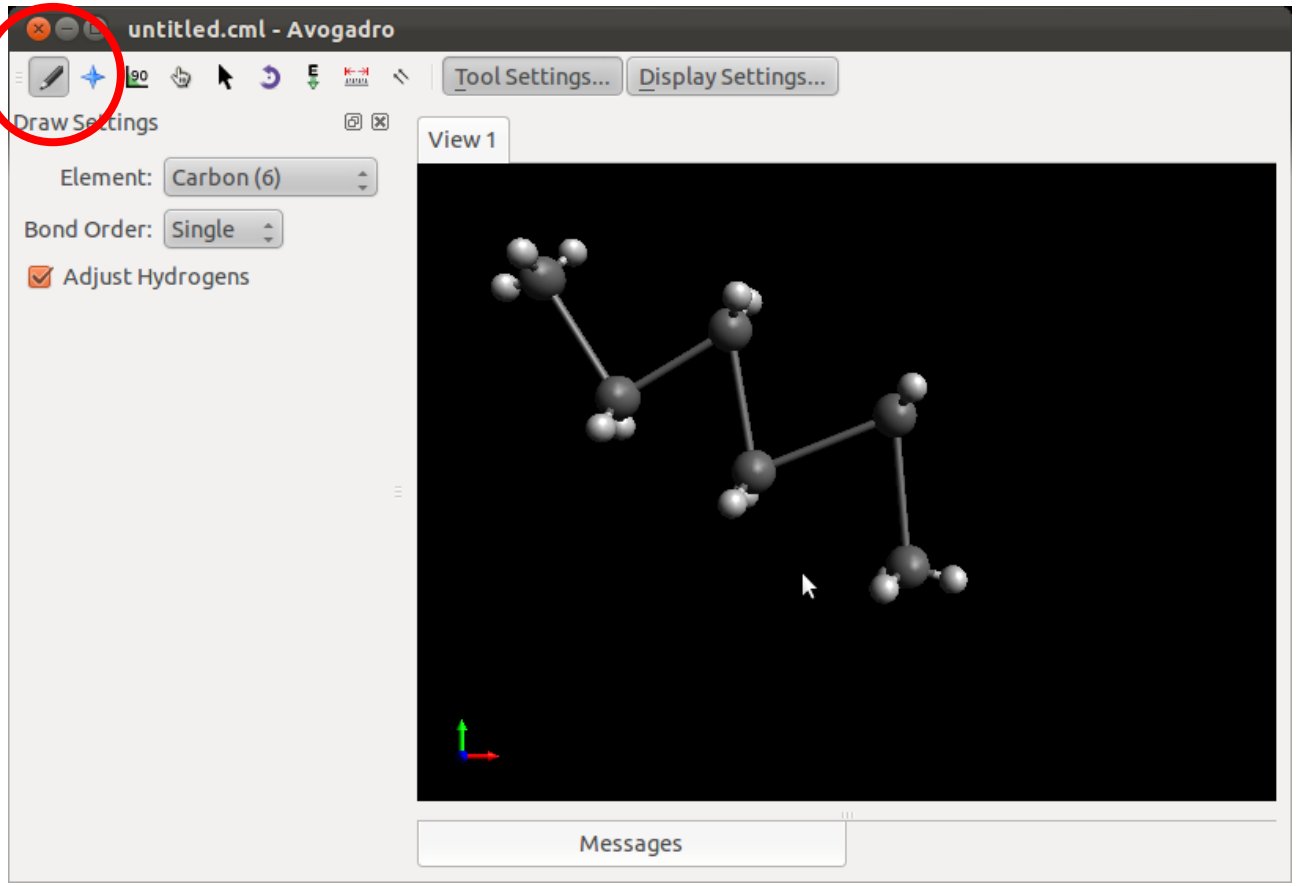
```
$ avogadro
```

- Or open terminal and run Avogadro from modules (not recommended)

```
$ module add avogadro
$ avogadro
```

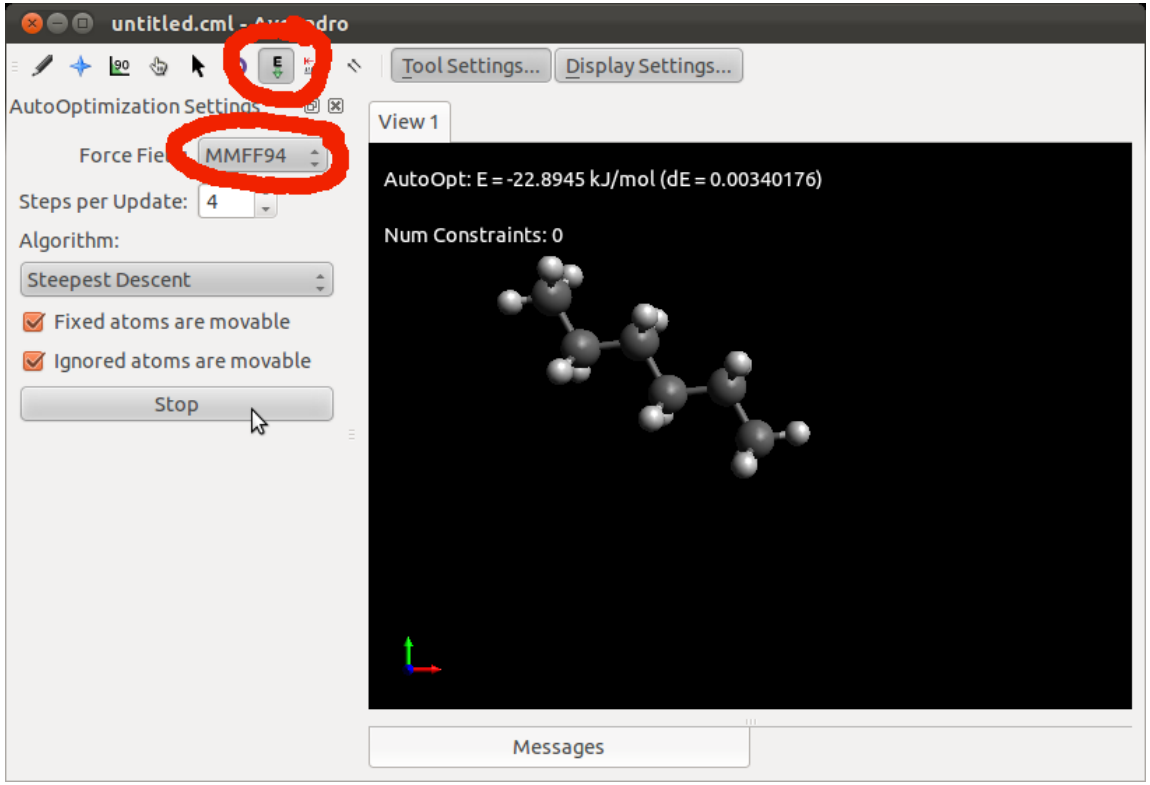
Draft model

- In edit mode, you can draft a model.
- This model does not have proper bond distances and angles. It needs to be optimized before further use.



Model optimization

- Avogadro uses molecular mechanics (force field) for geometry optimization.
- For proper usage, the model must have correct topology with right bond orders.
- Force field methods are empirical. Therefore, it is necessary to select proper parametrization such as MMFF94.

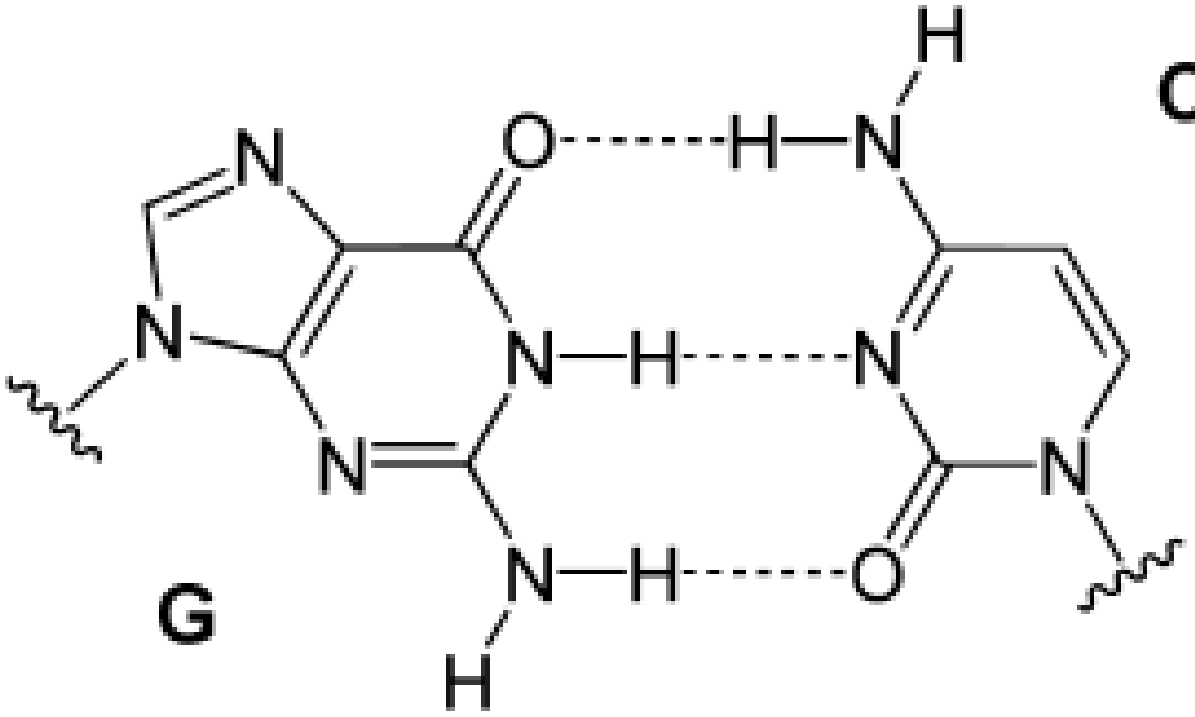


Exercise 1

1. Step by step, create models of the following molecules:
   - methane
   - ethene, ethyne
   - benzene
   - adamantane
   - benzoic acid
   - trinitrotoluene
   - salicylic acid
   - optionally building C_{60}

Exercise 2

1. Create a model containing G:C base pair, according to the scheme below. Use a hydrogen atom to saturate the free valences. For geometry optimization, use the MMFF94 force field.



https://en.wikipedia.org/wiki/Base_pair

Model building

Nemesis program

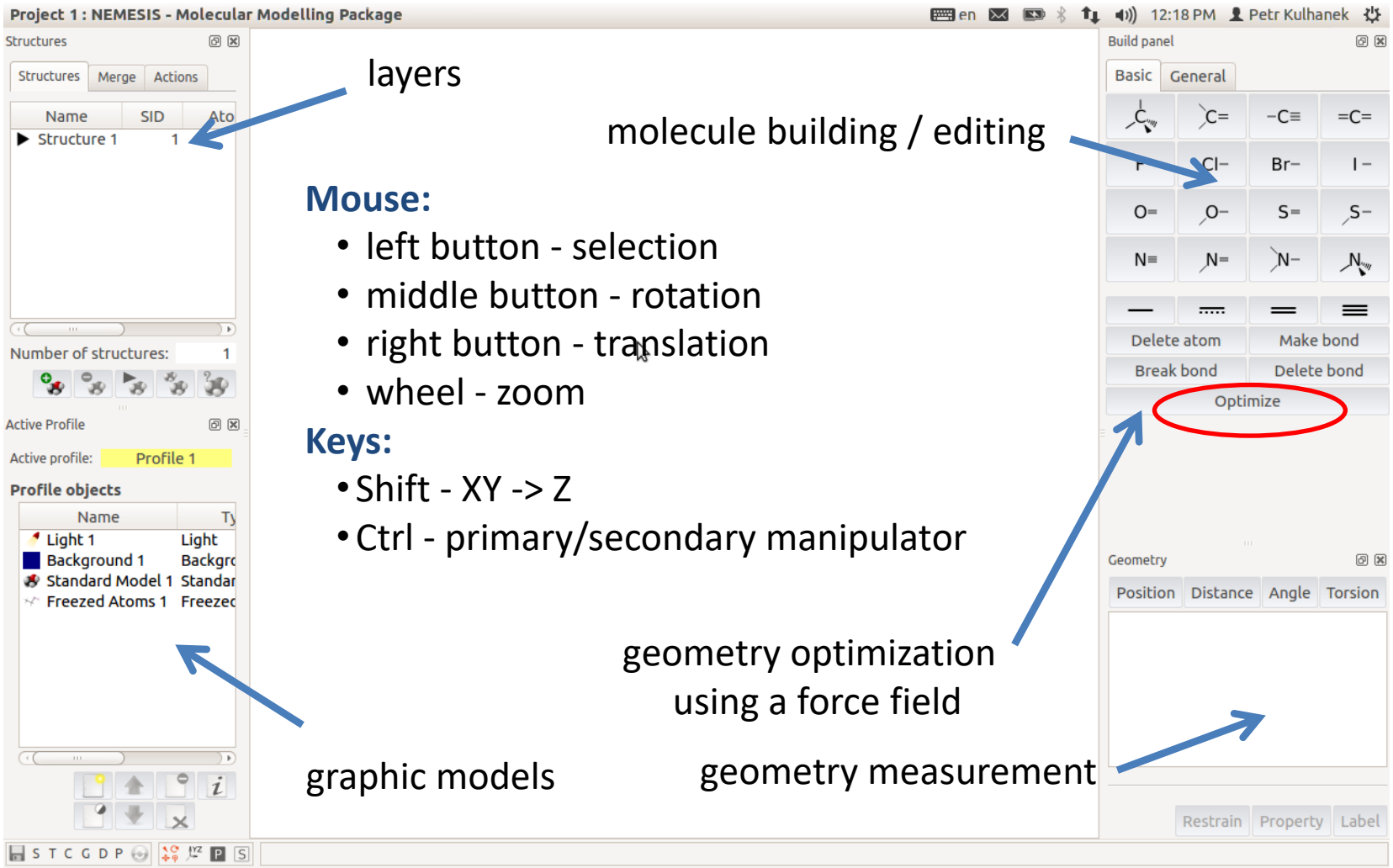
Starting Nemesis

How to start Nemesis?

- Open terminal and run Nemesis from modules:

```
$ module add nemesis
$ nemesis
```

Nemesis - Build Project



Force field settings for optimization: menu Geometry-> Optimizer Setup

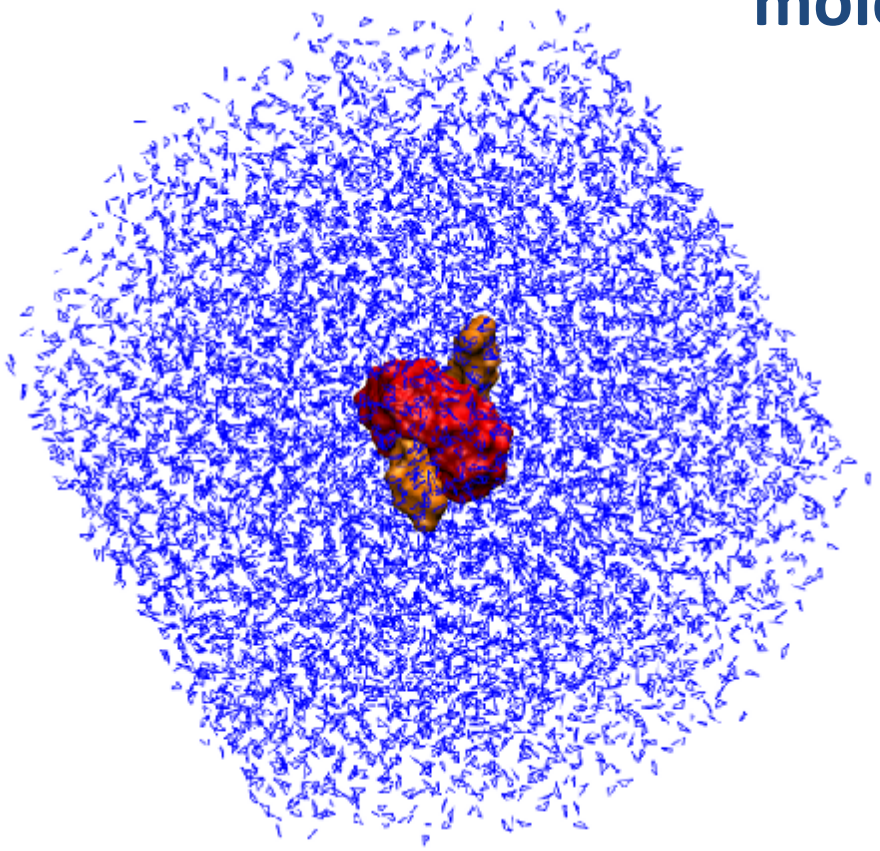
Exercise 3

1. Step by step, create models of the following molecules:
   - methane
   - ethene, ethyne
   - benzene
   - adamantane
   - benzoic acid
   - trinitrotoluene
   - salicylic acid

Visualization of molecular dynamics simulations

VMD program

Exercise 4



molecular dynamic simulation of a molecular switch

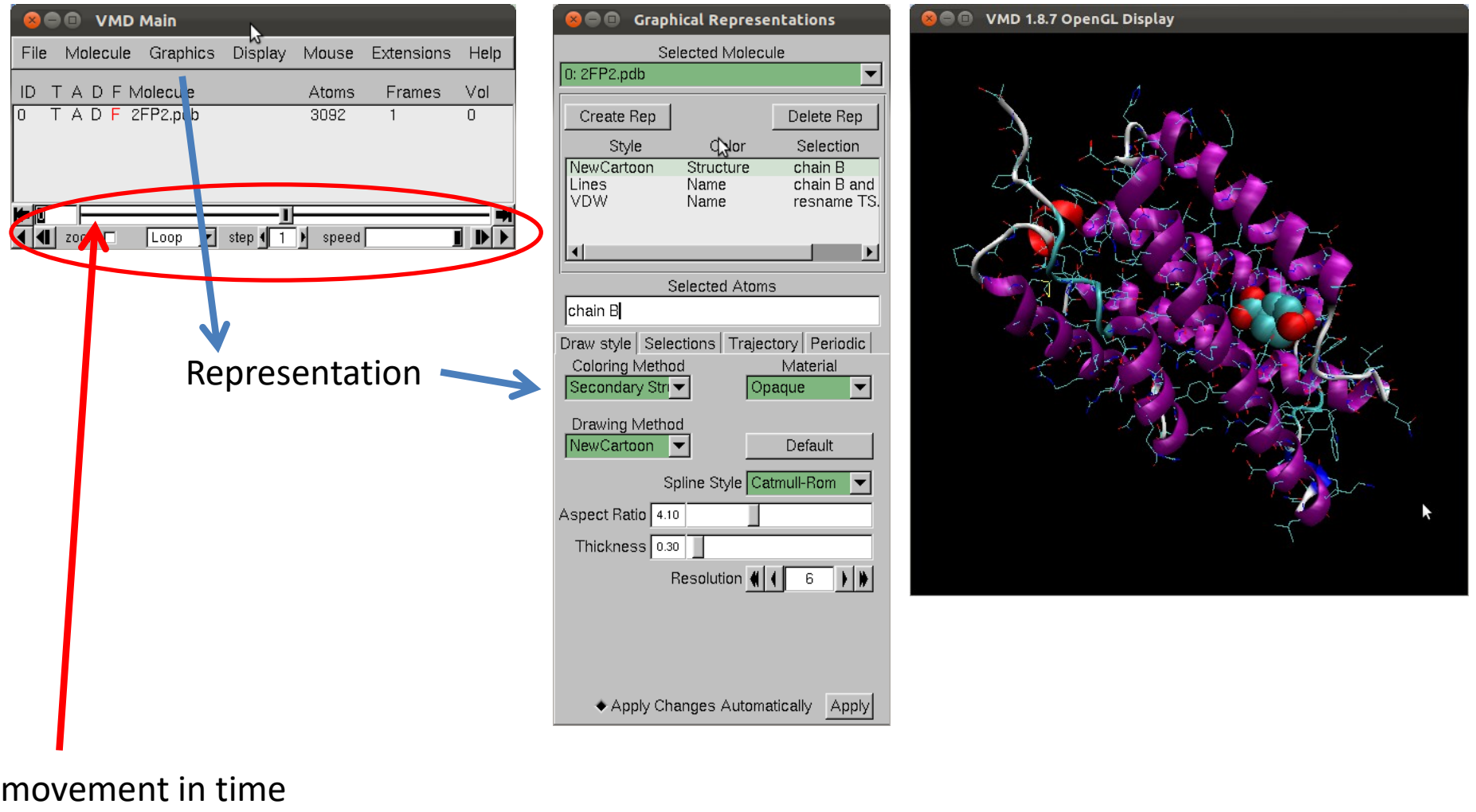
red - rotor
orange - axis
blue - water

Display simulation in VMD

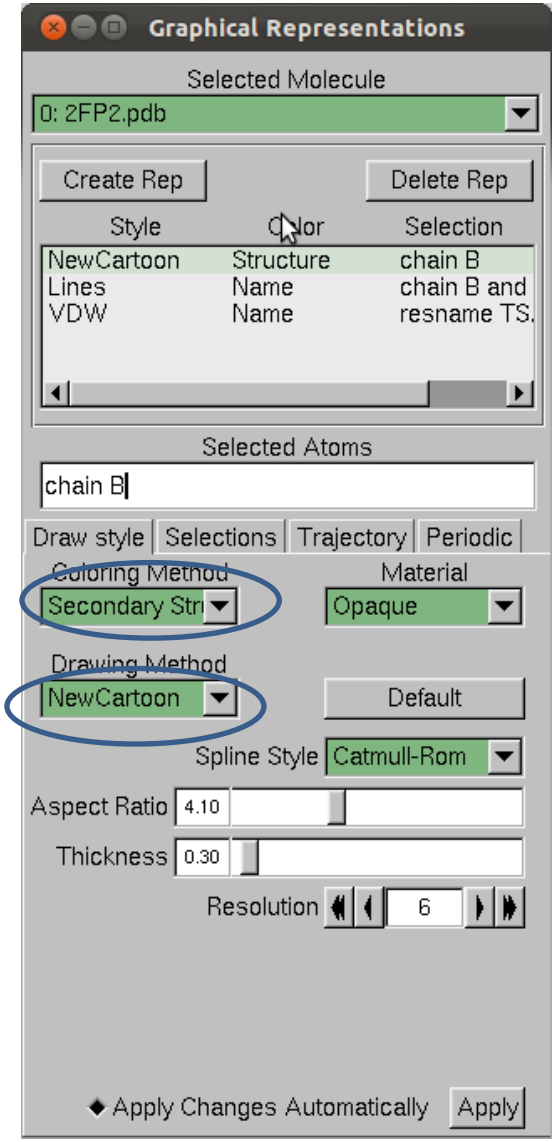
- Open terminal and run the following script

```
$ ~kulhanek/start-vmd-3
```

VMD


VMD Main
File Molecule Graphics Display Mouse Extensions Help
ID T A D F Molecule Atoms Frames Vol
0 T A D F 2FP2.pdb 3092 1 0
Loop
step 1
speed
Representation
movement in time
Graphical Representations
Selected Molecule
0: 2FP2.pdb
Create Rep
Delete Rep
Style Color Selection
NewCartoon Structure chain B
Lines Name chain B and
VDW Name resname TS
Selected Atoms
chain B
Draw style Selections Trajectory Periodic
Coloring Method
Secondary Str
Material
Opaque
Drawing Method
NewCartoon
Default
Spline Style Catmull-Rom
Aspect Ratio 4.10
Thickness 0.30
Resolution 6
Apply Changes Automatically
Apply
VMD 1.8.7 OpenGL Display

VMD program - visualization



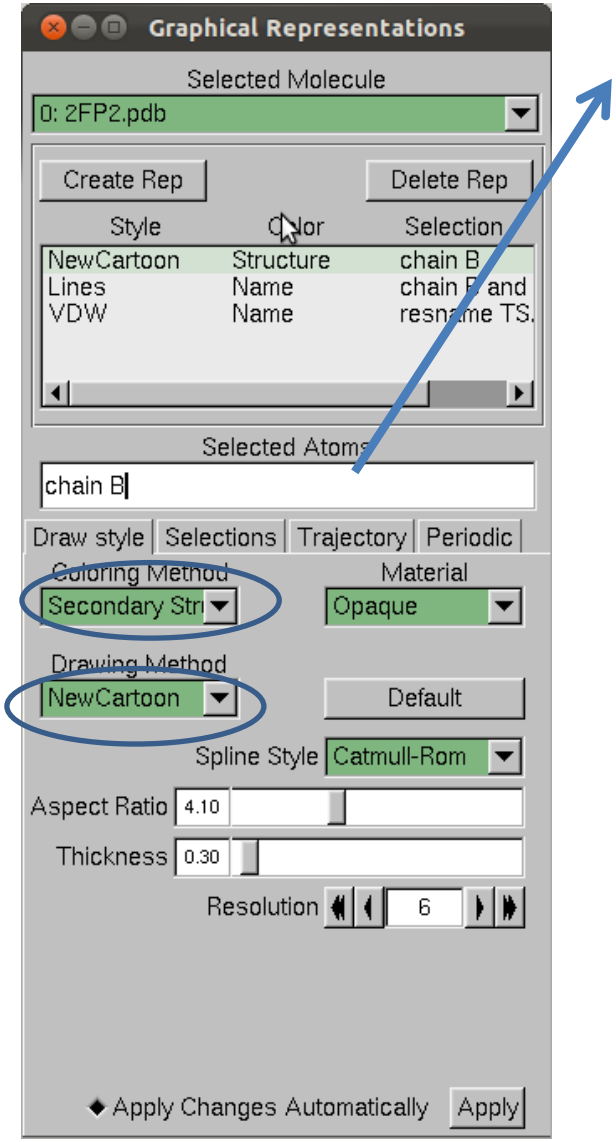
1 2 Create/Delete representation

3 Representation List
double click - activate/deactivate

4 Selection (what part of model is visualized)

5 Coloring method and drawing method

VMD program - selection



Selection for visualization (examples):

water - selects all water molecules
resname X - selects a residue named X
resid X - selects a residue with the number X
not hydrogen - do not display hydrogen atoms

Examples:

resid 1 to 7
resid 8 9 10

Exercise 4

1. How many atoms does the model contain?
2. How many units contains cucurbit[n]uril?
3. What happens to water molecules at the interface of the simulation box?
4. What functional groups contains the axis?
5. What is the total charge of the axis?
6. Try to visualize the model as it is shown on the page 15.