

C7800 Introduction to molecular modelling - exercise

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=xdmLoBILmq5>

Nemesis

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

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

WOLF Cluster - GNOME Desktop

The image shows two screenshots of the GNOME desktop environment. The top screenshot shows a terminal window with the text "Terminal" overlaid. A yellow circle highlights the system tray in the top right corner, and a yellow arrow points from the text "type 'terminal'" to the terminal window. The bottom screenshot shows the application overview (dash) with a search bar at the top. A green circle highlights the application icon grid in the bottom left corner, and a green arrow points from the text "Dock (running applications, frequently used applications)" to the dock area. A yellow arrow also points from the search bar to the terminal window in the top screenshot.

Settings, logout, shutdown

type "terminal"

Terminal

Dock (running applications, frequently used applications)

Standard applications

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!!!**)

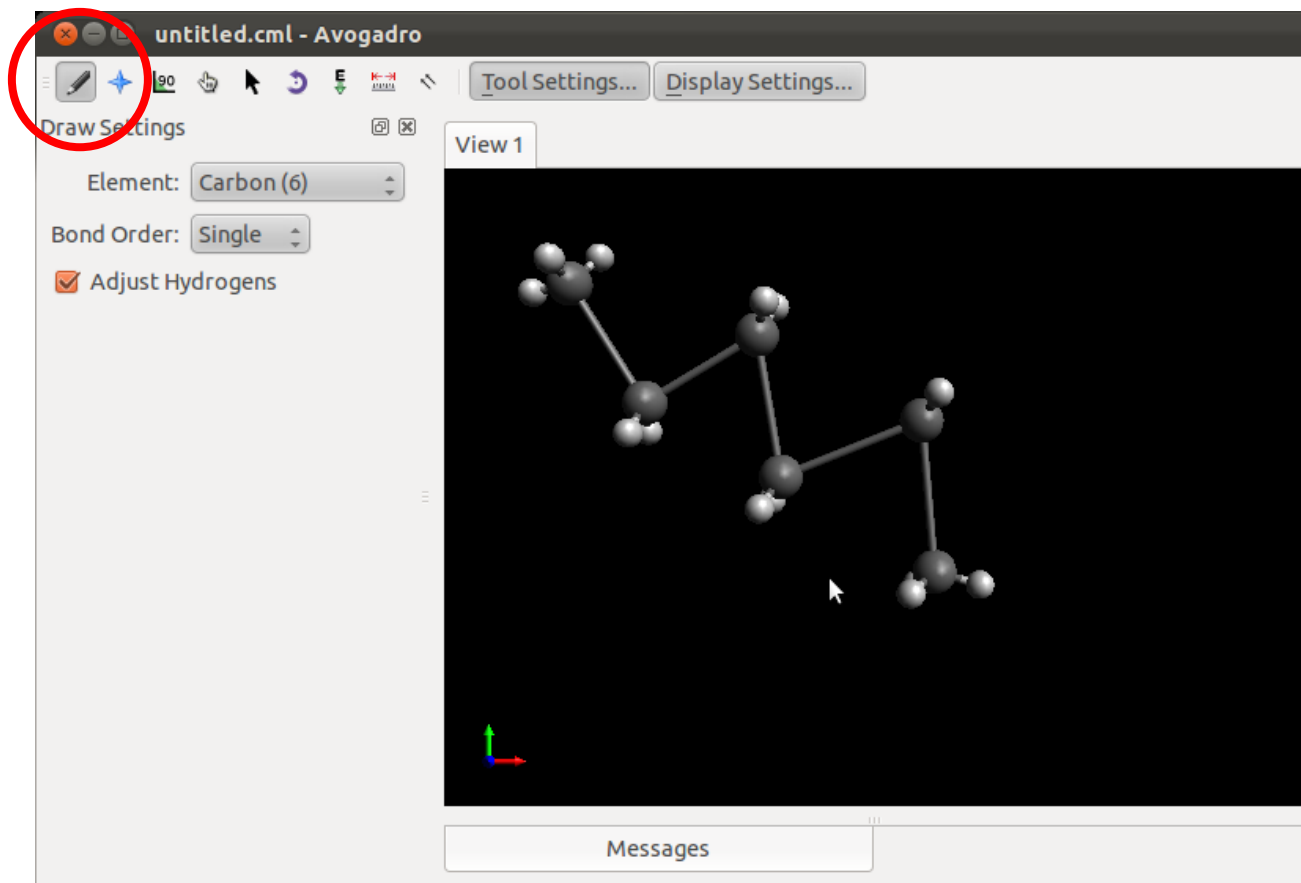
```
$ avogadro
```

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

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

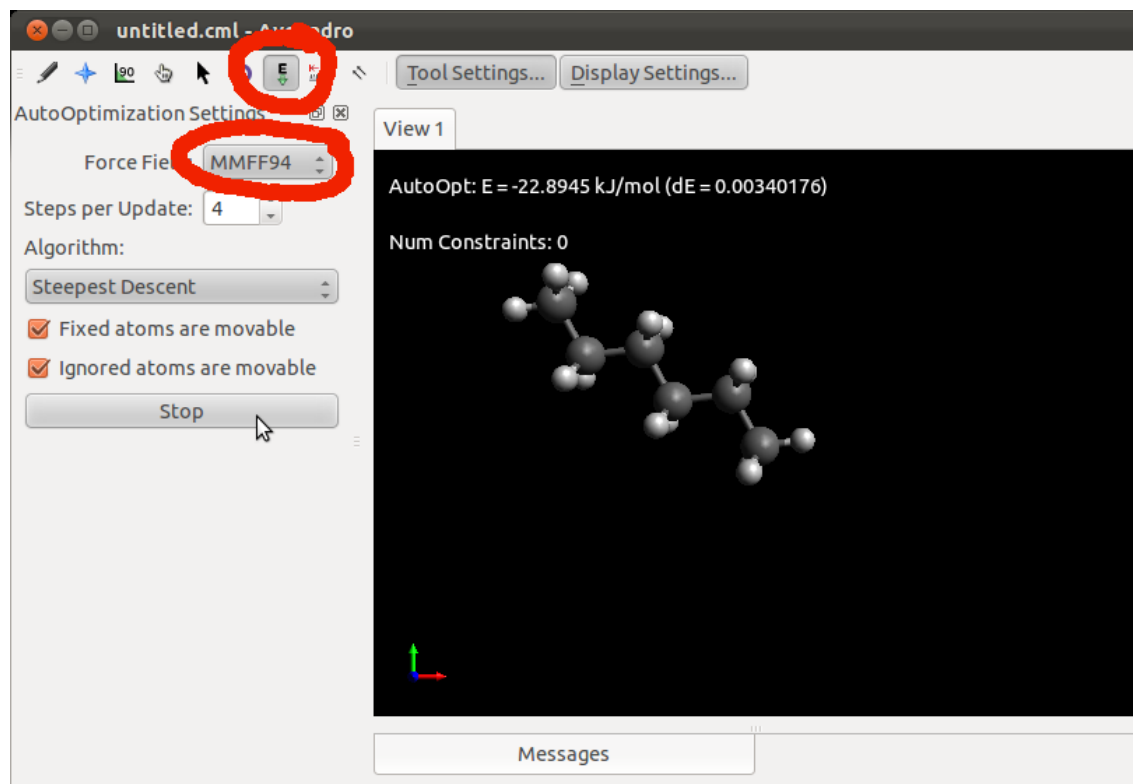
Draft model

- 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.

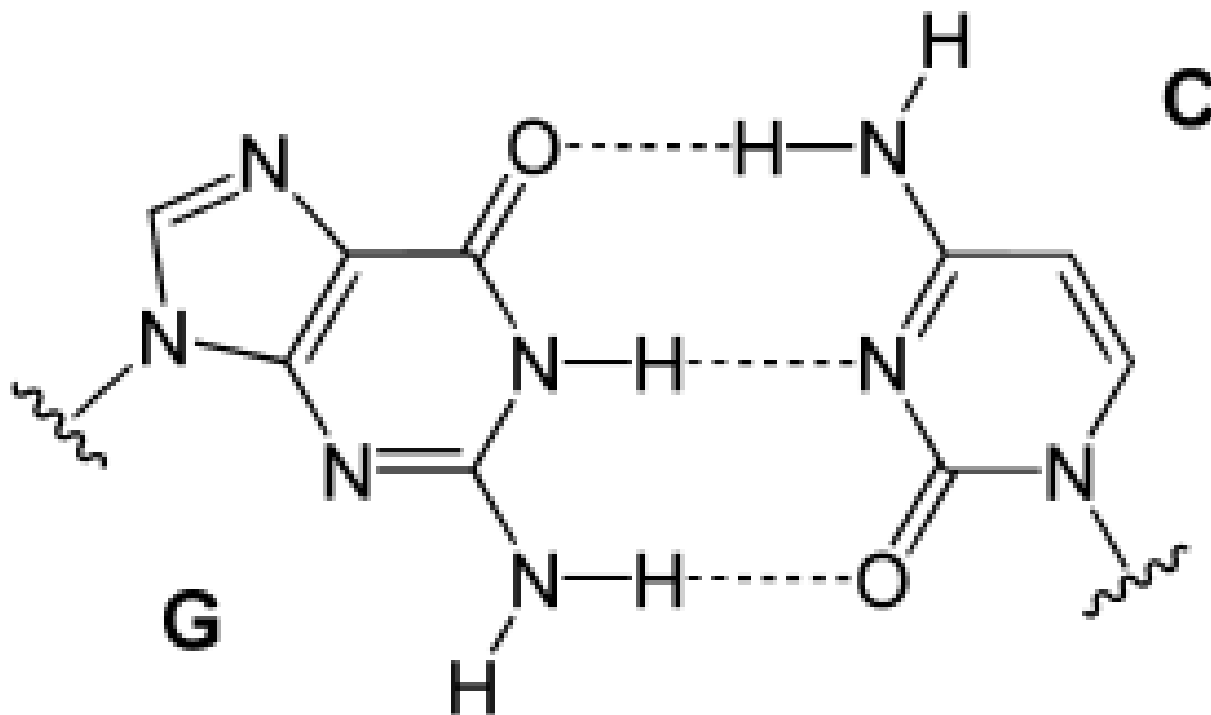


Exercise 1

1. Step by step, create models of the following molecules:
 - methane
 - ethene, ethyne
 - benzene
 - adamantane
 - benzoic acid
 - trinitrotoluene
 - salicylic acid
 - optionally building C₆₀

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

The screenshot shows the Nemesis Molecular Modelling Package interface. The main window is titled "Project 1 : NEMESIS - Molecular Modelling Package". The interface is divided into several panels:

- Structures panel:** Contains a table with columns "Name", "SID", and "Ato". It lists "Structure 1" with SID "1". An arrow points to this table with the label "layers".
- Build panel:** Contains a "Basic" tab and a "General" tab. It features a grid of chemical symbols for building molecules (C, O, N, S, Cl, Br, I, etc.) and buttons for "Delete atom", "Make bond", "Break bond", "Delete bond", and "Optimize". The "Optimize" button is circled in red. An arrow points to this panel with the label "molecule building / editing".
- Profile objects panel:** Contains a table with columns "Name" and "Type". It lists "Light 1", "Background 1", "Standard Model 1", and "Freezed Atoms 1". An arrow points to this panel with the label "graphic models".
- Geometry panel:** Contains tabs for "Position", "Distance", "Angle", and "Torsion". An arrow points to this panel with the label "geometry measurement".

Mouse:

- left button - selection
- middle button - rotation
- right button - translation
- wheel - zoom

Keys:

- Shift - XY -> Z
- Ctrl - primary/secondary manipulator

Annotations:

- "layers" points to the Structures panel.
- "molecule building / editing" points to the Build panel.
- "graphic models" points to the Profile objects panel.
- "geometry optimization using a force field" points to the Optimize button.
- "geometry measurement" points to the Geometry panel.

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

Exercise 3

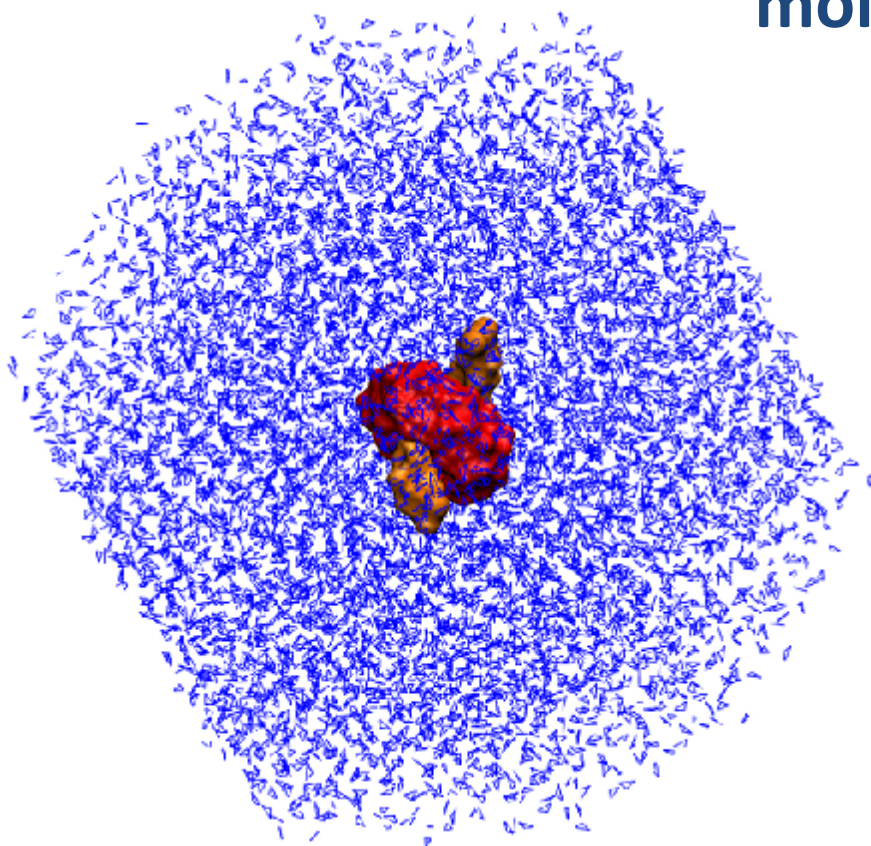
1. Step by step, create models of the following molecules:
 - methane
 - ethene, ethyne
 - benzene
 - adamantane
 - benzoic acid
 - trinitrotoluene
 - salicylic acid

Visualization of molecular dynamics simulations

VMD program

Exercise 4

molecular dynamic simulation of a molecular switch



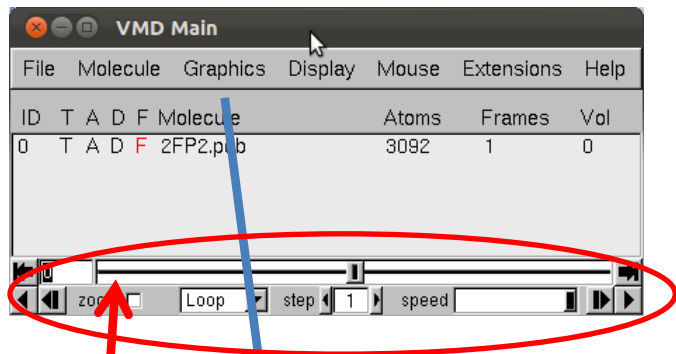
red - rotor
orange - axis
blue - water

Display simulation in VMD

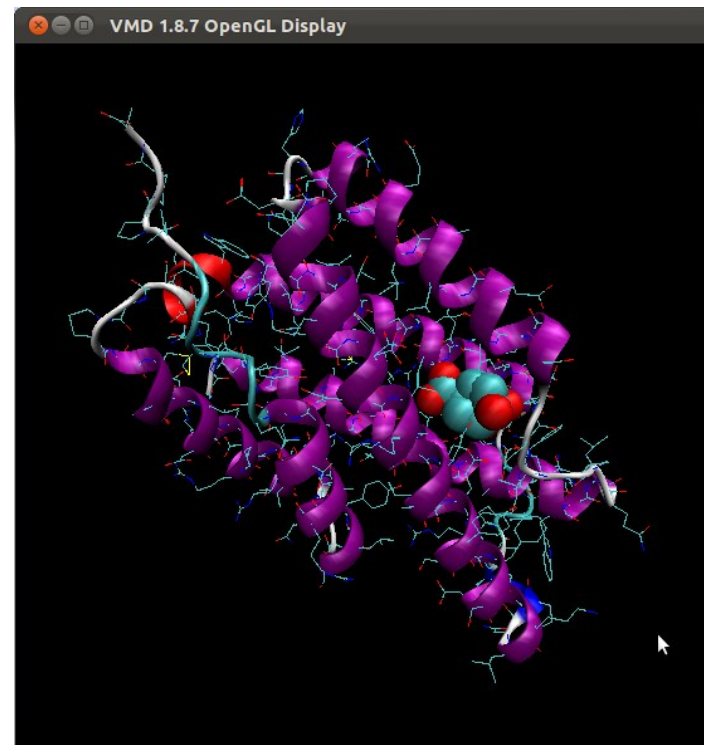
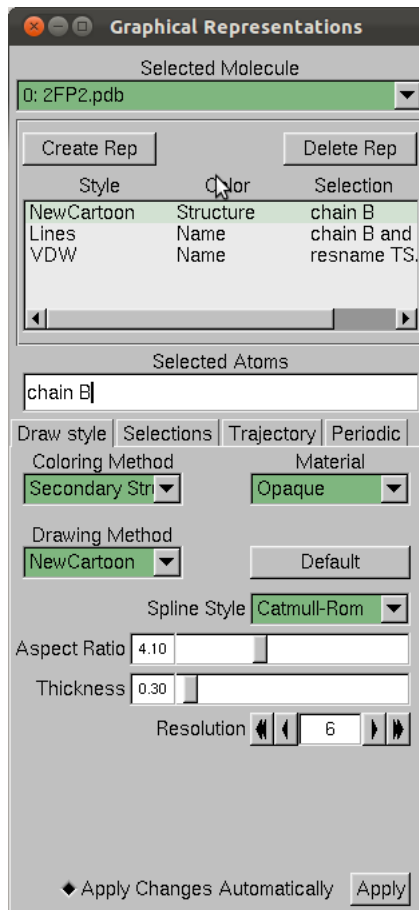
- Open terminal and run the following script

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


VMD

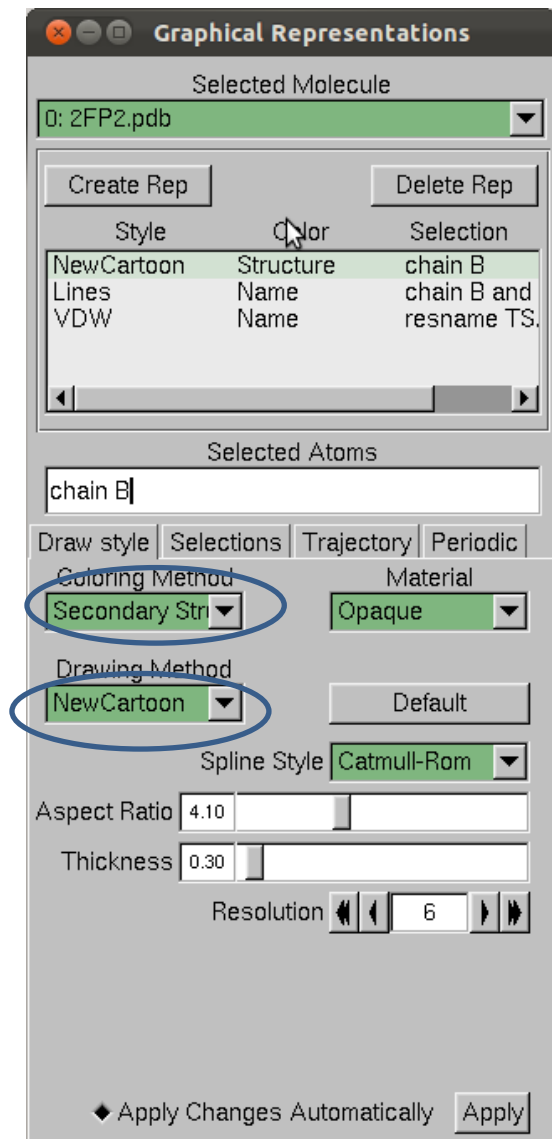


Representation



movement in time

VMD program - visualization



Create/Delete representation



Representation List

double click - activate/deactivate

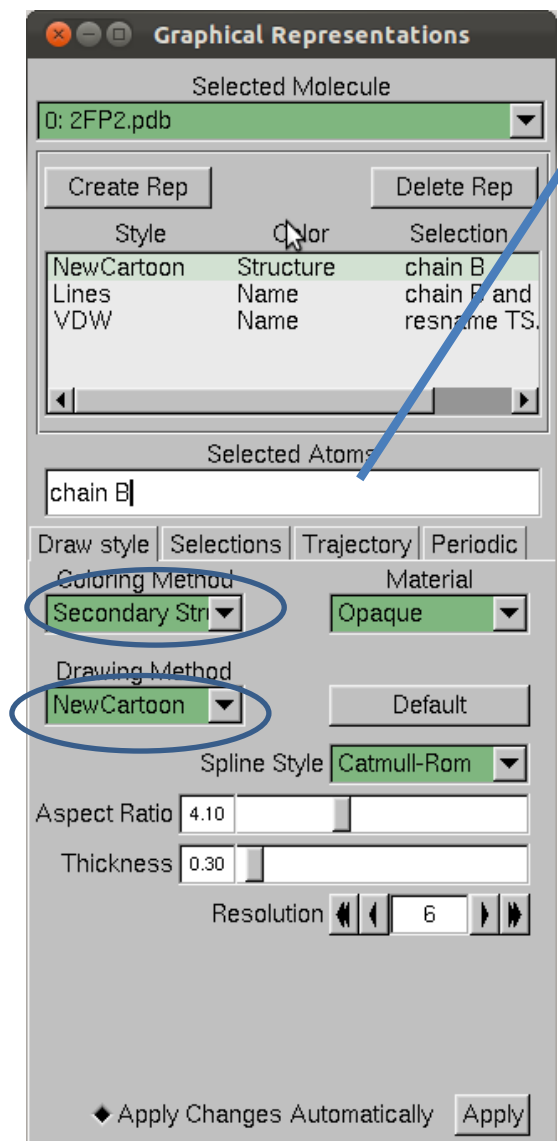


Selection (what part of model is visualized)



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.