Reference manuals

AMBER

Petr Kulhanek

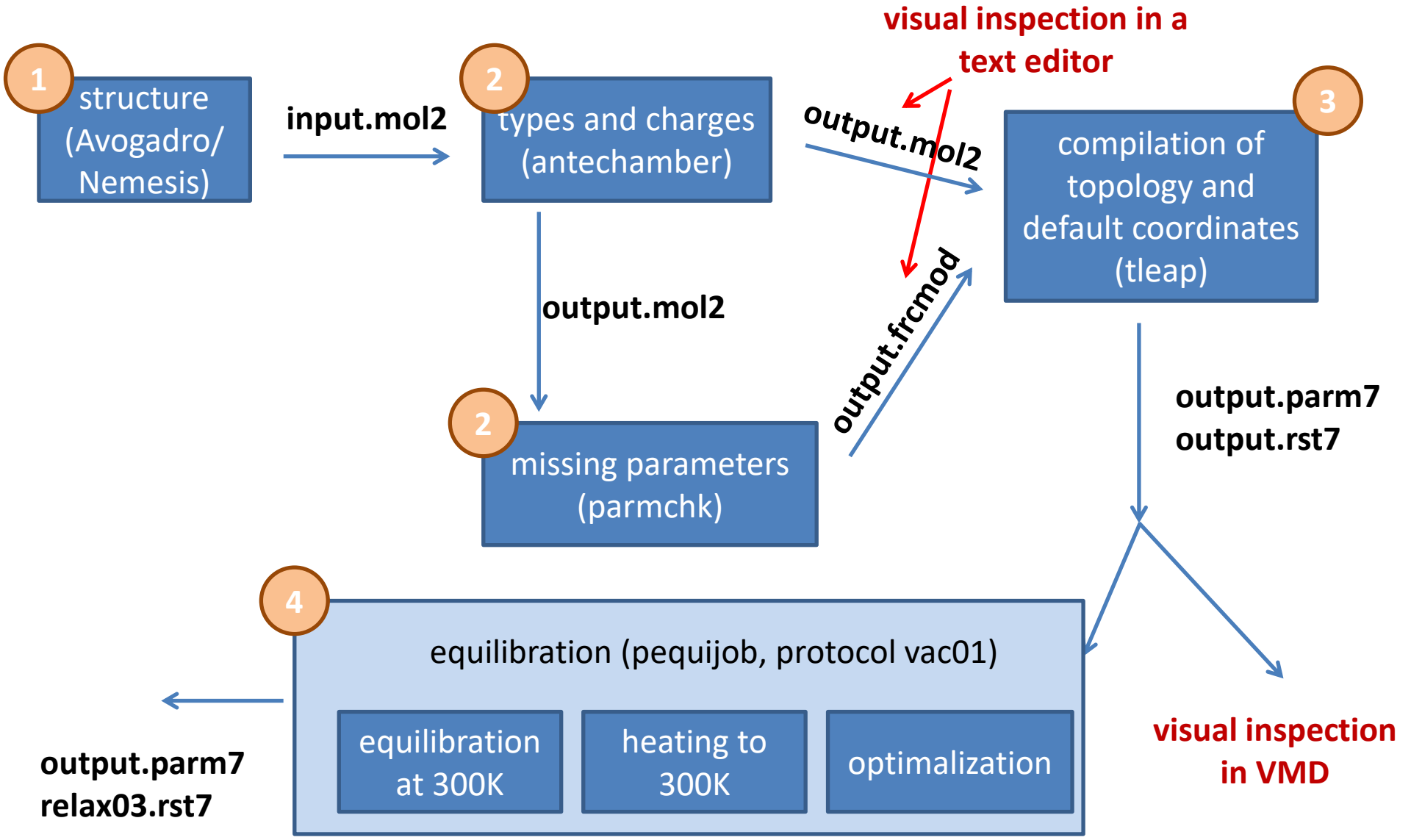
kulhanek@chemi.muni.cz

National Center for Biomolecular Research, Faculty of Science
Masaryk University, Kotlářská 2, CZ-61137 Brno

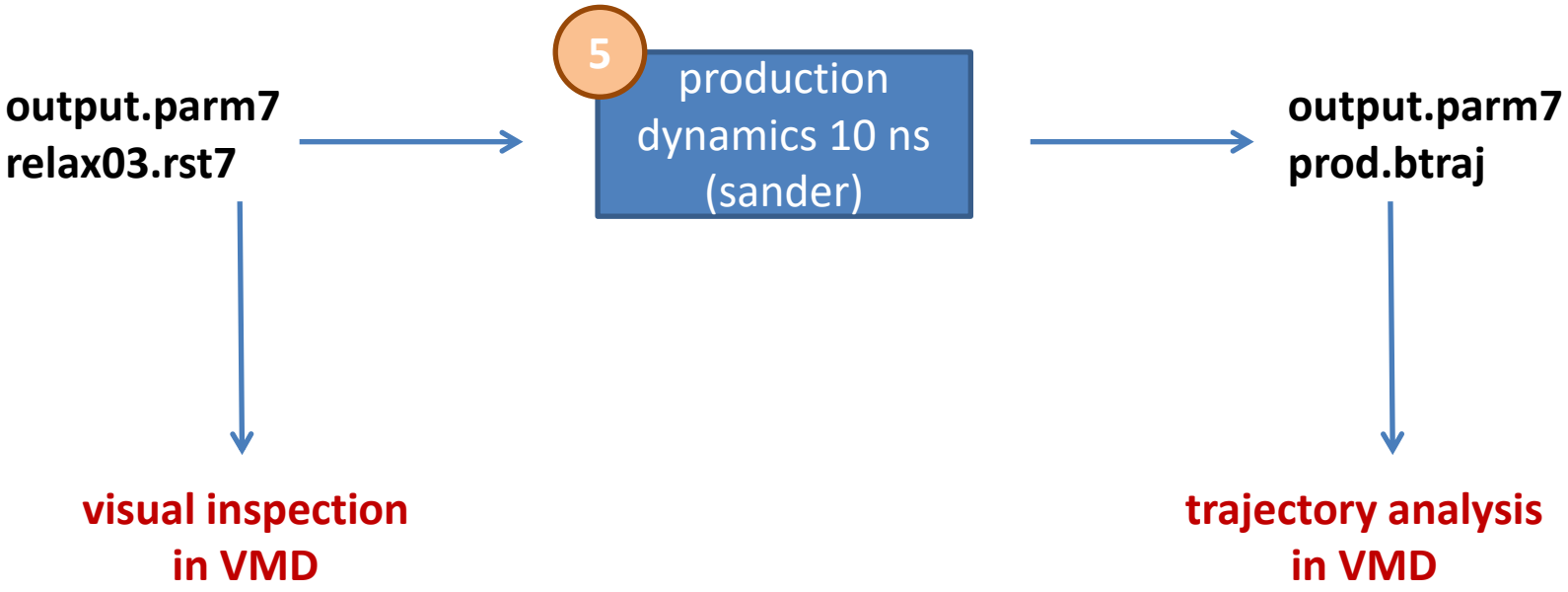
AMBER

http://ambermd.org

Flowchart, MD in vacuum



Flowchart, vacuum, ...

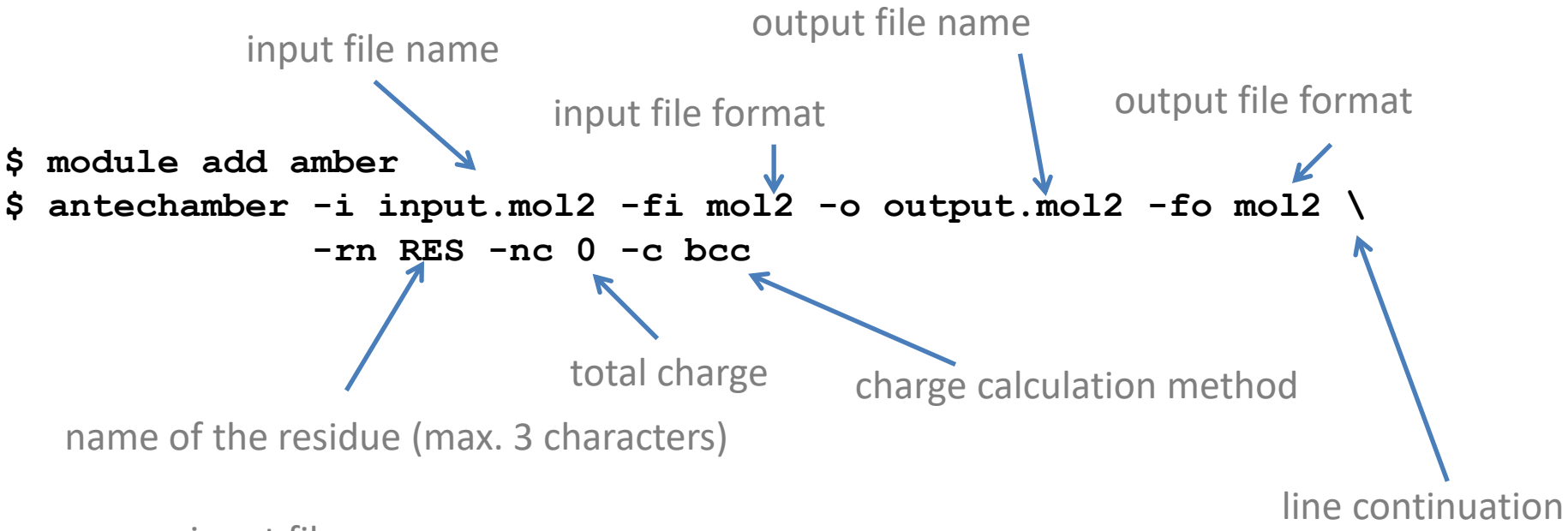


1. Building a molecule

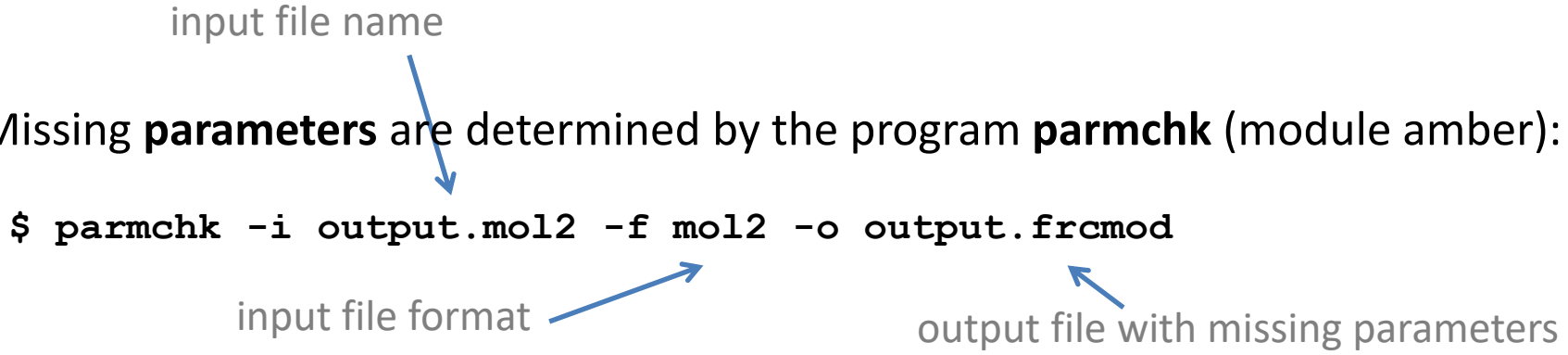
1. The molecule will be built in the program Avogadro/Nemesis.
2. The molecule geometry **will be optimized** (using force field MMFF94).
3. The optimized geometry will be saved in the format **mol2** (input.mol2).

2. Types, charges and FF parameters

Types and charges of individual atoms are determined by the program **antechamber** (module amber):



Missing **parameters** are determined by the program **parmchk** (module amber):



3. Building a topology

Create a script (**script.in**) for the program **tleap**. The script describes how to build the final topology (contains a list of constraints, angles, dihedral angles and parameters of bonding and non-boding interactions) and system coordinates.

```
# loading parameters of force field (GAFF)
source leaprc.gaff

# loading missing parameter
loadamberparams output.frcmod

# loading template with structure
LIG = loadmol2 output.mol2

# saving topology and coordinates
saveamberparm LIG output.parm7 output.rst7
```

We will execute the script by the interpreter **tleap**:

```
$ module add amber
$ tleap -f script.in
```

go through the entire output displayed on the screen to see if an error has occurred somewhere

4. Equilibration

1. Make a separate directory and copy the **output.parm7** and **output.rst7** files there. Set the directory as the current directory.

2. Create templates for equilibration, use the protocol **vac01** from the dynutil module.

```
$ module add dynutil
$ small-prep vac01
```

3. Open the file **pequiJob** in text editor and edit the items containing names of the topology and coordinate files.

```
# input topology ------------------------------------------------------------
# file name without path, this file has to be presented in working directory
export PEQUI_TOP="output.parm7"

# input coordinates ---------------------------------------------------------
# file name without path, this file has to be presented in working directory
export PEQUI_CRD="output.rst7"
```

4. Submit job **pequiJob** into the batch system.

5. Production dynamics

1. Create a separate directory and copy **output.parm7** and **relax03.rst7** files there (result from equilibration). Set the directory as the current directory.

2. Copy the contents of the directory **/home/kulhanek/Vibuch/2011/prod-vac** to the directory.

3. If other file names were used, it is necessary to edit the script **prodJob** .

4. Check the contents of the prod.in file.

5. Submit the job **prodJob** into the batch system.

The goal of the production dynamics is to create **trajectory** which is used for calculation of **system properties**.

We will display the resulting trajectory in the VMD program:

```
$ vmd -parm7 output.parm7 -netcdf prod.btraj
```

5. Production dynamics, ...

```
# production dynamics at 300 K

&cntrl
 imin=0,
 nstlim=10000000,
 dt=0.001,
 irest=1,
 ntx=5,

 ntpr=1000,
 ntwx=1000,
 ntwr=1000,
 ioutfm=1,

 ntf=2,
 ntb=0,
 cut=999,

 ig=-1,
 temp0=300.0,
 ntt=3,
 gamma_ln=2.0,

 ntc=2,
&end
```

control file **prod.in** determines under what conditions the production dynamics takes place

total number of steps

the size of the integration step (in ps)

temperature in K

Settings of Langevin thermostat

the meaning of other parameters can be found in the manual of sander program