Running a simulation

in Gromacs

Gromacs

Originally developed at Groningen University (the Netherlands)

Now actively developed internationally (mostly Sweden and the US)

Aim: to be *fast,* in real time to result

- hand-coded assembly interaction kernels
- high scalability to parallel systems

Gromacs 4.6

- Support for GPUs
- Also faster for CPUs,
  - especially on modern hardware
- Many more free energy options

A typical (biomolecular) simulation

- Get a structure (PDB or homology modeling)
- Fix missing segments, side chains. Determine protonation states, etc.
- Prepare a (Gromacs) topology
- Add solvent (water), ions
- Energy minimization
- Equilibration
- Run production simulation
- Analyze trajectory data

Starting structures

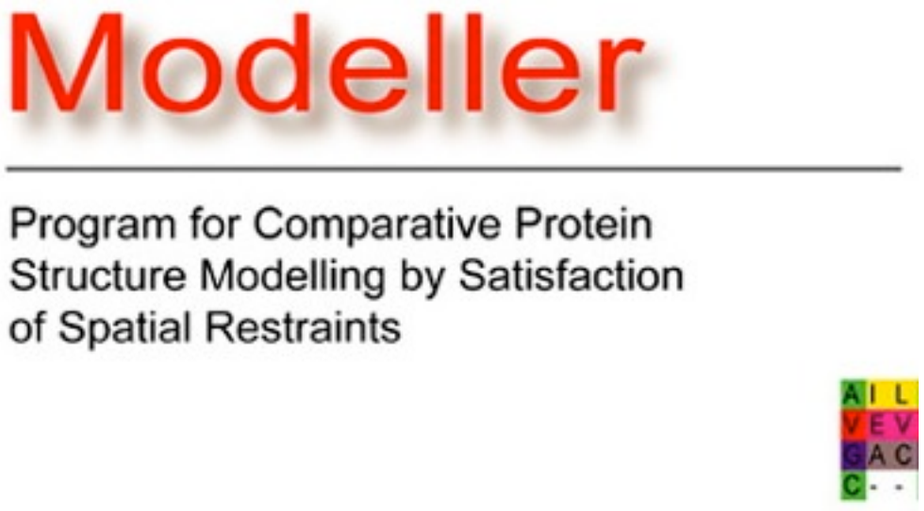
We need something to start with

Simulations are too slow to wait for protein folding

X-ray structure

or

Homology modeling



Starting structures

- With X-ray crystallography structures:
  - Usually high resolution
  - Maybe missing atoms/residues
  - Can have ligands bound

- Homology modeling structures
  - *Can* work with homology >~30%
  - Works well with higher homology

Topologies & configurations

Topology:
doesn't change during simulation

Bonds
Interaction strengths
Interaction ranges

Configuration:
changes during simulation

Coordinates
Box size & shape

Preparing a topology

- This is where we choose the force field
- Go from structure to chemical bonds & interactions
- Can be quite *messy* (we're taking experimental data and are making a potentially unstable simulation model)
- In Gromacs, done with `pdb2gmx`

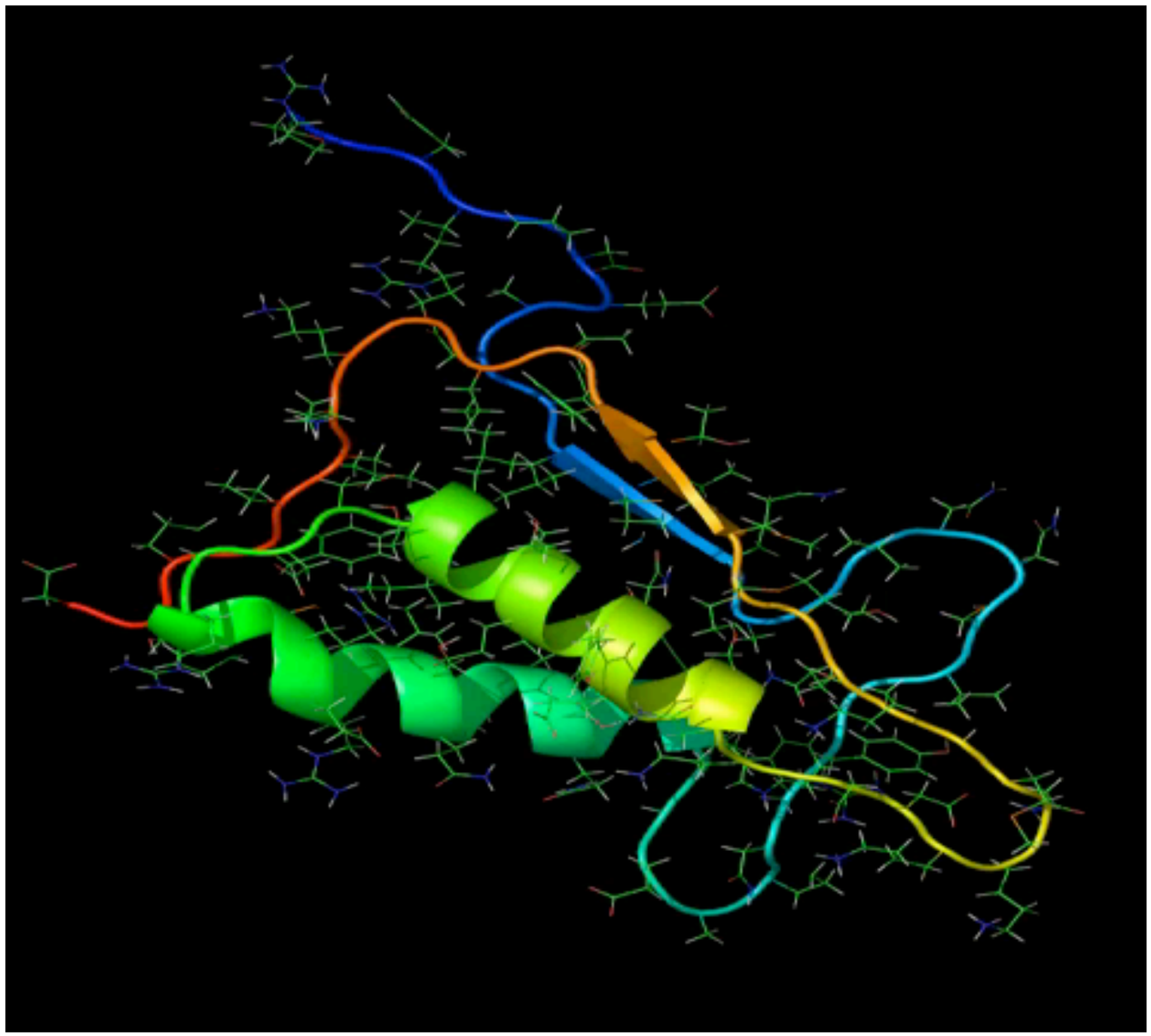
Energy minimization

Find local energy minimum, where force=0

Normally small changes

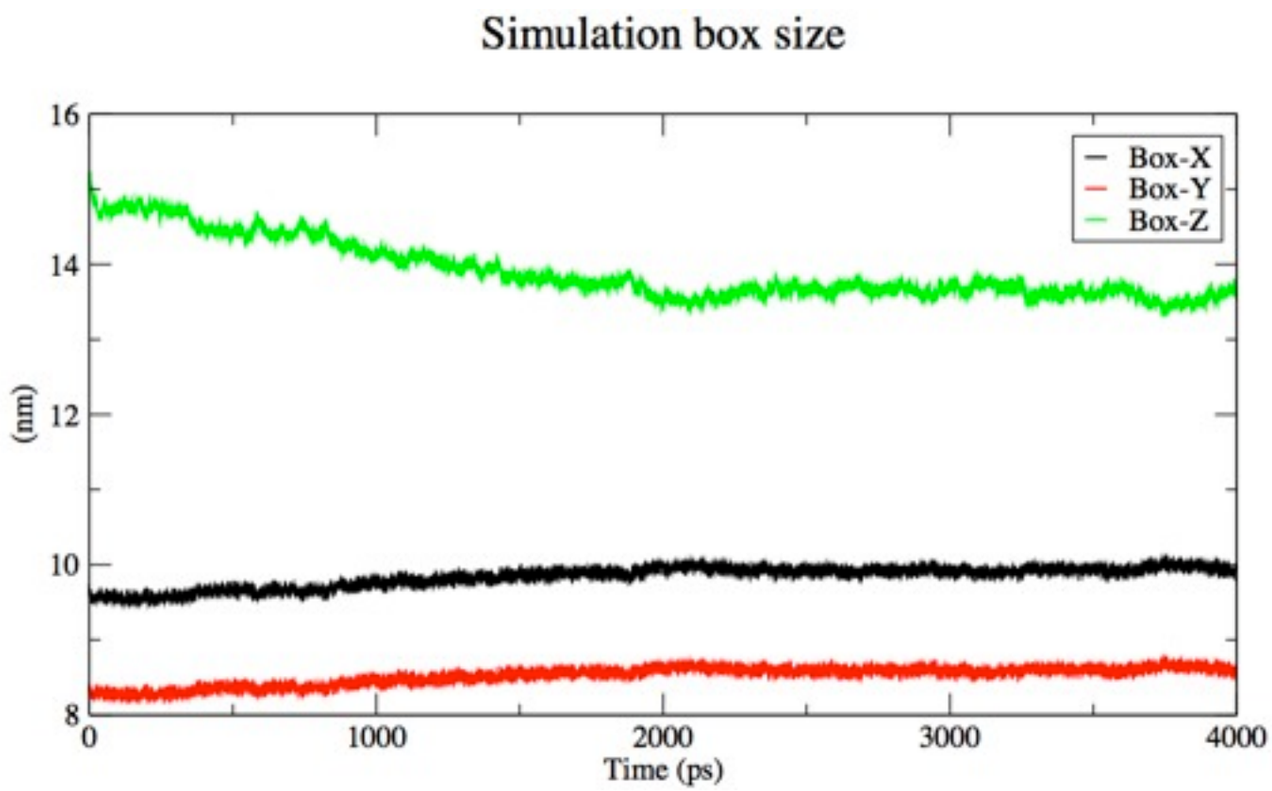
Removes obvious instabilities from configuration

In Gromacs, done with `mdrun`



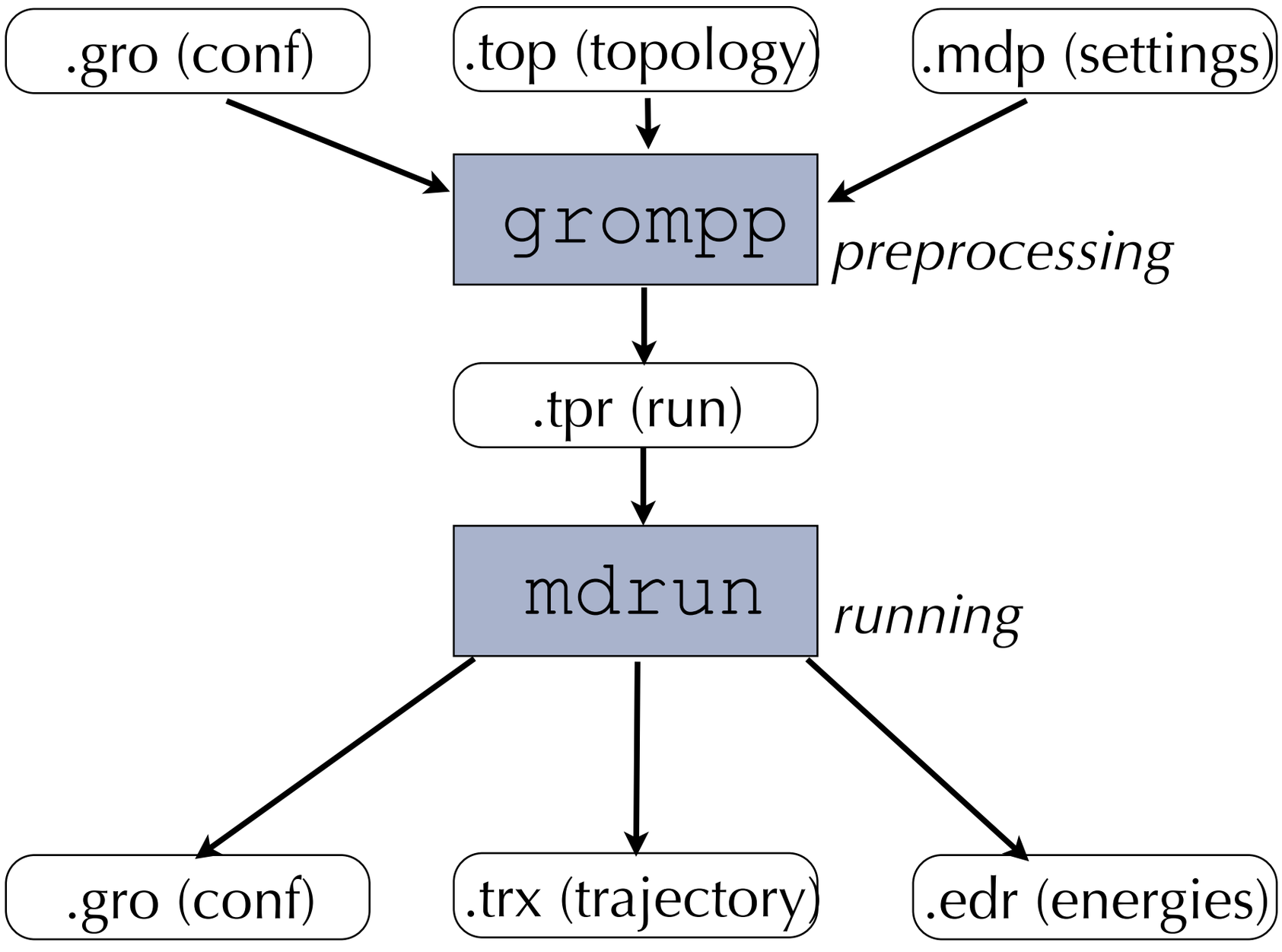
Equilibration

- Starting configuration usually not representative of our *ensemble*
- Equilibration fixes this
- How long should we equilibrate?



Running the simulation

In Gromacs, with `mdrun`



After the simulation

- Many, *many* postprocessing tools
- Will be covered tomorrow

Now, an example

Chicken villin headpiece