

# 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

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- 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



The image shows a screenshot of the RCSB Protein Data Bank (PDB) website. At the top left, the logo reads "RCSB PDB PROTEIN DATA BANK". Below the logo is a blue navigation bar with "HELP | PRINT" in white text. On the left side, there is a sidebar menu with a "Home" button and a "Hide" button. The menu items include: "News & Publications", "Usage/Reference Policies", "Deposition Policies", "Website FAQ", "Deposition FAQ", "Contact Us", and "About Us". To the right of the sidebar, the text "A Resource" is visible, followed by a paragraph: "The PDB archive contains... according to agreed..." and another paragraph: "The RCSB PDB also provides... downloaded, and analyzed..."

## Modeller

Program for Comparative Protein Structure Modelling by Satisfaction of Spatial Restraints



# 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  $> \sim 30\%$
  - 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`



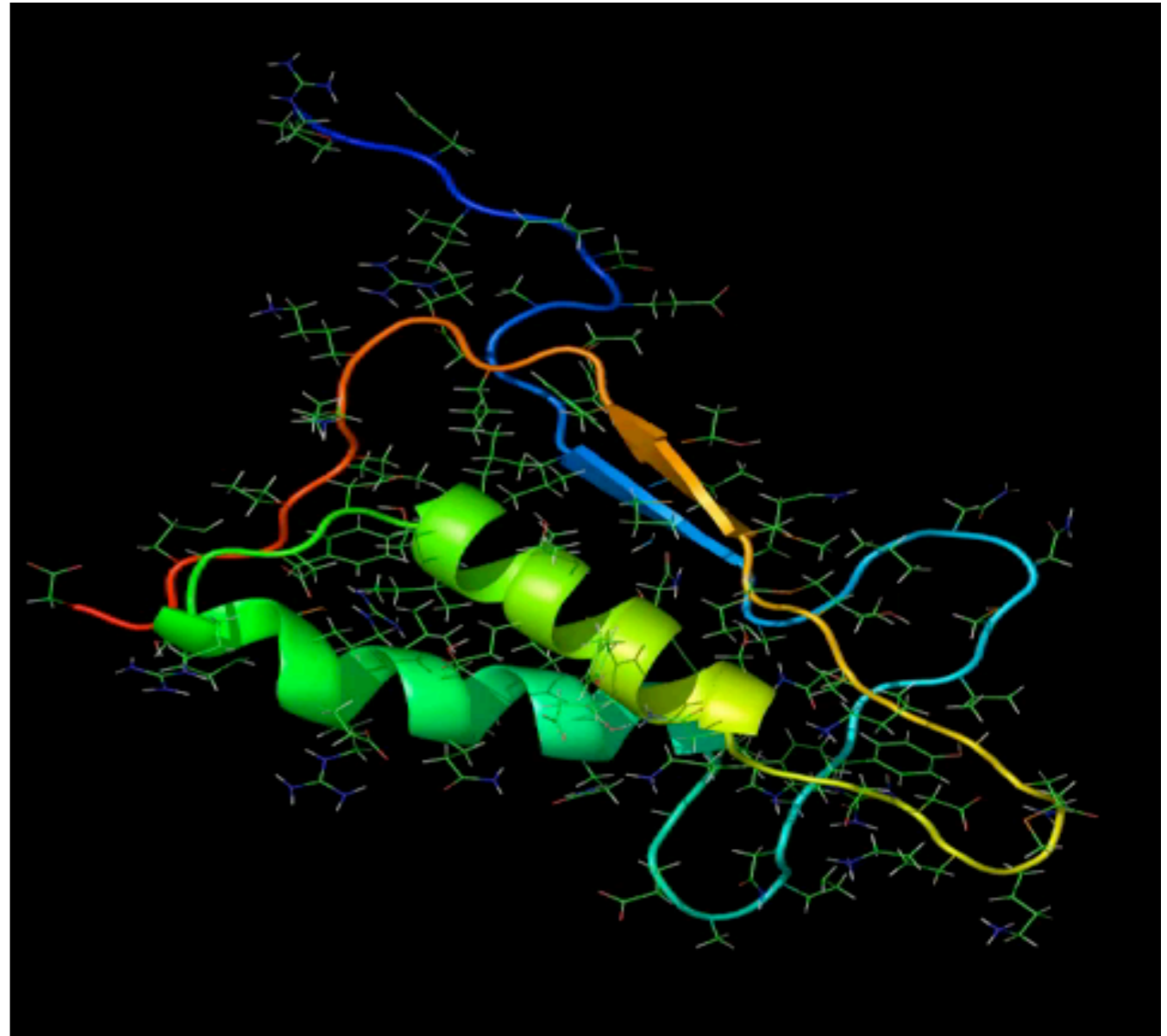
# Energy minimization

Find local energy minimum, where  $\text{force}=0$

Normally small changes

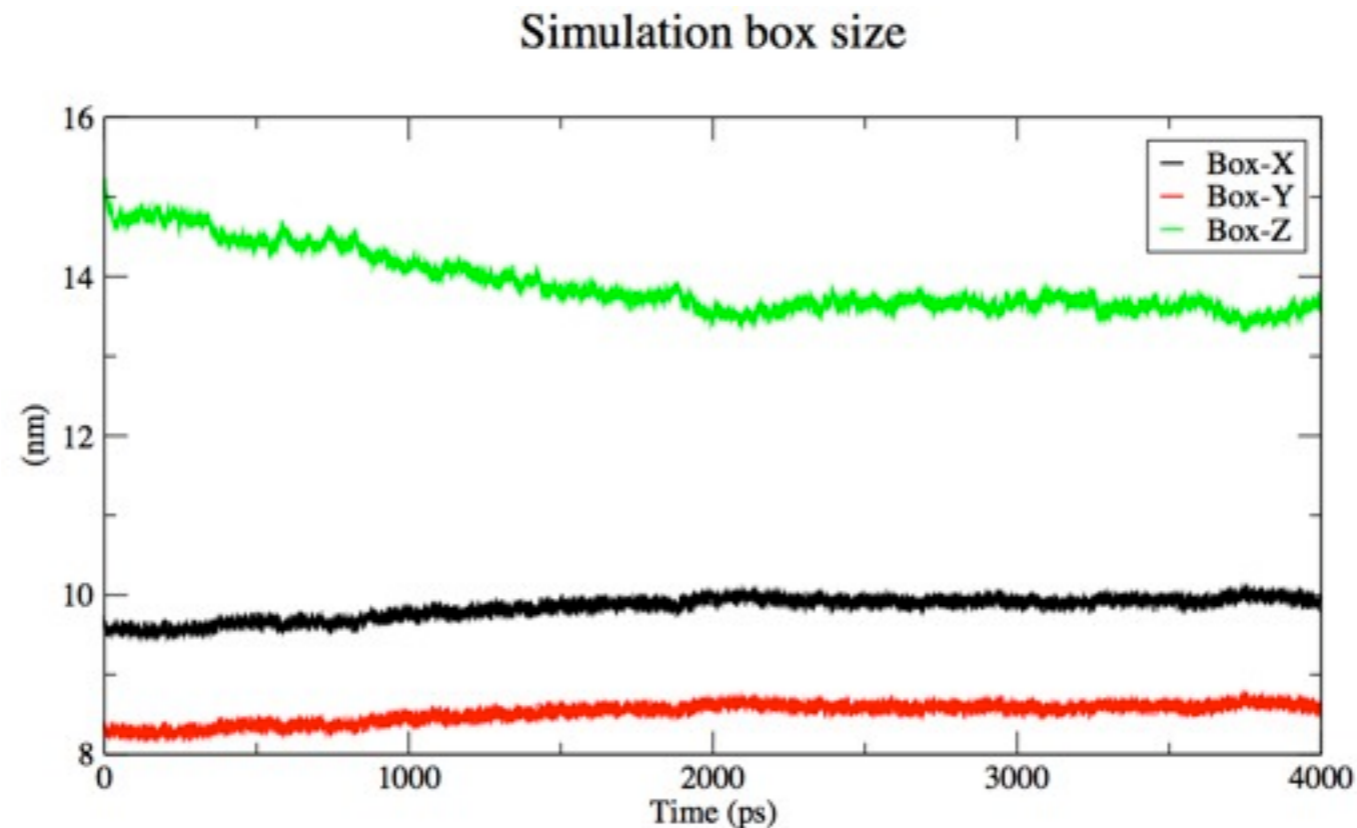
Removes obvious instabilities from configuration

In Gromacs, done with `mdrun`



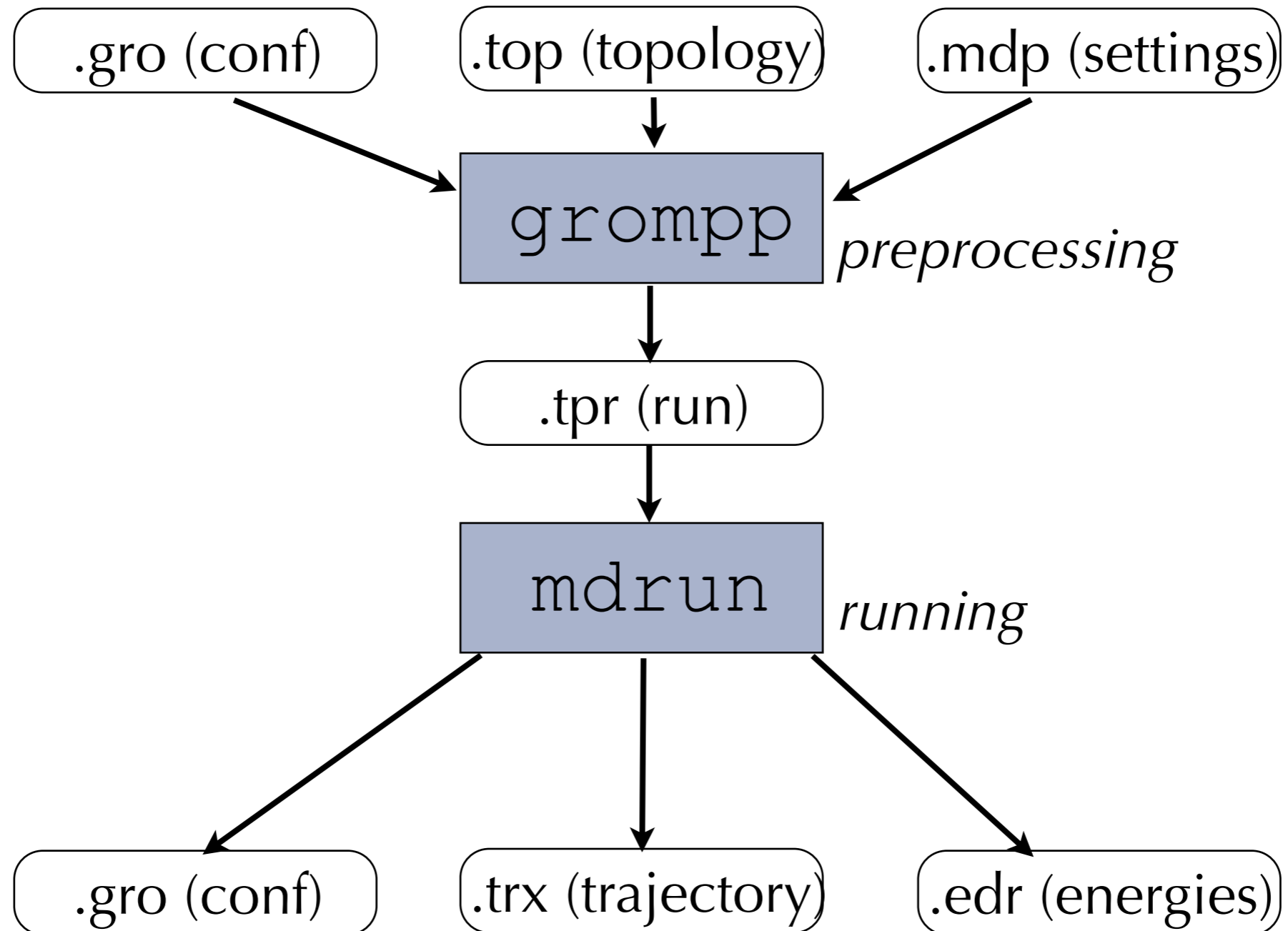
# Equilibration

- 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

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

# Now, an example

## Chicken villin headpiece

