Preparing an MD simulation

the procedures – briefly

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Work plan

1. build the initial structure
2. bring the system into thermodynamic equilibrium
3. perform the productive simulation
4. analyze the trajectory

Tools to build the structure

- do it yourself
- specific programs within simulation packages
- ‘universal’ visualization programs – VMD, Molden, Pymol

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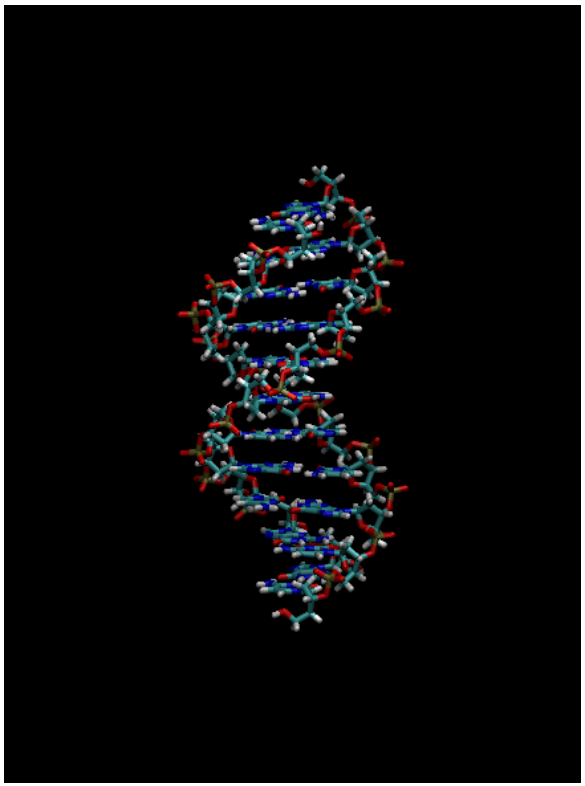
- specialized web services – Make-NA
- tools to create periodic box and hydrate system

Tools to build the structure

build the solute, solvate it and add counterions



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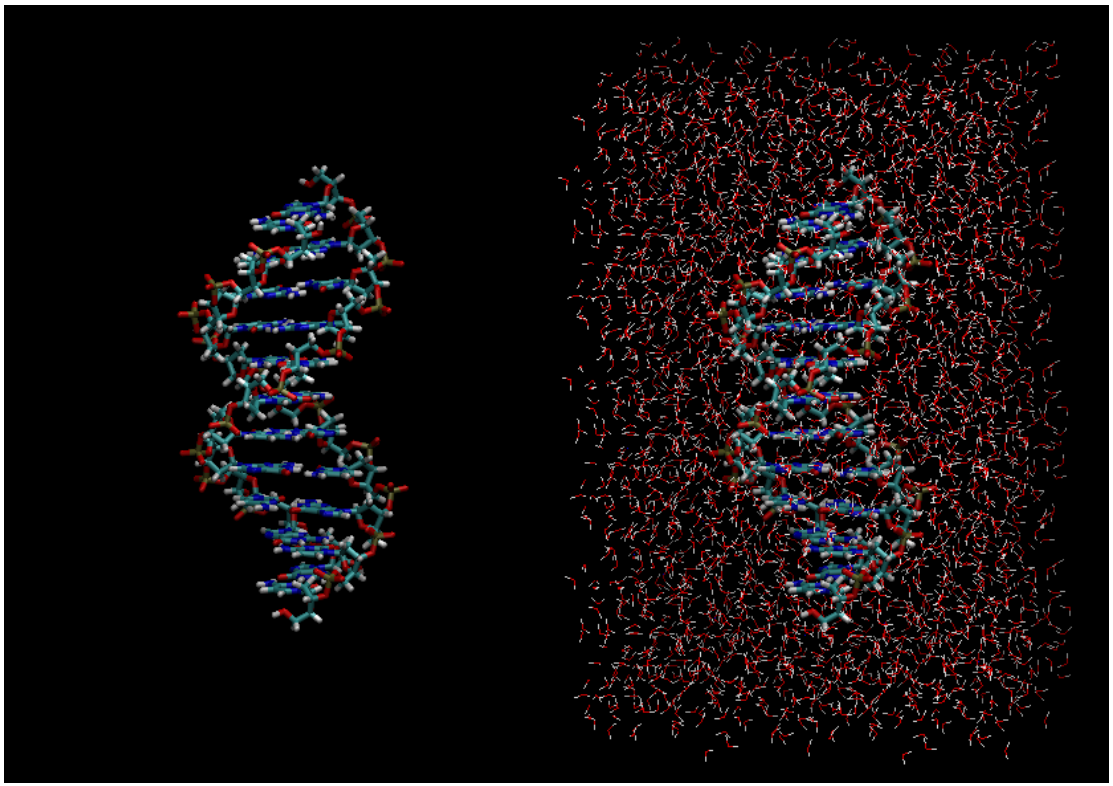

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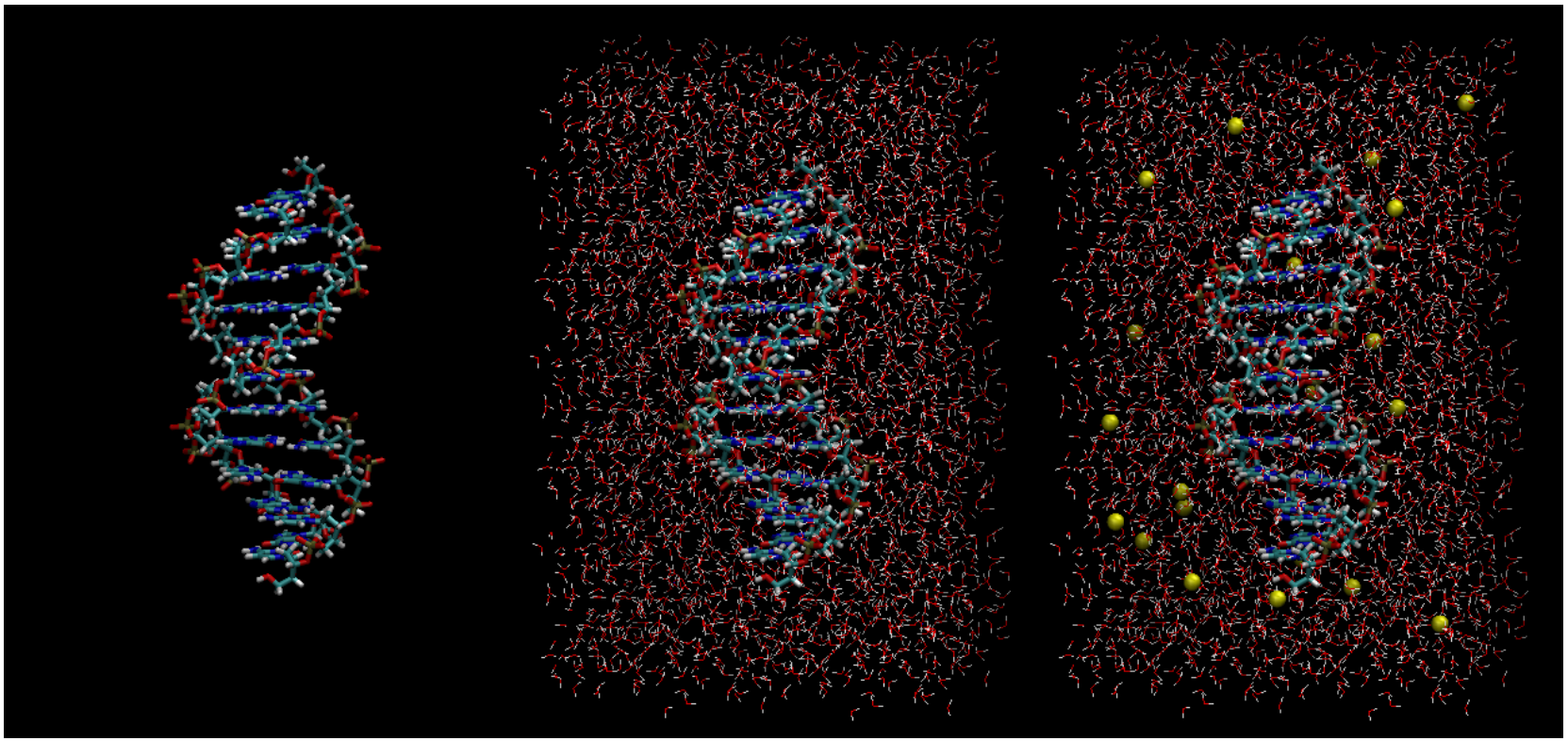

Why equilibrate?

- the initial structure may have high potential energy – dangerous – remove ‘close contacts’
- often, static structure available – velocities missing
- often, structure resolved at different conditions (xtal)
- structure of solvent artificially regular – entropy wrong

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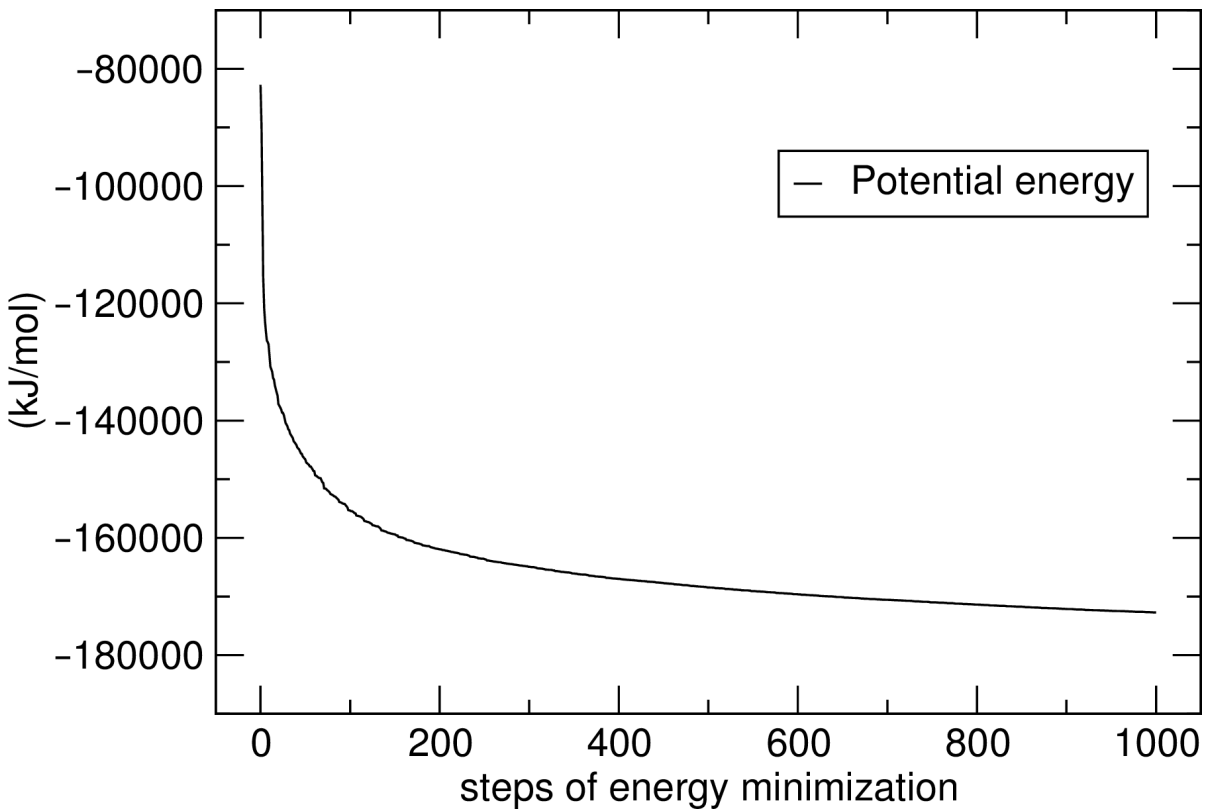
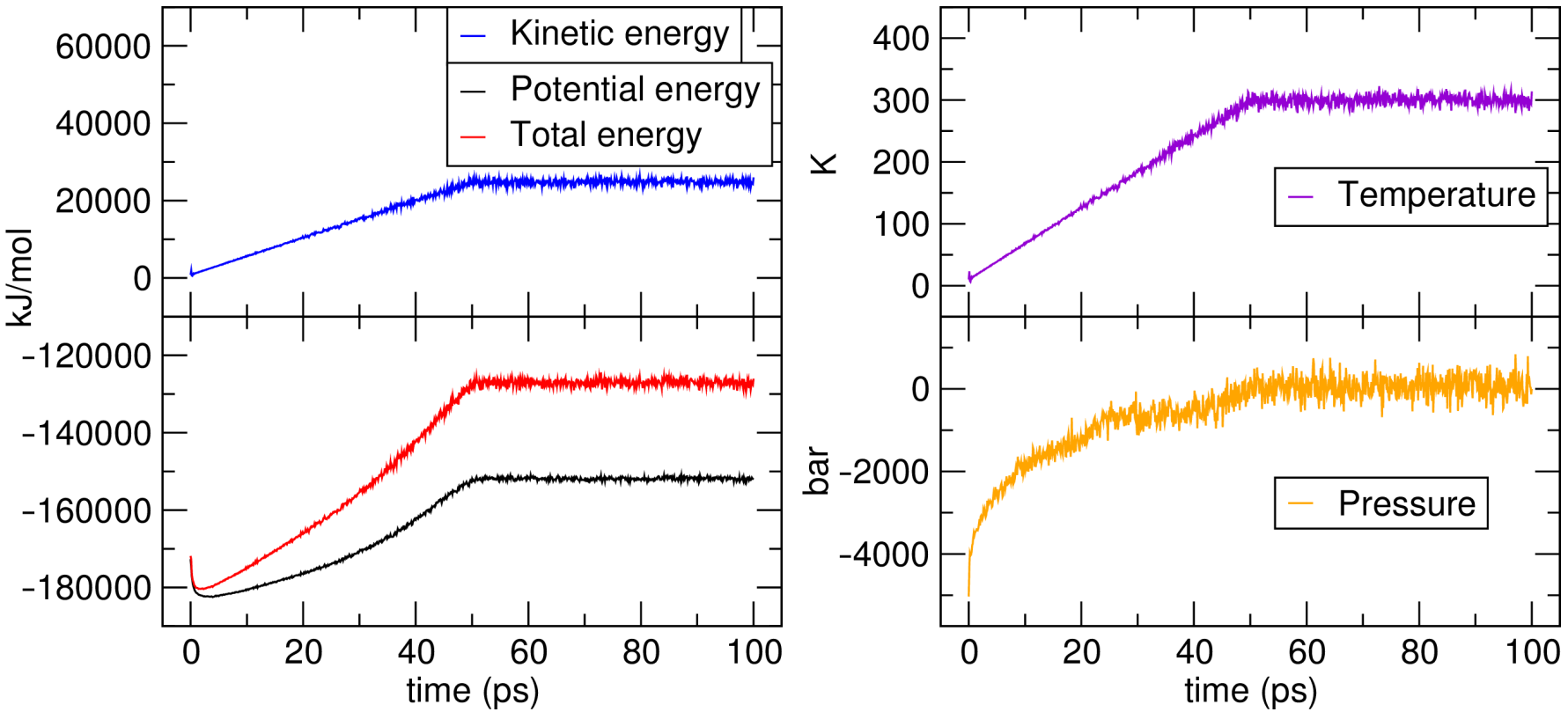
4. simulation with the same setup as the production – probably NPT, with appropriate thermostat and barostat

Short optimization

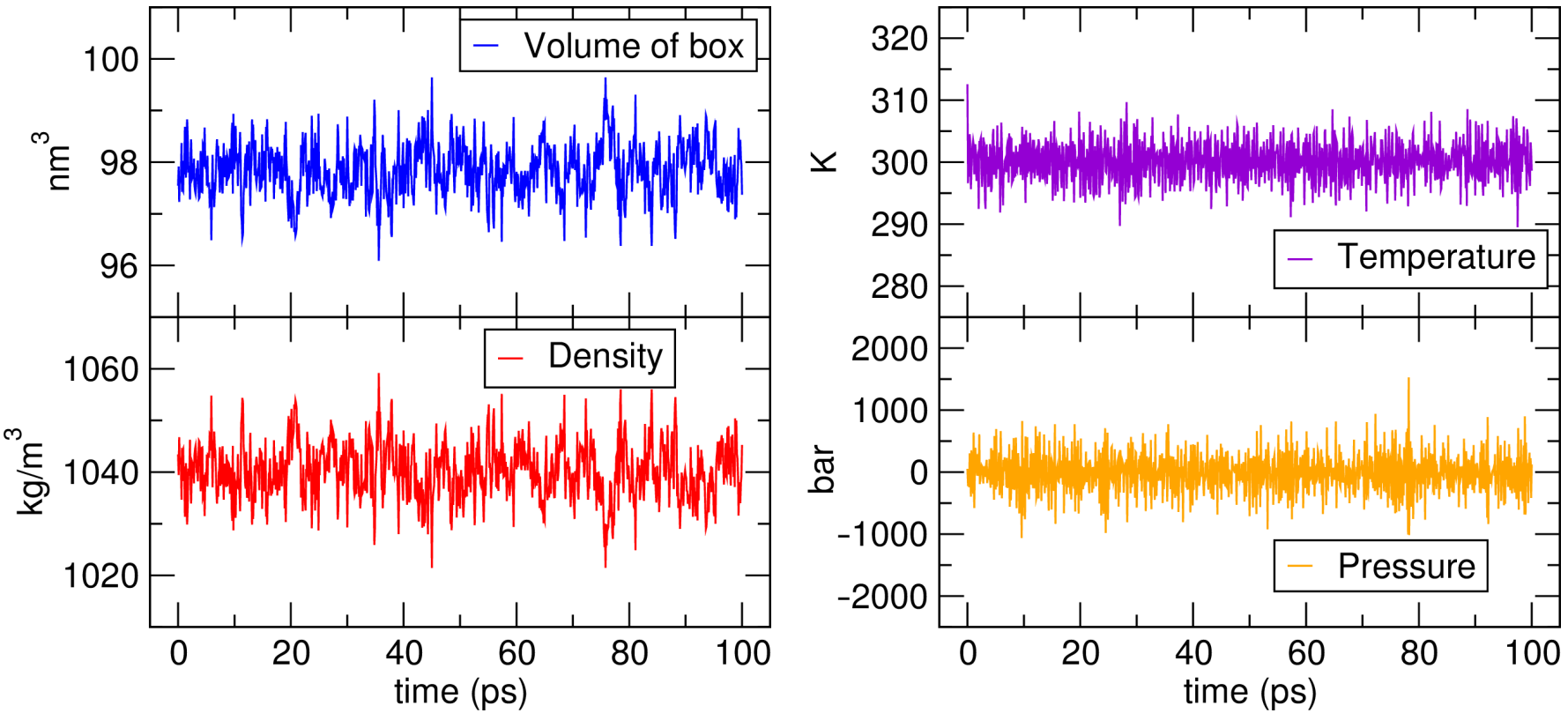


Thermalization



last 40 ps: $T = 300 \pm 7$ K, $p = 64 \pm 266$ bar

Equilibration



last 40 ps: $T = 300 \pm 3$ K, $p = -11 \pm 331$ bar

What comes then?

Productive simulation
- easy ☺

Analysis of the trajectory
- let us see...