**Level 1: main information**

* gromacs version
  + gmx dump -s .tpr → VERSION
* type of simulation - determined by the "integrator" option
  + energy minimization - "steep" or "cg" values
  + molecular dynamics - "md\*" or "sd" values
* statistical ensemble - determined by the combination of "tcoupl" and "pcoupl" options
  + NVE (microcanonical)
    - tcoupl = "no"
    - pcoupl = "no"
  + NVT (canonical)
    - tcoupl = usually "nose-hoover" or "v-rescale"; less common "berendsen", "andersen", "andersen-massive"
    - pcoupl = "no"
    - include the reference temperature of the system: "ref-t" in [K] - IVO
  + NpT (isothermal-isobaric)
    - tcoupl = usually "nose-hoover" or "v-rescale"; other options "berendsen", "andersen", "andersen-massive"
    - pcoupl = usually "Berendsen" or "Parrinello-Rahman"
    - include the reference temperature of the system: "ref-t" in [K] IVO
    - include the reference pressure of the system: "ref-p" in [bar] IVO
* simulation time step
  + dt in [ps]
  + only when the type of simulation is “molecular dynamics”
* simulation length
  + single run: dt \* nsteps
  + extended simulations: gmx check -f .cpt → "Last frame" in [ps]

force field

* + probably has to be set by the user
* list of molecules (with their counts) in the system
  + listed in a "\*.top" file, section [ molecules ]
  + gmx dump -s "\*.tpr" → topology: → molblock → moltype + #molecules
    - in the case of proteins, also include its sequence
* size and shape of the simulation box
  + last line of a coordinate file (e.g., “\*.gro”)
* free energy calculation - option "free-energy"
  + values "yes"/"no"
* umbrella sampling - option "pull"
  + values "yes"/"no"
    - before gromacs 5.x, the options were "umbrella"/"constraint"/"constant-force"/"no"
  + only if AWH is not set (options: "awh", "pull-coord\*-potential-provider")
* AWH adaptive biasing – "awh"
  + values "yes"/"no"

**Level 2: published information**

* if the type of simulation is energy minimization
  + options: "emtol" and "emstep"
* preferably group into "thermostat"
  + in case that "tcoupl" is not set to "no"
  + "tcoupl", "nsttcouple", "tc-grps" , "tau-t"
* preferably group into "barostat"
  + in case that "pcoupl" is not set to "no"
  + "pcoupl", "refcoord-scaling", "compressibility" (3x3 matice), "pcoupltype", "tau-p"
* preferably group into "van der Waals interactions"
  + options "rvdw", "vdwtype", "rvdw-switch", "vdw-modifier", "dispcorr"
    - note that both "cut-off" and "cutoff" are accepted for vdwtype
* preferably group into "electrostatic interactions"
  + "coulombtype", "coulomb-modifier", "rcoulomb", "epsilon-r", "epsilon-rf"
* preferably group into "neighbour list"
  + "cutoff-scheme", "nstlist", "ns-type" (odebráno – email od Iva 30.4. 2022), "pbc", "rlist"
* preferably group into "umbrella sampling"
  + only in case that "pull" is not set to "no"; options:
    - "pull-ncoords", "pull-ngroups"
    - "pull-coord\*-dim", "pull-coord\*-vec", "pull-coord\*-geometry", "pull-coord\*-type", "pull-group\*-name", "pull-coord\*-k", "pull-coord\*-rate", "pull-coord\*-groups"
    - only if the geometry is set to "cylinder"
      * add: "pull-cylinder-r"
  + note that pull options are numbered (starting from 1); here denoted with \*
* preferably group into "AWH adaptive biasing"
  + in case that "awh" is set to "yes"; options:
    - "awh\*-dim\*-cover-diameter", "awh-nbias", "awh\*-ndim", "awh\*-dim\*-diffusion", "awh\*-dim\*-coord-index", "awh\*-dim\*-force-constant", "awh\*-dim\*-start", "awh\*-dim\*-end", "awh\*-error-init"
  + these options are numbered (starting from 1); "awh" and "dim" is numbered independently

**Level 3: detailed information**

* generate initial velocities, options:
  + "gen-vel", "gen-temp" (odebráno – email od Iva 30.4. 2022)
* constraint settings, options:
  + "constraints", "constraint-algorithm", "lincs-order", "lincs-iter"
* center-of-mass motion removal, options:
  + "comm-grps", "nstcomm", "comm-mode"
* in case that "coulombtype" is set to "pme":
  + "fourierspacing"
* in case that "pull" is not set to "no"; options:
  + "pull-coord\*-start", "pull-coord\*-init"
* in case that "free-energy" is set to "yes":
  + options: "init-lambda", "delta-lambda", "sc-alpha", "sc-power", "sc-sigma"
* in case that "awh" is set to "yes"; options:
  + "awh-potential", "awh-share-multisim", "awh\*-target", "awh\*-growth", "awh\*-equilibrate-histogram"

NOTE: in some cases "\_" and "-" can be used interchangeably