C Input file example

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 # Example of full input file for MDProgram
# The line starting with '#' are comments, which are ignored by the parser.

topology file.top # path to topology file, mandatory
coords file.xyz # path to XYZ coordinates file, mandatory
debug 0 # Enables different levels of debug printing, values: 0, 1, 2
pbc 10.0 # Request Periodic Boundary Conditions with a cubic box length of 10 Å

  [minimize] # Request a minimization
method cg # Request a minimization with conjugate gradients, alternative: st (steepest descent)
etol 1e-6 # Set the energy convergence criteria
ftol 1e-4 # Set the force convergence criteria
maxiter 1000 # Set the maximum number of iterations
alpha 1e-4 # change the alpha parameter for the line search

  [run_md] # Request a MD simulation
ts 1.0 # Set the timestep in fs
nsteps 5000 # Set the number of simulation steps
integrator Verlet # Select the integrator to use between Verlet and velocity Verlet
ensemble NVE # Choose the ensemble between NVE, NVT and NPT
temp 298.0 # Set the simulation temperature in K, valid for initialization and thermostat (if present)
press 100000.0 # Set the simulation temperature in Pa, valid for the barostat (if present)
fix_com true # Request to keep the center of mass momentum fixed along the simulation
traj_dump 10 # Set the number of steps between two saved snapshots
bussi_tau 50.0 # Set Bussi thermostat time constant τ in fs
berendsen_tau 5000.0 # Set Berendsen barostat time constant τ in fs
berendsen_k 4.6e-10 # Set Berendsen barostat isothermal compressibility constant k in Pa^-1


  [run_meta] # Requests a metadynamics simulation
cv distance 3 5 #Set the CV type (distance, angle, dihedral) and the index of the atoms involved
nsteps 100 # Set the number of bias potential deposition in the simulation time
tau 10.0 # Set the deposition time interval in fs
sigma 0.2 # Set the width of the Gaussian bias potential terms
omega 1 # Set the initial bias deposition rate
dT 2700 # Determines the bias factor
```