

NODE_salt

SERVER

NODE_gel

INITIALIZATION

set timestep
set langevin
set non-bonded interaction

set timestep
set langevin
set non-bonded inter
set bonded interaction

charge gel segments
add counterions

minimize energy
by steepest descent
optimization of
particles position

compress/expand
to target volume

populate with ion pairs

populate with ion pairs

EQUILIBRATION

integrate MD equations
to stationary
pressure

integrate MD equations
to stationary
end-to-end distances

exchange ion pairs
to stationary
particle count

repeat till all variables
are stationary between runs

SAMPLING

integrate MD equations
subsample pressure
to effective samle size

integrate MD equations
subsample pressure
to effective samle size

exchange ion pairs
to subsample particle
count to effective sample
size

repeat 200 times, subsample effective size 50

STORING

compress and store data
to pickle format