Energy

INTRODUCTION

With Gromacs it is easy to calculate intermolecular interaction energies, for static lists of atoms. When the demand is to calculate the energies for waters occupying a nanopore or protein active site, the list of water molecules dynamically change between each timestep, requiring the user to perform the following Gromacs (versions <5.0) commands for each timestep in their simulation.

a) g_select. Generates index file for pore water.

b) tpbvonv. Generates topology file for pore water at each timestep.

c) trjconv. Generates compressed trajectory file for pore water at each timestep.

d) mdrun. Recalculate energy functions for solute-solvent or solvent-solvent interactions.

e) g_energy. Calculates short range LJ and Coulomb intermolecular energy for pore water.

f) A nested loop to acquire the energies from the output file of g_energy.

Solenergy and Ligenergy are program written in C, wrapped around the Gromacs API. The output is either the average solvent-solvent interaction energy, or solvent-solute interaction energy.

REQUIRMENTS

1) Simulation data in compressed trajectory format. Example simulation.xtc.

2) Simulation topology file. Example simulation.tpr

3) Distance file (.txt). See Structure manual for instructions on how to use g_dist. The distance file for this calculation are a list of the distances of the solvent atoms with respect to the solute center-of-mass, at each timestep.

4) (Only required for calculating solute-solvent interaction enegy)Index file for the solute(.ndx), generated using Gromacs command make_ndx.

INSTALLATION

clang solenergy_v4.5.c -o sole

and

clang ligsolenergy_v4.5.c -o ligsole

USING

Perform the following commands on your terminal of choice, or in a shell script.

./sole simulation.xtc simulation.tpr distance.txt Nsol NatomsperSol Simlength(ps) Timestep(ps) Poreradius(nm) output

./ligsole simulation.xtc simulation.tpr distance.txt Nsol NatomsperSol Simlength(ps) Timestep(ps) Poreradius(nm) output