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 a dynamic list of atoms, like waters occupying a nanopore or active site, the following Gromacs (versions ¡ 5.0) commands have to be repeated for each timestep.

a) g_select. Generates index file for pore water at timestep i.

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

c) trjconv. Generates compressed trajectory file for pore water at timestep i, porewater.xtc

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

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

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

Solenergy and Ligenergy are a wrapper programs composed of a C program plus several shell scripts, that repeat this procedure for the all of the simulation timesteps. 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 is the distances of the solvent atoms with respect to the solute center-of-mass at timestep i.

4) 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

Execute the following commands on the command line, or in a shell script to use the programs.

```
( ./sole full.xtc full.tpr sol_data.txt NSol NatomsperSol Simlength(ps) Timestep(ps) poreradius(nm) output)
```

```
( ./ligsole full.xtc full.tpr sol_data.txt solute.ndx NSol NatomsperSolvent NatomsperSolute Simlength(ps) timetsep(ps) poreradius(nm) output)
```