Coarse Grain Force Field
for
Protein Simulations.

Version 2.1

Derived from the Martini 2.0 force field

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How to go from a PDB structure to a pdb and itp files compatible with the force field CG2.1 and running in gromacs.

1. All the files necessary can be found in:
   ~periole/FILES_CG2.1/Version_2.1+ElNeDyn
2. Get the pdb file in the protein data base.
3. Clean the pdb file from any header, title line, etc …, Hydrogens, water or other molecules. You should end up with a file containing only the ATOM lines relative to the protein and no hydrogens.
   Note: - all residues MUST be complete.
   - save the file under a name, here we use pdbfile-4CG.pdb
4. Introduce at the top of the file (first line) the number of residues followed by the number of atoms
   e.g.: 64 390
   ATOM …
   ATOM …
5. Place the files AA.dat and cg-2.1.dat in the working directory.
6. Run the program pdb2cg2.1.f with the command line command line:
   pdb2CG2.1 < pdbfile-4CG.pdb
7. The standard output gives the pdb file transformed according to the geometrization Redirect the file to a file name "pdb-CG.pdb"
8. Run the program topol-CG-2.1 on the working directory. It will ask you:
   a. The force constant for the CA i-i+4 interactions. Choose the desired value or 0 (zero) to exclude them.
   b. The force constant for the ElNeDyn bonds
   c. The cutoff distance at which the Ca will be considered interacting under the ElNeDyn bonds.
9. The output is a file called "protein.itp", which is the topology according to CGFF-2.1

One final step is required it consists in modifying the backbone bead according to the secondary. This step has the aim to reduce the polarity of backbone beads when they are involved in a secondary structure element.

10. All the files can be found in: ~periole/FILES_CG2.0/
11. Use the original (complete) pdb file of the protein and generate a file ssdump using do_dssp. The file should be renamed ssdump.ssd
12. Download the sequence of the protein in the PDB with the fasta format. Rename this file XXX.seq
13. Run the command: seq2itp_martini_test-LYS2.pl –h everything is then explained.
14. You got in output a file.itp from which you can extract the column with the bead type (second in the atom list) and paste it to the protein.itp file you got before (step9). Note: the program nedit allows to copy and paste by columns. Select pressing on the Ctrl key. And paste using the Edit menu.

How to run a simulation.

Here we describe the protocol that allows getting smoothly from the pdb-CG.pdb file to a run of the protein under the CG2.1 FF.

Run:

a. editconf –f pdb-CG.pdb –c –dt 1.2 –o pdb-CG-editconf.gro
b. genbox –cp pdb-CG-editconf.gro –cs ~periole/NEW_FF –vdwd 0.19 –o pdb-CG-genbox.gro
   Notes: - the vdwd value was determined empirically and gives a good approximate number of water in the box for the proteins simulated.
   - the force field file (martini.itp can be found in ~periole/FILEs/martini.itp
c. Preparative:
   a. make_ndx, the name of the solvent should SOL as in the mdp files.
   b. genpr, two sets of position restrains should be build 1) all atoms of the protein with 1000 kJ mol^{-1} force, 2) only CA atoms with 1000 kJ mol^{-1}.
   c. In the topol.top file replace 10% of the water molecules (name W) by the name WF, which is an antifreeze particle!
d. Minimization: minimize using the mini.mdp file:
   cp posre-all-1000.itp posre.itp
   grompp –f mini.mdp –c pdb-CG-genbox.gro –n index.ndx –p topol.top –o mini.tpr
   mdrun –v –deffnm mini
e. Run 50 ps (50000 steps) at dt=0.001ps to relax the side chains because they are constrained:
   grompp –f md-PR.mdp –c mini.gro –r mini.gro –n index.ndx –o md-PR.tpr
   mdrun –deffnm md-PR
f. Run 1 ns (50000 steps) at dt=0.02 ps: equilibrate the solvent and mix the antifree particules:
   cp posre-CA-1000.itp posre.itp
   grompp –f md-PR2.mdp –c md-PR.gro –r mini.gro –n index.ndx –o md-PR2.tpr
   mdrun –deffnm md-PR2
g. Run free at dt=0.02 ps:
   grompp –f md.mdp –c md-PR2.gro –n index.ndx –o md.tpr
   mdrun –deffnm md