Topology File Description for GROMACS

Atom types

Each force field defines a set of atom types, which have a characteristic name or number, and mass (in a.m.u.). These listings are found in the ***atomtypes.atp*** file (.atp = atom type parameter file). Therefore, it is in this file that you can begin to change and/or add an atom type whereas the charge is listed in ****.rtp*** file (.rtp = residue topology parameter file). This implies that the charges are only defined in the building blocks of amino acids, nucleic acids or otherwise, as defined by the user. When generating a topology (*.top) using the pdb2gmx program, the information from these files is combined.

> Example:
> ls /usr/share/gromacs/top/amber03.ff

Non-bonded parameters

The non-bonded parameters consist of the van derWaals parameters V (c6 or σ, depending on the combination rule) and W (c12 or ε), as listed in the file ***ffnonbonded.itp***.

Bonded parameters

The bonded parameters (i.e. bonds, bond angles, improper and proper dihedrals) are listed in ***ffbonded.itp.*** The entries in this database describe, respectively, the atom types in the interactions, the type of the interaction, and the parameters associated with that interaction. These parameters are then read by grompp when processing a topology and applied to the relevant bonded parameters, i.e. bondtypes are applied to entries in the [bonds] directive, etc. Any bonded parameter that is missing from the relevant [*type] directive generates a fatal error.

Intramolecular pair interactions

Extra Lennard-Jones and electrostatic interactions between pairs of atoms in a molecule can be added in the [pairs] section of a molecule definition. The parameters for these interactions can be set independently from the non-bonded interaction parameters. In the GROMOS force fields, pairs are only used to modify the 1-4 interactions (interactions of atoms separated by three bonds). In these force fields the 1-4 interactions are excluded from the non-bonded interactions. The pair interaction parameters for the atom types in ffnonbonded.itp are listed in the [pairtypes] section. The GROMOS force fields list all these interaction parameters explicitly, but this section might be empty for force fields like OPLS that calculate the 1-4 interactions by uniformly scaling the parameters.

Exclusions

The exclusions for non-bonded interactions are generated by grompp for neighboring atoms up to a certain number of bonds away, as defined in the [moleculetype] section in the topology file.

Constraints

Constraints are defined in the [constraints] section. The format is two atom numbers followed by the function type, which can be 1 or 2, and the constraint distance. The only difference between the two types is that type 1 is used for generating exclusions and type 2 is not. The distances are

constrained using the LINCS or the SHAKE algorithm, which can be selected in the *.mdp file. SETTLE algorithm, which is an analytical solution of SHAKE, specifically for water. SETTLE can be selected in the topology file.

pdb2gmx input files

The GROMACS program pdb2gmx generates a topology for the input coordinate file. Several formats are supported for that coordinate file, but *.pdb is the most commonly-used format (hence the name pdb2gmx). pdb2gmx searches for force fields in subdirectories of the GROMACS share/top directory and your working directory. Force fields are recognized from the file ***forcefield.itp*** in a directory with the extension ***.ff.*** Two general files are read by pdb2gmx: an atom type file (extension ***.atp***) from the force field directory, and a file called ***residuetypes.dat*** from either the working directory, or the GROMACS share/top directory. residuetypes.dat determines which residue names are considered protein, DNA, RNA, water, and ions.

Residue database

The files holding the residue databases have the extension ***.rtp.*** So the residue database file contains information (bonds, charges, charge groups, and improper dihedrals) for a frequently-used building block.

Residue to building block database

Each force field has its own naming convention for residues. Most residues have consistent naming, but some, especially those with different protonation states, can have many different names. The ***.r2b*** files are used to convert standard residue names to the force field build block names. If no .r2b is present in the force field directory or a residue is not listed, the building block name is assumed to be identical to the residue name.

Atom renaming database

Force fields often use atom names that do not follow IUPAC or PDB convention. The ***.arn*** database is used to translate the atom names in the coordinate file to the force field names. Atoms that are not listed keep their names. The file has three columns: the building block name, the old atom name, and the new atom name, respectively.

Hydrogen database

The hydrogen database is stored in ***.hdb*** files. It contains information for the pdb2gmx program on how to connect hydrogen atoms to existing atoms.

Termini database

The termini databases are stored in ***aminoacids.n.tdb*** and ***aminoacids.c.tdb*** for the N and C-termini respectively. They contain information for the pdb2gmx program on how to connect new atoms to existing ones, which atoms should be removed or changed, and which bonded interactions should be added.