My report about the fudge parameter in Gromacs

Petra Bačová*

Departamento de Ciencia de los Materiales e Ingeniería Metalúrgica y Química Inorgánica, Facultad de Ciencias, IMEYMAT, Campus Universitario Río San Pedro s/n., Puerto Real, Cádiz 11510, Spain

E-mail: petra.bacova@uca.es

Material elaborated for students and/or users of Gromacs simulation package, free to use and share. For any comments, objections and/or questions, please, contact me per email. May these notes help you in your journey!

FugdeLJ and FugdeQQ: The fudge factors are used (only) as scaling factors for the 1-4 interactions (LJ or Coulomb). In order to specify these 1-4 interactions, the GROMACS implementation uses an explicit pairs list, called [pairs]. All the 1-4 pairs should be included in the [pairs] section (pdb2gmx makes it automatically, if you prepare the input files by yourself you need to include it manually). If there is no pairs list, for GROMACS it means that there are no 1-4 interactions and it ignores the fudge parameters (no matter what the value of gen-pairs is).

Pairs: The interactions for the explicit pairs in the [pairs] list are always computed - even though they are computed through the non-bonded kernels, they are not subject to cutoffs (may slow down a bit the simulation).

Gen-pairs: These 1-4 interactions also need parameters. The parameters are automatically generated when gen-pairs = yes from the topology data, based on the combination rules and the fudge (=scaling) factors. If gen-pairs = no, then the [pairs] section should contain both the atom indices and the parameters (otherwise you will get an error message from grompp). Again, notice that if no [pairs] list is present in the .itp file, then the value of gen-pairs is irrelevant.

Example n.1: one chain of PEO in a vacuum, pairs defined

nrexcl	fudge(LJ & QQ)	LJ(SR)	LJ(1-4)	Coul(SR)	Coul(1-4)	Coul.reciprocal
2	0.5	7.93776e+01	4.80775e+01	1.78400e+02	7.21037e+02	6.54038e+02
2	1	7.93776e+01	9.61550e+01	1.78400e+02	1.44207e+03	6.54038e+02
3	0.5	-1.67775e+01	4.80775e+01	-5.67645e+01	7.21037e+02	-5.52872e+02
3	1	-1.67775e+01	9.61550e+01	-5.67645e+01	1.44207e+03	-5.52872e+02

LJ(SR) includes short-range LJ interactions, LJ(1-4) represents the contribution from the explicitly specified 1-4 interactions (the same in the case of Coulomb interaction). Coul. Reciprocal is the reciprocal part of Coulomb interaction in PME algorithm.

The scaling in 1-4 interactions works as it's expected (compare the data for the fudge=1 and fudge=0.5). The total LJ energy (LJ(SR) + LJ-14) in the case of nrexcl 3 and scale factor 1.0 is 79.3775 that is equal to the LJ(SR) in the case of nrexcl 2 and no pairs list defined (see below). Similar for Coulombic interactions.

In case of the nrexl=2 the pairs list of 1-4 interactions is redundant, because these interactions are already included in the definition of nrexcl, so we basically calculate the same interaction twice. Therefore we get higher total LJ energy in comparison to the other systems.

Example n.2: one chain of PEO in a vacuum, no pairs defined (simulation with a pairs list included and fudge=0 would give the same results).

nrexcl	fudge(LJ & QQ)	LJ(SR)	LJ(1-4)	Coul(SR)	Coul(1-4)	Coul.reciprocal
2	1	7.93776e+01	0	1.78400e+02	0	6.54038e+02
2	0.5	7.93776e+01	0	1.78400e+02	0	6.54038e+02

Again, no specific 1-4 interaction, GROMACS ignores the value of fudge.

Note: In case of nrexcl=4, the pairs list has to contain also 1-5 pairs in order to get the same energy as in case of nrexcl=2. So we always define in the [pairs] the interactions, that are not already present through the nrexcl setting.