GROMACS - Bug #1569

Unreasonable energy with "coulombtype=Switch"

07/24/2014 12:37 AM - Igor Leontyev

Status:	Rejected		
Priority:	Normal		
Assignee:	Erik Lindahl		
Category:	mdrun		
Target version:	5.0		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	5.0		

Description

Testing with gmx-5.0 different schemes of Long-Range electrostatics for
NMA liquid I noticed unreasonable behavior with "coulombtype=Switch".
Electrostatic energies calculated for the same configuration (i.e. at 0
MD step) with PME and Cut-off coulombtype reasonably agree between each
other. But once I use coulombtype=Switch, the electrostatic energy jumps
by the order of magnitude. All input and output files are attached. See the results for 0-step in corresponding log-files.

<coulombtype=PME, rcoulomb=1.3>
Coulomb-14 LJ (SR) Disper. corr. Coulomb(SR)+Recipr. Potential
-1.29147e+04 -3.28852e+03 -1.28735e+02 -3.54258e+03 -7.86555e+03

<coulombtype=Cut-off, rcoulomb=1.3>
Coulomb-14 LJ (SR) Disper. corr. Coulomb (SR) Potential
-1.29147e+04 -3.28852e+03 -1.28735e+02 -3.53416e+03 -7.85714e+03

<coulombtype=Switch, rcoulomb=1.3, rcoulomb-switch=1.2>
Coulomb-14 LJ (SR) Disper. corr. Coulomb (SR) Potential
-1.29147e+04 -3.28852e+03 -1.28735e+02 -5.25858e+04 -5.69088e+04

History

#1 - 07/26/2014 09:35 AM - Erik Lindahl

- Status changed from New to Accepted

- Assignee set to Erik Lindahl

#2 - 07/26/2014 04:14 PM - Erik Lindahl

- Status changed from Accepted to Rejected

I don't see any bug in the switched coulomb interaction, and in particular I have checked that switched PME produces fine results.

Instead, this result is a consequence of using gigantic energy groups consisting of the entire molecule in combination with switched plain coulomb. Since your molecules are neutral this will effectively give you a dipole-dipole (or almost quadropole-quadropole interaction, since the dipole in the molecule is small) since the cutoff is based on the charge group - either all atoms in two molecules interact, or none of them. As a check, you can try to disable the large charge group, which will give you a big change in the energy even without enabling any switch.

By definition, that will give you a total energy quite similar to PME, where we include all interactions. In principle you are only missing quadropole interactions outside of 1.3nm, which will be a very small component of the energy.

In contrast, when you apply a switch to the coulomb interactions the switch factor is computed based on the atom-atom distance, NOT the group distance. This will violate the effective dipole-dipole interactions you had by using the charge groups, and is pretty much the reason why both switched plain coulomb and large charge groups are bad ideas.

Grompp does emit a note that the plain cut-off can produce artifacts, and recommends PME instead; we might want to turn that into a more stern warning in the future.

Files

Cut-off.log	21.9 KB	07/23/2014	Igor Leontyev

Methylacetamide.mdp	1.65 KB	07/23/2014	Igor Leontyev
Methylacetamide.gro	160 KB	07/23/2014	Igor Leontyev
Methylacetamide.top	3.59 KB	07/23/2014	Igor Leontyev
PME.log	23.8 KB	07/23/2014	Igor Leontyev
oplsaaff.itp	287 KB	07/23/2014	Igor Leontyev
Switch.log	22.1 KB	07/23/2014	Igor Leontyev