GROMACS - Bug #2640

coul-lambda affects the pressure computation of a ligand with zero partial charge

09/07/2018 02:54 PM - zhiyi wu

Status:	Closed		
Priority:	High		
Assignee:	Berk Hess		
Category:	mdrun		
Target version:	2018.4		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	2018.2		

Description

This is a simplified and corrected version of the issue 2600.
I'm trying to compute the decoupling free energy of vdw interactions of a ligand which has zero partial changes.
Since the ligand has zero partial, changing coul-lambda shouldn't have any effect on anything.
However, setting coul-lambda to 0 yields a pressure 2.13121e+02 bar of whereas setting coul-lambda to 1 yeilds a pressure of 1.07168e+02 bar.
The commands to reproduce the results are
gmx grompp -f coul-lambdas_0.mdp -c prod.gro -o coul-lambdas_0.tpr
gmx mdrun -deffnm coul-lambdas_0 -rerun prod.gro
gmx grompp -f coul-lambdas_1.mdp -c prod.gro -o coul-lambdas_1.tpr
gmx mdrun -deffnm coul-lambdas_1 -rerun prod.gro

If you compare the pressure in coul-lambdas_1.edr and coul-lambdas_0.edr, you will notice that the pressure are different whereas they should be the same.

Related issues:

Related to GROMACS - Bug #2849: Free energy discrepancies between GROMACS ver...	**Closed**

Associated revisions

Revision 12f01f79 - 09/10/2018 09:55 PM - Berk Hess

Fix PME forces with FE without perturbed q/LJ

PME would incorrectly scale the mesh forces with lambda when no
charges or LJ atom types were actually perturbed.

Fixes #2640

Change-Id: I193d55cf76d842f5b04d3a220411282c06b08a90

History

#1 - 09/10/2018 05:58 PM - Berk Hess

- Category set to mdrun

- Status changed from New to Accepted

- Target version set to 2018.4

I reproduced this issue.
Also the force on non-perturbed, charged atoms differ significantly with coul-lambda, even though the Coulomb energies do not.

#2 - 09/10/2018 06:02 PM - Berk Hess

The issue disappears when not using LJ-PME. So this looks like some incorrect interaction between the Coulomb and LJ-PNE FE code.

#3 - 09/10/2018 09:57 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2640.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018~I193d55cf76d842f5b04d3a220411282c06b08a90
Gerrit URL: https://gerrit.gromacs.org/8333

#4 - 09/10/2018 09:59 PM - Berk Hess

- Status changed from Accepted to Fix uploaded

- Assignee set to Berk Hess

The Coulomb forces were, incorrectly, scaled with lambda.
This bug (only) occurs when no charges are actually perturbed. Or, analogously, for LJ-PME when no atom types are actually perturbed.

#5 - 09/11/2018 03:15 PM - Berk Hess

- Status changed from Fix uploaded to Resolved

Applied in changeset 12f01f7917dec5863bf76437fc470bc3b45484b2.

#6 - 09/27/2018 12:30 PM - Berk Hess

- Status changed from Resolved to Closed

#7 - 01/30/2019 12:08 PM - Mark Abraham

- Related to Bug #2849: Free energy discrepancies between GROMACS versions added

Files

pressure.tgz	6.16 MB	09/07/2018	zhiyi wu