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

Revision a507acbc - 02/04/2020 11:05 AM - Berk Hess

Actually fix PME forces with FE without perturbed q/LJ

PME would incorrectly ignore the mesh forces on perturbed atoms when
no charges or LJ atom types were actually perturbed.
This is because the "fix" in commit 12f01f79 incorrectly changed the
lambda value used for the PME forces from the actual lambda value
to 1 instead of to 0 as it should have been.

Fixes #2640
Fixes #3359

Change-Id: Ib19565bf017ddbd2fddc66c52be0ff9efc7e707c

Revision 7387a098 - 02/05/2020 08:14 AM - Berk Hess

Actually fix PME forces with FE without perturbed q/LJ

PME would incorrectly ignore the mesh forces on perturbed atoms when
no charges or LJ atom types were actually perturbed.
This is because the "fix" in commit 12f01f79 incorrectly changed the
lambda value used for the PME forces from the actual lambda value

to 1 instead of to 0 as it should have been.

Fixes #2640
Fixes #3359

Change-Id: Ib19565bf017ddbd2fddc66c52be0ff9efc7e707c

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