GROMACS - Bug #2174

LJPME should not accept VDW modifiers it does not support

05/08/2017 11:58 PM - Mark Abraham

Status:	Closed			
Priority:	Normal			
Assignee:	Berk Hess			
Category:	preprocessing (pdb2gmx,grompp)			
Target version:	2016.4			
Affected version - extra info:		**Difficulty:**	uncategorized	
Affected version:	2016.3			

Description

An .mdp including the fragment

```
vdwtype = pme
vdw-modifier = force-switch
```

is accepted, produces a .tpr that is different from that with vdw-modifer = potential-shift, and IMO is mal-formed. I'm not sure what it computes in practice.

IIRC the only supported modifiers with the Verlet scheme are potential-shift and (maybe) none, so grompp should only accept supported combinations (ie probably not potential-switch, either). We should not just ignore a modifier that can't be implemented for the vdwtype, because we don't know whether the user's error was in choosing the vdwtype or its modifier.

Check this for electrostatic PME, also.

Associated revisions

Revision 4bc38d9e - 05/15/2017 10:49 AM - Berk Hess

Fix LJPME + switch grompp error

An error call was missing in grompp when LJPME was requested in combination with a force or potential switch modifier.

Fixes #2174.

Change-Id: I92bc718869bf98b17efef1bab16c6457e07d0544

History

#1 - 05/15/2017 10:55 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2174.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2016~I92bc718869bf98b17efef1bab16c6457e07d0544
Gerrit URL: https://gerrit.gromacs.org/6634

#2 - 05/15/2017 10:55 AM - Berk Hess

- Status changed from New to Fix uploaded

- Assignee set to Berk Hess

- Target version set to 2016.4

The check was actually implemented in grompp, but the warning_error() call was missing.
Coulomb PME is checked properly.

#3 - 05/15/2017 11:38 AM - Mark Abraham

Thanks!

#4 - 05/15/2017 02:33 PM - Berk Hess

- Status changed from Fix uploaded to Resolved

Applied in changeset [4bc38d9eaf226dd4d907093b44718bc800f561a8](#).

#5 - 05/31/2017 08:39 PM - Szilárd Páll

- Status changed from Resolved to Closed