**GROMACS - Bug #2174**

**LJPME should not accept VDW modifiers it does not support**

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

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**Status:** Closed

**Priority:** Normal

**Assignee:** Berk Hess

**Category:** preprocessing (pdb2gmx,grompp)

**Target version:** 2016.4

**Affected version - extra info:**

**Affected version:** 2016.3

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**Description**

An .mdp including the fragment

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

is accepted, produces a .tpr that is different from that with vdw-modifier = 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.

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**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: I92bc718669bf98b17efef1bab16c6457e07d0544

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**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~I92bc718669bf98b17efef1bab16c6457e07d0544

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