An .mdp including the fragment

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.

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: l92bc718869bf98b17eef1bab16c6457e07d0544

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~I92bc718869bf98b17eef1bab16c6457e07d0544
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 4be38d9eaf226dd4d907093b44718bc800f561a8.

#5 - 05/31/2017 08:39 PM - Szilárd Páll
- Status changed from Resolved to Closed