GROMACS - Bug #2332
verlet + pme-user should give grompp and mdrun fatal error
12/06/2017 02:04 AM - Mark Abraham

| Status:    | Closed       |
| Priority:  | Normal       |
| Assignee:  | Mark Abraham |
| Category:  | core library |
| Target version: | 2016.5 |
| Affected version - extra info: | probably all since 4.6 |
| Affected version: | 2016.4 |

Difficulty: uncategorized

Description
A report on gmx-users mentioned this combination and that of course they got the energies from a normal run. We should be giving a fatal error for this combination.

Associated revisions
Revision 9283b607 - 12/11/2017 09:55 AM - Paul Bauer
Disallow combination of PME-user and verlet cutoff

Fixes #2332
Change-id: 1127a5680a0a83b7e5f8163b99619a6cc3729a992

History
#1 - 12/06/2017 02:04 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2332.
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-id: gromacs~release-2016~I127a5680a0a83b7e5f8163b99619a6cc3729a992
Gerrit URL: https://gerrit.gromacs.org/7297

#2 - 12/06/2017 03:12 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2332.
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-id: gromacs~master~I127a5680a0a83b7e5f8163b99619a6cc3729a992
Gerrit URL: https://gerrit.gromacs.org/7298

#3 - 12/11/2017 12:59 PM - Paul Bauer
- Status changed from New to Resolved
Applied in changeset 9283b607c18aa22923b950553a43e08ea861b574.

#4 - 12/12/2017 11:50 AM - Mark Abraham
- Status changed from Resolved to Closed