GROMACS - Bug #2332

verlet + pme-user should give grompp and mdrun fatal error

12/06/2017 02:04 AM - Mark Abraham

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Mark Abraham</td>
</tr>
<tr>
<td>Category:</td>
<td>core library</td>
</tr>
<tr>
<td>Target version:</td>
<td>2016.5</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>probably all since 4.6</td>
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<tr>
<td>Affected version:</td>
<td>2016.4</td>
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**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-2016~1127a5680a0a83b7e5f8163b99619a6cc3729a992
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~1127a5680a0a83b7e5f8163b99619a6cc3729a992
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