GROMACS - Bug #1289

EEL_USER is true when eelPMESWITCH is true

06/23/2013 09:37 PM - Mark Abraham

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
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</tr>
<tr>
<td>Assignee:</td>
<td>Mark Abraham</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>4.6.4</td>
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<tr>
<td>Affected version - extra info:</td>
<td>4.6-4.6.2</td>
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<tr>
<td>Affected version:</td>
<td>4.6.2</td>
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<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
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Description
The monster Verlet kernel patch included

#define EEL_USER(e) ((e) == eelUSER || (e) == eelPMEUSER || (e) == (eelPMESWITCH))
(see [http://redmine.gromacs.org/projects/gromacs/repository/revisions/release-4-6/entry/include/types/enums.h#L120](http://redmine.gromacs.org/projects/gromacs/repository/revisions/release-4-6/entry/include/types/enums.h#L120))

I think it should be

#define EEL_USER(e) ((e) == eelUSER || (e) == eelPMEUSER || (e) == (eelPMEUSERSWITCH))

Associated revisions
Revision 242f9f63 - 07/01/2013 08:04 PM - Mark Abraham
Corrected definition of EEL_USER

Looks like a copy-paste typo occured at some point in the nbnxn development. EEL_USER is only used in runner.c, and only to issue a fatal error with user-supplied non-bonded potentials. That clearly should be not applicable to eelPMESWITCH.

Fixes #1289
Change-Id: I4e987c81aec81a920779dd29d7c52e8b6d233b45

History
#1 - 06/24/2013 10:13 PM - Mark Abraham
- Description updated

#2 - 06/24/2013 10:14 PM - Mark Abraham
- Description updated

#3 - 06/26/2013 01:22 AM - Mark Abraham
- Status changed from New to Fix uploaded
- Assignee changed from Berk Hess to Mark Abraham

#4 - 07/17/2013 01:21 PM - Teemu Murtola
- Status changed from Fix uploaded to Resolved
- Affected version - extra info set to 4.6-4.6.2

Was fixed in [https://gerrit.gromacs.org/#/c/2459/](https://gerrit.gromacs.org/#/c/2459/) for 4.6.3 (not possible to set that target version any longer). For some reason, the commit wasn't linked here.

#5 - 08/13/2013 08:55 PM - Mark Abraham
- % Done changed from 0 to 100
#6 - 10/16/2013 03:36 PM - Mark Abraham

- Status changed from Resolved to Closed
- Target version changed from 4.6.x to 4.6.4