GROMACS - Bug #1238

g_hydorder does not set PBC

05/01/2013 11:58 PM - Justin Lemkul

<table>
<thead>
<tr>
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<th>Closed</th>
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<tr>
<td>Priority:</td>
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</tr>
<tr>
<td>Assignee:</td>
<td>David van der Spoel</td>
</tr>
<tr>
<td>Category:</td>
<td>analysis tools</td>
</tr>
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<td>Target version:</td>
<td>4.6.2</td>
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<td>Affected version - extra info:</td>
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<td>4.6.2</td>
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Description

As reported to gmx-users (http://lists.gromacs.org/pipermail/gmx-users/2013-April/080837.html), it appears that gmx_hydorder.c does not call set_pbc() before pbc_dx(). The problem exists in the latest git version of pre-4.6.2.

Associated revisions

Revision bfc70c3c - 05/02/2013 08:30 AM - David van der Spoel
Fixes #1238 g_hydorder does not call set_pbc.
Now it does.
Change-id: 1085ca9ad8e8eca1803feee605d39932483a771f9

Revision 9aa32fd7 - 06/13/2013 09:45 AM - David van der Spoel
Fixes #1238 g_hydorder does not call set_pbc.
Now it does.
Change-id: 1085ca9ad8e8eca1803feee605d39932483a771f9

History

#1 - 05/02/2013 08:31 AM - David van der Spoel
Fix in gerrit https://gerrit.gromacs.org/#/c/2356/

#2 - 05/03/2013 04:25 PM - David van der Spoel
- Status changed from New to Resolved
- % Done changed from 0 to 100

Applied in changeset bfc70c3c92fd922a8320ee158243f2ab94177db8.

#3 - 05/03/2013 04:26 PM - David van der Spoel
Applied in changeset bfc70c3c92fd922a8320ee158243f2ab94177db8.

#4 - 05/03/2013 04:27 PM - David van der Spoel
Applied in changeset bfc70c3c92fd922a8320ee158243f2ab94177db8.

#5 - 05/30/2013 06:23 AM - Teemu Murtola
- Target version changed from 4.6.3 to 4.6.2

Changed target version as was already fixed for 4.6.2.

#6 - 05/31/2013 10:41 AM - Mark Abraham
- Status changed from Resolved to Closed