**GROMACS - Bug #2245**

**Swap code does not do PBC correctly**

09/08/2017 02:49 PM - Berk Hess

<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>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>2016.4</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>any version with swap</td>
</tr>
<tr>
<td>Affected version:</td>
<td>2016</td>
</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
</tr>
</tbody>
</table>

**Description**

The swap (computational electrophysiology) code uses the initial box instead of the current box to correct distances for PBC. For checking distance to a channel, this likely went unnoticed if the channel doesn't cross the periodic boundary. For making molecules whole this would certainly be an issue, but maybe only single atomic ions have been used.

**Associated revisions**

Revision 149c6633 - 09/11/2017 03:51 PM - Berk Hess

Fix PBC bugs in the swap code

Fixes #2245

Change-id: l90e2bed71a2499c63794e420dca383d91e6fc86c

**History**

#1 - 09/08/2017 02:50 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2245.
Uploader: Berk Hess (hess@kth.se)
Change-id: gromacs~release-2016~I90e2bed71a2499c63794e420dca383d91e6fc86c
Gerrit URL: https://gerrit.gromacs.org/6910

#2 - 09/08/2017 02:50 PM - Berk Hess

- Status changed from New to Fix uploaded

#3 - 09/11/2017 05:09 PM - Berk Hess

- Status changed from Fix uploaded to Resolved

Applied in changeset 149c6633b5f9372a8b0143889b014ba2de411fce

#4 - 09/12/2017 11:42 AM - Mark Abraham

- Status changed from Resolved to Closed