### g_sas computes incorrect values with -nopbc

**02/28/2014 05:33 AM - Teemu Murtola**

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<tr>
<td>Assignee:</td>
<td>Teemu Murtola</td>
</tr>
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<td>Category:</td>
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**Description**

`g_sas` computes incorrect surface areas if `-nopbc` is specified. The problem has been introduced some time in the 4.0.x series, probably between 4.0 and 4.0.3 (`e2045413`, merged to development version in `1437fac0`). The cell size of the grid used to search for neighboring atoms is determined as the radius of the first atom instead of double the maximum radius as it should.

Additionally, the 4.0.x series `g_sas` always triggers the `-nopbc` option (`ed04b50`), irrespective of what is provided on the command line (and thus always produces the incorrect result).

This explains at least some of the results reported on gmx-users: https://mailman-1.sys.kth.se/pipermail/gromacs.org_gmx-users/2014-February/087460.html

**Associated revisions**

**Revision a56228ac - 03/02/2014 02:49 AM - Teemu Murtola**

Fix incorrect grid cell size in `g_sas -nopbc`

Fixes #1445

Change-Id: I798fc8fe96608633lf2ed9a3500f83f39b44af008

**History**

**#1 - 02/28/2014 05:34 AM - Gerrit Code Review Bot**

Gerrit received a related patchset '1' for Issue #1445

Uploader: Teemu Murtola (teemu.murtola@gmail.com)

Change-id: I798fc8fe96608633lf2ed9a3500f83f39b44af008

Gerrit URL: https://gerrit.gromacs.org/3199

**#2 - 02/28/2014 05:41 AM - Teemu Murtola**

- Status changed from In Progress to Fix uploaded

**#3 - 03/02/2014 03:00 AM - Teemu Murtola**

- Status changed from Fix uploaded to Resolved

- % Done changed from 0 to 100

Applied in changeset a56228accb8dc04c7ef08fe6bfc7518da43c218d.

**#4 - 03/04/2014 04:57 AM - João M. Damas**

Teemu Murtola wrote:

Applied in changeset a56228accb8dc04c7ef08fe6bfc7518da43c218d.

Conclusion on this issue: https://mailman-1.sys.kth.se/pipermail/gromacs.org_gmx-users/2014-March/087665.html

**#5 - 04/03/2014 07:47 PM - Roland Schulz**

- Status changed from Resolved to Closed

Conclusion on this issue: https://mailman-1.sys.kth.se/pipermail/gromacs.org_gmx-users/2014-March/087665.html