g_sas computes incorrect values with -nopbc

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

Status: Closed
Priority: Normal
Assignee: Teemu Murtola
Category: analysis tools
Target version: 4.6.6
Affected version - extra info: 4.0.7-4.6.5
Affected version: 4.6.5

Difficulty: uncategorized

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: I798fc8fe9660863f26d9a3500f83f39b44af008

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: I798fc8fe9660863f26d9a3500f83f39b44af008
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 a56228acce8dc04c7e7f07fe6b83f751bda43c218d.

#4 - 03/04/2014 04:57 AM - João M. Damas
Teemu Murtola wrote:

Applied in changeset a56228acce8dc04c7e7f07fe6b83f751bda43c218d.

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