g_sham needs more documentation

09/15/2011 05:43 AM - Mark Abraham

Description
-map and -mdata inputs are not discussed in the help text or any code comments.

It would be useful if there was a suggestion in the documentation that the log file contains an ordered set of indices of energy minima that are useful for going and looking at low-energy structures, after using trjconv -sub bindex.ndx.

I'd assign this to David van der Spoel, who seems to have written g_sham, but he's not a member of this project.

Associated revisions

Revision 3a52686e - 06/12/2014 10:54 AM - Erik Lindahl
Removed undocumented -map and -mdata options from g_sham.

Both options and code were completely undocumented, and nobody seemed interested in helping document them for the last two years, so for now they are gone.

Fixes #812.

Change-Id: l4d60cf3d58da89d76a4461cddc2e75f031676d2c9

History

#1 - 09/20/2011 04:06 PM - Rossen Apostolov
- Assignee set to David van der Spoel
Assigning to David.

#2 - 09/21/2011 11:19 AM - David van der Spoel
- Target version changed from 4.5.5 to 4.6

Updated target version.

#3 - 04/19/2012 04:41 PM - Rossen Apostolov
David, could you add info before the 4.6-beta next week?

#4 - 03/04/2014 03:00 PM - Rossen Apostolov
- Target version changed from 4.6 to 4.6.x
- Affected version set to 4.6

#5 - 05/22/2014 04:59 PM - Erik Lindahl
- Target version changed from 4.6.x to 5.x
- Affected version changed from 4.6 to 4.6

Unless somebody looks into it the next few days, we should consider removing undocumented options (and corresponding code) from 5.0.
the issue was moved to project "Gromacs", category "documentation", and the original sub-project "Documentation" was removed.

#7 - 06/12/2014 12:13 AM - Erik Lindahl
Time to remove the options & code.

#8 - 06/12/2014 12:26 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #812.
Uploader: Erik Lindahl (erik@kth.se)
Change-Id: I4d60cf3d58da89d76a4461cdc2e75f031676d2c9
Gerrit URL: https://gerrit.gromacs.org/3575

#9 - 06/12/2014 12:26 AM - Erik Lindahl
- Status changed from New to Fix uploaded

"Fix", meaning "kill" uploaded :-)

#10 - 06/12/2014 12:15 PM - Erik Lindahl
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 3a52686eb02334c843e2c2063699cdaab7b8e3e0.

#11 - 06/12/2014 02:42 PM - Erik Lindahl
- Status changed from Resolved to Closed

#12 - 07/15/2014 06:43 AM - Teemu Murtola
- Target version changed from 5.x to 5.0