GROMACS - Bug #812

_g_sham needs more documentation_

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

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>David van der Spoel</td>
</tr>
<tr>
<td>Category:</td>
<td>documentation</td>
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<tr>
<td>Target version:</td>
<td>5.0</td>
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<tr>
<td>Affected version - extra info:</td>
<td>4.6</td>
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<tr>
<td>Affected version:</td>
<td>4.6</td>
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**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: l4d60cf3d58da89d76a4461cdc2e75f031676d2c9

**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.
#6 - 05/23/2014 02:02 PM - Rossen Apostolov
- Project changed from Documentation to GROMACS
- Category changed from manual and in-source to documentation

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: 4d60cf3d58da89d76a4461cdc2e75f031676d2c9
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