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>
</tr>
</thead>
<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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**Affected version:** 4.6

**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
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.

"Fix", meaning “kill” uploaded :-)

Applied in changeset 3a52686eb02334c843e2c2063699cdaab7b8e3e0.

- Target version changed from 5.x to 5.0