**GROMACS - Bug #2903**

gmx wham doesn't compute profile with pull=angle-axis

03/22/2019 06:32 PM - Kevin Boyd

<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></td>
</tr>
<tr>
<td>Category:</td>
<td>analysis tools</td>
</tr>
<tr>
<td>Target version:</td>
<td>2020</td>
</tr>
<tr>
<td>Affected version</td>
<td>2019.1</td>
</tr>
<tr>
<td>Extra info:</td>
<td></td>
</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
</tr>
</tbody>
</table>

**Description**

Given correct tprs and pull files on a set of umbrella windows maintained using angle-axis, the histogram is computed correctly but the profile is a bunch of Nans.

**Related issues:**

Is duplicate of GROMACS - Bug #2609: Evaluating PMF for angle rotations using...  Closed

**History**

#1 - 03/25/2019 01:26 PM - Berk Hess
- Status changed from New to Feedback wanted

Can you upload input and a command line?

#2 - 06/02/2019 09:17 PM - Kevin Boyd
- File gwham_error_sample.tar.gz added

Here's a simplified system, with a sample command run.

#3 - 06/09/2019 03:58 PM - Krzysztof Makuch

Kevin Boyd wrote:

Given correct tprs and pull files on a set of umbrella windows maintained using angle-axis, the histogram is computed correctly but the profile is a bunch of Nans

I have the same bug. It was reported by several people:

https://mailman-1.sys.kth.se/pipermail/gromacs.org_gmx-users/2016-August/108093.html

With possible solution for gromacs 2016:

https://redmine.gromacs.org/issues/2609

If solving it soon is a problem, could you please add an explanation inside gmx wham manpage, what exactly should we modify in xvg output files or in tpr binary to make it work? Also it might be a good idea to mention this bug in umbrella tutorials.

#4 - 06/10/2019 11:19 AM - Berk Hess
- Is duplicate of Bug #2609: Evaluating PMF for angle rotations using gmx WHAM added

#5 - 06/10/2019 11:21 AM - Berk Hess
- Status changed from Feedback wanted to Fix uploaded

I uploaded a fix, please check:

https://gerrit.gromacs.org/c/gromacs/+/11458

#6 - 06/11/2019 12:02 PM - Paul Bauer
- Status changed from Fix uploaded to Closed

#7 - 08/14/2019 04:35 PM - Krzysztof Makuch

Berk Hess wrote:
I uploaded a fix, please check:
https://gerrit.gromacs.org/c/gromacs/+/11458

I had a moment to check it out and unfortunately it still doesn't work. As I understand (and as I've checked the part of the code mentioned in bug-fix) the change was incorporated in v. 2019.3. Histograms are still ok and profile is still column of '-nan'.

#8 - 08/14/2019 04:37 PM - Krzysztof Makuch
By the way, if we use pullf files instead of pullx we get bunch of sharp peaks instead of -nan.

#9 - 09/17/2019 09:28 AM - yujie liu
I also found this bug in gromacs 2019.3, when I calculate the PMF of dihedral angle rotation. I pose a question on maillist https://mailman-1.sys.kth.se/pipermail/gromacs.org_gmx-users/2019-September/126614.html

Files

<table>
<thead>
<tr>
<th>File Name</th>
<th>Size</th>
<th>Date</th>
<th>Author</th>
</tr>
</thead>
<tbody>
<tr>
<td>gwham_error_sample.tar.gz</td>
<td>45.2 MB</td>
<td>06/02/2019</td>
<td>Kevin Boyd</td>
</tr>
</tbody>
</table>