Evaluating PMF for angle rotations using gmx WHAM

08/14/2018 03:15 AM - Jonathan Sheavly

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>Low</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>analysis tools</td>
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<tr>
<td>Target version:</td>
<td>2019.3</td>
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<td>Affected version:</td>
<td>2016</td>
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<td>Extra info:</td>
<td>Difficulty:</td>
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<td>simple</td>
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Description
I had been trying to evaluate a PMF using umbrella sampling (GROMACS 2016) for rotating an object. The mdp option I used was:
```
pull_coord1_geometry     = angle-axis
```

The .mdp options page says the input units are in degrees, and the simulation runs fine with this. However, when evaluating the PMF using gmx WHAM, the histograms seemed to overlap in x space, but not in force space which yields "nan" PMF results.

After troubleshooting, I found that the tpr file input for WHAM is required to be in radians (but is read in degrees within GROMACS simulations) and the pull-f files then can be used to get reasonable PMFs. Right now my workflow is fully functional, but I thought other would like to know how to fix this.

The only fix would be some conversion within WHAM from degrees to radians when reading the tpr files. I hope this helps to continue to improve GROMACS analysis tools

Related issues:
Has duplicate GROMACS - Bug #2903: gmx wham doesn't compute profile with pull...
Closed

Associated revisions

Revision 7e3521c2 - 06/10/2019 11:43 AM - Berk Hess
Fix gmx wham with angle geometries
Fixes #2609
Change-id: l36156e1d8bb98499e4357eadc4ca56384da433a5

Revision 92be1a9 - 09/30/2019 10:11 AM - Berk Hess
Actually fix gmx wham with angle geometries
A previous fix for converting the force constant in gmx wham for angle and dihedral geometry applied an incorrect conversion factor.
Fixes #2609 and #3094
Change-id: l0aa9b848c7fa62306ccf15b327a650b1ad88e03f

History

#1 - 06/10/2019 11:19 AM - Berk Hess
- Has duplicate Bug #2903: gmx wham doesn't compute profile with pull=angle-axis added

#2 - 06/10/2019 11:20 AM - Berk Hess
- Status changed from New to Fix uploaded
- Assignee set to Berk Hess
- Target version changed from future to 2019.3

I uploaded a fix, please check:
https://gerrit.gromacs.org/c/gromacs/+/11458
#3 - 06/10/2019 05:30 PM - Berk Hess
- Status changed from Fix uploaded to Resolved

Applied in changeset 7e3521c2dd4d57f1cd730f45afac12dcb2abd8e.

#4 - 06/11/2019 12:02 PM - Paul Bauer
- Status changed from Resolved to Closed