

GROMACS - Bug #3094

gmx wham doesn't compute profile.xvg with dihedral angle

09/18/2019 11:41 AM - yujie liu

Status: Closed	
Priority: High	
Assignee:	
Category: analysis tools	
Target version: 2019.4	
Affected version - extra info: all version	Difficulty: uncategorized
Affected version: 2019.3	

Description

As previous mentioned <https://redmine.gromacs.org/issues/2903> . 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

Associated revisions

Revision 592be1a9 - 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: I0aa9b848c7fa62306ccf15b327a650b1ad88e03f

History

#1 - 09/27/2019 12:34 PM - Paul Bauer

I started debugging this, and it looks like the issue is that the calculated force constant is too high, leading to the result of an exponential function being nan

#2 - 09/27/2019 10:37 PM - Berk Hess

Could this be a radian/degree unit issue?

#3 - 09/28/2019 12:39 AM - yujie liu

- File 4.jpg added

- File 5.jpg added

Berk Hess wrote:

Could this be a radian/degree unit issue?

I think it is. If I change the source code of g_wham.cpp by add a conversion factors $((\pi/180)^2)$, the result may be fine. But only use to calculate PMF of angle. Please see attachment.

#4 - 09/30/2019 12:49 PM - Paul Bauer

please try the fix here: <https://gerrit.gromacs.org/c/gromacs/+/13477>

#5 - 09/30/2019 01:33 PM - yujie liu

Paul Bauer wrote:

please try the fix here: <https://gerrit.gromacs.org/c/gromacs/+/13477>

Yes, it is correct.

#6 - 10/01/2019 11:10 AM - Paul Bauer

- Status changed from *New* to *Resolved*

#7 - 10/01/2019 11:10 AM - Paul Bauer

- Status changed from *Resolved* to *Closed*

Files

4.jpg	23.3 KB	09/27/2019	yujie liu
5.jpg	25.1 KB	09/27/2019	yujie liu