GROMACS - Bug #2439

AWH deconvolution not working for sharing simulations

03/09/2018 09:47 PM - Viveca Lindahl

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: 2018.1
Affected version: 2018.1
Affected version -
extra info: GROMACS version: 2018.1-dev-20180306-33093601f
Difficulty: uncategorized

Description
The AWH PMF, extracted with gmx awh -s topol.tpr -f ener.edr -more, looks extremely "irregular" for awh-share-multisim=yes (see attached fig). When comparing to single-replica runs it's clear that this cannot be due to statistical noise. In this simulation there where 4 sharing simulations (-multidir walker-{1..4}).

Associated revisions
Revision 229c8f63 - 03/13/2018 12:13 PM - Berk Hess
Fix AWH deconvolution when sharing a bias

When sharing an AWH bias over multiple simulations, the PMF output was garbage due to a missing minus sign in the reduction.
Note that this only affected the PMF output, not the sampling.

Fixes #2439
Change-Id: l688cda045f5e757e58b392d64384705b3ac73a17

Revision 22e00d62 - 03/16/2018 01:34 PM - Berk Hess
Correct PMF sign error in AWH bias sharing

Recent commit 229c8f63 was though to fix a sign error in the calculation of the deconvolution of the AWH PMF when sharing the bias over multiple simulations, but this sign was misplaced.

Fixes #2439
Change-Id: l67ec06ff4d832a857467b58b362f9f6f88671aa8

History
#1 - 03/12/2018 09:38 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2439.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018~I688cda045f5e757e58b392d64384705b3ac73a17
Gerrit URL: https://gerrit.gromacs.org/7666

#2 - 03/12/2018 09:40 PM - Berk Hess
- Status changed from New to Fix uploaded
- Assignee set to Berk Hess
- Target version set to 2018.1

It seems that a minus went missing during refactoring. We need a module test for bias sharing.

#3 - 03/13/2018 12:15 PM - Berk Hess
- Status changed from Fix uploaded to Resolved

Applied in changeset 229c8f63f6b9d9a7b0eeced16b093852781eab605.
#4 - 03/13/2018 02:03 PM - Mark Abraham
- Status changed from Resolved to Closed

#5 - 03/16/2018 11:11 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2439.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018~I67ec06f4d832a857487b58b362f9f688671aa8
Gerrit URL: https://gerrit.gromacs.org/7685

Files

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