GROMACS - Bug #2703
constraint and mass contributions missing from foreign Hamiltonian values
10/18/2018 02:59 PM - Berk Hess

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: 2018.6
Affected version - extra info: all versions
Affected version: 2018

Difficulty: uncategorized

Description
The foreign Hamiltonian values only contain the potential energy terms. The constraint and kinetic energy contributions are missing.

Related issues:
Related to GROMACS - Bug #2849: Free energy discrepancies between GROMACS ver... Closed

Associated revisions
Revision 1d8678d9 - 10/23/2018 09:01 PM - Berk Hess
Add missing constraint term to deltaH

The constraint contribution was missing from foreign Hamiltonian difference output from mdrun used for BAR.

Refs #2703
Change-Id: l00fb88bed76f9ff03faed7543e90adfa163b99f08

Revision b51dbae2 - 10/26/2018 01:25 PM - Berk Hess
Add missing mass term to deltaH

The mass contribution was missing from foreign Hamiltonian difference output from mdrun used for BAR.

Refs #2703
Change-Id: l415c835e9e1a8473243041be004013af7141a1cc

Revision a741d07b - 02/15/2019 10:35 AM - Berk Hess
Fix mass Delta H double counting

With separate mass lambda parameters, the perturbed mass contribution to Delta H (not dH/dlambda) was double counted. This was due to an incorrect fix for issue #2703 for missing Delta H contribution.

Refs #2703
Fixes #2849
Change-Id: l1349260e1e90a17a6b7dbe0d239d9474dca928c

Revision 499ab90c - 02/20/2019 09:00 AM - Berk Hess
Fix mass Delta H double counting

With separate mass lambda parameters, the perturbed mass contribution to Delta H (not dH/dlambda) was double counted. This was due to an incorrect fix for issue #2703 for missing Delta H contribution.

Refs #2703
Fixes #2849
Change-Id: l1349260e1e90a17a6b7dbe0d239d9474dca928c
History

#1 - 10/18/2018 03:03 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2703.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018~I00fb88bed76f9f03faed7543e90adf163b99f08
Gerrit URL: https://gerrit.gromacs.org/8569

#2 - 10/18/2018 03:22 PM - Mark Abraham
Reasonable also to fix in release-2016

#3 - 10/18/2018 03:25 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2703.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018~I415c835e9e1a8473243041be004013af7f141a1cc
Gerrit URL: https://gerrit.gromacs.org/8570

#4 - 10/18/2018 03:28 PM - Berk Hess
- Subject changed from constraint contribution missing from foreign Hamiltonian values to constraint and mass contributions missing from foreign Hamiltonian values
- Status changed from In Progress to Fix uploaded

#5 - 11/05/2018 01:18 PM - Paul Bauer
- Status changed from Fix uploaded to Closed

#6 - 01/30/2019 12:09 PM - Mark Abraham
- Related to Bug #2849: Free energy discrepancies between GROMACS versions added

#7 - 02/13/2019 09:57 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2703.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2019~I1349260e1e90a17a6b7dbe0d239d9474dca928c
Gerrit URL: https://gerrit.gromacs.org/9141

#8 - 02/18/2019 01:22 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2703.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2018~I1349260e1e90a17a6b7dbe0d239d9474dca928c
Gerrit URL: https://gerrit.gromacs.org/9172

#9 - 02/18/2019 02:09 PM - Paul Bauer
- Target version changed from 2018.4 to 2018.6