

## GROMACS - Bug #2703

### constraint and mass contributions missing from foreign Hamiltonian values

10/18/2018 02:59 PM - Berk Hess

<b>Status:</b> Closed	
<b>Priority:</b> Normal	
<b>Assignee:</b> Berk Hess	
<b>Category:</b> mdrun	
<b>Target version:</b> 2018.6	
<b>Affected version - extra info:</b> all versions	<b>Difficulty:</b> uncategorized
<b>Affected version:</b> 2018	
<b>Description</b>	
The foreign Hamiltonian values only contain the potential energy terms. The constraint and kinetic energy contributions are missing.	
<b>Related issues:</b>	
Related to GROMACS - Bug #2849: Free energy discrepancies between GROMACS ver...	<b>Closed</b>

#### 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: I00fb88bed76f9ff03faed7543e90adf163b99f08

##### 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: I415c835e9e1a8473243041be004013af7141a1cc

##### 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: I1349260e1e90a17a6b7dbe0d239d9474dcfa928c

##### 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: I1349260e1e90a17a6b7dbe0d239d9474dcfa928c

## History

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### #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](mailto:hess@kth.se))  
Change-Id: gromacs~release-2018~100fb88bed76f9ff03faed7543e90adf163b99f08  
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](mailto:hess@kth.se))  
Change-Id: gromacs~release-2018~1415c835e9e1a8473243041be004013af7141a1cc  
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](mailto:hess@kth.se))  
Change-Id: gromacs~release-2019~11349260e1e90a17a6b7dbe0d239d9474dcfa928c  
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](mailto:hess@kth.se))  
Change-Id: gromacs~release-2018~11349260e1e90a17a6b7dbe0d239d9474dcfa928c  
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*