**GROMACS - Bug #2434**

**wrong values accumulated to dvdlambda in SHAKE with FE calcs**

03/02/2018 11:37 AM - Mark Abraham

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Mark Abraham</td>
</tr>
<tr>
<td>Category:</td>
<td>core library</td>
</tr>
<tr>
<td>Target version:</td>
<td>2018.1</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>all 5.1.x and 2016.x before 2016.6</td>
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<tr>
<td>Affected version:</td>
<td>5.1</td>
</tr>
<tr>
<td>Difficulty:</td>
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### Description

513813b514 refactored bshake() to remove the use of lam as a temporary iteration variable. This was wrong, but worked fine for non-FE calcs. FE calcs will have accumulated arbitrary values to dvdlambda.

This could have been prevented in many ways, including declaring the original parameter as

```plaintext
real *const lagr
```

and having SHAKE tests that cover a wider scope than cshake().

### Related issues:

Related to GROMACS - Task #2423: modernize constraints code

### Associated revisions

**Revision 33093601 - 03/06/2018 02:07 PM - Mark Abraham**

Fixed dvdlambda for SHAKE + FE

Garbage values have been accumulated to dvdlambda whenever SHAKE was used.

Refactoring in 513813b514 removed the lam variable. Previously, it was used as a temporary iteration variable over SHAKE blocks, but that refactoring to use the main variable changed the logic of the following loop.

Fixes #2434

Change-Id: la9642f50358ab31ec98f8317f7a1dcd8622a9f1

**Revision 17967ef5 - 05/23/2019 03:50 PM - Berk Hess**

Fix SHAKE dH/dlambda contributions

The constraint contributions to dH/dlambda would be incorrect with more than one SHAKE block.

Refs #2434 abd #2879

Change-Id: l0cb30a9f61893ce57d76bac34e7352fe307efe4e

### History

**#1 - 03/02/2018 11:37 AM - Mark Abraham**

- Target version changed from 2016.6 to 2018.1

For now, we should fix in 2018.1, but we should back port to release-2016 also.

**#2 - 03/02/2018 11:52 AM - Mark Abraham**

**Edit:** this test case probably doesn't enter the relevant code that would show a bug
regressiontests freeenergy/simtemp dhdl.xvg output of 2016.2:

```
@ title "dH/dxl and \xD\f{}H"
@ xaxis label "Time (ps)"
@ yaxis label "dH/dxl and \xD\f{}H (kJ/mol \[xl\f{}])\S-1\N"
@TYPE xy
@ subtitle "\xl\f{} state 1:  = "
@ view 0.15, 0.15, 0.75, 0.85
@ legend on
@ legend box on
@ legend loctype view
@ legend 0.78, 0.8
@ legend length 2
@ s0 legend "Thermodynamic state"
@ s1 legend "Total Energy (kJ/mol)"
@ s2 legend "\xdl\f{}H \xl\f{} to T = 300 (K)"
@ s3 legend "\xdl\f{}H \xl\f{} to T = 311.787 (K)"
@ s4 legend "\xdl\f{}H \xl\f{} to T = 324.037 (K)"
@ s5 legend "\xdl\f{}H \xl\f{} to T = 336.768 (K)"
@ s6 legend "\xdl\f{}H \xl\f{} to T = 350 (K)"

0.0000 1 -29093.266 -255.84591 0.0000000 265.89774 542.24302 829.44569
0.0200 0 -29372.768 0.0000000 261.88091 534.05154 816.91553 1110.8932
0.0400 0 -29376.373 0.0000000 257.37702 524.86680 802.86604 1091.7878
```

And 2018 branch with the incoming fix:

```
@ title "dH/dxl\f{} and \xD\f{}H"
@ xaxis label "Time (ps)"
@ yaxis label "dH/dxl\f{} and \xD\f{}H (kJ/mol \[xl\f{}])\S-1\N"
@TYPE xy
@ subtitle "\xl\f{} state 1:  = "
@ view 0.15, 0.15, 0.75, 0.85
@ legend on
@ legend box on
@ legend loctype view
@ legend 0.78, 0.8
@ legend length 2
@ s0 legend "Thermodynamic state"
@ s1 legend "Total Energy (kJ/mol)"
@ s2 legend "\xdl\f{}H \xl\f{} to T = 300 (K)"
@ s3 legend "\xdl\f{}H \xl\f{} to T = 311.787 (K)"
@ s4 legend "\xdl\f{}H \xl\f{} to T = 324.037 (K)"
@ s5 legend "\xdl\f{}H \xl\f{} to T = 336.768 (K)"
@ s6 legend "\xdl\f{}H \xl\f{} to T = 350 (K)"

0.0000 1 -29093.281 -255.84591 0.0000000 265.89774 542.24302 829.44569
0.0200 0 -29372.785 0.0000000 261.88089 534.05150 816.91547 1110.8931
0.0400 0 -29376.383 0.0000000 257.37712 524.86670 802.86634 1091.7882
```

In this trivial case (SHAKE on a single methane in water), the impact was negligible. So even if we were testing on the contents of dhdl.xvg, we might not have caught this.

#3 - 03/02/2018 11:54 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2434.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~release-2018~Ia9642f50358ab31ec98f8317f7a1dcd8622af9f1
Gerrit URL: https://gerrit.gromacs.org/7642

#4 - 03/02/2018 11:56 AM - Mark Abraham

- Status changed from New to Fix uploaded

#5 - 03/02/2018 12:02 PM - Gerrit Code Review Bot

Gerrit received a related patchset '4' for Issue #2434.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: gromacs~master~I09b7a719b58f8f8192762431edc139674eaf23ae
Gerrit URL: https://gerrit.gromacs.org/7610

#6 - 03/02/2018 04:09 PM - Mark Abraham

Actually that test case is never going to show the issue, since it does simulated tempering, rather than perturbing the system.

#7 - 03/06/2018 02:15 PM - Mark Abraham
- Status changed from Fix uploaded to Resolved

Applied in changeset 33093601ff229ed8c8a40e73866a7ff351e8963b.

#8 - 03/06/2018 04:31 PM - Mark Abraham
- Status changed from Resolved to Closed

#9 - 03/06/2018 05:10 PM - Mark Abraham
- Related to Task #2423: modernize constraints code added