wrong values accumulated to dvdlambda in SHAKE with FE calcs

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

```c
real *const lagr
```

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

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: Ia9642f50358ab31ec98f8317f7a1dcda8622a9f1

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
And 2018 branch with the incoming fix:

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.

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