Virial and pressure completely incorrect with SHAKE

The SHAKE constraint contribution to the virial is off leading to a large error in the pressure. Since the error is so large, this likely would have not gone unnoticed. The issue is due to incorrect incrementing of the scaled_lagrange_multiplier pointer.

This also indicates that our tests for SHAKE are inadequate.

Only version 2018 is affected, not 2016 or 2019.

Associated revisions

Revision de3a2cac - 05/23/2019 03:02 PM - Mark Abraham
Revert "Fixed dvdlambda for SHAKE + FE"
This broke normal simulations with SHAKE and does not seem to fix anything with FEP simulations either.
This reverts commit 33093601ff229ed8c8a40e73866a7ff351e8963b.
Fixes #2879
Change-Id: Ib6e9b4fe2b65811e9f64c37e842fd0ed9c0b055c

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: l0cb30a9f61893ce57d76bac34e7352fe307e4e

History

#1 - 03/06/2019 07:13 PM - Artem Zhmurov
Virial is not tested in SHAKE tests. We do test it in new LINCS/SHAKE test (in master branch), but only for the case of one bond. I was planning to improve that.

#2 - 03/11/2019 11:30 AM - Mark Abraham
Yes, for simplicity in implementing the old tests, I didn't consider the virial (and then never got back to it). I will look into solving this.

#3 - 03/19/2019 10:57 AM - Artem Zhmurov
I think I found the bug:

In bshakef(...) function in shakef.cpp, when the computations are split to blocks, all blocks are given the same pointer to save scaled Lagrange multipliers. I.e., the function vec_shakef(...) should have lam in its arguments, not scaled_lagrange_multiplier. lam is incremented in the loop over blocks, scaled_lagrange_multiplier is not. As a result, when virial components are computed, the Lagrange multipliers are convoluted with wrong rij vectors, giving the wrong result.
#4 - 03/19/2019 10:34 PM - Berk Hess
Thanks Artem, but I/we already knew this is the issue. This is what Mark changed when fixing dV/dlambda for SHAKE. We need to have both correct.

#5 - 03/20/2019 11:21 AM - Mark Abraham
Berk Hess wrote:

Thanks Artem, but I/we already knew this is the issue. This is what Mark changed when fixing dV/dlambda for SHAKE. We need to have both correct.

It's good to know that we will have test coverage for it when fixed!

#6 - 03/20/2019 02:17 PM - Artem Zhmurov
Mark Abraham wrote:

Berk Hess wrote:

Thanks Artem, but I/we already knew this is the issue. This is what Mark changed when fixing dV/dlambda for SHAKE. We need to have both correct.

It's good to know that we will have test coverage for it when fixed!

If I re-introduce the bug into the latest version and the tests indeed fail in a way it should. But this happens only after change 9193, which is CUDA version of LINCS (https://gerrit.gromacs.org/#/c/9193/). Did not want to make another separate patch set for the constraints test at the time. The question is: shall I extract the constraints test improvements for virial into a separate patch or we can wait until the CUDA LINCS will make it in?

#7 - 03/20/2019 04:01 PM - Mark Abraham
Artem Zhmurov wrote:

Mark Abraham wrote:

Berk Hess wrote:

Thanks Artem, but I/we already knew this is the issue. This is what Mark changed when fixing dV/dlambda for SHAKE. We need to have both correct.

It's good to know that we will have test coverage for it when fixed!

If I re-introduce the bug into the latest version and the tests indeed fail in a way it should. But this happens only after change 9193, which is CUDA version of LINCS (https://gerrit.gromacs.org/#/c/9193/). Did not want to make another separate patch set for the constraints test at the time. The question is: shall I extract the constraints test improvements for virial into a separate patch or we can wait until the CUDA LINCS will make it in?

No need to extract. If we need to use them to test a fix, then someone can do a hack job.

#8 - 05/07/2019 03:49 PM - Berk Hess
- File 2_dt_allbonds_216_meth_npt.tpr added
- Target version set to 2018.7

The issue is worse, some (or all?) systems with shake explode, likely due to 33093601ff229ed8c8a40e73866a7ff351e8963b

Simple test system attached.

#9 - 05/23/2019 03:45 PM - Mark Abraham
- Status changed from New to Resolved

Applied in changeset de3a2cac77bf57447fe07826b6972b60389845.

#10 - 05/27/2019 02:44 PM - Mark Abraham
- Status changed from Resolved to Closed