

GROMACS - Bug #2338

ShakeTest.ConstrainsThreeBondsWithCommonAtoms tolerance

12/07/2017 11:37 AM - Roland Schulz

Status: Closed	
Priority: Normal	
Assignee: Berk Hess	
Category: testing	
Target version: 2018-beta2	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2018-beta1	
Description	
With ICC 18.1, no-simd, Release:	
<pre>ShakeTest.ConstrainsThreeBondsWithCommonAtoms ./src/gromacs/mdlib/tests/shake.cpp:222: Failure Value of: finalDistancesSquared[i] Actual: 1.0000100135803223 Expected: constrainedDistancesSquared[i] Which is: 1 Difference: 1.00136e-05 (84 single-prec. ULPs, rel. 1e-05) Tolerance: abs. 1e-05, rel. 1e-05</pre>	

Associated revisions

Revision cbea06cf - 12/09/2017 12:44 AM - Berk Hess

Correct Shake test tolerances

The shake test used a tolerance on the square of the distance instead of the distance itself as the documentation says. Added tolerance for rounding errors due to the absolute size of the coordinate values involved.

Fixes #2338

Change-Id: I1a771c0682fd694b2672986b46c58d4888d5a4a2

Revision 80dd3f5b - 12/21/2017 10:54 AM - Mark Abraham

Update double-precision test configurations

These changes improve coverage of double precision, using more release mode, particularly with latest gcc and icc, and using 128-bit SIMD, which have been cases that were buggy recently. The other aspects of the configurations that have been modified have been non-critical. Where appropriate, brief rationales are recorded. This resolves an old TODO item in the post-submit matrix.

Fixed a sign mismatch in initializing an OpenCL variable that didn't need to be initialized.

Noted relevant new TODOs.

Refs #2300, #2325, #2326, #2334, #2335, #2336, #2337, #2338

Change-Id: I131fa1a6776d1e7809799c3f931a1fc8100fcdc9

History

#1 - 12/08/2017 03:35 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2338](#).

Uploader: Berk Hess (hess@kth.se)

#2 - 12/08/2017 03:45 PM - Berk Hess

- *Category set to testing*
- *Status changed from New to Fix uploaded*
- *Assignee set to Berk Hess*
- *Target version set to 2018-beta2*

I think this is because the distance calculation during Shake and in the check might not be binary identical, so we need to add a tolerance of $\text{real_eps} * \max(\text{coord})$.

I also noticed that the test checks distance^2 instead of distance like the documentation says.

#3 - 12/09/2017 12:58 AM - Roland Schulz

- *Status changed from Fix uploaded to Closed*