

GROMACS - Bug #2334

AWH WithParameters/BiasStateTest.InitializesFromFile test fails with ICC

12/06/2017 10:51 PM - Roland Schulz

Status: Closed	
Priority: Normal	
Assignee:	
Category:	
Target version:	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2018-beta1	
Description	
Fails with ICC 17.4 and 18.1 on HSW and KNL (probably on BDW on SKL too). Fine in Debug but fails in Release.	
Output (17.4 double on HSW):	
<pre>../src/gromacs/awh/tests/biasstate.cpp:174: Failure Value of: msdTarget Actual: 1.02315e-35 Expected: 0.0 Which is: 0 [FAILED] WithParameters/BiasStateTest.InitializesFromFile/0, where GetParam() = "pmf_target_format0.xvg" (1 ms) [RUN] WithParameters/BiasStateTest.InitializesFromFile/1 ../src/gromacs/awh/tests/biasstate.cpp:174: Failure Value of: msdTarget Actual: 1.02315e-35 Expected: 0.0 Which is: 0 [FAILED] WithParameters/BiasStateTest.InitializesFromFile/1, where GetParam() = "pmf_target_format1.xvg" (0 ms)</pre>	

Associated revisions

Revision 4846540b - 12/07/2017 07:40 PM - Roland Schulz

Fix AWH test accuracy

Fixes #2334

Change-Id: Ieda604a3dbd1c253302214559e169581dfc02fe1

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 - 12/06/2017 10:52 PM - Roland Schulz

- Description updated

#2 - 12/06/2017 10:54 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2334](#).

Uploader: Roland Schulz (roland.schulz@intel.com)

Change-Id: gromacs~release-2018~leda604a3dbd1c253302214559e169581dfc02fe1

Gerrit URL: <https://gerrit.gromacs.org/7300>

#3 - 12/07/2017 03:11 AM - Roland Schulz

- Status changed from New to Fix uploaded

#4 - 12/07/2017 06:04 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2334](#).

Uploader: Mark Abraham (mark.j.abraham@gmail.com)

Change-Id: gromacs~release-2018~1131fa1a6776d1e7809799c3f931a1fc8100fcdc9

Gerrit URL: <https://gerrit.gromacs.org/7303>

#5 - 12/07/2017 07:53 PM - Roland Schulz

- Status changed from Fix uploaded to Closed