GROMACS - Bug #1716

TrajectoryAnalysisUnitTests are failing on i686 openmpi double precision

04/18/2015 04:48 PM - Dominik Mierzejewski

Status: Closed
Priority: Normal
Assignee: Teemu Murtola
Category: testing
Target version: 5.0.5
Affected version: 5.0.4

Difficulty: uncategorized

Description

One of TrajectoryAnalysisUnitTests is failing in the following configuration:

- os: Fedora rawhide
- arch: i686
- gcc-5.0.1
- openmpi-1.8.5

Cmake command line:

```
-DCMAKE_Fortran_FLAGS_RELEASE= -DCMAKE_INSTALL_PREFIX:PATH=/usr -DSYSCONF_INSTALL_DIR:PATH=/etc -DSHARE_INSTALL_PREFIX:PATH=/usr/share -DBUILD_SHARED_LIBS:BOOL=ON -DBUILD_SHARED_LIBS=ON -DBUILD_TESTING:BOOL=ON
```

Failed subtest log:

```
14:  [ RUN      ] AngleModuleTest.HandlesOneVsMultipleVectorGroupsAngles
14:  WARNING: If there are molecules in the input trajectory file that are broken across periodic boundaries, they cannot be made whole (or treated as whole) without you providing a run input file.
14:  Analyzed topology coordinates
14:  WARNING: Masses and atomic (Van der Waals) radii will be guessed based on residue and atom names, since they could not be definitively assigned from the information in your input files. These guessed numbers might deviate from the mass and radius of the atom type. Please check the output files if necessary.
14:  
14:  [/buildir/build/BUILD/gromacs-5.0.4/src/testutils/refdata.cpp:931: Failure]
14:     Value of: value
14:     Actual: 0.016666666666666666
14:     Expected: refValue
14:     Which is: 0.0083333333333333332
14:     Difference: 0.00833333 (4503599627370495856 double-prec. ULPs)
14:     Tolerance: abs. 8.88178e-16, 4 ULPs
14:     Google Test trace:
14:     [/buildir/build/BUILD/gromacs-5.0.4/src/testutils/refdata.cpp:931: Failure]
```

04/05/2020
14: Tolerance: abs. 8.88178e-16, 4 ULPs
14: Google Test trace:
14: /builddir/build/BUILD/gromacs-5.0.4/src/testutils/refdata.cpp:912: Checking '/Data/histogram/Frame2/[1]/[1]/Value'
14: [ FAILED ] AngleModuleTest.HandlesOneVsMultipleVectorGroupsAngles (3 ms)

Associated revisions
Revision f42a9e9a - 05/05/2015 05:44 PM - Teemu Murtola
Avoid rounding errors affecting results in one test

Change the input for one of 'gmx gangle' tests such that it does not produce angles that are exactly at an edge of the three-bin histogram used in the test. Rounding could affect the bin into which the angle was assigned to, causing the test to fail erroneously.

Fixes #1716
Change-Id: l9979a8dfee0b870b3904fa28e274540f892f542d

History
#1 - 04/18/2015 04:58 PM - Dominik Mierzejewski
Update: the same test is failing with mpich-3.1.4, output is exactly the same.

#2 - 04/18/2015 05:23 PM - Dominik Mierzejewski
And another update: the same test is failing in a serial build, without MPI.
For reference, fftw and atlas versions used (in all configurations):
fftw-3.3.4
atlas-3.10.1

#3 - 04/20/2015 02:25 PM - Mark Abraham
I haven't been able to reproduce this on x86_64, and don't think I have an i686 to try. Are you able to reproduce it on an x86_64 machine, Dominik?

#4 - 04/20/2015 03:01 PM - Dominik Mierzejewski
You can reproduce it in a 32bit chroot or container environment, for example using mock on Fedora. At least, that's how I'm doing it. Also, a new bit of information: it works just fine on ARM 32bit: http://koji.fedoraproject.org/koji/taskinfo?taskId=9506969 so it isn't an issue of 64bit vs 32bit.

#5 - 04/20/2015 05:59 PM - Teemu Murtola
- Category set to testing
- Status changed from New to Accepted

Most likely the issue gets fixed by changing the coordinate file used in the test to not produce an exact 120 degree angle (which falls exactly at a histogram bin edge and can get rounded differently depending on three compiler, architecture, etc.).

#6 - 04/23/2015 01:57 PM - Berk Hess
But we shouldn't have tests that require exact matching of histograms.
Can this test be changed to look at the value of the angle instead (with a margin)?

#7 - 04/23/2015 04:20 PM - Teemu Murtola
Berk Hess wrote:

But we shouldn't have tests that require exact matching of histograms.
Can this test be changed to look at the value of the angle instead (with a margin)?

The test already tests the actual angles (with a margin) in addition to the histogram. And the histogram is one that is computed with a 60 degree bin width from two angle values, so testing it directly with existing code instead of writing elaborate extra code to test, e.g., the integral of the histogram is much more straightforward to actually check the basic histogramming in this case. We can of course just throw out testing the entire histogram and just trust that it might work without any testing, but then we will potentially miss issues.

#8 - 04/30/2015 11:56 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1716.
Uploader: Teemu Murtola (teemu.murtola@gmail.com)
Change-Id: l9979a8dfee0b870b3904fa28e274540f892f542d
Gerrit URL: https://gerrit.gromacs.org/4539
#9 - 04/30/2015 11:56 AM - Teemu Murtola
- Status changed from Accepted to Fix uploaded
- Assignee set to Teemu Murtola
- Target version set to 5.0.5

#10 - 05/05/2015 07:33 PM - Teemu Murtola
- Status changed from Fix uploaded to Resolved

Fix has been merged.

#11 - 05/05/2015 08:12 PM - Teemu Murtola
- Affected version - extra info set to 5.0-5.0.4

#12 - 05/06/2015 04:49 PM - Mark Abraham
- Status changed from Resolved to Closed