GROMACS - Bug #1542

two unit tests fail on 32-bit ARM

06/30/2014 07:47 PM - Szilárd Páll

Status: Closed
Priority: Normal
Assignee: Magnus Lundborg
Category: core library
Target version: 5.1
Affected version - 
extra info: 5.0.1-dev-20140629-ed48a3c
Affected version: 5.0

Description
On a 32-bit ARM (Tegra 3) platform with up-to-date Ubuntu 12.04.4 LTS the LegacyToolsTests and MdrunTests unit tests fail with segfault.

Attached are the CMake cache, make check output, and mdrun -version output. The configure command used:

```
CC=gcc-4.7  CXX=g++-4.7 cmake ../ -DGMX_GPU=OFF  -DGMX_BUILD_OWN_FFTW=ON
```

Note that the version is flagged "dirty" because the Random123 library does not officially support ARM and the #error at src/external/Random123-1.08/include/Random123/features/gccfeatures.h:38 preventing compilation needs to be disabled.

Related issues:
Related to GROMACS - Task #1545: test Random123 on unsupported platforms
    Closed 07/01/2014
Related to GROMACS - Bug #1559: Writing TNG files fails on Xeon Phi
    Closed 07/10/2014
Has duplicate GROMACS - Bug #1546: Legacy tools tests failed on armv7a with S...
    Closed 07/02/2014
Has duplicate GROMACS - Bug #1547: MDRUN tools tests failed on armv7a with SI...
    Closed 07/02/2014

Associated revisions
Revision 898166c3 - 08/21/2014 05:33 PM - Magnus Lundborg

Fixed TNG memory alignment problem and reset pointers.

This is a temporary fix to the memory alignment problems on some platforms. In the main TNG repository the whole I/O system is rewritten to address this problem. This fix is to avoid the problems without making too large changes.

There are also some pointers that were not reset after memory was freed. This is also fixed in here.

This commit does not correspond to any commit in the TNG repository.

Fixes #1542, #1546, #1547 and #1559.

Change-Id: I90a6406cccbc43fd57d4423c2b661019cf7763e8

History
#1 - 06/30/2014 07:51 PM - Szilárd Páll
- File gmx-version.out added
- File CMakeCache.txt added
- File make-check.log added

#2 - 07/01/2014 08:52 AM - Roland Schulz
Can you add a stacktrace?

#3 - 07/01/2014 03:00 PM - Szilárd Páll
Both tests fail with "Bus error".

With the LegacyToolsTests the crash happens at the 6th test:

```
[----------] 5 tests from NoFatalErrorWhenWritingFrom/TrjconvWithIndexGroupSubset
[ RUN ] NoFatalErrorWhenWritingFrom/TrjconvWithIndexGroupSubset.WithDifferentInputFormats/0
Will write tng: Trajectory file (tng format)
Select group for output
Group 0 (System) has 6 elements
Group 1 (FirstWaterMolecule) has 3 elements
Group 2 (SecondWaterMolecule) has 3 elements
Select a group: Selected 2: 'SecondWaterMolecule'

Bus error

bateframe 1 time 0.000 --> frame 1 time 0.000
```

The MdrunTest fails right after the following output:

```
starting mdrun 'spc-and-methanol'
6 steps, 0.0 ps.
```

I suspect that both of these may be related to TNG, but let me get some backtraces to confirm.

```
Program received signal SIGBUS, Bus error.
0x005e78f2 in quantize_float (x=0x25b6323, natoms=3, nframes=2, precision=0.000999999931, quant=0x25b6323) at /home/pszilard/data/gromacs-5.0/src/external/tng_io/src/compression/tng_compress.c:91
91 quant[frame*natoms*3+i*3+j]=(int)floor((x[frame*natoms*3+i*3+j]/precision)+0.5);
(gdb) (gdb) (gdb)
(gdb) bt
#0 0x005e78f2 in quantize_float (x=0x25b6323, natoms=3, nframes=2, precision=0.000999999931, quant=0x25b6323) at /home/pszilard/data/gromacs-5.0/src/external/tng_io/src/compression/tng_compress.c:91
#1 0x005e9d34 in tng_compress_pos_float (pos=0x25b6323, natoms=3, nframes=2, desired_precision=0.001000000005, speed=0, algo=0x16129e8, nitems=0xbe7c11ec) at /home/pszilard/data/gromacs-5.0/src/external/tng_io/src/compression/tng_compress.c:1248
#2 0x005e9e2e in tng_compress_pos_float_find_algo (pos=0x25b6323, natoms=3, nframes=2, desired_precision=0.001000000005, speed=0, algo=0x16129e8, nitems=0xbe7c11ec) at /home/pszilard/data/gromacs-5.0/src/external/tng_io/src/compression/tng_compress.c:1279
#3 0x005b691a in tng_compress (tng_data=0x24ee4c8, block=0x26d7450, n_frames=2, n_particles=3, type=2 '\002', start_pos=0x25b6323) at /home/pszilard/data/gromacs-5.0/src/external/tng_io/src/lib/tng_io.c:4837
#4 0x005b901e in tng_particle_data_block_write (tng_data=0x24ee4c8, block=0x26d7450, block_index=0, mapping=0, x=0, hash_mode=1 '\001') at /home/pszilard/data/gromacs-5.0/src/external/tng_io/src/lib/tng_io.c:6311
#5 0x005c7622 in tng_frame_set_write (tng_data=0x24ee4c8, hash_mode=1 '\001') at /home/pszilard/data/gromacs-5.0/src/external/tng_io/src/lib/tng_io.c:13153
#6 0x005c76f4 in tng_frame_set_premature_write (tng_data=0x24ee4c8, hash_mode=1 '\001') at /home/pszilard/data/gromacs-5.0/src/external/tng_io/src/lib/tng_io.c:13192
#7 0x0004429a in fflush_tng (tng=0x24ee4c8) at /home/pszilard/data/gromacs-5.0/src/gromacs/fileio/tngio.cpp:84
#8 0x0019f5f7a in mdoutf_write_to_trajectory_files (fplog=0x2458c58, cr=0x15a2be0, of=0x24ecaa0, mdflags=0, global=0x16117b0, step=6, t=0.006000000000000000, state_local=0x16117b0, state_global=0x2458fd8, f_local=0x16117b0, f_global=0x16117b0) at /home/pszilard/data/gromacs-5.0/src/gromacs/fileio/mdoutf.c:298
#9 0x0018e40c in do_md_trajectory_writing (fplog=0x2458c58, cr=0x15a2be0, nfile=35, f_local=0x161f7c26a8, step=6, st tep_rel=6, t=0.0060000000000000000000001, state_local=0x1613170, state_global=0x2458fd8, f_local=0x16117b0, f_global=0x16117b0) at /home/pszilard/data/gromacs-5.0/src/gromacs/fileio/mdoutf.c:298
```

Below is the backtrace for mdrun-test. This indicates that the issue is in the TNG compression function and based on the SIGBUS, my guess is that this is perhaps an alignment issue.

```
```

05/04/2020
#6 - 07/02/2014 12:00 PM - Teemu Murtola
- Has duplicate Bug #1546: Legacy tools tests failed on armv7a with SIGBUS added

#7 - 07/02/2014 12:00 PM - Teemu Murtola
- Has duplicate Bug #1547: MDRUN tools tests failed on armv7a with SIGBUS added

#8 - 07/02/2014 01:01 PM - Magnus Lundborg
- Assignee set to Magnus Lundborg

I'm working on this. There should be a fix within a few days.

#9 - 07/02/2014 01:03 PM - Magnus Lundborg
- Status changed from New to In Progress

#10 - 07/11/2014 10:32 AM - Magnus Lundborg
- Related to Bug #1559: Writing TNG files fails on Xeon Phi added

Gerrit received a related patchset '1' for Issue #1542.
Uploader: Magnus Lundborg (magnus.lundborg@scilifelab.se)
Change-Id: i96e0704d3858264ca918603bf1d7e3b27b4db7ea
Gerrit URL: https://gerrit.gromacs.org/3799

#12 - 07/11/2014 12:37 PM - Magnus Lundborg
- Status changed from In Progress to Fix uploaded

#13 - 07/15/2014 09:12 AM - Teemu Murtola
- Category set to core library
- Target version set to 5.1

#14 - 08/25/2014 06:15 AM - Roland Schulz
- Status changed from Fix uploaded to Closed
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<td>Szilárd Páll</td>
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<tr>
<td>CMakeCache.txt</td>
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<td>make-check.log</td>
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<td>06/30/2014</td>
<td>Szilárd Páll</td>
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