GROMACS - Bug #1546
Legacy tools tests failed on armv7a with SIGBUS
07/02/2014 11:03 AM - Alexey Shvetsov

Status: Closed
Priority: Normal
Assignee: Magnus Lundborg
Category: core library
Target version: 5.1
Affected version: git master

Description
Backtrace for latest master branch code
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'
Reading frame 1 time 0.000 -> frame 1 time 0.000
Program received signal SIGBUS, Bus error.
0xb682b6e0 in quantize_float (x=0x24, x@entry=0x87543, natoms=natoms@entry=3, nframes=nframes@entry=1, precision=0.000999999931, quant=0xl, quant@entry=0x8efa0)
   at /home/alexxy/Develop/gromacs/src/external/tng_io/src/compression/tng_compress.c:91
91 quant[iframe*natoms*3+i*3+j]=(int)floor((x[iframe*natoms*3+i*3+j]/precision)+0.5);
(gdb)
(gdb) bt
#0 0xb682b6e0 in quantize_float (x=0x24, x@entry=0x87543, natoms=natoms@entry=3, nframes=nframes@entry=1, precision=0.000999999931, quant=0xl, quant@entry=0x8efa0)
   at /home/alexxy/Develop/gromacs/src/external/tng_io/src/compression/tng_compress.c:91
#1 0xb682c7c0 in tng_compress_pos_float (pos=pos@entry=0x87543, natoms=3, nframes=nframes@entry=1, desired_precision=desired_precision@entry=0.00100000005, speed=speed@entry=0, algo=0x8b6f8, nitems=0xbeff5bc) at /home/alexxy/Develop/gromacs/src/external/tng_io/src/compression/tng_compress.c:1248
#2 0xb682c874 in tng_compress_pos_float_find_algo (pos=pos@entry=0x87543, natoms=3, nframes=nframes@entry=1, desired_precision=desired_precision@entry=0.00100000005, speed=speed@entry=0, algo=0x8b6f8, nitems=0xbeff5bc, nitems@entry=0xbeff5b4) at /home/alexxy/Develop/gromacs/src/external/tng_io/src/compression/tng_compress.c:1279
#3 0xb6847cd4 in tng_compress (start_pos=<optimized out>, type=2 \"\002\", n_particles=1, n_frames=2468575403623720, block=0x88f00, tng_data=0x88f00)
at /home/alexxy/Develop/gromacs/src/external/tng_io/src/lib/tng_io.c:4837
#4 tng_particle_data_block_write (tng_data=0x88f00, tng_data@entry=0x8c528, block=0x88f00, block_index=<optimized out>, mapping=mapping@entry=0x0, hash_mode=hash_mode@entry=1 '001')
at /home/alexxy/Develop/gromacs/src/external/tng_io/src/lib/tng_io.c:6311
#5 0xb685661c in tng_frame_set_write (tng_data=0x8c528, hash_mode=<optimized out>) at /home/alexxy/Develop/gromacs/src/external/tng_io/src/lib/tng_io.c:1310
#6 0xb685190c in tng_util_generic_write (tng_data=tng_data@entry=0x8c528, frame_nr=<optimized out>, values=values@entry=0x8bf50, n_values_per_frame=n_values_per_frame@entry=3, block_id=block_id@entry=268435457, block_name=0xb6f0c810 "POSITIONS", block_name@entry=0x100001, compression=2 '002', particle_dependency=1 '001', particle_dependency@entry=0 '000', compression=2 '002', compression@entry=16 '020') at /home/alexxy/Develop/gromacs/src/external/tng_io/src/lib/tng_io.c:1815
dl #7 0xb68526f4 in tng_util_generic_with_time_write (tng_data=0x8c528, frame_nr=<optimized out>, time=time@entry=0, values=values@entry=0x8bf50, n_values_per_frame=n_values_per_frame@entry=3, block_id=268435457, block_name=0xb6f0c810 "POSITIONS", particle_dependency=1 '001', compression=2 '002') at /home/alexxy/Develop/gromacs/src/external/tng_io/src/lib/tng_io.c:18662
#8 0xb6b44204 in gmx_fwrite_tng (tng=0x8c528, bUseLossyCompression=optimized out, step=1, elapsed=elapsed, edPicoSeconds=optimized out) at /home/alexxy/Develop/gromacs/src/external/tng_io/src/lib/tng_io.c:1851

05/03/2020
In your project, the error occurred in the function `tng_compress_pos_float` located in the file `compression/tng_compress.c`. This function is responsible for compressing position data. The error trace points to a call to this function where the input parameters are: `pos=pos@entry=0x87543`, `natoms=3`, and `nframes=nframes@entry=1`. The call occurs in the file `external/tng_io/src/compression/tng_compress.c`. The error happens when the function attempts to quantize the float precision to a desired precision. The error is thrown when the quantization fails, indicating that the precision might not be achievable within the given constraints.
```c
#include <iostream>
#include <vector>

int main(int argc, char* argv[])
{
    std::vector<int> v;
    v.push_back(1);
    v.push_back(2);
    v.push_back(3);
    return 0;
}
```

**Related issues:**

- Related to GROMACS - Bug #1559: Writing TNG files fails on Xeon Phi
  - Closed 07/10/2014
- Is duplicate of GROMACS - Bug #1542: two unit tests fail on 32-bit ARM
  - Closed 06/30/2014

**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: I90a6406cccbc43fd57d4423c2861019cf7763e8

**History**

- #1 - 07/02/2014 12:00 PM - Teemu Murtola

05/03/2020
- Is duplicate of Bug #1542: two unit tests fail on 32-bit ARM added

#2 - 07/02/2014 01:02 PM - Magnus Lundborg
- Status changed from New to In Progress
- Assignee set to Magnus Lundborg

#3 - 07/02/2014 08:56 PM - Mark Abraham
- Description updated

#4 - 07/11/2014 10:32 AM - Magnus Lundborg
- Related to Bug #1559: Writing TNG files fails on Xeon Phi added

#5 - 07/11/2014 11:53 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1546:
Uploader: Magnus Lundborg (magnus.lundborg@scilifelab.se)
Change-id: I96e0704d3858264ca918603bf1d7e3b27b4db7ea
Gerrit URL: https://gerrit.gromacs.org/3799

#6 - 07/11/2014 12:38 PM - Magnus Lundborg
- Status changed from In Progress to Fix uploaded

#7 - 07/15/2014 09:12 AM - Teemu Murtola
- Category changed from testing to core library
- Target version changed from 5.x to 5.1

#8 - 08/25/2014 06:15 AM - Roland Schulz
- Status changed from Fix uploaded to Closed