GROMACS - Bug #1547

MDRUN tools tests failed on armv7a with SIGBUS

07/02/2014 11:08 AM - Alexey Shvetsov

Status: Closed
Priority: Normal
Assignee: Magnus Lundborg
Category: core library
Target version: 5.1
Affected version - extra info:

Difficulty: uncategorized

Description
Also backtrace for mdrun-test

WARNING: Using the slow plain C kernels. This should not happen during routine usage on supported platforms.

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

Program received signal SIGBUS, Bus error.
0xb682b6e0 in quantize_float (x=0x24, x@entry=0x9591bb, natoms=natoms@entry=3, nframes=1, nframes@entry=2, precision=0.000999999931, quant=0x2, quant@entry=0x959208)
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) bt
#0 0xb682b6e0 in quantize_float (x=0x24, x@entry=0x9591bb, natoms=natoms@entry=3, nframes=1, nframes@entry=2, precision=0.000999999931, quant=0x2, quant@entry=0x959208)
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=0x9591bb, natoms=3, nframes=2, desired_precision=desired_precision@entry=0.00100000005, speed=speed@entry=0, algo=0x2017728, nitems=0xbeffc30c) at /home/alexxy/Develop/gromacs/src/external/tng_io/src/compression/tng_compress.c:1279
#2 0xb682c874 in tng_compress_pos_float_find_algo (pos=pos@entry=0x9591bb, natoms=<optimized out>, nframes=<optimized out>, desired_precision=desired_precision@entry=0.00100000005, speed=speed@entry=0, algo=0x2017728, nitems=0xbeffc30c, nitems@entry=0xbeffc304) at /home/alexxy/Develop/gromacs/src/external/tng_io/src/compression/tng_compress.c:1279
#3 0xb6847cb0 in tng_compress (start_pos=<optimized out>, type='\002', n_particles=2, n_frames=3151178625676096, block=0x9590c8, tng_data=0x9590c8)
at /home/alexxy/Develop/gromacs/src/external/tng_io/src/lib/tng_io.c:4837
#4 tng_particle_data_block_write (tng_data=0x9590c8, tng_data@entry=0x6ff340, block=0x9590c8, 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=0x6ff340, hash_mode=<optimized out>) at /home/alexxy/Develop/gromacs/src/external/tng_io/src/lib/tng_io.c:13107
#6 0xb6b5c56c in mdoutf_write_to_trajectory_files (fplog=0x200a7d0, cr=0x1df1b60, of=0x200e0e40, mdo_flags=19, top_global=0x1ffe298, step=6, step_rel=6, t=0.0060000000000000001, ir=0x1df0d20, state_local=0x20101f0, state_global=0x1df1328, f_local=0x702e0e8, f_global=0x702e0e8) at /home/alexxy/Develop/gromacs/src/gromacs/fileio/mdoutf.c:299
#7 0xb6b5c3b8 in do_md_trajectory_writing (fplog=0x1ffe138, cr=0x1df1b60, nfile=7351896, fnm=0x0, step=6, step_rel=6, t=0.0060000000000000001, ir=0x1df0d20, state_local=0x20101f0, state_global=0x1df1328, topglobal=0x1ffe138, ofr=0x200e0e40, mdebin=0x701d30, ekind=0x702e58, f=0x702e0e8, f_global=0x702e0e8, wcycle=0x0, nchkpt=0xbeff6c64, bCPT=1, bRerunMD=0, bLastStep=1, bDoConfOut=4096, bSumEkinhOld=0) at /home/alexxy/Develop/gromacs/src/gromacs/fileio/trajfactory.c:146
#8 0x000045078 in do_md (fplog=0x6, cr=0x1df1b60, nfile=0, fnm=0x0, oenv=0x200e0e40, bVerbose=0, bCompact=1, nstglobalcomm=1, viscosity=0x0, constr=0x200ed0e0, stepout=100, ir=0x1df0d20, topglobal=0x1ffe138, fcd=0x1ffe298, stateglobal=0x1df1328, mdatoms=0x200ed38, nnb=0x200d4a8, wcycle=0x0, ed=0x0, fr=0x200e0e40, repl_ex_nst=0, repl_ex_nex=0, repl_ex_seed=1, membed=0x0, cpt_period=15, max_hours=1, deviceOptions=0x93f98 "", imdport=8888, Flags=1055744...
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: I90a6406ccc4c34fd57d4423c2b661019cf7763e8

History

#1 - 07/02/2014 12:00 PM - Teemu Murtola
- Is duplicate of Bug #1542: two unit tests fail on 32-bit ARM added

#2 - 07/02/2014 01:01 PM - Magnus Lundborg
- Assignee set to Magnus Lundborg

#3 - 07/02/2014 01:02 PM - Magnus Lundborg
- Status changed from New to In Progress

#4 - 07/03/2014 02:35 PM - Mark Abraham
- Description updated

#5 - 07/11/2014 10:32 AM - Magnus Lundborg
- Related to Bug #1559: Writing TNG files fails on Xeon Phi added

#6 - 07/11/2014 11:53 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1547.
Uploader: Magnus Lundborg (magnus.lundborg@scilifelab.se)
Change-Id: i96e0704d3858264ca918603b1f1d769b27b4d7e8a
Gerrit URL: https://gerrit.gromacs.org/3799

#7 - 07/11/2014 12:38 PM - Magnus Lundborg
- Status changed from In Progress to Fix uploaded

#8 - 07/15/2014 09:11 AM - Teemu Murtola
- Category changed from testing to core library
- Target version changed from 5.x to 5.1

#9 - 08/25/2014 06:15 AM - Roland Schulz
- Status changed from Fix uploaded to Closed