### GROMACS - Bug #1559

#### Writing TNG files fails on Xeon Phi

07/10/2014 08:57 AM - Roland Schulz

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Magnus Lundborg</td>
</tr>
<tr>
<td>Category:</td>
<td>core library</td>
</tr>
<tr>
<td>Target version:</td>
<td>5.1</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>5.0</td>
</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
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#### Description

The unit tests:

- mdrun-test CanWrite/Trajectories.ThatDifferInNstxout/*
- legacy-tools-test NoFatalErrorWhenWritingFrom/TrjconvWithIndexGroupSubset.WithDifferentInputFormats/*

fail. And "gmx trjconv" fails with segfault if the output is TNG. This is without zlib. But running the tests with the same compiler (ICC14.0.2) on the CPU or without zlib seems fine.

#### Related issues:

- Related to GROMACS - Bug #1542: two unit tests fail on 32-bit ARM
- Related to GROMACS - Bug #1546: Legacy tools tests failed on armv7a with SIGBUS
- Related to GROMACS - Bug #1547: MDRUN tools tests failed on armv7a with SIGBUS

<table>
<thead>
<tr>
<th>Revision</th>
<th>Date</th>
<th>Status</th>
<th>Message</th>
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</thead>
<tbody>
<tr>
<td>898166c3</td>
<td>08/21/2014</td>
<td>Closed</td>
<td>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: l90a6406ccbc43td57d4423c2b661019cf7763e8</td>
</tr>
</tbody>
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#### History

**#1 - 07/10/2014 10:14 AM - Mark Abraham**

Roland Schulz wrote:

The unit tests:

- mdrun-test CanWrite/Trajectories.ThatDifferInNstxout/*
- legacy-tools-test NoFatalErrorWhenWritingFrom/TrjconvWithIndexGroupSubset.WithDifferentInputFormats/*

fail. And "gmx trjconv" fails with segfault if the output is TNG.

I don't think it makes sense to have I/O code run anywhere near a Phi. Presumably to reproduce one needs to do cmake .. -DCMAKE_TOOLCHAIN_FILE=Platform/XeonPhi, but what was the run-time setup?

This is without zlib. But running the tests with the same compiler (ICC14.0.2) on the CPU or without zlib seems fine.
One of those "without" should be "with?"

#2 - 07/10/2014 04:34 PM - Roland Schulz
Mark Abraham wrote:

I don't think it makes sense to have I/O code run anywhere near a Phi. Presumably to reproduce one needs to do cmake ..
-DCMAKE_TOOLCHAIN_FILE=Platform/XeonPhi, but what was the run-time setup?

In native mode the I/O has to happen on the Phi. And native mode is currently the only supported option (we are still working on offload). Also the next generation will be self hosted. And even if we think that we don't care about TNG on Phi, the fact that this isn't working is hinting to some bug which probably will be present on some other architectures too. The Phi card has a standard Linux environment and I'm actually surprised that it isn't working. All other Gromacs I/O, unit- and regression tests work without any problems (with no changes). No special run-time setup is needed. To make it easy to run the unit-tests, the source and build folders should be located in a directory which is mounted to the same location on the Phi (e.g. /data/gromacs or /home/.../gromacs on both host and MIC - the reason is that the reftdata classes use the CMAKE_SOURCE_DIR to find its xml files).

This is without zlib. But running the tests with the same compiler (ICC14.0.2) on the CPU or without zlib seems fine.

no. I tested on a standard CPU that the unit tests pass when one disables zlib. I also tested that the same compiler version is fine on a standard CPU.

#3 - 07/11/2014 10:32 AM - Magnus Lundborg
- Assignee set to Magnus Lundborg

Hopefully this is related to the other TNG issues. I hope to have a fix ready quite soon.

#4 - 07/11/2014 10:32 AM - Magnus Lundborg
- Related to Bug #1542: two unit tests fail on 32-bit ARM added

#5 - 07/11/2014 10:32 AM - Magnus Lundborg
- Related to Bug #1546: Legacy tools tests failed on armv7a with SIGBUS added

#6 - 07/11/2014 10:32 AM - Magnus Lundborg
- Related to Bug #1547: MDRUN tools tests failed on armv7a with SIGBUS added

#7 - 07/11/2014 11:53 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1559.
Uploader: Magnus Lundborg (magnus.lundborg@scilifelab.se)
Change-Id: I96e0704d3858264ca918603bf1d7e3b27b4db7ea
Gerrit URL: https://gerrit.gromacs.org/3799

#8 - 07/11/2014 12:29 PM - Roland Schulz
Yes this patch fixes it. It segfaulted in quantize_float because the compiler assumed that the float* passed to it is 4-byte aligned.

#9 - 07/11/2014 12:36 PM - Magnus Lundborg
- Status changed from New to Fix uploaded

Thanks for the feedback.

#10 - 07/11/2014 12:50 PM - Roland Schulz
Was the previous code valid C code or is OK for the C compiler to assume 4-byte alignment? If it was valid it might be good to report a compiler bug.

#11 - 07/15/2014 09:11 AM - Teemu Murtola
- Category set to core library
- Target version set to 5.1

#12 - 08/25/2014 06:14 AM - Roland Schulz
- Status changed from Fix uploaded to Closed