GROMACS - Bug #1540

tng unit test shows errors

06/29/2014 11:36 PM - 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>5.0.1</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>5.0</td>
</tr>
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<td>Affected version:</td>
<td>5.0</td>
</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
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**Description**
The tng unit tests shows errors:
23:03:10 8: TNG library: Cannot read header size.
D:\jenkins-build\workspace\Gromacs_Gerrit_5_0@2\f9e84682\gromacs\src\external\tng_io\src\lib\tng_io.c: 818
23:03:10 8: TNG library: Cannot read block header at pos -1.
D:\jenkins-build\workspace\Gromacs_Gerrit_5_0@2\f9e84682\gromacs\src\external\tng_io\src\lib\tng_io.c: 11553

Without failing. Not sure whether these errors are actually a problem.
- If they are, they need to fixed and also the unit test fixed so that it fails if an error occur
- If it is an problem, they need to be silent to not confuse.

**Associated revisions**

Revision ece402b9 - 07/05/2014 02:37 PM - Magnus Lundborg
Fix tng_num_frame_sets_get() with no frame sets.
When there are no frame sets the function returned an error.
This corresponds to commit 6f7862c7406b in the TNG repository.
Fixes #1540
Change-Id: I3df04d84ebd8fcdc6be76a446efa3209df363d23

**History**

#1 - 06/30/2014 09:18 AM - Magnus Lundborg
- Status changed from New to Accepted

The tests should indeed fail at that stage, since somethings is apparently a problem. I guess this is from running bin/tests/tng_testing, right? Could you give the whole output of the tests so that I can see where it fails. I think I know, but it's good to be sure.

The next question is why the test(s) fail(s).

#2 - 06/30/2014 09:47 AM - Magnus Lundborg

Sorry, now I've realised where the error occurs. There's nothing that actually fails, there was just a poor handling of TNG files without any trajectory data.

#3 - 06/30/2014 10:07 AM - Gerrit Code Review Bot

Gerrit received a related patchset `1` for Issue #1540.
Uploader: Magnus Lundborg (magnus.lundborg@scilifelab.se)
Change-Id: l3df04d84ebd8fcdc6be76a446efa3209df363d23
Gerrit URL: https://gerrit.gromacs.org/3729

#4 - 06/30/2014 10:10 AM - Magnus Lundborg
- Status changed from Accepted to Fix uploaded

#5 - 07/05/2014 08:51 AM - Roland Schulz

Shouldn't the unit test have failed? I understand that it wasn't an error. But I'm wondering that if an error was (wrongly) detected, it seems odd that the
unit test passed. I just want to make sure that if a real error happens in the future it isn't missed because the error isn't propagated incorrectly.

#6 - 07/11/2014 11:58 AM - Magnus Lundborg
I think that the TNG unit tests in GROMACS currently only check that there are no fatal errors, but Mark might know more about that.

#7 - 07/11/2014 11:11 PM - Mark Abraham
Magnus Lundborg wrote:

I think that the TNG unit tests in GROMACS currently only check that there are no fatal errors, but Mark might know more about that.

GROMACS doesn't use the TNG unit tests at all - though there's probably a todo about that somewhere. The integration-style tests for various trajectory handling exercise the TNG code, of course, but don't do anything more interesting than wrap trjconv or such, and report on its return code. Some unit style tests on the GROMACS functions that wrap calls to TNG might well be a good idea, but if there's not constructors for stuff that work decently, that should come first!

#8 - 07/15/2014 09:21 AM - Teemu Murtola
- Category set to core library
- Target version set to 5.0.1

#9 - 08/10/2014 08:18 PM - Roland Schulz
- Status changed from Fix uploaded to Closed