GROMACS - Bug #2813
regressiontests/complex fails on Fedora30 with x86_64, i686 and other archs.
12/20/2018 06:12 PM - Christoph Junghans

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: testing
Target version: 2019.1
Affected version - extra info: Difficulty: uncategorized
Affected version: 2019-rc1

Description
I did a test build on version 2019-rc1 on Fedora 30 with the following result:

Thanx for Using GROMACS - Have a Nice Day
Mdrun cannot use the requested (or automatic) number of ranks, retrying with 8.
Abnormal return value for ' gmx mdrun -nb cpu -notunepme >mdrun.out 2>&1' was 1
Retrying mdrun with better settings...
sh: line 1: 4161 Aborted                    (core dumped) gmx mdrun -nb cpu -notunepme > mdrun.out 2 >&1
Abnormal return value for ' gmx mdrun -nb cpu -notunepme >mdrun.out 2>&1' was -1
FAILED. Check mdrun.out, md.log file(s) in urea for urea
1 out of 51 complex tests FAILED
Details build log for x86 and i686 attached.

Associated revisions
Revision 3911191a - 01/03/2019 02:18 PM - Berk Hess
Fix segmentation fault in DD code
mdrun could exit with a segmentation fault in DD when DLB was disabled.
Fixes #2813
Change-Id: Ie20ca1995c93fa74f41d8db5becfce1cb20348a3

Revision c5c3743d - 02/06/2019 05:58 PM - Berk Hess
Fix segfault with EM, DD and group scheme
Resetting to an old DD state during EM would leave the cg sorting array
used with the group scheme in an invalid state. This could cause
out of bounds vector access one DD step after rejecting an EM step.
When merging this into master branch, prefer to change to use ssize
rather than the static_cast.
Fixes #2813
Change-Id: I7f13b46d7ff5352ce41838b13c46f2e90c93b1c

History
#1 - 12/21/2018 09:19 AM - Paul Bauer
Error occurs in the serial build with openblas according to the log for x86 (so that other people don't need to dig through it)

02/21/2020
Does this also show up in Fedora 29 or before?

#2 - 12/21/2018 01:14 PM - Paul Bauer
I tried reproducing this on my machine, but it doesn't have gcc-8.2.1 and I couldn't trigger the same error.

#3 - 12/21/2018 04:12 PM - Paul Bauer
- Target version changed from 2019-rc2 to 2019

no second release candidate is planned

#4 - 12/21/2018 10:43 PM - Christoph Junghans
Paul Bauer wrote:

Does this also show up in Fedora 29 or before?

I didn't see it it on Fedora 29, but I also didn't see with gromacs-2018.4 on Fedora 30.

#5 - 12/21/2018 11:24 PM - Christoph Junghans
To reproduce this (using Fedora):

- Get Fedora account: https://admin.fedoraproject.org/accounts/
- git clone -b v2019 https://src.fedoraproject.org/rpms/gromacs.git
- cd gromacs
- spectool -g gromacs.spec
- rpmbuild -bs gromacs.spec
- kinit <USER>@FEDORAPROJECT.ORG
- koji build --nowait --scratch f30 gromacs-2019-0.1rc1.fc30.src.rpm

#6 - 12/22/2018 12:59 PM - Paul Bauer
We would still need to have access to the build host to try to reproduce this. As I said, I can't reproduce it with gcc-8.2.0-12 on Debian Unstable.

#7 - 12/22/2018 04:53 PM - Christoph Junghans
Paul Bauer wrote:

We would still need to have access to the build host to try to reproduce this. As I said, I can't reproduce it with gcc-8.2.0-12 on Debian Unstable.

Accessing koji directly is not possible! Maybe one can reproduce this in the fedora:rawhide docker container?

#8 - 12/23/2018 09:15 PM - Christoph Junghans
I was able to reproduce this in docker starting from the fedora:rawhide container:

docker run -it fedora:rawhide /bin/bash
and then:

dnf install -y rpm-build git bash-completion cmake fftw-devel gcc-c++ gsl-devel hwloc-devel libX11-devel lmfit-devel motif-devel mpich-devel ocl-icd-devel openblas-devel opencl-devel openmpi-devel tng-devel hwloc make spectool adduser user su - user
- git clone -b v2019 https://src.fedoraproject.org/rpms/gromacs.git
- cd gromacs/
- spectool -g gromacs.spec
- mkdir -p /home/user/rpmbuild/SOURCES
for i in *2019-rc1* *.patch *.fedora; do ln -s $PWD/$i /home/user/rpmbuild/SOURCES; done

```
#!/etc/profile.d/modules.sh
```

rpmbuild -ba gromacs.spec

**#9 - 12/28/2018 12:12 PM - Paul Bauer**

- Status changed from New to Feedback wanted

Tried building a debug version in the docker container

```
/home/user/rpmbuild/BUILD/gromacs-2019-rc1/src/gromacs/correlationfunctions/gmx_lmcurve.cpp: In function 'void gmx_lmcurve(int, double*, int, const double*, const double*, const double*, double (*)(double, const double*), const lm_control_struct*, lm_status_struct*)':
  lmmin(n_par, par, m_dat, nullptr, &data, lmcurve_evaluate,
^~~~~
In file included from /home/user/rpmbuild/BUILD/gromacs-2019-rc1/src/gromacs/correlationfunctions/gmx_lmcurve.cpp:53:
/usr/include/lmmin.h:33:20: note: initializing argument 5 of 'void lmmin(int, double*, int, const void*, void (*)(const double*, int, const void*, double*, int*), const lm_control_struct*, lm_status_struct*)'
  void (*evaluate) (const double* par, const int m_dat, const void* data,
  ~~~~~~~~~~~~~~~~~~~~~~~~~~
    double* fvec, int* userbreak),
```

**#10 - 12/28/2018 12:48 PM - Paul Bauer**

- Status changed from Feedback wanted to Blocked, need info
- Target version changed from 2019 to 2019.1

I think this might be related to Fedora not having the bundled lmfit?

When building directly from git everything passes, so the error gets introduced in the process of preparing the Fedora version. I bumped this to 2019.1, because whatever the issue is I don't think it will get fixed before the release.

**#11 - 12/28/2018 06:30 PM - Christoph Junghans**

I did a test build with the external lmfit here: [https://koji.fedoraproject.org/koji/taskinfo?taskId=31709353](https://koji.fedoraproject.org/koji/taskinfo?taskId=31709353), let's see what happens.

**#12 - 12/31/2018 09:14 PM - Christoph Junghans**

- Status changed from Blocked, need info to Accepted

Ok the problem persists even with the internal lmfit.

**#13 - 01/02/2019 06:07 AM - Paul Bauer**

- Status changed from Accepted to Blocked, need info

I tried it just right now again in the docker container. Building straight from gromacs.git with internal lmfit works perfectly fine.

docker run -it fedora:rawhide /bin/bash
dnf install -y rpm-build git bash-completion cmake fftw-devel gcc-c++ gsl-devel hwloc-devel libX11-devel lmfit-devel motif-devel mpich-devel occi-icd-devel openblas-devel opencv-devel openmpi-devel tng-devel hwloc make spectool adduser user su - user
git clone https://github.com/gromacs/gromacs.git -b release-2019
git clone https://github.com/gromacs/regressiontests.git -b release-2019
cd gromacs
mkdir build
cd build
-DBUILD_SHARED_LIBS:BOOL=ON -DBUILD_TESTING:BOOL=ON -DCMAKE_SKIP_RPATH:BOOL=ON -DCMAKE_SKIP_BUILD_RPATH:BOOL=ON \  
-N -DGXX_BLAS_USER=openblas -DGXX_EXTERNAL_TNG:BOOL=ON -DGXX_EXTERNAL_TINYXML2:BOOL=OFF -DGXX_LAPACK_USER=openblas -DGXX_USE_RDTSCP=OFF -D
What are the changes applied to the code in order to prepare the Fedora package?

#14 - 01/02/2019 12:26 PM - Mark Abraham

Note that the lmfit package did not have reasonable packaging or versioning last time I looked at it, so it may not be reasonable to try to support it in a distro.

#15 - 01/02/2019 03:44 PM - Christoph Junghans

Mark Abraham wrote:

Note that the lmfit package did not have reasonable packaging or versioning last time I looked at it, so it may not be reasonable to try to support it in a distro.

I think that discussion before, fedora has something against bundle libraries (https://fedoraproject.org/wiki/Bundled_Libraries?rd=Packaging:Bundled_Libraries). The main problem is that libgromacs provide the same lmfit symbols as liblmfit for the lmfit package itself, which could lead to some unwanted effect if an executable links both.

Also I am not sure what you mean by reasonable packaging, lmfit uses autotools and don't use anything fancy like mpi hence has the most simplest packaging process even: https://src.fedoraproject.org/rpms/lmfit/blob/master/f/lmfit.spec.

Paul's build issue with lmfit above, which doesn't show up in my original build ("Found lmfit: /usr/include (found version "6.4") is still unclear to me, but an lmfit-7 update is on the way, too: https://src.fedoraproject.org/rpms/lmfit/pull-request/2

#16 - 01/02/2019 03:52 PM - Paul Bauer

GROMACS depends on lmfit 7.0, so it can't work with the lower versions (see cmake/gmxManageLmfit.cmake). So the bug might be that it didn't pick up the requirements for lmfit correctly.

#17 - 01/02/2019 03:53 PM - Christoph Junghans

Paul Bauer wrote:

What are the changes applied to the code in order to prepare the Fedora package?

in spec (see https://src.fedoraproject.org/rpms/gromacs/blob/v2019/f/gromacs.spec#_234) we do:

```
%patch0 -p1
%if 0%{?fedora} <= 29
%patch1 -p1
%endif
rm -r src/external/{fftpack,tng_io,lmfit}
```

Patch0 changes the path of dssp: https://src.fedoraproject.org/rpms/gromacs/blob/v2019/f/gromacs-dssp-path.patch
Patch1, which only get applied for Fedora 29 and below (so not in the original build posted here): https://src.fedoraproject.org/rpms/gromacs/blob/v2019/f/gromacs-issue-2366.patch, disables a piece of a test on aarch64 only. See #2366, which seemed to have been an issue in earlier version of hwloc.

#18 - 01/02/2019 04:03 PM - Christoph Junghans

By the end of the day, I could simply disable the regressiontests in the rpm build, but I just don't want to deploy a possibly broken binary to all of Fedora's userbase.

#19 - 01/02/2019 04:05 PM - Christoph Junghans

Paul Bauer wrote:

GROMACS depends on lmfit 7.0, so it can't work with the lower versions (see cmake/gmxManageLmfit.cmake). So the bug might be that it didn't pick up the requirements for lmfit correctly.

It built with lmfit-6.4 not sure if this was intended, but anyhow this should be discussed on a different issue as the test still fail with the internal lmfit library as well.
I saw that the build fails in debug mode for the packaged version as well, likely related to the wrong version of lmfit.
I just now build the packaged version with the modifications to the gromacs.spec file needed to turn off external lmfit.
I managed to get a backtrace for the bug

```
==7680== Process terminating with default action of signal 6 (SIGABRT): dumping core
==7680== at 0x5B7E00F: raise (in /usr/lib64/libc-2.28.9000.so)
==7680== by 0x5B68894: abort (in /usr/lib64/libc-2.28.9000.so)
==7680== by 0x449F1F7: std::__replacement_assert(char const*, int, char const*, char const*) (c++config.h:2391)
==7680== by 0x44A4515E: operator[] (stl_vector.h:932)
==7680== by 0x44A4515E: get_load_distribution(gmx_domdec_t*, gmx_wallcycle*) (partition.cpp:882)
==7680== by 0x44A4BD05: dd_partition_system(_IO_FILE*, gmx::MDLogger const&, long, t_commrec const*, bool, int, t_state*, gmx_mtop_t const*, t_inputrec const*, t_state*, gmx::PaddedVector<gmx::BasicVector<float>, gmx::Allocator<gmx::BasicVector<float>, gmx::AlignedAllocationPolicy>*, gmx::BasicVector<float>*>, gmx::AlignedAllocationPolicy>*, gmx::MDAtoms*, gmx::localtop_t*, t_forcerec*, gmx::swalkstate_t*, gmx::Constraints*, t_nrb*, gmx::wallcycle*, bool) (partition.cpp:3104)
==7680== by 0x525A512B: em_dd_partition_system(_IO_FILE*, gmx::MDLogger const&, int, t_commrec const*, gmx_mtop_t*, t_inputrec*, em_state_t*, gmx::localtop_t*, gmx::MDAtoms*, t_forcerec*, gmx::swalkstate_t*, gmx::Constraints*, t_nrb*, gmx::wallcycle*) (partition.cpp:3104)
==7680== by 0x525B52D6: gmx::Integrator::do_steeep() (minimize.cpp:2610)
==7680== by 0x525B8D014: gmx::Integrator::run(unsigned int, bool) (integrator.cpp:86)
==7680== by 0x525C707B: gmx::md_runner::start_fn(void const*) (runner.cpp:219)
==7680== by 0x5334985: tMPI_Thread_starter(void*) (tmpi_init.cpp:399)
==7680== by 0x82F2582: start_thread (in /usr/lib64/libpthread-2.28.9000.so)
```

#21 - 01/02/2019 07:36 PM - Paul Bauer

- Status changed from Blocked, need info to Accepted

#22 - 01/03/2019 10:54 AM - Mark Abraham

Christoph Junghans wrote:

Mark Abraham wrote:

Note that the lmfit package did not have reasonable packaging or versioning last time I looked at it, so it may not be reasonable to try to support it in a distro.

I think that discussion before, fedora has something against bundle libraries (https://fedoraproject.org/wiki/Bundled_Libraries?rd=Packaging:Bundled_Libraries). The main problem is that libgromacs provide the same lmfit symbols as liblmfit for the lmfit package itself, which could lead to some unwanted effect if an executable links both.

Sure. Lmfit is not very easy to write a cmake find_package for, because there’s no explicit way to discover the version (and the only implicit way is to see if test or real code compiles and runs).

Also I am not sure what you mean by reasonable packaging. Lmfit uses autotools and don’t use anything fancy like mpi hence has the most simplest packaging process even: https://src.fedoraproject.org/rpms/lmfit/blob/master/f/lmfit.spec.

See 13410c301f5af. They made breaking API changes and have provided no way for anyone to discover the version of the code in liblmfit.so or its headers. So we can’t spend the effort to support more than one version of it, and have to bundle that one, and provide for distros to be able to provide their own version of it.

Paul’s build issue with lmfit above, which doesn’t show up in my original build ("Found Lmfit: /usr/include (found version "6.4") is still unclear to me, but an Lmfit-7 update is on the way, too: https://src.fedoraproject.org/rpms/lmfit/pull-request/2

"GROMACS 2019 requires Lmfit 7" is one of our boundary conditions :-)"

#23 - 01/03/2019 11:12 AM - Mark Abraham

- Related to Bug #2584: regressiontests/complex fails on i686 added

#24 - 01/03/2019 11:45 AM - Christoph Junghans

Mark Abraham wrote:

Christoph Junghans wrote:

Paul's build issue with Lmfit above, which doesn't show up in my original build ("Found Lmfit: /usr/include (found version "6.4") is still unclear to me, but an Lmfit-7 update is on the way, too: https://src.fedoraproject.org/rpms/lmfit/pull-request/2

02/21/2020
"GROMACS 2019 requires lmfit 7" is one of our boundary conditions :-)

The problem of lmfit-6.4 not give an error is attacked here: https://gerrit.gromacs.org/#/c/8916/

#25 - 01/03/2019 02:20 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2813.
Uploader: Berk Hess (hess@kth.se)
Change-id: gromacs~release-2019~iae20ca1995c93fa74f41d8db5becf1e1cb20348a3
Gerrit URL: https://gerrit.gromacs.org/8917

#26 - 01/03/2019 02:21 PM - Berk Hess
- Status changed from Accepted to Fix uploaded
- Assignee changed from Paul Bauer to Berk Hess

#27 - 01/03/2019 03:12 PM - Szilárd Páll
- Related to deleted (Bug #2584: regressiontests/complex fails on i686)

#28 - 01/03/2019 03:12 PM - Szilárd Páll
Not related to #2584, that has been shown to be a 32-bit only issue in AWH.

#29 - 01/03/2019 04:40 PM - Christoph Junghans
- File build.log.txt added

I patched https://gerrit.gromacs.org/8917 in, but it didn't help, build log attached.

#30 - 01/04/2019 02:00 PM - Berk Hess
- Status changed from Fix uploaded to Resolved

Applied in changeset 3911191a537a2597522432680395e99735e6cb32.

#31 - 01/04/2019 04:27 PM - Christoph Junghans
- Status changed from Resolved to Accepted

Problem persists.

#32 - 01/04/2019 06:39 PM - Mark Abraham
I can't reproduce this with SSE2+OpenCL build with gcc 8.2 on ubuntu 18.02

#33 - 01/04/2019 08:00 PM - Christoph Junghans

Mark Abraham wrote:

I can't reproduce this with SSE2+OpenCL build with gcc 8.2 on ubuntu 18.02

The gcc version basically doesn't mean anything as Ubuntu and Fedora both patch their gcc heavily.

#34 - 01/11/2019 01:31 PM - Mark Abraham
- Assignee deleted (Berk Hess)

#35 - 01/14/2019 01:23 PM - Mark Abraham
We might come back to this in a week or two, no assignee for now

#36 - 01/16/2019 02:04 PM - Mark Abraham

In master, we just converted this test to run with the verlet scheme. It used no constraints and steepest descent. We observed TSAN find a race with steep+Verlet, and it wasn't stable when converted to leapfrog+Verlet, so we switched it to no temperature coupling and a small timestep, and now it seems stable.

So my guess is that if we run urea on x86 for a tsan build then we will find a race.
#37 - 02/04/2019 01:52 PM - Paul Bauer
- Related to Bug #2858: Group scheme C kernels fail in complex tests added

#38 - 02/04/2019 02:48 PM - Paul Bauer
So, just tried reproducing this again in the docker container. The error again did not show up when building GROMACS directly from source, but I got this error while running the rpm build script

/home/user/rpmbuild/BUILD/gromacs-2019/src/gromacs/gpu_utils/gpu_utils_ocl.cpp:279:107: error: format not a string literal and no format arguments [-Werror=format-security]
  279 | gmx_warning((formatString("While sanity checking device %zu, ", deviceId) + errorMessage).c_str());
     | ^
cc1plus: some warnings being treated as errors

Does not show up on a different build under Debian as well, so I'm not sure where this one comes from now.

#39 - 02/04/2019 02:58 PM - Szilárd Páll
That's fixed, see [dabd3b9d](#)

#40 - 02/04/2019 03:13 PM - Paul Bauer
Thanks for pointing it out!

#41 - 02/04/2019 04:26 PM - Paul Bauer
so, after patching the issue above, I got this error message now when running gmx mdrun on its own.

/usr/include/c++/9/bits/stl_vector.h:1009: std::vector<_Tp, _Alloc>::reference std::vector<_Tp, _Alloc>::operator[] (std::vector<_Tp, _Alloc>::size_type) [with _Tp = DDCellsizesWithDlb; _Alloc = std::allocator<DDCellsizesWithDlb>; std::vector<_Tp, _Alloc>::reference = DDCellsizesWithDlb&; std::vector<_Tp, _Alloc>::size_type = long unsigned int]: Assertion '_built_in_expect(_n < this->size(), true)' failed.
/usr/include/c++/9/bits/stl_vector.h:1009: std::vector<_Tp, _Alloc>::reference std::vector<_Tp, _Alloc>::operator[] (std::vector<_Tp, _Alloc>::size_type) [with _Tp = DDCellsizesWithDlb; _Alloc = std::allocator<DDCellsizesWithDlb>; std::vector<_Tp, _Alloc>::reference = DDCellsizesWithDlb&; std::vector<_Tp, _Alloc>::size_type = long unsigned int]: Assertion '_built_in_expect(_n < this->size(), true)' failed.
/usr/include/c++/9/bits/stl_vector.h:1009: std::vector<_Tp, _Alloc>::reference std::vector<_Tp, _Alloc>::operator[] (std::vector<_Tp, _Alloc>::size_type) [with _Tp = DDCellsizesWithDlb; _Alloc = std::allocator<DDCellsizesWithDlb>; std::vector<_Tp, _Alloc>::reference = DDCellsizesWithDlb&; std::vector<_Tp, _Alloc>::size_type = long unsigned int]: Assertion '_built_in_expect(_n < this->size(), true)' failed.
/usr/include/c++/9/bits/stl_vector.h:1009: std::vector<_Tp, _Alloc>::reference std::vector<_Tp, _Alloc>::operator[] (std::vector<_Tp, _Alloc>::size_type) [with _Tp = DDCellsizesWithDlb; _Alloc = std::allocator<DDCellsizesWithDlb>; std::vector<_Tp, _Alloc>::reference = DDCellsizesWithDlb&; std::vector<_Tp, _Alloc>::size_type = long unsigned int]: Assertion '_built_in_expect(_n < this->size(), true)' failed.

and this when running under valgrind

==7689== Process terminating with default action of signal 6 (SIGABRT): dumping core
==7689== at 0x5E100F5: raise (in /usr/lib64/libc-2.29.so)
==7689== by 0x5DA95D: abort (in /usr/lib64/libc-2.29.so)
==7689== by 0x4A116E7: __replacement_assert (char const*, int, char const*, char const*) (c++config.h:2493)
==7689== by 0x4A629BE: operator[] (std::vector<_Tp, _Alloc>::reference std::vector<_Tp, _Alloc>::operator[] (std::vector<_Tp, _Alloc>::size_type) [with _Tp = DDCellsizesWithDlb; _Alloc = std::allocator<DDCellsizesWithDlb>; std::vector<_Tp, _Alloc>::reference = DDCellsizesWithDlb&; std::vector<_Tp, _Alloc>::size_type = long unsigned int]: Assertion '_built_in_expect(_n < this->size(), true)' failed.
==7689== by 0x4A67819: dd_partition_system (_IO_FILE*, gmx::MDLogger const&, long, t_commrec const*, int, t_state*, gmx::Constraints*, t_nrnb*, gmx::wallcycle*, bool) (partition.cpp:882)
==7689== by 0x527DF5B: em_dd_partition_system (_IO_FILE*, gmx::MDLogger const&, int, t_commrec const*, gmx::Constraints*, int, t_commrec const*, gmx::Constraints*, t_nrnb*, gmx::wallcycle*, bool) (transition.cpp:3104)
==7689== by 0x527DF5B: em_dd_partition_system (_IO_FILE*, gmx::MDLogger const&, int, t_commrec const*, gmx::Constraints*, t_nrnb*, gmx::wallcycle*, bool) (partition.cpp:3104)
==7689== by 0x528DD5E: gmx::Integrator::do_steep () (integrator.cpp:2610)
==7689== by 0x52C6864: gmx::Import::run (unsigned int, bool) (integrator.cpp:86)
==7689== by 0x52A1C5B: gmx::Mdrunner::mdrunner () (runner.cpp:1438)
==7689== by 0x52A3207: gmx::Mdrunner_start_fn (void const*) (runner.cpp:219)
==7689== by 0x5309F95: tMPI_Thread_terminate (void*) (tmpi_init.cpp:399)
==7689== by 0x8575555: start_thread (in /usr/lib64/libpthread-2.29.so)
/usr/include/c++/9/bits/stl_vector.h:1009: std::vector<_Tp, _Alloc>::reference std::vector<_Tp, _Alloc>::operator[] (std::vector<_Tp, _Alloc>::size_type) [with _Tp = DDCellsizesWithDlb; _Alloc = std::allocator<DDCellsizesWithDlb>; std::vector<_Tp, _Alloc>::reference = DDCellsizesWithDlb&; std::vector<_Tp, _Alloc>::size_type = long unsigned int]: Assertion '_built_in_expect(_n < this->size(), true)' failed.
WithDlb(); std::vector<Tp, _Alloc>::reference = DDCellsizesWithDlb; std::vector<Tp, _Alloc>::size_type = long unsigned int]: Assertion '_builtin_expect(__n < this->size(), true)' failed.

#42 - 02/04/2019 04:27 PM - Paul Bauer
my fault, did not apply the other patch yet, ignore last message

#43 - 02/04/2019 04:45 PM - Paul Bauer
- Related to deleted (Bug #2858: Group scheme C kernels fail in complext tests)

#44 - 02/05/2019 07:59 AM - Paul Bauer
So, now I managed to trigger it again

rt_t>; std::vector<Tp, _Alloc>::reference = gmx_cgsort_t&; std::vector<Tp, _Alloc>::size_type = long unsigned int]: Assertion '_builtin_expect(__n < this->size(), true)' failed.
/usr/include/c++/9/bits/stl_vector.h:1009: std::vector<Tp, _Alloc>::reference std::vector<Tp, _Alloc>::operator[](std::vector<Tp, _Alloc>::size_type) [with _Tp = gmx_cgsort_t; _Alloc = std::allocator<gmx_cgsort_t>; std::vector<Tp, _Alloc>::reference = gmx_cgsort_t&; std::vector<Tp, _Alloc>::size_type = long unsigned int]: Assertion '_builtin_expect(__n < this->size(), true)' failed.
==12805== Process terminating with default action of signal 6 (SIGABRT): dumping core
==12805== at 0x5E100F5: raise (in /usr/lib64/libc-2.29.so)
==12805== by 0x5DFA95D: abort (in /usr/lib64/libc-2.29.so)
==12805== by 0x4A116E7: std::__replacement_assert(char const*, int, char const*, char const*) (c++config.h:2493)
==12805== by 0x4A6B1A1: operator[] (stl_vector.h:1009)
==12805== by 0x4A6B1A1: dd_sort_order (partition.cpp:2735)
==12805== by 0x4A6B1A1: dd_sort_state(gmx_domdec_t*, float (*) [3], t_forcerec*, t_state*, int) (partition.cpp:2819)
==12805== by 0x4A6C097: dd_partition_system(_IO_FILE*, gmx::MDLogger const*, long, t_commerc const*, bool, int, t_state*, gmx_mtop_t const*, t_inputrec const*, t_state*, gmx::PaddedVector<gmx::BasicVector<float>, gmx::Allocator<gmx::BasicVector<float>>, gmx::AlignedAllocationPolicy>*, gmx::MDatoms*, gmx::MDlocaltop_t*, t_forcerc*, gmx::vstate_t*, gmx::Constraints*, t_nrn*, gmx::wallcycle*) (partition.cpp:3458)
==12805== by 0x527DF68: em_dd_partition_system(_IO_FILE*, gmx::MDLogger const&, int, t_commerc const*, gmx_mtop_t*, t_inputrec*, em_state_t*, gmx::MDlocaltop_t*, gmx::MDatoms*, t_forcerc*, gmx::vstate_t*, gmx::Constraints*, t_nrn*, gmx::wallcycle*) (minimize.cpp:738)
==12805== by 0x527F5AB: (anonymous namespace)::EnergyEvaluator::run(em_state_t*, float*, float (*) [3], float at (*) [3], long, bool) (minimize.cpp:860)
==12805== by 0x528D89F: gmx::Integrator::do_steep() (minimize.cpp:2525)
==12805== by 0x52A1C7B: gmx::mdrunner_start_fn(void*) (runner.cpp:219)
/usr/include/c++/9/bits/stl_vector.h:1009: std::vector<Tp, _Alloc>::reference std::vector<Tp, _Alloc>::operator[](std::vector<Tp, _Alloc>::size_type) [with _Tp = gmx_cgsort_t; _Alloc = std::allocator<gmx_cgsort_t>; std::vector<Tp, _Alloc>::reference = gmx_cgsort_t&; std::vector<Tp, _Alloc>::size_type = long unsigned int]: Assertion '_builtin_expect(__n < this->size(), true)' failed.

#45 - 02/05/2019 09:51 AM - Paul Bauer
Checking the different variables it looks like the issue is that sort->sorted[i] in line 2735 gets accessed with an invalid value for i because the previous check of i >= ncg_home_old gets optimized away

#46 - 02/05/2019 04:07 PM - Berk Hess
- Assignee set to Berk Hess

What system and setting did you use to trigger this?
I can't reproduce it. I added an assertion which should fail if your conclusion is correct:

diff --git a/src/gromacs/domdec/partition.cpp b/src/gromacs/domdec/partition.cpp
index 96ae04536..353a5686a 100644
--- a/src/gromacs/domdec/partition.cpp
+++ b/src/gromacs/domdec/partition.cpp
@@ -2712,6 +2712,9 @@ static void dd_sort_order(const gmx_domdec_t *dd,
     +GMX_RELEASE_ASSERT(sort->sorted.size() >= static_cast<size_t>(ncg_home_old),
             +"The sorting buffer should contain the old home charge group indices");
     +std::vector<gmx_cgsort_t, &stationary = sort->stationary;

02/21/2020
std::vector<gmx_cgsort_t> &moved = sort->moved;

#47 - 02/05/2019 04:19 PM - Paul Bauer
I was only able to trigger this from within the fedora rawhide docker container when running rpmbuild

#48 - 02/05/2019 04:21 PM - Berk Hess
Can you try with this assertion then?
To me this starts looking like a compiler bug. I would think the assertion would fail if there is an actual bug in my code.

#49 - 02/05/2019 04:33 PM - Paul Bauer
Just reset the container ;)
Need some time to set it up again, but I'll try it as soon as possible.

#50 - 02/06/2019 01:42 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2813.
Uploader: Berk Hess (hess@kth.se)
Change-Id: gromacs~release-2019~I7f13b46d7ff5352ce41838b813c46f2e90c93b1c
Gerrit URL: https://gerrit.gromacs.org/9097

#51 - 02/06/2019 01:42 PM - Berk Hess
- Status changed from Accepted to Fix uploaded

#52 - 02/06/2019 07:00 PM - Berk Hess
- Status changed from Fix uploaded to Resolved

Applied in changeset c5c3743d3a5dfe0d90f5940815e94a9e6cd332d6.

#53 - 02/06/2019 09:22 PM - Christoph Junghans
- File build.log.txt added

I patched c5c3743.diff into v2019, but it still fails, see attached build log.
But I am not sure if I am missing another patch here, so I will retest after the 2019.1 release.

#54 - 02/07/2019 06:37 AM - Paul Bauer
- Status changed from Resolved to Accepted

It is missing this one as well

Szilárd Páll wrote:

That's fixed, see dabd3bf9d

#55 - 02/07/2019 06:37 AM - Paul Bauer
- Status changed from Accepted to Resolved

#56 - 02/07/2019 08:26 PM - Christoph Junghans
Paul Bauer wrote:

It is missing this one as well

Yeah, let me rerun on top of 2019.1!

#57 - 02/08/2019 06:53 AM - Mark Abraham
- Status changed from Resolved to Feedback wanted

#58 - 02/14/2019 04:42 PM - Paul Bauer
should we bump this now or leave for fixing later?
Target version changed from 2019.1 to 2019.2  
Christoph will get us a new round of feedback after 2019.1

Fixed confirmed in 2019.1

Target version changed from 2019.2 to 2019.1

Status changed from Feedback wanted to Resolved

Status changed from Resolved to Closed

How do things look with 2019.1 please, Christoph?

Files

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<th>Date</th>
<th>Author</th>
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