GROMACS - Bug #2653

gmindist (GMX5.14, 2018 vesrions) crashes with segmentation fault

09/26/2018 11:11 AM - Stéphane Abel

Status:	Closed		
Priority:	Normal		
Assignee:			
Category:	analysis tools		
Target version:			
Affected version - extra info:	5.1.4	**Difficulty:**	uncategorized
Affected version:	2018		

Description

I report an issue with gmx mindist of gromacs (v 4.6.7, 5.1.4 and 2018+). The program crashes with the following command

echo 0 1 > Protein_AlkylChain.txt

- gmx_mpi mindist -f myXTC.xtc -s MYPDB.pdb -n Hydratation_Protein_OGNG.ndx -b 215000 -e 215000 -dt 4 -d 0.4 -respertime -printresname -group -od 3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_min_res.xvg -on 3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_Number.xvg < Protein_AlkylChain.txt

With GMX4.6.7 --> OK

With GMX5.1.4 (segmentation fault) ----------

Group 0 (Protein_HeavyAtoms) has 4976 elements
Group 1 (OGNG_AlkylChain) has 1530 elements
Group 2 (OGNG_Headgroup) has 2244 elements
Group 3 (OGNG_All_HeavyAtoms) has 3774 elements
Group 4 (Water_oxygen) has 60000 elements
Select a group: Select a group: ^MReading frame 0 time 0.000 ^MReading frame 0 time 200000.000
Back Off! I just backed up 3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_min_res.xvg to ./#3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_min_res.xvg.2#

Back Off! I just backed up 3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_Number.xvg to ./#3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_Number.xvg.2#
[irene1022:52095:0] Caught signal 11 (Segmentation fault) ==== backtrace ====
2 0x0000000000068d1c mxm_handle_error() /var/tmp/OFED_topdir/BUILD/mxm-3.6.3102/src/mxm/util/debug/debug.c:641
3 0x000000000006926c mxm_error_signal_handler() /var/tmp/OFED_topdir/BUILD/mxm-3.6.3102/src/mxm/util/debug/debug.c:616
4 0x0000000000035270 killpg() ??:0
5 0x00000000000471ad _IO_vfprintf_internal() :0
6 0x0000000000051827 __GI_fprintf() :0
7 0x00000000003b3cd8 xvgr_header() ??:0
8 0x00000000003b3c70 xvgropen_type() ??:0
9 0x0000000000545400 dist_plot.a() gmx_mindist.c:0
10 0x0000000000543990 gmx_mindist() ??:0
11 0x00000000001e1ff3 _ZN3gmx24Comman

With GMX2018 and 2018.2 (fatal error) ----------

Group 0 (Protein_HeavyAtoms) has 4976 elements
Group 1 (OGNG_AlkylChain) has 1530 elements
Group 2 (OGNG_Headgroup) has 2244 elements
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Group 4 (Water_oxygen) has 60000 elements
Select a group: Select a group: ^MReading frame 0 time 0.000 ^MReading frame 0 time 200000.000
Back Off! I just backed up 3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_min_res.xvg to ./#3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_min_res.xvg.1#

Back Off! I just backed up 3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_Number.xvg to ./#3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_Number.xvg.1#

Program: gmx mindist, version 2018
Source file: src/gromacs/fileio/gmxfio.cpp (line 345)

Fatal error:
Cannot open file with NULL filename string

For more information and tips for troubleshooting, please check the GROMACS
website at http://www.gromacs.org/Documentation/Errors

+ echo 0 2
+ echo 0 3
+ echo 0 4
+ exit 0

Please note that if I remove the "-group" and "-printresname" arguments all the tested version (except for 4.6.7) crashes.

I have included three files for the tests

MYXTC.xtc (1 snapshot 215ns)
MYNDX.ndx
MYPDB.pdb

Thank you

Associated revisions

Revision 034183c8 - 09/27/2018 04:37 PM - Paul Bauer

Add mindist output file check

gmx mindist would not check if the output file for an analysis options
was actually present, leading to cryptic error messages. Added the
corresponding check.

Fixes #2653

Change-Id: I26ccc7df37e5cc6a0276ecce50036aba452e0a45

History

#1 - 09/26/2018 12:22 PM - Stéphane Abel

- File MYNDX.ndx added

- File MYXTC.xtc added

- File MYPDB.pdb added

Below report two issues with the mindist analysis tool of gromacs (v 4.6.7, 5.1.4 and 2018+). The program crashes with the following command

gmx_mpi mindist -f myXTC.xtc -s MYPDB.pdb -n Hydratation_Protein_OGNG.ndx -b 200000 -e 215000 -dt 4 -d 0.4 -respertime -printresname -group -od 3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_min_res.xvg -on 3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_Number.xvg < Protein_AlkylChain.txt

With GMX4.6.7 --> OK

With GMX5.1.4 (segmentation fault) ----------

Group   0 (Protein_HeavyAtoms) has 4976 elements
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Group   3 (OGNG_All_HeavyAtoms) has 3774 elements
Group   4 (Water_oxygen) has 60000 elements
Select a group: Select a group: ^MReading frame   0 time   0.000   ^MReading frame   0 time 200000.000
Back Off! I just backed up 3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_min_res.xvg to ./#3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_min_res.xvg.2#

Back Off! I just backed up 3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_Number.xvg to ./#3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_Number.xvg.2#
[irene1022:52095:0] Caught signal 11 (Segmentation fault) ==== backtrace ====
2 0x0000000000068d1c mxm_handle_error() /var/tmp/OFED_topdir/BUILD/mxm-3.6.3102/src/mxm/util/debug/debug.c:641
3 0x000000000006926c mxm_error_signal_handler() /var/tmp/OFED_topdir/BUILD/mxm-3.6.3102/src/mxm/util/debug/debug.c:616

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11 0x00000000001e1ff3 _ZN3gmx24Comman

With GMX2018 and 2018.2 (fatal error) ----------

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Group   4 (Water_oxygen) has 60000 elements
Select a group: Select a group: ^MReading frame   0 time   0.000   ^MReading frame   0 time 200000.000
Back Off! I just backed up 3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_min_res.xvg to
./#3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_min_res.xvg.1#

Back Off! I just backed up 3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_Number.xvg to
./#3FHH_102OGNG_complex_CHARMM36_TIP3P_Protein_AlkylChain_Contact_Number.xvg.1#

Program: gmx mindist, version 2018
Source file: src/gromacs/fileio/gmxfio.cpp (line 345)

Fatal error:
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For more information and tips for troubleshooting, please check the GROMACS
website at http://www.gromacs.org/Documentation/Errors

+ echo 0 2
+ echo 0 3
+ echo 0 4
+ exit 0

Please note that if I remove the "-group" and "-printresname" arguments the program also crashes

And other possible bug in the tool is that you add -printresname, no output files contains the residue names (tested with GMX4.6.7)

Thank you

#2 - 09/27/2018 12:15 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2653.
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~release-2018~I26ccc7df37e5cc6a0276ecce50036aba452e0a45
Gerrit URL: https://gerrit.gromacs.org/8439

#3 - 09/27/2018 12:16 PM - Paul Bauer

Hello, the issue here is that mindist expects to get all the output files defined at least with the default filename.
I added a check that makes sure the program complains about missing the output file in this case.

#4 - 09/27/2018 06:15 PM - Paul Bauer

- Status changed from New to Resolved

Applied in changeset 034183c82d46d45981ef9543a77c80193b3f72ac.

#5 - 09/28/2018 01:34 PM - Stéphane Abel

Paul Bauer wrote:

> Applied in changeset 034183c82d46d45981ef9543a77c80193b3f72ac.

OK Paul by adding the missing file name (here with the -od with the "mindist.xvg") it works for all the gromacs versions I have. Thanks

#6 - 10/04/2018 10:59 AM - Paul Bauer

- Status changed from Resolved to Closed

Files

MYPDB.pdb	15 MB	09/26/2018	Stéphane Abel
MYXTC.xtc	715 KB	09/26/2018	Stéphane Abel
MYNDX.ndx	457 KB	09/26/2018	Stéphane Abel
MYNDX.ndx	457 KB	09/26/2018	Stéphane Abel
MYXTC.xtc	715 KB	09/26/2018	Stéphane Abel
MYPDB.pdb	15 MB	09/26/2018	Stéphane Abel