

GROMACS - Bug #2493

Command line file passing no longer works for gmxana tools

04/26/2018 06:44 PM - Joe Jordan

Status: Closed	
Priority: High	
Assignee:	
Category:	
Target version: 2019	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2019	

Description

The legacy gmx analysis tools no longer are able to read files passed from the command line such as trajectory or topology information. I am pretty sure this is the result of #7620 where `t_filenm` is changed from arrays of chars to `std::arrays`. As proof, I cite that this patch updated `gmx_sans` which is now broken, but left untouched `gmx_saxs` which still works. I have only tested about half of the `gmx_*` tools changed in patch #7620 but none of them worked so I suspect all are broken.

Associated revisions

Revision 249ed9e2 - 04/27/2018 05:45 PM - Paul Bauer

Fix file reading in gmx sans

Fixes #2493

Change-Id: Ia48008e476b1cf1a6d5e32a06103d16f92f18064

History

#1 - 04/27/2018 09:46 AM - Paul Bauer

so, I just tried running `trjconv` yesterday with master and it worked without any issues, so I'm not sure what is happening here. Can you provide an example that is broken, together with the git version you are using?
Thanks!

#2 - 04/27/2018 11:08 AM - Joe Jordan

- File `lysozyme-water.xtc` added
- File `lysozyme-water.tpr` added
- Priority changed from High to Low

Here are an `xtc/tpr` combo that I have been using for testing. It looks like I was premature last night in saying that several tools were not working, but `gmx sans` is indeed broken. I am wondering now why the many other tools in `gmxana` that use `t_filenm` were not also C++ified.

Command line:

```
gmx sans -f lysozyme-water.xtc -s lysozyme-water.tpr
```

```
-----  
Program: gmx sans, version 2019-dev-20180426-53b561f  
Source file: src/gromacs/commandline/cmdlineparser.cpp (line 276)  
Function: void gmx::CommandLineParser::parse(int*, char**)
```

```
Error in user input:  
Invalid command-line options  
Unknown command-line option -f  
Unknown command-line option -s
```

#3 - 04/27/2018 12:06 PM - Paul Bauer

- Priority changed from Low to High

Confirmed now. After discussing with Aleksei, the issue seems to be that the `asize` macro used to determine the number of files is not typesafe and is passed the pointer to `fnm` instead of the static array.

#4 - 04/27/2018 12:53 PM - Gerrit Code Review Bot

Gerrit received a related patchset '5' for Issue [#2493](#).
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~master~laa75b650a3af07c8ddf4b238d2cc3a9a5ddecaaa
Gerrit URL: <https://gerrit.gromacs.org/7803>

#5 - 04/27/2018 03:46 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2493](#).
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~master~la48008e476b1cf1a6d5e32a06103d16f92f18064
Gerrit URL: <https://gerrit.gromacs.org/7804>

#6 - 04/27/2018 06:00 PM - Paul Bauer

- Status changed from New to Resolved

Applied in changeset [249ed9e27f939f252f16e01476343ba7c7ba313d](#).

#7 - 04/30/2018 10:44 AM - Paul Bauer

- Status changed from Resolved to Closed

Files

lysozyme-water.xtc	25.6 KB	04/27/2018	Joe Jordan
lysozyme-water.tpr	202 KB	04/27/2018	Joe Jordan