GROMACS - Bug #1813

gmx dos

08/26/2015 12:10 AM - Marcelo Depolo Poleto

Status:	Closed		
Priority:	Normal		
Assignee:	David van der Spoel		
Category:	analysis tools		
Target version:			
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	5.0.6		

Description

gmx dos (version 5.0.6) yields in a fatal error, even though previous versions (5.0.1 and 5.0.4) can run the command line below.

@echo BEN | gmx dos -s ben.DOS.tpr -f ben.DOS.trr -g ben.log -dos dos.xvg -vacf vacf.xvg -mvacf mvacf.xvg

/home/marcelodepolo/Downloads/BACKUP-softwares/gromacs-5.0.6/src/gromacs/gmxana/gmx_dos.c, line: 93
Fatal error:Index contains atom numbers larger than the topology*
@

Looking into gmx_dos.c on 5.0.6 and 5.0.4 versions, I've found many modifications, but this insertion might be the issue:

(line 67 on 5.0.6v)

@static int calcMoleculesInIndexGroup(t_block *mols, int natoms, atom_id *index, int nindex) {
int i = 0;
int mol = 0;
int nMol = 0;
int j;

```
while (i < nindex)
    {
        while (index[i] > mols->index[mol])
        {
            mol++;
            if (mol >= mols->nr)
            {
                gmx_fatal(FARGS, "Atom index out of range: %d", index[i]+1);
            }
        }
        for (j = mols->index[mol]; j < mols->index[mol+1]; j++)
        {
            if (index[i] != j)
            {
                gmx_fatal(FARGS, "The index group does not consist of whole molecules");
            }
            i++;
            if (i == natoms)
            {
                gmx_fatal(FARGS, "Index contains atom numbers larger than the topology");
            }
        }
        nMol++;
    }
    return nMol;
}@
```

I would upload a trajectory, but it demands a .trr and it is quite large. Is there anything else I could provide for this case?

Associated revisions

Revision 2a1052e2 - 07/08/2016 03:39 PM - David van der Spoel

Introduce fatal error for too few frames in gmx dos.

To prevent gmx dos from crashing with an incomprehensible error
message when there are too few frames, test for this.

Part of #1813

Change-Id: Ie2f23d68cb3d4570944c4ade5ced49873dc98a29

History

#1 - 08/26/2015 12:13 AM - Justin Lemkul

A single frame of the .trr should suffice to reproduce it, in concert with the .tpr file.

#2 - 08/26/2015 12:21 AM - Marcelo Depolo Poleto

- File ben.DOS.tpr added

- File ben.DOS.trr added

Respective .trr and .tpr uploaded

#3 - 09/29/2015 04:16 PM - David van der Spoel

- Assignee set to David van der Spoel

#4 - 05/09/2016 02:05 PM - Marvin Bernhardt

This bug seems to be still around in 5.1.2.

I fixed it locally by putting the incrementor "i++;" behind the "if (i == natoms)" block. I am not entirely sure, but i think it belongs there.

#5 - 07/08/2016 02:14 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1813.
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-Id: Ie2f23d68cb3d4570944c4ade5ced49873dc98a29
Gerrit URL: https://gerrit.gromacs.org/6025

#6 - 07/08/2016 02:15 PM - David van der Spoel

The original bug was fixed already.

#7 - 07/08/2016 02:56 PM - Erik Lindahl

- Status changed from New to Fix uploaded

#8 - 07/08/2016 04:28 PM - David van der Spoel

- Status changed from Fix uploaded to Closed

Files

bad_run.txt	2.15 KB	08/25/2015	Marcelo Depolo Poleto
ben.DOS.trr	563 KB	08/25/2015	Marcelo Depolo Poleto
ben.DOS.tpr	286 KB	08/25/2015	Marcelo Depolo Poleto