I am having problems when running "gmx_order" utility. When I give the command -sl to divide the box into slices the utility works properly only for certain values and for others not.

If option -sl 200 is selected the error presents but if a greater number as 250 is put in, the utility runs without any problem.

Hope to find a solution in the meanwhile by myself.

Associated revisions
Revision 48d68b70 - 02/03/2017 10:42 PM - David van der Spoel
Fixes SEGV in gmx order.
gmx order used a cumbersome floating point method to compute an index in a histogram leading to index -1. The present code is simpler and robust, in fact the old code was likely wrong.
Fixes #2104
Change-Id: Ic3c15917eebe6c4964cd5cb053dfa4f05781cb73

History
#1 - 01/31/2017 04:06 PM - Mark Abraham
- Status changed from New to Accepted

I can reproduce this with release-5-1 HEAD with gmx -s nvt3mix.tpr -n order.ndx -sl 200 -f nvt3mix.trr. The indexing of slCount[slice] at line 650 goes out of bounds, specifically slice is -1 for the frame with time 19062.

My first thought was that’s because the trajectory doesn’t conform to whatever (undocumented) PBC preconditions this tool has, but actually line 649 looks problematic. slice must be negative for any sufficiently small z_ave. I don’t know whether the slices are intended to start at the box edge, or the box edge is the middle of the first slice, so I can’t suggest a fix.

For that frame:

```
Breakpoint 2, calc_order (fn=0x65cec0 "nvt3mix.trr", index=0x65cf70, a=0x6ce7b0, order=0x7ffffffffd0, s1Order =0x7ffffffffd0, s1Width=0x7ffffffffd0, nslices=200, bSliced=1, bUnsat=0, top=0x65af0, ePBC=0, ngrps=7, axis =2, permolecule=0, radial=0, distcalc=0, radfn=0x0, distvals=0x7ffffffffd0, oenv=0x65ce80) at /home/marklocal/git/r51/src/gromacs/gmxana/gmx_order.c:650
650 slCount[slice]++; /* determine slice, increase count */
```

Breakpoint 2, calc_order (fn=0x65cec0 "nvt3mix.trr", index=0x65cf70, a=0x6ce7b0, order=0x7ffffffffd0, s1Order =0x7ffffffffd0, s1Width=0x7ffffffffd0, nslices=200, bSliced=1, bUnsat=0, top=0x65af0, ePBC=0, ngrps=7, axis =2, permolecule=0, radial=0, distcalc=0, radfn=0x0, distvals=0x7ffffffffd0, oenv=0x65ce80) at /home/marklocal/git/r51/src/gromacs/gmxana/gmx_order.c:650
650 slCount[slice]++; /* determine slice, increase count */

(gdb) print slice
$1 = -1
(gdb) print t
$2 = 19062
(gdb) print axis
$3 = 2
(gdb) print box[axis][axis]
$4 = 20
(gdb) print z_ave
$5 = 0.0176316798
(gdb) print z1
$6 = 0.132036507
(gdb) print z2
$7 = -0.0967731476
(gdb) print *slWidth
$8 = 0.100000001

#2 - 01/31/2017 04:06 PM - Mark Abraham
- Subject changed from gmx_order deallocation to gmx_order -sl indexing out of bounds

#3 - 02/01/2017 08:12 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #2104.
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-Id: gromacs-release-5-1~lc3c15917eebe6c4964cd5cb053dfa4f05781cb73
Gerrit URL: https://gerrit.gromacs.org/6445

#4 - 02/03/2017 07:24 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #2104.
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-Id: gromacs~master~Ic3c15917eebe6c4964cd5cb053dfa4f05781cb73
Gerrit URL: https://gerrit.gromacs.org/6450

#5 - 02/06/2017 04:14 PM - Mark Abraham
- Status changed from Accepted to Resolved
- Target version set to 5.1.5

2016.2 will likely include this fix (via merge from release-5-1 branch)

#6 - 02/06/2017 11:35 PM - David van der Spoel
Applied in changeset 48d68b706614fd1dc5c432c0d570f00c7097fbdc.

#7 - 03/17/2017 05:58 PM - Mark Abraham
- Status changed from Resolved to Closed

Files

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