

GROMACS - Bug #2701

GMX Helix Segmentation Fault

10/17/2018 02:18 PM - Budheswar Dehury

Status: Closed	
Priority: High	
Assignee: Paul Bauer	
Category: analysis tools	
Target version: 2018.4	
Affected version - extra info: The same problem also lies with GROMACS 2018.2 version	Difficulty: hard
Affected version: 2016.4	
Description	
<p>Dear GROMACS Development Team,</p> <p>Hello everybody. I am doing analysis of helix properties using GMX helix command in Gromacs 2016.4 as well as in 2018.2. While running the command I have the following issue after executing the following command..</p> <pre>GROMACS: gmx helix, version 2016.4 Executable: /usr/bin/gmx Data prefix: /usr Working dir: /storage/home/local/bude-loc/Desktop/PS2/Seed1/TM1 Command line: gmx helix -f ../md1.xtc -s ../md.tpr -n index.ndx Reading file ../md.tpr, VERSION 2018.2 (single precision) Reading frame 0 time 490000.000 Please select a group containing the entire backbone Group 0 (System) has 201382 elements Group 1 (Protein) has 22327 elements Group 2 (Protein-H) has 11159 elements Group 3 (C-alpha) has 1414 elements Group 4 (Backbone) has 4242 elements Group 5 (MainChain) has 5651 elements Group 6 (MainChain+Cb) has 6978 elements Group 7 (MainChain+H) has 6986 elements Group 8 (SideChain) has 15341 elements Group 9 (SideChain-H) has 5508 elements Group 10 (Prot-Masses) has 22327 elements Group 11 (non-Protein) has 179055 elements Group 12 (Other) has 179055 elements Group 13 (POPC) has 40468 elements Group 14 (TIP3) has 138315 elements Group 15 (SOD) has 146 elements Group 16 (CLA) has 126 elements Group 17 (a_10635-11031) has 397 elements Select a group: 17 Selected 17: 'a_10635-11031' Checking group a_10635-11031 There are 25 residues There are 23 complete backbone residues (from 2 to 24) nall=397 Reading file ../md.tpr, VERSION 2018.2 (single precision) helix from: 8 through 23</pre> <p>The same problem also in case of 2018.2 . Though the other helix properties including gmx helixorient and gmx bundle works fine in both the versions...</p> <p>I have attached the last ns trajectory with 10 snapshots for your kind perusal and necessary input.</p> <p>Thanking You With Warm regards</p>	

Associated revisions

Revision 76c65770 - 10/18/2018 12:21 PM - Paul Bauer

Fix segmentation fault in gmx helix

Changed the logic in tpxio to only try to access the mtop datastructure if it is actually present.

Fixes #2701

Change-Id: I268af10dc125a57758f5f3e79e4b14a25050b3b3

Revision 93bea6f4 - 11/08/2018 07:22 PM - Paul Bauer

Actually fix gmx helix segmentation fault

The residue indexing in hxprops was wrong because the residue indices used for residue name lookup were wrong.

Added some documentation to clarify what this code does.

Fixes #2701

Change-Id: Ie6c002be6ff2139f6af27c7b891a180338ae5b20

History

#1 - 10/17/2018 02:49 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2701](#).

Uploader: Paul Bauer (paul.bauer.q@gmail.com)

Change-Id: gromacs~release-2018~I268af10dc125a57758f5f3e79e4b14a25050b3b3

Gerrit URL: <https://gerrit.gromacs.org/8566>

#2 - 10/23/2018 09:30 AM - Paul Bauer

- Status changed from New to Resolved

Applied in changeset [76c65770f8d31b0a9194311c5c0384d897fd0bae](#).

#3 - 10/29/2018 11:01 AM - Paul Bauer

- Status changed from Resolved to Closed

Fixed in 2018.

#4 - 10/31/2018 11:03 AM - Paul Bauer

- Status changed from Closed to Accepted

not fixed yet, there is a separate memory violation going on that was masked by the first, more obvious one.

#5 - 10/31/2018 04:34 PM - Gerrit Code Review Bot

Gerrit received a related patchset '2' for Issue [#2701](#).

Uploader: Paul Bauer (paul.bauer.q@gmail.com)

Change-Id: gromacs~release-2018~Ie6c002be6ff2139f6af27c7b891a180338ae5b20

Gerrit URL: <https://gerrit.gromacs.org/8633>

#6 - 11/08/2018 07:30 PM - Paul Bauer

- Status changed from Accepted to Resolved

Applied in changeset [93bea6f4ccc34e24c69647e77e560b9100a55831](#).

#7 - 11/28/2018 03:32 PM - Paul Bauer

- Status changed from Resolved to Closed

#8 - 11/28/2018 03:44 PM - Mark Abraham

- Target version set to 2018.4

Files

md.gro	13.3 MB	10/17/2018	Budheswar Dehury
index.ndx	5.2 MB	10/17/2018	Budheswar Dehury
md.tpr	11.3 MB	10/17/2018	Budheswar Dehury
md1.xtc	15.1 MB	10/17/2018	Budheswar Dehury