

GROMACS - Bug #2962

Segmentation fault, core dumped error

05/30/2019 05:09 AM - Neena Eappen

Status:	Closed	
Priority:	Normal	
Assignee:	Paul Bauer	
Category:	analysis tools	
Target version:	2019.3	
Affected version - extra info:		Difficulty: uncategorized
Affected version:	2018.4	

Description

I saw this error on using gmx hbond command (described in detailed in the attached file)

Associated revisions

Revision d886cc08 - 06/11/2019 09:20 AM - Paul Bauer

Add check for too many grid points in hbond

Fixes #2962

Change-Id: I61e80f8f254f1b5a0d968af087a87361fe4554ae

History

#1 - 06/02/2019 09:32 PM - Kevin Boyd

I looked into it, it looks like we're running out of memory. Your trr file box size is ~1000 nm, so I think something is wrong with your input files. Given that box size, the search grid has a size of ~13 billion elements.

Edit - confirmed this is the issue with Neena. We can close this, or add a check for excessive boxdims/gridding?

#2 - 06/03/2019 05:33 PM - Paul Bauer

- Status changed from New to Fix uploaded

- Assignee set to Paul Bauer

- Target version set to 2019.3

Uploaded a check for too many interactions.

#3 - 06/07/2019 06:22 PM - Mark Abraham

One would need a hierarchical grid to cope with such extremes of scale, like the multipole methods' octrees, which the implementation hasn't tried to do. So all we can do is give the clue that the box size to cutoff ratio is unsuitable

#4 - 06/11/2019 09:30 AM - Paul Bauer

- Status changed from Fix uploaded to Resolved

Applied in changeset [d886cc0820aa862f20aa4cb546d6de789f031b31](#).

#5 - 06/11/2019 12:02 PM - Paul Bauer

- Status changed from Resolved to Closed

Files

Segmentation fault error.docx	16.1 KB	05/30/2019	Neena Eappen
md_0_1.tpr	50.6 KB	05/30/2019	Neena Eappen
md_0_1.trr	3.09 MB	05/30/2019	Neena Eappen