

GROMACS - Bug #2508

gmx enemat segment faults

05/21/2018 05:43 PM - Mark Abraham

Status: Closed	
Priority: Low	
Assignee: Mark Abraham	
Category: analysis tools	
Target version: 2018.2	
Affected version - extra info:	Difficulty: simple
Affected version: 2016.3	
Description	
According to https://mailman-1.sys.kth.se/pipermail/gromacs.org_gmx-users/2018-May/120400.html it seems that gmx enemat is not robust to being supplied an energy file that does not have energygrps. It should give a graceful message that it can't do its job with such input.	

Associated revisions

Revision f76f70fb - 06/05/2018 02:32 PM - Mark Abraham

Fixed enemat when .edr had no matching energy groups

Removed some debug output that obscured both the code and the useful user-facing warnings.

Used a simpler bool construct to decide whether to issue the warning.

Fixes #2508

Change-Id: Ife56264991e365f8f5ca3b1285caea8033da7584

History

#1 - 05/21/2018 07:21 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2508](#).

Uploader: Mark Abraham (mark.j.abraham@gmail.com)

Change-Id: gromacs~release-2018~Ife56264991e365f8f5ca3b1285caea8033da7584

Gerrit URL: <https://gerrit.gromacs.org/7925>

#2 - 05/21/2018 07:22 PM - Mark Abraham

- Status changed from New to Fix uploaded

- Assignee set to Mark Abraham

- Target version set to 2018.2

More generally, it segfaulted whenever the .edr file does not have the energy groups that the user asked for.

#3 - 06/05/2018 02:45 PM - Mark Abraham

- Status changed from Fix uploaded to Resolved

Applied in changeset [f76f70fba009395839e2dae0dcd81db8865698dd](https://gerrit.gromacs.org/7925).

#4 - 06/05/2018 04:26 PM - Mark Abraham

- Status changed from Resolved to Closed