GROMACS - Bug #2918

mdrun segfaults with group scheme .tpr

04/04/2019 03:14 PM - Carsten Kutzner

Status: Closed
Priority: Normal
Assignee: Carsten Kutzner
Category: 
Target version: 2020-beta1
Affected version - extra info:
Affected version: git master

Difficulty: simple

Description
Due to a small glitch, commit ce17e81d93d7416c0e2d "Initial deactivation of group scheme" does not give a fatal error with group scheme .tpr files, but segfaults. The problem is in line 1631 of forcerec.cpp (init_forcerec): the condition "if (fr->cutoff_scheme ecutsGROUP)" can never be true at this point: ecutsGROUP is the second entry in the list of cutoff schemes and will thus be 1. Since fr has just been build using new t_forcerec before entering init_forcerec, its contents will be zero, including fr->cutoff_scheme.

A solution would be to use the condition "if (ir->cutoff_scheme ecutsGROUP)" instead.

A maybe better solution would be to move checking for the group scheme directly after .tpr file reading to runner.cpp:682.

Associated revisions
Revision 8080617f - 04/04/2019 05:27 PM - Carsten Kutzner
Early exit from mdrun if group scheme is detected in .tpr
Fixes #2918
Change-Id: I37566623c3ed4613f8b4e69f9f74882656772d1d

History
#1 - 04/04/2019 04:29 PM - Carsten Kutzner
- Assignee set to Carsten Kutzner

#2 - 04/04/2019 05:20 PM - Mark Abraham
- Status changed from New to Fix uploaded

#3 - 04/04/2019 05:20 PM - Mark Abraham
- Target version set to 2020-beta1

#4 - 04/04/2019 05:30 PM - Carsten Kutzner
- Status changed from Fix uploaded to Resolved

Applied in changeset 8080617f2cffc22223a3ed4613f8b4e69f9f74882656772d1d.

#5 - 04/05/2019 12:15 PM - Paul Bauer
- Status changed from Resolved to Closed