

GROMACS - Bug #2483

gmx dump writes mdp files that can not be parsed by grompp

04/18/2018 06:52 PM - Paul Bauer

Status:	New	
Priority:	Low	
Assignee:	Paul Bauer	
Category:	preprocessing (pdb2gmx,grompp)	
Target version:	future	
Affected version - extra info:	properly affecting a number of versions previously as well, but haven't checked this	Difficulty: uncategorized
Affected version:	2018.1	

Description

While checking some tpr files for an unrelated bug I found out that grompp is unable to process mdp files provided by gmx dump -om.
The issue seems to be with some (now unrecognised) fields being written to the file, as well as using the wrong name syntax for a number of options.

History

#1 - 04/19/2018 03:10 PM - Paul Bauer

From checking the code for readir and pr_inputrec it seems to be a conflict between the input bool values accepted ("yes" or "no", as defined by yesno_names), and what is written out as a result of the EBOOL macro (and the boolToString function) that is either "true" or "false".
One proposed fix would be to update the definitions for yesno_names, or refactor the variable reading to use the boolFromString function instead.

#2 - 05/25/2018 01:55 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2483](#).
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~master~18e0540c415eceddf43db1a243509f8a4c22b50b
Gerrit URL: <https://gerrit.gromacs.org/7949>

#3 - 05/25/2018 02:43 PM - Mark Abraham

If we want this to continue to work, then we need e.g. an integration test case that shows that grompp then dump produces a valid input to grompp.

#4 - 10/07/2018 01:20 PM - Mark Abraham

- Target version set to 2019

Can we fix this before the final release?

#5 - 10/08/2018 10:50 AM - Paul Bauer

- Target version changed from 2019 to future

I don't think so. The issue was that the writing needs info about the group names being used, and I couldn't find any reasonable way to get the information into the write method. Also, it looks like the group names are not stored properly in the symtab (as far as my offline work for modifying this has shown).