

GROMACS - Bug #1893

grompp fails to warn about .mdp values with the wrong type

01/27/2016 03:16 PM - Mark Abraham

Status: Closed	
Priority: Normal	
Assignee: Mark Abraham	
Category: preprocessing (pdb2gmx,grompp)	
Target version: 5.1.2	
Affected version - extra info: at least 5 and 5.1	Difficulty: uncategorized
Affected version: 5.0	
Description For example, init_lambda_values = 0.35 is silently interpreted as 0.	
Related issues: Related to GROMACS - Feature #1026: request for gen_vel to work with multiple... New	

Associated revisions

Revision 937fd932 - 01/27/2016 10:54 PM - Mark Abraham

Make sc-power an integer like it needs to be

This means it can pass the new check.

Refs #1893

Change-Id: I652f383e5914a6475e1640ec8842b7b6cfc8f1d3

Revision d0071abf - 02/03/2016 01:41 PM - Mark Abraham

Fix grompp not warning when .mdp values have wrong types

With old code, e.g. init_lambda_state = 0.35 was silently interpreted as 0.

Added some comments and TODOs.

Added unit tests for some simple parts of the the functionality that needed to be fixed. Extended the interface of warninp_t to permit sound testing.

Fixes #1893

Change-Id: I425798daa8ed3a391cde49ba4a2d3d352d682f8f

Revision fe436f74 - 02/02/2017 10:35 PM - Mark Abraham

Clarify use of tau-p and pcoupltype

grompp used to permit "tau-p = 5 5" which is misleading. The recent fix for #1893 leads to the user receiving a grompp warning, so this improves the docs to make clear that pressure coupling is not implemented like temperature coupling (where different time constants might be used).

Refs #1893

Change-Id: I8328b30a12689795c7af2d12dfc94db11b78a03a

History

#1 - 01/27/2016 03:22 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1893](#).
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I425798daa8ed3a391cde49ba4a2d3d352d682f8f
Gerrit URL: <https://gerrit.gromacs.org/5588>

#2 - 01/27/2016 10:54 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#1893](#).
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I652f383e5914a6475e1640ec8842b7b6cfc8f1d3
Gerrit URL: <https://gerrit.gromacs.org/5590>

#3 - 02/03/2016 01:45 PM - Mark Abraham

- Status changed from New to Resolved

Applied in changeset [d0071abfbcbdc0a14c184707acf09737f4c4c832](#).

#4 - 02/03/2016 01:50 PM - Mark Abraham

- Status changed from Resolved to Closed

#5 - 02/05/2016 06:57 PM - Gerrit Code Review Bot

Gerrit received a related patchset '2' for Issue [#1893](#).
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I8328b30a12689795c7af2d12dfc94db11b78a03a
Gerrit URL: <https://gerrit.gromacs.org/5618>

#6 - 11/17/2016 04:38 PM - Mark Abraham

- Related to Feature #1026: request for *gen_vel* to work with multiple temperature coupling groups at different temperatures added

#7 - 02/02/2017 10:35 PM - Gerrit Code Review Bot

Gerrit received a related patchset '3' for Issue [#1893](#).
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-Id: gromacs~release-5-1~I8328b30a12689795c7af2d12dfc94db11b78a03a
Gerrit URL: <https://gerrit.gromacs.org/5618>