

GROMACS - Bug #2489

Handle mdp-option case "awh-nsamples-update = 0"

04/25/2018 02:34 PM - Viveca Lindahl

Status: Closed	
Priority: Low	
Assignee: Viveca Lindahl	
Category: preprocessing (pdb2gmx,grompp)	
Target version: 2018.2	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2018.1	
Description Setting "awh-nsamples-update = 0" is accepted by grompp but leads to a floating point exception because the variable is later (in mdrun) used in a modulo operator.	

Associated revisions

Revision cb1ac9a9 - 06/06/2018 12:51 PM - Viveca Lindahl

Make sure that the value of awh-nsamples-update is allowed

Previously, awh-nsamples-update could be set to zero, leading to division by zero. Now it results in a fatal error.

Fixes #2489

Change-Id: I65aae5d5c533b9aab7ea9aae3e317e92a926c18c

History

#1 - 04/25/2018 04:04 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2489](#).
Uploader: Viveca Lindahl (vivecalindahl@gmail.com)
Change-Id: gromacs~master~I23dbc80992e130a28af413754d12f8fd167e7bde
Gerrit URL: <https://gerrit.gromacs.org/7794>

#2 - 06/05/2018 10:55 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2489](#).
Uploader: Viveca Lindahl (vivecalindahl@gmail.com)
Change-Id: gromacs~release-2018~I65aae5d5c533b9aab7ea9aae3e317e92a926c18c
Gerrit URL: <https://gerrit.gromacs.org/7980>

#3 - 06/05/2018 11:03 PM - Viveca Lindahl

- Status changed from New to Fix uploaded

#4 - 06/06/2018 01:00 PM - Anonymous

- Status changed from Fix uploaded to Resolved

Applied in changeset [cb1ac9a98d49468dc3019882dfc279281ce82ca5](#).

#5 - 06/07/2018 01:50 AM - Mark Abraham

- Status changed from Resolved to Closed