GROMACS - Bug #2058

GROMACS does not honor when GMX_MAXCONSTRWARN is set to -1

10/11/2016 03:20 PM - James Barnett

Status: Closed
Priority: Normal
Assignee: 
Category: mdrun
Target version: 2016.1
Affected version:

Difficulty: uncategorized

Description

Only one SETTLE error is enough to cause the program to halt when GMX_MAXCONSTRWARN is set to -1. There is no check that I can find that checks if maxwarn is -1. I will add a patch.

Associated revisions

Revision 5844c8b0 - 10/12/2016 10:03 PM - James Barnett
Set maxwarn to INT_MAX if GMX_MAXCONSTRWARN < 0

maxwarn is set to the value of the environmental variable GMX_MAXCONSTRWARN, and we tell users to set that variable to -1 to have no maximum. This condition was not being checked, so when set to -1 just 1 SETTLE warning was enough to halt the program. This commit fixes that behavior by setting maxwarn to INT_MAX if GMX_MAXCONSTRWARN is -1 (or any other negative number).

Fixes #2058.

Change-Id: Ie6e2cb57f8402dd9a327f72f7fad36db19b8bb68

History

#1 - 10/11/2016 03:25 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2058.
Uploader: James "Wes" Barnett (<jbarnet4@tulane.edu>)
Change-Id: Ie6e2cb57f8402dd9a327f72f7fad36db19b8bb68
Gerrit URL: https://gerrit.gromacs.org/6254

#2 - 10/13/2016 12:26 PM - Berk Hess
- Category set to mdrun
- Status changed from New to Resolved
- Target version set to 2016.1

#3 - 10/13/2016 11:43 PM - James Barnett
Applied in changeset 5844c8b02f2abf8adc9887f7fad36db19b8bb68

#4 - 10/19/2016 02:08 PM - Szilárd Páll
- Status changed from Resolved to Closed