GROMACS - Bug #1690

Lack of reproducibility with 5.04 even when run on one thread, same machine, etc.

02/16/2015 07:31 PM - Michael Shirts

Status: Closed
Priority: Low
Assignee: mdrun
Category: mdrun
Target version: 
Affected version - 
extra info: 
Affected version: 5.0.4

Description
Command run with is:

$MDRUN -nt 1 -s runone.save2.tpr -reprod -deffnm runone -cpt 1000 -dhdl runone.dhdl.xvg

Crash sometimes occurs after 980 steps, but sometimes after 3000 steps, sometimes later, once after 740 steps, once went to 5000 steps w/o crashing

Haven't tested double precision yet; this was in single precision.

Associated revisions
Revision 52e33110 - 06/20/2015 07:57 PM - Erik Lindahl
Fix reproducibility bug in fft5d

fft5d has been accessing FFTW directly instead of using the Gromacs FFT interface, and while doing so the estimate flag was not correctly set for reproducible runs. For now we have just fixed it, but this FFTW-specific code should be removed from fft5d, or we will likely see more fft bugs due to duplicated code paths.

Fixes #1690.

Change-Id: Ib03f7af710ed208d2824f105bd15712d32632cfa

History
#1 - 06/16/2015 11:39 PM - Erik Lindahl
- Status changed from New to Feedback wanted

Please provide all input files so we can debug by altering settings!

#2 - 06/19/2015 12:19 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1690.
Uploader: Erik Lindahl (erik.lindahl@gmail.com)
Change-Id: lb03f7af710ed208d2824f105bd15712d32632cfa
Gerrit URL: https://gerrit.gromacs.org/4748

#3 - 06/19/2015 12:21 PM - Erik Lindahl
- Status changed from Feedback wanted to Fix uploaded

Fixed. fft5d has been doing monkey business by reimplementing its own FFTW interface, and in doing so it did not set flags correctly.

#4 - 06/22/2015 12:35 PM - Rossen Apostolov
- Status changed from Fix uploaded to Closed

Files
runone.save2.tpr 215 KB 02/16/2015 Michael Shirts