GROMACS - Bug #1740
invalid use of gmx_simd_check_and_reset_overflow

05/19/2015 09:10 PM - Mark Abraham

Status: Closed
Priority: Normal
Assignee: Mark Abraham
Category: mdrun
Target version: 5.0.6
Affected version: 5.0.5
Difficulty: uncategorized

Description
I try to compile GROMACS 5.0.5 on Fujitsu PRIMEHPC FX-10 with the command
from installation instruction page
http://www.gromacs.org/Documentation/Installation_Instructions_5.0#linear-algebra-libraries
I use the Fujitsu compiler with the custom build toolchain as suggestion from the GROMACS webpage.
The command is:

>> ~/software/cmake/bin/cmake ../
-DCMAKE_INSTALL_PREFIX=/home/k0055/k005503/software/gromacs -DGMX_MPI=ON
-DCMAKE_TOOLCHAIN_FILE=../cmake/Platform/Toolchain-Fujitsu-Sparc64-mpi.cmake
-DCMAKE_PREFIX_PATH=/usr/local/fftw/3.3 -DGMX_BUILD_MDRUN_ONLY=ON
-DCMAKE_RELAXED_DOUBLE_PRECISION=ON

But unfortunately, I got this message after running make.

../../../../lib/libgromacs_mdrun_mpi_d.a(tpi.c.o): In function `do_tpi':
tpi.c:(.text+0x2130): undefined reference to `gmx_simd_check_and_reset_overflow'
made[2]: *** [bin/mdrun_mpi_d] Error 1
made[1]: *** [src/programs/CMakeFiles/mdrun.dir/all] Error 2
made: *** [all] Error 2

Associated revisions
Revision 47b12697 - 05/23/2015 11:36 PM - Mark Abraham
Fix misuse of gmx_simd_check_and_reset_overflow
Only x86 has useful definitions of this function. The check will be entirely removed in master branch.
Fixes #1740
Change-Id: Ida1bc43201f44dffbd64d94bc485d4d882167b

Revision 8e46784a - 06/05/2015 07:46 PM - Mark Abraham
Remove gmx_simd_check_and_reset_overflow
We think this can only be implemented on x86, was only used for TPI, and protected against an issue Berk can't reproduce. Thus best removed.
Refs #1740
Change-Id: la8ca50b67683dab5a0e5e4a8b8485946edld922a

History
#1 - 05/19/2015 09:17 PM - Gerrit Code Review Bot
Gerrit received a related patchset '2' for Issue #1740
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: Ida1bc4320144dfffbd64d94bc485d4d6d882167b
Gerrit URL: https://gerrit.gromacs.org/4624

#2 - 05/19/2015 09:18 PM - Mark Abraham
- Status changed from New to Fix uploaded

#3 - 05/19/2015 09:23 PM - Mark Abraham
- Description updated

#4 - 06/04/2015 01:56 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1740
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: Ia8ca50b67f83dab5a0e5e4a8b8485946edfd922a
Gerrit URL: https://gerrit.gromacs.org/4690

#5 - 06/04/2015 02:00 PM - Mark Abraham
- Status changed from Fix uploaded to Closed