Gromacs - Task #1263

Test Gromacs with X32 ABI

05/23/2013 09:18 PM - Roland Schulz

Status: Closed
Priority: Low
Assignee: Erik Lindahl
Category: mdrun
Target version: 5.0

Description
Given that we never need more than 4GB, X32 ABI (http://en.wikipedia.org/wiki/X32_ABI) shouldn't have any disadvantage and it could give us very slightly better performance. So it might be worth testing it.

Associated revisions
Revision 72e3e8f5 - 06/25/2014 07:26 PM - Erik Lindahl

Make source compile under Linux X32 ABI

The X32 ABI uses 32-bit pointers in combination with all other features of x86-64 to save memory. This requires two minor changes to x86 inline assembly macro checks, where we need check for LP64 (64-bit pointers) rather than x86_64 (which is set for X32). The resulting binaries run approximately 2% faster, but since it requires all dependent libraries to be available in X32 format it is not something we will enable with a simple setting for now.
To use it manually, set CFLAGS and CXXFLAGS to "-O3 -mx32".

Fixes #1263.

Change-Id: I2555b2c68d4bba24f4e581268c472a47e7d1531

History
#1 - 05/29/2013 02:30 PM - Berk Hess
- Status changed from New to Accepted

It seems floating point performance is nearly unaffected and we avoid pointer operations as much as possible in Gromacs, so I expect very little gain. But if it's easy to try, we should. On OpenSuse x32 libraries are not readily available. But for Ubuntu the situation seems to be better:
http://www.phoronix.com/scan.php?page=news_item&px=MTM1OTA

#2 - 05/30/2013 11:22 AM - Mark Abraham

If there was a benefit, it seems like we'd just need to detect it exists and is supported by the tool chain, and give the right GCC flag, yes?

#3 - 07/14/2013 11:04 PM - Alexey Shvetsov

Seems like easiest way to test it is to run a minimal x32 system in LXC container (e.g. gentoo or may be debian build)
#4 - 06/23/2014 09:35 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1263.
Uploader: Erik Lindahl (erik@kth.se)
Change-id: i2555b2c68d4bb24f4e581268c472a47e7d1531
Gerrit URL: https://gerrit.gromacs.org/3668

#5 - 06/23/2014 09:35 PM - Erik Lindahl
- Status changed from Accepted to Fix uploaded

#6 - 06/26/2014 10:14 PM - Erik Lindahl
- Status changed from Fix uploaded to Resolved

#7 - 06/26/2014 10:14 PM - Erik Lindahl
- Status changed from Resolved to Closed

#8 - 07/15/2014 11:57 AM - Teemu Murtola
- Assignee changed from Berk Hess to Erik Lindahl
- Target version set to 5.0