

GROMACS - Bug #195

MDRUN segfaults on Intel64 platform due to using wrong data type in MKL FFT

05/14/2008 12:17 PM - Hirokazu Kobayashi

Status: Closed	
Priority: Normal	
Assignee: Erik Lindahl	
Category: mdrun	
Target version: 3.3.1	
Affected version - extra info:	Difficulty: uncategorized
Affected version:	
Description	
<p>I faced segfault in MDRUN on Intel64 platform with MKL FFT. I think why it crashes is MKL FFT expects "long" as some arguments while Gromacs passes "int" as arguments. On 32bit Linux machine, Both "int" and "long" are 32bit and it will run without problem. But 64bit Linux machine often defines "int" as 32bit while "long" as 64bit.</p> <p>I fixed gmx_fft_mkl.c file and attached it. I tested this fix with MKL 9.0 and MKL 10.0. MKL10.0 defines "MKL_LONG" datatype in include file to support ILP64 mode of MKL. In ILP64 mode MKL_LONG is defined as 64bit int. In LP64 mode (MKL default) it is defined as long. In MKL 9.0 or lower version, "MKL_LONG" is not defined. So I defined MKL_LONG as long in gms_fft_mkl.c if MKL_LONG is not defined.</p> <p>The file may violate coding rule of Gromacs, So it need to be reviewed and to be rewritten.</p> <p>Thanks. --- Kobayashi</p>	
Related issues:	
Has duplicate GROMACS - Bug #174: MDRUN segfaults on an AMD64 system using In...	Closed 10/26/2007

Associated revisions

Revision db48b317 - 10/08/2008 01:52 AM - Erik Lindahl

Bugfix from bugzilla #195: Intel MKL is sensitive to long being 64 bits on some x86 platforms.

History

#1 - 05/14/2008 12:20 PM - Hirokazu Kobayashi

Created an attachment (id=279)
fixed wrong datatype

#3 - 10/08/2008 01:51 AM - Erik Lindahl

Committed to the release branch.

Files

gmx_fft_mkl.c	34 KB	05/14/2008	Hirokazu Kobayashi
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