GROMACS - Bug #1186

install guide should mention how to configure blas and lapack

03/11/2013 02:16 PM - Mark Abraham

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
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<tr>
<td>Assignee:</td>
<td>Mark Abraham</td>
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<tr>
<td>Category:</td>
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<tr>
<td>Target version:</td>
<td>4.6.2</td>
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<td>Difficulty:</td>
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<td>Affected version - extra info:</td>
<td>4.6.1</td>
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Description

Related issues:
- Related to GROMACS - Bug #771: cmake overwrites BLAS_LIBRARIES and LAPACK_LIB... Closed 07/05/2011
- Related to GROMACS - Bug #1110: GMX_FFT_LIBRARY=mkl does not work Closed 01/09/2013
- Related to GROMACS - Bug #1067: ICC links against FFTW-MKL wrapper instead of... Closed 12/11/2012

Associated revisions

Revision 2f5dcb06 - 03/11/2013 03:46 PM - Mark Abraham
Added install guide section for BLAS/LAPACK
Fixes #1186
Change-Id: If9e95f93cd216b86143685fd0ae9fbc5d26792e

Revision 28d2a6d1 - 04/26/2013 08:37 AM - Mark Abraham
Update linking to MKL and document same
Works using nifty feature from icc 11 and up, or any other compiler if the user does the legwork (which is all we ever used to offer).
Code that used HAVE_LIBMKL had a bug, which we never saw because the top-level CMakeLists.txt set HAVE_MKL. Fixed that.
Removed unused TextMKL.c code - check_function_exists() is sufficient.
Refs #1110,#1186
Change-Id: l39a66673e5fe571a5f8b0691bbe2ec619cd60778

Revision 1fd10dcd - 06/13/2013 09:45 AM - Mark Abraham
Added install guide section for BLAS/LAPACK
Fixes #1186
Change-Id: l9f9f93cd216b86143685fd0ae9fbc5d26792e

Revision 99fd3d66 - 07/25/2013 01:40 PM - Mark Abraham
Update management of linear algebra libraries
Management of detection and/or linking to BLAS and LAPACK libraries is re-organized. The code has migrated to its own module. This will help future extension and maintenance. This version communicates things that are newsworthy and stays out of the way when nothing is changing.
We no longer over-write the values specified by the user for GMX_EXTERNAL_(BLAS|LAPACK). Previously, this was used to signal
whether detection succeeded, but that does not really get the job done. Instead, the user is notified that detection failed (repeatedly, if they deliberately set such an option on).

Correct usage and expected behaviour in all cases is documented both in the code and the install guide.

The user interface is pretty much unchanged. We still don't offer full configurability (e.g. MKL for FFTs must use MKL for linear algebra unless GMX_\_*_USER is used, and the only way to get MKL for linear algebra is to use it for FFTs). The size of any performance difference is probably very small, and if the user really needs mdrun with certain FFT and tools with certain linear algebra library, they can do two configurations. Note that mdrun never calls any linear algebra routines (tested empirically)!

Expanded the solution of #771 by testing that the user supplied libraries that actually work. If not, we emit a warning and try to use them anyway.

We also now check that MKL really does provide linear algebra routines, and fall back to the default treatment if it does not.

Refs #771,#1186

Change-Id: Ife5c59694e29a3ce73fc55975e26f6c083317d9b

History

#1 - 04/19/2013 06:37 PM - Mark Abraham
- Status changed from New to Accepted
- Affected version set to 4.6.1

#2 - 04/19/2013 06:38 PM - Mark Abraham
- Status changed from Accepted to In Progress

#3 - 05/24/2013 07:49 PM - Mark Abraham
- Status changed from In Progress to Resolved
- Target version set to 4.6.2

#4 - 05/31/2013 10:44 AM - Mark Abraham
- Status changed from Resolved to Closed