Gromacs - Bug #771

cmake overwrites BLAS_LIBRARIES and LAPACK_LIBRARIES

07/05/2011 09:56 AM - Christoph Junghans

Status: Closed
Priority: Normal
Assignee: Rossen Apostolov
Category: build system
Target version: 4.5.5

Affected version - extra info:

Description
If the blas / lapack libraries have funny names, like lapack on AIX (lapack-essl_O3_qstrict), cmake will not find them. Setting them by hand in the common way (LAPACK_LIBRARIES) does not work as LAPACK_LIBRARIES gets overwritten in FindLAPACK.cmake (line 132).

The same problem with FindBLAS.cmake

My first try for a workaround was something like -DBLA_VENDOR=Generic -DBLAS_blas_LIBRARIES="path/to/libsomeblas.so", which is a bit clumsy.

Related issues:
Related to Gromacs - Bug #1186: install guide should mention how to configure...

Closing date: 03/11/2013

Associated revisions

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

11/19/2015 1/3
The Find*.cmake modules in the latest cmake 2.8.5 still don't have support for AIX. I found something here: http://code.google.com/p/hpccodelets/source/browse/trunk/CMake/addNumerics.cmake?spec=svn1&r=1. But this probably won't solve your problem.

A better solution would be to change CMakeLists.txt like

```cmake
... find_package(BLAS REQUIRED) list(APPEND GMX_EXTRA_LIBRARIES ${BLAS_LIBRARIES}) endif(GMX_EXTERNAL_BLAS)

to
... find_package(BLAS REQUIRED) if(BLAS_FOUND) list(APPEND GMX_EXTRA_LIBRARIES ${BLAS_LIBRARIES}) else(BLAS_FOUND) list(APPEND GMX_EXTRA_LIBRARIES ${GMX_BLAS_USER}) endif(BLAS_FOUND) endif(GMX_EXTERNAL_BLAS)

where GMX_BLAS_USER would be a new CMake variable

And same for LAPACK.

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#2 - 09/01/2011 09:53 AM - Christoph Junghans

I would prefer

```cmake
if (GMX_BLAS_USER)
    list(APPEND GMX_EXTRA_LIBRARIES ${GMX_BLAS_USER})
else(GMX_BLAS_USER)
    find_package(BLAS REQUIRED)
    list(APPEND GMX_EXTRA_LIBRARIES ${BLAS_LIBRARIES})
endif (GMX_BLAS_USER)
```

as it gives GMX_BLAS_USER priority over BLAS_LIBRARIES.
Right, that's better. I'm gonna make a patch for that.

I pushed a patch, gerrit ID I4ca1c4ca, but then I saw that Mark has applied a fix to FindLAPACK.cmake, ID I6fefed83 but those don't conflict.

Christoph, can you check whether my patch works on AIX?

Christoph confirmed for Change-Id: I4ca1c4ca365788fcafc4219934fdfe8758db84f1 that it works, so closing. Thanks!