

## GROMACS - Bug #771

### cmake overwrites BLAS\_LIBRARIES and LAPACK\_LIBRARIES

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

<b>Status:</b> Closed	
<b>Priority:</b> Normal	
<b>Assignee:</b> Rossen Apostolov	
<b>Category:</b> build system	
<b>Target version:</b> 4.5.5	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b>	
<b>Description</b>	
<p>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).</p> <p>The same problem with FindBLAS.cmake</p> <p>My first try for a workaround was something like -DBLA_VENDOR=Generic -DBLAS_blas_LIBRARIES="path/to/libsomeblas.so", which is a bit clumsy.</p>	
<b>Related issues:</b>	
Related to GROMACS - Bug #1186: install guide should mention how to configure...	<b>Closed</b> <b>03/11/2013</b>

#### 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

## History

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### #1 - 08/31/2011 09:53 PM - Rossen Apostolov

- Assignee changed from Sander Pronk to Rossen Apostolov

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

```
...
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.

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

I would prefer

```
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.

### #3 - 09/01/2011 02:26 PM - Rossen Apostolov

Right, that's better. I'm gonna make a patch for that.

### #4 - 09/09/2011 04:38 PM - Rossen Apostolov

I pushed a patch, Gerrit ID I4ca1c4ca, but then I saw that Mark has applied a fix to FindLAPACK.cmake, ID I6fefd83 but those don't conflict.

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

### #5 - 09/12/2011 01:29 PM - Rossen Apostolov

- Status changed from New to In Progress

### #6 - 09/12/2011 02:03 PM - Rossen Apostolov

- Status changed from In Progress to Closed

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