### Gromacs - Feature #911

**implement CMake option to enable fully static binaries**

04/03/2012 03:22 PM - Sziárd Páll

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<thead>
<tr>
<th>Status</th>
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<tr>
<td>Priority</td>
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<tr>
<td>Assignee</td>
<td>Sziárd Páll</td>
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**Description**

On some systems like Cray statically linked binaries are either a must or highly recommended. Below are the steps required to get static linking to work; the method is not foolproof, it can fail in some cases (e.g. if some external libraries get shared version detected). We should attempt to automate this as much as possible.

- set the target properties `LINK_SEARCH_START_STATIC` and `LINK_SEARCH_END_STATIC`, e.g:

  ```
  set_target_properties(mdrun PROPERTIES LINK_SEARCH_START_STATIC ON)
  set_target_properties(mdrun PROPERTIES LINK_SEARCH_END_STATIC ON)
  ```

- configure with `-static` and disable CMake `RPATH`:

  ```
  cmake /path/to/gromacs/source -DCMAKE_PREFIX_PATH=/path/to/fftw -DGMX_PREFER_STATIC_LIBS=ON
  -DCMAKE_C_FLAGS=-static -DCMAKE_CXX_FLAGS=-static -DCMAKE_SKIP_RPATH=YES
  ```

**Related issues:**

Related to Gromacs - Feature #1641: Add toolchain file for Cray systems  
New  
11/11/2014

**Associated revisions**

**Revision 88fda475 - 05/13/2015 10:45 AM - Roland Schulz**

Facilitate linking of static binaries

Minimal solution. The user has to manually set both
- `DBUILD_SHARED_EXE=no` and `CFLAGS=CXXFLAGS=static`, perhaps manage their own toolchain, and certainly make static libraries available for all dependencies. Also does not auto-detect if compiler defaults to static (Cray). Works better than `LINK_SEARCH_END_STATIC` because otherwise dynamic flags can be added to the middle if some libraries in default search path exist as both dynamic and shared.

Fixes #911  
Related to #1641

Change-Id: If7b8192b44c33c861f126e3422df04388d2f2be5

**History**

#1 - 04/03/2012 03:22 PM - Sziárd Páll

- Assignee deleted (Rossen Apostolov)
#2 - 08/04/2012 08:33 PM - Roland Schulz

For GMX_PREFER_STATIC_LIBS we use

```
SET(CMAKE_FIND_LIBRARY_SUFFIXES .a ${CMAKE_FIND_LIBRARY_SUFFIXES})
```

Any reason not to use

```
SET(CMAKE_FIND_LIBRARY_SUFFIXES .a)
```

for fully static libraries?

LINK_SEARCH_END_STATIC is only available starting with cmake 2.8.5. In what cases are LINK_SEARCH_START_STATIC/LINK_SEARCH_END_STATIC needed? For me it always worked without. I thought that giving "-static" automatically makes it work.

While the rpath is not necessary for static binaries I don't think it hurts. Again it just works for me.

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#3 - 10/08/2012 03:07 PM - Szilárd Páll

Roland Schulz wrote:

```
For GMX_PREFER_STATIC_LIBS we use
[...]
Any reason not to use
[...]
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Hmm, I didn't want to just override the content of CMAKE_FIND_LIBRARY_SUFFIXES. Would that be always safe?

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Those are needed to link system libraries statically:


Now, what I'm not sure about anymore whether both are always needed or it's better to set both because in some cases the former, in other cases the latter is needed.

While the rpath is not necessary for static binaries I don't think it hurts. Again it just works for me.

Not sure about the exact source of the idea of disabling RPATH, but as far as I remember it was recommended on the CMake mailing list.
Szilárd Pál wrote:

Roland Schulz wrote:

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That means it is not a proper solution if we want it to work with 2.8.0. Also there are other problems:

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I guess it doesn't hurt since it is obviously not needed.
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Yeah, that looks familiar, it's my thread after all :) I have not seen the -lgcc_s errors for a year or so.

Anyway, my point was not to implement a rock-solid feature because that's simply not possible (the build will fail if not all external dependencies are detected as static archives), but to make a fair attempt to build a fully static mdrun (perhaps tools as well) and control it through an advanced variable.

And my question was whether this is useful or not. For me and a handful of other working on quirky Crays it would be useful to not have to patch CMake sources before compiling static binaries.

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Not sure about the exact source of the idea of disabling RPATH, but as far as I remember it was recommended on the CMake mailing list.

I guess it doesn't hurt since it is obviously not needed.
#6 - 10/09/2012 12:25 AM - Roland Schulz

Yeah, that looks familiar, it's my thread after all :) I have not seen the -lgcc_s errors for a year or so.

Didn't see that :-(

And my question was whether this is useful or not. For me and a handful of other working on quirky Crays it would be useful to not have to patch CMake sources before compiling static binaries.

I'm surprised you need to do anything special on Cray. All the Cray I have access to automatically add the "-static" in the "cc" compiler wrapper and it just works for me.

#7 - 10/09/2012 12:30 AM - Szilárd Páll

And my question was whether this is useful or not. For me and a handful of other working on quirky Crays it would be useful to not have to patch CMake sources before compiling static binaries.

I'm surprised you need to do anything special on Cray. All the Cray I have access to automatically add the "-static" in the "cc" compiler wrapper and it just works for me.

Newer Crays don't, in particular on an XK6 (where it would even be impossible due to CUDA not being distributed statically) and both XE6 machines I have access to. I guess I'll have to ask the question differently: do you have anything against such a feature?

#8 - 10/09/2012 12:34 AM - Roland Schulz

No. Since it is anyhow only for a small group of people it might be OK if it only works with >=2.8.5 or it doesn't always work. As long as it doesn't have any effect when it is disabled.
Somehow they changed something on Hopper and now you need the `LINK_SEARCH_END_STATIC` there too. And it works by itself without problems. So I think it is a good idea to have a option which enables it. I don't think it should be enabled by `GMX_PREFER_STATIC_LIBS` (I don't think you suggested that - instead I thought originally this would be a good idea). Instead we need a separate flag for this (e.g. `GMX_FULLY_STATIC`). This should also add `"-static"`. This later isn't needed on Cray because it already gets added by their compiler wrapper but is useful in general. E.g. if avoid the gcc_s problem on non Cray machines. We should print a warning on cmake <2.8.5 that the option `GMX_FULLY_STATIC` isn't working.

I looked it up incorrectly 3 months ago for comment #2. `LINK_SEARCH_END_STATIC` is available in 2.8.0 - only `LINK_SEARCH_START_STATIC` was added in 2.8.5 (http://www.cmake.org/Wiki/CMake_Version_Compatibility_Matrix/Properties#Properties_on_Targets). But I don't think we actually need `LINK_SEARCH_START_STATIC`. So fixing this issue should be as simple as adding a new option which activates `LINK_SEARCH_START_STATIC` and adds `"-static"`.

I was just looking at that earlier today. What I don't understand is how does the `-Bstatic` affect the linking when at the beginning or end of the library list?

What I assume (inferred from the behavior without really knowing how it works) is that the libraries added by the linker by default (e.g. `libgcc`, `glibc`,...) are added to the end, and are affected by the last `Bdynamic/Bstatic` in the list. Thus without the `LINK_SEARCH_END_STATIC` the default libs are linked dynamic and with it they are linked static. I don't think `LINK_SEARCH_START_STATIC` has any effect for any of the compilers we use. The only place it seems to matter is for odd custom tool-chains: http://cmake.3232098.n2.nabble.com/To-avoid-target-link-libraries-magic-td6192280.html . But I don't think it hurts either (neither with version which support it nor with those which don't). So I would simply set it and don't worry about that it isn't supported with older cmake because 99% of users probably don't need it anyhow.

I'm starting to get it now. The `LINK_SEARCH_END_STATIC` affects system libs while the `LINK_SEARCH_START__` affects the `-lXXX` library list. Assuming that this is the case, we should use both (if supported).
Well if cmake finds static libraries with PREFER_STATIC then it already adds the Bstatic before those libraries (and if it doesn't find the static library something is anyhow wrong). That's why I think it isn't necessary to have LINK_SEARCH_START_STATIC. But as I wrote it shouldn't hurt and might be helpful in some odd cases.

Are we able to get something done here for 4.6?

I think we agreed on:
- add a new option GMX_STATIC_BINARY (probably better name than GMX_FULLY_STATIC)
- add -static (if supported compiler option), LINK_SEARCH_END_STATIC and LINK_SEARCH_START_STATIC (if cmake>=2.8.5)

So should be very easy. Who wants to do it?

Roland Schulz wrote:

I think we agreed on:
- add a new option GMX_STATIC_BINARY (probably better name than GMX_FULLY_STATIC)
- add -static (if supported compiler option), LINK_SEARCH_END_STATIC and LINK_SEARCH_START_STATIC (if cmake>=2.8.5)

Yes, that is the plan.

So should be very easy. Who wants to do it?

I wanted to do it, but have been quite busy with other stuff and forgot about it. Will do it asap.

- Status changed from New to In Progress
- Assignee set to Szilárd Páll

- Target version changed from 4.6 to future

The reason why LINK_SEARCH_END_STATIC sometimes is required and sometimes not, seems to be related to whether any library in standard
locations is used. In that case cmake uses "-Wl,-Bstatic -lsomelib" instead of "/usr/lib/libsomelib.a". Now that xml is removed and fftw isn't in the default location on Cray, it seems to be no problem on Cray.

#21 - 05/22/2013 05:56 AM - Mark Abraham
- Target version changed from future to 4.6.x

#22 - 11/07/2013 09:34 PM - Mark Abraham
- Target version changed from 4.6.x to future

I seem to be able to build on Cray without problems, but my libraries were standard or own-fftw.

#23 - 11/11/2013 09:03 PM - Szilárd Páll
Mark Abraham wrote:

I seem to be able to build on Cray without problems, but my libraries were standard or own-fftw.

That's because on Crays the compiler wrappers force static builds whenever they can without being asked to do so, but this of course only works if all external libraries in their static form. However, even on Crays without turning off RPATH you won't be able to do make install because cmake thinks that it built dynamically linked binaries.

Note that you may not even be using the "own" FFTW because the Cray toolchain will link binaries against the scientific libs which contain Cray's own FFTW (which is anyway tuned and typically faster than the standard FFTW). Hence, I guess it's a matter or linking order whether you get to use your or Cray's FFTW.

#24 - 11/11/2013 09:57 PM - Mark Abraham
So we should expect/design the CMake detection to pick up that the toolchain provides FFTW even if there's nothing specific in any of the the paths? Does anybody know this happens?

#25 - 11/11/2013 10:20 PM - Roland Schulz
Currently it isn't checked. But it could be easily added by testing with CHECK_FUNCTION_EXISTS before looking for the library. But I think it isn't strictly related to the issue of having a static binary.

#26 - 11/12/2013 02:33 PM - Szilárd Páll
Mark Abraham wrote:

So we should expect/design the CMake detection to pick up that the toolchain provides FFTW even if there's nothing specific in any of the the paths? Does anybody know this happens?

Given that it will be a rare thing that compiler toolchains silently pull in loads of libraries "thought to be good for you" (does it happen on other HPC machine besides Cray?), unless it's trivial I would considere such an issue (if filed) a low priority one.

Note that I know this happens (at least on the CSCS XE6 Rosa and XK7 Toedi) because a while ago I wanted to benchmark standard FFTW against Cray's modified FFTW and after some struggling I gave up because I could not get the linking order tweaked appropriately.
...and indeed, this aspect is not really related to the current issue.

#27 - 11/13/2013 01:36 PM - Rossen Apostolov
Regarding the linking order - if you need to add a library right at the end of the link line, at least on some systems (e.g. SuperMUC) CMAKE_EXE_LINKER_FLAGS doesn't help. Instead one needs to use CMAKE_C_STANDARD_LIBRARIES to pass the arguments.

#28 - 06/12/2014 04:08 PM - Rossen Apostolov
Update - in 5.0.x and master one needs to use CMAKE_C_STANDARD_LIBRARIES_INIT instead.

#29 - 06/13/2014 12:12 PM - Szilárd Páll
- Status changed from In Progress to Accepted

#30 - 10/29/2014 10:21 AM - Mark Abraham
A somewhat related issue is that on Cray systems, the early tests by CMake for a functional compiler will pick up the CMake-standard Modules/Platform/Linux-xyz-lang.cmake files, which fails completely when Intel is the base compiler for the Cray wrapper, because these files hardcore the use of CMAKE_SHARED_LIBRARY_LINK_CXX_FLAGS=-rdynamic. Fix for 5.0 in progress

#31 - 10/29/2014 11:29 AM - Gerrit Code Review Bot
Gerrit received a related DRAFT patchset '1' for Issue #911.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: Id5e9f6594bb481617e58d1ed4e79f9dc692689ece
Gerrit URL: https://gerrit.gromacs.org/4188

#32 - 11/18/2014 04:26 PM - Mark Abraham
- Related to Feature #1641: Add toolchain file for Cray systems added

#33 - 11/18/2014 05:55 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #911.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I47b4524e9c33f52f20b0f54082d290ee22d9993b
Gerrit URL: https://gerrit.gromacs.org/4227

#34 - 11/26/2014 07:27 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #911.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I47b4524e9c33f52f20b0f54082d290ee22d9993b
Gerrit URL: https://gerrit.gromacs.org/4242

#35 - 12/12/2014 04:19 PM - Mark Abraham
- Description updated

#36 - 03/17/2015 05:12 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #911.
Uploader: Roland Schulz (roland@rschulz.eu)
Change-Id: If7b8192bb44c33c861126e3422df04388d2f2be5
Gerrit URL: https://gerrit.gromacs.org/4496
- Status changed from Accepted to Closed
- Target version changed from future to 5.1