

## GROMACS - Task #1013

### Library division for tools and generic Gromacs code

09/30/2012 06:37 AM - Teemu Murtola

<b>Status:</b>	Closed
<b>Priority:</b>	Normal
<b>Assignee:</b>	Teemu Murtola
<b>Category:</b>	build system
<b>Target version:</b>	5.0
<b>Difficulty:</b>	uncategorized
<b>Description</b>	
<p>Currently, <a href="http://www.gromacs.org/Developer_Zone/Programming_Guide/Library_Structure">http://www.gromacs.org/Developer_Zone/Programming_Guide/Library_Structure</a> states that there will be only one library, <i>libgromacs</i>. In the source code, there are still two built: <i>libgromacs</i> and <i>libgmxana</i>. Do we want to merge also all the analysis tool code into <i>libgromacs</i>? I think that some concerns have been raised regarding the size of the library for platforms where memory is limited (e.g., BlueGene). If we merge the libraries and the size is a problem, we could possibly just add some build system features that allow building only parts of Gromacs, so that users could build a stripped-down version that runs only mdrun, for use on such platforms. In particular if we have a modular system for building the different old binaries into a single binary with <a href="#">#685</a>, it shouldn't be too difficult to skip building some parts.</p> <p>Even if we want to keep a separate analysis library, the division needs some work, as currently tools using the new analysis framework are built as part of <i>libgromacs</i> and not <i>libgmxana</i>. It also needs to be considered where do other parts of the framework belong (the generic runner code, the selection library, other utility functions). With the new framework, most code in the tools is part of the framework, and not in the tool-specific code.</p> <p>The division has an effect on <a href="#">#988</a> and <a href="#">#701</a>, in particular in placing constraints what symbols we must export from the shared libraries.</p>	
<b>Related issues:</b>	
Related to GROMACS - Task #988: Definition of "public API"	<b>New</b>
Related to GROMACS - Task #701: Add symbol visibility macros	<b>New</b>

#### Associated revisions

##### Revision 8421fa36 - 03/24/2013 07:28 PM - Teemu Murtola

Merge libgmxana into libgromacs.

- Move contents of `src/tools/` into `src/gromacs/gmxana/`, except for `g_tune_pme.c` and `g_pme_error.c`.
- Delete unused `src/tools/g_membed.c`.
- Adjust the build system accordingly, removing references to `gmxana`.
- Merge contents of `libgmxana.pc` into `libgromacs.pc` and remove the former.
- Move `src/gromacs/legacyheaders/gmx_ana.h` into `src/gromacs/gmxana/` and adjust files that include it accordingly. Removed a few unnecessary inclusions of this header. Don't install it, as it doesn't do much good.
- Merge `src/contrib/g_sdf.c` into `src/contrib/gmx_sdf.c` to make it independent of `gmx_ana.h`. Remove `gmx_sdf()` from `gmx_ana.h`.

Closes #1013.

Change-Id: I34ba52fc938823833103123c8ada06d169abf7de

##### Revision 9734c9fa - 06/13/2013 09:45 AM - Teemu Murtola

Merge libgmxana into libgromacs.

- Move contents of `src/tools/` into `src/gromacs/gmxana/`, except for `g_tune_pme.c` and `g_pme_error.c`.
- Delete unused `src/tools/g_membed.c`.
- Adjust the build system accordingly, removing references to `gmxana`.
- Merge contents of `libgmxana.pc` into `libgromacs.pc` and remove the former.
- Move `src/gromacs/legacyheaders/gmx_ana.h` into `src/gromacs/gmxana/` and adjust files that include it accordingly. Removed a few unnecessary

inclusions of this header. Don't install it, as it doesn't do much good.  
- Merge src/contrib/g\_sdf.c into src/contrib/gmx\_sdf.c to make it independent of gmx\_ana.h. Remove gmx\_sdf() from gmx\_ana.h.

Closes #1013.

Change-Id: I34ba52fc938823833103123c8ada06d169abf7de

## History

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### #1 - 02/12/2013 01:40 PM - Teemu Murtola

- Assignee set to *Teemu Murtola*

I assume from a few e-mails in different mailing lists that the decision is to go at least initially with a single monolithic library, i.e., merging libgmxana to libgromacs. I can volunteer to do the initial merge, after all the 4.6 merges into master are merged in and uncrustify and copyright changes have been applied.

I think this issue can be closed after libgmxana no longer exists; any additional implementation or additional build system features as suggested in the description can be implemented as separate tasks.

### #2 - 04/11/2013 05:38 AM - Teemu Murtola

- Description updated

- Status changed from *New* to *Closed*

### #3 - 02/14/2014 08:10 PM - Teemu Murtola

- Project changed from *Source code reorganization* to *GROMACS*

- Description updated

- Category set to *build system*