

GROMACS - Task #637

Reorganize code from src/kernel/

01/08/2011 10:04 AM - Teemu Murtola

Status:	Closed
Priority:	Normal
Assignee:	Teemu Murtola
Category:	build system
Target version:	5.0
Difficulty:	uncategorized
Description	
Move code for programs that are built from src/kernel/ into separate subdirectories under src/programs/ and update CMake files accordingly. Code used in multiple programs can go for now under src/gromacs/gmxpreprocess/, and get linked into libgromacs. Only minimal if any changes should be needed to the source files themselves.	

Associated revisions

Revision 01491632 - 01/09/2011 01:32 PM - Teemu Murtola

Moved mdrun from src/kernel/ to src/programs/mdrun/.

compute_io.* were moved to src/gromacs/gmxpreprocess/ because they are used by both grompp and mdrun. No other changes were necessary.

IssueID #637

Revision 36ab4073 - 01/09/2011 01:55 PM - Teemu Murtola

Moved grompp from src/kernel/ to src/programs/grompp/.

Functions related to topology IO were moved to src/gromacs/gmxpreprocess/ because they were also referenced by pdb2gmx.

IssueID #637

Revision 9c7e4e67 - 01/09/2011 02:13 PM - Teemu Murtola

Moved pdb2gmx from src/kernel/ to src/programs/pdb2gmx/.

Functionality shared with g_x2top and/or g_protonate was moved to src/gromacs/gmxpreprocess/.

IssueID #637

Revision ec666d52 - 01/09/2011 02:26 PM - Teemu Murtola

Moved x2top, gmxcheck and gmxdump to src/programs/.

IssueID #637

Revision d48cc76d - 01/09/2011 02:31 PM - Teemu Murtola

Removed libgmxpreprocess from CMake.

All shared content has been moved to src/gromacs/gmxpreprocess/, and it was no longer referenced by any of the existing code.

IssueID #637

Revision cf22b656 - 01/09/2011 02:40 PM - Teemu Murtola

Moved protonate and tpbconv to src/programs/.

IssueID #637

Revision eed611d5 - 05/02/2012 08:25 PM - Teemu Murtola

Removed unused code from src/kernel/.

When code from src/kernel/ was originally moved to the new file hierarchy, these were left over as not necessary for building any of the binaries. They haven't been included in the build for master for over a year.

IssueID #637

Change-Id: I37dadf1a77239e554c5968a2c61c163183af65b7

Revision ea83bf89 - 05/03/2012 06:24 PM - Teemu Murtola

Remove g_luck.

Also removed any references found with grepping for "luck" in the tree. With this, there is nothing left in src/kernel/.

Closes #637.

Change-Id: I4f1f229ea7f9a98eed94aa2b891112b3db2bd062

History

#1 - 01/09/2011 03:47 PM - Teemu Murtola

- Status changed from *New* to *Feedback wanted*
- % Done changed from 0 to 90

Most of the task is now completed. Now, there remains only g_luck in src/kernel/, and a bunch of dead code that was not included in the build. I would vote for just removing g_luck while where are doing this clean-up, but for the rest of the code, other people are more likely able to say whether they should be retained, moved to contrib, or removed.

It should also be checked that everything works after these file renames. I've only tested a non-MPI build on Macs, but any problems on other platforms should be easy to fix.

#2 - 04/13/2012 05:38 PM - Teemu Murtola

- Target version set to 5.0

#3 - 05/08/2012 01:55 PM - Teemu Murtola

- Status changed from *Feedback wanted* to *Closed*
- Assignee set to *Teemu Murtola*

All mentioned code has now been removed.

#4 - 02/15/2014 09:37 PM - Teemu Murtola

- Project changed from *Source code reorganization* to *GROMACS*
- Category set to *build system*