The legacyheaders/ directory was meant as a temporary workaround to be able to move files to the new directory layout gradually, while keeping the build and the installed headers working all the time. The original idea (when the discussion started back in 2010 or so) was that this would be more or less gone by 5.0, but it has been quite persistently alive. So the goal would be to have all the headers from src/gromacs/legacyheaders/ moved into subdirectories like src/gromacs/domdec/ or src/gromacs/nbnxn/ or something, together with the source files that implement those functions and anything that belongs naturally together with them. Large parts of this should not be rocket science, and if people would contribute on the areas that they know, we could then see what are the problematic areas. The initial division can also be adjusted later as we grow wiser.

There are currently about 150 headers remaining, plus 38 from thread_mpi (the latter should be easy to move, once there is some clarify for #1411). Large parts of this will be easy, but the types/ subdirectory can be challenging.

This would allow us to clearly see the dependencies between the modules and draw reasonable division lines for the different libraries required for, e.g., #1165. Visualizing the dependencies between the parts with something like https://gerrit.gromacs.org/#/c/2908/ would provide a much clearer picture of where we are and what could be done to clarify the structure of the code.

Associated revisions

Revision fdbd0916 - 01/11/2014 02:41 PM - Carsten Kutzner
Move essential dynamics / flooding code to separate directory

Part of #1415 Get rid of legacyheaders.

Additional changes:
- provided doxygen-style documentation for functions in edsam.h
  (partly copied over from edsam.c and removed there to avoid duplication)
- uncrustified edsam.c and edsam.h

Change-Id: If4af498470c5200d50ac1d1b5537917c873380b5

Revision 904e082b - 01/13/2014 08:06 PM - Carsten Kutzner
Move pull code to separate subdirectory

Another part of #1415 Get rid of legacy headers.

Other changes:
- updated pulling-related include guards to new format
- updated documentation for doxygen
- updated .h includes
- uncrustified pull.h and pull_rotation.h
- updated copyright year for all files touched by this commit

Change-Id: Ief1ed3543b84f651d1bff011952b342850f5c22

Revision 2b85adec - 01/21/2014 07:37 PM - Mark Abraham
Move more preprocessing files into the module

This removes the need for the gmx_objlib CMake object library, because there is no longer random functionality orphaned in src/programs/gmx (which is there because it was orphaned in src/kernel in release-4-8).
Moved legacyheaders/grompp.h to gmxpreprocess/grompp-impl.h since it only declared structures that are (now) only used in that module (and it no longer #includes stdio.h). gmxpreprocess/grompp.h now only declares gmx_grompp().

Likewise, pdb2gmx, protonate and x2top now have their own single-function headers.

Removed useless declaration of ncontrol from h_db.h

Removed grompp.h-related useless dependencies, declarations and definitions from Generalized Born files.

Updated include and added C++ guards for files already within the module (and new ones). Uncrusted, bumped copyrights

Refs #1415

Change-Id: le7967d7d7f61df684d530e3c2d982486a3cd128f

Revision d3ac3c5b - 04/01/2014 02:00 AM - Teemu Murtola

Move smalloc.h to utility/

One common header away from legacyheaders/.
 Mostly mechanical replacement for the include paths, but removed a few instances where the header was included more than once. Also, reordered the headers a bit, mainly in C++ files.

Part of #1415.

Change-Id: lc438d501ebf5ecccc285655a9e8f2f625eb12f1d1

Revision 2ca0f555 - 04/02/2014 03:11 PM - Teemu Murtola

Move string2.* to utility/cstringutil.*

Another common header away from legacyheaders/.
 Some associated #include cleanup.
 This reintroduces some unwanted dependencies (like utility -> fileio), but those need to be fixed separately.

Part of #1415.

Change-Id: lfffb2820019e2b41ef74bcabcc202364917e43d58

Revision 1fe1fb54 - 04/08/2014 05:38 PM - Teemu Murtola

Move gmx_fatal.* to utility/fatalerror.*

One more included-by-all header to utility/.
 Mainly mechanical replacement of include paths, some reordering in C++ files. Minor clean-up in the moved files.
 gmx_fatal_collective.h not moved at this point, as it is unclear whether it should go here, or somewhere else (utility/ should not depend on t_commrec...).

Now, it's mainly types/simple.h that prevents removing some module-level dependencies to legacyheaders/.
 Finding a good location for that (or its contents, if it needs to be split), and reorganizing the code a bit more should now allow really putting utility/ at the bottom of the dependency stack where it belongs.

Part of #1415.

Change-Id: l6e487566d5bd7c9ec7a1455a2d31bd6d645bada3

Revision 83847a3c - 04/16/2014 03:45 AM - Teemu Murtola

Remove sysstuff.h

Replace this with those standard headers that are actually necessary for the source files. There are likely several transitively covered header dependencies now, but those can be resolved when they give problems. One more header off from legacyheaders/.
Most of the changes are scripted replacement of include paths. Exceptions:
- #includes in the moved file were cleaned up slightly, and include guards adjusted.
- Places where it was included as "gromacs/legacyheaders/vec.h" were handled manually and the include order adjusted.
- Removal of unnecessary #include "vec.h" from update.h revealed some transitive dependencies that were fixed. Some associated include order cleanup in these files.
- Removed some duplicate includes.
- Remove dependency from linearalgebra/matrix.c to vec.h (only needed for a single sqr()) to avoid a cyclic math <-> linearalgebra dependency.

In the long run, this may be better outside utility/ to better distinguish code that depends on 'real' from parts that do not. Currently, it would create a lot of cyclic dependencies everywhere else.
Revision 2cc6cb6 - 04/28/2014 04:24 AM - Roland Schulz
Reduced usage of typedefs.h

Preliminary step to move types out of legacyheader.

Renamed parameter called "matrix" because cppcheck gets confused if a parameter is called the same as a type.

Part of #1415
Change-Id: i9207a7b8de7f092bab890da128abb48a8d97b79

Revision 604cd696 - 05/14/2014 09:33 PM - Teemu Murtola
Move physics.* to math/units.*

- Remove some unnecessary #includes.
- Remove the dummy tests; easy to rewrite as usable tests using GTest if someone needs those. They were anyways testing code that no one is still calling, even though it was introduced several years ago.
Now gmxlib is free of *_test.c files.

Now, only one file using atom_id is keeping math/ dependent on legacyheaders/.

Part of #1415.
Change-Id: i31312b92cf95d5129fbd90f311cf27be217aaf

Revision 2b5c9ac3 - 09/22/2015 01:34 PM - David van der Spoel
Removed legacyheaders/types/commrec_fwd.h from typedefs.h

Related to #1415
Change-Id: i9a9dd7f1e62cfd040d183370d187f6a23ede78fa

Revision 6cc44d3e - 11/03/2015 09:26 PM - David van der Spoel
Moved df_history utility routines from typedefs to new file.

Part of #1415.
Change-Id: ia2b99e6e5342cb3bb5820894fb82ef2908d969bc6

Revision 2a9f0384 - 11/11/2015 12:53 AM - David van der Spoel
Removed legacyheaders/typedefs.h

More cleaning up in legacyheaders. Mostly this patch involves shuffling around include files, and adding a couple of forward declarations. Renames gmxlib/typedefs.* to mdtypes/state.* and introduces new utility/init64_to_int.cpp with header.
Introduced new directory mdtypes to resolve circular dependencies. Right now state.* and history files are the only files living there.

Part of #1415
Change-Id: i5dc59a2ca3bd1f9c539f4b9fde9f116b30106fc

Revision 890ce4a8 - 11/11/2015 10:10 PM - David van der Spoel
Moved inputrec.* from gmxlib and legacyheaders to mdtypes.

Part of #1415
Change-Id: ldb00712d1b6ea9648a36d349f670790aaaf2c6d4

Revision e4034c03 - 11/12/2015 08:44 AM - David van der Spoel
Moved copyrite.* to fileio from gmxlib and legacyheaders.

Part of #1415
Change-Id: ld6cfb84cc683f88731fac7d80053aadcc9b828806
Revision 56a31f36 - 11/12/2015 04:37 PM - David van der Spoel
Moved txtdump.* to fileio.

Some cleanups in edsam.cpp too.

Part of #1415
Change-Id: l6cd58951eff1bac0dad75dbd448a958e57c767e7

Revision 99e5a7cc - 11/13/2015 08:05 AM - David van der Spoel
Moved genborn.h to mdlib

Part of #1415
Change-Id: la2d734be40df97426348a153040cf311a3abf7a3

Revision e8e13a0e - 11/15/2015 10:21 AM - David van der Spoel
Merged legacyheaders/types/state.h into mdtypes/state.h

Also merged swap/enum.h into legacyheaders/types/enums.h
to be moved later out of legacyheaders.
Part of #1415, #1854.
Change-Id: le53f190d6798b81c531896de80ef25c060836479

Revision a3be7872 - 11/15/2015 01:46 PM - David van der Spoel
Merged legacyheaders/types/inputrec.h into mdtypes/inputrec.h

Part of #1415.
Change-Id: l9985a01474173170bc6a7a7c2e54e7f21d64370

Revision a8a355f0 - 11/20/2015 02:02 AM - David van der Spoel
Moved legacyheaders/types/energy.h to mdtypes.

Part of #1415
Change-Id: l65a00cc49110a09edfa7c7520a7a480f73b5165c

Revision 386dedc8 - 11/20/2015 09:19 AM - David van der Spoel
Moved mdatom.h from legacyheader/types to mdtypes.

Add doxygen comments to the elements of the structure.

Part of #1415.
Change-Id: l811ad4782dd482ac7fe198c85c85b91a6e20b67

Revision ca3bb88c - 11/20/2015 09:51 AM - David van der Spoel
Merged legacyheaders/nrnb.h and types/nrnb.h to gmxlib.

Part of #1415
Change-Id: l33922419a6a5a79976bda12fd81e2d752eb0c5c6d

Revision f75bc658 - 11/20/2015 03:44 PM - David van der Spoel
Combine enums.h and names*.

Combined enums.h and names* to mdtypes/md Enums.cpp/h.
Added doxygen comments to md Enums.h.
Removed macros in inputrec.h to reduce cyclic dependencies.

Clean up of legacyheaders. By removing some unnecessary includes
from the files names.h and enums.h (now md Enums.h)
a lot of 'freeriders' showed up, therefore had to include
topology.h in many files.

Part of #1415
Revision e5a42060 - 11/20/2015 06:18 PM - David van der Spoel
Merged legacyheaders/types/ns.h and nblist.h to mdtypes/nblist.h
Also parts moved out of forcerec.h.
In order to make this work some parts of the forcerec structure
had to be made pointers, and the same for nblist structures.
Part of #1415.

Change-Id: I12b8ef4f82b7aec806aea2eee7d77604e86dc576

Revision 806e77b1 - 11/20/2015 08:19 PM - David van der Spoel
Moved legacyheaders/types/group.h to mdtypes.
Part of #1415.

Change-Id: Iaaadd76ccca001a11371b9a0ad1b75a727732f00

Revision 87f0b419 - 11/21/2015 11:51 AM - David van der Spoel
Merged genborn.h from legacyheaders/types into mdlib/genborn.h
Part of #1415.

Change-Id: I959941cf586b990e97359e8ec028dc923ff78aa5

Revision 6abe0013 - 11/22/2015 02:15 PM - David van der Spoel
Cleanups in legacyheader/types/commrec.h
Removed superfluous typedefs from above file.
Part of #1415.

Change-Id: If3d99dc24864d21dbbfa2eaf57fd52647d3d9ec

Revision 1cd9683a - 11/23/2015 03:11 PM - David van der Spoel
Moved domdec structures out of commrec.h.
In order to clean up the legacyheaders directory here the
structures relating to domain decomposition are taken out of
commrec.h and moved to a new file domdec/domdec_struct.h
To not introduce new cyclic dependencies modified the
interface of write_checkpoint and gmx_fatal_collective.
Part of #1415

Change-Id: I485a03eddbb87dccc236b7e2e7d85d03383d86f61

Revision ca26ed98 - 11/30/2015 11:52 AM - Teemu Murtola
Merge remaining legacyheaders/ to mdtypes/
One cyclic dependency suppressed for now.
legacyheaders/ is no more.
Closes #1415 (but this just moves us to the next phase of the clean-up)
Change-Id: le80d24d347acb61216002a309cb41181f8d99b6b

Revision 5922c55f - 12/12/2015 04:17 AM - Mark Abraham
Broke up copyright.*
Split unrelated content into binaryinformation.*, and pleasecite.*, and
move them to utility/. This removes functionality from fileio that does
not really belong there, and helps in removing cyclic dependencies.
One new cyclic dependency suppressed for now; it will disappear with
simplification of gmx_invsqrt().

Part of #1415.
Change-Id: i65f07768d46852783d30cf1a28dd22d614dde125

History

#1 - 01/07/2014 06:52 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1415.
Uploader: Carsten Kutzner (dkutzne@gwdg.de)
Change-Id: if4af498470c5200d50ac1d1b5537917c873380b5
Gerrit URL: https://gerrit.gromacs.org/2961

#2 - 01/13/2014 05:20 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1415.
Uploader: Carsten Kutzner (dkutzne@gwdg.de)
Change-Id: le1ed354384f651d1bf011952b342850f5c22
Gerrit URL: https://gerrit.gromacs.org/2979

#3 - 01/17/2014 06:38 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1415.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: le7967d77161d684d530e30c2d962486a3cd128f
Gerrit URL: https://gerrit.gromacs.org/2993

#4 - 03/31/2014 08:23 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1415.
Uploader: Teemu Murtola (teemu.murtola@gmail.com)
Change-Id: lc438d501eb5f5ecc285655a9e81df625eb12f1d1
Gerrit URL: https://gerrit.gromacs.org/3311

#5 - 04/01/2014 06:10 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1415.
Uploader: Teemu Murtola (teemu.murtola@gmail.com)
Change-Id: lfb2820019e2b41ef74bcabc202364917e43d58
Gerrit URL: https://gerrit.gromacs.org/3318

#6 - 04/05/2014 05:32 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1415.
Uploader: Teemu Murtola (teemu.murtola@gmail.com)
Change-Id: l6e4875f6d5bd7c9ec7a1455a2d31bd6d645bada3
Gerrit URL: https://gerrit.gromacs.org/3328

#7 - 04/13/2014 07:19 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1415.
Uploader: Teemu Murtola (teemu.murtola@gmail.com)
Change-Id: l4cc3f0eaec0f546ddad929512e532d6efb11da3694
Gerrit URL: https://gerrit.gromacs.org/3355

#8 - 04/15/2014 05:55 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1415.
Uploader: Teemu Murtola (teemu.murtola@gmail.com)
Change-Id: lb3d79bce65a2c03e4d7d001164921edd56657a2
Gerrit URL: https://gerrit.gromacs.org/3362

#9 - 04/16/2014 06:03 AM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1415.
Uploader: Teemu Murtola (teemu.murtola@gmail.com)
Change-Id: if7e0e6af22139215510148807c5979f6950a885
Gerrit URL: https://gerrit.gromacs.org/3363

#10 - 04/16/2014 08:00 AM - Roland Schulz
I think we shouldn't have a new top level folder for each simulation method. This is getting quickly out of hand. We already have: imd, pulling, swap, essentialdynamics. Not as problematic (because the list probably wont grow quickly) but also quite long of a list is math related top-level folders (math, fft, linearalgebra, statistics). Would it make sense to make the last 3 subfolders?
I'm still a bit confused about the dependency checking scripts. What is the easiest approach to use them to know whether moving files into different (sub)folders will create cyclic dependencies?

#11 - 04/16/2014 09:12 AM - Teemu Murtola

In general, I agree that the current subdirectories are possibly too fine-grained. But it is easier to first create smaller units and then combine them, than to try to figure out in advance what kind of bigger units make most sense. So I think that the current approach is reasonable, but we should aim for a smaller amount of top-level folders once it is clear what can be combined and makes sense to combine. Folders with just one or a few files don't really make much sense.

Roland Schulz wrote:

I think we shouldn't have a new top level folder for each simulation method. This is getting quickly out of hand. We already have: imd, pulling, swap, essentialdynamics.

I agree. My initial thought was to put all these special methods under a specialmd/ folder or similar.

Not as problematic (because the list probably wont grow quickly) but also quite long of a list is math related top-level folders (math, fft, linearalgebra, statistics). Would it make sense to make the last 3 subfolders?

Possibly, fft/ and linearalgebra/ have a special purpose of wrapping external libraries, and as such, have some relatively complex internal logic. But it would be simpler if there could be dependencies in both directions. This would, e.g., allow putting the definition of real and rvec into math/.

I'm still a bit confused about the dependency checking scripts. What is the easiest approach to use them to know whether moving files into different (sub)folders will create cyclic dependencies?

Currently, you need to run make dep-graphs and view doxygen/depgrahs/module-deps.dot.png. It currently only shows folders one level below src/gromacs/, but that is possible to change (but requires some thinking to keep things clear, both in the graph and elsewhere). I've been thinking of adding a proper cycle detection into the script, but that is complicated by the currently existing cycles. I'll see whether that would still be possible.

#12 - 04/18/2014 04:21 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1415.
Uploader: Teemu Murtola (teemu.murtola@gmail.com)
Change-Id: l2aa1890357377d0d14c05b3968e1b36e1023458f
Gerrit URL: https://gerrit.gromacs.org/3378

#13 - 04/20/2014 08:09 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1415.
Uploader: Roland Schulz (roland@rschulz.eu)
Change-Id: l360ae1f220b651e90edbbbe136053f02e1c0ad5b
Gerrit URL: https://gerrit.gromacs.org/3382

#14 - 04/20/2014 08:40 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1415.
Uploader: Teemu Murtola (teemu.murtola@gmail.com)
Change-Id: lffeafa4fa5c5e0c744cf6deecac4e1deae2c5f
Gerrit URL: https://gerrit.gromacs.org/3383

#15 - 04/21/2014 02:59 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1415.
Uploader: Roland Schulz (roland@rschulz.eu)
Change-Id: l9207a7b9de7f092bab899da129abbb48a8d97b79
Gerrit URL: https://gerrit.gromacs.org/3384

#16 - 04/22/2014 06:17 AM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1415.
Uploader: Teemu Murtola (teemu.murtola@gmail.com)
Change-Id: l31312b92cf95d5129fbd90e31cf27be27afaf
Gerrit URL: https://gerrit.gromacs.org/3388

#17 - 05/20/2014 09:03 PM - Teemu Murtola

Roland Schulz wrote:

I'm still a bit confused about the dependency checking scripts. What is the easiest approach to use them to know whether moving files into different (sub)folders will create cyclic dependencies?
As a reference, [https://gerrit.gromacs.org/#/c/3380/](https://gerrit.gromacs.org/#/c/3380/) now allows you to run make doc-check, and it will report any new cyclic dependencies that the changes create. Hopefully, existing cycles will not lead to too many confusing results with the algorithm that is currently used. Until it gets merged, you can just cherry-pick it on top of any change (it shouldn't conflict with much of anything). Just try not to push the cherry-picked version. ;)

#18 - 09/18/2015 08:58 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘4’ for Issue #1415.
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-id: l9a9d7d71e62cfd040d183370d1877f6a23ede7f9a
Gerrit URL: https://gerrit.gromacs.org/5082

#19 - 11/03/2015 05:17 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1415.
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-id: la2b9e6e5342cb3b5820894f2e2f2906d969bc6
Gerrit URL: https://gerrit.gromacs.org/5291

#20 - 11/04/2015 01:30 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1415.
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-id: ld5c59a2ca1bd1f9c53914b9de8f116b3906d969bc6
Gerrit URL: https://gerrit.gromacs.org/5267

Gerrit received a related patchset ‘1’ for Issue #1415.
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-id: ld6c884c683f88731fac7d80053aadcc9b828806
Gerrit URL: https://gerrit.gromacs.org/5315

#22 - 11/11/2015 01:24 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1415.
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-id: ld8b00712d1b8ea9645836d349f670790aaaf26d4
Gerrit URL: https://gerrit.gromacs.org/5317

Gerrit received a related patchset ‘1’ for Issue #1415.
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-id: ld86c598f51e61fbc0d97c75d4d448a958e57c767e7
Gerrit URL: https://gerrit.gromacs.org/5319

#24 - 11/11/2015 10:00 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1415.
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-id: la2d734e4bdf74726348a153040cf311a3ab7fa3
Gerrit URL: https://gerrit.gromacs.org/5320

Gerrit received a related patchset ‘1’ for Issue #1415.
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-id: 12b8df4f82b7eac8068e2e6ee7d77604e86d6576
Gerrit URL: https://gerrit.gromacs.org/5321

Gerrit received a related patchset ‘1’ for Issue #1415.
Uploader: Mark Abraham (mark.i.abraham@gmail.com)
Change-id: 16507758d468527853d0cf1a26d222d64d14d125
Gerrit URL: https://gerrit.gromacs.org/5322

#27 - 11/12/2015 08:35 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1415.
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-id: I39885a01474173170bcb7a7c2e54e7212d84370
Gerrit URL: https://gerrit.gromacs.org/5325
#39 - 12/01/2015 09:15 AM - Teemu Murtola
- Status changed from Fix uploaded to Resolved

Applied in changeset ca26ed983d1d628b0b7ccf603d9c7a68a4e8c91a.

#40 - 01/12/2016 08:25 PM - Teemu Murtola
- Status changed from Resolved to Closed