Refactor pdb2gmx into c++ framework

In order to have better with external callers (e.g. python API) having pdb2gmx implemented as a real c++ class structure will be beneficial. The first step is to re-implement pdb2gmx as an ICommandLineOptionsModule. Ideally, this should be coupled with a move away from pointers and towards references. Eventually I have some interest in taking this in a direction similar to the IForceProvider framework where there would be a sort of [structureFileFormat]2gmx functionality that can accommodate heterogeneous data and maybe handle some basic modeling tasks like combining pdbs or adding a few missing residues. Before that can happen though, a number of changes will be necessary.

Related issues:
Related to GROMACS - Task #1587: improve the configurability of regression tests

Associated revisions
Revision 27a4d57c - 07/16/2018 05:35 PM - Mark Abraham
Replacement for pdb2gmx tests

This test directly asserts upon the .top and .gro files that are written out, using fragments of the regressiontests/complex/aminoacids/conf.gro because these cover all basic amino acid types. It also adds testing for hydrogen vsites for amber and charmm.

We now omit doing an energy minimization after the string checks, which was always a doubtful way to test pdb2gmx. These tests are still too slow to run with other pre- and post-submit testing, so a newCTest category has been made for them, and that category is excluded from Jenkins builds by default. Developers will still run these by default with "make check" or "ctest" but that should be fast enough on a workstation. Later we can probably refactor them to use in-memory buffers and be fast enough to put with the other tests.

Modified pdb2gmx to avoid writing fractional charges for every atom in the [atoms] output, which isn't very useful for users and makes writing tests more difficult.

Fixed unstable sorting of dihedrals whose parameters are strings that identify macros.

Added new capability for refdata tests to filter out lines that vary at run time by supplying a regex that matches the lines to skip. That's not ideal, but useful for now. Better would be to refactor tools so that e.g. header output can go to a different stream, but first we should have basic tests in place.

Added tests for Regex. Fixed minor bug in c++ stdlib regex implementation of Regex. Noted the remaining reason why we have Regex supported by two different implementations.

Minor updates to use compat::make_unique

Extended functionality of CommandLine for convenient use.

Refs #1587, #2566

Change-Id: I6a4aeb1a4c460621ca89a0dc6177567fa09d9200
Revision e47c992c - 07/30/2018 06:44 PM - Joe Jordan

remove most debug flags from gmxpreprocess

To make pdb2gmx more readable as part of #2566 I removed the debug info. I went ahead and removed most debug info from other gmxpreprocess tools as well.

Change-Id: l88919d11f16d7f44508b4fcfae156fa051b4d70

Revision 2363a20f - 08/24/2018 09:41 AM - Joe Jordan

change some char to string in gmxpreprocess

Related to #2566 and #2570. As part of the refactoring of pdb2gmx one thing that becomes clear is that a lot of variables could have better defined scope and readability could be improved if some char’s are converted to string’s. This can ripple through the code base of gmxpreprocess. I have followed some of those ripples here and will continue to follow in later changes.

Change-Id: l0d12704ef27c06a4f64f8d1e8638760c8c7019ae

History

#1 - 07/06/2018 11:22 AM - Gerrit Code Review Bot
Gerrit received a related patchset ‘2’ for Issue #2566.
Uploader: Joe Jordan (e.jjordan12@gmail.com)
Change-Id: gromacs~master~I6dd750d0761c474415c02e9ae36d7db1fbdda10
Gerrit URL: https://gerrit.gromacs.org/8061

#2 - 07/06/2018 01:35 PM - Joe Jordan
- Tracker changed from Bug to Task
- Affected version deleted (future)

#3 - 07/06/2018 06:46 PM - Mark Abraham
- Related to Task #1587: improve the configurability of regression tests added

#4 - 07/19/2018 01:58 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #2566.
Uploader: Joe Jordan (e.jjordan12@gmail.com)
Change-Id: gromacs~master~I88919d11f16d7f44508b4fcfae156fa051b4d70
Gerrit URL: https://gerrit.gromacs.org/8105

#5 - 08/05/2018 08:08 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #2566.
Uploader: Joe Jordan (e.jjordan12@gmail.com)
Change-Id: gromacs~master~I0d12704ef27c06a4f64f8d1e8638760c8c7019ae
Gerrit URL: https://gerrit.gromacs.org/8134

#6 - 09/24/2018 02:19 PM - Joe Jordan
- Status changed from Feedback wanted to Closed

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