

GROMACS - Task #920

Task # 665 (New): Port existing trajectory analysis tools to use the new framework

Add test framework for trajectory analysis modules

04/13/2012 05:52 PM - Teemu Murtola

Status:	In Progress
Priority:	Normal
Assignee:	Teemu Murtola
Category:	testing
Target version:	
Difficulty:	uncategorized
Description	
<p>It should be straightforward to write a Google Test fixture that takes a trajectory analysis module (derived from <code>gmx::TrajectoryAnalysisModule</code>) and provides functionality for executing the analysis on a given trajectory and topology, with given options. Output from the modules should be accessible through <code>datasetFromName()</code>, and can be verified with the test classes written for the <code>analysisdata</code> subdirectory.</p> <p>So this task consists of:</p> <ul style="list-style-type: none">• Moving common code from <code>src/gromacs/analysisdata/tests/</code> to a separate library (<code>src/testutils/</code> probably works fine).• Writing the test fixture class. Initially, the test fixture can probably use <code>gmx::TrajectoryAnalysisCommandLineRunner</code>. If common parts of the runner are split into a separate class as part of #868, it may be possible to also write a simpler runner for the tests only, and test the command-line runner separately.• Writing some simple test cases to check that it works.	

Associated revisions

Revision 34e0eaa7 - 05/24/2012 11:03 AM - Teemu Murtola

Move common test code to `testutils`.

- Move test fixture for `AbstractAnalysisData` classes from `analysisdata/` to `testutils/`.
- Some renaming to make file and class names more descriptive.
- Move `gmx::test::CommandLine` from `commandline/` to `testutils/`.

Prerequisite for #920.

Change-Id: I2d4c8aaf87db03fe6c170856ba5b41eae05c483b

Revision 691bc21d - 05/24/2012 05:26 PM - Teemu Murtola

Improve `analysisdata` reference checks.

The reference checking for `AnalysisData` objects now supports more scenarios with multipoint data, i.e., cases where there are point sets that do not cover all columns.

Supporting changes:

- Add a `TestReferenceChecker::checkPresent()` method that allows to assign meaning to absence of a reference data item (and to check for that).
- Split common `analysisdata` XML stylesheet elements to a separate xsl file.
- Add a script for copying the XML stylesheets to the reference data directories for easier maintenance. Master copies of shared stylesheets are now kept in `src/testutils/`.

Needed for #920, but split from the main change to keep it smaller.

Change-Id: I108c013833052c37a4f2e6c73be6161c0dae1c78

Revision bccb1693 - 05/24/2012 05:26 PM - Teemu Murtola

Improve `gmx::test::CommandLine`.

- Make the class properly copyable for easier use in tests that need to manipulate it.
- Make the class manage its memory using `std::vector` and prevent memory leaks if the `argv` array is modified outside the class (the internal state of the class is still not correctly maintained, though).
- Add methods to append arguments.

Needed for #920, but split from the main change to keep it smaller.

Change-Id: I66ebe9d48936d35bce9e0b4fc1d6246d3d5ec07d

Revision b9a48ab2 - 07/06/2012 05:59 AM - Teemu Murtola

Test framework for TrajectoryAnalysisModules.

- Add a test fixture that makes it simple to test analysis tools that are implemented as TrajectoryAnalysisModule subclasses (moduletest.*).
 - Add tests using the new fixture for most of the functionality of the Select module.
 - Minor adjustment to reference data test fixture to make it more usable in this context.
 - Move all dataset registration calls to trajectory analysis module constructors from `initAnalysis()`. Also moved static initialization of the datasets, in particular calls to `setMultipoint()`.
- In addition to enabling the tests to access the datasets before any initialization of the module is done, this also makes the modules easier to use for other interfacing than the command-line runner.

Main part of #920, may need some additional features.

Change-Id: I67e123f8361fe7710e936d9b4a880e65a3dc89c5

History

#1 - 05/22/2012 09:16 AM - Teemu Murtola

- *Status changed from New to In Progress*
- *Assignee set to Teemu Murtola*

#2 - 06/20/2014 10:45 AM - Erik Lindahl

- *Target version changed from 5.0 to 5.x*

#3 - 07/14/2014 11:31 AM - Teemu Murtola

- *Category set to testing*

#4 - 07/11/2016 08:27 PM - Mark Abraham

- *Target version deleted (5.x)*