

GROMACS - Task #2396

Refactor trajectoryanalysis module to allow handling of trajectory frame manipulation

02/01/2018 11:52 AM - Paul Bauer

Status:	New
Priority:	Normal
Assignee:	Paul Bauer
Category:	analysis tools
Target version:	2021-infrastructure-stable
Difficulty:	uncategorized
Description	
<p>The trajectoryanalysis module works currently with the assumption that all data sets are of a type such as</p> <ul style="list-style-type: none">• index , value , deviation <p>This makes it more difficult to use the machinery for something like trajectory file manipulation or internal manipulation of coordinate frames.</p> <p>A proposed change is to move the declaration of the per-frame data structures to the individual analysis modules, so that each module could declare different kinds of data handlers that are distinct from the currently implemented types in analysisdata.h.</p> <p>One issue that Teemu has already raised is that this would remove the option to run the analysis in parallel, which should be avoided. I don't know if there would be a way around this by keeping the original structure and adding a different abstraction layer between the different kinds of data handled during the analysis.</p>	

Associated revisions

Revision b3e33ada - 09/09/2019 02:32 PM - Paul Bauer

Add gmx convert-trj

Adds a new module gmx convert-trj, aimed at providing the minimal functionality to convert different GROMACS supported trajectory formats into each other, as well as supporting selections to chose atoms for writing to disk.

The tool is based on the OutputManager and OutputAdapter framework for writing new trajectory files and for setting meta information in the coordinate datastructures.

Refs #2115, #2396

Change-Id: I1413721faa1383a9d3b8f14cdbea2bcc3089273f

History

#1 - 02/01/2018 12:16 PM - Gerrit Code Review Bot

Gerrit received a related patchset '4' for Issue [#2396](#).

Uploader: Paul Bauer (paul.bauer.q@gmail.com)

Change-Id: gromacs~master~l6bbb5c803c246cbea66470bccbd0d00d0bad0931

Gerrit URL: <https://gerrit.gromacs.org/7529>

#2 - 02/01/2018 04:20 PM - Teemu Murtola

I don't understand what your problem is. Using any of analysisdata, or even the per-frame data objects, is completely opt-in in the framework. You can perfectly well put arbitrary objects in your analysis module, or in a custom per-frame data structure, and at most you will lose the ability to run that particular tool with the simple parallelism scheme that is in the background (but has never been implemented). None of this should require removing any existing code or functionality.

#3 - 02/05/2018 04:01 PM - Paul Bauer

ok, then I didn't understand the code good enough for this, sorry.

I'll remove the linked change then again and will upload a proposal for a change that will introduce coordinate data handling and internal storage to the general framework.

Thanks for your advice and for setting me right on this.

#4 - 02/09/2018 01:30 PM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '1' for Issue [#2396](#).
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~master~19d8717c7a6a708f9bdd83e3a8cc478b5a8725be6
Gerrit URL: <https://gerrit.gromacs.org/7561>

#5 - 02/27/2018 03:30 PM - Gerrit Code Review Bot

Gerrit received a related patchset '3' for Issue [#2396](#).
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~master~1b9040c37d4b3b3d7ff2a83bfe356dbedc32b6403
Gerrit URL: <https://gerrit.gromacs.org/7627>

#6 - 10/02/2018 09:04 AM - Gerrit Code Review Bot

Gerrit received a related patchset '13' for Issue [#2396](#).
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~master~11413721faa1383a9d3b8f14cdbea2bcc3089273f
Gerrit URL: <https://gerrit.gromacs.org/8285>

#7 - 10/08/2018 07:29 PM - Mark Abraham

- Target version changed from 2019 to 2020

#8 - 12/02/2019 01:24 PM - Paul Bauer

- Target version changed from 2020 to 2021-infrastructure-stable

only halfway done