GROMACS - Task #2115

trjconv does too many things, and combinations of them work poorly

02/06/2017 04:20 PM - Mark Abraham

Status:	New	
Priority:	Normal	
Assignee:		
Category:	analysis tools	
Target version:		
Difficulty:	uncategorized	

Description

For now, this issue is just collecting links to related Redmine issues (including fixed and unfixed bugs, and feature requests).

How we want this to work via modular components will likely need to consider the needs of a future (e.g. python) API.

Related issues:

Related to GROMACS - Bug #2052: trjconv does not recognize periodic molecules	**New**	
Related to GROMACS - Bug #1832: 'gmx trjconv -dump t' gives no output if t ...	**Closed**	
Related to GROMACS - Bug #2114: gmx trjconv -pbc cluster claims to have -clus...	**Closed**	
Related to GROMACS - Bug #1705: trjcat append feature is broken	**Closed**	
Related to GROMACS - Feature #1167: trjconv -center would be more intuitive i...	**New**	02/28/2013
Related to GROMACS - Bug #2081: trjconv should respect "-pbc whole" when anot...	**Closed**	
Related to GROMACS - Task #2166: gmx trjconv functionality should check for m...	**Accepted**	
Related to GROMACS - Bug #2225: gmx trjcat -o pdb doesn't work	**Closed**	

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 - 02/06/2017 04:20 PM - Mark Abraham

- Related to Bug #2052: trjconv does not recognize periodic molecules added

#2 - 02/06/2017 04:20 PM - Mark Abraham

- Related to Bug #1832: 'gmx trjconv -dump t'   gives no output if t < frame timestep added

#3 - 02/06/2017 04:20 PM - Mark Abraham

- Related to Bug #2114: gmx trjconv -pbc cluster claims to have -clustercenter option but does not (5.1.2) added

#4 - 02/06/2017 04:21 PM - Mark Abraham

Many commits have just fixed things without referencing an issue, including 91fd36e3

#5 - 02/06/2017 04:21 PM - Mark Abraham

- Related to Bug #1705: trjcat append feature is broken added

#6 - 02/06/2017 04:21 PM - Mark Abraham

- Related to Feature #1167: trjconv -center would be more intuitive if it centered the center of mass, not the midpoint between minimum and maximum values added

#7 - 02/06/2017 04:22 PM - Mark Abraham

- Related to Bug #2081: trjconv should respect "-pbc whole" when another flag "-sep" is used added

#8 - 05/05/2017 04:16 PM - Mark Abraham

- Related to Task #2166: gmx trjconv functionality should check for mismatch between the tpr and the trajectory added

#9 - 08/03/2017 11:35 PM - Mark Abraham

- Related to Bug #2225: gmx trjcat -o pdb doesn't work added

#10 - 01/19/2018 04:48 PM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '1' for Issue [#2115](#).
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~master~I0e7a761ecd1b425254fa027675b528c4e3c3b39e
Gerrit URL: https://gerrit.gromacs.org/7500

#11 - 02/09/2018 01:30 PM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '1' for Issue [#2115](#).
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~master~I9d8717c7a6a708f9bdd83e3a8cc478b5a8725be6
Gerrit URL: https://gerrit.gromacs.org/7561

#12 - 02/09/2018 04:13 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2115](#).
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~master~Ie91d620c0ea25b7436f5745626b973ec97175d29
Gerrit URL: https://gerrit.gromacs.org/7562

#13 - 10/02/2018 09:04 AM - Gerrit Code Review Bot

Gerrit received a related patchset '13' for Issue [#2115](#).
Uploader: Paul Bauer (paul.bauer.q@gmail.com)
Change-Id: gromacs~master~I1413721faa1383a9d3b8f14cdbea2bcc3089273f
Gerrit URL: https://gerrit.gromacs.org/8285