GROMACS - Feature #2597

gmx cluster improuvement

08/07/2018 10:05 AM - Boris Timofeev

Status:	Closed	
Priority:	Normal	
Assignee:	David van der Spoel	
Category:	analysis tools	
Target version:	2019	
Difficulty:	simple	

Description

In processing of results of REMD there were inconveniences which, I think,
it will be easy to eliminate in future versions of Gromacs.
1. Command
gmx cluster ... -cl somefile.pdb ...
unlike command
gmx trjconv ... -o somefile.pdb ...
doesn't form record about the box sizes in the PDB file:
CRYST1 boxx boxy boxz ...
As a result, subsequent call
gmx hbond .. -f somefile.pdb ....
deals to the error:
Program: gmx hbond, version 2016.2
Source file: src\gromacs\gmxana\gmx_hbond.cpp (line 947)
Fatal error:
Your computational box has shrunk too much.
gmx hbond can not handle this situation, sorry.
Manual addition the record CRYST1 to pdb-file solves this problem.
I suggest to add formation of the record CRYST1 to output pdb,
formed by the gmx cluster command.
2. The gmx trjconv command can select parts of a trajectory by means of the index file: - sub index.ndx:
"Use option -sub. This assumes that the entries in the index file are frame numbers and
dumps each group in the index file to a separate trajectory file."
It would be very convenient if the "gmx cluster" command could form,
optionally, index files for the found clusters.
Now this problem is solved by copying of times from gmx cluster command's log-file
and transformation of times to indexes of frames manually. This is very uncomfortable.

I have already made changes in gmx_cluster.cpp code, having solved both problems. An array of boxes and an array of frame numbers are formed similar to the array of frames times at extraction of trajectories. Please, revise it.

Associated revisions

Revision c1c230e9 - 08/28/2018 04:10 PM - boristim

Updates to gmx cluster

As proposed by Boris Timofeev on redmine, this adds to ability
of writing CRYST information to output pdb files, as well as
writing index files for generated clusters.

Fixes #2597

Change-Id: I991889d4116f096a58a22d5482420f0ddc6d0ef9

History

#1 - 08/13/2018 04:19 PM - Paul Bauer

Hello, please upload your change to gerrit.gromacs.org for code review! :) Or if you did so already, please link the redmine issue in the code commit.

#2 - 08/25/2018 12:43 PM - Gerrit Code Review Bot

Gerrit received a related patchset '2' for Issue #2597.
Uploader: Paul Bauer (paul.bauer.q@gmail.com)

Change-Id: gromacs~master~I991889d4116f096a58a22d5482420f0ddc6d0ef9
Gerrit URL: https://gerrit.gromacs.org/8253

#3 - 08/27/2018 11:56 AM - Mark Abraham

- Target version changed from 2016.6 to 2019

Thanks for the suggestion. Features need to be targeted no earlier than the next release, ie 2019. But the idea and implementation seems pretty good :-)

#4 - 08/28/2018 04:11 PM - Mark Abraham

- Status changed from New to Resolved

#5 - 08/28/2018 04:15 PM - Anonymous

Applied in changeset c1c230e934c6af939258ace0423b23151a970e35.

#6 - 09/03/2018 02:03 PM - Paul Bauer

- Status changed from Resolved to Closed

Files

gmx_cluster.cpp	61.2 KB	08/07/2018	Boris Timofeev