GROMACS - Task #2133

GMX TRAJ NEEDS REFORM
03/07/2017 12:03 PM - Mark Abraham

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

Description
GMX TRAJ DOES TOO MANY THINGS THAT CONFLICT WITH EACH OTHER.

THE XVG WRITTEN BY -AV AND -AX DOES NOT DESCRIBE THE Y AXIS ADEQUATELY.

THE IMPLMENTS OF THINGS LIKE -AV AND -CV ARE CONFLATED TO THE POINT THAT YOU CANT DUMP THE AVERAGE VELOCITIES OF A GROUP PER FRAME TO XVG UNLESS YOU PROVIDE A TOPOLOGY (BECAUSE YOU NEED THAT FOR IMPLEMENTING -CV). SAME FOR -AF AND -CF.

THERE SHOULD NOT BE A DISTINCT IMPLEMENTATION OF PBC HANDLING IN REMOVE_JUMP.

THE -VD OPTION SHOULD PROBABLY NOT ROLL ITS OWN HISTOGRAM IMPLEMENTATION.

Associated revisions
Revision a2d8c56c - 03/07/2017 02:01 PM - Mark Abraham
Fix minor issues in gmx traj -av -af

Made the description of the xvg y-axis more useful. Also works for option -af.

Refs #2133

Change-Id: If3796ddbd9841fc442b765afab9ad249954f9316

History
#1 - 03/07/2017 01:15 PM - Mark Abraham
- Description updated

#2 - 03/07/2017 01:19 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2133.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: If3796ddbd9841fc442b765afab9ad249954f9316
Gerrit URL: https://gerrit.gromacs.org/6500

#3 - 03/07/2017 02:02 PM - Teemu Murtola
This should also be compared with gmx trajectory. Probably some of the existing functionality in gmx traj would fit there (I just put the bare minimum to support writing out trajectories from selections), but some of the existing options would probably better fit into a separate tool. And generic abilities like removing jumps would probably better go into the framework instead of individual tools.