GROMACS - Task #2133

**gmx traj needs reform**

03/07/2017 12:03 PM - Mark Abraham

<table>
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<th>Status:</th>
<th>New</th>
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**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 implementations of things like `-av` and `-cv` are conflated to the point that you can't 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: lfl3796ddbd9841fc442b765afab9ad249954f9316

**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: gromacs~release-2016-lfl3796ddbd9841fc442b765afab9ad249954f9316
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.