GROMACS - Feature #609

suggestion to add titles to columns in g_principal output files

11/03/2010 04:37 AM - Chris Neale

Status: Closed
Priority: Low
Assignee: Erik Lindahl
Category: analysis tools
Target version: 5.0
Difficulty: uncategorized

Description
Suggestion to add comments with titles for each column to axis1.dat axis2.dat axis3.dat and moi.dat out of g_principal.

See, for example, the following post that outlines how, without titles, the current output is counter-intuitive:


Related issues:
Related to GROMACS - Bug #1441: g_principal - bug in output files axis{1,2,3}...
Closed 02/19/2014

Associated revisions
Revision 97c3c3a9 - 06/09/2014 07:48 PM - Erik Lindahl
Fixed the output format of g_principal
Gromacs-4.6 and earlier versions had the output transposed. This patch fixes it such that paxisN.dat contains the x/y/z components of the N:th prinicipal axis. The default file output names have been changed to paxisN.dat to increase the probability that users who rely on old scripts will need to read the help text and find the changed format.
Fixes #1441, related to #609.
Change-Id: lc1ed9370145d3389ae8f43c2a419765dabf3a66f

Revision c72006a0 - 06/23/2014 02:13 PM - Erik Lindahl
Enable xvgr output and labels for g_principal

g_principal now writes proper xgr files instead of raw data files, and the output has more explanatory axis labels as well as legends for the data sets.
Fixes #609.
Change-Id: l1eb7914a25661734e6a95e70413194ef723f9635

History
#1 - 09/22/2011 04:14 PM - Rossen Apostolov
- Description updated
- Assignee changed from Erik Lindahl to David van der Spoel
- Priority changed from Normal to Low
- Target version changed from 4.0.7 to 4.5.6

#2 - 01/09/2013 02:37 AM - Erik Lindahl
- Target version changed from 4.5.6 to 5.0

#3 - 05/22/2014 04:46 PM - Erik Lindahl
- Tracker changed from Bug to Feature
- Target version changed from 5.0 to 5.x
#4 - 05/23/2014 03:55 PM - Rossen Apostolov
- Description updated

#5 - 05/26/2014 03:23 PM - Rossen Apostolov
- Related to Bug #1441: g_principal - bug in output files axis[1,2,3].dat added

#6 - 05/26/2014 03:24 PM - Rossen Apostolov
- Status changed from New to Feedback wanted

related patch in gerrit: https://gerrit.gromacs.org/#/c/3509/

#7 - 06/23/2014 01:02 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #609.
Uploader: Erik Lindahl (erik@kth.se)
Change-Id: I1eb7914a25561734e6a95e70413194ef723f9635
Gerrit URL: https://gerrit.gromacs.org/3661

#8 - 06/23/2014 01:02 PM - Erik Lindahl
- Status changed from Feedback wanted to Fix uploaded

#9 - 06/23/2014 02:15 PM - Erik Lindahl
- Status changed from Fix uploaded to Resolved

#10 - 06/23/2014 02:15 PM - Erik Lindahl
- Status changed from Resolved to Closed

#11 - 07/15/2014 06:40 AM - Teemu Murtola
- Assignee changed from David van der Spoel to Erik Lindahl
- Target version changed from 5.x to 5.0