GROMACS - Bug #783

g_mdmat invalid xvg output for legend. OR: g_mdmat, g_analyze, g_enemat output xmgr xvg format for xmgrace?


Status: Closed
Priority: Low
Assignee: David van der Spoel
Category: analysis tools
Target version: Attached
Affected version - extra info: 4.5.4
Affected version: 4.6.x

Description
Using g_mdmat from GROMACS 4.5.4, the xvg output file formats the legend metadata in a way that xmgrace 5.1.22 does not understand, complaining of "Unallocated set: LEGEND STRING ..." for each legend entry.

Example g_mdmat command:

g_mdmat \
-f testout/20110720-1614/trajectory.trr \
-s tpr/hasyn_0001.tpr \
-n gro/hasyn_0001.ndx \
-mean testout/20110720-1614/mdmat_mean.xpm \
-frames testout/20110720-1614/mdmat_frames.xpm \ 
-no testout/20110720-1614/mdmat_num.xvg

The xvg file produced formats the legend as:

@ legend string 0 "Total/mean"
@ legend string 1 "Total"
@ legend string 2 "Mean"
@ legend string 3 "# atoms"
@ legend string 4 "Mean/# atoms"

but xmgrace wants

@ s0 legend "Total/mean"
@ s1 legend "Total"
@ s2 legend "Mean"
@ s3 legend "# atoms"
@ s4 legend "Mean/# atoms"

... which is how the other g_. utilities that I've used generate it.

I'm not confident enough to suggest a diff, but the string "legend string" appears in these files:
src/tools/gmx_analyze.c lines 552 553
src/tools/gmx_enemat.c lines 417 419 421
src/tools/gmx_mdmat.c lines 324-328
src/gmxlib/xvgr.c line 358 -- again, only for xmgr

My guess is that g_analyze, g_enemat and g_mdmat are producing xmgr format xvg files when they should output xmgrace files.

Associated revisions

Revision 71b52b1b - 04/14/2011 06:05 PM - Mark Abraham
Moved heuristic neighbor-list code into mdlib
Moved heuristic neighbor-list code into mdlib

Moved iterated-constraints code into mdlib

Moved iterated-constraints code into mdlib

Moved various support functions for do_md into mdlib

Make sure figure legends are adapted to xmgr/xmgrace
A few programs were not using the xvgr_legend call. g_mdmat has been modified to use it, and for g_analyse and g_enemat I at least fixed the existing direct-writing code by adding a conditional.
Fixes #783.
Change-Id: I782af539b93737b570f266ba744e718fbd846e5f

Yes you are correct. Those tools should use the function xvgr_legend instead of printing directly. That way the format is correct for both programs.
Could you please upload a patch to gerrit.gromacs.org?

- Priority changed from Normal to Low

Gerrit received a related patchset '1' for Issue #783.
Uploader: Erik Lindahl (erik@kth.se)
Change-Id: I782af539b93737b570f266ba744e718fbd846e5f
Gerrit URL: https://gerrit.gromacs.org/3583

- Status changed from New to Fix uploaded
- Affected version set to 4.6.x

- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 75f84652037affa3e28fbcb651a8769c62f738a9.
- Status changed from Resolved to Closed