GROMACS - Bug #783

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


<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Low</td>
</tr>
<tr>
<td>Assignee:</td>
<td>David van der Spoel</td>
</tr>
<tr>
<td>Category:</td>
<td>analysis tools</td>
</tr>
<tr>
<td>Target version:</td>
<td></td>
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<tr>
<td>Affected version - extra info:</td>
<td>4.5.4</td>
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<tr>
<td>Affected version:</td>
<td>4.6.x</td>
</tr>
<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
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</table>

**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:**

```plaintext
$ 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:

```plaintext
@ legend string 0 "Total/mean"
@ legend string 1 "Total"
@ legend string 2 "Mean"
@ legend string 3 "# atoms"
@ legend string 4 "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
Revision 71b52b1b - 04/14/2011 06:05 PM - Mark Abraham
Moved heuristic neighbor-list code into mdlib

Revision c6619dee - 04/14/2011 06:06 PM - Mark Abraham
Moved iterated-constraints code into mdlib

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Revision 865dd11c - 04/14/2011 06:06 PM - Mark Abraham
Moved various support functions for do_md into mdlib

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Revision 75f84652 - 06/14/2014 06:29 AM - Erik Lindahl
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

History

#1 - 08/05/2012 06:16 AM - Roland Schulz
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?

#2 - 10/17/2012 10:48 PM - Roland Schulz
- Priority changed from Normal to Low

#3 - 06/12/2014 02:41 PM - Gerrit Code Review Bot
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

#4 - 06/12/2014 02:58 PM - Erik Lindahl
- Status changed from New to Fix uploaded
- Affected version set to 4.6.x

#5 - 06/14/2014 06:30 AM - Erik Lindahl
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 75f84652037affa3e28fcb651a8769c672f736a9.
- Status changed from Resolved to Closed