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>
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<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>
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<td>Target version:</td>
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<table>
<thead>
<tr>
<th>Affected version - extra info:</th>
<th>4.5.4</th>
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| 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:

```bash
  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"
```

but xmgrace wants

```plaintext
@ s0 legend "Total/mean"
@ s1 legend "Total"
@ s3 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/tools/gmx_saltbr.c line 252 -- this seems to only be output for xmgr, as (I think) is correct. Maybe that's the problem with g_mdmat?
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
IssueID #783

**Revision 71b52b1b - 04/14/2011 06:05 PM - Mark Abraham**
Moved heuristic neighbor-list code into mdlib
IssueID #783

**Revision c6619dee - 04/14/2011 06:06 PM - Mark Abraham**
Moved iterated-constraints code into mdlib
IssueID #783

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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
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: I782af539b93737b570f266ba744e718fb846e5f
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 75f84652037af539a3e20fcb851a8760c6727736a0.

- Status changed from Resolved to Closed