GROMACS - Bug #1479

g_rama and g_chi print some xvg headers even when -xvg none is set

04/11/2014 04:55 PM - Chris Neale

<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>
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<tr>
<td>Target version:</td>
<td></td>
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<tr>
<td>Affected version - extra info:</td>
<td>5.0-rc1 and 4.6.5</td>
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<tr>
<td>Affected version:</td>
<td>5.0-rc1</td>
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<tr>
<td>Difficulty:</td>
<td>uncategorized</td>
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Description

In gmx_rama.c, should probably protect:

```c
fprintf(out, "@ xaxis tick on\n@ xaxis tick major 60\n@ xaxis tick minor 30\n";
fprintf(out, "@ yaxis tick on\n@ yaxis tick major 60\n@ yaxis tick minor 30\n";
fprintf(out, "@ s0 symbol 2\n@ s0 symbol size 0.4\n@ s0 symbol fill 1\n");
```

with:

```c
if (output_env_get_print_xvgr_codes(oenv))
```

Same thing goes for the following code in gmx_chi.c:

```c
fprintf(fp, "# this effort to set graph size fails unless you run with -autoscale none or -autoscale y flags\n");
fprintf(fp, "@ xaxis tick on\n");
fprintf(fp, "@ xaxis tick major 90\n");
fprintf(fp, "@ xaxis tick minor 30\n");
fprintf(fp, "@ xaxis ticklabel prec 0\n");
fprintf(fp, "@ yaxis tick off\n");
fprintf(fp, "@ yaxis ticklabel off\n");
fprintf(fp, "@ type xy\n");
```

I didn't check all analysis tools, but the same problem likely exists elsewhere as well.

Related issues:

- Related to GROMACS - Bug #1407: xvg information leaks through -xvg none in g_... [Closed 12/13/2013]

Associated revisions

Revision 82f6f587 - 06/11/2014 08:43 PM - Erik Lindahl

Avoid writing xvgr formatting with -xvg none

Several tools were writing xvgr formatting code directly to output files, even when the users selects -xvg none as a command line option.

Fixes #1407, #1479.

Change-Id: 1db1b0c2ad7455332e2a415a922885cddaec5efd1

History

#1 - 04/18/2014 05:42 AM - Teemu Murtola

- Related to Bug #1407: xvg information leaks through -xvg none in g_cluster added

#2 - 06/09/2014 07:59 PM - Gerrit Code Review Bot

Gerrit received a related patchset ‘1’ for Issue #1479.
#3 - 06/09/2014 08:06 PM - Erik Lindahl
- Status changed from New to Fix uploaded

#4 - 06/11/2014 08:45 PM - Erik Lindahl
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 82f6f587e5b29ba0455e02c8e3581dafa72bf554.

#5 - 06/11/2014 11:36 PM - Erik Lindahl
- Status changed from Resolved to Closed