## GROMACS - Bug #785

**Entropy calculation using g_anaeig**  
07/27/2011 12:23 AM - Justin Lemkul

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</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>4.5.6</td>
</tr>
<tr>
<td>Affected version</td>
<td></td>
</tr>
</tbody>
</table>

### Description

There appear to be some issues with the code used to calculate entropy in `g_anaeig`, as reported to the list this morning:


### Associated revisions

**Revision 80a3b80e - 03/05/2012 12:18 PM - Berk Hess**  
added check for mass-weighting with `g_anaeig -entropy`, fixes #785  
Change-Id: I7a1623ba7a7c7987078901876fb4717d8c0a7261

**Revision 80a3b80e - 03/05/2012 12:18 PM - Berk Hess**  
added check for mass-weighting with `g_anaeig -entropy`, fixes #785  
Change-Id: I7a1623ba7a7c7987078901876fb4717d8c0a7261

### History

**#1 - 07/27/2011 12:23 AM - Justin Lemkul**  
- Assignee deleted (David van der Spoel)

**#2 - 08/22/2011 05:03 PM - Berk Hess**  
- Assignee set to David van der Spoel

The `g_anaeig` entropy calculation code seems to assume one unit for the eigenvales, whereas `g_covar` can produce two (length^2 and mass*length^2). This gives unit errors, but also only one of the two would give correct entropies, I assume the masses should not come into play here. Furthermore, the original report complained about possible incorrect use of `g_nmeig` eigenvalues.

**#3 - 09/22/2011 03:49 PM - Rossen Apostolov**  
- Target version changed from 4.5.5 to 4.5.6

**#4 - 03/05/2012 11:57 AM - Rossen Apostolov**  
- Status changed from New to Closed

Berk fixed it in commit:98333af8