### Gromacs - Bug #1387

**Wrong return value in topsort.c**

11/22/2013 11:57 AM - Manuel Luitz

<table>
<thead>
<tr>
<th>Status</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee</td>
<td>Berk Hess</td>
</tr>
<tr>
<td>Category</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version</td>
<td>4.6.5</td>
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<td>Affected version</td>
<td>4.6</td>
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**Description**

Function `gmx_bool gmx_mtop_bondeds_free_energy(const gmx_mtop_t *mtop)` in `src/gmxlib/topsort.c` returns always true. I think the correct return statement should be

```c
return (bPert ? ilsortUNKNOWN : ilsortNO_FE);
```

instead. Please comment.

**Associated revisions**

Revision 99f228b0 - 11/26/2013 11:22 PM - Berk Hess

Fixed return value of `gmx_mtop_bondeds_free_energy`

The return value was always true, which was harmless, since it could only cause a small performance hit of useless sorting.

Fixes #1387

Change-Id: I088a3747ddb3517fbb5e416b791bd542bd49fed2

**History**

#1 - 11/22/2013 12:00 PM - Manuel Luitz

Typo,

return bPert;

should be the correct return statement

#2 - 11/23/2013 01:43 AM - Mark Abraham

- Category set to mdrun
- Status changed from New to Accepted
- Assignee set to Berk Hess
- Target version changed from 4.6.x to 4.6.5

Yes, that looks like a bug introduced in `ec5d23831a6217a92ac4e3dc36d75e93be5236a9` in [http://redmine.gromacs.org/projects/gromacs/repository/revisions/ec5d23831a6217a92ac4e3dc36d75e93be5236a9/diff/src/gmxlib/topsort.c](http://redmine.gromacs.org/projects/gromacs/repository/revisions/ec5d23831a6217a92ac4e3dc36d75e93be5236a9/diff/src/gmxlib/topsort.c)
I uploaded the fix to gerrit.
But this was a harmless issue, since it only caused systems with free-energy on, but no perturbed bondeds to sort the bondeds, without any effect on the order, only a little effect on performance.

Applied in changeset 99f228b04707e025a0fd60518c575c1e974ed162.

#5 - 11/28/2013 07:52 PM - Mark Abraham
- Status changed from Resolved to Closed