GROMACS - Bug #825

pull constraining not functional

10/13/2011 10:04 AM - Berk Hess

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
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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>
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<tr>
<td>Target version:</td>
<td>4.5.6</td>
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<tr>
<td>Affected version - extra info:</td>
<td>4.5.5</td>
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<tr>
<td>Affected version:</td>
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**Difficulty:** uncategorized

**Description**

In version 4.5.5 the constraint pulling is not functional, the pull constraint(s) is/are simply ignored. I introduced this bug when fixing Bug #657.

The simple solution is to change line 527 of src/mdlib/constr.c from

```
bConverged_all = TRUE;
```

to

```
bConverged_all = FALSE;
```

**Associated revisions**

**Revision 633388c6 - 10/13/2011 10:16 AM - Berk Hess**

fixed pull constraining doing nothing, fixes #825

Change-Id: lefadc0bb34241f91998e8d9f974150da54397045

**Revision 633388c6 - 10/13/2011 10:16 AM - Berk Hess**

fixed pull constraining doing nothing, fixes #825

Change-Id: lefadc0bb34241f91998e8d9f974150da54397045

**Revision 4e059f57 - 10/19/2011 05:30 PM - Teemu Murtola**

Merge "fixed pull constraining doing nothing, fixes #825" into release-4-5-patches

**Revision 4e059f57 - 10/19/2011 05:30 PM - Teemu Murtola**

Merge "fixed pull constraining doing nothing, fixes #825" into release-4-5-patches

**History**

#1 - 11/28/2011 09:10 AM - Berk Hess

- Status changed from New to Closed

Fixed.