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>
</thead>
<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</td>
<td>4.5.5</td>
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**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: lefadc0bb34241f191998e8d9f974150da54397045

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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.