## Gromacs - Bug #1316

### distance restraints with multiple pairs segv with OpenMP

08/07/2013 05:35 PM - Berk Hess

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
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</tr>
<tr>
<td>Assignee:</td>
<td>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td></td>
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<tr>
<td>Affected version - extra info:</td>
<td>Affected version: 4.6.3</td>
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### Description

When distance restraints are used with multiple pair distances contributing to one restraint, mdrun will produce a segmentation fault when such pairs in such restraints end up on different OpenMP threads.

### Associated revisions

Revision 1bc53107 - 09/21/2013 09:49 PM - Berk Hess

fixed multiple distance restraints with OpenMP

Distance restraints with multiple pairs (the same label) are no longer split over multiple OpenMP threads. Some (beneficial) reorganization of the bonded thread division was required to do this, most importantly: removed calc_one_bond_foreign.

Fixes #1316

Change-Id: l88d8eafede5cbc26c26c19026a9272639e652f7abd7

### History

**#1 - 09/21/2013 09:50 PM - Berk Hess**

- Status changed from New to Resolved
- % Done changed from 0 to 100

Applied in changeset 1bc531070a94a4d967ad209df71a53069145a85e.

**#2 - 12/03/2013 04:23 PM - Rossen Apostolov**

- Status changed from Resolved to Closed