GROMACS - Bug #1316

distance restraints with multiple pairs segv with OpenMP

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

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version:
Affected version - extra info:
Affected version: 4.6.3

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.

Related issues:
Related to GROMACS - Bug #1917: Bug in calculation of Distance Restraints energy by gmx energy

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: I88d8eafede5cbc26c19026a9272639e652717ab7d

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 1bc53107a94a4d967ad209df71a53069145a85e.

#2 - 12/03/2013 04:23 PM - Rossen Apostolov
- Status changed from Resolved to Closed

#3 - 05/06/2016 09:38 PM - Mark Abraham
- Related to Bug #1917: Bug in calculation of Distance Restraints energy by gmx energy added