simple distance restraints should work with REMD and multiple ranks per simulation

06/12/2016 04:46 PM - Mark Abraham

| Status:    | Closed       |
| Priority:  | Low          |
| Assignee:  | Mark Abraham |
| Category:  | mdrun        |
| Target version: | 5.1.3       |
| Affected version - extra info: | all subsequent versions |
| Affected version: | 4.6          |
| Difficulty: | uncategorized |

Description
This should work just like a non-multi simulation

Related issues:
Related to GROMACS - Bug #1117: ensemble-averaged distance restraints is probably broken
Closed
Related to GROMACS - Bug #2029: mdrun gives different distance restraint pote... Closed

Associated revisions
Revision 58331988 - 06/17/2016 09:08 AM - Mark Abraham
Fix multi-sim + DD + simple distance restraints

The check should not look for the existence of a multi-sim, because the user must also set GMX_DISRE_ENSEMBLE_SIZE in order to get ensemble restraints.

Fixes #1989
Change-Id: ld8c9aeefb17583a6ef9ef5caf46232bc384f2ecd

Revision c1364cf4 - 09/16/2016 10:04 AM - Berk Hess
Made distance restraints work with threads and DD

The NMR distance restraints use several buffers for summing distances that were indexed based on the index of the thread+domain local list force atoms. This gives incorrect results with OpenMP and/or domain decomposition. Using the type index for the restraint and a domain-local, but not thread-local index for the pair resolves these issues. The are now only two limitations left:

- Time-averaged restraint don't work with DD.
- Multiple copies of molecules in the same system without ensemble averaging does not work with DD.

Fixes #1117.
Fixes #1989.
Fixes #2029.
Change-Id: lc51230aa19a4640caca29a7d7ff471e30a3d9f09

History
#1 - 06/12/2016 04:46 PM - Mark Abraham
- Related to Bug #1117: ensemble-averaged distance restraints is probably broken added

#2 - 06/12/2016 04:47 PM - Mark Abraham
reported on gmx-users at https://mailman-1.sys.kth.se/pipermail/gromacs.org_gmx-users/2016-June/106349.html

#3 - 06/12/2016 04:49 PM - Gerrit Code Review Bot
Gerrit received a related patchset ‘1’ for Issue #1989.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: ld8c9aefb17583a6e9e5ca5f4f6232bc384f2ecd
Gerrit URL: https://gerrit.gromacs.org/5950

#4 - 06/17/2016 01:00 PM - Mark Abraham
- Status changed from New to Resolved

Applied in changeset 5833196845cd99accf1a204cf5725233dbed3ef5b.

#5 - 06/22/2016 11:56 PM - Mark Abraham
- Status changed from Resolved to Closed

#6 - 08/10/2016 12:31 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1989.
Uploader: Berk Hess (hess@kth.se)
Change-Id: lc51230aa19a4640caca29a7d7f471e30a3d9f09
Gerrit URL: https://gerrit.gromacs.org/6108

#7 - 08/11/2016 11:25 AM - Szilárd Páll
- Related to Bug #2029: mdrun gives different distance restraint potential energies depending on the number of openMP threads added