Hi,

I got spuriously large distance restraint potential energy when running mdrun with multiple OpenMP threads and the system adopts a weird configuration sooner or later (depending on the restraint force constant) while the same simulation (same tpr file) runs fine. Here are the Dis. Res. related mdp option I used (see the uploaded tpr file for details):

disre = simple
disre-weighting = conservative
disre-tau = 0
disre-fc = 1e-5
nstdisreout = 10000

and I tried mdrun using a single MPI rank and giving 1, 2, 4 to -ntomp and only -ntomp = 1 gave sane results. The log file from the 1 OpenMP thread looks like:

```
Step   Time   Lambda
       0   0.000000   0.00000

Energies (kJ/mol)  
Bond   Angle   G96Angle   LJ (SR)   Coulomb (SR)  
2.16662e+01  0.000000e+00  1.96570e+03   9.15548e+03   0.00000e+00
5.56697e+04  2.90805e+04  6.68126e+04   1.57240e+04   8.25365e+04
Temperature Pressure (bar)  
2.99970e+02  -6.28303e-07
```

while that from 2 OpenMP threads looks like:

```
Step   Time   Lambda
       0   0.000000   0.00000

Energies (kJ/mol)  
Bond   Angle   G96Angle   LJ (SR)   Coulomb (SR)  
2.16662e+01  0.000000e+00  1.96571e+03   9.15548e+03   0.00000e+00
1.96610e+07  4.12632e+05  1.96722e+07   1.57284e+04   1.96879e+07
Temperature Pressure (bar)  
3.00055e+02   5.46943e-06
```

It looks like all the other potential energy terms are the same independent of the number of OpenMP threads except for Dis. Rest.. Can anyone tell me if I'm hitting a bug in GROMACS or if there's something I missed in setting up distance restraint?

Thanks,
Tim
Related to GROMACS - Bug #1117: ensemble-averaged distance restraints is prob...

Closed

Associated revisions

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: lc51230aa19ae640caca29a77ef471e30a3d9f09

History

#1 - 08/10/2016 10:17 AM - Berk Hess
- Category set to mdrun
- Status changed from New to Accepted
- Assignee set to Berk Hess
- Priority changed from High to Normal

I have found the source of this issue.
But it seems to me that you're don't want to do NMR distance restraints, but rather simply restrain distances using a simple potential. For that bonds type 10 is simpler, faster and will work with threads.

#2 - 08/10/2016 12:31 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2029.
Uploader: Berk Hess (hess@kth.se)
Change-Id: lc51230aa19ae640caca29a77ef471e30a3d9f09
Gerrit URL: https://gerrit.gromacs.org/6108

#3 - 08/10/2016 12:32 PM - Berk Hess
- Status changed from Accepted to Fix uploaded
- Target version set to 2016.1

I uploaded a fix for v2016.
But using bonds type 10 is probably the best solution for you.

#4 - 08/11/2016 11:25 AM - Szilárd Páll
- Related to Bug #1989: simple distance restraints should work with REMD and multiple ranks per simulation added

#5 - 08/11/2016 11:25 AM - Szilárd Páll
- Related to Bug #1117: ensemble-averaged distance restraints is probably broken added

#6 - 09/16/2016 05:36 PM - Berk Hess
- Status changed from Fix uploaded to Resolved

Applied in changeset c1364cf4e4b14d3726ed7bcb7caa5c17afbecf7.

#7 - 10/31/2016 11:22 AM - Mark Abraham
- Status changed from Resolved to Closed