

GROMACS - Bug #267

distance restraints and domain decomposition error

12/09/2008 11:47 PM - Anonymous

Status: Closed	
Priority: Normal	
Assignee: Erik Lindahl	
Category: mdrun	
Target version: 4.0	
Affected version - extra info:	Difficulty: uncategorized
Affected version:	
Description	
Created an attachment (id=329) This is the tpr file for the full 1 ns md simulation	
Several attempts have been made to run a simulation on a 13 residue peptide fragment with distance restraints, in parallel. After typing this exact command line for mdrun:	
nohup mpiexec -n 4 nice -19 mdrunmpi -s md.tpr -c md.gro -o md.trr -x md.xtc -e md.edr -g md.log < /dev/null &	
The simulation stopped almost immediately, generating this nohup.out file:	
NNODES=4, MYRANK=0, HOSTNAME=chong06.chem.pitt.edu NNODES=4, MYRANK=1, HOSTNAME=chong06.chem.pitt.edu NNODES=4, MYRANK=3, HOSTNAME=chong06.chem.pitt.edu NNODES=4, MYRANK=2, HOSTNAME=chong06.chem.pitt.edu NODEID=0 argc=13 NODEID=1 argc=13 NODEID=2 argc=13 NODEID=3 argc=13 :-) G R O M A C S (-:	
Great Red Oystich Makes All Chemists Sane	
:-) VERSION 4.0 (-:	
Written by David van der Spoel, Erik Lindahl, Berk Hess, and others. Copyright (c) 1991-2000, University of Groningen, The Netherlands. Copyright (c) 2001-2008, The GROMACS development team, check out http://www.gromacs.org for more information.	
This program is free software; you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation; either version 2 of the License, or (at your option) any later version.	
:-) mdrunmpi (-:	
Option	Filename Type Description

-s	md.tpr Input Run input file: tpr tpb tpa
-o	md.trr Output Full precision trajectory: trr trj cpt
-x	md.xtc Output, Opt! Compressed trajectory (portable xdr format)
-cpi	state.cpt Input, Opt. Checkpoint file
-cpo	state.cpt Output, Opt. Checkpoint file
-c	md.gro Output Structure file: gro g96 pdb
-e	md.edr Output Energy file: edr ene
-g	md.log Output Log file
-dgdl	dgdl.xvg Output, Opt. xvgr/xmgr file
-field	field.xvg Output, Opt. xvgr/xmgr file

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-table  table.svg Input, Opt. xvgr/xmgr file
-tablep tablep.svg Input, Opt. xvgr/xmgr file
-tableb table.svg Input, Opt. xvgr/xmgr file
-rerun  rerun.xtc Input, Opt. Trajectory: xtc trr trj gro g96 pdb cpt
-tpi    tpi.svg Output, Opt. xvgr/xmgr file
-tpid   tpidist.svg Output, Opt. xvgr/xmgr file
-ei     sam.edi Input, Opt. ED sampling input
-eo     sam.edo Output, Opt. ED sampling output
-j      wham.gct Input, Opt. General coupling stuff
-jo     bam.gct Output, Opt. General coupling stuff
-ffout  gct.svg Output, Opt. xvgr/xmgr file
-devout deviatie.svg Output, Opt. xvgr/xmgr file
-runav  runaver.svg Output, Opt. xvgr/xmgr file
-px     pullx.svg Output, Opt. xvgr/xmgr file
-pf     pullf.svg Output, Opt. xvgr/xmgr file
-mtx    nm.mtx Output, Opt. Hessian matrix
-dn     dipole.ndx Output, Opt. Index file

```

Option Type Value Description

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h      bool  no      Print help info and quit
-nice  int    0      Set the nicelevel
-defnm  string  Set the default filename for all file options
[no]xvgr bool  yes    Add specific codes (legends etc.) in the output
xvg files for the xmgrace program
pd     bool  no      Use particle decomposition
-dd    vector  0 0 0  Domain decomposition grid, 0 is optimize
-npme  int    1      Number of separate nodes to be used for PME, -1
is guess
-ddorder enum  interleave DD node order: interleave, pp_pme or cartesian
[no]ddcheck bool  yes    Check for all bonded interactions with DD
rdd    real  0      The maximum distance for bonded interactions with
DD (nm), 0 is determine from initial coordinates
-reon  real  0      Maximum distance for P-LINCS (nm), 0 is estimate
-dlb   enum  auto    Dynamic load balancing (with DD): auto, no or yes
-dds   real  0.8    Minimum allowed dlb scaling of the DD cell size
[no]sum bool  yes    Sum the energies at every step
v      bool  no      Be loud and noisy
[no]compact bool  yes    Write a compact log file
seppot bool  no      Write separate V and dV/dl terms for each
interaction type and node to the log file(s)
-pforce real  1      Print all forces larger than this (kJ/mol nm)
[no]reprod bool  no     Try to avoid optimizations that affect binary
reproducibility
ept    real  15     Checkpoint interval (minutes)
[no]append bool  no     Append to previous output files when restarting
from checkpoint
maxh   real  1      Terminate after 0.99 times this time (hours)
-multi int    0      Do multiple simulations in parallel
-replex int    0      Attempt replica exchange every # steps
-reseed int    1      Seed for replica exchange, 1 is generate a seed
[no]glas bool  no     Do glass simulation with special long range
corrections
-[no]ionize bool  no     Do a simulation including the effect of an X-Ray
bombardment on your system

```

Reading file md.tpr, VERSION 4.0 (single precision)

NOTE: atoms involved in distance restraints should be within the longest cut-off distance, if this is not the case mdrun generates a fatal error, in that case use particle decomposition (mdrun option -pd)

WARNING: Can not write distance restraint data to energy file with domain decomposition
rank 0 in job 57 chong06.chem.pitt.edu_35438 caused collective abort of all ranks
exit status of rank 0: killed by signal 9

As you can see there is only a warning generated but no "fatal error" written anywhere in the output file.

History

#1 - 12/11/2008 10:47 AM - Berk Hess

There are several issues here.

The crash is because of a bug where mdrun wants to print an error, but the log file is not present on all processors and the code does not check for this.

Running mdrun on one processor will give this (cryptic) error/warning in the log file:

There were 14 inconsistent shifts. Check your topology

The problem is that you have distance restraints at 3 nm distance. You said on gmx-users that all restraint distances are within 1 nm, but I this does not seem to be true.

In principle this should work (although not with domain decomposition, since 3 nm is more than half the box length). But the current graph code can not handle bonded interactions that are at more than half the box length.

We should come up with a solution for this.

David and Erik:

Currently the graph is built up in two steps, first the chembond interactions, then all bonded interactions. Currently this is useless, since the end results is simply a graph with all interactions.

What we should do is implement an algorithm that walks over the graph with only the chembonds, so we know if it consists of multiple unlinked parts.

Then we should only add the non-chembond bonded interactions if they connect two different parts.

Berk

#2 - 12/11/2008 03:26 PM - Berk Hess

Created an attachment (id=330)
fixed src/gmxlib/mshift.c

#3 - 12/11/2008 03:27 PM - Berk Hess

Hi,

I fixed the error print bug,
as well as the actual problem that previously
caused the inconsistent shift warnings.

I have attached the fixed mshift.c file.

Berk

#4 - 12/11/2008 04:21 PM - Anonymous

Thanks for all your attention to this bug! I'm just not sure about why the distance restraints are coming up to be 3 nm apart. I'm fairly certain that they are all under 1 nm apart. This is an excerpt of the distance restraints I added to the topology file:

[distance_restraints]

```
;ai aj type index type' low up1 up2 fac
1 72 1 0 1 0.55 0.60 0.65 1.0
5 67 1 1 1 0.52 0.57 0.62 1.0
5 70 1 2 1 0.54 0.59 0.64 1.0
5 72 1 3 1 0.46 0.51 0.56 1.0
16 67 1 4 1 0.51 0.56 0.61 1.0
16 70 1 5 1 0.52 0.57 0.62 1.0
16 72 1 6 1 0.45 0.50 0.55 1.0
5 82 1 7 1 0.54 0.59 0.64 1.0
5 84 1 8 1 0.47 0.52 0.57 1.0
5 88 1 9 1 0.48 0.53 0.58 1.0
16 82 1 10 1 0.51 0.56 0.61 1.0
```

I keep the force constant at 1.0 throughout and I have increased up1 and up2 from the low value by 0.5 nm and 0.1 nm, respectively. My low value is

the distance to which I want the atoms to be restrained. And the cut-off distance I'm using for restraining atoms is 0.55 nm. Also, the atoms pairs are at least 3 residues apart. Maybe I am doing something wrong when I add the restraints into the topology file? But I'm still not sure why it says the distance restraints are 3 nm apart.

Maria

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Berk

#5 - 12/11/2008 05:05 PM - Berk Hess

The upcoming version of mdrun adds more information about bonded distances:
For your system:

Initial maximum inter charge-group distances:
two-body bonded interactions: 2.231 nm, Dis. Rest., atoms 48 114

So your bounds might be small, but the distance restraint still has to work beyond the bound (at least up to 2.23 nm in this case).

Berk

Files

md.tpr	284 KB	12/09/2008	Anonymous
mshift.c	20.9 KB	12/11/2008	Berk Hess