GROMACS - Bug #956

Unit cell expands in X/Y during semiisotropic simulation of an octane slab with 8 threads and -pd but not with 2 threads or when using -dd on 8 threads

06/14/2012 06:59 PM - Chris Neale

<table>
<thead>
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<th>Status:</th>
<th>Closed</th>
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<td>Priority:</td>
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<td>Assignee:</td>
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<td>Category:</td>
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<td>Target version:</td>
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<td>Affected version:</td>
<td>4.5.3 and 4.5.5</td>
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<td>Difficulty:</td>
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Description

The simulation system consists of protein helices embedded in a hydrated octane slab. Pressure coupling is semi-isotropic with the z-dimension fixed by setting its compressibility to zero. This setup is necessary to maintain the octane slab. Furthermore, the use of particle decomposition is necessary because it is our intention to use long distance restraints. Note that the issue occurs in the absence of distance restraints, which are not included in the submitted test system.

The issue is that the box expands without limit (but does not explode or crash) when using particle decomposition on sufficient threads or MPI processes.

In the following, all results were obtained with both version 4.5.3 and 4.5.5, except where noted.

The box is stable with:
- serial simulations (nt=1)
- domain decomposition on 2, 8, or 16 threads or MPI processes
- particle decomposition on 2 threads or MPI processes
- particle decomposition on 8 threads of MPI processes

The box expands without limit with:
- particle decomposition on 8 threads or MPI processes

The simulation crashes with LINCS errors with:
- particle decomposition on 16 threads or MPI processes

I have included everything that you need to reproduce this issue. I have also included the .tpr, .xtc, .edr from a short run in which the simulation box expands. I have also included the output from g_energy selecting volume to show that the box expands.

Note that the .gro file that I have been using for my tests (and that I have included here) is taken from the end of a stable simulation run under gromacs 4.0.7.

This test can be completed in 5 minutes on 8 cores. The number of steps in the .mdp file may take longer to complete, but the box expansion is evident within a few ps.

Please note: This is not my simulation system. It is the system of a colleague of mine that I have been attempting to debug for them. I have, however, looked through the files and believe that they do not contain any obvious errors. Furthermore, the fact that the simulations are stable with domain decomposition or with -pd in gromacs 4.0.7 leads me to believe that this is not an issue with the simulation setup itself.

History

#1 - 06/14/2012 07:14 PM - Chris Neale

Note that I have also tested a few more conditions that do not affect box expansion:

- using the SD integrator
- using ns-type=simple and nstlist=1

#2 - 06/25/2012 04:19 PM - Berk Hess

I reproduced this issue.

Up to 6 MPI threads with PD the results are correct. With -nt 7 or 8 the pressure is off at step 0. Most, but not all, of the virial tensor elements are far...
off and the tensor is asymmetric, quite weird. But I currently don't have time to look further into this.
Note that domain decomposition works fine.

#3 - 07/05/2012 06:45 PM - Berk Hess
I think it has to do with the graph code. I changed the setup of the graphs for 4.6 and in release-4-6 the virial is correct. I don't know if we want to backport this somewhat extensive change to 4.5.

#4 - 10/17/2012 10:22 PM - Roland Schulz
- Status changed from New to Closed
I don't think it makes sense to backport it if it only affects pd and if we anyhow release 4.5.6 and 4.6 at the same time. Please reopen if you disagree.

Files
EXPANDING_BOX.tar.gz 3.81 MB 06/14/2012 Chris Neale