Gromacs - Bug #1467

8-way parallel run of small system does not match forces of single-thread run after first step

03/23/2014 02:58 PM - Erik Lindahl

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>High</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>4.6.6</td>
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<tr>
<td>Affected version - extra info:</td>
<td>Affected version: 4.6.6</td>
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**Description**
When checking energy conservation for a pretty small system (~900 atoms) for different free energy settings, I noticed that the energy conservation appears to depend on the number of cores used, and this is present for non-free-energy runs too. The attached system is a single ethanol in water, 939 atoms, and a rhombic dodecahedron box with side=2.4nm. When running with verlet kernels, reaction-field, lincs-order=3, and DLB, only simulations with a single thread appears to conserve energy, and with 8 cores the drift is horrible.

Even when limiting it to a single step and running with -reprod and -dlb no, there are large differences in forces after the first step. In this case it only appears to affect the 8-core simulation, though the others seem to match the single-core-run. The error is present for group kernels too, and with PME (although the energy drift is smaller there, likely because the direct-space interactions are lower magnitude).

This is using the release-4-6 branch of git, and running on amd1.theophys.kth.se with acceleration enabled.

**Associated revisions**

Revision a586b416 - 03/24/2014 07:26 PM - Berk Hess

    Adds cut-off checks for triclinic domain decomposition

    With domain decomposition and 2 decomposition cells in a trilinic dimension, the cut-off could be longer than the size of the communicated domains. This could lead to some pairs close to cut-off distance to be ignored in the force/energy calculations.
    Fixes #1467

    Change-Id: ld7e16d778fa0796d6add548ad6e8bblb88039ff

**History**

#1 - 03/24/2014 03:47 PM - Berk Hess

    - Priority changed from High to 6

The issue here is that the domain decomposition code does not check if the chosen domain decomposition grid ensures that all atoms required for pairs within the cut-off distance can be communicated. With rectangular boxes or with 3 or more domains in a dimension, the standard check of the cut-off being shorter than half the box size ensures all pairs are available. So this issue only appears for triclinic dimensions with exactly 2 domains. Here some non-bonded energies/forces of pairs close to the cut-off distance could be missing, which can lead to silent errors.

#2 - 03/24/2014 03:47 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #1467.
#3 - 03/28/2014 02:15 AM - Berk Hess
- Status changed from New to Resolved
- % Done changed from 0 to 100

Applied in changeset a586b4168d35113cb5e9f3315aa73bebcf20b1c3.

#4 - 04/03/2014 07:32 PM - Roland Schulz
- Status changed from Resolved to Closed

Files

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<td>380 KB</td>
<td>03/23/2014</td>
<td>Erik Lindahl</td>
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