GROMACS - Bug #2274

Mega - Flops accounting

10/17/2017 05:00 PM - Marie-Madeleine Walz

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>David van der Spoel</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>2016.5</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td>Still a bug in gromacs 2016</td>
</tr>
<tr>
<td>Affected version:</td>
<td>4.6.7</td>
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<tr>
<td>Difficulty:</td>
<td>simple</td>
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</tbody>
</table>

**Description**

In the .log file there is a section called Mega-Flops accounting. Here the "NB VdW [V&F]" counts also the polarization interactions (core-shell model) even though it should not. Even for 0 steps and niter = 0 it counts 1 polarization interaction per particle in the system. The error seems to be in the ifunc.cpp file, where a zero is hard-coded (zero is assigned via enum to "NB VdW [V&F]"). This way the number of polarization interactions ends up in the category of "NB VdW [V&F]."

**Associated revisions**

Revision bd8f4371 - 10/17/2017 10:28 PM - David van der Spoel

Fixed missing entries in nrnb arrays.

Some nrnb index entries were missing in the interaction_function array, others were zero leading to that the wrong megaflops accounting was printed.

Fixes #2274

Change-Id: lc0b05d30eb5fdfeb7f3e822b42ec7ca4cda58bc5

**History**

#1 - 10/17/2017 09:37 PM - Mark Abraham

I'm not sure if we have a relevant category to which accumulate? David or Justin, do you happen to know?

#2 - 10/17/2017 09:40 PM - David van der Spoel

The relevant field in ifunc.cpp is 0 for F_POLARIZE and F_ANHARM_POL, this is used to index the nrnb struct. I can make a fix, but what branch should it be in? This is not crucial so maybe just in master?

#3 - 10/17/2017 09:48 PM - Mark Abraham

David van der Spoel wrote:

The relevant field in ifunc.cpp is 0 for F_POLARIZE and F_ANHARM_POL, this is used to index the nrnb struct. I can make a fix, but what branch should it be in? This is not crucial so maybe just in master?

Indeed, not critical. release-2016 is still open for fixes for anything, but master is fine too

#4 - 10/17/2017 09:52 PM - David van der Spoel

While we're at it, I found this mathematic with indices into an enum in mdlib/sim_util.cpp:

```c
inc_nrb(nrb, enr_nbnnx_kernel_ljc-eNR_NBNXN_LJ_RF+eNR_NBNXN_RF,
inc_nrb(nrb, eNR_NBNXN_ADD_LJ_FSW+(flags & GMX_FORCE_ENERGY) ? 1 : 0),
inc_nrb(nrb, eNR_NBNXN_ADD_LJ_PSW+(flags & GMX_FORCE_ENERGY) ? 1 : 0),
in_nrb(nrb, eNR_NBNXN_ADD_LJ_EWALD+(flags & GMX_FORCE_ENERGY) ? 1 : 0),
```

especially the top one is interesting :)

#5 - 10/17/2017 10:09 PM - David van der Spoel
There are already eNRNB terms for eNR_POLARIZE and eNR_ANHARM_POL.

eNR_UREY_BRADLEY, eNR_CROSS_BOND_BOND, eNR_CROSS_BOND_ANGLE are missing too.

#6 - 10/17/2017 10:28 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #2274.
Uploader: David van der Spoel (davidvanderspoel@gmail.com)
Change-id: gromacs~release-2016~Ic0b05d30eb5fdfeb7f3e822b42ec7ca4cda58bc5
Gerrit URL: https://gerrit.gromacs.org/7949

#7 - 10/19/2017 01:24 PM - David van der Spoel
- Status changed from New to Resolved

Applied in changeset bd8f4371d44e61849405a1262502b57c11cb5d3a.

#8 - 11/12/2017 06:51 PM - Sziárd Páll
- Assignee set to David van der Spoel
- Target version set to 2016.5

#9 - 12/11/2017 12:16 PM - Erik Lindahl
- Status changed from Resolved to Closed