GROMACS - Bug #1873
dEkin/dl parallelization issue
12/10/2015 11:07 AM - Igor Leontyev

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>Mark Abraham</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>5.0.8</td>
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<td>Affected version:</td>
<td></td>
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<tr>
<td>extra info:</td>
<td>probably all versions since about GROMACS 4.0</td>
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<tr>
<td>Affected version:</td>
<td>5.1</td>
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**Difficulty:** uncategorized

**Description**

It looks there is a parallelization bug in computation of "dEkin/dl" term in free energy simulations.

I simulate ddG with gromacs 5.1 and mixed topology, i.e. need dG in protein and in water:

$$ddG = dG(\text{InProtein}) - dG(\text{InWater})$$

The alchemical transformation involves only one atom mutation H->Cl. I expect that dEkin/dl terms InProtein and InWater cancel each other. But it is not always true.

In simulations with 1 or 2 OMP threads thread-MPI ranks I get <dEkin/dl> value about 130 kJ/mol, with 4 or 8 threads <dEkin/dl> drops down to ~ 65 kJ/mol and with 16 threads it drops down again about twice.

Attached are tpr-file and log-files for 2, 4 and 8 thread simulations. 30 ps which I ran these short tests is not totally sufficient to get completely converged <dEkin/dl> value, but enough to see the qualitative difference between 2 and 4-8 thread simulations.

**Associated revisions**

Revision 414747c9 - 02/03/2016 01:02 PM - Mark Abraham

Fix dEkin/dl handling with multiple ranks

With non-vv integrators, enerd->dekindl was computed at nstglobalcomm-1 step, but not accumulated across ranks unless bGStat also happened to be true. Then at the next (ie nstglobalcomm) step, bGStat and bEkinhOld were true, so calc_ke_part copied the values into enerd->ekindl_old. These were then not accumulated, so sum_ekin averaged the accumulated enerd->ekind with the non-accumulated enerd->ekind_old to store in enerd->dvdl_lin[efptMASS]. So, it seems likely that mass-perturbed free-energy calculations with multiple ranks have been broken with (at least) non-vv integrators for a long time (perhaps since 031a8b58f).

Fixes #1873

Change-Id: i262e3cfc97a50e1a343563134c7ba89539bba59a

**History**

#1 - 01/13/2016 04:42 PM - Mark Abraham

- Description updated
- Status changed from New to Accepted

There's definitely problems here, Igor, can you please also share a tarball of grompp inputs? I would like to be able to change the integrator and cutoff scheme while diagnosing what is wrong with the code. (Side point Igor, you using the group scheme, which does not support OpenMP, so your threads are those of thread-MPI, creating multiple ranks.)

With your .tpr (SD + FE, group scheme with nstlist 10) and release-5-1 branch HEAD (double, MPI), doing gmx_mpi_d mdrun -np [124] -nsteps 1 everything agrees. With -nsteps 2, I see

<table>
<thead>
<tr>
<th>ranks_01.log:</th>
<th>Step</th>
<th>Time</th>
<th>Lambda</th>
</tr>
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<tr>
<td></td>
<td>0</td>
<td>0.00000</td>
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<tbody>
<tr>
<td></td>
<td>-4.78635e+04</td>
<td>8.29309e+01</td>
<td>-1.31394e+05</td>
<td>2.88844e+04</td>
</tr>
</tbody>
</table>

02/23/2020 1/3
ie. the KE and Temperature on step 2 is wrong with multiple ranks but eKin/dl is OK. (Same pattern for -nsteps 9, of course.)

With -nsteps 10,

```
ranks_01.log: Step Time Lambda
ranks_01.log-  0  0.00000  0.00000
--
ranks_01.log- -4.78635e+04  8.29309e+01 -1.31394e+05  2.88844e+04 -1.02510e+05
--
ranks_01.log: Temperature Pres. DC (bar) Pressure (bar) dEkin/dl dBVoul/dl
ranks_01.log-  7.45598e+02 -3.44867e+02  4.72019e+03  6.80340e+01  1.01129e+02
--
ranks_01.log: Step Time Lambda
ranks_01.log-  10  0.01000  0.00000
--
ranks_01.log- -4.79354e+04  7.98044e+01 -1.31746e+05  2.91660e+04 -1.02580e+05
--
ranks_01.log: Temperature Pres. DC (bar) Pressure (bar) dEkin/dl dBVoul/dl
ranks_01.log-  3.00742e+02 -3.44277e+02 -8.55108e+02  4.70784e+01 -6.86837e+01
--
ranks_01.log: Step Time Lambda
ranks_01.log-  10  0.01000  0.00000
--
ranks_02.log: Step Time Lambda
ranks_02.log-  0  0.00000  0.00000
--
ranks_02.log- -4.78635e+04  8.29309e+01 -1.31394e+05  2.88844e+04 -1.02510e+05
--
ranks_02.log: Temperature Pres. DC (bar) Pressure (bar) dEkin/dl dBVoul/dl
ranks_02.log-  7.45598e+02 -3.44867e+02  4.72019e+03  6.80340e+01  1.01129e+02
--
ranks_02.log: Step Time Lambda
ranks_02.log-  10  0.01000  0.00000
--
ranks_04.log: Step Time Lambda
ranks_04.log-  0  0.00000  0.00000
--
ranks_04.log- -4.78635e+04  8.29309e+01 -1.31394e+05  2.88844e+04 -1.02510e+05
--
ranks_04.log: Temperature Pres. DC (bar) Pressure (bar) dEkin/dl dBVoul/dl
ranks_04.log-  7.45598e+02 -3.44867e+02  4.72019e+03  6.80340e+01  1.01129e+02
--
ranks_04.log: Step Time Lambda
ranks_04.log-  10  0.01000  0.00000
--
```
ie, the KE and Temperature are now fine, but deEkin/dl has problems once there are more than 2 ranks (confirmed with 3, 5, 6 and 8 ranks also). 3-6 ranks still use a 1D decomposition, 8 uses 2D, and all report the same value for eKin/dl at step 10.

So, it looks like the reduction of KE is wrong for terminating non-nstlist steps, and the reduction of deEkin/dl is wrong for nstlist steps.

#2 - 01/14/2016 08:14 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1873.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I262e3cfc97a50e1a343563134c7ba89539bba59a
Gerrit URL: https://gerrit.gromacs.org/5550

#3 - 01/14/2016 08:16 PM - Mark Abraham
- Assignee set to Mark Abraham
- Target version set to 5.0.8
- Affected version - extra info set to probably all versions since about GROMACS 4.0

Yeah, the handling of enerd->dekindl is not right with multiple ranks. At step 9, it isn't accumulated (because !bGStat), then at step 10 it's immediately copied to enerd->dekindl_old. This issue seems to have been present for a long time.

I've uploaded a candidate fix, but I need to try some other integrators and stuff before we can feel any confidence about this.

#4 - 01/18/2016 12:50 PM - Gerrit Code Review Bot
Gerrit received a related patchset '1' for Issue #1873.
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: I8d4d69de2ceabe0b13b5aaeea31edb988b100a3
Gerrit URL: https://gerrit.gromacs.org/5554

#5 - 02/01/2016 10:13 PM - Mark Abraham
- Status changed from Accepted to Fix uploaded

#6 - 02/03/2016 01:15 PM - Mark Abraham
- Status changed from Fix uploaded to Resolved

Applied in changeset 414747c947e130ac0dc58f0a587a95016dcf2e5d.

#7 - 02/03/2016 01:50 PM - Mark Abraham
- Status changed from Resolved to Closed