GROMACS - Bug #3396
Gromacs 2019.4 extreme high potential energy
02/25/2020 01:52 AM - Chenou Zhang

<table>
<thead>
<tr>
<th>Status:</th>
<th>Rejected</th>
</tr>
</thead>
<tbody>
<tr>
<td>Priority:</td>
<td>Normal</td>
</tr>
<tr>
<td>Assignee:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td></td>
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<tr>
<td>Affected version:</td>
<td>2019.4</td>
</tr>
<tr>
<td>Affected version - extra info:</td>
<td></td>
</tr>
<tr>
<td>Difficulty:</td>
<td>Uncategorized</td>
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Description

Issue:
Running gromacs over multiple GPUs sometimes produce weird high potential energy and the code seems to be still happy to run with it.

Here is a example one step output from one of those runs (md_seed_fixed.part0001.log):

```
Energies (kJ/mol)
Bond          U-B    Proper Dih.  Improper Dih.      CMAP Dih.
3.74931e+04    1.79391e+05    1.23103e+05    3.00044e+03   -7.96174e+02
2.59184e+04    5.11243e+05    1.04424e+04   -2.06586e+06    5.35435e+03
Potential    Kinetic En.   Total Energy  Conserved En.    Temperature
*-7.62391e+12*    4.83443e+05   *-7.62391e+12*   *-7.62391e+12*    3.61030e+02
Pressure (bar)   Constr. rmsd
1.00485e+02    4.53814e-06
```

Here is the example run command for gromacs (benchmark.slurm)
```
gmx mdrun -v -s $TPR -deffnm md_seed_fixed -ntmpi 8 -pin on -nb gpu -ntomp 3 -pme gpu -pmefft gpu -npme 1 -gputasks 00112233 -maxh $HOURS -cpt 60 -cpi -noappend
```

Given the fact that we've tested different protein systems on different computing clusters (say ASU agave and PSC Bridges), we believe this issue is not related to specific hardware.

We tested same system on single GPU, with run command:
```
gmx mdrun -v -s $TPR -deffnm md -maxh $HOURS -cpt 60 -cpi -noappend
```

No such issue observed.

Expected behavior:
Yielding at me for producing such high potential energy and exit the simulation.
Or produce regular potential energy.

Related issues:
Is duplicate of GROMACS - Bug #3120: Uninitialized energy and virial contribu...  Closed

History

#1 - 02/25/2020 03:56 PM - Paul Bauer
- Is duplicate of Bug #3120: Uninitialized energy and virial contributions with PME on GPU on PME-only rank added

#2 - 02/25/2020 03:56 PM - Paul Bauer
- Status changed from New to Rejected

this should have been fixed already

Files

<table>
<thead>
<tr>
<th>File</th>
<th>Size</th>
<th>Date</th>
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<tbody>
<tr>
<td>md_seed_fixed.tpr</td>
<td>7.28 MB</td>
<td>02/25/2020</td>
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