GROMACS - Bug #2950

wrong temperature reported at end of sim with uneven number of steps

05/13/2019 03:13 PM - Marvin Bernhardt

Status:	Closed		
Priority:	Normal		
Assignee:	Berk Hess		
Category:	mdrun		
Target version:	2019.4		
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	2019.2		

Description

For one of my simulations i get a temperature of 3000 K reported for the last bit of 333333 steps, where it was equilibrated around 298.15 K before.

I tried to reproduce this with 333 steps, but that did not result in a spike. Therefore I include the ener.edr file. Using gmx dump, one sees the spike is in the .edr file, so this is not a problem of gmx energy.

Associated revisions

Revision 147f664d - 10/01/2019 09:03 AM - Pascal Merz

Output correct kinetic at last step (modular simulator)

This replicates the fix in I9a0bc228 for the modular simulator.

Fixes a bug which would write an incorrect kinetic energy and
temperature to the energy and log files when using the leap-frog
integrator and having a last step not coinciding with an energy
calculation step.

Refs #2950

Change-Id: I9969fa8114240145d9aa84f381a898bbb7570b75

Revision a2afb057 - 10/01/2019 09:03 AM - Berk Hess

Always output correct kinetic at last step

When the last step did not coincide with an energy calculation step,
the kinetic energy and temperature written to the energy and log
file were incorrect when using the leap frog integrator.

Fixes #2950

Change-Id: I9a0bc2280235f233a37cd3b2cd03d9d5067bd4f9

History

#1 - 07/08/2019 12:59 PM - Paul Bauer

- File ener_3333steps.edr added

- Category set to mdrun

- Status changed from New to Accepted

- Assignee set to Paul Bauer

- Target version set to 2019.4

I just reproduced this with 3333 steps in a debug build on my machine.

#2 - 07/08/2019 01:44 PM - Paul Bauer

- File 3355.tpr added

- File ener_3355steps.edr added

- File md_3355steps.log added

so, investigating further I found that the only thing significantly diverging between the average and final write step energies is the kinetic energy contribution

The results here are from extending the previous 3333 step run to 3355 steps to have a fast reproducer

```
   Energies (kJ/mol)
           Bond           Angle Ryckaert-Bell.          LJ-14     Coulomb-14
    5.87965e+03    3.71328e+04    6.73000e+03    0.00000e+00    6.87208e+04
        LJ (SR)   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.
   -8.25315e+03   -2.94160e+05    2.65487e+03   -1.81295e+05    1.66365e+06
   Total Energy  Conserved En.    Temperature Pressure (bar)   Constr. rmsd
    1.48235e+06    1.48278e+06    4.63189e+03    4.11956e+04    1.81575e-06

        <======  ###############  ==>
        <====  A V E R A G E S  ====>
        <==  ###############  ======>

        Statistics over 3356 steps using 34 frames

   Energies (kJ/mol)
           Bond           Angle Ryckaert-Bell.          LJ-14     Coulomb-14
    6.11285e+03    3.70713e+04    6.90941e+03    0.00000e+00    6.86842e+04
        LJ (SR)   Coulomb (SR)   Coul. recip.      Potential    Kinetic En.
   -8.27930e+03   -2.93863e+05    2.67504e+03   -1.80689e+05    1.07054e+05
   Total Energy  Conserved En.    Temperature Pressure (bar)   Constr. rmsd
   -7.36357e+04   -7.37932e+04    2.98057e+02   -2.11207e+01    0.00000e+00
```

The kinetic energy seems to be wrong by a factor of 10.

#3 - 09/25/2019 11:54 AM - Paul Bauer

@Berk, could this just be an issue with the summation?

#4 - 09/30/2019 11:54 AM - Paul Bauer

- Status changed from Accepted to Fix uploaded

- Assignee changed from Paul Bauer to Berk Hess

#5 - 09/30/2019 12:49 PM - Paul Bauer

please try the fix here: https://gerrit.gromacs.org/c/gromacs/+/13478

#6 - 09/30/2019 03:59 PM - Marvin Bernhardt

Any tip on how to provoke the wrong temperature without running all 333333 steps?
I tried with 3333 steps, but don't get a spike with a not-fixed-2019.3
I also had a look at the fix, but I do not really get what the expression

```
step_rel + 1 == ir->nsteps
```

does.

#7 - 10/01/2019 09:15 AM - Berk Hess

- Status changed from Fix uploaded to Resolved

Applied in changeset a2afb057bea44951f1ec71c617ea3231346ec5e0.

#8 - 10/01/2019 11:10 AM - Paul Bauer

- Status changed from Resolved to Closed

#9 - 10/01/2019 11:13 AM - Marvin Bernhardt

Thanks for taking care of this.

Files

ener.edr	822 KB	05/13/2019	Marvin Bernhardt
grompp.mdp	540 Bytes	05/13/2019	Marvin Bernhardt

conf.gro	3.05 MB	05/13/2019	Marvin Bernhardt
ffbonded.itp	205 KB	05/13/2019	Marvin Bernhardt
ffnonbonded.itp	61.5 KB	05/13/2019	Marvin Bernhardt
forcefield.itp	862 Bytes	05/13/2019	Marvin Bernhardt
MET.itp	880 Bytes	05/13/2019	Marvin Bernhardt
SOL.itp	1.09 KB	05/13/2019	Marvin Bernhardt
topol.top	135 Bytes	05/13/2019	Marvin Bernhardt
ener_3333steps.edr	9.67 KB	07/08/2019	Paul Bauer
3355.tpr	1.08 MB	07/08/2019	Paul Bauer
ener_3355steps.edr	9.67 KB	07/08/2019	Paul Bauer
md_3355steps.log	52.1 KB	07/08/2019	Paul Bauer