Strange Fluctuations with NH+PR coupling in GROMACS 2018.3

I recently bought a workstation with Intel Xeon CPUs and 3 Nvidia Tesla P100 GPUs. I inteded to perform simulations on pure water. Since I also run water simulations on a CPU-HPC cluster using GROMACS 5.1.4 I wanted to use also this version on the workstation. I could, however, not compile this version on the workstation. Therefore, I decided to use the most recent GROMACS version (2018.3). It compiled fine, but test simulations produced drastically different fluctuations than the simulations using 5.1.4 (same mdp files used).

I also tried with 2018.3 (without GPU support), where I find similarly strange results, and 2016.5, where everything worked fine. The simulations I ran were
- NPT of 1000 TIP4P/2005 molecules at 1bar, 300K
- NPT of 1000 TIP4P/2005 molecules at 1bar, 240K
- Simulated annealing (-30K/ns) of 1000 TIP4P/2005 molecules at 1 bar, starting from 240 K (Nose-Hoover and Parrinello-Rahman thermo- and barostats used.)

Attached you find simulation data of all runs showing potential energy (U), T, P, and density. At 300 K the results are similar for all versions used (T300.png). At 240 K (T240K.png) and when cooling (COOLING.png) the data obtained from 2018.3 (with and without GPU support) differ markedly from the results obtained with 5.1.4 and 2016.5.

I also performed the 2018.3 tests (including physical validation), which produced 1 error for the GPU version in the complex regression test (see 2018-GPU.txt attached) and 1 error for the CPU only version in the physical validation test ens_water_md_verlet_settle_pme_vr_pr (see 2018-CPU.txt attached). I however, have the feeling that these fails are not responsible for the immensely large fluctuations I find in the simulations.

In the meantime I use 2016.5 for my simulations, but I still tought I'll let you know of this strange behaviour in the 2018.3 version.

In case you need additional information from my side, do not hesitate to contact me.

Best,
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This looks strange.
Could you attach all input files needed to run grompp?

I uploaded archives containing the necessary input files for the three runs performed.

The large fluctuations seem to be caused by using the same resonance time for Nose-Hoover and Parrinello-Rahman. We generally advise against this. Setting tau_p to 2 ps significantly reduces the fluctuations in gmx2018. You might need a larger distance to get acceptable fluctuations. But I have not yet found out why there is a difference in the fluctuations between 2016 and 2018.

I suppose we should add a warning in grompp for setting tau_p equal for Nose-Hoover and Parrinello-Rahman (or four tau_p <= 1.5*tau_t) and advise to have tau_p at least twice as large as tau_t.

Actually the gmx2018 behavior is technically correct, as your gmx2016 runs are affected by bugs #2031 and #2032. Of course gmx2018 is still physically incorrect. For that the only solution is separation between tau_t and tau_p.

I uploaded a fix for gmx 2018.5.
I thought we already had a check for this, but apparently not.

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- Status changed from Resolved to Closed

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