GROMACS - Bug #2416

Task # 2391 (Closed): re-enable TPI test

TPI producing invalid results with nsteps too small

02/19/2018 12:58 PM - Aleksei Iupinov

Status:	Closed			
Priority:	Low			
Assignee:	Berk Hess			
Category:	mdrun			
Target version:	2019			
Affected version - extra info:			**Difficulty:**	uncategorized
Affected version:	2016.4			

Description

Running TPI on a sample system (spc216 with methane) will quietly produce infs/nans if -nsteps argument is set to anything but default value.

gmx mdrun -rerun spc216.gro

or

gmx mdrun -rerun spc216.gro -nsteps -2

```
Reading frame       0 time    0.000   mu  1.368e+01 <mu>  1.368e+01
```

gmx mdrun -rerun spc216.gro -nsteps 20
(value is the same as in the initial mdp)

```
Reading frame       0 time    0.000   mu        inf <mu>        inf
```

(This is likely not the last of it since I'm also getting infs without nsteps but with some other arguments specified)

Associated revisions

Revision 40d8c458 - 02/26/2018 11:31 AM - Aleksei Iupinov

Advice users on infinite output of TPI

Fixes #2416

Change-Id: I6202154bc2a24377d036e5c115f2c90b1c678dda

History

#1 - 02/19/2018 01:50 PM - Aleksei Iupinov

Alright, so Berk has explained to me how this is a feature and not a bug - not getting enough samples with low number of nsteps.
I would still think the output could be a bit more user-friendly.
By the way, nsteps 0 is the special case that prints nan.

#2 - 02/19/2018 04:22 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue #2416.
Uploader: Aleksei Iupinov (a.yupinov@gmail.com)
Change-Id: gromacs~master~I6202154bc2a24377d036e5c115f2c90b1c678dda
Gerrit URL: https://gerrit.gromacs.org/7597

#3 - 02/19/2018 09:24 PM - Berk Hess

- Status changed from New to Fix uploaded

- Priority changed from Normal to Low

- Target version changed from 2016.6 to 2019

#4 - 02/20/2018 11:35 AM - Berk Hess

- Subject changed from TPI producing invalid results with nsteps specified to TPI producing invalid results with nsteps too small

#5 - 02/26/2018 11:45 AM - Aleksei Iupinov

- Status changed from Fix uploaded to Resolved

Applied in changeset 40d8c458c584892f4c263143eb4a479ead1e00dc.

#6 - 03/05/2018 01:35 PM - Mark Abraham

- Status changed from Resolved to Closed