

## GROMACS - Bug #2394

### energy average printing segfaults when no data sets are recorded

01/31/2018 08:52 AM - Mark Abraham

<b>Status:</b>	Closed		
<b>Priority:</b>	Low		
<b>Assignee:</b>	Mark Abraham		
<b>Category:</b>	mdrun		
<b>Target version:</b>	2018.1		
<b>Affected version - extra info:</b>	probably all of them	<b>Difficulty:</b>	uncategorized
<b>Affected version:</b>	2016.5		

#### Description

If no calcenergy steps have added data to mdebin, the printing divides by zero when computing the averages. That's unlikely to be a problem in practice.

#### Associated revisions

##### Revision fb33d1ce - 02/06/2018 04:27 PM - Mark Abraham

Prevent log file energy average printing dividing by zero

If there's not enough data for averages, skip the average printing entirely. In principle, pr\_ekin could be called from elsewhere than print\_ekin, so now we print "N/A" rather than "nan" or segfaulting.

Added some const correctness. Added some tests. Unfortunately they currently have to write a file to disk, but we should have the test before refactoring it to run in memory. The tests needed to be able to clean up their memory, so runner can now also call done\_ekin but for stability we'll leave that off for now.

TODO When merging to master branch enable the call to done\_ekin in runner().

Fixes #2394

Change-Id: Id2e151664dd4553e49880f96bdd90aacc945f992

#### History

##### #1 - 01/31/2018 09:38 AM - Mark Abraham

- Status changed from New to In Progress

##### #2 - 01/31/2018 11:06 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2394](#).  
Uploader: Mark Abraham ([mark.j.abraham@gmail.com](mailto:mark.j.abraham@gmail.com))

**#3 - 01/31/2018 11:10 PM - Mark Abraham**

- Status changed from *In Progress* to *Fix uploaded*

**#4 - 02/06/2018 04:30 PM - Mark Abraham**

- Status changed from *Fix uploaded* to *Resolved*

Applied in changeset [fb33d1ced794c511839d21ed3444325d2db9b728](#).

**#5 - 02/06/2018 04:34 PM - Mark Abraham**

- Status changed from *Resolved* to *Closed*