

## GROMACS - Bug #2781

### mdrun 2018 using SD integrator segfaults when attempting to read from checkpoint file

11/29/2018 02:01 PM - Carsten Kutzner

<b>Status:</b> Closed	
<b>Priority:</b> Normal	
<b>Assignee:</b> Paul Bauer	
<b>Category:</b> mdrun	
<b>Target version:</b> 2019-rc1	
<b>Affected version - extra info:</b> also in the current HEAD of release-2019	<b>Difficulty:</b> uncategorized
<b>Affected version:</b> 2018.3	
<b>Description</b>	
<p>We have a small mixture system of water/alkanol using the SD integrator. It runs fine and stable in v. 2018, however it immediately segfaults when trying to restart from .cpt.</p> <p>Can be reproduced with the attached .tpr:</p> <pre>gmx mdrun -nt 1 -s md.tpr -nsteps 10 gmx mdrun -nt 1 -s md.tpr -cpi</pre> <p>The segv happens in <code>restore_energyhistory_from_state()</code> where the program accesses <code>enerhist-&gt;...</code>, however <code>enerhist</code> is a null pointer.</p>	

#### Associated revisions

##### Revision d5972f77 - 11/29/2018 03:30 PM - Paul Bauer

Fix energy history reading

The energy history could be read as a nullptr from a checkpoint file, leading to issues when trying to restart a simulation. Fixed the logic issue and added an assertion to catch it in the future.

Also removed redundant comparisons to nullptr.

Separate commit on 2018 as per #2770.

Refs #2781

Change-Id: lc584dc92c110065c1650cc1ab0d7ff0a8960fb3a

##### Revision ad77000a - 12/03/2018 10:02 AM - Paul Bauer

Fix energy history reading

The energy history could be read as a nullptr from a checkpoint file, leading to issues when trying to restart a simulation. Fixed the logic issue and added an assertion to catch it in the future.

Also removed redundant comparisons to nullptr.

Fixes #2781

Change-Id: I99ce1a2b932046cab6918ec24b267fc8ff3850ad

#### History

##### #1 - 11/29/2018 02:50 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2781](#).

Uploader: Paul Bauer ([paul.bauer.q@gmail.com](mailto:paul.bauer.q@gmail.com))

Change-Id: gromacs~release-2019~I99ce1a2b932046cab6918ec24b267fc8ff3850ad

Gerrit URL: <https://gerrit.gromacs.org/8759>

##### #2 - 11/29/2018 02:50 PM - Paul Bauer

- Assignee set to Paul Bauer
- Target version set to 2019-rc1
- Affected version - extra info set to also in the current HEAD of release-2019

This is also still present in release 2019. I have a possible fix prepared and will upload it shortly.

**#3 - 11/29/2018 02:51 PM - Gerrit Code Review Bot**

Gerrit received a related patchset '1' for Issue [#2781](#).  
Uploader: Paul Bauer ([paul.bauer.q@gmail.com](mailto:paul.bauer.q@gmail.com))  
Change-Id: gromacs~release-2018~lc584dc92c110065c1650cc1ab0d7ff0a8960fb3a  
Gerrit URL: <https://gerrit.gromacs.org/8760>

**#4 - 12/03/2018 10:15 AM - Paul Bauer**

- Status changed from New to Resolved

Applied in changeset [ad77000af9af50267c9e22891832658e6fdeafa3](#).

**#5 - 12/03/2018 10:55 AM - Paul Bauer**

- Status changed from Resolved to Closed

**Files**

---

md.tpr	275 KB	11/29/2018	Carsten Kutzner
--------	--------	------------	-----------------