

## GROMACS - Feature #1131

### Checkpoint file compatibility 4.5 and 4.6

01/25/2013 12:43 PM - Carsten Kutzner

<b>Status:</b>	Closed
<b>Priority:</b>	Low
<b>Assignee:</b>	Michael Shirts
<b>Category:</b>	mdrun
<b>Target version:</b>	
<b>Difficulty:</b>	uncategorized
<b>Description</b>	
<p>we have a .tpr file here produced with Gromacs 4.0 that runs fine with Gromacs 4.0, 4.5, and 4.6. Also restarts from checkpoint work if one sticks to the same version. However, if I produce a .cpt with Gromacs 4.5 and try to read that into 4.6 I get</p> <p>-----</p> <p>Program mdrun, VERSION 4.6-dev-20130121-bfef29c Source code file: /home/ckutzne/installations/git-gromacs-4-6-department/src/gmxlib/checkpoint.c, line: 405</p> <p>Fatal error: Count mismatch for state entry FE-lambda, code count is 7, file count is 1</p> <p>For more information and tips for troubleshooting, please check the GROMACS website at <a href="http://www.gromacs.org/Documentation/Errors">http://www.gromacs.org/Documentation/Errors</a></p> <p>-----</p> <p>although this is not generally the case, just with this system (which uses free energy).</p>	
<b>Related issues:</b>	
Related to GROMACS - Feature #1230: Addition of Mu-x/y/z to .edr file makes i...	<b>Closed</b> <b>04/24/2013</b>

#### History

##### #1 - 02/26/2013 07:28 PM - Roland Schulz

Could you check whether <https://gerrit.gromacs.org/#/c/2196/> fixes the problem?

##### #2 - 02/27/2013 04:32 PM - Carsten Kutzner

Just checked, it's still the same problem (same error message).

##### #3 - 03/06/2013 02:41 PM - Berk Hess

- Assignee changed from Berk Hess to Michael Shirts

##### #4 - 04/24/2013 10:53 PM - Mark Abraham

- Affected version set to 4.6

Per comment by Berk to the thread on gmx-core that lead to this, we don't guarantee checkpoint file inter-operability between minor releases. I don't know if there is any reasonable work-around here, or even if one would be advisable to use if it existed.

##### #5 - 04/29/2013 07:50 PM - Mark Abraham

- Target version deleted (4.6.1)

##### #6 - 05/23/2014 01:03 AM - Erik Lindahl

- Tracker changed from Bug to Feature

- Status changed from New to Closed

We explicitly don't guarantee checkpoint compatibility between releases, so closing this for now.

