

## GROMACS - Bug #452

### eneconv error with -dt: missing energy sums

06/22/2010 10:41 AM - Teemu Murtola

<b>Status:</b> Closed	
<b>Priority:</b> Normal	
<b>Assignee:</b> Erik Lindahl	
<b>Category:</b> analysis tools	
<b>Target version:</b> CVS	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b>	

#### Description

If one tries to use eneconv -dt with git master (tested with 4.0.99-dev-20100621-d101dcc) to remove some frames from an .edr file, one gets a lot of warnings about missing energy sums, but only for every second frame or so. gmxdump on the original .edr file shows that all sums are present in the file for all frames, so this seems like a bug in eneconv. This also affects the output: the sums are not accumulated over the skipped frames as they should. If -dt is not used, no warnings occur.

I'll attach a .tpr file generated from spc216.gro that runs for 1000 steps and writes energies every 100 frames. Running that, and then running

```
eneconv -f ener.edr -dt 1
outputs (initial parts skipped):
```

```
Reading energy frame 0 time 0.000
Continue writing frames from t=0, step=0
Reading energy frame 2 time 0.400
WARNING: missing energy sums at time 0.400000
Reading energy frame 4 time 0.800
WARNING: missing energy sums at time 0.800000
Reading energy frame 7 time 1.400
WARNING: missing energy sums at time 1.400000
Reading energy frame 9 time 1.800
WARNING: missing energy sums at time 1.800000
Last energy frame read 10 time 2.000
Last step written from test.edr: t 2, step 1000
```

```
Last frame written was at step 1000, time 2.000000
Wrote 3 frames
```

```
gmxdump -e fixed.edr shows that for the last frame, the sums are identical as in the original .edr.
```

#### History

##### #1 - 06/22/2010 11:23 AM - Teemu Murtola

Created an attachment (id=479)  
Simple .tpr file for reproducing the bug.

##### #2 - 06/23/2010 11:31 AM - Berk Hess

I fixed it.

Berk

##### #3 - 06/23/2010 11:44 AM - Rossen Apostolov

Thanks Berk, closing the bug.

#### Files

test.tpr	31 KB	06/22/2010	Teemu Murtola
----------	-------	------------	---------------