

## GROMACS - Bug #3068

### Misleading warning on rerun

08/26/2019 03:44 PM - Semen Yesylevskyy

<b>Status:</b> New	
<b>Priority:</b> Normal	
<b>Assignee:</b>	
<b>Category:</b>	
<b>Target version:</b>	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b> 2019.2	
<b>Description</b>	
<p>When doing `mdrun -rerun` with multiple energy groups the following warning is issued:</p>	
<pre>Multiple energy groups is not implemented for GPUs, falling back to the CPU. For better performance, run on the GPU without energy groups and then do gmx mdrun -rerun option on the trajectory with an energy group .tpr file.</pre>	
<p>However, this is <i>already</i> a rerun i.e. this warning ask one to do what the user is already doing. This is misleading, especially for inexperienced users. This warning should not be issued when `-rerun` flag is used.</p>	