

GROMACS - Task #1246

expanded ensemble .tpr cannot be rerun

05/10/2013 11:44 AM - Mark Abraham

Status:	New	
Priority:	Normal	
Assignee:	Michael Shirts	
Category:	mdrun	
Target version:		
Difficulty:	uncategorized	
Description		
Discussion in https://gerrit.gromacs.org/2368 suggests this is true.		
Sander suggested "Shouldn't there be a corresponding fix in src/gmxlib/trnheader.c? I don't see fep_state being read/written there."		
Michael agreed there was an issue to resolve, and suggested the statement in the title of this issue is true.		
Related issues:		
Related to GROMACS - Task #1868: implement mdrun -rerun better, simplifying d...		Closed

History

#1 - 05/10/2013 04:41 PM - Michael Shirts

When you say "can't be rerun" do you mean crashes, or gives the wrong energies because it is evaluated at the wrong thermodynamics state? I will assume "gives wrong energies" in the rest of this discussion.

rerun with expanded ensemble with a single lambda variable using .trr should work (let me know if it no longer does). fep-state has not been added to the .trr to avoid changing the .trr format as requested by other developers. I would argue it should be added in 5.0.

expanded ensemble with .gro or .xtc cannot work since lambda is not stored in the frame. I don't know if this will ever be changed (might be nice since in a sense lambda / fep state is a coordinate of the frame).

#2 - 05/10/2013 10:58 PM - Mark Abraham

I have no idea. I'm just quoting you in the issue I linked, and trying to avoid losing information when merging a patch!

#3 - 06/18/2015 08:46 PM - Erik Lindahl

Michael: In the commit above you wrote:

"Re Sander's comment -- hmm. I recall now that we didn't include fep state in the .trr because of concern about backportability, so at least for now I guess expanded ensemble runs cannot be -rerun. That should be fixed eventually (perhaps 5.0 if not 4.6.3). However, there is still the issue of fep_state being overwritten, which is fixable with a smaller change."

Could you look into this? There are starting to be a few too many bugs related to free energy that go unaddressed for years.

#4 - 06/19/2015 01:56 PM - Michael Shirts

- *Tracker changed from Bug to Task*

Could you look into this? There are starting to be a few too many bugs related to free energy that go unaddressed for years.

So, can we put the fep state into rerun? "resolve" in this cases is deciding whether or not fep_state can be put into the .trr so that the simulation has history dependence. I would argue that for any method that requires history, there should be a record of this in the .trr.

The alternate is that if it's an expanded ensemble run, a warning is issued that rerunning will not capture changes in lambda (or it fails to rerun).

Or is there some way to get backportability in the .trr that didn't exist earlier?

#5 - 03/06/2018 11:30 PM - Mark Abraham

- *Related to Task #1868: implement mdrun -rerun better, simplifying do_md added*