

GROMACS - Bug #1773

"Lambda" (value of fep-lambdas) is output to log at every step for every simulation

07/13/2015 12:16 AM - James Barnett

Status: Closed	
Priority: Normal	
Assignee: James Barnett	
Category:	
Target version: 2016	
Affected version - extra info:	Difficulty: uncategorized
Affected version: git master	

Description

"Lambda", which seems to be the current value of fep-lambdas, is output to log at every step of every simulation, even in non-free energy simulations and energy minimizations (next to "Time" and "Step"). In the non-free energy case it just outputs 0.00000 at every step, and even in free energy simulations where mdp options such as "coul-lambdas" and "vdw-lambdas" it just outputs zero if "fep-lambdas" is not used. Additionally in regular free energy simulations the lambda values are constant throughout the simulation, so it would be unnecessary to print it every step.

In expanded ensemble simulations it might make sense to print the value, except that it only prints the corresponding value from "fep-lambdas", not "coul-lambdas", "vdw-lambdas", etc. Additionally the expanded ensemble sims output more detail to the log that includes the current lambda values.

Associated revisions

Revision 04212d2b - 10/05/2015 09:30 PM - James Barnett

Remove lambda from print_ebin_header.

Fixes #1773.

Change-Id: I7392623e4ead2568c764847a06391f0ddee4ea2c

History

#1 - 07/13/2015 12:24 AM - Gerrit Code Review Bot

Gerrit received a related DRAFT patchset '2' for Issue [#1773](#).

Uploader: James "Wes" Barnett (jbarnet4@tulane.edu)

Change-Id: I7392623e4ead2568c764847a06391f0ddee4ea2c

Gerrit URL: <https://gerrit.gromacs.org/4889>

#2 - 07/13/2015 12:27 AM - James Barnett

I wasn't sure if the bot would link the draft (first time trying this out, so bear with me), but that's a possible solution (just not printing it at every step), but others may find printing it in some situations useful.

#3 - 07/14/2015 11:46 PM - Mark Abraham

Inasmuch as (hopefully better versions of) lambda values are written to the .edr file, there's no need to have it in the .log file.

If there's value in observing any transitions of the lambda value of the simulation reported in the .log file, then that transition event is reasonable to log independently. But frankly, I can't see that that is useful for more than debugging the .mdp input (except expanded ensemble, which takes care of itself).

So I'm fine with removing this

#4 - 10/05/2015 09:13 PM - Mark Abraham

- Target version set to 2016

#5 - 10/05/2015 09:45 PM - James Barnett

- Status changed from New to Resolved

Applied in changeset [04212d2b9ed83ab2527a8bc6f0813caec6a6300a](#).

#6 - 02/03/2016 01:53 PM - Mark Abraham

- Status changed from Resolved to Closed