GROMACS - Bug #1350

mdrun reinitializing the initial Wang-Landau delta for expanded ensemble simulations when starting from checkpoint

10/03/2013 01:58 AM - Michael Shirts

Status: Closed
Priority: High
Assignee: Michael Shirts
Category: mdrun
Target version: 4.6.4
Affected version: 4.6

Description

mdrun is reinitializing the initial Wang-Landau delta for expanded ensemble simulations, because the data turning it off was stored the expanded ensemble data structure (not saved in cpt) instead of the df_history structure (is saved in checkpoint).

A fix will be uploaded momentarily.

Associated revisions

Revision 771f674a - 10/17/2013 03:49 PM - Michael Shirts

Restarting from checkpoint no longer reinitializes WL weights.

Fixes a problem where mdrun was reinitializing the initial Wang-Landau delta for expanded ensemble simulations, because the flag turning it off was stored the expanded ensemble data structure (not saved in cpt) instead of the df_history structure (is saved in checkpoint). In the process, some moderate encapsulation of the df_history structure and the expanded ensemble methods.

Fixes #1350

Change-Id: I13492a7a9773fcb417fcd0ee106d851d9838ce25

History

#1 - 10/03/2013 02:02 AM - Michael Shirts
- Status changed from New to Fix uploaded

#2 - 10/17/2013 03:50 PM - Michael Shirts
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 771f674a5f7e89195b0c61e77f8db5ba9e6aa507

#3 - 10/17/2013 05:56 PM - Mark Abraham
- Status changed from Resolved to Closed