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