GROMACS - Bug #1321
expanded ensemble simulation using sd integrator
08/19/2013 09:15 PM - Dejun Lin

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

Description
As described here:
http://gromacs.5086.x6.nabble.com/gmx-4-6-1-Expanded-ensemble-weird-balancing-factors-td5007681.html#a5009892
The weighting factors are not calculated correctly when using sd integrator in gromacs 4.6.3.

Associated revisions
Revision 268cad9a - 10/16/2013 01:50 PM - Michael Shirts
turning off expanded ensemble for all integrators but md-vv.

Broke at some point, and somewhat tricky to turn back on
correctly for other integrators at this point; target for
5.0 when it should be more straightforward.

fixes #1321
Change-Id: i599b308800411e0cea111ff280487037d613755

History
#1 - 09/02/2013 05:43 AM - Michael Shirts
- Category set to mdrun
- Status changed from New to Fix uploaded
- Assignee set to Michael Shirts
- Priority changed from Normal to High
- Target version set to 4.6.4
- Affected version changed from 4.6.3 to 4.6

expanded ensemble not working for velocity-half step integrators. Fixes will be complicated to validate for 4.6 because of bookkeeping, better to restrict operation to md-vv for now, and make it work more generally for 5.0.

#2 - 10/16/2013 01:55 PM - Michael Shirts
- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 268cad9a14d7fe4650238b3d960aaab07f77ad3ce.

#3 - 10/16/2013 03:32 PM - Mark Abraham
- Status changed from Resolved to Closed