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

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
<tr>
<td>Priority:</td>
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</tr>
<tr>
<td>Assignee:</td>
<td>Michael Shirts</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>4.6.4</td>
</tr>
<tr>
<td>Difficulty:</td>
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<tr>
<td>Affected version -</td>
<td></td>
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<td>extra info:</td>
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<tr>
<td>Affected version:</td>
<td>4.6</td>
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**Description**

As described here: [http://gromacs.5086.x6.nabble.com/gmx-4-6-1-Expanded-ensemble-weird-balancing-factors-td5007681.html#a5009892](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: i599b308800411e0cea111fffd280487037d613755

**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 268cad9a14d7fe4650238b3d960aaab07f7ad3ce.

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