Expanded ensemble simulation died with fatal error: Something wrong in choosing new lambda state with a Gibbs move

08/02/2013 04:38 AM - Michael Shirts

<table>
<thead>
<tr>
<th>Status:</th>
<th>Closed</th>
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<tbody>
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<td>Priority:</td>
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<tr>
<td>Assignee:</td>
<td>Michael Shirts</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
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<td>Target version:</td>
<td>4.6.4</td>
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<td>Affected version:</td>
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Description

see:


Basic problem: logic was failing for single precision because of round off errors. Solution: convert some of the intermediate arrays into double. Solution is being tested and will be checked in in the next few minutes.

Associated revisions

Revision 0f52b0d0 - 08/02/2013 04:39 AM - Michael Shirts

Fixing problem caused by overflow in expanded ensemble.

Basic problem: logic was failing for single precision because of round off errors. Solution: convert some of the intermediate arrays into double.

Fixes redmine #1314

Change-Id: Id7e3771d257bbeebeed2f340593b817015a0cd4c

History

#1 - 08/02/2013 04:44 AM - Michael Shirts

- Status changed from New to Fix uploaded

OK fix uploaded.

#2 - 10/16/2013 01:49 PM - Mark Abraham

- Status changed from Fix uploaded to Closed