GROMACS - Bug #1138

sd integrator issues with OpenMP threading

02/06/2013 04:22 PM - Berk Hess

<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>Berk Hess</td>
</tr>
<tr>
<td>Category:</td>
<td>mdrun</td>
</tr>
<tr>
<td>Target version:</td>
<td>4.6.1</td>
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<td>Affected version</td>
<td>4.6</td>
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<td>Difficulty:</td>
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**Description**

The sd integrator reallocates the same pointer on multiple OpenMP threads. This can lead to small errors in the integrator or a segmentation fault. This bug was introduced with the fix of #1121.

**Associated revisions**

Revision fe27c346 - 02/06/2013 04:21 PM - Berk Hess
fixed bug with sd integrator and OpenMP threading
This could cause small error in the integration or a segv.
This bug was introduced with d120c370
Fixes #1138
Change-Id: l4ae2c0c857cb68e796d01c5b2e0ea42beaf13d4a

Revision a2be6564 - 02/28/2013 08:49 AM - Berk Hess
fixed bug with sd integrator and OpenMP threading
This could cause small error in the integration or a segv.
This bug was introduced with d120c370
Fixes #1138
Change-Id: l4ae2c0c857cb68e796d01c5b2e0ea42beaf13d4a

**History**

#1 - 02/14/2013 02:04 PM - Berk Hess
- Status changed from New to Closed