

## GROMACS - Bug #1138

### sd integrator issues with OpenMP threading

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

<b>Status:</b> Closed	
<b>Priority:</b> High	
<b>Assignee:</b> Berk Hess	
<b>Category:</b> mdrun	
<b>Target version:</b> 4.6.1	
<b>Affected version - extra info:</b> 4.6	<b>Difficulty:</b> uncategorized
<b>Affected version:</b>	
<b>Description</b>	
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 <a href="#">#1121</a>	

#### 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: I4ae2c0c857cb68e796d01c5b2e0ea42beaf13d4a

##### 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: I4ae2c0c857cb68e796d01c5b2e0ea42beaf13d4a

#### History

##### #1 - 02/14/2013 02:04 PM - Berk Hess

- Status changed from New to Closed