sd integrator issues with OpenMP threading

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

Status: Closed
Priority: High
Assignee: Berk Hess
Category: mdrun
Target version: 4.6.1
Affected version - extra info: 4.6
Affected version:
Difficulty: uncategorized

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: 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