Gromacs - Bug #1697

rare replica-exchange problem

03/04/2015 11:04 AM - Mark Abraham

Status: Closed
Priority: Normal
Assignee: Michael Shirts
Category: mdrun
Target version: 5.0.5
Affected version: 5.0.4

Description
If a series of multiple replica exchanges at a single attempt led to permutations of all replicas that formed a single cycle, problems ensued.

Associated revisions
Revision 3e1fc90f - 04/30/2015 10:54 AM - Michael Shirts
Fix for rarely occurring replica exchange error.

It could write to unallocated memory when permutations of all replicas formed a single cycle (which is rare except for very low numbers of replicas)

Fixes #1697
Change-Id: I23e8f7213572d3e8b9461cfd7cb1eb790b45fe3

History
#1 - 03/04/2015 11:05 AM - Gerrit Code Review Bot
Gerrit received a related patchset '2' for Issue #1697
Uploader: Mark Abraham (mark.j.abraham@gmail.com)
Change-Id: l23e8f7213572d3e8b9461cfd7cb1eb790b45fe3
Gerrit URL: https://gerrit.gromacs.org/4483

#2 - 04/09/2015 10:58 AM - Mark Abraham
- Status changed from New to Fix uploaded

#3 - 05/06/2015 04:52 PM - Mark Abraham
- Status changed from Fix uploaded to Closed