GROMACS - Bug #1314

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

Status: Closed
Priority: Normal
Assignee: Michael Shirts
Category: mdrun
Target version: 4.6.4
Affected version - extra info:
Affected version: 4.6
Difficulty: uncategorized

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: Id7e3771d257beebeed2f340593b817015a0cd4c

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