GROMACS - Bug #1244

cos-acceleration viscosity output incorrect

05/08/2013 05:29 PM - Berk Hess

Status: Closed
Priority: Normal
Assignee: Berk Hess
Category: mdrun
Target version: 4.6.2
Affected version - extra info: 
Affected version: 4.6.1

Difficulty: uncategorized

Description
The viscosity output with cos-acceleration is off by a factor of the box volume. For version 4.5.4 I ADDED a missing factor of density instead of REPLACING the volume. Note that the incorrect viscosity value you get can be simply corrected by dividing by the box volume.

Associated revisions
Revision 25a78ecb - 05/08/2013 06:07 PM - Berk Hess
fixed incorrect scaling of cos-acceleration viscosity
The cos-acceleration 1/viscosity output contained an anomalous factor 1/volume. This factor is now removed.
Fixes #1244
Change-Id: I9bf318b4e6557720683d50a0c2e887e306bacc3f

Revision 0eeab7c0 - 06/13/2013 09:45 AM - Berk Hess
fixed incorrect scaling of cos-acceleration viscosity
The cos-acceleration 1/viscosity output contained an anomalous factor 1/volume. This factor is now removed.
Fixes #1244
Change-Id: I9bf318b4e6557720683d50a0c2e887e306bacc3f

History
#1 - 05/15/2013 09:55 PM - Berk Hess
- Status changed from New to Resolved
- % Done changed from 0 to 100

Applied in changeset 25a78ecb812d56ffcd82bb212b1a28c578dd9371f.

#2 - 05/31/2013 10:40 AM - Mark Abraham
- Status changed from Resolved to Closed