GROMACS - Bug #2972

small bug in anaeig when comparing two eigenvector files

06/10/2019 10:22 PM - Carlo Camilloni

Status: Closed
Priority: Normal
Assignee:
Category:
Target version:
Affected version - extra info: 2018.x, 2019.x
Affected version: 2019

Difficulty: uncategorized

Description

is src/gromacs/gmxana/gmx_anaeig.cpp

1172: neig2 = DIM*neig2;
should be
1172: neig2 = std::min(nvec2, DIM*neig2);
otherwise the comparison between eigenvector files may fail

Associated revisions

Revision 41a44e7a - 07/09/2019 11:05 PM - David van der Spoel
Fixed small bug in gmx anaeig
Poor use of variable names led to a small bug.
Fixes #2972
Change-Id: I244eac13dbaeeb0eac2be6531e579a125f4a66d3

History

#1 - 07/08/2019 10:01 AM - Paul Bauer
Hello, could you upload a test case here for this? Also, has this always been an issue or has it been recently introduced?

@David, can you comment on this?

#2 - 07/08/2019 10:29 AM - David van der Spoel
For some reason the patch does not show here.
https://gerrit.gromacs.org/c/gromacs/-/11958

#3 - 07/09/2019 11:15 PM - David van der Spoel
- Status changed from New to Resolved

Applied in changeset 41a44e7a8660d0bbbc5f4d23e6ee91d37023c9eb.

#4 - 07/10/2019 09:40 AM - Paul Bauer
- Status changed from Resolved to Closed