

GROMACS - Bug #1702

Segmentation fault g_covar

03/06/2015 10:52 AM - Fernando Martin

| | |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------|
| Status: Closed | |
| Priority: Low | |
| Assignee: Peter Kasson | |
| Category: analysis tools | |
| Target version: 5.0.5 | |
| Affected version - extra info: | Difficulty: uncategorized |
| Affected version: 5.0.2 | |
| Description | |
| <p>When I perform a g_covar on a bundle of PDBs, a get a segmentation fault. However, the same command, executed with g_covar of gromacs 4.6.5 works perfectly.</p> <p>The command line is:</p> <pre>g_covar -f NMR.xtc -s p5c5NEWfit_1.pdb -n -o -v</pre> <p>where NMR.xtc is the bundle of PDBs generated with trjcat:</p> <pre>trjcat -f p5c5NEWfit_?.pdb p5c5NEWfit_???.pdb -o NMR.xtc -settime</pre> | |

History

#1 - 06/20/2015 02:23 AM - Peter Kasson

- Status changed from New to Blocked, need info

Trying to reproduce on master:
empty -n and -o arguments will produce an error. Running with:
gmxcovar -f NMR.xtc -s p5c5NEWfit_1.pdb -v

Cannot reproduce if I select Protein for lsq fit and for covariance analysis. Program completes successfully.

Can also run successfully on v5.0.2, although the eigenvalue output differs substantially.

At this point, I cannot reproduce the reported error. Can you provide more info?

#2 - 06/22/2015 09:29 PM - Peter Kasson

- Assignee set to Peter Kasson

#3 - 06/24/2015 10:26 PM - Berk Hess

Is this the same issue as [#1733](#) (with number of 3*atoms in the analysis group < #frames), which was fixed for 5.0.5?

#4 - 06/27/2015 03:56 PM - Berk Hess

- Status changed from Blocked, need info to Closed

Duplicate of [#1733](#), fixed in 5.0.5.

#5 - 07/11/2016 07:44 PM - Mark Abraham

- Target version changed from 5.x to 5.0.5

Files

| | | | |
|------------------|--------|------------|-----------------|
| NMR.xtc | 104 KB | 03/06/2015 | Fernando Martin |
| p5c5NEWfit_1.pdb | 105 KB | 03/06/2015 | Fernando Martin |