

## GROMACS - Bug #30

### g\_anaeig

11/04/2005 11:37 AM - Jens Krüger

<b>Status:</b> Closed	
<b>Priority:</b> High	
<b>Assignee:</b> Erik Lindahl	
<b>Category:</b> analysis tools	
<b>Target version:</b> CVS	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b>	

#### Description

We tried to make a standard PCA using CVS 3.3.99\_20050909 on a 64-bit linux box (cluster front end). g\_covar runs smooth, but when we try to use whatever function of g\_anaeig, it crashes with a memory failure (see below). With 3.2.1 on the same system or with CVS 3.3.99\_20050909 on a 32bit machine no error occurs.

We assume that it is a 32bit 64bit thing. Maybe somewhere in the code a fixed 32bit pointer length had been used?

Greetings,

Jens Krüger

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paderborn.de:/scratch/mercutio/AChE/3.3/series01/1DX6/BOTH/covar\$ /opt/pc2/gromacs-3.3/bin/g\_anaeig first 1 -last 1 -extr extreme\_vec\_01.pdb -nframes 25  
:) G R O M A C S (-:

GRoups of Organic Molecules in ACTion for Science

:-) VERSION 3.3.99\_20050909 (-:

Written by David van der Spoel, Erik Lindahl, Berk Hess, and others.  
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:-) /opt/pc2/gromacs-3.3/bin/g\_anaeig (-:

Option	Filename	Type	Description
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-v	eigenvec.trr	Input	Full precision trajectory: trr trj
-v2	eigenvec2.trr	Input, Opt.	Full precision trajectory: trr trj
-f	traj.xtc	Input, Opt.	Generic trajectory: xtc trr trj gro g96 pdb
-s	topol.tpr	Input, Opt.	Structure+mass(db): tpr tpb tpa gro g96 pdb xml
-n	index.ndx	Input, Opt.	Index file
-eig	eigenval.xvg	Input, Opt.	xvgr/xmgr file
-eig2	eigenval2.xvg	Input, Opt.	xvgr/xmgr file
-comp	eigcomp.xvg	Output, Opt.	xvgr/xmgr file
-rmsf	eigrmsf.xvg	Output, Opt.	xvgr/xmgr file
-proj	proj.xvg	Output, Opt.	xvgr/xmgr file
-2d	2dproj.xvg	Output, Opt.	xvgr/xmgr file

-3d 3dproj.pdb Output, Opt. Generic structure: gro g96 pdb xml  
 -filt filtered.xtc Output, Opt. Generic trajectory: xtc trr trj gro g96 pdb  
 -extr extreme\_vec\_01.pdb Output, Opt! Generic trajectory: xtc trr trj gro g96 pdb  
 -over overlap.xvg Output, Opt. xvgr/xmgr file  
 -inpr inprod.xpm Output, Opt. X PixMap compatible matrix file

Option	Type	Value	Description
-[no]h	bool	no	Print help info and quit
-[no]X	bool	no	Use dialog box GUI to edit command line options
-nice	int	19	Set the nicelevel
-b	time	0	First frame (ps) to read from trajectory
-e	time	0	Last frame (ps) to read from trajectory
-dt	time	0	Only use frame when t MOD dt = first time (ps)
-tu	enum	ps	Time unit: ps, fs, ns, us, ms, s, m or h
-[no]w	bool	no	View output xvg, xpm, eps and pdb files
-[no]xvgr	bool	yes	Add specific codes (legends etc.) in the output xvg files for the xmgrace program
-first	int	1	First eigenvector for analysis (-1 is select)
-last	int	1	Last eigenvector for analysis (-1 is till the last)
-skip	int	1	Only analyse every nr-th frame
-max	real	0	Maximum for projection of the eigenvector on the average structure, max=0 gives the extremes
-nframes	int	25	Number of frames for the extremes output
-[no]split	bool	no	Split eigenvector projections where time is zero

trn version: GMX\_trn\_file (single precision)

Read non mass weighted reference structure with 528 atoms from eigenvec.trr

Read non mass weighted average/minimum structure with 528 atoms from eigenvec.trr

- glibc detected \* realloc(): invalid pointer: 0x0000000004006e8 \*  
 zsh: abort /opt/pc2/gromacs-3.3/bin/g\_anaeig -first 1 -last 1 -extr extreme\_vec\_01.pdb

## History

### #1 - 02/26/2006 01:42 AM - Tyler Luchko

I have come across what I believe is the same bug using GROMACS 3.3 on my Mac dual 2.7 GHz G5 running OS 10.4.5. I have seen the same thing on a quad G5 mac as well. These are both 64 bit machines but I have also tried it on a AMD Opteron box, which is also 64 bit, and have experieced no problems. The error message I got was:

Read mass weighted average/minimum structure with 247 atoms from 0/pca/eigenvec.trj

g\_anaeig(644) malloc: \* error for object 0x8fe5e718: pointer being reallocated was not allocated

g\_anaeig(644) malloc: \* set a breakpoint in szone\_error to debug

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 Program g\_anaeig, VERSION 3.3  
 Source code file: smalloc.c, line: 137

Fatal error:  
 realloc for \*eigval (40 bytes, file eigio.c, line 118, \*eigval=0x0x8fe5e718)

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 I looked at the code and I have found a solution to the problem, at least to the one that I was experiecing. The solution is a one line fix. Line 779 of gmx\_anaeig.c was

```
real      *eigval1,*eigval2;
```

and should be

```
real      *eigval1=NULL,*eigval2=NULL;
```

Tyler

#2 - 03/30/2006 05:32 PM - Erik Lindahl

Fixed, according to the suggestion.