

## GROMACS - Bug #455

### Weird g\_sorient failure

06/25/2010 02:51 PM - Justin Lemkul

<b>Status:</b> Closed	
<b>Priority:</b> Normal	
<b>Assignee:</b> Erik Lindahl	
<b>Category:</b> analysis tools	
<b>Target version:</b> 4.0	
<b>Affected version - extra info:</b>	<b>Difficulty:</b> uncategorized
<b>Affected version:</b>	

#### Description

As posted to gmx-users, 6/24/2010 (with slight modifications to reflect the filenames in the attachment):

I'm trying to use g\_sorient to calculate some solvent properties in a few systems I'm simulating. It's the first time I've used the tool, so if I've missed something obvious, please let me know. I'm getting a very weird error when I execute the command:

```
echo 1 13 | g_sorient_4.0.7_s -s md_0_20.tpr -f 1ns.xtc -rmin 0 -rmax 1 -com
```

Groups 1 and 13 represent Protein (which is a single amino acid, dipeptide form) and SOL, respectively. The error is:

```
-----  
Program g_sorient_4.0.7_s, VERSION 4.0.7  
Source code file: mshift.c, line: 635
```

```
Fatal error:  
No GREY nodes found while nG=1
```

I think I have tracked the problem down to time 958 ps. If I supply -e 956 to the above command, the program finishes. If I use -e 958, it crashes with the error. However, if I run:

```
echo 1 13 | g_sorient_4.0.7_s -s md_0_20.tpr -f 1ns.xtc -rmin 0 -rmax 1 -com -b 950 -e 1000
```

The program completes. Very weird. Using gmxcheck indicates no abnormality in the trajectory, and other analysis tools work just fine (g\_hbond, g\_traj, g\_rdf, etc). Processing the frame at 958 ps (as a .gro file) also works fine, i.e.:

```
echo 1 13 | g_sorient_4.0.7_s -s md_0_20.tpr -f 958.gro -rmin 0 -rmax 1 -com
```

Works without a problem.

#### History

##### #1 - 06/25/2010 02:53 PM - Justin Lemkul

Created an attachment (id=482)  
run input file and trajectory

##### #2 - 07/02/2010 09:51 AM - David van der Spoel

Fixed bug [http://bugzilla.gromacs.org/show\\_bug.cgi?id=455](http://bugzilla.gromacs.org/show_bug.cgi?id=455) which was due to a histogram writing out of boundaries. While debugging introduced a structure in the rmpbc code that does not use static variables. This is however used only in g\_sorient. The other programs that use this functionality still use a convenience function that calls new functionality under the hood and in the convenience function a static variable is used. This I will fix as well.

The fix is in the head branch.

#### Files

test.tgz	17.1 MB	06/25/2010	Justin Lemkul
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