

GROMACS - Bug #151

g_msd -type -nomw yields D=0.0 for all systems

06/04/2007 11:10 PM - Chris Neale

Status: Closed	
Priority: Low	
Assignee: Erik Lindahl	
Category: analysis tools	
Target version: 3.3.1	
Affected version - extra info:	Difficulty: uncategorized
Affected version:	

Description

A line is missing in the code. Addition of the proper line fixes the bug.
Add the following line between line 220 and line 221 in 3.3.1 gm_x_msd.c:
r2+=r*r;

More info:

Line 220 in calc1_norm() gives r for -type <x|y|z> -nomw. However, r2 is never calculated for -type in calc1_norm() and therefore for -nomw.

Line 220 should be followed by the line:

```
r2+=r*r;
```

as is the case for line 214 and 226 in calc1_norm() and also on line 362 in calc_one_mw() for -type.

Chris.

History

#1 - 06/07/2007 10:35 PM - David van der Spoel

Fixed as per your suggestion. Thanks for your report.