GROMACS - Bug #1592

Manual of trjconv is unclear about precision.

09/07/2014 09:42 AM - David van der Spoel

Status:	Rejected		
Priority:	Low		
Assignee:	David van der Spoel		
Category:	analysis tools		
Target version:			
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	5.0.1		

Description

The manual says:
The precision of .xtc and .gro output is taken from the input file for .xtc, .gro and .pdb, and from the -ndec option for other input formats. The precision is always taken from -ndec, when this option is set. All other formats have fixed precision.

It is not clear from this whether a transfer from .pdb to .xtc results in higher precision than .gro to .xtc. The command line help suggests that .gro file can be written with different number of decimals.

History

#1 - 09/09/2014 04:02 PM - Norbert Jeszenoi

- *File trjconv_precision.tar.gz added*

David van der Spoel wrote:

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>
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The input and output files can be found in the attached zip file (trjconv_precision.tar.gz). GMX commands are in the commands.txt text file (also in the zip file), the latest Gromacs version (5.0.1) was used.
According to the manual, trjconv uses ndec = 3 by default, however when .pdb were created from .xtc the last decimal of the coordinate digits are not zero (as they should be). When .gro files were written as output with ndec > 3 the last decimals are also not zeros.

The .xtc was converted from .trr with default settings (ndec = 3).

#2 - 10/01/2014 04:24 PM - Mark Abraham

- *Target version deleted (5.0.2)*

#3 - 06/22/2015 06:13 AM - Erik Lindahl

- *Status changed from New to Rejected*

The commands in the example all use the -center option, which will cause the system to be translated after the coordinates have been read from the xtc file. Without that option the output files will have zeros in positions beyound the 4th decimal.

Files

trjconv_precision.tar.gz	11.3 MB	09/09/2014	Norbert Jeszenoi