

GROMACS - Feature #846

Warning messages should be added to programs reducing the precision of coordinates/velocities etc.

11/27/2011 12:56 PM - David van der Spoel

Status:	Closed
Priority:	Low
Assignee:	David van der Spoel
Category:	
Target version:	
Difficulty:	uncategorized
Description	
When pdb2gmx processes a pdb file to a gro file precision is lost. The same can happen in editconf or trjconv. A warning message should be issued when this occurs.	

History

#1 - 04/11/2012 12:36 PM - Rossen Apostolov

- Priority changed from Normal to Low

#2 - 05/22/2014 06:51 PM - Erik Lindahl

- Tracker changed from Bug to Feature

- Assignee set to David van der Spoel

- Target version set to 5.x

#3 - 06/22/2014 10:50 AM - Erik Lindahl

In principle this would be neat to have for the user, but it might run contrary to the idea of increasing modularization if the highest-level user program needs to be aware of the implementation detail of every single possible output format (what future sub-option to TNG will preserve vs. reduce precision, for instance?).

In particular, many of these minor features start out as nice-to-have, but a couple of years later they lead to lots of extra code we need to maintain. I think a better solution would be to have a text-based description of each output format available in an output module, and then leave it up to the user to decide. If they pick a file format that does lossy compression, that is simply what they will get.

#4 - 06/18/2015 03:13 PM - Erik Lindahl

- Status changed from New to Closed

- Target version changed from 5.x to future

Three year old feature, but with no activity whatsoever, so I'll assume even David doesn't think it isn't very important. Closing for now - feel free to reopen when somebody plans to actually work on it.

#5 - 07/11/2016 08:44 PM - Mark Abraham

- Target version deleted (future)