

GROMACS - Task #2603

Add ability to properly check coordinate files during testing

08/08/2018 05:57 PM - Paul Bauer

Status:	New
Priority:	Normal
Assignee:	Paul Bauer
Category:	testing
Target version:	future
Difficulty:	uncategorized
Description	
<p>At the current state, the testing code is only able to check that the first two lines of a GRO file written by a tool are identical to a reference. This means that coordinate file writing in any other format, or even properly checking a complete GRO file is not possible and tools that do so may silently fail on that task.</p> <p>The ConfMatch option for the TestReferenceChecker should be extended to check that all fields and their formatting are identical to a reference file.</p> <p>For now the old behaviour of only checking a GRO file and then only the first two lines should be left as a default, with the more in depth checking available on demand.</p>	

History

#1 - 08/08/2018 05:58 PM - Gerrit Code Review Bot

Gerrit received a related patchset '7' for Issue [#2603](#).

Uploader: Paul Bauer (paul.bauer.q@gmail.com)

Change-Id: gromacs~master~1726f973e2c0b6207a8a53c2e2e443ffbb8275ab4

Gerrit URL: <https://gerrit.gromacs.org/8142>

#2 - 10/15/2018 01:16 PM - Paul Bauer

- Target version changed from 2019 to future

not going to happen for 2019