

GROMACS - Task #2353

improve on relative tolerance for constructing tables

12/19/2017 02:33 AM - Mark Abraham

Status:	New	
Priority:	Normal	
Assignee:		
Category:	core library	
Target version:	2021	
Difficulty:	uncategorized	
Description		
The existing approach is not robust with respect to function or derivative values near zero, and can fail in double precision for different compilers, build types, and number of data points tested. We need an approach to testing that our functions do that right job that is more resilient to the kinds of arbitrarily curved functions users might want to use, e.g. from Boltzmann inversion.		
Related issues:		
Related to GROMACS - Task #2336: improve on relative tolerance tests for tabu...		Closed
Related to GROMACS - Feature #1347: future of tables		New

History

#1 - 12/19/2017 02:34 AM - Mark Abraham

- Related to Task #2336: improve on relative tolerance tests for tabulated interaction added

#2 - 12/19/2017 02:38 AM - Mark Abraham

- Related to Feature #1347: future of tables added

#3 - 12/19/2017 08:07 AM - Erik Lindahl

- Subject changed from improve on relative tolerance for testing implementation of tabulated interaction tables to improve on relative tolerance for constructing tables

This is not mainly related to testing, but how to construct the tables, since we presently use relative tolerances to decide the table density. Once we have a robust solution there, we should just apply the same one during testing.

#4 - 10/30/2018 04:17 AM - Erik Lindahl

- Target version changed from 2019 to 2020

#5 - 12/20/2019 12:12 PM - Paul Bauer

- Target version changed from 2020 to 2021