

GROMACS - Bug #3388

NMR restraints not working in modular simulator

02/21/2020 12:21 AM - Pascal Merz

Status: Closed	
Priority: Normal	
Assignee: Pascal Merz	
Category: mdrun	
Target version: 2020.1	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2020	

Description

The NMR restraints are not properly working using modular simulator, but are not explicitly excluded from using the new code path.

Distance restraints

- Are not working when time-averaging is used (because `t_history` is disabled), will cause an error for accessing a nullptr (no wrong results possible).
- Works correctly when no time-averaging is used, but output only happens on `nstenergy` steps (results are correct, but output might not be as expected).

Orientation restraints

- Are never working - they depend on a `t_graph` object, which is currently disabled in modular simulator. Will cause an error (assertion in debug mode, access to nullptr in non-debug mode), no wrong results possible.
- Also, time-averaging would not work as a `t_history` object is missing.
- Output would currently only happen on `nstenergy` steps.

Proposed solution

As the required amount of additional functionality (`t_history`, `t_graph`, energy printing) is relatively large, I suggest to disable distance and orientation restraints from being used with modular simulator for GROMACS 2020 and plan to properly implement this functionality for modular simulator in GROMACS 2021.

Associated revisions

Revision 3ccb0ef1 - 02/21/2020 11:25 PM - Pascal Merz

Use legacy code path for NMR restraints (modular simulator)

Fixes #3388

Change-Id: I03db8af35d71c7405716e73516c4235fc089334c

History

#1 - 02/21/2020 07:36 AM - Pascal Merz

- Status changed from New to Fix uploaded

- Private changed from Yes to No

#2 - 02/24/2020 05:15 PM - Anonymous

- Status changed from Fix uploaded to Resolved

Applied in changeset [3ccb0ef14912728eca68cdfd8161a082a85b40e9](#).

#3 - 02/25/2020 10:12 AM - Paul Bauer

- Status changed from Resolved to Closed