

GROMACS - Bug #2883

essentialdynamics fail with Intel MPI

03/08/2019 03:10 AM - Roland Schulz

Status: New	
Priority: Normal	
Assignee:	
Category:	
Target version:	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2019.1	
Description - If one compiles with Intel MPI but doesn't run with mpirun than the application can't read from stdin - Line 1361 of gmxtest.pl does that. It pipes one of the required inputs into the stdin and calls make_edi without mpirun. Possible solutions: - Have make_edi take the input by command line argument rather than stdin - call make_edi with mpirun (but even then MPI doesn't guarantee that you can read from stdin). - Exclude that test from those run with MPI	
Related issues: Related to GROMACS - Bug #2876: 2019.1 make check fails on AVX and AVX2 (Inte... New	

History

#1 - 03/08/2019 03:12 AM - Roland Schulz

- Related to Bug #2876: 2019.1 make check fails on AVX and AVX2 (Intel 2018u3) added