

GROMACS - Task #2979

Reconsider default 1 OpenMP thread per thread-MPI rank

06/17/2019 01:28 PM - Berk Hess

Status:	Accepted	
Priority:	Normal	
Assignee:	Berk Hess	
Category:	mdrun	
Target version:	2020-beta2	
Difficulty:	uncategorized	
Description		
<p>We always have 1 OpenMP thread per thread-MPI rank by default. This is best at small/medium rank and simple. But with 128 core nodes, this might no longer be the best. It might even limit the system size when we will soon communicate the whole tpr as one chunk of memory.</p>		

History

#1 - 09/24/2019 03:22 PM - Paul Bauer

- Target version changed from 2020-beta1 to 2020-beta2