

GROMACS - Task #3420

Task # 3418 (New): Infrastructure improvements for modular simulator

Unify force and shellfc elements for modular simulator

03/10/2020 09:49 PM - Pascal Merz

Status:	New	
Priority:	Normal	
Assignee:	Pascal Merz	
Category:	mdrun	
Target version:	2021-infrastructure-stable	
Difficulty:	uncategorized	
Description		
In the GROMACS 2020 implementation, ForceElement is handling the call to do_force, while ShellFCElement is handling the call to relax_shell_flexcon. This lead to two nearly identical elements with a large amount of code duplication, which can easily be merged into one.		

History

#1 - 03/10/2020 09:50 PM - Pascal Merz

- Tracker changed from Feature to Task