

GROMACS - Task #3162

Feature # 3114 (New): Improve GPU update-constraints module

Feature # 3352 (New): GPU update-constraints feature support

Add virtual site support to GPU version of update-constraints.

10/18/2019 02:28 PM - Artem Zhmurov

Status:	New
Priority:	Normal
Assignee:	Artem Zhmurov
Category:	
Target version:	2021-infrastructure-stable
Difficulty:	uncategorized
Description	
<p>The virtual sites require forces to be distributed among normal atoms. Hence, all forces has to be copied to the host on every step if vsites are on. Since this defeats the purpose of offloading all computations to the device and introduces additional logical expressions into the main MD loop, the vsite support is removed. Consider moving force redistribution for virtual sites to the device so that no extra copy will be needed.</p>	
<p>Gerrit patch with the vsite support: https://gerrit.gromacs.org/#/c/gromacs/+13781/ Gerrit patch that removes the support: https://gerrit.gromacs.org/#/c/gromacs/+13799/</p>	

History

#1 - 10/18/2019 02:29 PM - Artem Zhmurov

- Description updated

#2 - 10/21/2019 03:59 PM - Artem Zhmurov

- Parent task changed from #2816 to #2888

#3 - 01/22/2020 11:36 AM - Artem Zhmurov

- Tracker changed from Feature to Task

- Assignee set to Artem Zhmurov

- Target version set to 2021-infrastructure-stable

- Parent task changed from #2888 to #3114

#4 - 01/23/2020 11:52 AM - Artem Zhmurov

- Parent task changed from #3114 to #3352