

GROMACS - Feature #2510

Implement update groups

05/22/2018 01:06 PM - Berk Hess

Status:	Closed
Priority:	Normal
Assignee:	Berk Hess
Category:	mdrun
Target version:	2019
Difficulty:	uncategorized

Description

Performance of mdrun can be improved by using "update groups" as the smallest indivisible unit. There are planned to be groups of atoms connected by (H-bond only) constraints and virtual sites. By using such groups on the nbxn grid and in the domain decomposition instead of individual atoms, update, constraints and vsites become completely independent tasks which don't require MPI communication and OpenMP barriers. This improves performance by itself. More performance can be gained by running the update out of sync on different domains to decrease the GPU idle time.

History

#1 - 10/12/2018 02:35 PM - Mark Abraham

- Status changed from *In Progress* to *Resolved*

There were many refactoring and functionality commits here, the feature is now live.

#2 - 10/12/2018 02:35 PM - Mark Abraham

- Status changed from *Resolved* to *Closed*