

GROMACS - Task #2997

improve performance of alchemical free energy calculations

06/24/2019 03:07 PM - Szilárd Páll

Status:	New
Priority:	Normal
Assignee:	
Category:	mdrun
Target version:	2020
Difficulty:	uncategorized
Description	
Top-level task for SIMD and GPU-accelerated alchemical free energy calculations work.	

Associated revisions

Revision acb7e888 - 07/01/2019 12:01 AM - Szilárd Páll

Create dedicated subcounter for nonbonded FEP

Now all nonbonded work has their own separate subcounters which allows measuring the performance of each task separately.

Refs #2997

Change-Id: I601445364592923d08087a858da4629b0b58ae76

Revision b72a2df2 - 09/04/2019 12:14 PM - Magnus Lundborg

Inline functions of calculations of FE interaction types.

The functions are so far only templated on the real requirements of the softcore that is used.

This is one step towards templating the calculations for SIMD.

Refs #2997.

Change-Id: I3fd119dce30f95eba4f8cd6f139f99260acf0e22

Revision 01b3e2e4 - 09/10/2019 04:19 PM - Magnus Lundborg

More templating of `gmx_nb_free_energy_kernel()`

Kernel templated on interaction types.

Refs #2997.

Change-Id: Id02a6daab817705bdaca2ef610b793f1ddab6829