Supporting Information

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non PFF performance

The present package also proposes non-polarizable force fields simlation capabilities. The following Table displays the performances of the initial portage of the Tinker-HP CPUs subroutines for force fields like CHARMM, AMBER or OPLS (same scaling). We are currently working on the HPC optimization of these approaches but the present implementation already allow to perform production simulations.

Table 1: Tinker-*HP* Mixed Precision benchmarks (standard setup) with the Charmm Force-field on a single device with RESPA 2 fs (full flexibility, no shake

	DHFR	COX	STMV
V100 (ns/j)	130	28.74	4.71
RTX 2080 Ti	95.5	14.34	2.37

Comparison between device architectures

Given the device specifications, the overall computation analysis made with the Nvidia Profiler indicates a peak performance of 9, 8 and 5% respectively from GV100, RTX-2080 Ti and RTX 3090 after measuring the total number of Flops and duration on a 100 steps MP simulation. In other words, each of these devices performs on average 6 7 and 8 floating point operations after every access to a 32bits floating point from global memory. Thus, it remains possible to add extra computational instructions which is encouraging regarding future developments. For the current generation of Geforce *GPUs* , it seems that reaching peak performance will represent a considerable challenge as memory technologies do not evolve proportionally as processors.