

128 nodes: Piz Daint Supercomputer (Cray XC50)

	CPU-ONLY			GPU ACCELERATED	
ALGORITHM	CRAY-LIBSCI	MKL	COSMA-CPU	CRAY-LIBSCI_ACC	COSMA-GPU
CONFIGURATION	1MPI x 12T	1MPI x 12T	1MPI x 12T	1MPI x 12T	1MPI x 12T
CP2K RPA-RI 128-H20 [s]	6379.14	2305.41	2238.94	865.73	781.60
46 x PDGEMM [s]	5896.45	1836.85	1723.62	338.47	257.99
NODE GFLOP/s	128.30	411.87	438.92	2235.19	2932.44
% PEAK PERF.	25.70%	82.51%	87.92%	49.67%	65.17%
NODE TYPE (128 nodes)	Intel® Xeon® E5-2690 v3 @ 2.60GHz (12 cores, 64GB RAM)			NVIDIA® Tesla® P100 16GB	
NODE PEAK PERF[GFLOP/s]	499.2			4500	
	This is only using CPU nodes on the GPU partition of Piz Daint. However, CPU node peak perf is much higher on the CPU partition.			Max peak assumes the data is already on GPU, which explains why it is not fully achieved.	

~10% faster

~25% faster