

1024 nodes: Piz Daint Supercomputer (Cray XC50)

ALGORITHM	GPU ACCELERATED	
	CRAY-LIBSCI_ACC	COSMA-GPU
CONFIGURATION	1MPI x 12T	1MPI x 12T
CP2K RPA-RI 128-H2O [s]	317.68	175.12
46 x PDGEMM [s]	139.82	75.26
NODE GFLOP/s	676.37	1256.49
% PEAK PERF.	15.03%	27.92%
NODE TYPE (1024 nodes)	NVIDIA® Tesla® P100 16GB	
NODE PEAK PERF[GFLOP/s]	4500	

~2× faster