

|                          | 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-H2O [ms] | 6379.14  | 2305.41    | 2238.94    | 865.73  | 781.60     |
| 46 x PDGEMM [ms]         | 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. |            |