

Examining Performance Portability with Kokkos for an Ewald Sum Coulomb Solver

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Abstract. We have implemented the computation of Coulomb interactions in particle systems using the performance portable C++ framework Kokkos. Coulomb interactions are evaluated with an Ewald-sum-based solver, where the interactions are split into long- and short-range contributions. The short-range contributions are calculated using pair-wise contributions of particles while long-range interactions are calculated using Fourier sums. We evaluate the performance portability of the implementation on Intel CPUs, including Intel Xeon Phi, and Nvidia GPUs.

1 Introduction

The development of modern computer architectures shows a clear trend towards increased complexity and heterogeneity. This increases the complexity of efficient code development for multiple architectures that takes advantage of all available components. GPUs, for example, are powerful processors available in cell phones as well as supercomputers usually requiring their own programming model. As a matter of fact GPUs have become more and more important as a source of computing power in supercomputers, as can be seen in the increase of systems using GPUs in the Top500 list [17] over the past ten years. While in November 2008 there was no system that included GPUs, in November 2013 there were 39 systems, and in the current list from November 2018 126 systems contained GPUs. There are many ways of programming GPUs but unfortunately few are even function portable without large changes to the source code [10]. This matter becomes even worse if we want to write code for different kind of accelerators, e.g., Intel’s Xeon Phi series.

In the domain of particle simulation methods of complex systems, electrostatic interactions represent a class of algorithms of high computational complexity. This arises as a result of pair-wise interactions between all particles in a system, which basically scale as $\mathcal{O}(N^2)$. More efficient methods can be reduced to $\mathcal{O}(N \log(N))$ or even $\mathcal{O}(N)$ but come with a large implementation effort [6,13,15,19,3]. In the present paper we consider the Ewald summation method, which is suitable for particle systems in three dimensions under periodic boundary conditions and which can be optimised by proper choice of

parameters to $\mathcal{O}(N^{3/2})$ (essentially there are also formulations for one- or two-dimensional systems, which we do not consider here). The basic structure of the Ewald summation is sufficiently transparent and not too complex, allowing an analysis of the operational count and providing insight into the procedure to measure performance portability.

Performance portable approaches have been supported recently by the US department of Energy and have resulted in frameworks like Kokkos [5,1] or Raja [4,2], which offer C++ software abstractions for code execution and memory management.

In this paper, we compare the performance of an Ewald sum implemented in Kokkos on various Intel CPUs including Intel Xeon Phi Knights Landing and Nvidia GPUs. We start with a quick overview of Kokkos and its main features (Sec. 3). Then we introduce the problem of a system of electric charges with periodic boundary conditions and show how the Ewald sum can be used to calculate it efficiently (Sec. 2). In Sec. 4 we establish a base line for the achievable performance. Afterwards we present our implementation and show our performance benchmarks (Sec. 5).

2 Calculating Long-range Interactions with Periodic Boundaries

When computing energies and forces in particle systems composed of N particles, which are dominated by long range interactions, each particle i gets partial contributions of each other particle $j \in [1, N]$. Long range interactions arise when the potential energy function $\phi(r)$ decays slower than $1/r^d$, where d is the dimension of the system and r is the distance from a point in space to a particle. Here, we consider electrostatic potentials created by point charges, for which the potential energy at a point r in free space is given by $\phi(r) = q_j/|r - r_j|$ which leads to a total electrostatic energy $U = 1/2 \sum_{i,j} q_i \phi(r_{ij})$. When simulating bulk systems, the number of particles in a simulation is always small, compared with laboratory samples and therefore, in order to avoid surface effects, periodic boundary conditions are often applied [9] and the electrostatic potential energy at particle position $\mathbf{r}_i$ can formally be written as

$$\phi(\mathbf{r}_i) = \sum_{\mathbf{n}} \dagger \sum_{j=1}^N \frac{q_j}{\|\mathbf{r}_{ij} + \mathbf{n}L\|_2}$$

where $\mathbf{n} \in \mathbb{Z}^3$ is a so called lattice vector, L the length of the (cubic) system and " $\dagger$ " indicates that $j \neq i$ for $\|\mathbf{n}\|_2 = 0$. This sum cannot be evaluated by a straightforward summation rule, since (i) the first sum is formally over an infinite number of lattice vectors; and (ii) the lattice sum is conditionally convergent, i.e., the result depends on the order of summation. Ewald proposed [7] a way to overcome the conditional convergence by subdividing the expression into a short range and a long range part, which is introduced via a splitting function, $f(r)$, which decays to zero within a finite range. A function $u(r) = 1/r$ can then be

rewritten as $u(r) = f(r)/r + (1 - f(r))/r$. The first term is short range (since it decays to zero), while the second one is long range (since asymptotically it decays as $1/r$). This reformulation has the advantage that it can be transformed into an unconditionally convergent sum for a proper choice of f . Originally, $f(r) = \text{erfc}(\alpha r)$ was chosen, where α is a splitting parameter, controlling the width of the short range part. The long range part can be elegantly computed in Fourier space, which leads to [9]

$$\phi(\mathbf{r}_i) = \sum_{j=1}^N \sum_{\mathbf{n}} q_j \frac{\text{erfc}(\alpha \|\mathbf{r}_{ij} + \mathbf{n}L\|)}{\|\mathbf{r}_{ij} + \mathbf{n}L\|_2} + \frac{4\pi}{L} \sum_{|\mathbf{k}| \neq 0} \sum_{j=1}^N \frac{q_j}{|\mathbf{k}|^2} e^{-\frac{|\mathbf{k}|^2}{4\alpha^2}} e^{i\mathbf{k}\mathbf{r}_{ij}} - q_i \frac{2\alpha}{\sqrt{\pi}} \quad (1)$$

The last term corresponds to a correction for particle i , which also appears in the k-space summation (second term). For practical computations the infinite sums (over $\mathbf{n}$ and $\mathbf{k}$) have to be approximated. For large arguments $\text{erfc}(x)$ decays as a Gaussian, as it does the k-space summation. Therefore, both sums can be limited to a finite range of values, which still allows for control of approximation error. In most cases, due to the spherical symmetry of $\text{erfc}(x)$ and a fast decay, the first sum can be restricted to contributions within a spherical region of radius R_c . Furthermore, it can be shown that via a proper set of parameters [8,16], the computational complexity is reduced from $\mathcal{O}(N^2)$ to $\mathcal{O}(N^{3/2})$.

3 Kokkos at a Glance

Kokkos uses C++ to provide an abstraction of parallel algorithms, their execution and memory spaces. The basic algorithms include `parallel_for`, `parallel_reduce`, and `parallel_scan`. Each of these algorithms can be executed in different execution spaces, for example, using an OpenMP execution space on the CPU or a CUDA execution space on an Nvidia GPU.

CPUs and GPUs use different approaches to vectorization. CPUs use a single instruction multiple data paradigm. GPUs use a single instruction multiple threads paradigm. These two approaches lead to different preferred memory layouts. To accommodate different memory layouts and memory locations Kokkos introduces so called *Views*.

A **View** is a thin wrapper around the data. It knows its dimensionality, its sizes, its layout, and its memory space. `Kokkos::View<double*> v(n);`, for example, initializes a one dimensional array of doubles of size n in the default execution space, which can be set at compile time. A **View** can be mirrored on the host side. In GPU computing it is not uncommon to initialize data on the host, transfer them to the GPU, perform computations, and transfer the results back. A mirrored **View** can do just that. Any transfer between a **View** and its mirror needs to be done explicitly using `Kokkos::deep_copy`. The code shown in Listing 1.1 creates a 1d **View** and a host mirror of it, fills the mirrored **View** with random numbers, copies the numbers to the **View**, sums them up in parallel, and gets the result.

Listing 1.1. Reduction using Kokkos. This program can be executed using OpenMP on a CPU or on a GPU. Second level curly brackets are needed to ensure deallocation of views before calling `Kokkos::finalize`.

```
#include <random>
#include <Kokkos_Core.hpp>

int main(int argc, char* argv[]) {
    Kokkos::initialize(argc, argv);
    {
        std::default_random_engine generator;
        std::uniform_real_distribution<double> uniform_dist(0, 1);
        auto uniform = [&]{return uniform_dist(generator);};
        int n = 1024;
        double sum = 0;
        // Create a view in the default execution space
        Kokkos::View<double*> v("v", n);
        // Create a mirror of v in host memory
        auto h_v = Kokkos::create_mirror_view(v);
        for(int i = 0; i < n; ++i) h_v(i) = uniform();
        // Copy data from host to device if necessary
        Kokkos::deep_copy(v, h_v);
        // Parallel reduction in default execution space
        Kokkos::parallel_reduce(n, KOKKOS_LAMBDA(int i, double&
            localSum){
            localSum += v(i);
        }, sum);
        std::cout << "The average value of the elements of v is "
            << (sum / n) << ".\n";
    }
    Kokkos::finalize();
}
```

If the program is compiled for OpenMP, the mirror view becomes an alias and the deep copy does not have to do anything, but if the program is compiled for CUDA, the original View lives on the GPU and the deep copy transfers the data from the CPU to the GPU.

On GPUs neighboring threads should access consecutive memory. Thread `i` should access `a[i]` and thread `i+1` `a[i+1]`, but on a CPU this prevents *vectorization* and can introduce an unnecessary dependency. If `a[i]` and `a[i+1]` belong to the same cache line and thread `i` writes to `a[i]` it invalidates the entire cache line. If thread `i+1` wants to access `a[i+1]` it first needs to read the entire cache line again. This effect is called false sharing [18]. So for CPUs a single thread should deal with a chunk of data. The effects due to different memory layout requirements become even more pronounced for multi-dimensional data. Note that in Kokkos, the left-most index is assumed to be the one over which parallelization is performed.

4 Achievable Performance

To determine how well our implementation takes advantage of the available hardware, we need to know what the hardware is capable of. Theoretical peak performance is *not* a good measure of the performance that is achievable for a particular algorithm. If the calculation is dominated by square roots or exponentials, for example, it does not matter how quickly a compute device can calculate multiplications and additions. To estimate the number of cycles needed for the Ewald summation (Eq. 1), we use vendor information and mini benchmarks.

We first initialize an array of elements to some range of values and then loop over this array applying the operation in question one to a few times. The idea is to access data from cache or registers to minimize the effect of memory bandwidth and latency. We check that vectorized versions of the functions are used where available. The important operations are multiplication, division, square roots, exponentials (exp), sine (sin) and cosine (cos), and the error function (erfc). Table 1 lists the duration of an operation in cycles and its inverse (throughput per cycle) for each device. For operations for which we found information from the vendors, the values are listed in parenthesis as well.

Table 1. Average duration in cycles per core or streaming multiprocessor (SMs) for additions, multiplication, (fused) multiply-add, division, square roots, exponentials, sin and cos, and the error function. All values are approximate. The number of cycles is calculated as the number of cycles per vector instruction divided by the width of the vector. A division using AVX512 instruction on Skylake-X, for example, takes 16 cycles and does 8 division in parallel during those 16 cycles. We therefore have 2 cycles per division. The numbers in parenthesis are from [11,14]. The line for Skylake (zmm) shows results when the compiler was asked for a high usage of zmm registers. On the CPU architectures, we used a single core for the measurements. On the GPUs, we used all SMs and divided the throughput by the number of SMs.

	add	mul	(f)ma	div	sqrt	exp	sin	cos	erfc
Skylake	$(\frac{1}{16})$	$(\frac{1}{16})$	$(\frac{1}{16})$	2.0 (2)	3.06 (3)	12.5	11.58	12.63	16.77
Skylake (zmm)	$(\frac{1}{16})$	$(\frac{1}{16})$	$(\frac{1}{16})$	0.96	1.20	6.32	6.51	6.76	9.25
Haswell	$(\frac{1}{8})$	$(\frac{1}{8})$	$(\frac{1}{8})$	3.97	3.97	2.66	2.84	3.35	5.85
KNL	$(\frac{1}{16})$	$(\frac{1}{16})$	$(\frac{1}{16})$	1.12	2.04	3.82	6.94	7.09	9.20
Kepler	$(\frac{1}{64})$	$(\frac{1}{64})$	$(\frac{1}{64})$	0.15	0.21	0.37	0.55	0.55	1.25
Volta	$(\frac{1}{32})$	$(\frac{1}{32})$	$(\frac{1}{32})$	0.30	0.31	0.57	0.84	0.84	2.04

In the following sections we look at the number of instructions performed by the Ewald solver.

4.1 Ewald Solver

The Ewald solver consists of a k-space (Fourier space) and a real-space part. Let N be the number of particles in the central cell and N_k be the number of wave vectors.

Real-space Contributions To calculate a single particle-particle interaction energy, we first need to calculate the distance between the particles (c.f. first term of Eq. 1). In our implementation the central cell is large enough that we do not need to add additional image cells and thus do not have contributions of the type nL . A distance calculation consists of 3 subtraction, 2 multiply-adds, 1 multiplication and a square root (sqrt). For the particles within a cutoff radius defined by a tunable parameter α , we then calculate the error function (erfc) of the distance, divide by it, and multiply the result by the charge of particle j . All these partial results need to be added up for each particle i and the result is multiplied by the charge of particle i and a constant. Finally, the potential energy of all particles needs to be summed up to get the total energy. This leads to a total of $N^2((3 \text{ sub} + 2 \text{ multiply-add} + 1 \text{ mul} + 1 \text{ sqrt}) + V_f (2 \text{ mul} + 1 \text{ div} + 1 \text{ erfc})) + N \text{ multiply-adds}$, where V_f is the fraction of the total volume within the cutoff radius. For Skylake (zmm) this becomes

$$(1.58 + 10.34V_f)N^2 + N/16 \quad (2)$$

cycles. On a Volta GPU we need

$$(0.50 + 2.40V_f)N^2 + N/32 \quad (3)$$

cycles.

K-space Contributions The second term of Eq. 1 contains 2 nested sums. The outer sum is over $N_k = (2k_{\text{int}} + 1)^3$, where k_{int} is the integer ceiling of k_{max} and k_{max} is determined by the required precision and the factor α mentioned in the Sec. 2. It requires the calculation of the square of the length of the k-vector (2 multiply-add, 1 multiplication), which is used twice. Only wave vectors with a length less than k_{max} are included for the remaining calculations. There are 3 divisions, 7 multiplication, 2 multiply-adds, and 1 exponential. The argument of the inner sum includes the dot product between $\mathbf{k}$ and $\mathbf{r}_i$ (2 multiply-add, 1 multiplication). The exponential of the complex argument is calculated using 1 sin and 1 cos. This is then multiplied by q_i and summed up (1 multiply-add). The argument of the inner sum is executed NN_kV_f times, where $V_f = \frac{4\pi}{3} \frac{k_{\text{max}}^3}{N_k}$. In total this becomes $N_k(3 (\text{sub,multiply-add,mul}) + V_f(9 (\text{sub,multiply-add,mul}) + 3 \text{ div} + 1 \text{ exp} + N(\sin + \cos + 3 (\text{sub,multiply-add,mul})))$. For Skylake (zmm) this becomes

$$(0.19 + (9.76 + 13.46N)V_f)N_k \quad (4)$$

cycles. On a Volta GPU we need

$$(0.09 + (1.75 + 1.77N)V_f)N_k \quad (5)$$

cycles.

5 Results

The program was benchmarked on five different architectures: three different Intel CPUs and two different Nvidia GPUs. The benchmarks were performed on the JURECA and JUWELS clusters at the Jülich Supercomputing Centre [12]. On JURECA the tests were run on i) a CPU compute node, equipped with two Intel Xeon E5-2680 v3 Haswell CPUs, ii) a GPU node equipped with two NVIDIA K80 (Kepler) cards, of which only a single one was used, and iii) a booster node consisting of a single Xeon-Phi 7250-F Knights Landing (KNL) processor. The nodes used on JUWELS are i) a CPU node containing two Intel Xeon Platinum 8168 Skylake-X (SKX) processors and ii) a GPU node with four NVIDIA V100 (Volta) cards, of which again only one is used for the benchmarks.

For each benchmark the same source code was used, containing only minor adjustments concerning the used ExecutionSpace and MemorySpace, depending on the use of i) a GPU architecture and ii) the use of the host_mirror mechanic of Kokkos. The possibility to change the memory layout is also included. For the CPU benchmark runs a complete node was used, i.e., two processors of Haswell and Skylake and one KNL processor, while for the GPU benchmarks only a single GPU was used, i.e., 'half' a K80 and a single Volta V100 card. Therefore the presented runtimes are per-node runtimes, not per processor runtimes.

For the benchmarks a cubic NaCl crystal was simulated, for which the exact solution to the Coulomb potential is known, so that the accuracy of the computed solution could be compared to the exact solution. During the benchmark the size of the crystal was increased by increasing the edge length L of the crystal, thereby increasing the number of particles by L^3 . Due to the nature of the system, the contribution of the Fourier-space is much smaller than the real-space contribution, due to screening effects. This does not decrease the computational demand of the algorithm if a given accuracy has to be achieved.

In the optimal case the Ewald solver shows an complexity of $\mathcal{O}(N^{3/2})$, which depends on an optimal choice of the splitting parameter α , the real-space cut-off radius r_c and the k-space cut-off $k_{\max}$. Due to the implementation of the real-space computation, which is basically a direct solver of complexity $\mathcal{O}(N^2)$, in our results it can be seen that for larger systems sizes the resulting runtimes behave more like $\mathcal{O}(N^2)$ than $\mathcal{O}(N^{3/2})$ (see Fig. 1). The figure also shows the expected relations of runtime to architecture, as the more powerful architectures shows faster runtimes than the less powerful ones. Another detail that can be seen is that the GPUs show the same scaling behavior as the CPUs, with the Volta card resulting in the shortest runtimes of all architectures.

In order to achieve some more insight into the performance portability between the same types of architectures, i.e., CPU-CPU, GPU-GPU, and across types of architectures, i.e., CPU-GPU, we consider the peak-performance normalized runtime on the architectures. The runtime can be expressed by the number of operations divided by a fraction γ , where γ is a measure for the proximity to maximum performance, $t_{\text{run}} = \frac{N_{\text{instruc}}}{\gamma P_{\text{peak}}}$; $\gamma \in [0, 1]$. This can be rewritten as

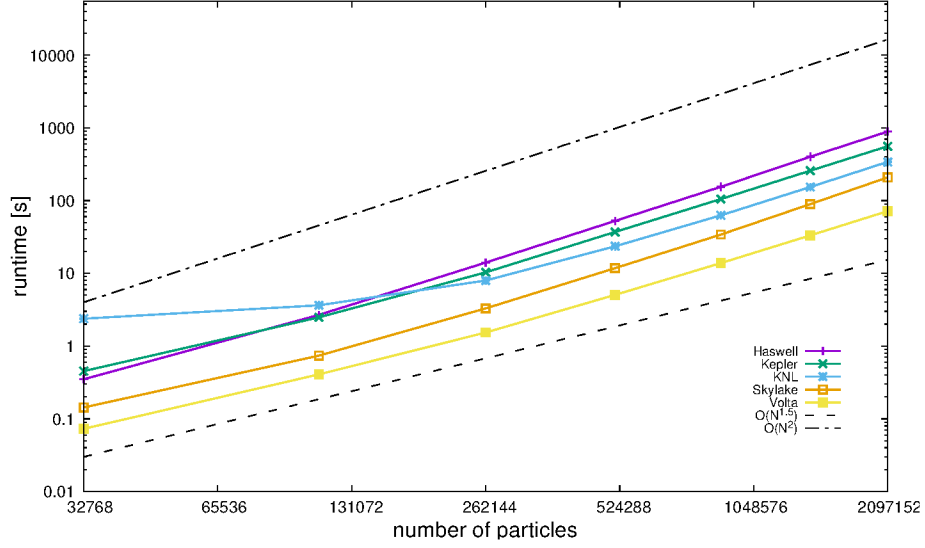


Fig. 1. Comparison of the runtime for different systems sizes on all tested architectures. For reference two guide lines showing a complexity of $\mathcal{O}(N^{3/2})$ and $\mathcal{O}(N^2)$ are shown.

Table 2. Nominal peak performance data for each of the architectures used in the benchmarks

architecture	note	nominal peak performance [TFlops/sec]
Haswell	complete node (two processors)	0.9
Kepler	single GPU (half a K80 card)	0.945
KNL	one processor	3.05
Skylake	complete node (two processors)	4.1
Volta	single GPU	7.8

$$t_{run} \cdot P_{peak} = N_{instruct}/\gamma. \quad (6)$$

To compare the performance portability of the implementation the runtimes need to be compared between the different architectures. Assuming that on each architecture a comparable number of instructions are executed for a given simulation, one can assume that the product of runtime t_{run} and the nominal peak performance P_{peak} will be equal across all platforms, if the reached relative performance γ is equal (equation 6).

For a qualitative comparison based on this thought, the runtimes are multiplied with the nominal peak performance for each of the architectures given in table 2. All peak performance data is with regard to double precision computations, which are used in the code. The resulting plot (Fig. 2) shows that the normalized number of instructions computed for each of the different architectures is similar. It can also be seen that the lines for the same type of architecture (CPU, GPU) are nearly identical to each other, indicating on a qualitative level, that the achieved relative performance is similar within a given type of architecture (with the exception of KNL).

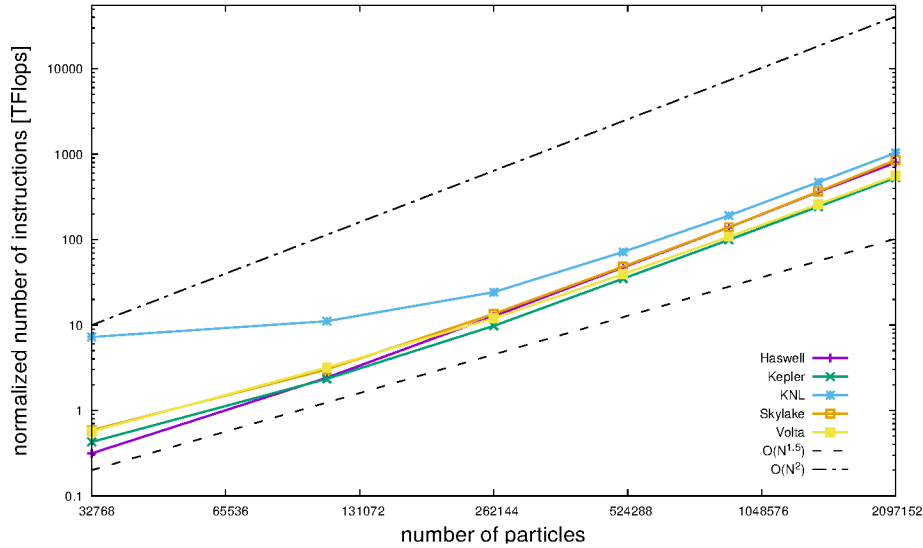


Fig. 2. Runtime on each architecture normalized by the nominal peak performance of the architecture. If the achieved performance on two architectures relative to the nominal peak performance is equal, the lines should be overlapping.

No significant difference could be measured between the variants of the code using the Kokkos `host_mirror` functionality and using the option with unified memory. While this was expected on CPU architectures, it was interesting to

see that required hard copies of data between devices were handled in a very efficient way on GPU architectures independent of the GPU model.

We can do a quantitative analysis of the performance based on the results from Sec. 4. As an example, for $N = 128^3$ we obtain an optimal runtime of 56.44 s based on Eqns. 2 and 4 for the Skylake system. The measured runtime is 206.74 s. This corresponds to a relative performance γ_{SKX} of 0.27. For Volta we get an optimal runtime of 18.61 s and a measured runtime of 71.56 s resulting in a relative performance γ_{SKX} of 0.26. While the scaling with the nominal peak performance P_{peak} (Fig. 2) suggests that γ_{Volta} is larger than γ_{SKX} , above analysis shows that they are nearly equal.

6 Discussion and Conclusions

The performed benchmarks indicate that it is possible to write a performance portable Ewald solver code with Kokkos that can utilize different architectures without the requirement of intensive code adaptations for each of the architectures. Of course it might be possible to write more efficient code specialized for certain architectures, but this kind of code would lose the advantage of versatility concerning architectures it could usefully run on. The quantitative analysis shows that the expected runtime for Skylake is three times longer than for Volta, which our measurement confirm. On the other hand, the nominal peak performance predicts only a factor of two leading to the discrepancy with Fig. 2.

It is noticeable that the performance of the KNL is worse than the performance of the other architectures when using smaller number of particles. This could be related to a massive overhead in the administration of threads, as each thread might not be fully utilized due to the smaller amount of work for each thread. For larger system sizes, it can be seen that the KNL behaves comparable to the other architectures, with regard to the scaling behavior.

Implementing the Ewald solver with Kokkos was slightly more difficult than implementing the code with OpenMP, as the correct usage of the corresponding *parallel_for* and *parallel_reduce* constructs is a bit more intricate than the usage of OpenMP pragmas. The advantage is that they can be used on GPUs as well if certain restrictions regarding memory access are obeyed. As can be seen from our benchmarks this can be done with nearly no loss of relative performance on the different architectures.

Our first results indicate that implementations of algorithms based on Kokkos on a given architecture allows a simplified way of porting to other architectures without a redesign of code (e.g., porting an efficient code for GPUs from standard C++ to CUDA). This allows for an easier transition to other (future) architectures and to investigate and utilise this hardware in an earlier stage of their availability.

For the future it needs to be examined, if the $\mathcal{O}(N^{3/2})$ complexity can be achieved for the Kokkos implementation, e.g., by implementing nearest-neighbor lists for the real-space contribution computation. Also, it would be beneficial to implement more advanced Coulomb solvers, like PEM, P3M or the fast multipole

method, with Kokkos to see if the solvers can also be used performance portable. With regard to Kokkos features, it will also be investigated how large the impact is of choosing an unsuitable memory layout for a given architecture.

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