Challenges Porting a C++ Template-Metaprogramming Abstraction Layer to Directive-based Offloading

Jeffrey Kelling, Sergei Bastrakov, Alexander Debus, Thomas Kluge, Matt Leinheiser, Richard Pausch, Klaus Steiniger, Jan Stephan, René Widera, Michael Bussmann, Sunita Chandrasekaran, and Guido Juckeland

1 Department of Information Services and Computing, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Bautzner Landstr. 400, 01328 Dresden, Germany
2 Institute of Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Bautzner Landstr. 400, 01328 Dresden, Germany
3 Department of CIS, University of Delaware, Newark, Delaware, 19716, USA
4 Center for Advance Systems Understanding (CASUS), Am Untermarkt 20 02826 Görlitz, Germany
5 Georgia Tech, School of Computer Science, Atlanta, GA 30332, USA

Abstract. HPC systems employ a growing variety of compute accelerators with different architectures and from different vendors. Large scientific applications are required to run efficiently across these systems but need to retain a single code-base in order to not stifle development. Directive-based offloading programming models set out to provide the required portability, but, to existing codes, they themselves represent yet another API to port to. Here, we present our approach of porting the GPU-accelerated particle-in-cell code PIConGPU to OpenACC and OpenMP target by adding two new backends to its existing C++ template metaprogramming-based offloading abstraction layer alpaka and avoiding other modifications to the application code. We introduce our approach in the face of conflicts between requirements and available features in the standards as well as practical hurdles posed by immature compiler support.

Keywords: C++ · OpenACC · OpenMP · Offloading.

1 Introduction

Contemporary scientific applications are often written with accelerators, like GPUs, in mind. This approach is required to make use of many modern compute clusters and supercomputers, but it brings a dilemma of choice from a zoo
of proprietary and open offloading APIs coming with varying degrees of support form hardware vendors. While vendor specific, proprietary APIs usually promise best performance and hardware support, their use limits an application to one vendor’s ecosystem. Open APIs offer portability, but cannot guarantee support on future hardware. Committing to any particular offloading API may thus necessitate future rewrites of software when new hardware or architectures become available or the chosen API loses support, which may be unfeasible with the limited time-budged for software development available within the scientific community. Porting even between similar offloading APIs has in the past also proven to be a non-trivial task.

With C++ being very prevalent in contemporary HPC, one approach to mitigate this problem of choice is to use this language’s strength in zero-overhead abstraction via templates and template metaprogramming (TMP) to create an abstraction layer which applications can use to formulate parallelism in an API agnostic way. At first glance this only moves the support problem from the offloading API to the abstraction layer, however, in relation to a large scientific application such an abstraction layer is much smaller and thus requires much less work to port to new parallel APIs. Thus, such an abstraction layer is first conceived as a part of one or a group of scientific applications rather than a library for a general audience. Despite this focus, it will lend itself to other applications, with support being guaranteed as long as the primary applications fuel its developer’s interest.

Another breed of open-standard APIs for parallelization and offloading are directive-based approaches which try to minimize changes to an existing, sequential code base by employing directives for marking code regions which may be offloaded by the compiler without modifying the code in it base-language to the eyes of a compiler with support not enabled. Like with any other API, their practical portability depends on the development afforded by compiler and hardware vendors, too. Currently two competing directive-based model that target accelerator offloading are being developed: OpenMP, which has been around since 1997 as a parallel model for multi-core CPUs, has been extended with target directives in version 4.0 of its standard, while OpenACC was initially created to provide offloading to accelerators exclusively.

This paper presents our efforts and experiences in porting the computational radiation physics code PIConGPU to both OpenACC and OpenMP. PIConGPU uses alpaka, which was first developed to provide portable between different accelerator architectures, including GPUs and Intel MIC, as well as multi-core CPUs to PIConGPU. Even though the primary purpose of OpenMP and OpenACC is to simplify porting of existing codes, porting a code like PIConGPU, with alpaka, as a C++ abstraction layer, already in place, the code for two new alpaka back-ends requires much less effort than porting the whole of PIConGPU directly. Thus, the majority of this paper is dedicated to documenting our efforts to create alpaka back-ends for both OpenACC and OpenMP. Some of the lessons learned here will also apply to using direc-
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PIConGPU is an extremely scalable, heterogeneous, fully relativistic particle-in-cell (PIC) C++ code. This code has been chosen as one of the eight CAAR codes across the United States by the Oak Ridge National Laboratory. CAAR stands for Center for Acceleration Application Readiness - a program at ORNL that is created to ready applications for their next generation computing system, Frontier, the first exascale system to be in place later this year, 2021. Work in this paper narrates challenges and potential solutions to prepare such large scale applications for the ever changing hardware platforms.

This paper discusses the aspects of programmability, portability and performance via the following contributions:

- challenges porting PIConGPU to a directive-based programming model,
- creating alpaka back-ends for OpenMP and OpenACC and evaluating the functionalities of the available compilers, and
- highlighting compiler and runtime issues throughout the PIConGPU code migration process.

We provide an overview of various offloading APIs and abstraction libraries in Section 2. In Section 3 the employed APIs and alpaka are reviewed and compared. During the porting process, various issues with both standards and compiler support were encountered which are described in Section 4. In Section 5 we first discuss the major obstacles we faced during this effort, then provide a short overview of which examples already work using our OpenMP target and OpenACC alpaka backends and current compilers. Finally, Section 6 concludes with an outlook on the developments in the OpenMP and OpenACC ecosystems.

2 Related Work

Since the dawn of general purpose computing on GPUs (GPGPU), quite a few offloading APIs have come and gone. One notable open, cross vendor entry is the Khronos Group’s OpenCL [9] which is barely used anymore in HPC mostly due to some vendor support in this space and partly due to its choice of having device code separate from the host source. Other APIs use a single-source approach, where offloaded code is integrated into the host language. NVIDIA’s proprietary compute unified device architecture (CUDA) [4], which is older than the OpenCL standard, is a C/C++ dialect which offers single-source offloading. It is the most widely used API for scientific codes today, having evolved into the go-to API for many scientific application developers. In response to CUDA’s popularity, AMD created Heterogeneous-compute Interface for Portability (HIP) [13] which mimics the CUDA API to simplify porting CUDA codes. Later single-source approaches aimed at integrating offloading into standard C++ without creating a dialect. This was first attempted by Microsoft introducing C++ AMP [6], which inspired Khronos’ SYCL [15]. The do concurrent construct introduced
to Fortran in version 2008, which can also be offloaded to GPUs by some compilers [24], is a more mature example of the drive to include offloading support directly into base languages.

With these and more offloading APIs, including OpenMP target and OpenACC, available to choose from obsolescence is always looming and can not only be caused by a vendor dropping support for an API, but also by technical developments: With the prevalence NVIDIA GPUs in supercomputers, CUDA looked like a safe choice not long ago. A switch to an AMD-based machine could be addressed by an, in theory, not too demanding port to HIP. However, both of these APIs can only target GPUs not the host CPUs which are the primary compute resource installed on the currently fastest supercomputer Fugaku [17], meaning a code based on these APIs would not be able to run in such a system. Therefore, C++ abstraction layers do not only aim to be a bridge between accelerator architectures and APIs, but also include sequential and parallel execution on the host.

Sandia National Laboratories started the development of Kokkos [21] to achieve performance portability for scientific codes written in C++. It currently supports CUDA OpenMP (host), native POSIX threads and HPX. Another library is RAJA [13], developed at Lawrence Livermore National Laboratory, which offers support of CUDA HIP, Thread Building Blocks (TBB) and OpenMP (including target). RAJA also specifically aims to provide parallel algorithms like Thrust [16]. These libraries, just like alpaka, are single-source, passing user code as a predicate to templates which encapsulate the underlying back-end APIs. In contrast to these examples, alpaka aims to be lightweight low-level abstraction, providing generic access to the basic parallel hierarchies of accelerators without shaping user code prescribing memory layout or algorithms [23].

Another approach that should be mentioned is that of a template expression library, where user code is not directly passed to a back-end but written in template-based domain specific language which then generates backend-compatible code. VexCL [19] used this approach to generate code for just-in-time compilation (JIT) to support OpenCL, next to CUDA and OpenMP.

3 Methods and APIs

3.1 Alpaka and PIConGPU

PIConGPU is a plasma physics code that simulates the dynamics of fast charged particles in electromagnetic fields taking into account relativistic effects and fields generated by moving particles. The employed particle-in-cell approach does store electric and magnetic fields on a regular grid but also must keep track of quickly moving particles. Particles are stored on a per-supercell basis using a dynamic collection of fixed-sized particle vectors. Kernels implementing particle-grid operations on GPUs collectively copy nearby field values between device memory and on-chip scratch memory (e.g. __shared__ in CUDA) to facilitate
efficient parallel processing of particles. This approach takes the hierarchical architecture of GPUs into account and was initially implemented using CUDA directly.

PIConGPU uses templates and [TMPL] to provide a domain-specific language (DSL) for the user to describe the types of particles, interactions and external fields present in the simulation. Some numerical parameters of these are also fixed at compile time. This incurs a large number of constexpr variables of static lifetime, either as static class members or global inside namespaces, to be defined as part of the simulation definition.

Alpaka was introduced to make PIConGPU portable without duplicating code for different target architectures while retaining the present performance on GPUs. To this end, alpaka provides abstract forms of all major concepts present in CUDA, including the execution hierarchy, atomics, block-level synchronization primitives and shared memory as well as a generalize device and memory management API. To generalize these concepts alpaka provides a rather verbose API. To simplify porting codes from CUDA to alpaka the wrapper library cupla [5] was created which provides a simplified API which is more similar to CUDA. Other applications also adopted alpaka as their abstraction for offloading, such as a ptychography code and a high-level trigger software in a large-scale particle detector.

Alpaka currently provides a backend targeting sequential execution, backends for parallel execution on the host via OpenMP and [TBB] as well as on GPUs using CUDA and HIP. A SYCL backend is also under development [2]. Alpaka’s codebase [1] contains some examples, ranging from a parallel “Hello World” to Euler integration. All backends are also covered by a suite of tests, each of which tests a different aspect of offloading. One test focuses on transferring memory between buffers on host and device, including multiple cases covering different source and device locations and buffer sizes. Other tests cover aspects of kernel execution on the device, like trivial kernels, variables in block-shared memory, synchronization between threads or atomic operations.

3.2 Review of OpenACC and OpenMP target

Both OpenACC and OpenMP target have been designed with GPUs or similar accelerators as offload target devices in mind. Both expose the same two main layers of parallelization on target devices as known from GPUs: A work grid is first decomposed into loosely coupled blocks executing independently, which in turn decompose into threads which execute in at least such a way that data sharing may be exclusively between threads of the same block. Both models can also target CPUs, where implementations tend to limit the number of threads per block, often to one, in order to effectively map blocks to CPU threads. An overview on the names the different models assign to these layers is provided in table [1]. We will stick to the CUDA/Alpaka naming scheme.

OpenACC adds a third innermost layer called vector as a straight continuation of this concept, which could conceivably be translated in the same way
Table 1. Rosetta-stone for the names of parallel execution layers. The element/simd layer is only listed for completeness. Each model using a different set of terms pollutes the name space, which is why we stick to the CUDA/Alpaka terminology in the text. Where the word “worker” is used it refers to a scheduled unit executing some work on any parallel level, not to the OpenACC worker.

| CUDA   | Alpaka | OpenMP 5.0 | OpenACC 3.0 |
|--------|--------|-----------|-------------|
| grid   | grid   | (target)  | (parallel)  |
| block  | block  | team      | gang        |
| thread | thread | thread    | worker      |
| _      | element| simd      | (vector)    |

as OpenMP’s simd loop on some architectures. While alpaka does provide an element layer inside threads, no abstraction is provided beyond offering a work-partitioning concept to support canonical for loops, ideally with compile-time length which a compiler can automatically vectorize. As this layer is not going to be mapped explicitly we are not covering it further.

Both models provide directives to control parallel execution and data movement between host and device. Directives start with

```plaintext
#pragma acc ...
``` in OpenACC and

```plaintext
#pragma omp ...
``` in OpenMP.

Here, we shall briefly review the basic primitives of the OpenACC 3.0 and OpenMP 5.0 APIs to highlight their primary design aspects that affect our porting efforts.

Execution of code on the device is initiated using the directives acc parallel and omp target. OpenMP provides the directives teams and parallel which cause regions of code to be executed by multiple blocks or threads, but do not imply any distribution of work. Loops can be distributed in these regions using the distribute (blocks) and for (threads) directives. In OpenACC parallel execution and work distribution constructs are inseparably linked with work distribution provided by the loop gang and loop worker constructs. Herein lies the main conceptual difference between the OpenMP and OpenACC programming models: While OpenMP aims to support all types of parallelism, OpenACC is exclusively designed to describe data parallelism in device code.

On GPUs no assumptions about the execution order of blocks should be made, which is reflected in OpenMP not allowing synchronization and locks across blocks, it does, however, support them between threads of the same block, using barrier and critical, respectively. Following its exclusively data-parallel paradigm, OpenACC does not make any assumptions on execution order on any level and thus does not support explicit synchronization and locks.

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1 Alpaka is following the approach of very long instruction word (VLIW) architectures in OpenCL in this aspect.
|                | CUDA          | OpenMP 5.0          | OpenACC 3.0          |
|----------------|---------------|---------------------|----------------------|
| cudaMalloc    | omp_target_alloc | acc_malloc          |                      |
| cudaMemcpy    | omp_target_memcpy | acc_memcpy_to_device| acc_memcpy_from_device|
| cudaMemcpy    | acc_memcpy_device |                      |                      |
| cudaFree      | omp_target_free | acc_free            |                      |

Because a loop gang region may contain multiple loops in sequence marked with loop worker and loop vector synchronization can be achieved implicitly within blocks.

Both APIs support atomic operations through an atomic directive. OpenMP defines atomics as binding to the target device. OpenACC is less clear on this aspect, only stating that operations are atomic between gangs.

OpenMP provides the runtime API functions omp_get_team_num() to determine the id of a block in device code and omp_get_thread_num() determine the id of a thread within a block. OpenACC does not provide this functionality because in its strict map-reduce picture only the work items must be identified, the workers may remain anonymous to the application code.

### Data Management and Declarations

The canonical way of moving data between host and device in these models is by declaring host storage locations to be associated to locations in device memory and later, or in the same construct, instructing the runtime to copy data between the host and associated device locations. We will not elaborate on the omp target data and acc data directives because in our port we are using runtime API functions which allow for explicit memory management instead. These are listed in table 2.

Clauses related to data movement may also be present in omp target and acc parallel constructs where they declare how the listed variables should be handled before the start and after the end of the attached region. On the OpenACC side these include copy, copyin, copyout, create and others. OpenMP uses the map clause, which handles details through a map-type attribute.

Global variables, including compile-time constants, must be declared for presence on the device. In OpenACC this is done through the construct acc declare copyin( varList ), where varList is a list variables that are declared for the device. With OpenMP global variables can be made available to device code either, in a similar way, using the omp declare target( varList ) construct or by declaring them inside a declare target region. Implementations relax this requirement and only require declaration of compile time constants if they are not optimized out and the compiler places the value in run-time memory. Violations of this relaxed requirement get expressed as linker errors.
Similar constructs are also used to declare functions to be compiled for the device, so they can be called from offloaded code in other compilation units. Functions defined in the same compilation unit can be called without having been declared for the device.

3.3 Experimental Setup

Initially, we started out testing various compilers. For the OpenMP we tried Clang, AMD’s Clang-based development compiler AOMP version 0.7, AMD’s ROC variant of Clang version 4.3.0 (based on Clang 13) [14], GCC version 9, and IBM XL version 16.1.1-5. For OpenACC NVIDIA’s NVHPC toolkit versions from 20.3 to 21.7 and GCC versions 9 through 11 were used. We stopped testing with GCC and IBM XL due to fixes to reported bugs not becoming available timely enough to fit the scope of this work. In the case of IBM XL, debugging runtime errors also turned out to be infeasible due to prohibitively long compile times. We dropped AOMP due repeated difficulty building new releases and also most fixes to bugs AOMP inherited from upstream clang being available upstream first.

Extensive testing was done only for OpenMP using Clang version 10 and above, primarily tracking the main branch, targeting host (x86²) and AMD GPUs (HSA³) and for OpenACC using the latest NVHPC release, currently 21.7, targeting host (x86²) and NVIDIA GPUs⁴. We only used ROC Clang for a few tests prior to this paper. Our testing was strictly focussed on functionality and therefore performance was not measured.

4 Porting Alpaka

With PIConGPU using alpaka to abstract parallel execution models, the only viable way of porting it to OpenMP and OpenACC is to create two alpaka backends and, ideally, not touch PIConGPU itself at all. This severely reduces the amount of code required for the port because each alpaka feature only needs to be mapped to the respective target model once, resulting in most relevant OpenMP and OpenACC construct being used only once in the code.

Alpaka breaks down any offloading backend into a set of basic concepts which are separately implemented and tied together. Table 3 lists the most relevant of these.

Executing User Code on Device For each backend, alpaka provides a type TaskKernelBackendName which wraps a user-provided functor containing the payload code as well as the arguments that should be passed to the functor on-device for execution in a Queue. This is where alpaka’s parallel levels get mapped

² Intel i7-4930K, Ubuntu 18.04
³ Radeon Vega 64, Ubuntu 18.04
⁴ GTX Titan Black, Ubuntu 18.04
Table 3. List of selected primary concepts which need to be implemented by any Alpaka backend.

| Concept          | Description                                                                 |
|------------------|-----------------------------------------------------------------------------|
| Acc              | A type that acts as a handle for a backend. It can be used at compile time to select implementations of traits related to the backend and thus ties all parts of a backend together. |
| AtomicGrids      | Atomic operations which can be implemented differently for atomicity at each level of parallelization: on the whole target device, between block of a kernel, between threads of a block. |
| AtomicBlocks     | A block-shared memory buffer of a size that is set at run time.              |
| AtomicThreads    | A strategy to declare block-shared variable akin to CUDA’s __shared__.        |
| BlockSync        | A strategy by which to synchronize threads within a block.                   |
| Buf              | A RAII class managing a memory buffer in a target device.                    |
| Dev              | A handle for a target device.                                                |
| IdxBt            | A strategy by which a thread can determine its id within a block.            |
| IdxGb            | A strategy by which a block can determine its id within a kernel.            |
| Queue            | A type that implements an execution queue on a target device.                |
| TaskKernel       | A class that wraps user code for execution on a target device.               |
| WorkDiv          | A type holding information about the requested sizes of the grid, blocks and threads (number of elements) for kernel execution. |

onto the levels provided by the backend. The listing in Figure 1 illustrates the basic structure of what the Alpaka TaskKernel invocation could look like for both OpenMP and OpenACC.

A block-shared variable ctx is declared inside the teams, respectively loop gang, region, but outside of the omp parallel, respectively loop worker region, to represent a block-context handle to the thread. This context information includes the current block id. More details about this are provided in the following.

Memory Alpaka’s implementation adheres to the resource acquisition is initialization (RAII) principle and provides a buffer type for memory on each device, including the host. Therefore, Alpaka does not have a concept of fixed associations between host and device memory, but rather allows copying data between (sections of) any pair of buffers. One implication of this is, that the buffer types for OpenMP and OpenACC must be implemented using the manual management routines listed in Table 2, but more importantly, that any pointer to data used in device code, will be a device pointer with no associated host memory. This leads to different complications with each of the models.

By default both models map local variables, including function parameters to the device automatically if they are required in the device code. OpenMP assumes that any pointer it maps hence contains a host address and tries to
template<class Functor, class... Args>
void TaskKernel_OpenMP5_OpenACC(
  WorkDiv workDiv, // grid size
  Functor functor, // user functor
  Args ... args ) // user arguments
{

  // OpenMP
  #pragma omp target
  {
    #pragma omp teams distribute
    for ( int blockIdx = 0;
         blockIdx < workDiv.blocks;
         ++blockIdx )
    {
      AccOmp5 ctx ( workDiv, blockIdx ); // OpenMP backend handle
      #pragma omp parallel
      {
        functor ( ctx, args... );
      }
    }

  // OpenACC
  #pragma acc parallel
  {
    #pragma acc loop gang
    for ( int blockIdx = 0;
         blockIdx < workDiv.blocks;
         ++blockIdx )
    {
      CtxBlockOacc ctxBlock ( workDiv, blockIdx ); // OpenACC backend handle
      #pragma acc loop worker
      for ( int threadIdx = 0;
         threadIdx < workDiv.threads;
         ++threadIdx )
      {
        // need to add threadIdx to the context info
        AccOacc ctx ( ctxBlock, threadIdx );
        functor ( ctx, args... );
      }
    }
  }
}

Fig. 1. Sketch of the structure of a TaskKernel template which calls a user-provided functor with user-provided argument in a parallel context using OpenMP or OpenACC, also providing a handle ctx to enable the user to generically access abstracted backend features. Note, that in the actual implementation TaskKernel is a class template which stores the functor and the arguments as members and provides a call operator to provide the functionality sketched above.
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replace it by the associated device address. If no associated address exists the value copied to the device is 0x0, which also applies to original device pointers. The OpenMP runtime can be instructed to copy a device pointer verbatim using the \texttt{is\_device\_ptr(varName)} clause on the \texttt{target} directive in line 9 or on additional \texttt{omp target data} directives, which alpaka cannot use directly because any pointers are elements of a parameter pack and thus have no name. OpenMP will not perform this replacement on pointers which are enclosed in other data types. Thus, we can get around this problem by wrapping any kernel parameters, which are provided by the user in a C++ parameter pack, in an \texttt{std::tuple} or similar structure.

OpenACC performs a similar replacement of address values also for pointers found inside structures which are mapped, taking the wrapping-workaround off the table. Like in OpenMP, a variable can be explicitly declared as a device pointer using the \texttt{deviceptr(varName)} clause on the \texttt{parallel} directive in line 25 which is not possible because there is no way to know which parameters contain pointers without access to static reflection. The only other option is to add the clause \texttt{default(present)} telling the runtime to assume, that all variables referenced in the offloaded code are already present on the device and do not need to be mapped. Unfortunately this also disables automatic mapping of local variables, necessitating that all local host variables used in the \texttt{parallel} region occur in a \texttt{copyin} clause, which is feasible because they are named.

\textbf{Block and Thread Index} Each worker needs access to information about its position in the global execution grid in order for work distribution to work. The OpenACC variant below line 25 does basically show the canonical way of distributing work over blocks and threads verbatim. In alpaka, the indices of these two nested loops are passed to the user code in \texttt{ctx}. Because OpenMP provides a build-in way to retrieve the thread index via \texttt{omp get thread num()} we use a parallel region without loop to avoid the overhead passing another loop counter to the user code, while the compiler may use hardware intrinsics to supply the user code with this information.

\textbf{Atomic Operations} The set of atomic operations supported by alpaka follows the set provided by CUDA. This includes operations like atomic compare and swap (CAS) min and max next to binary operations. Both OpenMP and OpenACC support atomic load and store as well as binary operations with both a pure update and a capture semantic, i.e. atomically retrieving the stored value before applying the operation to the memory location. Only OpenMP 5.1 adds an atomic compare clause \cite{11}, which permits the ternary operator which is required to implement CAS min and max.

As a work-around these ternary operations can be implemented using a critical region, which, however, does not exist in OpenACC. Not supporting these operations is not an option as PIConGPU’s on-device dynamic memory allocator mallocMC \cite{6} requires them. Therefore we had to implement critical region in violation of the OpenACC standard using device-global, grid-level and
block-level locks based on more basic atomics to cover all levels at which atomic operations may be required.

**Block-Shared Memory** Alpaka provides block-shared variables in the same way CUDA does, i.e. declaration of them is allowed at any point inside kernel/thread code. This is not supported by our targeted models. This capability is implemented by providing a block-shared small-object allocator `BlockSharedSt` as part of the `ctx` object, which contains a fixed-size member array as underlying buffer. The size of this array can only be set at compile time. Allocations of such shared variables are carried out by a master thread, requiring synchronization between threads of a block, after which a reference to the allocated memory is returned to all threads. A part of aforementioned buffer can be reserved as a shared buffer of run time-size (`BlockSharedDyn`), analogous to CUDA dynamic shared memory.

Our expectation is, that implementations will in time be optimized to actually store block-shared variables which fit into on-chip memory there when targeting GPUs. As long as these variables are stored in global device memory our strategy will at least allow these variables to reside compactly in a cache close to executing block.

OpenMP 5.0 added the `omp allocate` directive which allows explicit allocation of memory through the OpenMP runtime, including an implementation-defined allocator `omp_pthread_mem_alloc` which may allow the declaration of block-shared memory akin to using CUDA’s `_shared_` attribute. We did not test this option yet, because functionally, albeit conceivably with lower performance, we can make due with the implementation described above, which is required for OpenACC either way, and using this feature could open another angle where incomplete OpenMP 5.0 compiler support may hit us.

**Block-Level Barrier** Alpaka provides a block-level barrier akin to CUDA’s `__syncthreads()` which can be implemented in OpenMP using the `omp barrier` directive.

OpenACC does not support any explicit synchronization, so we again violated the OpenACC standard by implementing a barrier using atomic operations and spin loops on counters stored in the block-shared context variable `ctx`. This implementation works on GPUs in practice as long as the OpenACC runtime executes exactly the number of threads per block the code expects it to.

### 4.1 Final Touches: PIConGPU

PIConGPU uses one global variable on the target device which is not abstracted by alpaka and thus must be declared by an `acc declare device_resident( varName )`, respectively `omp declare target( varName )`, directive in the PIC-onGPU code.

Global `constexpr` variables, used primarily as part of the simulation definition, for the most part only exist at compile time and influence what code is
generated for offloading. Constants whose value the compiler cannot optimize out do require explicit mapping to the device. This is the case for arrays which are dynamically indexed at run time and any other constant the address of which taken in any context, e.g. if it is used as this argument of a member function call. We chose to not map constants without run time storage explicitly to limit our changes to the application code outside of alpaka to a minimum.

5 Major Hurdles and Discussion

5.1 Standards Issues

OpenACC/OpenMP: Static constexpr Mapping Both OpenACC and OpenMP require global variables to be marked explicitly for availability in device code, making no exception for compile-time constants, so formally all compile time constants have to be declared for the target. In a code like PIConGPU this would effectively lead to each simulation definition file starting with omp declare target and ending with omp end declare target or, worse, acc declare copyin( listOfAllConstexpr ). While the OpenMP version of this only makes the declare construct devoid of meaning, the OpenACC version actually hurts the code maintainability because each addition or removal of a constant has to be mirrored in a second place.

Most available implementations only raise warnings when a constexpr variable is referenced in a target region without having been mapped because there is no problem unless the compiler determines, that a constexpr must be addressed at run time. In this case a reference to a symbol is generated, but no definition, eventually leading to errors during dynamic linking at run time.

For compile time constants, the standards should require symbols to be generated for constexpr variables that are defined inline if needed, as it is easier for the compiler to determine if a given constexpr require a run time representation then for the programmer. This would be more consistent with inline functions, or functions defined within the same translation unit in general, not requiring a declare to be callable from an offloaded region. It would also better fit the C++-notion, that the compiler decides how to handle constexpr.

OpenMP: static constexpr Members We started this work with only OpenMP 4.5 being supported by compilers which required types to not contain any static data members for them to be considered mappable to target, with no exception for compile time constants. Most compilers would only warn if mapped types contained static compile time constants. However, GCC did throw an error here, which prevented us from performing any testing of GCC’s OpenMP or OpenACC implementations with PIConGPU where, as in any TMP code, static constexpr data members are too commonplace to be removed as a

5 In [10]: Section 2.10.4, Restrictions, bullet 5
6 OpenACC does not actually have this restriction, but GCC’s implementation is based on the OpenMP implementation and thus inherited this check.
workaround. OpenMP 5.0 solves this problem by removing the restriction on static data members altogether.

**OpenACC: Lack of Explicit Block-Level Synchronization** The lack of an explicit block-level thread barrier is the most prominent issue our OpenACC port faces in terms of production-readiness. Although we do have a functioning workaround for it, based on the standard not allowing any assumption on thread scheduling, it is correct in stating, that our solution using atomics and spin loops is not save. In practice this issue is exacerbated by the standard API not providing any way to ascertain the actual number of threads being run per block nor to force a certain number to be run, leaving it to the user to find the maximum number of threads the runtime will actually run per block on a given platform and instruct alpaka to not request more than this. If the number actually running threads is smaller than expected, our barrier implementation will dead-lock.

Any need for synchronization between threads could in theory be served using only the implicit barrier after a loop worker region, but this is not feasible in practice. On the surface this would require changing all kernels in PIConGPU which employ barriers to employ loops to describe block-level parallelism, circumventing the existing abstractions and introducing a second implementation incompatible with, e.g., the CUDA backend. Even deeper structural changes would be required where PIConGPU uses other libraries based on alpaka:MallocMC provides an alpaka device function which returns information about the allocator to all threads of a block using collective operations which require synchronization inside the function.

When targeting any hardware which does actually not allow any assumptions about thread execution but somehow still supports the implicit barrier after a loop worker region, a compiler could still implement an explicit barrier by first inlining the code surrounding the barrier and then reordering it to split it into one region before the barrier and one after. Some transformations required to achieve this may require assertions about the code to be made which the base language does not allow in general, e.g., swapping of inner and outer loops. Considering, that any code where data dependencies block the required transformations would be using the barrier in an invalid way, often leading to a dead-lock at run time, the compiler could raise an error when it fails to transform the code to make the barrier implicit.

**C++: std::tuple Trivial Copy** When it comes to offloading, it is very important, that types can be copied bit-wise in order to transfer instances to the target. The C++ standard template library (STL) defines the type trait std::is_trivially_copyable which, if true, guarantees that a bit-wise copy is safe for the given type. Composite types of trivially copyable types are trivially copyable if the move and copy constructors and assignment operators are trivial. For any type which is mapped to target, clang checks this condition and issues a warning when it is not met.
The C++ STL provides the type `std::tuple` which is very useful, among other things, when storing parameter packs for later use, or to sneak device pointers past the address mapping of the OpenMP runtime. Unfortunately, the C++ standard does not require implementations of `std::tuple` to be trivially copyable if all component types are. Both the GNU libstdc++ and LLVM’s libc++ implement `std::tuple` in a way that removes the `std::is_trivially_copyable` trait. While they can still be copied bit-wise in practice as long as all component types can be, this makes `std::tuple` effectively unusable for offloading, because its use turns an otherwise useful warning into noise. An active defect report against the C++ standard on this issue exists [20].

5.2 Compiler and Runtime Issues

PIConGPU is a rather large application, combing through almost all of the C++ core language and, while alpaka only requires a subset of OpenMP or OpenACC to implement its API, it probably happens to lean on aspects which are usually not a focus when porting legacy applications, such as a wide range of atomic operations, data sharing at block level and manual memory management. Hence, the main roadblock to this work was, and remains, an immaturity of the compilers around OpenMP target and OpenACC as the specifications are rather new. Previously ported applications may use a common set of patterns, predominantly straight parallel unrolling of loops over arrays, which is what current compilers support best. When straying off the trodden path we find a number of compiler bugs. With respect to C++ features especially, existing test suites appear to contain mainly small examples each only using a very limited set.

The compiler/runtime bugs can be grouped roughly into three categories: First, internal compiler errors (ICEs) triggered in the compilers by the occurrence of, usually, more complex C++ constructs, e.g. lambdas or parameter packs, occurring in or around target regions. The second are ICEs in the backend, where either intermediate representations from host and target appear to get mixed up or plain missing features, like missing code generation for some atomics. If a code gets past these two, there are run time errors triggered by faulty code generation or runtime behavior.

The largest issue arising from all of these is that further development of triggering code is blocked until the compiler gets fixed; unless a simple workaround is available, which turned out to be rare. Encountering a run time error is especially tricky, as, chances are, there is only one compiler successfully compiling an example for a specific target and thus there is no way to independently test whether the example code itself is correct.

Having only one large application, PIConGPU, that has to iterate with the compiler development and gets stuck at each encountered compiler bug would be too slow. In our work, we were able to take advantage of alpaka’s example codes and test suite. With each small application only using a subset of the backend’s features, some of which may trigger different errors first, we were able to report or debug those in parallel.
Close communication with compiler vendors also helps to alleviate the issue of code not being testable due a lack of reliable compilers. With the very fresh support of offloading, error messages raised by the compiler can often be misleading and fail to point at the actual issue. In some cases an ICE can be triggered by faulty user code, which is just handled badly inside the compiler. It is likely, that invalid code is not often part of compiler test suites. 

ICEs are rather simple to report and caused either by incomplete implementations or some compiler internals which we cannot comment on. Run time errors caused by compiler bugs require debugging on our part. Issues we encountered that lead to wrong run time behavior of our program include an atomic capture which falsely did not change the addressed value and variables declared at block-level being shared between all blocks instead of being private to a single block. Bugs leading to the runtime actively raising an error are simpler to pin down, such as, e.g., a case where accessing an element of a struct member array which is above a certain size in bytes would cause the runtime to report a “GPU memory error”.

**Compiler Error Messages** Another problem encountered when debugging issues in C++ codes in general, specifically when using vendor compilers backed by smaller development teams, is unspecific error reporting. The minor part of this can be unspecific messages of the form “invalid something”, which is almost useless information in the absence of a very verbose context description. The major problem is a lack of context information provided by non-mainstream compilers. There appears to be a strong focus on a procedural style of programming, leading to the assumption, that pointing to the line in the source code where an error occurs provides sufficient information—in C++ it does not: When a code instantiates a template, e.g., ten times, four of which contain something invalid, printing the same line number four times is not helpful. The fact, that gcc and clang++ compilers sometimes produce screens upon screens of a single error message in some template instantiation is a source of much ridicule of C++, but it is very important to have this information in any non-trivial application. Template instantiation generates code at compile time. Consequently, that one line may have four different meanings when the error occurs and six more different meanings where the template is instantiated without causing a compiler error. Thus, it is important for the programmer to know which instance of the template causes the error, otherwise they are left guessing.

We also observed bugs in the error reporting of compilers. For example, a compiler may print an error message pointing to the correct line number, but name the wrong file, specifically complaining about a line in a header, while giving the name of the main source file.

### 5.3 Preliminary Results

Despite complete alpaka backends for OpenMP target and OpenACC and explicit mappings of some bits of PIConGPU’s code which circumvented the abstraction layer, PIConGPU still cannot be successfully ported to GPUs using
OpenMP or OpenACC due to a number of open issues in compilers and run-
times as highlighted in the previous section. With Clang, we were able to use
host as offload target for OpenMP. We had the same option with NVHPC and
OpenACC. We successfully ran PIConGPU via alpaka’s OpenMP or OpenACC
backend using recent versions of the respective compiler on the host.

HelloWorld is the most basic example for an alpaka application in that is only
runs one kernel which does nothing but print the thread and block index of each
thread. Successful execution shows, that the block-shared variables in figure 1
lines 16 or 32 could be created and that they contain the correct block index
for each block. This works on GPU with OpenACC using NVHPC. There is one
major bit of complexity in this example though, in that it requires the runtime
to provide printf() on target. Clang’s offloading runtime for AMD GPUs does
not provide this yet.

VectorAdd performs a simple addition of two vectors filled with random values
on the device and checks the result on the host. This example includes copying
data between host and device in both directions, next to executing a kernel
containing a grid-strided loop. It is, however more portable than helloWorld in
that is does not require any c-stdlib functions in offloaded code. This example
works successfully on GPU with OpenACC using NVHPC. With OpenMP
targeting AMD GPUs this example works only with AMD’s ROC Clang version
4.3.0, while with clang’s main branch we see an issue where having large arrays
as members in structs causes a memory error, which makes starting any alpaka
kernel fail.

Alpaka test suite Targeting the host, all tests pass with OpenMP and Open-
ACC using clang 11+ and NVHPC 21.7, respectively.

Using the most current upstream clang most tests compile targeting AMD
GPUs, some fail with ICEs two due to missing cmath symbols for device code.
All tests fail at run time when using clang main because of the aforementioned
issue crashing any alpaka kernel. Using ROC clang, the linker hangs with most
of the tests.

With OpenACC, targeting NVIDIA GPUs, the majority of tests compile and
succeed at run time. Most notably, tests of the block-level thread synchronization
and block-shared memory succeed on GPU.

6 Conclusions and Outlook

This work attempted to map the feature set of the C++ template metaprogramming (TMP)-
based accelerator abstraction layer alpaka to the directive-based APIs OpenMP
target and OpenACC. The main conceptual difficulty is that alpaka’s API set
is heavily inspired by CUDA and thus requires some very specific capabilities

7 Git commit c20cb5547dd
to be implemented, such as the possibility for user code to declare block-shared variables anywhere instead of only up-front, which no existing API other than CUDA and its look-alikes supports. Here, alpaka could achieve better performance portability by relaxing its adherence to CUDA and instead providing a more general abstraction.

We described a number of problems with the present ecosystem encountered introducing directive-based models into a [TMP] based and heavily abstracted C++ code, which any other abstraction layer, such as Kokkos of RAJA, aiming to support these models would have to face, too. These issues highlight, that the main for OpenMP and OpenACC use-case for these programming models is to add accelerator-offloading to legacy code, which are usually large Fortran or C code-bases. These programming languages mostly support a procedural programming paradigm and only offer a limited options for abstraction beyond this. C++ allows very high levels of abstraction using templates, which provides a quite rigorous formalism for code generation and meta-programming. This lack of consideration for C++ [TMP] makes the standards treat compile time constants like any other (global) variable. This seems reasonable in C or Fortran, where a compile time constant is little more than a variable that is known to the compiler to not change a runtime and that has a static life time. In C++, they can affect code generation itself, leading to the expectation, that handling them is the responsibility of the compiler. They may sometimes become a variable at runtime which does not change, but mostly their storage is optimized out. A distinction should be made between static life time and compile-time life time, where in the latter case the compiler should be responsible for mapping any data still needed at run time.

OpenACC aims to distinguish itself from OpenMP by offering a less explicit way describe parallelism in code. As in this work it was our goal map a very explicit model onto it, we could not appreciate this. From our perspective, the main distinction is OpenACC’s strict adherence to data parallel principles. This is interesting from an academic perspective in that it might enforce a cleaner description of parallel code if fully embraced. When porting originally sequential code to OpenACC it may not be much of a problem to follow this path. We are, however, not aware of any hardware architecture in common use exhibiting the restrictions enforced by OpenACC. Likewise, no other offloading API enforces strict data parallelism, which causes existing parallel codes to be build around established features such as explicit barriers and accessible worker ids. Porting a code that relies on certain patterns to a programming model that does not offer them results in substantial changes to the code and may end up being more of a rewrite than a port, such as in the case of PIConGPU. In our view, this makes OpenACC not a viable general-purpose parallel programming model in its current form.

The primary issue we encountered was the immaturity of compilers both with respect to the support for OpenMP target and OpenACC as well the interaction of that support with C++ code. This forced us to follow a, nowadays, quite unusual development approach, were we had write our code without
the possibility to validate it by compiling, because the compiler would fail at
an [internal compiler error (ICE)]. In order to progress we shifted our focus to
compilers and targets where we saw the fastest development with respect to
the issues we encountered. For this reason, we followed the clang mainline
development on the OpenMP side. With OpenACC, we were only able to make
significant progress due to active support from the NVHPC developers with
finding and fixing bugs in their compiler and also testing our code with their
development compilers in between releases.

We continue to follow the compiler development on both the OpenMP and
OpenACC side to push towards improved compiler support and to address po-
tential issues in the backends presented here.

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