Performance and Optimization Abstractions for Large Scale Heterogeneous Systems in the Cactus/Chemora Framework

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***Abstract*—We describe a set of lower-level abstractions to improve performance on modern large scale heterogeneous systems. These provide portable access to system- and hardware-dependent features, automatically apply dynamic optimizations at run time, and target stencil-based codes used in finite differencing, finite volume, or block-structured adaptive mesh refinement codes.**

These abstractions include a novel data structure to manage refinement information for block-structured adaptive mesh refinement, an iterator mechanism to efficiently traverse multi-dimensional arrays in stencil-based codes, and a portable API and implementation for explicit SIMD vectorization.

These abstractions can either be employed manually, or be targeted by automated code generation, or be used via support libraries by compilers during code generation. The implementations described below are available in the Cactus framework, and are used e.g. in the Einstein Toolkit for relativistic astrophysics simulations.

I. Introduction

Cactus [16], [12] is a software framework for high performance computing, notably used e.g. in the Einstein Toolkit [20], [15] for relativistic astrophysics. The Chemora project [11] aims at significantly simplifying the steps necessary to move from a physics model to an efficient implementation on modern hardware. Starting from a set of partial differential equations expressed in a high level language, it automatically generates highly optimized code suitable for parallel execution on heterogeneous systems. The generated code is portable to many operating systems, and adopts widely used parallel programming standards and programming models (MPI, OpenMP, SIMD Vectorization, CUDA, OpenCL).

In this paper, we describe a set of lower-level abstractions available in the Cactus framework, and onto which Chemora is building. These abstractions are used by many Cactus components outside the Chemora project as well.

These abstractions are:

1) a novel data structure to manage refinement information for block-structured adaptive mesh refinement (section II),
2) an iterator mechanism to efficiently traverse multi-dimensional arrays in stencil-based codes, employing dynamic auto-tuning at run time (section III),
3) a portable API and implementation for explicit SIMD vectorization, including operations necessary for stencil-based kernels (section IV).

These abstractions address issues we encountered when porting Cactus-based applications to modern HPC systems such as Blue Waters (NCSA), Hopper (NERSC), Kraken (NICS), Mira (ALCF), or Stampede (TACC). Of course, these abstractions also improve performance on "regular" HPC systems, workstations, or laptops.

Below, we describe each of these abstractions in turn, and conclude with general observations and remarks.

II. Efficient Bounding Box Algebra

When using adaptive mesh refinement (AMR), one needs to specify which regions of a grid need to be refined. The shape of these regions can be highly irregular. Some AMR algorithms (called cell-based AMR) allow this decision to be made independently for every cell, others (called block-structured AMR) require that refined points be clustered into non-overlapping, rectangular regions for improved efficiency [10], [9]. These regions can then efficiently be represented e.g. via Fortran-style arrays on which loop kernels operate. While cell-based AMR algorithms require tree data structures to represent the refinement hierarchy, block-structured AMR algorithms (such as available in Carpet [22], [21], [13]) require data structures to represent *sets of bounding boxes* describing the regions that make up a particular refinement level.

A *bounding box* (`bbox`) describes the location and shape of a rectangular region, a *bounding box set* (`bboxset`) describes a set of non-overlapping bounding boxes. There is a direct connection between a bboxset and how data for grid points are stored in memory. While a bboxset can in principle describe any set of grid points (that may have arbitrary shape and may be disconnected), one assumes that a bboxset comprises just a few rectangular regions, which will then be handled more efficiently.

Since a bboxset is used to describe the grid points that make up a particular refinement level, its points lie on a uniform grid; see figure 1a below for an example. Each grid point can be described by its location, which can be expressed as

$x_0^i + n^i \cdot \Delta x^i$ where x_0^i and Δx^i describe origin and spacing of the grid, and n^i is a vector with integer elements. (The abstract index i denotes that these are vectors, where $i \in [1 \dots D]$ in D dimensions.)

Carpet not only uses bounding box sets to describe refined regions, it also offers a full algebra for bounding box sets. This includes operations such as set union, intersection, difference, complement, etc., and also includes additional operations enabled by the grid structure such as `shift` (to move a set by a certain offset) or `expand` (to grow a set in some directions), or to change the grid spacing. It is also possible to convert a bboxset into a normalized list of bboxes.

This full set algebra allows using bboxsets as a convenient base for implementing many other operations, such as determining the AMR operators for prolongation, boundary prolongation, restriction, or refluxing; distributing a refinement level's grid points onto MPI processes; determining the communication schedule; or performing consistency checks in a simple-to-express manner. The price one has to pay is that this requires an efficient data structure for these operations, such as we describe below.

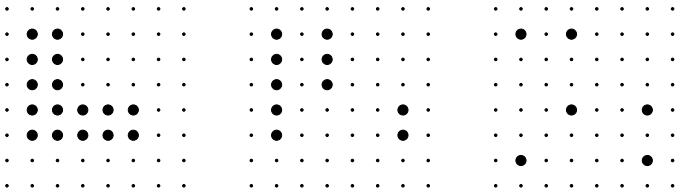
A. Background

There exist two simple approaches to describe sets: one can either enumerate the elements of the set (e.g. in a list or a tree), or one can view the set as a mapping from elements to a boolean (storing one boolean for each element e.g. in an array or a map). The former is efficient if the sets contain few elements and if the elements can be meaningfully ordered, the latter is efficient if the number of possible set elements is small.

Unfortunately, neither is the case here: We intend to handle a refinement level as a set of rectangular bboxes for efficiency; building a data structure that disregards this structure and manages points individually will be much less efficient. At the same time, the *possible* number of points can be many orders of magnitude larger than the *actual* number of points in a region. Thus neither enumerating the grid points making up a bboxset (e.g. via their integer coordinates) makes sense, nor using a boolean array to describe which points belong to a refinement. A more complex data structure is needed.

The literature describes a host of data structures for holding sets of points, or to describe sets of regions. For example, GIS (Geographic Information Systems) heavily rely on such data structures, and R-trees or R^*-trees [23] find applications there. While it would be possible to design an efficient bboxset data structure based on these, they do not quite fit our problem description: They assume that the points making up the set are unstructured (i.e. do not need to be located on a uniform grid), and make no attempt to cluster these points into bboxes. On the other hand, R^*-trees are able to handle regions with varying point density, which is not relevant for a uniform grid.

Other block-structured AMR packages introduce data structure to handle sets of points on uniform grids, but do not provide a full set algebra. Internally, these bboxsets are often represented as a list of bounding boxes. For example, AMROC [1] calls this structure `BBoxList`. (AMROC is a successor of DAGH, which is in turn the intellectual predecessor of Carpet.) Efficient operations may include creating a bboxset from a list of non-overlapping bboxes, while adding an individual bbox to an existing bboxset may not be an efficient operation. Specific operations required for an AMR algorithm are then implemented efficiently, but other operations – such as calculating the intersection between two bboxsets – are not. Most AMR operations acting on bboxsets are then implemented in an ad-hoc fashion and may introduce arbitrary restrictions, e.g. regarding the size of the individual bboxes, or the number of ghost zones for inter-process communication.



(a) L-shaped region (b) x-derivative of this region (c) xy-derivative of this region

Fig. 1: An L-shaped region and its derivatives. The xy-derivative consists only of the "key points" of this shape, and can be stored very efficiently.

Carpet's previous bboxset data structure was based on a list of non-overlapping bboxes. It did provide a full algebra of set operations, but with reduced efficiency. For example, the list of bboxes was kept normalized, requiring an $O(n^2)$ normalization step after each set operation, where n is the number of bboxes in the list. Many other set operations also had an $O(n^2)$ cost, as is common for set implementations based on lists. This cost was acceptable for small numbers of bboxes (say, less than 1,000), but began to dominate the grid setup time when using more than 1,000 MPI processes, as the regions owned by MPI processes are described by bboxes.

An earlier attempt to improve the efficiency of bboxsets is described in [25]. Unfortunately, this work never left the demonstration stage.

We are not aware of other literature or source code describing a generic, efficient data structure to handle sets of points lying on a uniform grid. To our knowledge, this is a novel data structure for AMR applications.

B. Discrete Derivatives of Bounding Box Sets

Our data structure is based on storing the *discrete derivative* of a bboxset. An example is shown in figure 1. Algebraically, the discrete derivative in the i-direction of a bboxset R is given by

$$\partial_i R \quad := \quad R \veebar \operatorname{shift}(R, -e^i) \tag{1}$$

where $\veebar$ is the symmetric set difference (exclusive or), $\operatorname{shift}(R, v)$ shifts the bboxset R by a certain offset v, and e^i is the unit vector in direction i (ith component is 1, all other components are 0).

This discrete derivative is equivalent to a finite difference derivative, applied to the boolean values describing the set interpreted as integer values modulo 2, i.e. using the following arithmetic rules for addition: $0 \oplus 0 = 0$, $0 \oplus 1 = 1$, $1 \oplus 1 = 0$.

Note that we choose to use a leftward finite difference; this is a convention only and has no other relevance. We also note that these discrete derivatives commute, so that the order in which they are applied does not matter. Given a set derivative, the anti-derivative is uniquely defined, and the original set can be readily recovered:

$$R \quad := \quad \partial_i R \veebar \text{shift}(R, -e^i) \tag{2}$$

This implies that the anti-derivative should be calculated by scanning from left to right.

The salient point about taking the derivative is that it reduces the number of elements in a set, assuming that the set has a "regular" structure. For example, in two dimensions (as shown above), an L-shaped region is described by just six points, and in three dimensions, a cuboid ("3D rectangle") is described by just eight points. In fact, the number of points in the derivative of a set increases with the number of bboxes required to describe it – this is exactly the property we are looking for, as the efficiency of a block-structured AMR algorithm already depends on the number of bboxes required to represent the bboxset.

Since the number of elements in the derivative of a set is small, we store these points (i.e. their locations) directly in a tree structure.

Instead of taking derivatives to identify boundaries, one could also use a run-length encoding; the resulting algorithm would be very similar.

C. Implementation

We now describe an efficient algorithm for set operations based on storing bboxsets as derivatives.

Most set operations cannot directly be applied to bboxsets stored as derivatives. The notable exception for this is the symmetric difference, which can directly be applied to derivatives:

$$R \veebar S \quad = \quad \partial R \veebar \partial S \tag{3}$$

where we introduce the notation ∂R to denote subsequent derivatives in all direction, i.e. $\partial R := \partial_0 \partial_1 R$ in two dimensions, and $\partial R := \partial_0 \partial_1 \partial_2 R$ in three dimensions. Property (3) follows directly from the definition of the derivative above and the properties of the exclusive-or operator.

To efficiently reconstruct a bboxset from its derivative, we employ a *sweeping algorithm* [24]. Instead of directly taking the derivative of a bboxset R in all directions, we employ dimensional recursion. We represent a d-dimensional bboxset by taking its derivative in direction d, and storing the resulting set of $d-1$-dimensional bboxsets in a tree structure. We do this recursively, until we arrive at 0-dimensional bboxsets. These are single points, corresponding to a single boolean value that we store directly, ending the recursion.

Since this data structure represents a bboxset, it is irrelevant how the bboxset is represented internally. In particular, from the d-dimensional bboxset's representation, it does not matter how the $d-1$-dimensional bboxsets are internally represented, and from an algorithm design point of view, the $d-1$-dimensional bboxsets are directly available for processing.

$R_{d-1} := \{\}$
$S_{d-1} := \{\}$
$T_{d-1} := \{\}$
$n := 0$
while find next n for which $\partial_d R_d$ or $\partial_d S_d$ **do**
  if $\partial_d R_d$ contains an element at n **then**
    $R_{d_1} := R_{d-1} \veebar \partial_d R_d[n]$
  end if
  if $\partial_d S_d$ contains an element at n **then**
    $S_{d_1} := S_{d-1} \veebar \partial_d S_d[n]$
  end if
  $T'_{d-1} := T_{d-1}$
  $T_{d-1} := R_{d-1} \odot S_{d-1}$
  $\partial_d T_d[n] := T_{d-1} \veebar T'_{d-1}$
  if $\partial_d T_d[n]$ not empty **then**
    store $\partial_d T_d[n]$
  end if
end while

Fig. 2: Algorithm for traversing two bboxsets R and S, calculating $T := R \odot S$ where $\odot$ is an arbitrary set operation. This algorithm applies to a d-dimensional set, recursing to $d-1$ dimensions.

We now describe how to efficiently evaluate the result of a set operation acting on two bboxsets R and S, calculating $T := R \odot S$ for an arbitrary set operation $\odot$. The main idea is to sweep the domain in direction d, keeping track of of the *current state* of the $d-1$-dimensional subsets R_{d-1}, S_{d-1}, and T_{d-1} on the sweep line. (This "line" is a $d-1$-dimensional hypersurface in general.) As the sweep line progresses, we update R_{d-1} and S_{d-1} by calculating the anti-derivative from our stored derivatives, calculate $T_{d-1} := R_{d-1} \odot S_{d-1}$, and then calculate and store the derivate of T_{d-1} in a new bboxset structure.

The operation $T_{d-1} := R_{d-1} \odot S_{d-1}$ needs to be re-evaluated whenever R_{d-1} or S_{d-1} change, i.e. once for each element in the stored derivatives of R_d and S_d. Figure 2 lists the respective algorithm.

Given that accessing set elements stored in a tree has a cost of $O(\log n)$, set operations implemented via the algorithm above have a cost that can be bounded by $O([n_d \log n_d]^d)$, where d is the number of dimensions, and n_d is the maximum number of bboxes encountered by a scan line in direction d. In non-pathological cases, $n_d \approx n^{1/d}$, leading to a log-linear cost. Figure 3 demonstrates then scalability of Carpet for a weak scaling benchmark, when this bboxset algorithm is used for all set operations.

D. Future Work

This derivative bboxset data structure and its associated algorithms are serial, as the sweeping algorithm is sequential

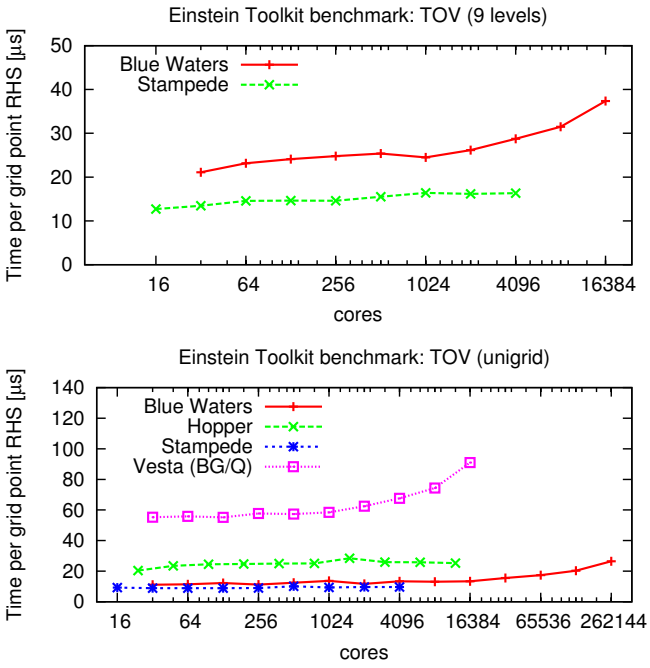


Fig. 3: Weak scaling benchmarks for a relativistic astrophysics application with Carpet, using nine refinement levels (top) and a uniform grid (bottom). Smaller times are better, ideal scaling is a horizontal line. Carpet's AMR implementation scales to 10k+ cores. With a uniform grid, Carpet scales to 250k+ cores.

and does not lead to a natural parallelization. (Of course, different sets can still be processed in parallel.)

One parallelization approach would be to break each bboxset into several independent pieces and to process these in parallel. This would then also require stitching the results together after each set operation.

III. Dynamic Loop Optimizations

Most CPUs and accelerators (if present) of modern HPC systems are multi-core systems with a deep memory hierarchy, where each core requires SIMD vectorization to obtain the highest performance. In addition, in-order-execution systems (i.e. accelerators, including Blue Gene/Q) require SMT (symmetric multi-threading) to hide memory access and instruction latencies. These architectures require significant programmer effort to achieve good single-node performance, even when leaving distributed memory MPI programming aside.[1]

Ignoring the issues of SIMD vectorization here (see section IV below), one would hope that language standards and implementations such as OpenMP or OpenCL allow programmers to ensure efficiency. However, this is not so, for several reasons:

- neither OpenMP nor OpenCL allow distinguishing between SMT, where threads share all caches, and coarse-grained multi-threading, where most cache levels are not shared;
- it is very difficult, if not impossible to reliably predict performance of compute kernels, so that dynamic (run-time) decisions regarding optimizations are necessary;
- the most efficient multi-threading algorithms need to be aware of cache line boundaries, which also needs to factor into how multi-dimensional arrays are allocated; neither OpenMP nor OpenCL provide support for this.

Here we present *LoopControl*, an iterator mechanism to efficiently loop over multi-dimensional arrays for stencil-based loop kernels. LoopControl parallelizes iterations across multiple threads, across multiple SMT threads, performs loop tiling to improve cache efficiency, and honours SIMD vector sizes to ensure an efficient SIMD vectorization is possible.

LoopControl monitors the performance of its loops, and dynamically adjusts its parameters to improve performance. This not only immediately adapts to different machines and to code modifications, but also to differing conditions at run time such as changes to array sizes (e.g. due to AMR) or changes to the physics behaviour in loop kernels. LoopControl uses a *random-restart hill-climbing* algorithm for this dynamic optimization.

The multi-threading is based on OpenMP threads, but employs a dynamic region selection and load distribution mechanism to handle kernels with non-uniform cost per iteration.

LoopControl employs *hwloc* [6] to query the system hardware, and also queries MPI and OpenMP about process/thread setups. hwloc also reports thread-to-core and thread-to-cache bindings that are relevant for performance. All information is gathered automatically, requiring no user setup to achieve good performance.

LoopControl dynamically auto-tunes stencil codes at run time. This is fundamentally different from traditional auto-tuning, which surveys the parameter space for a set of optimizations ahead of time, and then re-uses these survey results at run time. See e.g. [14] for a description of ahead-of-time auto-tuning of stencil-based codes, or [8] for a description of ahead-of-time auto-tuning search algorithms.

Ahead-of-time surveys have the disadvantage that they need to be repeated for each machine on which the code runs, for each compiler version/optimization setting, for each modification to the loop kernel, and also for different array sizes. This makes it prohibitively expensive to use in a code that undergoes rapid development, or where adaptive features such as AMR are used. LoopControl does not have these limitations, and to our knowledge, LoopControl's dynamic auto-tuning algorithm is novel.

A. Loop Traversal

LoopControl assumes that each loop iteration is independent of the others, and can thus be executed in parallel or in an arbitrary order.

Most architectures have several levels of caches. LoopControl implicitly chooses one cache level for which it optimizes.

[1] Single-*core* performance is not really relevant here, since (a) applications will use more than one core per node, and (b) the individual cores interact at run time e.g. via cache access patterns.

The random-restart algorithm (see below) will explore optimizing for other cache levels as well, and will settle for that level that yields the largest performance gain. It would be straightforward to implement support for multiple cache levels, but it is not clear that this would significantly improve performance in practice.

LoopControl uses the following mechanisms, in this order, to split the index space of a loop:

1) coarse-grained (non-SMT) multithreading (expecting no shared caches)
2) iterating over loop tiles (each expected to be small enough to fit into the cache)
3) iterating within loop tiles
4) fine-grained (SMT) multithreading (expecting to share the finest cache level)
5) SIMD vectorization (see section IV below).

The index space is only known at run time. It is split multiple times to find respective smaller index spaces for each of the mechanisms described above. Each index space is an integer multiple of the next smaller index space, up to boundary effects.

Certain index space sizes and offsets have to obey certain constraints:

- SIMD vectorization requires that its index space to be aligned with and have the same size as the SIMD hardware vector size.
- The SMT multithreading index space should be a multiple of the vector size, so that partial vector store operations are not required except at loop boundaries (as some hardware does not offer thread-safe partial vector stores).
- The number of SMT and non-SMT threads is determined by the operating system upon program start, and are not modified (i.e. all threads are used).
- Loop tiles should be aligned with cache lines for efficiency.

Since LoopControl cannot influence how arrays are allocated, the programmer needs to specify the array alignment, if any. The first array element is expected be aligned with the vector size or the cache line size (which can always be ensured when the array is allocated), and the array dimensions may or may not be padded to multiples of the vector size or cache line size. Higher alignment leads to more efficient execution on some hardware, since edge effects such as partial vector stores or partial cache line writes can be avoided. LoopControl offers support for all cases.

B. Random-Restart Hill-Climbing

Since each loop behaves differently (obviously), and since this performance behaviour also depends on the loop bounds, LoopControl optimizes each *loop setup* independently. A loop setup includes the loop's source code location, index space, array alignment, and number of threads available.

Several execution parameters describe how a loop setup is executed, describing how the index space is split according to the mechanisms described above.

Each newly encountered loop setup has its initial execution parameters chosen heuristically. As timing measurements of the loop setup's execution become available, these parameter settings are optimized. It is well known that the execution time of a loop kernel depends on optimization parameters in a highly non-linear and irregular manner, with many threshold effects present. Simplistic optimization algorithms will thus fail. For this optimization, we use a random-restart hill-climbing algorithm as described in the following.

Our optimization algorithm has two competing goals: (1) for a given execution parameter setting, quickly find the nearby local optimum, and (2) do not get stuck in local optima; instead, explore the whole parameter space. To find a local optimum, we use a *hill climbing* algorithm: we explore the local neighbourhood of a given parameter setting, and move to any setting that leads to a shorter run time, discarding parameter settings that lead to longer execution times. To explore the whole parameter space, we use a *random restart* method: once we arrived in a local optimum, we decide with a certain, small probability to chose a random new parameter setting. After exploring the neighbourhood of this new parameter setting, we either remain there (if it is better), or return to the currently known best setting.

There is one major difference between an ahead-of-time exploration of the parameter space, and a dynamic optimization at run time: The goal of an ahead-of-time exploration is to find the best possible parameter setting, while the goal of a run-time optimization is to reduce the overall run time. A bad parameter setting can be significantly worse than a mediocre parameter setting, and can easily have a running time that is an order of magnitude higher. That means that exploring even one such bad parameter setting has a cost that is only amortized if one executes hundreds of loops with good parameter settings.

This makes it important to be cautious about exploring the parameter space, and to very quickly abort any excursion that significantly worsens the run time. It is much more important to find a mediocre improvement and to find it quickly, than to find the optimum parameter choice and incurring a large overhead. In particular, we find that genetic algorithms or simulated annealing spend much too much time on bad parameter settings, and while they may ultimately find good parameter settings, this comes at too great a cost to be useful for a dynamic optimization to be applied at run-time.

For the relatively large kernels present in our astrophysics application, we observe roughly a 10% improvement over a naive OpenMP parallelization via `#pragma omp parallel for` for the first loop executions via our heuristic parameter choices, and an additional approximately 10% improvement in the long run via LoopControl's dynamic optimizations.

C. Future Work

It may be worthwhile to save and restore execution parameter settings and their respective timings. Although these may be invalidated by code modifications or changes to the build setup, this would provide a way to remember exceptionally

good parameter settings that may otherwise be difficult to re-discover.

In particular in conjunction with OpenCL, where it is simple to dynamically re-compile a loop kernel, LoopControl's optimizations could also include compile-time parameter settings such as loop unrolling or prefetching.

In addition to these low-level loop execution optimizations, one can also introduce optimizations at a higher level, such as e.g. loop fission or loop fusion. These optimizations can have large impacts on performance if they make code fit into instruction- or data-caches. Combining LoopControl's optimizer with a way to select between different (sets of) loop kernels would be straightforward.

IV. SIMD Vectorization

Modern CPUs offer SIMD (short vector) instructions that operate on a small number of floating point values simultaneously; the exact number (e.g. 2, 4, or 8) is determined by the hardware architecture. To achieve good performance, it is essential that SIMD instructions are used when compiling compute kernels; not doing so will generally reduce the possible theoretical peak performance by this factor. Of course, this is relevant only for compute-bound kernels.

A. Background

However, using SIMD instructions typically comes with a set of restrictions that need to be satisfied; if not, SIMD instructions either cannot be used, or lose a significant fraction of their performance. One of these restrictions is that it is efficient to perform element-wise operations, but quite inefficient to reduce across a vector. That is, while e.g. $a_i := b_i + c_i$ is highly efficient, the operation $s := \sum_i a_i$ will be relatively expensive. This means that one should aim to vectorize across calculations that are mutually independent. As a rule of thumb, it is better to vectorize across different loop iterations than to try and find independent operations within a single iteration.

Another restriction concerns memory access patterns. Memory and cache subsystems are these days highly vectorized themselves (with typical vector sizes of e.g. 64 bytes), and efficient load/store operations for SIMD vectors require that these vectors are *aligned* in memory. Usually, a SIMD vector with a size of N bytes needs to be located at an address that is a multiple of N. Unaligned memory accesses are either slower, or are not possible at all and then need to be split into two aligned memory accesses and shift operations.

Finally, if one vectorizes across loop iterations, the number of iterations may not be a multiple of the vector size. Similarly, if one accesses an array in a loop, then the first accessed array element may not be aligned with the vector size. In both cases, one needs to perform operations involving only a subset of the elements of an SIMD vector. This is known as *masking* the vector operations. The alternative – using scalar operations for these edge cases – is very expensive if the vector size is large.

Unfortunately, the programming languages that are widely used in HPC today (C, C++, Fortran) do not offer any constructs that would directly map to these SIMD machine instructions, nor do they offer declarations that would ensure the necessary alignment of data structure. It is left to the compiler to identify kernels where SIMD instructions can be used to increase efficiency, and to determine whether data structures have the necessary alignment. Often, system-dependent source code annotations can be used to help the compiler, such as e.g. `#pragma ivdep` or `#pragma simd` for loops, or `__builtin_assume_aligned` for pointers.

Generally, compiler-based vectorization works fine for small loop kernels, surrounded by simple loop constructs, contained in small functions. This simplifies the task of analyzing the code, proving that vectorization does not alter the meaning, and allowing estimating the performance of the generated code to ensure that vectorization provides a benefit. However, we find that the converse is also true: large compute kernels, kernels containing non-trivial control flow (if statements), or using non-trivial math functions (exp, log) will simply not be vectorized by a given compiler. "Convincing" a certain compiler that a loop should be vectorized remains a highly system-specific and vendor-specific (i.e. non-portable) task. In addition, if a loop is vectorized, then the generated code may make pessimistic assumptions regarding memory alignment that lead to sub-ideal performance, in particular when stencil operations in multi-dimensional arrays are involved.

The root of the problem seems to be that the compiler's optimizer does not have access to sufficiently rich, high-level information about the employed algorithms and their implementation to make good decisions regarding vectorization. (The same often holds true for other optimizations as well, such as e.g. loop fission/fusion, or cloning functions to modify their interfaces.) We hope that the coming years will lead to widely accepted ways to pass such information to the compiler, either via new languages or via source code annotations. For example, the upcoming OpenMP 4.0 standard will provide a `#pragma omp simd` to enforce vectorization, GCC is already providing `__builtin_assume_aligned` for pointers, and Clang's vectorizer has as of version 3.3 arguably surpassed that of GCC 4.8, justifying our hope that things are improving.

B. Manual Vectorization

The hope for future compiler features expressed in the previous section does not help performance today. Today, vectorizing a non-trivial code requires using architecture-specific and sometimes compiler-specific *intrinsics* that provide C/C++ datatypes and function calls mapping directly to respective vector types and vector instructions that are directly supported by the hardware. This allows achieving very high performance, at the cost of portability.

For example, the simple loop

```
for (int i=0; i<N; ++i) {
  a[i] = b[i] * c[i] + d[i];
}
```

can be manually vectorized with Intel/AMD's SSE2 intrinsics (for all 64-bit Intel and AMD CPUs) as

```
#include <emmintrin.h>
for (int i=0; i<N; i+=2) {
  __m128d ai, bi, ci, di;
  bi = _mm_load_pd(&b[i]);
  ci = _mm_load_pd(&c[i]);
  di = _mm_load_pd(&d[i]);
  ai = _mm_add_pd(_mm_mul_pd(bi, ci), ci);
  _mm_store_pd(&a[i], ai);
}
```

or with IBM's QPX intrinsics (for the Blue Gene/Q) as

```
#include <builtins.h>
for (int i=0; i<N; i+=4) {
  vector4double ai, bi, ci, di;
  bi = vec_lda(0, &b[i]);
  ci = vec_lda(0, &c[i]);
  di = vec_lda(0, &d[i]);
  ai = vec_madd(bi, ci, di);
  vec_sta(ai, 0, &a[i]);
}
```

These vectorized loops assume that the array size N is a multiple of the vector size, and that the arrays are aligned with the vector size. If this is not the case, the respective vectorized code is more complex.

While the *syntax* of the vectorized kernels looks quite different, the *semantic* transformations applied to the original kernel are quite similar. Vector values are stored in variables that have a specific type (`__mm128d`, `vector4double`), memory access operations have to be denoted explicitly (`_mm_load_pd`, `vec_lda`), and arithmetic operations become function calls (`_mm_add_pd`, `vec_madd`). Other architectures require code transformations along the very same lines.

Note that QPX intrinsics support a fused multiply-add (*fma*) instruction that calculates $a \cdot b + c$ in a single instruction (and presumably also in a single cycle). Regular C or C++ code would express these via separate multiply and add operations, and it would be the task of the compiler to synthesize such fma operations when beneficial. When writing vectorized code manually, the compiler will generally not synthesize vector fma instructions, and this transformation has to be applied explicitly. Today, most CPU architectures support fma instructions.

Vector architectures relevant for high-performance computing these days include Intel's and AMD's SSE instructions, Intel and AMD's AVX instructions (both SSE and AVX exist in several variants), Intel's Xeon Phi vector instructions, IBM's Altivec and VSX instructions for Power CPUs, and IBM's QPX instructions for the Blue Gene/Q. On low-power devices, ARM's NEON instructions are also important.

C. An API for Explicit Vectorization

Based on architecture- and compiler-dependent intrinsics, we have designed and implemented a portable, efficient API for explicit loop vectorization. This API targets stencil-based loop kernels, as can e.g. be found in codes using finite differences or finite volumes, possibly via block-structured adaptive mesh refinement. Our implementation `LSUThorns/Vectors` uses C++ and supports all major current HPC architectures [20], [15].

The API is intended to be applied to existing scalar codes in a relatively straightforward manner. Data structures do not need to be reorganized, although it may provide a performance benefit if they are, e.g. ensuring alignment of data accessed by vector instructions, or choosing integer sizes compatible with the available vector instructions.

The API consists of the following parts:

- data types holding vectors of real numbers (float/double), integers, and booleans (e.g. for results of comparison operators, or for masks);
- the usual arithmetic operations (+ - * /, copysign, fma, isnan, signbit, sqrt, etc.), including comparisons, boolean operations, and an if-then construct;
- "expensive" math functions, such as cos, exp, log, sin, etc. that are typically not available as hardware instructions;
- memory load/store operations, supporting both aligned and unaligned access, supporting masks, and possibly offering to bypass the cache to improve efficiency;
- helper functions to iterate over a index ranges, generating masks, and ensuring efficient array access, suitable in particular for stencil-based kernels.

We describe these parts in more detail below.

The OpenCL C language already provides all but the last item. Once mature OpenCL implementations become available for HPC platforms – that is, for the CPUs on which the applications will be running, not only for accelerators that may be available there – this API could be replaced by programming in OpenCL C instead. We are actively involved in the *pocl* (*Portable Computing Language*) project [5] which develops a portable OpenCL implementation based on the LLVM infrastructure [2].

1) Data Types and Arithmetic Operations: The first two items – data types and arithmetic operations – can be directly mapped to the vector intrinsics available on the particular architecture. We remark that vectorized integer operations are often not available, and that vectorized boolean values are internally often represented and handled quite differently from C or C++.

For each architecture, the available vector instruction set and vector sizes are determined automatically at compile time, and the most efficient vector size available is chosen. Both double and single precision vectors are supported.

For several architectures, this API is implemented via macros instead of via inline functions. Surprisingly, several widely used compilers for HPC systems cannot handle inline functions efficiently. The most prominent consequence of this is that operator overloading is not possible; instead, arithmetic operations have to be expressed in a function call syntax such as `vec_add(a,b)`. While straightforward, this unfortunately reduces readability somewhat.

A trivial implementation, useful e.g. for debugging, maps this API to scalar operations without any loss of efficiency.

Using our API, the example from above becomes

```
#include <vectors.h>
for (int i=0; i<N; i+=CCTK_REAL_VEC_SIZE) {
  CCTK_REAL_VEC ai, bi, ci, ci;
  bi = vec_load(&b[i]);
  ci = vec_load(&c[i]);
  di = vec_load(&d[i]);
  ai = vec_madd(bi, ci, di);
  vec_store(&a[i], ai);
}
```

This code is portable across many architectures. However, this example still assumes that all arrays are aligned with the vector size, that the array size is a multiple of the vector size, and does not include any cache optimizations.

`if` statements require further attention when vectorizing, since different elements of a vector may lead to different paths through the code. Similarly, the logical operators `&&` and `||` cannot have shortcut semantics with vector operands (see e.g. the OpenCL standard [3]). To translate `if` statements, we provide a function `ifthen(cond, then, else)` with a definition very similar to the `?:` operator, but without shortcut semantics. (This corresponds to the OpenCL `select` function, except for the order of the arguments.)

To vectorize an `if` statement, it needs to be rewritten using this `ifthen` function, taking into account that both the *then* and the *else* branches will be evaluated for all vector elements. Often, declaring separate local variables for the *then* and the *else* branches and moving all memory store operations (if any) out of the `if` statement (and turning them into masked store operations if necessary) make this transformation straightforward.

2) "Expensive" Math Functions: Some compilers (IBM, Intel) offer efficient implementations of the "expensive" math functions that can be used (`mass_simd`, `mkl_vml`), while other compilers (GCC, Clang) do not. To support system architectures other than IBM's and Intel's, we have implemented an open-source library *Vecmathlib* [7], [18] providing portable, efficient, vectorized math functions.[2]

The OpenCL C language standard requires that these math functions be available for vector types. For the pocl project's OpenCL compiler, we thus use Vecmathlib to implement these where no vendor library is available.

3) Memory Access: The API supports a variety of access modes for memory load/store operations that are likely to occur in stencil-based codes. In particular, great care has been taken to ensure that the most efficient code is generated depending on either compile-time or run-time guarantees that the code can make regarding alignment. Some code transformations, such as array padding of multi-dimensional arrays, enable such guarantees and can thus improve performance.

Let us consider a slightly more complex example using stencil operations. The code below calculates a derivative via a forward finite difference:

```
for (int i=0; i<N-1; ++i) {
  a[i] = b[i+1] - b[i];
}
```

[2]Under some circumstances, this library is for scalar code faster than glibc on Intel/AMD CPUs.

We assume that the arrays `a` and `b` are aligned with the vector size, and that $N-1$ is a multiple of the vector size. This code can then be vectorized to

```
#include <vectors.h>
for (int i=0; i<N-1; i+=CCTK_REAL_VEC_SIZE) {
  CCTK_REAL_VEC ai, bi, bip;
  bi  = vec_load(&b[i]);
  bip = vec_loadu_off(+1, &b[i+1]);
  ai  = vec_sub(bip, bi);
  vec_store(&a[i], ai);
}
```

Here, the function `vec_loadu_off(offset, ptr)` loads a value from memory that is located at an offset of $+1$ from an aligned value. This specification expects that the offset is known at compile time, and allows the compiler to generate the most efficient code for this case. A similar function `vec_loadu(ptr)` allows loading unaligned values if the offset is unknown at compile time. Equivalent functions exist for storing values.

4) Iterators: Finally, our API provides an "iterator" to simplify looping over index ranges. Typically, only the innermost loop of a loop nest is vectorized, and it is expected that this loop has unit stride. This iterator also sets a mask to handle edge cases at the beginning and end of the index range. This is also connected to shared memory parallelization such as via OpenMP, where one wants to ensure that an OpenMP parallelization of the innermost loop does not introduce unaligned loop bounds.

The scalar code below evaluates a centered finite difference:

```
for (int i=1; i<N-1; ++i) {
  a[i] = 0.5 * (b[i+1] - b[i-1]);
}
```

We assume again that the arrays `a` and `b` are aligned with the vector size. We also assume that the array is padded, so that we can access elements that are "slightly" out of bounds without causing a segmentation fault. Both conditions can easily be guaranteed by allocating the arrays correspondingly, e.g. via `posix_memalign`. If the arrays' alignment is not known at compile time, then they need to be accessed via `vec_loadu` and `vec_storeu` functions instead. We make no other assumptions, and the array can have an arbitrary size. This leads to the following vectorized code:

```
#include <vectors.h>
VEC_ITERATE(i, 1, N-1) {
  CCTK_REAL_VEC ai, bim, bip;
  bim = vec_loadu_off(-1, &b[i-1]);
  bip = vec_loadu_off(+1, &b[i+1]);
  ai  = vec_mul(vec_set1(0.5), vec_sub(bip, bim));
  vec_store_nta_partial(&a[i], ai);
}
```

The macro `VEC_ITERATE(i, imin, imax)` expands to a loop that iterates the variable `i` from `imin` to `imax` with a stride of the vector size. It also ensures that `i` is always a multiple of the vector size, starting from a lower value

than `imin` if necessary. Additionally, it prepares an (implicitly declared) mask in each iteration.

The suffix `_partial` in the vector store operation indicates that this mask is taken into account when storing. The code is optimized for the case where all vector elements are stored. The suffix `_nta` invokes a possible cache optimization, if available. It indicates that the stored value will in the near future not be accessed again ("non-temporal access"). This hint can be used by the implementation to bypass the cache when storing the value.

Most CPU architectures do not support masking arbitrary vector operations, while masking load/store operations may be supported. In the examples given here, we only mask store operations, assuming that arrays are sufficiently padded for load operations to always succeed. The unused vector elements are still participating in calculations, but this does not introduce an overhead.

This iterator provides provides a generic mechanism to traverse arrays holding scalar values via vectorized operations. It thus provides the basic framework to enable vectorization for a loop, corresponding to a `#pragma simd` statement. By implicitly providing masks that can be used when storing values, aligned and padded arrays are handled efficiently.

Different from the previous items, this iterator is applicable even for OpenCL C code, since no equivalent constructs exist in the language.

D. Applications

The API described above allows explicitly vectorizing C++ code. While somewhat tedious, it is in our experience straightforward to vectorize a large class of scalar codes where vectorization is beneficial. There is special support for efficient support of stencil-based codes on block-structured grids using multi-dimensional arrays.

While manual vectorization is possible, this API also lends itself for automated code generation. We use Kranc [17], [19] to create Cactus components from partial differential equations written in Mathematica notation, and have modified Kranc's back-end to emit vectorized code. Mathematica's pattern matching capabilities are ideal to apply optimizations to the generated vector expressions that the compiler is unwilling to perform.

V. Conclusion

This paper describes a set of abstractions to improve performance on modern large scale heterogeneous systems targetting stencil-based codes. These abstractions are available in the Cactus framework, and are used in "real-world" applications, such as in relativistic astrophysics simulations via the Einstein Toolkit.

Our implementations of these abstractions require access to low-level system information. Especially hwloc [6] and PAPI [4] provide valuable information. While hwloc is very portable and easy to use, we are less satisfied with the state of PAPI installations; these are often not available (and neither are alternatives), not even on freshly installed cutting-edge systems. We are highly dissatisfied with this situation, which forces us to resort to crude overall timing measurements to evaluate performance.

While our performance and optimization abstractions are portable, they are by their very nature somewhat low-level, and using them directly e.g. from C++ code can be tedious, although straightforward. We anticipate that they will see most use either via automated code generation (e.g. via Kranc [17], [19]), or via including them into compiler support libraries (e.g. via pocl [5]).

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