Automatic Parallelization of Python Programs for Distributed Heterogeneous Computing

Jun Shirako, Akihiro Hayashi, Sri Raj Paul, Alexey Tumanov, and Vivek Sarkar

School of Computer Science, Georgia Institute of Technology

Abstract. This paper introduces a novel approach to automatic aheadof-time (AOT) parallelization and optimization of sequential Python programs for execution on distributed heterogeneous platforms. Our approach enables AOT source-to-source transformation of Python programs, driven by the inclusion of type hints for function parameters and return values. These hints can be supplied by the programmer or obtained by dynamic profiler tools; multi-version code generation guarantees the correctness of our AOT transformation in all cases.

Our compilation framework performs automatic parallelization and sophisticated high-level code optimizations for the target distributed heterogeneous hardware platform. It includes extensions to the polyhedral framework that unify user-written loops and implicit loops present in matrix/tensor operators, as well as automated section of CPU vs. GPU code variants. Further, our polyhedral optimizations enable both intranode and inter-node parallelism. Finally, the optimized output code is deployed using the Ray runtime for scheduling distributed tasks across multiple heterogeneous nodes in a cluster.

Our empirical evaluation shows significant performance improvements relative to sequential Python in both single-node and multi-node experiments, with a performance improvement of over $20,000 \times$ when using 24 nodes and 144 GPUs in the OLCF Summit supercomputer for the Space-Time Adaptive Processing (STAP) radar application.

1 Introduction

Multiple simultaneous disruptions are currently under way in both hardware and software, as we consider the implications for future parallel systems. In hardware, "extreme heterogeneity" has become critical to sustaining cost and performance improvements with the end of Moore's Law, but poses significant productivity challenges for developers. In software, the rise of large-scale data science and AI applications is being driven by domain scientists from diverse backgrounds who demand the programmability that they have come to expect from high-level languages like Python [14]. While this paper focuses on Python as an exemplar of modern high-productivity programming, the approach in this paper is equally applicable to other high-productivity languages such as Julia [7].

A key challenge facing domain scientists is determining how to enable their Python-based applications to use the parallelism inherent in both distributed

and heterogeneous computing. A typical workflow for domain scientists is to experiment with new algorithms by starting with smaller datasets and then moving on to larger datasets. A tipping point is reached when the dataset size becomes too large to be processed within a single node, and another tipping point is reached when there is a need to use accelerators such as GPUs.

One approach to dealing with these tipping points is to rely on experienced programmers with a deep ("ninja level") expertise in computer architecture and code optimization for accelerators and inter-node communication. However, this approach is a non-starter for many domain scientists due to its complexity and the skills required. For example, even though Python bindings for MPI [9] have been available for many years, there has been very little adoption of these bindings by domain scientists. An alternate approach is to augment a highproductivity language with native libraries that include high-performance implementations of commonly used functions, e.g., functions in the NumPy [2] and SciPy [1] libraries for Python. However, fixed library interfaces and implementations do not address the needs of new applications and algorithms. Yet another approach is to develop and use Domain Specific Languages (DSLs); this approach has recently begun showing promise for certain target domains, e.g., PyTorch and TensorFlow for machine learning, Halide for image processing computations, and TACO for tensor kernels. However, the deliberate lack of generality in DSLs poses significant challenges in requiring domain scientists to learn multiple DSLs and to integrate DSL kernels into their overall programming workflow, while also addressing corner cases that may not be supported by DSLs.

In this paper, we make the case for new advances to enable productivity and programmability of future HPC platforms for domain scientists. The goal of our system, named AutoMPHC, is Automation of Massively Parallel and Heterogeneous Computing, obtained by delivering the benefits of distributed heterogeneous hardware platforms to domain scientists without requiring them to undergo any new training. As a first step towards this goal, this paper introduces a novel approach to automatic ahead-of-time (AOT) parallelization and optimization of sequential Python programs for execution on distributed heterogeneous platforms, and supports program multi-versioning for specializing code generation to different input data types and different target processors. The optimized code is deployed using the Python-based Ray runtime [11] for scheduling distributed tasks across multiple heterogeneous nodes in a cluster.

As a simple illustration of our approach, consider two versions of the Poly-Bench [6] correlation benchmark shown in Figures 1 and 2. The first case represents a list-based pattern implemented using three explicit Python loops that access elements of lists (as surrogates for arrays), which might have been written by a domain scientist familiar with classical books on algorithms such as [13]. The second case represents a NumPy-based pattern with one explicit loop and a two-dimensional array statement in line 7 of Figure 2, which might have been written by a domain scientist familiar with matrix operations. A unique feature of our approach is the ability to support both explicit Python loops and implicit loops from NumPy operators and library calls in a unified optimization

```
1
     def kernel(self, float_n: float, data: list, corr: list, mean: list, stddev: list):
2
         for i in range(0, self.M-1):
3
             corr[i][i] = 1.0
4
             for j in range(i+1, self.M):
5
                 corr[i][j] = 0.0
6
                 for k in range(0, self.N):
7
                     corr[i][j] += (data[k][i] * data[k][j])
8
9
                 corr[j][i] = corr[i][j]
10
         corr[self.M-1][self.M-1] = 1.0
```

Fig. 1. PolyBench-Python correlation: List version (default)

```
from numpy.core.multiarray import ndarray
1
2
    def kernel(self, float_n: float, data: ndarray, corr: ndarray, mean: ndarray, stddev: ndarray):
3
4
        corr[np.diag_indices(corr.shape[0])] = 1.0
5
        for i in range(0, self.M - 1):
6
            corr[i,i+1:self.M] = (data[0:self.N,i] * data[0:self.N,i+1:self.M].T).sum(axis=1)
7
        tril_indices = np.tril_indices( n=self.M, m=self.M, k=-1 )
8
        corr[tril_indices] = corr[triu_indices]
9
        corr[self.M - 1, self.M - 1] = 1.0
10
```

Fig. 2. PolyBench-Python correlation: NumPy version

Table 1. Execution time of correlation (dataset = large)

Ι	List version	NumPy version	Our optimization (Figure 6c)
	$152.5 \; [sec]$	$2.212 \; [sec]$	$0.07163 \; [sec]$

framework. Table 1 shows that the NumPy-based version of the correlation benchmark performs better than the list version, while our approach (which can be applied to either style of input) performs significantly better than both. Additional performance results are discussed in Section 5.

In summary, this paper makes the following contributions:

- A novel approach to automatic ahead-of-time (AOT) parallelization and optimization of sequential Python programs for execution on distributed heterogeneous platforms. Our approach is driven by the inclusion of type hints for function parameters and return values, which can be supplied by the programmer or obtained by dynamic profiler tools; multi-version code generation guarantees the correctness of our AOT transformation in all cases.
- Automatic parallelization and high-level code optimizations for the target distributed heterogeneous hardware platform, based on extensions to the polyhedral framework that unify user-written loops and implicit loops present in matrix/tensor operators, as well as automated selection of CPU vs. GPU code variants.
- Automatic code generation for targeting the Ray runtime to schedule distributed tasks across multiple heterogeneous nodes in a cluster.
- An empirical evaluation for 15 Python-based benchmarks from the Polybench suite on a single node with multiple GPUs, and another evaluation of the Space-Time Adaptive Processing (STAP) radar application in Python.

Both evaluations show significant performance improvements due to the use of AutoMPHC. In the case of STAP, the performance improvement relative to the original Python code was over $20,000 \times$ when using 24 nodes and 144 GPUs (6 GPUs/node) in the OLCF Summit supercomputer.

2 Background

2.1 Intrepydd Compiler

The Intropydd programming language [23] introduced a subset of Python that is amenable to ahead-of-time (AOT) compilation into C++. It is intended for writing kernel functions rather than complete or main programs. The C++ code generated from Intropydd kernels can be imported into a Python application or a C++ application.

A key constraint in the Intrepydd subset of Python is the requirement that Intrepydd function definitions include type annotations for parameters and return values. Given these type annotations, the Intrepydd compiler statically infers the types of local variables and expressions. The Intrepydd tool chain includes a library knowledge base, which specifies type rules for a wide range of standard library functions used by Python programs. As discussed in the following sections, the AutoMPHC system extends the Intrepydd tool chain to serve as a Python-to-Python optimization and parallelization system; there is no C++ code generated by AutoMPHC.

It is important to note that Intrepydd also includes extensions to standard Python to enable C++ code generation. These extensions include statements with explicit parallelism (e.g., pfor for parallel loops) and special library functions. In contrast, AutoMPHC does not rely on any of these extensions. All input code to AutoMPHC and all output code generated by AutoMPHC can be executed on standard Python implementations.

2.2 AutoMPHC Runtime

We use Ray [11] as the base distributed runtime framework. Ray features a number of properties beneficial for AutoMPHC. First, the ability to simultaneously support both *stateless* and *stateful* computation—one of its key research contributions useful for a heterogeneous mix of CPU and GPU compute. Stateless computation, in the form of side effect free tasks, is best suited for processing large data objects or partitions on numerous CPU resources. Stateful computation is beneficial for GPU tasks. We create tasks for this distributed runtime by *automatically* compiling chunks of code into Ray tasks. Each Ray task then can be spawned asynchronously. A full directed acyclic graph (DAG) of such task instantiations is dynamically constructed and submitted for execution without waiting for intermediate computation results. It enables AutoMPHC to (a) hide the latency of task instantiation and propagation to workers for execution, (b) extract pipeline parallelism, and, (c) extract parallelism from the partial order of

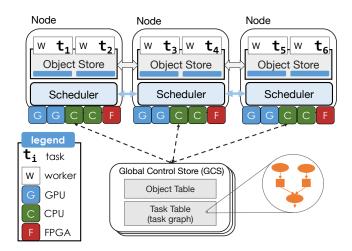


Fig. 3. AutoMPHC distributed runtime architecture.

the dynamically constructed directed acyclic task graph. As Ray tasks are instantiated, they return immediately with a future-like construct, called an ObjectID — an object handle that refers to a globally addressable object. The object is eventually fulfilled and can be extracted with a blocking ray.get(object_id) API. We note that the distributed object store (Fig. 3 used for the lifecycle of these objects is immutable—a property that elides the need for expensive consistency protocols, state coherence protocols, and other synchronization overheads needed for data correctness. Critically, this alleviates the need for expensive MPI-style distributed barriers and, therefore, does not suffer from the otherwise common straggler challenges—an important property for heterogeneous compute at scale. Finally, data store immutability, combined with the deterministic nature of the task graph, enable fault tolerance, as any missing object in the graph can be recomputed by simply replaying the sub-graph leading up to and including the object's parent vertex. This mechanism can be triggered automatically and comes with minimal overhead on the critical path of a task [22].

3 Overview of our Approach

Figure 4 summarizes the overall design of our proposed AutoMPHC system. Userdeveloped code is a combination of main program code and kernel code, where the former is executed unchanged and the latter is optimized by AutoMPHC via automatic ahead-of-time (AOT) source-to-source transformations. There are two forms of kernel code supported by our system — one in which type annotations are manually provided by the user, and another in which type annotations are obtained by a type profiler such as MonkeyType. In both cases, the type annotations serve as *hints* since the multi-version code generation guarantees the correctness of our AOT transformations in all cases (whether or not the actual inputs match the type annotations).

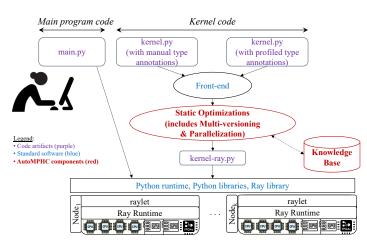


Fig. 4. Overall Design of AutoMPHC system

The kernel functions with type annotations (hints) are first translated by the Front-end to an Abstract Syntax Tree (AST) representation implemented using the standard Python Typed AST package. The core optimizations in AutoMPHC are then performed on the AST, including multi-version code specialization (Section 4.1), polyhedral optimizations (Section 4.2), and generation of distributed parallel code using Ray tasking APIs along with generation of heterogeneous code using selective NumPy-to-CuPy conversion (Section 4.3). These Static Optimizations benefit from the use of the AutoMPHC Knowledge Base, which includes dataflow and type information for many commonly used library functions. The transformed code is then executed on a distributed heterogeneous platform using standard Python libraries in addition to Ray.

4 Optimizations

The AutoMPHC compiler is the extension of Intrepydd compiler [23], which supports type inference and basic optimizations including loop invariant code motion, sparsity optimization, and array allocation/slicing optimizations. In the following sections, we present newly developed optimizations for automatic parallelization targeting distributed heterogeneous systems.

4.1 Program Multi-versioning for Specialized Code Optimizations

Multi-versioning is an approach to data-aware optimizations, which generates multiple code versions specialized under certain conditions at compile-time and selects a proper code version at runtime. In our framework, we consider two classes of conditions, *legality-based* and *profitability-based*. All the conditions are organized as decision trees, where legality conditions are located at higher levels while profitability conditions are at lower levels in general.

```
1
    def kernel(self, float_n: float, data: ndarray, ...
                                                              .):
         if type(float_n) == float and type(data) == ndarray and ...:
if data.ndim == 2 and ...:
2
3
                  ... # Code with type-specific and rank-specific optimizations
4
              else:
5
                       # Code with type-specific optimizations
6
         else:
7
                  # Code without type-specific optimizations
8
```

Fig. 5. Multi-versioning for PolyBench-Python correlation

The legality conditions are mainly used to verify the data type annotations attached on function parameters and returns. In our approach, the type annotations are used as hints and can be different from actual types given at runtime. Further, the correctness of array rank/dimensionality inference is critical to the polyhedral optimizations (Section 4.2). The multi-versioning serves as runtime checks of annotated/inferred types and ranks for specialized code version while ensuring correct behavior for others, as shown in Figure 5.

The profitability conditions can cover a broad range of conditions/scenarios related to runtime performance rather than correctness. As described later, the AutoMPHC compiler can generate two versions of optimized kernels, one for CPUs and the other for GPUs. The runtime condition between these two versions is a typical example of profitability conditions (Section 4.3).

4.2 Polyhedral Optimizations

Polyhedral compilation has provided significant advances in the unification of affine loop transformations combined with powerful code generation techniques [8,21,24]. However, despite these strengths in program transformation, the polyhedral frameworks lack support for: 1) dynamic control flow and non-affine access patterns; and 2) library function calls in general. To address the first limitation, we have extended the polyhedral representation, Static Control Parts (SCoP), to represent unanalyzable expressions as a compound "black-box" statement with approximated input/output relations. To address the second limitation, we took advantage of our library knowledge base to obtain element-wise dataflow relations among function arguments and return values, whose examples are shown in Table 2. These unique features enable the co-optimization of both explicit loops and implicit loops from operators and library calls in a unified optimization framework, as detailed in the following sections.

Given SCoP representation extracted from the Python IR, the AutoMPHC polyhedral optimizer, which is built on PolyAST [16,15] framework, computes dependence constraints and performs program transformations. Finally, the optimized SCoP representation is converted back to Python IR with the help of library knowledge base for efficient library mapping.

Intra-node parallelization: The optimization policy for intra-node level is to provide sufficient parallelism to fully utilize the efficient multithreaded implementations such as BLAS-based NumPy and CuPy. Our modified PolyAST [16] algorithm applies loop distribution to split different library calls while maximiz-

Library function	Domain	Semantics and dataflow
$transpose_{2D}$	(i_0, i_1)	$R[i_0, i_1] := A_1[i_1, i_0]$
$\operatorname{mult}_{1D,2D}$	(i_0, i_1)	$R[i_0, i_1] := A_1[i_1] \times A_2[i_0, i_1]$
sum_{1D}	(0)	$R := \Sigma_k A_1[k]$
$sum_{2D,axis=1}$	(i_0)	$R[i_0] := sum_{1D}(A_1[i_0,:])$
$dot_{2D,2D}$	(i_0, i_1)	$R[i_0, i_1] := sum_{1D}(mult_{1D, 1D}(A_1[i_0, :], A_2[:, i_1]))$
$fft_{2D,axis=1}$	(i_0)	$R[i_0,:] := fft_{1D}(A_1[i_0,:])$

Table 2. NumPy examples in library knowledge base

1 for i in range(0, M-1):

corr[i, i+1:M] = (data[0:N, i] * data[0:N, i+1:M].T).sum(axis=1)

(a) Original code fragment

Domain:	{S[i0.	i1] : 0 <= i0 < M - 1 and i0 + 1 <= i1 < M}
Read:	{S[i0,	<pre>i1] -> data[any1, i0], data[any2, i1] : 0 <= any1, any2 < N}</pre>
Write:		i1] -> corr[i0, i1]}
Body:	S[i0,	<pre>i1] :: corr[i0, i1] = sum(mult(data[:, i0], data[:, i1]))</pre>

(b) Extracted polyhedral information (SCoP)

1 tmp1 = np.dot(data[0:N, 0:M].T, data[0:N, 0:M])

corr[0:M-1, 0:M] = np.triu(tmp1[0:M-1, 0:M], k=1)

(c) Transformed code fragment by intra-node polyhedral optimization

Fig. 6. Kernel from the PolyBench-Python correlation

ing the iteration domain (i.e., amount of computation) that can be mapped to a single library function call. The SCoP-to-Python-IR generation stage leverages the library knowledge base to select the efficient combination of available library functions for each statement whenever possible. The maximal matching strategy is currently employed if multiple choices are available.

Figure 6a shows the computationally heavy code fragment of PolyBench-Python correlation NumPy version, which has a for loop enclosing a sequence of NumPy function calls: 2-D array transpose overlapping T operator; $1-D\times2-D$ array multiply overlapping * operator, and 2-D array summation sum to produce 1-D result. Based on the type inference results, the polyhedral phase first identifies these library functions with specific types and array ranks. As summarized in Table 2, the library knowledge base provides the element-wise dataflow information and operational semantics of these functions, which are used to extract the SCoP information and semantics of each statement (Figure 6b). Both explicit and implicit loops are unified in a triangular iteration domain; and the same loop order is selected by the transformation stage. Given statement body of sum(mult(data[:, i0], data[:, i1])), the SCoP-to-Python-IR generation stage selects the combination of matrix-matrix multiplication numpy.dot and 2-D transpose T as the best mapping, followed by numpy.triu to update only the triangular iteration domain (Figure 6c). As evaluated in Section 5.2,

1 for idx in range(numPulses):
2 ...
3 beamforming[idx,:] = np.squeeze(np.matmul(steerVector11, dataCube)) # S
4 d_X = np.fft.fft(beamforming, fftSize, axis=1) # T
5 d_Y = d_X * d_matchFilterMultiply # U

(a) Original code fragment

Domain:		: 0 <= i0 < numPulses} : 0 <= i0 < numPulses}
Body:	S[i0] T[i0]	<pre>: 0 <= i0 < numPulses and 0 <= i1 < fftSize} :: beamforming[i0, :] = :: d_X[i0, :] = fft(beamforming[i0, :]) :: d_Y[i0, i1] = d_X[i0, i1] * d_matchFilterMultiply[i0, i1]</pre>

(b) Extracted polyhedral information (read/write omitted due to space)

1

2

3

5

```
pfor t1 in range(0, numPulses, __tile_size): # Parallel loop across nodes
up1 = min(t1 + __tile_size, numPulses)
for c1 in range(t1, up1):
...
beamforming[c1,:] = np.squeeze(np.matmul(steerVector11, dataCube)) # S
d_X = np.fft.fft(beamforming[t1:up1, :], fftSize, axis=1) # T
d_Y = d_X * d_matchFilterMultiply # U
(c) Transformed code fragment by inter-node polyhedral parallelization
```

(c) Hundronneu eoue hughten of mer noue porficerur privilendur

Fig. 7. Kernel from the STAP Signal Processing Application

this transformation sufficiently increases the intra-node parallelism per library call and resulted in significant improvements for several benchmarks.

When the input program is written only with explicit loops, e.g., List version in Figure 2, our approach extracts similar SCoP and generates the same code with additional conversions between List and NumPy array.

Inter-node parallelization: The optimization policy for inter-node level is equivalent to the original PolyAST [16] algorithm that maximizes outermost level parallelism, while incorporated with our data layout transformation approach [17,18] to reduce the total allocated array sizes and data movement across Ray tasks. Analogous to the GPU two-level parallelization [15], our polyhedral optimizer selects different *schedules* – i.e., compositions of loop transformations and parallelization – for inter-node and intra-node levels individually; and integrates them into the final schedule via loop tiling.

Figures 7a and 7b respectively show the computational kernel of the STAP radar application and the extracted SCoP information. The explicit loop with statement S and the fft call of statement T are handled as 1-D iteration domains while 2-D×2-D array multiply of statement U is handled as a 2-D iteration domain. The polyhedral optimizer identifies the outermost level parallelism and computes the inter-node schedule that fuses these statements into a single parallel loop. The transformed code after integrating the inter-node and intra-node schedules is shown in Figure 7c, where pfor is the parallel loop construct to be distributed across Ray tasks.

4.3 NumPy-to-CuPy Conversion and Parallelized Code Generation

After the polyhedral phase, the program multi-versioning (Section 4.1) is applied to the *pfor* parallel loops and generates both sequential and parallel versions. The profitability condition, which makes the decision on whether the loop to be distributed across nodes via Ray runtime, is generated by a simple cost-based analysis and summarized as a threshold expression using loop counts. This analysis also includes the feasibility and profitability check of the CuPy conversion for given sequence of NumPy library calls. The current implementation takes an all-or-nothing approach for the NumPy-to-CuPy conversion, and more finegrained control, e.g., per-array decision, will be addressed in future work.

To generate Ray-based distributed code from high-level *pfor* loop, the polyhedral phase provides the following data access information.

pfor (output = { var_{out_1} : $type_{out_1}$, var_{out_2} : $type_{out_2}$, ...}, input = { var_{in_1} : $type_{in_1}$, var_{in_2} : $type_{in_2}$, ...}, transfer = module_name)

The output and input clauses respectively specify the produced and referenced variables by the *pfor* loop and their corresponding types, while transfer clause indicates the possibility of NumPy-to-CuPy conversion based on the polyhedral dataflow analysis and library compatibility. Due to the space limit, the generated code with Ray tasking APIs is omitted.

4.4 Important Packages Used in Tool Chain Implementations

Our AutoMPHC compilation flow is built on top of the Python Typed AST package [5], which serves as the baseline IR to perform fundamental program analyses and transformations such as type inference, loop invariant code motions, and constant propagations. For the polyhedral optimizations presented in Section 4.2, we employ islpy package, the Python interface to the Integer Set Library (ISL) [20] for manipulating sets and relations of integer points bounded by linear constraints. Beside the polyhedral representations using islpy, we employ sympy [19] to manage symolic expressions observed in the Typed AST.

5 Experimental Results

5.1 Experimental Setup

We use a standard GPU-equipped workstation, Titan Xp, for single-node experiments (Section 5.2) and two leading HPC platforms, NERSC Cori [3] and OLCF Summit [4] supercomputers, for multi-node experiments (Section 5.3). The single-node specification for each platform is summarized in Table 3. For Summit, we manually build Ray and its dependencies from scratch because there is currently no out-of-the-box Python Ray package for POWER.

Per node	Cori-GPU	Summit	Titan Xp (workstation)
CPU	$2 \times$ Intel Xeon Gold 6148	$2 \times IBM POWER9$	$1 \times \text{Intel i5-7600 CPU}$
	@ 2.40 GHz (40 cores/node)	@ 3.1 GHz (44 cores/node)	@ 3.50GHz (4cores)
GPU	$8 \times \text{NVIDIA Tesla V100}$	$6 \times \text{NVIDIA Tesla V100}$	$1 \times \text{NVIDIA Pascal}$
Memory	384GB	512GB	15GB
Interconnect	InfiniBand + PCIe (CPUs-GPUs)	InfiniBand	N/A
	+ NVLink(GPUs)	+ NVLink (CPUs-GPUs, GPUs)	
Python / NumPy / CuPy	3.7.3 / 1.16.4 / 7.4.0	3.7.3 / 1.16.0 / 7.4.0	3.6.9 / 1.19.5 / 7.2.0
Ray	0.8.4	0.7.7	0.8.4

Table 3. Hardware Platform Information (per node) and software versions

Table 4. PolyBench-Python baselines: Execution time in second (dataset = large)

	2mm	3mm	atax	bicg	correlation	covariance	doitgen	gemm
List Default [sec]	224.4	356.2	0.6578	0.6730	152.5	305.7	54.46	147.4
List Pluto [sec]	205.2	337.9	0.8381	0.8304	152.1	153.8	54.45	191.5
NumPy [sec]	0.0214	0.03252	0.002516	0.002447	2.212	3.813	0.1250	0.01789
	gemver	gesummv	mvt	symm	syr2k	syrk	trmm	
List Default [sec]	1.510	0.3068	0.8710	140.4	171.4	96.66	91.10	
List Pluto [sec]	1.453	0.3154	0.8714	140.5	137.9	81.73	93.27	
NumPy [sec]	0.04676	0.001074	0.002537	1.656	2.667	0.7839	0.8499	

5.2 Single-node Results (Polybench)

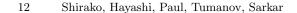
We first evaluate the impact of our polyhedral optimizations using PolyBench-Python [6], which is the Python implementation of PolyBench [12], a widely used benchmark kernels for compiler evaluations. We use total 15 benchmarks shown in Table 4, which are appropriate to evaluate the current library-oriented optimization strategy, while the evaluation of other 15 benchmarks will be addressed in our on-going work on hybrid Python/C++ code generation.

PolyBench Python provides a variety of benchmark implementations, including default List version, optimized List version by the Pluto polyhedral compiler [8], and NumPy version. Table 4 shows the execution time of these versions using "large" dataset. While the Pluto optimization improves the performance, NumPy version largely outperforms List versions for all benchmarks.

In the following experiments, we use NumPy version as the baseline of our comparison, and "extra large" dataset to ensure sufficient execution time. Figure 8 shows the GFLOP/s of three experimental variants:

- NumPy baseline: the original NumPy implementation from PolyBench.
- AutoMPHC opt-CPU: the CPU optimized version by AutoMPHC framework.
- AutoMPHC opt-GPU: the GPU optimized version by AutoMPHC framework enabling NumPy-to-CuPy conversion.

Comparing the NumPy and AutoMPHC opt-CPU versions, our polyhedral optimization gives $8.7 \times -212.4 \times$ performance improvements for correlation, covariance, doitgen, symm, syr2k, syrk, and trmm, while showing comparable performance for other benchmarks. Enabling NumPy-to-CuPy conversion further improves the performance for most benchmarks, with two exceptions of



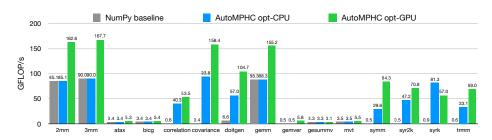


Fig. 8. PolyBench-Python performance on NVIDIA Titan Xp (dataset = extra large)

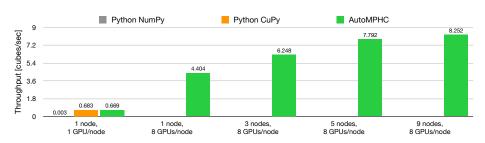
gesummv and syrk. In this evaluation, our profitability conditions always selected GPU variants. The improvement of CPU/GPU selection based on offline profiling is an important future work.

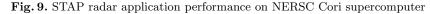
5.3 Multi-node Results (STAP)

We demonstrate the multi-node performance of our AutoMPHC compiler framework using one of our target applications in the signal processing domain, namely the Space-Time Adaptive Processing (STAP) application for radar systems [10]. The problem size used for STAP is to evaluate the analysis of 144 data cubes for the CPU case; and 2304 data cubes for the GPU case, where each data cube has # pulses per cube = 100, # channels = 1000, and # samples per pulse = 30000. The throughput required for real-time execution is 33.3 [cubes/sec]. There are three experimental variants as listed below:

- Python NumPy: The original single-node CPU implementation.
- Python CuPy: CuPy-based single-node GPU implementation, manually ported from the original Python NumPy version.
- AutoMPHC: Automatic parallelization by the AutoMPHC compiler of the original Python NumPy version, running on the Ray distributed runtime.

Figures 9 and 10 show the throughput performance, i.e., number of data cubes processed per second, respectively on Cori and Summit. Given the Python NumPy version as input, the AutoMPHC compiler automatically parallelized the major computation kernel and mapped to GPUs via NumPy-to-CuPy conversions. This significantly improves the throughput performance of the baseline Python NumPy version, while obtaining comparable performance with the manually ported CuPy implementation when using a single GPU. The AutoMPHC version also shows good multi-node scalability based on the Ray distributed runtime up to 44.58 [cubes/sec] using 24 nodes on Summit, which satisfies the domain-specific throughput requirement of 33.3 [cubes/sec] in the real-time scenario of actual radar systems. The AutoMPHC version also shows good single-node performance on Cori, 4.40 [cubes/sec], but the multi-node scalability on Cori is more limited than on Summit. One reason for this could be the difference in networks, i.e., Summit's NVLink (50GB/s) vs. Cori's PCIe 3.0 (16GB/s). In the





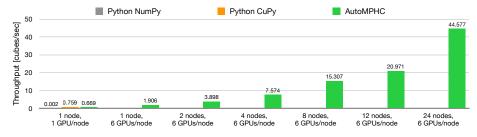


Fig. 10. STAP radar application performance on OLCF Summit supercomputer

parallelized code by AutoMPHC, each parallel task performs the computation on the GPU-side and returns the result via the device-to-host data (D2H) transfers. We expect that the low-latency D2H transfer on NVLink contributed to the good scalability of the AutoMPHC-generated code on the Summit system.

6 Conclusions

This paper describes AutoMPHC — a programming system designed to deliver the benefits of distributed heterogeneous hardware platforms to domain scientists who naturally use high-productivity languages like Python. In our approach, the parameters and return values of kernel Python functions are annotated with type hints, manually by users or automatically by profiling tools. Based on these type hints, the AutoMPHC compiler performs automatic AOT parallelization, based on advanced polyhedral optimizations, CuPy-driven GPU code generation, and Ray-targeted heterogeneous distributed code generation and execution. The correctness of our AOT parallelization is guaranteed by multiversion code generation, since code versions with type-specific optimizations are executed only when the actual runtime types match the type hints. Our empirical evaluations using PolyBench-Python for workstation performance and the STAP radar application for heterogeneous distributed performance show significant performance improvements, e.g., up to $358 \times$ improvement for PolyBench and up to $20,000 \times$ improvement for the STAP radar application, relative to baseline NumPy-based implementations. Opportunities for future work include hybrid Python/C++ code generation, fine-grained NumPy-to-CuPy conversion, and profile-based CPU/GPU runtime selection.

References

- 1. Scipy. https://www.scipy.org/ (2001)
- 2. Numpy. https://numpy.org/ (2006)
- 3. NERSC Cori Supercomputer. https://docs.nersc.gov/systems/cori/ (2016)
- 4. Lcf summit supercomputer. https://www.olcf.ornl.gov/olcf-resources/computesystems/summit/ (2019)
- 5. Python typed ast package. https://pypi.org/project/typed-ast/ (2019)
- Abella-González, et al.: Polybench/python: Benchmarking python environments with polyhedral optimizations. In: Proc. of CC 2021 (2021)
- Bezanson, J., Karpinski, S., Shah, V.B., Edelman, A.: Julia: A fast dynamic language for technical computing. CoRR abs/1209.5145 (2012)
- Bondhugula, U., Acharya, A., Cohen, A.: The pluto+ algorithm: A practical approach for parallelization and locality optimization of affine loop nests. ACM Trans. Program. Lang. Syst. 38(3) (Apr 2016)
- Dalcin, L., Fang, Y.L.L.: mpi4py: Status update after 12 years of development. Computing in Science Engineering (2021)
- 10. Melvin, W.L.: Chapter 12: Space-time adaptive processing for radar. Academic Press Library in Signal Processing: Volume 2 Comm. and Radar Signal Proc. (2014)
- Moritz, P., Nishihara, R., Wang, S., Tumanov, A., Liaw, R., Liang, E., Elibol, M., Yang, Z., Paul, W., Jordan, M.I., Stoica, I.: Ray: A distributed framework for emerging ai applications. In: Proc. of OSDI'18 (2018)
- PolyBench: The polyhedral benchmark suite, http://www.cse.ohio-state.edu/ ~pouchet/software/polybench/
- Press, W.H., Teukolsky, S.A., Vetterling, W.T., Flannery, B.P.: Numerical Recipes 3rd Edition: The Art of Scientific Computing. 3 edn. (2007)
- 14. Python. https://www.python.org/ (1991)
- Shirako, J., Hayashi, A., Sarkar, V.: Optimized Two-Level Parallelization for GPU Accelerators using the Polyhedral Model. In: Proc. of CC 2017 (2017)
- Shirako, J., Pouchet, L.N., Sarkar, V.: Oil and Water Can Mix: An Integration of Polyhedral and AST-based Transformations. In: Proc. of SC'14 (2014)
- 17. Shirako, J., Sarkar, V.: Integrating Data Layout Transformations with the Polyhedral Model. In: Proc. of IMPACT 2019 (2019)
- 18. Shirako, J., Sarkar, V.: An affine scheduling framework for integrating data layout and loop transformations. In: Proc. of LCPC 2020 (2020)
- 19. Sympy. https://www.sympy.org (2017)
- Verdoolaege, S.: isl: An Integer Set Library for the Polyhedral Model. In: Mathematical Software ICMS 2010 (2010)
- Verdoolaege, S., et al.: Polyhedral parallel code generation for CUDA. ACM Trans. Archit. Code Optim. 9(4), 54:1–54:23 (2013)
- Wang, S., Liagouris, J., Nishihara, R., Moritz, P., Misra, U., Tumanov, A., Stoica, I.: Lineage stash: Fault tolerance off the critical path. In: Proc. of the ACM Symposium on Operating System Principles (SOSP'19). p. 338–352. SOSP '19 (2019)
- Zhou, T., Shirako, J., Jain, A., Srikanth, S., Conte, T.M., Vuduc, R., Sarkar, V.: Intrepydd: Performance, productivity and portability for data science application kernels. In: Proc. of Onward! '20 (2020)
- 24. Zinenko, O., et al.: Modeling the conflicting demands of parallelism and temporal/spatial locality in affine scheduling. In: Proc. of CC 2018 (2018)