Pricing Python Parallelism: A Dynamic Language Cost Model for Heterogeneous Platforms

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1 Introduction
Dynamic scripting languages like Python are increasingly popular, particularly for domain-specific scientific code written by end users. Meanwhile compute accelerators, such as GPUs, are increasingly available on commodity devices at all scales. Much recent research effort has focused on identifying parallelism in such end user programs and exploiting this parallel code on manycore hardware. Different approaches include embedding domain-specific parallel code in dynamic languages [20, 21] or using parallel APIs, patterns and libraries [8, 11]. However, there has been little focus on the automatic selective application of such parallel optimizations. In prior work, coders are left to choose manually which sections of their program should be parallelized. Such techniques rely on the risky assumption that the programmer knows best.

Rather than require that developers have parallel programming expertise, our approach is to automatically parallelize loop nests in vanilla Python on GPUs. The ALPyNA framework has demonstrated significant reduction in runtimes of large and moderately complex loop nests [14, 15] (Section 2). However offload overheads like kernel compilation and data transfer mean that offloading small loops is slower than CPU execution.

The key technical contribution of this paper is a new parameterized, lightweight and staged cost model, the ALPyNA Cost Model (ACM), that automatically and selectively applies loop parallelization to minimize runtime (Section 3). This is precisely what non-expert scripting programmers require on current commodity platforms with multiple heterogeneous compute resources.

While cost models for automatic compilation and parallelization are common for static languages (Section 6), modelling a dynamic language like Python poses significant challenges. Parallelizing compilers for static languages have far more program information, can use profiling or heavyweight...
offline analysis, and may speculatively generate code for alternative execution platforms. Such techniques are severely restricted in dynamic language implementations as so much program information is determined only at runtime. For example the parallel structure of a Python loop nest can only be determined dynamically when iteration domains are dynamic, and dependences cannot be resolved statically. Moreover in a dynamically typed language the array element types are dynamic, and these determine costs like GPU data transfer times.

Fortunately modern sophisticated dynamic language implementations now provide the technologies to address auto-parallelization challenges. For example the dynamically determined safe loop nest can be JIT compiled for CPU or GPU; likewise runtime introspection allows dynamic type information to be extracted and used to parameterise the cost model. To the best of our knowledge ACM is the first analytical cost model that supports the automatic runtime exploitation of GPUs in a dynamic language.

For each instance of a loop nest, ACM dynamically predicts the relative runtimes on alternative execution platforms so that ALPyNA can select the fastest. ACM is staged, combining compile-time analysis with runtime introspection in the CPython interpreter to parameterise the static model. The model is designed to be lightweight as it is evaluated at runtime. The ACM models for interpreted and JIT-compiled CPU execution are simple and relatively standard. In contrast the GPU model is both elaborate and more novel as it accounts for key device costs, including the time to transfer data to and from the device, block structured execution, starvation effects etc. All of the platform models are parametric in key characteristics of the devices in a heterogeneous platform, like warp size on the GPU.

An important scientific contribution is to show that a comparatively simple staged analytical model can effectively determine at runtime whether to offload a loop nest in a dynamic language (Section 5). Comparatively simple cost models for the parallel platforms suffice because the system does not attempt to accurately predict absolute loop runtimes, rather it compares the relative runtimes on the GPU and CPU with interpretation or JIT compilation. Of course such relative cost models are common for static languages (Section 6).

2 Parallelizing Python Loops with ALPyNA

ALPyNA is an auto-parallelizing framework for heterogeneous architectures that parallelizes dense linear loop nests written in vanilla Python [14, 15]. Linear loop nests consist of statements in which array subscripts are linear expressions of the loop iterator variables. While the examples below are very simple, ALPyNA can analyze loop nests that are moderately complex: the benchmarks in Section 5 demonstrate ALPyNA parallelizing multiple loops in a program, nested loops, perfect and imperfect loop nests, and nests with control flow divergence.

2.1 Runtime Dependence Analysis

ALPyNA parallelization relies on analyzing the dependence relationships between variables in the loop nests, as popularised by Allen and Kennedy [18] for FORTRAN. The dependence analysis uses standard techniques to solve systems of linear equations [38] determined by loop domain limits and array subscripts. When these domains are unknown at compile time, a static compiler must conservatively assume that dependences exist.

For simple loop nests, optimizing static compilers try and create parallel and sequential variants. Execution of such speculatively generated parallel variants is subject to guard conditions being satisfied. Such systems, like MegaGuards (Qunaibit et al[30]), are available for interpreted languages like Python. However, generating multiple variants of loop nests based on different combinations of dependence relationships quickly becomes unwieldy even if only a small number of factors are unknown at compile time.

```
def ln_func(arg_a, k, limits):
    im, jm = limits
    for i in range(0,im,1):
        for j in range(0,jm,1):
            # Statement - S1
            arg_a[i+k,j] = arg_a[i,j] + 4
            # Statement - S2
            arg_a[i+16,j] = arg_a[i,j]
```

Listing 1. ALPyNA loop nest parallelization example

Consider the loop nest in Listing 1. The dependence relationships between the two statements S1 and S2 is determined by loop bounds (im, jm), the loop invariant variable ‘k’ and the coefficients and constants in each array subscript. Due to the unresolved loop domain sizes and non-iterator variable within the array subscript on the LHS of S1, a purely static compiler must conservatively generate sequential code.

Figure 1 shows the dependence graph for an instance of the nested loops in Listing 1 having limits (im, jm) ← (32, 1024) and ($k$) ← (64). All 32 × 1024 execution instances of Statement S1 can safely be executed in parallel because $k > im$. For statement S2, executing the outer loop ($F_j$) sequentially allows 1024 execution instances (corresponding to the inner loop $F_j$) to be executed in parallel. Figure 2 shows the dependence graph for the same loop nest with domain limits (im, jm) ← (32, 1024) and variable ($k$) ← (8). As $k < im$ the inner loop ($F_j$) may only be executed in parallel if the outer loop ($F_i$) is executed sequentially. If the loop limits have the values (im, jm) ← (16, 1024) and ($k$) ← (16), all instances of statements S1 and S2 can be executed in parallel.
Primary contributions in this paper are the development of a hybrid cost model that estimates the relative execution time of such loops, and the integration of this cost model into the ALPyNA system (Figure 3).

2.2 ALPyNA System Architecture

ALPyNA is not a whole program compiler: users invoke loop analysis by passing marked functions with loop nests in them to the system. ALPyNA isolates and analyzes these loops and either JIT compiles for the CPU or generates GPU kernels and schedules them while preserving dependence relationships. Any Python statements between loop nests are executed within the interpreter. It first parses loop nests and performs loop normalization (i.e. transforms loops to increment by unit stride) to facilitate dependence analysis. Control flow divergence within loop nests is handled by converting computational statements to predicated statements using if-conversion. ALPyNA allows calls to pure intrinsic functions within the loop body to aid computation. These are mapped onto corresponding intrinsics supplied by the Numba compiler (Section 2.3) for a particular target device. A loop nest with computation that cannot be JIT compiled by Numba is executed by the interpreter.

Figure 3 provides an overview of ALPyNA’s architecture, incorporating the cost model extensions. The parser generates a very simple flat record structure of the loop nests which are grouped into ‘loop landmarks’. Any loop limits that cannot be statically determined are marked for runtime analysis. The presence of variables within array subscripts which are not loop iterators are also marked for runtime analysis.

If all dependence relationships can be determined at compile time, skeletal kernels and drivers are generated and cached. During runtime, when the loop nest is invoked, ALPyNA introspects the data types of the data being accessed within the loop nest and determines the types to be patched into the skeletal kernels that have been generated. These kernels are then compiled using Numba.

If a dependence relationship cannot be ascertained at compile time, any dependence that can be statically derived is memoized and the whole loop nest is marked for runtime analysis and optimization. At runtime, ALPyNA intercepts invocations of these loop nests. All relationships deferred to runtime analysis are computed for each loop nest instance.

In the presence of unknown loop limits and other variables (such as loop invariants), a static compiler would have to be conservative and assume that dependences exist. In contrast ALPyNA uses introspection to determine loop domain limits and other variable relationships at runtime to aggressively exploit potential parallelism. ALPyNA combines statically derived dependences and those determined at runtime to compute the overall dependence relationships in a loop nest.

The loop nest is then converted into a skeletal form to pass into the code generator for each target architecture. After the loop nest has been analyzed and transformed into a skeletal structure, code is custom generated for the dependence relationships that exist for an execution instance of the loop nest. Code generated by ALPyNA after dependence analysis is JIT compiled using Numba (Section 2.3).

2.3 Numba Compiler

ALPyNA uses the Numba [23] library to JIT compile and execute loop nests. Numba is an LLVM based framework that can dynamically compile Python functions. Normally, programmers add a @jit decorator to a Python function to compile it to CPU machine code. Numba also has the @cuda.jit decorator syntax to provide access to CUDA bindings. This enables programmers to write CUDA kernels for GPU using restricted Python semantics and CUDA idioms.

For ALPyNA, developers provide undecorated Python source code. After staged analysis/parallelization passes, ALPyNA will eventually invoke Numba to JIT compile synthesized Python code for the appropriate backend target device (CPU or GPU). Our new cost model (ACM) is intended to guide the dynamic selection of target devices.

Numba compiles code at runtime once the concrete data types of the variables within the code are determined. While automatic type inference is provided within Numba, the cost of compiling and type-checking is expensive. Numba allows programmers to optionally specify data types within the @jit and @cuda.jit decorators. A compiled kernel is cached to reduce execution time. Since ALPyNA generates a GPU kernel for each statement, each loop invocation of a GPU kernel (caused by sequential execution of a loop to maintain a loop-carried dependence) would trigger automatic type-inspection by Numba. This reduces performance by an order of magnitude, and to ameliorate this ALPyNA performs type inspection and supplies each kernel with the requisite types. This enables Numba to re-use a previously cached kernel without fresh type inspection.
2.4 GPGPU Programming Model

Current NVIDIA GPU architectures execute parallel threads on parallel cores called a Streaming Multiprocessor (SM) [12]. Each SM has a large number of CUDA cores and potentially multiple warp schedulers. Each warp scheduler schedules threads for execution on a warp sized subset of CUDA cores in an SM. Every thread within a warp executes an instruction in lock-step on CUDA cores. An SM may also have a number of shared caches [33].

This model is abstracted for the programmer as computational kernels executed in parallel on a GPU. An instance of kernel execution is identified with a threadIdx and threads are arranged into a threadblock. The number of threads in a threadblock are limited, e.g. to 1024. The number of threads executing instances of a kernel can be increased by executing grids of equal-sized thread blocks. In CUDA, threads are logically arranged along one, two, or three dimensional axes in a two tier structure of grids and blocks [12, 26]. The actual threadIdx along a particular axis can be dereferenced using simple two tier dereferencing semantics (blockidaxis × blocksizeaxis + threadIdxaxis). The three axis thread hierarchy (x, y, z) of GPGPU programming originate from 3D graphics computation. Parallel threads in a thread block are expected to be scheduled on the same SM [12].

Dependence theory states that if a dependence in a loop nest is *carried* by a loop, executing this loop sequentially allows any nested loops to be executed in parallel, so long as they do not carry any other loop dependences [18]. ALPyNA uses dependence analysis to parallelize such inner loops. It generates a single GPU kernel for each loop nest statement. This design enables the partial parallelization of (i) imperfect loop nests and (ii) loop nests with loop carried dependences requiring sequential execution of some loops.

3 ALPyNA Cost Model

The ALPyNA Cost Model (ACM) determines which device to execute a loop nest on, in a heterogeneous manycore compute environment. It does so by using staging and a family of lightweight models to compare the predicted relative runtimes of loop nest instances on each execution device.

ALPyNA analyzes dependence relationships in a staged manner. When all dependence relationships can be determined statically, untyped GPU kernels along with their domain sizes can be generated at compile time (Section 2.1). However, loop domain values are often not known until runtime, so the amount of potential parallelism in a loop nest cannot be statically determined.

The heavyweight dependence analysis, optimization, and cache access pattern analysis typically used in offline compilers is too expensive for JIT compilation. Hence we introduce a lightweight cost model to compile loop nests for heterogeneous environments featuring CPU+GPU compute devices. Execution on GPU is worthwhile if the interpreted execution time exceeds that of compiling for, transferring code and
The form is not restrictive as multiple top level loops can be executed in parallel. Loop interchange is used by parallelizing compilers to maximize parallel execution of loops [18].

### 3.1 Modelling Interpreter Execution

$L_{\text{int}}$ is a function that maps any individual loop nest statement $S_j$ to an abstract cost, effectively a predicted execution time in the CPython interpreter. Such values could be profiled ahead-of-time. However, a novel feature of ACM is that all costs are expressed relative to $L_{\text{int}}$, so the profiling never actually takes place. $C_{\text{int}}$ is a function that predicts the total cost of interpreting all instances of statement $S_j$ in the loop nest as the product of $L_{\text{int}}(S_j)$ and all of the iteration domain sizes, Equation 2. This requires loop limits to have been resolved to numerical constants, which may require runtime introspection. $T_{\text{int}}$ is a function that predicts the total execution cost of the entire loop nest with top-level for loop header $f$ as the sum of the total execution costs of all statements in the loop nest, Equation 3.

$$C_{\text{int}}(s) = L_{\text{int}}(s) \prod_{f \in D(s)} L(f) \quad (2)$$

$$T_{\text{int}}(f) = \sum_{s \in E(f)} C_{\text{int}}(s) \quad (3)$$

In our running example (Listing 3), all three loops $F_k, F_i$ and $F_j$ are executed sequentially in the interpreter. The overall abstract cost is proportional to the product of the loop domain sizes.

### 3.2 Modelling JIT Compiled CPU Execution

When ALPyNA JIT compiles a loop nest targeting the CPU, the cost model is very similar to that of the interpreter. $L_{\text{cpu}}$ maps a loop nest statement to an abstract cost, and we perform one-time profiling to express $L_{\text{cpu}}$ in terms of $L_{\text{int}}$ for each statement (Section 3.4). $C_{\text{cpu}}$ is a function that predicts the total cost of executing all instances of a statement in the loop nest as a product of the individual statement cost and the loop domain limits, Equation 4. $T_{\text{cpu}}$ is a function that predicts the total execution cost of the entire loop nest, Equation 5.

$$C_{\text{cpu}}(s) = L_{\text{cpu}}(s) \prod_{f \in D(s)} L(f) \quad (4)$$

$$T_{\text{cpu}}(f) = \sum_{s \in E(f)} C_{\text{cpu}}(s) \quad (5)$$

Relating $L_{\text{cpu}}$ and $L_{\text{int}}$ assumes that the JIT compiler only compiles the loop into sequential binary instructions, and does not vectorize the loop body for Single Instruction Multiple Data (SIMD) execution units on the CPU. We have also verified that Numba does not automatically parallelize loop nest execution to multiple cores on the CPU.

A single threaded JIT compiled CPU variant of the running example (Listing 3) executes loops $F_k, F_i$ and $F_j$ sequentially.
The abstract cost of execution is proportional to the product of loop domain sizes.

### 3.3 Modelling GPU Execution

Dependence analysis determines which loops to execute sequentially to maintain dependences between each statement. In theory, all other loops can be executed in parallel. Loops that *must* be executed sequentially are transformed into a GPU kernel call within the interpreter and called sequentially maintaining dependence relationships. Every loop instance of a statement which can be executed in parallel is executed within a GPU kernel. However, current GPGPU programming semantics restrict the number of dimensions along which we can schedule threads to three (Section 2.4). This means we can parallelize a triple nested for loop at best using CUDA thread semantics alone.

To model the cost of executing a loop nest that has been parallelized, the set of for loops enclosing each statement is split into distinct partitions:

1. \( D_{\text{seq}}(s) \) – the set of outer loop headers enclosing statement \( s \) which *must* be executed sequentially, due to dependences.
2. \( D_{\text{par}}(s) \) – the set of all loop headers enclosing statement \( s \) which can be executed in parallel because either there are no loop-carried dependences or all loops carrying dependences are executed sequentially (the set \( D_{\text{seq}}(s) \)). In general, the number of loops in \( D_{\text{par}}(s) \) may be greater than the number of parallel axes on the GPU (i.e. three). To model this we further partition the set \( D_{\text{par}}(s) \) into:
   a. \( D_{\text{gpu}}(s) \) – the set of loops that ALPyNA has mapped to hardware axes. ALPyNA transforms each instance of execution along these iteration domains into a GPU kernel execution instance. On NVIDIA GP104 (Pascal microarchitecture) GPUs for example, each block can only execute a maximum of 1024 threads. ALPyNA calculates a thread hierarchy from the loop domain sizes at run time and splits it into a tuple of grid sizes and block sizes. The loop domains scheduled along the logical \( x,y,z \) hardware axes are intended to maximize parallel work [15] while meeting the *threads per block* constraint.
   b. \( D_{\text{par}}(s) \) – the set of all remaining loops that cannot be mapped onto a GPU parallel axis, these are executed sequentially within each GPU kernel. This can be done safely without synchronization because ALPyNA transforms all loops which carry dependences into sequential kernel invocations in the interpreter.

In our running example (gemm–Listing 3) dependence analysis determines that loop \( F_k \) carries both true \(^1\) and *anti* \(^2\) dependences. Executing \( F_k \) sequentially enables the parallel execution of the inner loops \( F_i \) and \( F_j \). As there are only two parallel loops, ALPyNA does not execute any loops sequentially within the generated GPU kernel. The loop in \( D_{\text{seq}}(s) = \{ F_k \} \) is executed sequentially by the interpreter calling GPU kernels executing the computation represented by loops \( D_{\text{gpu}}(s) = \{ F_i,F_j \} \) and \( D_{\text{par}}(s) = \{ \emptyset \} \).

To model the parallel execution cost of a statement \( s \) on a GPU, we measure the number of executions as the product of the loop limits for the enclosing for loops, as before. However unlike the interpreter and CPU models, we now have a factor term to represent parallel execution, and hence reduce predicted execution time. The function \( \mathcal{G}(\mathcal{L}(f)) \), \( f \in D_{\text{gpu}}(s) \) calculates the grid size and maps a loop domain to a GPU hardware axis. \( \mathcal{G} \) maximizes threads-per-block to calculate the number of grids within a thread-hierarchy.

While the number of threads allocated to execute on an SM can be greater than the number of CUDA cores in the SM, the maximum number of threads executing in parallel at any one time in an SM is the product of the number of warp schedulers per SM (denoted \( v \)) and the warp size (denoted \( w \)). The block structure of parallelized GPU code means we need to take into account precisely how the execution is mapped onto SMs in a GPU (denoted \( \Omega \)). For a statement \( s \), we denote the amount of work done in each GPU kernel invocation as \( \lambda_{\text{exec}}(s) \) (Equation 6). Intuitively, if the GPU had an infinite number of SMs, then term \( g \cdot v \cdot w \) would provide the parallel speed-up. The ACM also calculates the cost of serializing execution of thread blocks in excess of the actual number of SMs.

\[
\lambda_{\text{exec}}(s) = \left[ \frac{g}{u} \right] \times \frac{1}{g \cdot v \cdot w} \times \prod_{f \in D_{\text{gpu}}(s)} \mathcal{L}(f) \times \prod_{f \in D_{\text{par}}(s)} \mathcal{L}(f) \\
g = \prod_{f \in D_{\text{gpu}}(s)} \mathcal{G}(\mathcal{L}(f))
\]

### Modelling GPU Starvation

ALPyNA maintains loop-carried dependences on code transformed for the GPU by scheduling the outermost loop iterations to execute in the CPython interpreter. The GPU executes JIT compiled binary code much faster than the interpreter. If the interpreter executes each kernel invocation faster than the GPU can execute the kernel, each kernel is queued for execution on the GPU and overall execution time is bound by kernel execution. Otherwise, the GPU will finish each kernel before the interpreter can schedule the next one, and the GPU is *starved* of work.

There are two cases to consider as shown in Equation 7. If all the loops around a statement \( s \) are parallelizable, i.e. \( D_{\text{seq}}(s) = \emptyset \), the code is transformed into a single invocation
of a kernel that executes all loop iterations of $D(s)$ on the GPU. Hence there is a single kernel invocation latency cost $C_{ki}$, otherwise $D_{seq}(s) \neq \emptyset$ and the execution cost is the greater of the kernel invocation or the GPU execution cost. Here $I_{gpu}(s)$ is the cost of executing a single instance of the compiled kernel that represents statement $s$. This scenario arises in the running example (Listing 3) where $D_{seq}(s) = \{T_k\}$.

$$C_{gpu}(s) = \max(C_{ki}, \lambda_{exec}(s)I_{gpu}(s))$$
if $D_{seq}(s) \neq \emptyset$ \hspace{1cm} (7)

$$C_{gpu}(s) = C_{ki} + \lambda_{exec}(s)I_{gpu}(s)$$
if $D_{seq}(s) = \emptyset$

Figure 4 depicts how for smaller amounts of parallel work, the GPU kernel completes early and the interpreter loop execution time dominates. However once there is enough work in each kernel invocation to keep the GPU busy, GPU execution time dominates. This threshold varies depending on the relative performance of the GPU and the interpreter.

To ascertain the GPU invocation cost threshold for each hardware setup, a very simple statement is profiled once at installation time. We use a two dimensional loop where only the inner loop can be parallelized. We profile this loop nest in ALPyNA using varying domain sizes to arrive at the GPU throttling threshold. The profiling starts at a parallel domain size $\{L(f) = w|f \in D_{par}(s)\}$ and the domain size is increased exponentially until the profiler detects execution time has gone beyond its inflection point. The profiler then interpolates the number of threads at the inflection point and calculates $\lambda_{exec}$ (Equation 7) for the domain size at the inflection point.

We seek to estimate the amount of GPU parallel work (in terms of domain sizes) required to overcome the kernel invocation cost $C_{ki}$, and designate this value $\lambda_X$. At the kernel invocation cost threshold, we assume the relationship

$$C_{ki} = \lambda_X \times I_{gpu}(s)$$ \hspace{1cm} (8)

Profiling the simplest statement $s$ to determine the crossover point $\lambda_X$, provides a maximal number of threads beyond which GPU execution time will dominate for any statement $s$. For a kernel representing more complex statements, this assumption leads to the ACM selecting a higher, (conservative), threshold of parallel work to offload to the GPU. Substituting $C_{ki}$ into Equation 7 the estimated cost of executing each kernel is shown in Equation 9.

$$C_{gpu}(s) = \max(\lambda_X, \lambda_{exec}(s))I_{gpu}(s) \cdot \prod_{f \in D_{seq}(s)} L(f)$$
if $D_{seq}(s) \neq \emptyset$ \hspace{1cm} (9)

$$C_{gpu}(s) = (\lambda_X + \lambda_{exec}(s))I_{gpu}(s)$$
if $D_{seq}(s) = \emptyset$

The full cost of executing the loop nest with outermost for loop $f$ on the GPU is the summation in Equation 10 where $C_{xfer}(GPU)$ is the data transfer cost outlined next.

$$T_{gpu}(f) = C_{xfer}(f) + \sum_{s \in D(f)} C_{gpu}(s)$$ \hspace{1cm} (10)

Modelling GPU transfer time. Executing on accelerators like GPUs incurs overhead for transferring data between the host CPU and the accelerator. We will see in Section 5 that loop nests with light computational work are especially sensitive to the overheads of data transfer.

Following common practice we normalize data transfer time against the estimated cost of executing a very simple statement in the CPython interpreter, $I_{int}(s)$. Bandwidth profiling of the PCIe bus on which the GPU resides is performed once at install time, along with the measurements of GPU starvation factor $\lambda_X$ (Section 3.3, Equation 8) and the CPU JIT speed-up factor $\mu$ (Section 3.4, Equation 11). While the transfer model is fairly standard, a novel feature is that it is staged. That is ALPyNA identifies the set of vectors to be transferred to/from the GPU, and resolves their types and sizes at runtime. These are combined with the ahead-of-time bandwidth measurements to estimate the transfer overhead, $C_{xfer}(GPU)$.

3.4 Calibrating ACM

Like many cost models ACM takes parameters that characterise the specific execution platform, e.g. CPython and the Numba JIT compiler on a specific CPU, and CUDA on a specific GPU. Specifically the key cost equations, 2, 4 and 7 take parameters representing the predicted runtime $I_{platform}(s)$ of executing a statement $s$ on a given platform, e.g. $I_{gpu}(s)$ in Equation 4. The platform costs for a statement $s$ are computed relative to the predicted interpreter cost $I_{int}(s)$. 

Calibration is required to determine the value of the model parameters for each execution platform, and this is achieved as follows.

The cost of executing a JIT compiled statement relative to the interpretation cost is profiled once at install time. A very simple kernel similar to the one used to profile $C_{kim}$ (Section 3.3) is used to relate the runtimes of JIT compiled, and CPython interpreted code. The array size in the loop nest is chosen to ensure that there is only one cache miss (on the first iteration). The relative performance factor obtained is designated as $\mu$ in Equation 11. This provides a close approximation of the relative runtimes of compiled and interpreted code without caching, and allows us to separately account for caches when comparing CPU and GPU runtimes.

$$\mu = \frac{I_{int}(s)}{I_{cpu}(s)} \tag{11}$$

The relative cost of GPU execution clearly depends on the relative clock frequencies of the CPU and GPU, $f_{cpu}$ and $f_{gpu}$. Moreover, Armih et al [1] and Belikov et al [6] both report the size of the last level cache as a significant factor while comparing relative performance of data intensive programs on heterogeneous platforms. The last level cache (L2) on the GPU $L_{c_{cpu}}$ is shared by all Symmetric Multiprocessors (SMs). Each SM has its own set of L1 caches. For example in the NVIDIA Pascal (GP104) each SM has two L1 caches [33]. This cache sharing is represented by the factor $\sigma = num_{SM} \times L_{1} \text{caches per SM}$ in Equation 12 that computes relative GPU/CPU performance. There is no cache sharing factor for the CPU as Numba JIT compiles code for a single core and we assume that this core has exclusive use of the L3 cache ($L_{c_{cpu}}$).

$$\frac{I_{cpu}(s)}{I_{gpu}(s)} = \psi \approx \frac{f_{gpu} \times (L_{c_{cpu}} / \sigma)}{f_{cpu} \times L_{c_{gpu}}} \tag{12}$$

Equation 13 shows how the cost of GPU execution relative to the interpreter is directly computed as the product of CPU/GPU cost and the interpreter/CPU ratio $\mu$ (Equation 11).

$$\frac{I_{int}(s)}{I_{gpu}(s)} \approx \mu \times \psi \tag{13}$$

Substituting Equations 11, 12 and 13 into Equations 2, 4 and 7 allows ALPyNA to compare the predicted runtimes on each execution platform and select the platform with minimum cost, i.e. $\min(T_{int}, T_{cpu}, T_{gpu})$.

3.5 ALPyNA Implementation

ACM is integrated into ALPyNA by annotating each statement with lightweight ‘loop landmarks’ data structure (Section 2.2) with its relative cost when loop nest dependence analysis takes place at runtime. ALPyNA’s runtime analysis and introspection capabilities enable aggressive discovery of opportunities to parallelize and estimate costs. This approach minimises overheads as the cost model is constructed while resolving runtime dependences.

4 Experimental Setup

4.1 Benchmarks

ACM is evaluated using 12 loop-intensive benchmarks from the BLAS routines in the Polybench suite [29], the Numba benchmarks, and from domains like finance (black-scholes) and digital signal processing (fbcorr).

The benchmarks represent a variety of characteristics that test ACM’s prediction capabilities for a variety of moderately complex loop nests as summarised in Table 1. Benchmarks like saxpy and vadd are extremely simple: a single loop with just a single statement, and are embarrassingly parallel. Control flow divergence is encountered in black-scholes and mandelbrot. These loop nests also have pure (math) function calls that are mapped onto CUDA intrinsics in GPU kernels. Matrix multiplication (gemm) and conv-2d are perfect loop nests (every statement is dominated by every loop in the loop nest) but must execute some loops sequentially to maintain dependence ordering. Imperfect loop nests occur in gemver and syr2k.

4.2 Hardware Platforms

The evaluation is conducted on a server grade machine (M1) and typical desktops (M2, M3). M1 has a Xeon E5-2620v4 octa core CPU with a 20MB L3 cache and a clock frequency of 2.1GHz that can be ‘Turboboost’ ed to 3GHz. It has 16GB (2x8GB) DDR4 RAM with a memory bus speed of 2133MHz.

M2 has a Core i7-6700 quad core CPU with an 8MB L3 cache clock and a clock frequency of 3.4GHz, that can be boosted to 3.9GHz. It has 16GB DDR4 (2x8GB) RAM with a

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<td>✓</td>
</tr>
<tr>
<td>Syr2k</td>
<td>(2,3)</td>
<td>(2,2)</td>
<td>✓</td>
</tr>
<tr>
<td>Vadd</td>
<td>1</td>
<td>1</td>
<td>✓</td>
</tr>
</tbody>
</table>

Table 1. Benchmark characteristics described as the set of loops surrounding each statement, e.g. syr2k has two loops around the first statement and three around the second. Only some loops are parallelized.
memory bus speed of 2133MHz. In a third machine configuration (M3) the CPU frequency of machine M2 is limited to 800MHz leaving all other parameters the same.

M1’s GPU is an NVIDIA Titan-XP (GP102) with a clock frequency of 1.4GHz and 12GB of GDDR5 RAM. It has 30 SMs and a 3MB last level cache (L2). M2/M3 have an NVIDIA GeForce GTX-1060 with a clock frequency of 1.5GHz and 3GB of GDDR5 RAM. It has 9 SMs and a 1.5MB L2 cache. In both GPUs each SM has 128 CUDA cores, 4 warp schedulers and two L1 caches [33]. Data transfer uses a PCI-Express (PCIe 3.0) bus with the GPU as the only peripheral, and it negotiates to use 16 channels (x16).

The experiments are conducted on similar software stacks as follows (M1, M2/M3). A native x86-64 Linux kernel (v4.15, v4.9); CPython interpreter (v3.6.9, v3.5.3); PyPy (v7.3.1); NumPy (v1.13.3, v1.13.3); Numba (v0.34, v0.33); and CUDA (v8.0.61, v8.0.44). We identify the combined hardware and software stacks as target platforms T1, T2 and T3.

4.3 ACM Usage

Before using ACM on a target CPU/GPU platform the values of $\alpha$, $\mu$ (Eqs. 11 and 8) and relative GPU bandwidth (Section 3.3) must be profiled. A 10% safety margin is used over the predicted inflection point where the interpreter is able to keep the GPU busy. The calculation of $\frac{BW_{CPU}}{BW_{GPU}}$, i.e. data transfer speeds in execution time units ($l_{int}$), is done while profiling for the value $\mu$ to ensure consistency.

The Numba compiler compiles and executes single threaded code. During experimentation no other cores execute computationally intensive code and hence the core can reach maximum frequencies without being throttled.

The selection of CPU or GPU to target for JIT compilation is dependent on the overall computation size, proportion of parallel computation, and data movement costs. The effectiveness of ACM’s device selection for JIT compilation is measured across a wide range of iteration domain sizes. Iteration domain sizes are increased by doubling the loop domain size of each loop within the benchmarks. Reported runtimes are the arithmetic mean of 5 executions.

4.4 Comparative Baselines

For each domain size, execution time on the ACM predicted device is compared with two baselines: (1) execution time on the optimal device identified by an ‘oracle’ predictor; (2) execution time on the device selected by a two-class support vector machine (SVM), i.e. a representative supervised learning model. The SVM is trained on the 12 benchmarks using per-benchmark leave-one-out cross-validation. We train separately for each of the three evaluation platforms. We use the oracle predictor value to label training set instances. The feature vector comprises static code structure metrics (cf. Table 1), input size and dimensions, and raw execution times on both target devices. All feature values are scaled with min-max normalization to the range [0, 1].
Table 2. Range of ALPyNA GPU speedups across iteration domain sizes. Some benchmarks have no speedup.

<table>
<thead>
<tr>
<th>Benchmark</th>
<th>GPU speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>T1: CPU/GPU</td>
</tr>
<tr>
<td></td>
<td>2960/1405MHz</td>
</tr>
<tr>
<td></td>
<td>T2: CPU/GPU</td>
</tr>
<tr>
<td></td>
<td>3900/1500MHz</td>
</tr>
<tr>
<td></td>
<td>T3: CPU/GPU</td>
</tr>
<tr>
<td></td>
<td>800/1500MHz</td>
</tr>
<tr>
<td>black-scholes</td>
<td>1.20 – 3.86</td>
</tr>
<tr>
<td>conv-2d</td>
<td>1.19 – 4.73</td>
</tr>
<tr>
<td>conway</td>
<td>na</td>
</tr>
<tr>
<td>fbcorr</td>
<td>8.59 – 17.89</td>
</tr>
<tr>
<td>gemm</td>
<td>2.49 – 8.64</td>
</tr>
<tr>
<td>gemver</td>
<td>1.23</td>
</tr>
<tr>
<td>hilbert</td>
<td>1.55</td>
</tr>
<tr>
<td>jacobi</td>
<td>na</td>
</tr>
<tr>
<td>mandelbrot</td>
<td>1.98 – 9.90</td>
</tr>
<tr>
<td>saxpy</td>
<td>na</td>
</tr>
<tr>
<td>syr2k</td>
<td>2.33 – 223.62</td>
</tr>
<tr>
<td>vadd</td>
<td>na</td>
</tr>
</tbody>
</table>

PyPy [3] is a tracing JIT compiler to speed-up Python execution. Execution time of CPU and GPU code generated by ALPyNA for the 12 benchmarks (Section 4.1) is compared to the execution time taken by PyPy with loop vectorization enabled. For each benchmark, PyPy is allowed to warm up to enable tracing and JIT compilation before timing measurements are taken. A timeout of five hours is used for benchmark execution with PyPy.

5 Evaluation

GPU Speedups. Table 2 shows the range of speedups obtained using the GPU for the benchmarks on each machine. It shows that most benchmarks benefit from exploiting the GPU at some iteration domain sizes; even those that show no benefit can be useful ACM test cases as outlined below.

ACM Misprediction Penalty is reported in Figure 5 for each of the 12 benchmarks on target platform T1. At each domain size it shows the platform device (CPU or GPU) selected by the cost model, along with any misprediction penalty. The misprediction penalty is the ratio between runtime on the selected device and runtime on the optimal device, so 1.0 is optimal. Note the logarithmic x-axis for relevant domain sizes. ACM delivers similar misprediction penalties for the benchmarks on T2 and T3, and corresponding misprediction penalty graphs are available in supplementary online materials [16].

For all benchmarks and platforms Table 3 shows the geometric mean penalties over all domain sizes and the maximum penalties. ACM provides entirely accurate predictions for four benchmarks on T2 and T3 and for three on T1. The mean penalties for different benchmarks vary from 1.0 (optimal) to 1.61, 1.39, and 1.86 for T1, T2, and T3 respectively. The last row of Table 3 shows the mean penalty and mean per-benchmark maximum penalty on each platform. The geometric mean penalty across all our experiments is 1.136.

We observe the SVM mean penalty is worse than ACM on each platform. Significant worst-case outliers for SVM maximum penalties contribute to high SVM mean per-benchmark maximum penalty on each platform. This may indicate limitations in the training set used for SVM classification.

Misprediction Intervals. Figure 6 shows CPU and GPU benchmark runtimes on T1 with ACM and SVM misprediction intervals highlighted. Between measured domain sizes the misprediction is interpolated. ACM delivers similar misprediction intervals for the benchmarks on T2 and T3 [16]. Table 4 shows the relative proportion of each input domain that is mispredicted. The mean misprediction proportion across all benchmarks is 0.143. ACM has the same or smaller misprediction intervals than the SVM predictor for 5, 6 and 9 of the 12 benchmarks on T1, T2 and T3 respectively.

The ACM misprediction intervals are generally small for benchmarks with sharply diverging CPU and GPU runtime curves like conv-2d, gemm, mandelbrot and syr2k. The exceptions are black-scholes on T2 and T3, where ACM mispredicts that the CPU execution will be faster over the initial range before correctly selecting the GPU at medium to large domain sizes. For the benchmarks that have no domain sizes where the GPU is faster, ACM correctly predicts this at all domain sizes for gemver and conway, but mispredicts at large domain sizes for saxpy and vadd.

Comparison with PyPy. Figure 6 also compares PyPy execution time with ALPyNA CPU and GPU execution times for each benchmark on platform T1. Both CPU and GPU code generated by ALPyNA is faster than PyPy across all domain sizes for 10 benchmarks on T1 and T3, and for 9 benchmarks on T2. For jacobi, PyPy is slower than ALPyNA CPU execution across all domain sizes on T1, T2 and T3.

For jacobi PyPy is slower than ALPyNA CPU execution at all domain sizes on T1, T2 and T3. It is faster than ALPyNA GPU but slower than ALPyNA CPU at the two smallest iteration domain sizes. For syr2k PyPy is slower than ALPyNA’s CPU code and faster than ALPyNA’s GPU code at the smallest four iteration domain sizes on all three platforms. The situation reverses at larger domain sizes where PyPy is slower than ALPyNA’s GPU code but faster than ALPyNA’s CPU code. For both jacobi and syr2k, utilising the device chosen by ACM at each domain size is faster than PyPy.

Loop Nest Characteristics. The benchmarks represent a range of different loop nests, and we investigate the impact of these on the cost model.

In embarrassingly parallel loop nests, every loop dominating a statement can safely be executed in parallel: black-scholes, conway, hilbert jacobi, saxpy and vadd are in this class. For some of these applications, the data transfer overhead is so large, relative to the actual computation, that GPU execution never outperforms CPU execution. This is particularly noticeable for single loops with tiny loop bodies that iterate linearly over input arrays. Referring back to Table 1, we observe that hilbert, jacobi, saxpy and vadd fall into this...
Figure 6. Misprediction intervals of ALPyNA Cost Model (shaded blue), an SVM predictor (shaded red), and both (shaded purple) for 12 loop-intensive benchmarks with varying domain sizes on platform T1. ACM’s domain crossover point is interpolated from the measured values. Execution time of ALPyNA’s CPU and GPU code is also compared with PyPy execution. Execution time (y-axis) is plotted on a logarithmic scale.

Table 3. ACM misprediction penalties for all benchmarks on all platforms: Geometric Mean Penalties across all input sizes, and Maximum Penalties.

<table>
<thead>
<tr>
<th>Benchmark</th>
<th>T1: CPU/GPU 2960/1405 MHz</th>
<th>T2: CPU/GPU 3900/1500 MHz</th>
<th>T3: CPU/GPU 800/1500 MHz</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ACM</td>
<td>SVM</td>
<td>ACM</td>
</tr>
<tr>
<td></td>
<td>mean</td>
<td>max</td>
<td>mean</td>
</tr>
<tr>
<td>black-scholes</td>
<td>1.16</td>
<td>2.36</td>
<td>1.03</td>
</tr>
<tr>
<td>conv-2d</td>
<td>1.07</td>
<td>2.20</td>
<td>1.68</td>
</tr>
<tr>
<td>conway</td>
<td>1.01</td>
<td>1.12</td>
<td>1.00</td>
</tr>
<tr>
<td>fbcorr</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>gemm</td>
<td>1.07</td>
<td>1.70</td>
<td>1.91</td>
</tr>
<tr>
<td>gemver</td>
<td>1.01</td>
<td>1.22</td>
<td>1.00</td>
</tr>
<tr>
<td>hilbert</td>
<td>1.02</td>
<td>1.23</td>
<td>1.05</td>
</tr>
<tr>
<td>jacobi</td>
<td>1.12</td>
<td>2.05</td>
<td>1.00</td>
</tr>
<tr>
<td>mandelbrot</td>
<td>1.00</td>
<td>1.00</td>
<td>7.10</td>
</tr>
<tr>
<td>saxpy</td>
<td>1.56</td>
<td>4.43</td>
<td>1.00</td>
</tr>
<tr>
<td>syr2k</td>
<td>1.00</td>
<td>1.00</td>
<td>2.08</td>
</tr>
<tr>
<td>vadd</td>
<td>1.61</td>
<td>5.56</td>
<td>1.00</td>
</tr>
<tr>
<td>Geo.Mean</td>
<td>1.17</td>
<td>1.73</td>
<td>1.39</td>
</tr>
</tbody>
</table>

category. This is reflected in these benchmarks’ performance on all three platforms, where CPU execution is optimal across all domain sizes. For instance, Figure 6 shows that parallel GPU execution cannot match sequential CPU execution for these simple embarrassingly parallel benchmarks, since data transfer overhead is included in total execution time. This interplay between data transfer overhead and GPU parallelism has motivated the design of ACM; similar ideas are seen in other cost models as outlined in Section 6.

Partially parallelizable loops have loop-carried dependences that constrain some loops to be executed sequentially in the CPython interpreter: conv-2d, fbcorr, gemm, gemver, mandelbrot and syr2k are in this class. For such loops the amount of parallelism obtained is dependent on the domain sizes of
Table 4. Ratio of mispredicted/correct ranges for all benchmarks on platforms T1, T2 and T3 using ACM and an SVM predictor

<table>
<thead>
<tr>
<th>Benchmarks</th>
<th>Misprediction Range</th>
<th>ACM</th>
<th>SVM</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>T1</td>
<td>T2</td>
<td>T3</td>
</tr>
<tr>
<td>black-scholes</td>
<td>0.30</td>
<td>0.60</td>
<td>0.60</td>
</tr>
<tr>
<td>conv-2d</td>
<td>0.09</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>conway</td>
<td>0.14</td>
<td>0.14</td>
<td>0.14</td>
</tr>
<tr>
<td>fbcorr</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>gemm</td>
<td>0.13</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>genver</td>
<td>0.08</td>
<td>0.08</td>
<td>0.00</td>
</tr>
<tr>
<td>hilbert</td>
<td>0.22</td>
<td>0.11</td>
<td>0.22</td>
</tr>
<tr>
<td>jacobi</td>
<td>0.20</td>
<td>0.10</td>
<td>0.10</td>
</tr>
<tr>
<td>mandelbrot</td>
<td>0.00</td>
<td>0.13</td>
<td>0.12</td>
</tr>
<tr>
<td>saxpy</td>
<td>0.43</td>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td>sylv2k</td>
<td>0.00</td>
<td>0.10</td>
<td>0.10</td>
</tr>
<tr>
<td>vadd</td>
<td>0.40</td>
<td>0.20</td>
<td>0.20</td>
</tr>
<tr>
<td>mean</td>
<td>0.16</td>
<td>0.13</td>
<td>0.14</td>
</tr>
</tbody>
</table>

the parallelizable loops and the amount of work scheduled on the GPU.

There is no clear difference between the ACM misprediction penalties and misprediction intervals for embarrassingly and partially parallelizable loops.

6 Related Work

Execution time prediction has a very long history. Worst case execution time (WCET) analysis aims to precisely and conservatively predict absolute runtime by static analysis or dynamic profiling [37]. To be lightweight ACM uses static analysis as far as possible. However rather than predicting absolute runtimes it compares the relative runtimes on a set of heterogeneous compute platforms.

Cost models, or resource analyses, are commonly used to predict runtimes in parallel systems, e.g. to inform task scheduling. Trinder et al present a wide-ranging survey [34], and using their classification ACM is an abstract relative parallel cost model, based on heuristic linear equations, and parameterized by a parallel implementation model of the underlying hardware.

Static Languages. Loop nests have been widely and successfully automatically parallelized in compiled languages, e.g. [7]. Many auto-parallelizing compilers use a cost model to determine what to parallelize. Compared with a dynamic language like Python, compilers for static languages have far more information about the loop nests.

A rapidly growing body of work studies GPU performance prediction. For example [22] models standard GPU architectures and, like ACM, derives parameterized mathematical equations to estimate GPU kernel runtimes. There are a variety of more sophisticated GPU performance prediction techniques making use of analytical models like [5, 32].

Another approaches rely on the program being written as algorithmic skeletons, e.g. the Grophecy tool [28] predicts GPU runtime based on CPU runtime. Other predictions of GPU runtime based on CPU profiling rely on machine learning, e.g. [2] that builds a regression model for cross-architecture performance prediction.

Using machine learning rather than derived analytical models for GPU runtime prediction has become increasingly common, e.g. [39]. However an empirical comparison with analytical cost models shows that the analytical models provide greater accuracy [1]. Analytic models are parameterised with hardware and program values, and ACM’s dynamic analytic system determines some of these at runtime.

Currently there is intense interest in automatically executing OpenMP loop nests on heterogeneous architectures. Here, as in other auto-parallelization the importance of augmenting static analysis with runtime values is recognised, e.g. [9]. This approach compiles parallel CPU and GPU code for the loop nest and uses a staged cost model to select what code to run. ACM is similarly staged, but ALPyNA uses JIT compilation to dynamically create custom GPU kernels that are tailored to the exact dependences that arise in each instance of the loop nest. ACM also reflects the idea that the execution schedule of the loops may change along with the structure of the kernels.

Speculative parallelization of tightly nested loops in managed language runtimes is an attractive approach to obtain speed ups [30, 31, 36]. Leung et al [25] attempt to cost potential execution on a GPU compared to a CPU. Extensive profiling of absolute time required for execution of a Java bytecode on CPU and GPU is used to arrive at an estimate for GPU execution time. ACM uses a predictor parameterised on the hardware characteristics of each device such as frequency, cache sharing and also model runtime bottlenecks such as starvation effects.

Some systems that target heterogeneous platforms exploit sophisticated managed language runtimes. For example TornadoVM operates on annotated loop-intensive Java [10]. It uses task graphs to express dependencies and selects between CPU, GPU and FPGA targets. It exhaustively samples loop execution profiles for all available targets and selects the best target for future scheduling. ACM and ALPyNA also exploit Python’s sophisticated managed runtime, but (1) use an analytical model where TornadoVM uses profiling and (2) avoid eagerly generating code for all targets. That is, code is only JIT compiled if ACM identifies the target as the best.

Some recent Dynamic Language compilers dynamically generate code for heterogeneous compute devices. There are various approaches to automatically select the most appropriate compute device at runtime for particular program fragments like methods or loop nests. Hayashi et al [13] and Kim et al [19] study CPU and GPU execution of Java code and advocate machine learning for selecting the target platform for parallel stream API calls. Extracted features for input to the trained machine learning model include the parallel loop
range, which must be acquired by runtime introspection as in ACM.

Other researchers have recognized the importance of Python for end user programming in scientific domains. For example the Selective Embedded Just-in-Time Specialization (SEJITS) project [17] enables expert users to embed domain-specific optimizations for key computational kernels such as matrix algebra. These optimizations are dynamically invoked and high-performance (typically native C) code is generated for the compute-intensive portions of the code. In contrast ALPyNA does not require expert ‘intervention’ to generate kernels and dynamically selects the execution platform.

7 Conclusions

This paper presents the design, implementation and evaluation of ACM, the first analytical cost model that supports the automatic runtime exploitation of GPUs in a dynamic language. The model is staged and lightweight, and is used to select between compute devices to effectively parallelize moderately complex Python loop nests on commodity heterogeneous platforms using the ALPyNA framework.

For each instance of a loop nest, ACM dynamically predicts the relative runtimes on alternative devices so that ALPyNa can select the fastest. The models for the CPython interpreter, and for JIT compiled CPU execution are relatively standard, but the GPU model is both novel and elaborate. It accounts for key costs like data transfer time, and for starvation effects etc. All of the platform models are parametric in key characteristics of the platforms, like cache size and sharing, and warp size on the GPU (Section 3).

We report a systematic evaluation of ACM on three heterogeneous platforms using 12 standard loop-intensive Python benchmarks, and covering a wide range of domain sizes (Section 4). The cost model proves to be effective, with small misprediction ranges (Table 3) and a mean misprediction penalty of just 13.6% slowdown, relative to optimal, across all benchmarks (Section 5). The cost model also outperforms a trained SVM.

Future Work An immediate avenue for future work is to evaluate the cost model on additional heterogeneous systems. Currently ACM does not account for the overhead of runtime compilation. Hence interpretive execution is never selected over JIT compilation even when it would reduce runtime for small iteration domains. For frequently executed kernels it helps that Numba persists generated code in a compilation cache. We expect it will be relatively easy to extend ACM to account for runtime compilation overheads, e.g. using models like [27].

ACM has been designed to be extensible and we envisage extending ACM as underlying technologies improve. An extension might model GPU kernel fusion [35] if ALPyNA adds support for this. A further extension might model vectorized execution on CPU or other parallel code generation.

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