Extracting Clean Performance Models from Tainted Programs

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Abstract

Performance models are well-known instruments to understand the scaling behavior of parallel applications. They express how performance changes as key execution parameters, such as the number of processes or the size of the input problem, vary. Besides reasoning about program behavior, such models can also be automatically derived from performance data. This is called empirical performance modeling. While this sounds simple at the first glance, this approach faces several serious interrelated challenges, including expensive performance measurements, inaccuracies inflicted by noisy benchmark data, and overall complex experiment design, starting with the selection of the right parameters. The more parameters one considers, the more experiments are needed and the stronger the impact of noise. In this paper, we show how taint analysis, a technique borrowed from the domain of computer security, can substantially improve the modeling process, lowering its cost, improving model quality, and help validate performance models and experimental setups.

CCS Concepts: • **Computing methodologies** → **Modeling methodologies**; *Model verification and validation*; • **Theory of computation** → *Program semantics*; *Concurrency*.

Keywords: performance modeling, high-performance computing, compiler techniques, taint analysis, LLVM

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1 Introduction

The increasing complexity of both hardware and scientific problems creates new challenges for developers of high-performance applications. The design process of a massively parallel program that can scale on modern architectures requires a deep understanding of computational kernels and communication patterns. Performance modeling has become a standard technique to solve problems such as locating scalability bottlenecks [11, 19, 47], estimating the execution time when the input size or the core count changes [51], or predicting application performance on a new architecture [9, 36].

The main goal of performance modeling is to express the performance of an application as a function of one or more execution parameters [22, 31]. Purely analytical performance modeling involves an expert who analyzes the source code and understands the underlying algorithms [22]. While very effective once the models have been created, the required person-hours and experience restrict its usability in practice. Empirical performance modeling, by contrast, generates similar performance models automatically by analyzing measurements taken from running an instrumented version of the application in different configurations. It follows three major steps: identifying parameters, designing an experiment to measure the influence of parameter changes on the application behavior, and learning the model that best fits the data. While generating models from existing data is automatic and resource efficient, running the experiments may require careful planning and extensive computational effort. In general, empirical performance modeling involves two important decisions: (1) choosing parameters that will affect application performance and (2) designing a set of experiments capable of accurately measuring their influence, while not exhausting the available computational budget.

Modern scientific applications use dozens of parameters that describe numerical properties, data size, or the degree of parallelism, making their selection extremely challenging. Without detailed insight into the application behavior, the

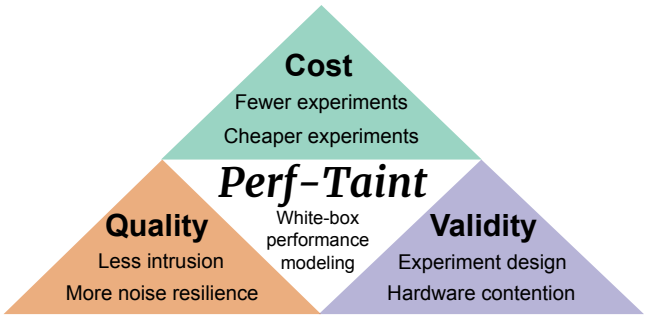


Figure 1. The basic concept of Perf-Taint. A tainted run of the program provides information that improves the empirical performance modeling process along the dimensions cost, quality, and validity of the resulting models.

user has to consider all possible combinations of the chosen parameters. The larger the number of parameters, the bigger is the number of experiments and the impact of noise on the quality of the resulting models [42]. Some performance effects are not measurable for the entire range of parameter values available in the experiment design, potentially invalidating some measurements. Another major difficulty arises from the black-box nature of empirical modeling. Without insight into function behavior beyond empirical data, the modeler cannot distinguish between actual runtime change because of parameter influence and the effects of noise on the measurements. This leads to overfitting, estimating false dependencies, and generating incorrect models for constant functions with negligible execution time.

In this paper, we show how taint analysis [14], a technique borrowed from the field of computer security, which reliably relates marked input values with the program parts they potentially affect, can provide this additional context, leading to the concept of *tainted performance modeling*. Performance tainting provides us with accurate performance parameter information and enables the design of a novel loop-based complexity analyzer. We integrate our complexity analyzer with Extra-P [11], an empirical performance-modeling tool, and derive a new hybrid performance modeling framework called *Perf-Taint*, whose underlying concept is illustrated in Figure 1. We make the following specific contributions:

- The application of taint analysis, which has originally been devised to track the flow of protected data through a program, to a new problem: the improvement of empirical performance models of HPC applications.
- The elaborate concept of tainted performance modeling, that can (1) reduce the cost of empirical performance models, (2) improve their quality, and (3) help validate them and the experimental setups used for their generation. An example of such a validation is the detection of contention as the source of measurements that contradict expected computational volumes.
- An open-source, LLVM-based tainted performance modeling tool, ready to use on HPC programs to provide the insights of a virtual performance expert[1].

After reviewing related work in Section 2, and the taint analysis in Section 3, we describe the theoretical and practical aspects of our method in Section 4 and Section 5, respectively. We then demonstrate the benefits it provides in Section 6 and present our conclusion in Section 7.

2 Related Work

The broad spectrum of existing methods and tools to support the creation of performance models documents their importance for understanding the performance influence of algorithms [57], the hardware [36, 37], and the operating system [21, 39, 57]. They are often used to extrapolate performance outside the known range of a single parameter [27, 54, 59] or even multiple parameters [19, 47], sometimes exploiting the properties of certain classes of algorithms such as stencil computations [55]. Some require the prior annotation of the code with performance expressions [49, 51]. Machine learning methods have also been successively used for performance modeling [26, 34].

There have been several attempts to enable performance modeling through static analysis of source code [20, 32, 35, 38]. Thanks to the dynamic nature of taint analysis, our method is not affected by fundamental limitations of static methods. The dependence of performance modeling tools on an entirely static dataflow analysis or a perfect loop modeling might prevent them from scaling to large scientific applications. A hybrid performance modeling tool was presented for online modeling by Bhattacharyya et al. [7].

A different aspect of performance modeling, dataflow analysis, is also well studied in high-performance computing: DfAnalyzer performs dynamic dataflow analysis of Spark high-performance applications [48]. Parallel control-flow graphs of MPI programs have been constructed with dataflow analysis [2]. Value influence analysis, a variant of taint analysis, has been used in message-passing applications [43].

3 Dynamic Taint Analysis

When trying to construct the performance model of a full application, one would hope that there is a way to automatically determine its runtime complexity (or complexity w.r.t. other metrics) by analyzing the program code with a sufficiently smart compiler. While previous research showed first results [24] towards this direction, these solutions are inherently limited to special cases or approximations and are hard to scale to non-trivial programs (Section 3.1), as even the simple problem of identifying which input parameter affects an arbitrary program variable is inherently difficult.

[1]The code is available on GitHub: `spcl/perf-taint`

Dynamic taint analysis (Section 3.2) has been successfully used in the context of computer security to reliably analyze data relations across complex programs. We introduce the major concepts and techniques and discuss how taint analysis provides precise knowledge as to how input parameters affect variables of the program. This gives us the instruments to introduce white-box performance modeling of non-recursive HPC programs (Section 4).

3.1 Static performance modeling is hard

Modeling performance statically is difficult from both a theoretical and a practical viewpoint. There are strict theoretical limitations of how accurate a static analysis can be or if an analysis can be computed at all. On the practical side, various levels of abstractions or indirections make program code easy to maintain, but make static analysis even less likely to succeed. We now outline several theoretical and practical considerations that make static performance modeling hard.

Theoretic limitations There are strong theoretic reasons why static program analysis techniques are often unable to provide precise answers even for seemingly simple analyses. The most well known is the halting problem [13] or its generalization, Rice's theorem [40], which we here rephrase in the terms of program analysis: any non-trivial semantic property of a program cannot be computed. A property such as "does a program contain a certain instruction sequence" is syntactic and might be decidable, but "does a program return 0" is a semantic property and is undecidable for arbitrary programs. As a result, the question "can the value stored in a given memory location affect an instruction that is run when executing a given program" is a semantic property. Hence, determining whether a configuration parameter affects certain parts of a program is undecidable.

Practical considerations While Rice's theorem shows that the proof of semantic properties to be impossible for all programs, there might still exist a sufficiently large set of programs where this is realistic. We now argue that even an approximate analysis for only a subset of programs is difficult in practice. The main culprits are abstraction overhead, complex abstract data types, and runtime configurability. Abstraction is important to ensure the maintainability of large software projects. To that end, class hierarchies, virtual dispatching, and many very fine-granular functions are commonly used. Pointer aliasing in general is a hard problem [44], and while some static analysis tools [50] can achieve a significant degree of precision in the inter-procedural context, the results are affected by over-approximation. Performance modeling needs precise program information, since proving the lack of a parameter dependency on computation is necessary to reduce the dimensionality of models. Another source of over-approximation is the hard-to-predict control-flow found in languages gaining popularity in scientific computing. The problem arises from virtual dispatch in statically typed languages (C++, Julia) and from duck typing (Python).

Message-passing and multithreading adds to the code nondeterminism that can lead to a combinatorial explosion of states. A common choice for the analysis of MPI programs is symbolic execution [17], but it suffers from the exponential number of paths it has to analyze, limiting its scalability [56].

3.2 Dynamic taint analysis

Dynamic taint analysis is a runtime analysis that *marks and tracks the movement of certain data elements and computed results depending on them through the execution of a program.* Taint analysis can compute semantic analyses while a program is executed, overcoming the limitations that prevent static (compile-time) analysis from providing precise results, at the price of narrowing the insights to a specific run and its input configuration. For many analyses – especially if the results anyhow depend on input data – this is often exactly what is desired. We introduce a general taint-analysis framework that can be used to instantiate problem-specific taint analyses. We define three major components described by Clause et al. [14] – (a) taint sources, (b) propagation policy, (c) taint sinks, which we discuss below with code examples.

Taint sources Taint sources are all components of a program that can represent some kind of program data. Typical taint sources are memory locations, variable names, or function return values, but almost any part of a program can be a taint source, including I/O interfaces, system calls, network devices, etc. Marking taint sources requires the specification of data to be tainted and taint labels used to mark it.

```
// Program input: taint with label "size"
scanf("%d", &size);
// Manual taint source: taint with label "p"
write_label(&p, sizeof(p), "p");
// Third-party library output: taint with label "ranks"
MPI_Comm_size(MPI_COMM_WORLD, &ranks);
```

Taint propagation policy The taint propagation policy defines how taint labels are moved through a program. We specify it by (1) defining a mapping function, and by (2) defining the affected data. The *mapping function* defines how two (or more) taint labels are joined. In the most trivial case, two sets of labels are joined by taking the union of the sets.

The *affected data* defines all data to which taint labels are propagated through data-flow and control-flow. Data-flow based propagation passes taint labels from inputs of operations to their outputs, including program instructions and propagation from function arguments to its return value. Control-flow based propagation captures the propagation of taint labels through control dependencies [15, 28].

```
int foo(int a,int b,int c) {//Input labels: "a","b","c"
  int d = 2 * a; //Dataflow tainting with label "a"
  if(b) d++; else d--; //Explicit tainting, label "b"
  if(c) d = pow(d, 2); //Implicit tainting, label "c"
  return d; //Taint labels of return: "a", "b", "c"
}
```

In the example above, the variable a taints the return value of the function through a data-flow propagation. Variable b taints d through a control-flow condition which controls the execution of code that changes the return value (explicit dependence). An implicit dependence occurs for c since the value depends on it even if the second branch is not taken.

Taint sinks Taint sinks are program code locations with an associated variable or memory location that may observe tainted program data. Sinks are used to determine which tainted values affect a given behavior. Each taint sink is defined by (1) a program code location, (2) the variable or memory location to check, and (3) a checking method that is invoked whenever the taint sink is executed.

4 Tainted Performance Modeling

Building on the concepts presented in Section 3.2, we introduce a *taint analysis for performance modeling* (Section 4.1), where the influence of input parameters on program variables is used to model the number of loop iterations. We show how this knowledge allows us to place a bound on the *volume of computation* (Section 4.2), defined as the number of operations executed in a non-recursive program run. An empirical black-box performance modeler uses the information of compute volumes to limit the space of potential complexity functions it considers (Section 4.5).

4.1 Loop count parameter identification

We solve the core data-flow problem behind performance modeling by formulating a suitable taint analysis. We assume that all target metrics, such as the program runtime or the number of operations, only vary with the iteration number of loop constructs in the code, since a control-flow decision not associated with a loop pattern will not affect asymptotic complexity of performance models. This assumption is intuitive because the source code is typically not changed (i.e., in complexity or size) when changing program input parameters. Our analysis computes how potential input parameters affect the iteration counts of all *natural* loops [3] in a program.[2] While the analysis does not support recursive functions, it warns of over-approximation when recursion is detected. Nevertheless, the core focus of performance modeling are HPC applications where the vast majority of computations are iterative anyway.

Sources The sources of our loop taint analysis are all potentially performance-relevant parameters of a program. Performance relevant parameters are all memory locations marked explicitly by the performance engineer with a parameter label. Parameters are typically read from the command line, but might also be provided through other means (e.g., a configuration file), as long as their value is eventually stored in a variable that the user has marked as a parameter.

Propagation policy To reliably produce accurate results, our analysis requires the propagation of taint across data flow and control flow. Because we need to know only the presence of a specific taint label in a performance-relevant variable, we choose the set union as mapping function. Each label will contain the set of input parameters that in some way affected the value marked by the taint label.

Sinks The sinks of our taint analysis are all loop exit conditions. For a given loop, the number of times it iterates depends only on loop exit branch conditions. Any further indirect dependencies will eventually taint these branch conditions through our taint analysis.

We summarize the concepts in an example. With automatic taint propagation, the dependency on input parameters is propagated through function calls and memory operations to the sink, where it is used by our loop-count analysis.

```
struct params = parse_args();
write_label(&params.size,"size", &params.step,"step");
iterate(pow(params.size, 2), optimize_step(params));
void iterate(int size, int step) {
 for(int i = 0; i < size; i += step) {
  compute();  sink({&i, &size}, register_loop);
 }
}
```

Assuming a loop L depends on taint labels $p_1, \ldots, p_n$, the number of loop iterations of L, $count(L)$, must then be a function $g(p_1, \ldots, p_n)$. While the parameters this function potentially depends on are clearly defined, no further information about function g can be derived through the taint analysis itself. Even if the taint label just contains a single taint mark p, it does not imply a number of loop iterations linear in p. $count(L)$ could also be $log(p)$, p^2, or any other function $g(p)$. As a result, we can state the following claim:

Claim 1. *Given an application with a set of input variables V and a set of n correctly marked potential performance variables $P = (p_1, \ldots, p_n) \subseteq V$, we derive for a given loop L a class of symbolic functions $g_i(p_1, \ldots, p_n)$ which only depend on parameters in P. If all program parameters that impact the iteration count of L have been marked, a performance taint analysis with full data and control flow propagation computes with $count(L) = p_i$ a class of functions which contain the function that exactly describes the number of loop iterations.*

4.2 Iteration volume of a loop nest

We now derive the iteration volume of a loop nest, that is, the accumulated number of times the body of a loop nest is executed. We define the iteration volume recursively. The base case of our recursion is a loop nest with just a

[2] Our analysis does not explicitly consider irreducible loops where control is transferred through multiple paths into the loop (no single loop header), as irreducible loops can easily be transformed into natural loops [53].

single loop L. In this case, the volume of computation $vol(L)$ is $count(L) = g(\vec{p})$, the result of our loop iteration count parameter identification. We now define the iteration volume of larger loop nests by combining existing loop nests.

Sequencing two loops Executing two child loops nests (LN_{c1} and LN_{c2}) in sequence forms a larger loop nest LN. The iteration volume of LN is over-approximated as the sum of the compute volumes of the child loop nests, $vol(LN) = vol(LN_{c1}) + vol(LN_{c2})$.

```
LN:  {
       for(int i = 0; i < count(LN_c1); i += 1) { ... }
       for(int i = 0; i < count(LN_c2); i += 1) { ... }
     }
```

Nesting of a loop and a loop nest Executing a child loop nest (LN_c) inside a loop L forms a larger loop nest LN. The iteration volume of LN is over-approximated by multiplying the iteration count of the outer loop with the iteration count of the loop nest, $vol(LN) = g(\vec{p}) \cdot vol(LN_c)$.

```
LN:  {
L_1:     for(int i = 0; i < count(L_0); i += 1)
           for(int j = 0; j < count(LN_child); j += 1)
             ...
     }
```

The power of these simple composition rules can be summarized in the following claim about asymptotic performance with respect to performance-critical variables.

Claim 2. *Given an application with a set of input variables V, a set of n correctly marked potential performance variables $P = (p_1, \ldots, p_n) \subseteq V$, and a loop nest built from natural loops L_i without irreducible control flow or recursion, we derive for the loop nest a class of symbolic functions $g_i(p_1, \ldots, p_n)$ which only depend on the parameters in P. If all variables that impact the loop iteration count have been marked, we derive an asymptotic upper bound on the maximal number of times any given basic block is executed in the loop.*

These functions may still contain unresolved functions $g(\vec{p})$ representing loops for which the runtime is not known statically. We will explain in Section 4.5 how we derive these functions empirically from performance measurements.

4.3 Compute volume of a full program

We calculate the compute volume of a full program without recursion. Any code not part of a loop can be ignored as it has only constant cost. Similarly, bodies of inner loops can be assumed to have only constant computational cost since the analysis is inter-procedural and loop nests are aggregated across function calls. Therefore, the asymptotic compute volume can be derived by looking only at the recursively accumulated cost of loop nests.

Theorem 1. *Given an application A with a set of input variables V, a set of n correctly marked potential performance variables $P = (p_1, \ldots, p_n) \subseteq V$, no irreducible control flow or recursion, the recursive accumulation of the iteration volume in each function of the call tree (due to no recursion) computes the asymptotic compute volume of A.*

The taint analysis therefore yields properties of the function space of possible performance models but it does not explicitly generate precise models. In this sense, it provides a "scaffolding" that defines some relations among loops. However, the precise function for each loop is not yet defined. To derive such functions, we first discuss how to include additional control-flow information into the model (4.4). We subsequently refine an empirical modeling approach to parametrize the missing loop models to derive accurate overall performance models for each function (4.5).

4.4 Algorithm selection

In addition to building a set of performance models for each function discussed earlier, we apply taint analysis to locate control-flow decisions unrelated to loop exit conditions that are affected by input parameters. Instrumenting conditional branches with taint sinks enables (1) the detection of tainted control-flow decisions affecting performance models for branches inside any loop nest and (2) the detection of code paths that are never visited, including the parameter-based selection of algorithms.

4.5 Empirical performance modeling is also hard

Our dynamic taint analysis provides us with information on how parameters influence the compute volume of individual functions, but does not provide specific functions that describe the asymptotic behavior very precisely. To close this gap, we build a hybrid analysis by combining the compute volume information from our compiler-based analysis with a black-box empirical performance modeler. This modeler runs a program multiple times with different parameter configurations. Using both the results of taint analysis and the observed execution times, it derives a performance-model function that (1) respects parameter dependencies derived during the taint analysis and (2) provides the best fit to empirical data. As a black-box performance prediction approach we use the performance modeling tool Extra-P [8, 12, 46].

Performance function A key concept of the Extra-P approach is the *performance model normal form* (PMNF), defined in Equation 1. It models the effect of parameters x_i on a variable of interest $f(x_1, \ldots, x_m)$, typically execution time or a performance counter. The PMNF is based on the assumption that performance, at least at the level of functions calls, can usually be expressed as a combination of polynomial and logarithmic terms. This flexibility in expressing behaviors is sufficient to cover most cases encountered in practice while keeping the modeling process fast enough to be viable.

$$f(x_1, \ldots, x_m) = \sum_{k=1}^{n} c_k \cdot \prod_{l=1}^{m} x_l^{i_{kl}} \cdot log_2^{j_{kl}}(x_l) \qquad (1)$$

The PMNF defines a function search space, which is traversed to find the function that comes closest to representing the set of measurements. This assumes that the true function is within the search space. A possible assignment of all i_k and j_k in a PMNF expression is called a *model hypothesis*. The sets $I, J \subset \mathbb{Q}$ from which the exponents i_k and j_k are chosen and the number of terms n define the model search space. The coefficients of all hypotheses are automatically derived using regression and the hypothesis with the smallest error is chosen to find the most likely model function. In this work, we use the configuration suggested by Ritter et al. [42].

This approach *always* generates a human-readable expression out of any given measurement data. It attempts to explain this data as well as possible by fitting the PMNF to the data. The more complex the PMNF is, such as by adding more terms or a wider range of exponents to the terms, the more freedom the modeling has to fit the data. This allows more behaviors to be expressed but risks overfitting the data—especially in the presence of noise.

Limitations A significant limitation of Extra-P is the black-box nature of the approach that uses only empirical measurements to generate performance models. This means that the models can be affected both by random noise, and by systemic interference such as network congestion caused by multiple applications sharing a physical system. While these effects can be mitigated by repeating measurements and trying to control the measurement infrastructure, they cannot be eliminated and their impact is larger the more parameters are considered [42]. In most applications, runtime is concentrated in a small number of routines, and while these routines are correctly modeled, the previously discussed disturbances disproportionately affect regions of code with short runtimes, and in some cases translate to Extra-P effectively modeling noise. Given the large number of such occurrences, in some the noise can randomly resemble a strong correlation between a parameter and a metric. Such false positives can, at the moment, only be eliminated by manual inspection of the code and cost users valuable time.

Hybrid modeler Our goal is to allow the PMNF to be as expressive as possible to accurately model different performance behaviors but wish to prevent this expressivity from generating false positives by overfitting. We therefore use taint analysis to define a prior for the modeling process in Extra-P. We use the results of the taint analysis to minimize the negative effects of measurement noise. The model of computational volume is applied to restrict the search space by removing parameters that could not affect performance. As a result, the black-box regression algorithm no longer uses non-existing parameter dependencies in models.

The immediate effect is pruning out parametric models for constant functions. These functions are notoriously hard to model since the variability of measurement data forces the modeler to favor functions that are not constant. The final model is overfitted and likely misleading. The second important result is the removal of false dependencies in performance models. We therefore automate the process of verifying empirical models by removing parameters not present in the code from the search space.

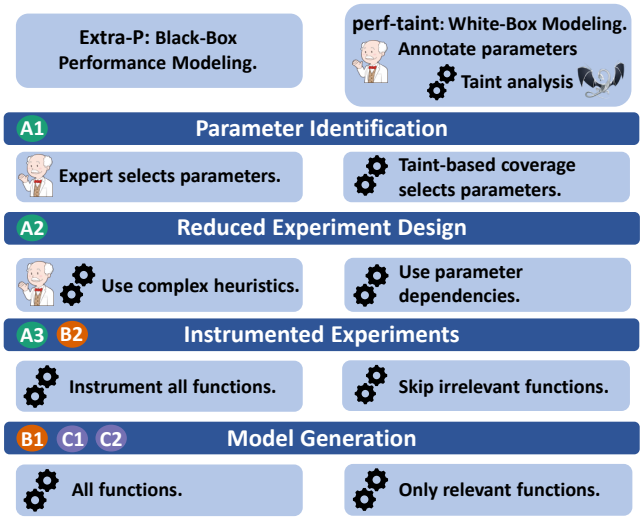


Figure 2. The processing pipeline of Perf-Taint. All four major steps of empirical modeling are improved with the program information provided by taint analysis.

5 Implementation of Perf-Taint

We provide with Perf-Taint an implementation of our performance tainting approach, as shown in Figure 2. Our processing pipeline includes the new step of tainted modeling that consists of three stages: (1) a static analysis, (2) a dynamic taint analysis; and (3) a database of performance-critical libraries, which we discuss in detail in the following subsections. Perf-Taint uses LLVM [33] and works on the level of the intermediate representation (IR), which makes Perf-Taint applicable to a range of languages, including C++, Fortran, Julia, etc. However, our taint-based modeling approach (Section 4) is independent of the taint implementation and can also be built using other taint-analysis frameworks [15, 28, 30, 45].

Figure 2 shows how performance modeling with Extra-P is improved with the program information provided via taint analysis. Without taint analysis expert knowledge is necessary to decide which parameters have the largest impact on performance and scalability, a difficult manual task. Perf-Taint leverages taint analysis to determine how many loops and functions are affected by each specific parameter, providing a simple yet intuitive coverage metric and removing from the analysis any parameters that have no effect on performance. The only user action is the annotation of each input parameter with one line of code in the program source, as illustrated in the example below. In contrast to many performance modeling tools [35, 38, 51], we do not require our

users to annotate regions of interests, functions, loop boundaries, or even to provide manually annotated performance models for each kernel.

```
struct cmdLineOpts opts;
ParseCommandLineOptions(argc, argv, myRank, &opts);
register_variable(&opts.nx, "size");
```

The next step determines the set of measurements used for empirical modeling. The user needs to provide the constraints on parameter values, which is a problem-specific part. The naïve approach considers all combinations of parameter values and therefore the number of samples scales exponentially with the number of parameters. While the original approach required sophisticated heuristics and a potential accuracy loss to reduce this number, taint analysis decides which parameter have multiplicative dependencies and which lead to additive effects. This means often not all combinations are required, therefore reducing the burden of the most computationally expensive part of the pipeline without sacrificing accuracy. Finally, Perf-Taint uses taint-based information on parameter dependencies to select only relevant functions for instrumentation and prune models with false dependencies, leading to better and cheaper models.

5.1 Static analysis

At compile time, we identify all functions that contain no loops or only loops with constant and statically resolvable trip counts since their performance models are known to be independent from any program parameter. To that end, we query an existing loop induction analysis (e.g., ScalarEvolution [18]). During this process, we include functions containing library calls that are known to be affected by performance parameters, such as MPI communication routines.

5.2 Dynamic taint analysis

We build our solution on top of the DataFlowSanitizer plugin [16] in LLVM, a data-flow taint system consisting of (1) a runtime implementing taint system, and (2) a transformation pass instrumenting each instruction with propagation of taint labels from its operands to the output. The sanitizer implementation trades efficiency in favor of versatility, supporting up to 2^{16} unique labels. We extended the plugin with support for explicit control-flow taint propagation.

Perf-Taint gathers information on the effects of tainted parameters on each non-constant loop in the program, by treating loop exit branch conditions as taint sinks. We store call-path information to distinguish between function calls that result in different dependencies, letting the empirical modeler Extra-P create calling-context-aware performance models. As part of post-processing after program execution, we parse loop nests with parameter dependencies and use this information to generate explicit multiplicative and additive dependencies for a function. The only source of over-approximation in our analysis is the presence of multiple labels in a single exit condition, where we conservatively report a multiplicative dependency. The latter requires more experiments to be accurately parametrized.

5.3 Global state libraries

Loop-based kernels are not the only way how parameters can affect the performance. The model has to include parametric effects of communication and synchronization routines. The performance parameter could affect their behavior in the following ways: (1) a value tainted by the parameter is exchanged between processes operating in disjoint memory spaces, (2) the parameter is passed to the routine explicitly, (3) the parameter is hidden from the user in the library runtime. We solve issues (2) and (3) by introducing a library database describing performance-relevant functions, implicit parameters provided by libraries, and sources of taint values.

We demonstrate the solution on MPI, the most widely-used library for distributed and high-performance applications. We declare the implicit parameter `p`, which denotes the size of the global communicator, and we include the function `MPI_Comm_size` as a source of tainted values, writing a label to the memory address passed as a second argument to the function. We derive parametric dependencies for MPI communication and synchronization routines from precise analytical models [23, 52], and provide them in the library database supplied with Perf-Taint. As an example, we consider the case of MPI peer–to–peer communication routines. When they appear in a function, our analysis introduces implicit dependence on `p`. Since performance of these functions depends on the network conditions and message size, we query the taint labels associated with `count` argument provided to the function and add them as additional parametric dependencies for this function call.

Taint labels could be transfered between processes withing MPI messages. The problem of tainting network communication has already been tackled [58], and an analogous solution for MPI would only have to cover standard MPI datatypes and the few, well-defined routines that create user-defined datatypes. We have found that the lack of support for data exchange across the network is not an obstacle for the applications we analyzed.

6 Taint Analysis in Action

We present the three major categories of improvements that our taint-supported framework brings to the empirical performance modeling process: decreased cost (Section A), improved quality (Section B), and the discovery of software and hardware phenomena the knowledge of which can help validate experiment design and modeling results (Section C). We support our claims by applying taint-supported performance modeling to two representative HPC benchmarks: LULESH [29] and MILC [6], summarized in Table 2

	Piz Daint	Skylake Cluster
CPU	Intel Xeon E5-2695 v4 2.10GHz	Intel Xeon 6154 3GHz
Cores	2 sockets, 18 cores each	36 cores
Memory	128 GB	384 GB
Software	GCC 8.3, Cray MPICH 7.7.2 Score-P 6.0 [4], Extra-P 3.0 [1], LLVM 9.0 [33]	GCC 8.3, OpenMPI 4.0.3

Table 1. Software and hardware configuration of Perf-Taint evaluation on Piz Daint and a local Skylake cluster.

	LULESH	MILC
Functions	356	629
Pruned Statically/Dynamically	296/11	364/188
Kernels/Comm. Routines/MPI	40/2/7	56/13/8
Loops	275	874
Pruned Statically	52	96
Relevant	78	196
Modeling		
p	$3^n(27, ..., 729)$	$2^n(4, ..., 64)$
size	25,30,35,40,45	32,64,128,256,512

Table 2. Overview of LULESH and MILC: the two-phase identification of computational kernels, communication routines and MPI functions used, and the manually specified parameter values for two-parameter modeling.

and discussed in the next two paragraphs. The hardware and software systems used are summarized in Table 1.

LULESH is a scientific application written in C++, implementing stencil computations for a hydrodynamic shock problem on a three-dimensional mesh. The code is structured around the main class `Domain` and contains multiple simple methods. Their expected constant computational effort is hard to capture empirically because the presence of noise makes timing data unreliable for such short functions. We run the taint analysis of this application with `size` 5 and 8 MPI ranks, leaving other parameters at the default value, since it provides a representative execution of the application that is close to parameter configurations used in modeling (Section B). If we choose the number of MPI ranks `p` and the grid size `size` as performance-model parameters, a typical use case, our analysis marks 86.2% of the functions as not influenced by these two parameters, allowing the immediate classification of their models as constant.

MILC We model the performance of the su3_rmd application from the MIMD Lattice Computation, a collection of scientific applications working on problems from the lattice quantum chromodynamics (QCD) fields. We analyze here the effects of two parameters frequently chosen for scaling studies: (1) the `size` of the space-time domain, which is computed from the four parameters `nx, ny, nz`, and `nt`, and

LULESH	Total	p	*size*	*regions*	*iters*	*balance*	*cost*	***p, size***
Functions	43	2	40	13	4	9	2	40
Loops	86	2	78	27	4	20	2	78

MILC	Total	p	*size*	*trajecs*	*warms steps*	*nrest. niter*	*mass,beta nfl. / u0*	***p, size***
Functions	56	54	53	12	9	6	1 / 4	56
Loops	196	187	161	39	31	15	1 / 7	196

Table 3. Computational kernels and loops in multi-parameter modeling. ***p, size*** is not equal to the sum of corresponding columns since multiple parameters can affect the same region.

(2) `p`, the number of MPI ranks. We apply the taint analysis of this application with a `size` of 128 on 32 MPI ranks. Again, the taint analysis identifies 87.7% of the functions as constant relative to these two parameters. This corrects 77% models previously indicating performance effects. Our analysis is confirmed by the preceding manual analysis and the validation with up to 512,000 processes [5].

A *Cost*

The cost of the modeling process is influenced by two major factors: the number of the required performance experiments, which significantly grows with the number of model parameters, and the cost of these experiments under instrumentation. Tainted performance modeling lowers these costs in multiple ways while reducing the dependence on human expertise. First, it supports automatic pruning of the parameter space (Section A1), avoiding many unnecessary experiments. It can expose parameter dependencies at an early stage (Section A2), allowing smarter experiment design with even less experiments. Finally, we show that the ability to judge the performance relevance of a function upfront can substantially decrease the instrumentation overhead (Section A3).

A1 *Parameter pruning*

```
int foo(int a, int b, int & result) {
  for(int i = 0 ; i < a; ++i)
    result += b * i;
}
```

Parameter a affects loop.
Prune **numerical** parameter b.

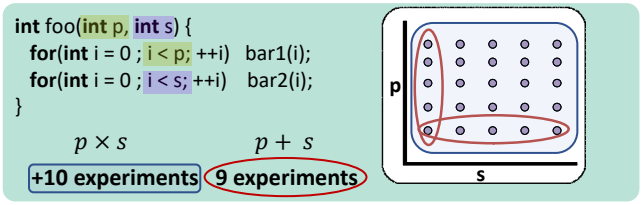
High-performance computing applications often involve a large set of execution parameters. In practice, limited compute budgets restrict the number of model parameters to three, and even with boundless resources one should not go much beyond, as the impact of noise would become too strong [41]. Tainting allows us to decide which parameter influences which part of the program. Programmers should mark program parameters found in routines parsing command-line arguments and configuration files. Our analysis determines all parameters without effect on the control flow and counts the number of loops and functions directly

affected by a specific parameter. Table 3 summarize parameter pruning on both benchmarks, excluding communication routines relevant only because of calls to MPI.

LULESH includes six major parameters: the problem size `size`, the number of MPI ranks `p`, `regions`, `balance`, `cost`, `iters`. To build a two-parameter model providing the broadest coverage of performance relevant functions our taint analysis suggests we select `size` and `p`.

In MILC, we detect the performance-relevant parameters `nx`, `ny`, `nz`, `nt`, `steps`, `niter`, `warms`, `trajecs` and the implicit parameter `p`. Our findings are identical with the ground truth established by experts in a laborious manual process [5].

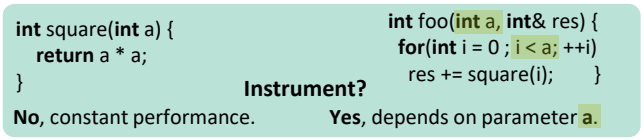
A2 *Parameter dependencies*



Taint analysis can find parameter dependencies, such as multiplicative dependencies between parameters influencing the iteration count in outer and inner loops, and additive dependencies between parameters influencing the iteration count of non-nested loops. For routines where parameter dependencies are detected as additive only, accurate performance models can be generated by creating single parameter models for each of the parameters involved. Should this be true for all routines in an applications, the experiment design as a whole can be simplified and its dimensionality reduced.

An interesting corner case of a multiplicative dependency is LULESH, where the taint-based modeling detects a single instance of the parameter `iters` in the main loop of the program. Through that we recover a multiplicative dependency with all other model parameters. The number of iterations therefore linearly affects the entire computation. We can reduce the dimensionality of sample space, since `iters` does not grant useful insights into application performance.

A3 *Instrumentation overhead*



In the default instrumentation mode, Score-P [4], a widely used measurement infrastructure and the default for Extra-P, estimates whether a function should be inlined and therefore excluded from instrumentation. This approach is inappropriate for empirical performance modeling because it might encourage the compiler to remove performance-critical functions through inlining, obscuring potential sources of bottlenecks and impeding effective performance analysis. Thus, without contextual information from the taint analysis, each function must be conservatively assumed to be influenced by changing parameter values, leading to instrumentation of all functions and significant runtime overhead.

Using the results of our analysis, we decrease the instrumentation overhead by instrumenting selectively, including only functions that are affected by a parameter change. In particular, we prune most of the simple constant functions, such as class getters and setters, which are irrelevant to scaling studies, without reducing the model quality for the remaining functions. We compare the overhead of Score-P with default, full, and our selective instrumentation.

The results for LULESH in Figure 3 clearly demonstrate how severe the overhead can become for C++ applications. Depending on the number of ranks and the problem size, removing constant and irrelevant functions *decreases the execution time by a factor of up to 45 times.* Although the overhead of the default Score-P instrumentation is manageable, the results may influence the models themselves. Our selective instrumentation contains 40 important application functions, while the default Score-P run instruments less than half of the performance-relevant functions but includes helper functions with constant runtime. For MILC, the geometric mean overheads are 1.6% for selective instrumentation and 23% for full and default instrumentation. We observe that selective instrumentation provides the most significant improvements in C++ applications, which are gaining popularity in the HPC community. The usage of object-oriented and metaprogramming abstractions has a negative effect on performance of instrumented runs.

Since the default Score-P instrumentation misses important functions, causing false-negative results, the modeling process can only use the selective or full instrumentation mode. Thus, we can compensate the cost of an additional step of tainted execution byt lower costs of instrumented executions. The core-hour costs of taint analysis are 1 and 16 hours for LULESH and MILC, respectively, while the costs of the experiment decreased from 20483 to 547 hours for LULESH (97.3%), and from 364 to 321 hours for MILC (13.4%), when switching from a *full* to *taint-based* instrumentation. The savings from reduced overhead significantly outweigh the costs of an additional analysis.

B *Quality*

We use tainting to mitigate the effects of measurement noise (Section **B1**), and the selective instrumentation discussed in Section **A3** to reduce the intrusion of instrumentation, improving the quality of the resulting models (Section **B2**).

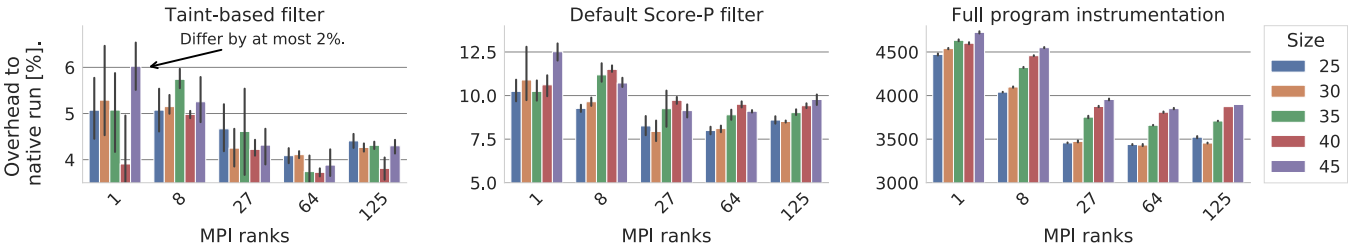


Figure 3. The Score-P instrumentation overhead of LULESH on the Skylake cluster. Plot scales are tuned to enhance visibility.

B1 *Noise resilience*

```
int foo(int a, int b, int& result) {
  for(int i = 0 ; i < a; ++i)
    result += b * i;                }
```

$0.5a + 10^{-3}b$

Seperate program from noise.

We apply the model obtained by the taint analysis to the model estimation in Extra-P, to prune models with false dependencies and evaluate the validity of experiments. We combine the five values of each parameter defined in Table 2 to construct a set of training data with 25 points, repeating each measurement five times to reduce the effects of random noise, resulting in 125 measurements, which we obtain by using up to 21 (LULESH) and 2 (MILC) Piz Daint nodes.

We compare the new models to black-box ones. We generally observe that models generated using taint analysis are closer to (nearly always exactly matching) the ground truth that we established with manual performance modeling techniques using code inspection [22]. We select for the comparison only those functions whose data sets do not contain values with a coefficient of variance larger than 0.1, as they are too affected by noise to be reliable.

We compare our findings for MILC with models created manually [5] as a ground truth. For the kernels manually studied, the taint analysis correctly identifies the dependencies on both `p` and `size` in accordance with the theoretical study. The empirical model also converges to the same model for each function. There are four `MPI_Comm_Rank` functions which we correctly detect as constant where measurement noise previously caused incorrect models to be generated.

B2 *Less intrusion*

```
int bar(int a) {
  instrument();
  return a * a;
}

int foo(int a, int& res) {
  instrument();
  for(int i = 0 ; i < a; ++i)
    res += bar(i);                }
```

$1.3a + 10^{-4}\sqrt{a}$

Separate program and instrumentation.

Empirical performance modeling relies on measurements. The instrumentation process introduces overhead, increasing the cost of the experiments, as discussed in the previous section. Yet, even more troubling is that the instrumentation perturbs the measurements, causing the resulting models

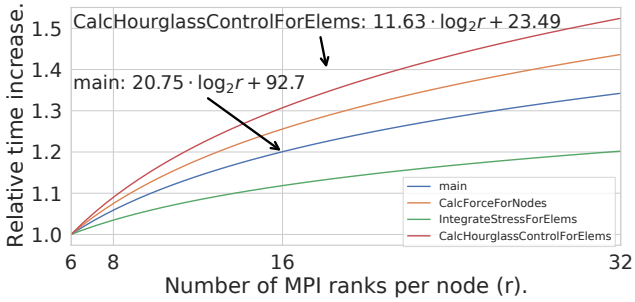


Figure 4. The one-parameter model of LULESH evaluating the effect of the number of MPI ranks `r` per node. Computational kernels experience slowdown because of hardware contention when many processes occupy the same socket.

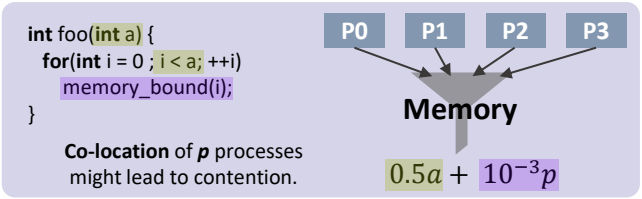
to change qualitatively. We compare models from the fully instrumented code with those from code where only the routines identified as performance relevant are instrumented. Beyond the observation that nearly all runtimes are almost two orders of magnitude bigger under full instrumentation, critical routines such as `CalcQForElems` show different models depending on the degree of instrumentation. The model derived from fully instrumented runs shows an additive dependency between p and $size$, $3 \cdot 10^{-3} \cdot p^{0.5} + 10^{-5} \cdot size^3$ while the filtered instrumentation shows a multiplicative dependency $2.4 \cdot 10^{-8} \cdot p^{0.25} \cdot size^3$. The second model is validated by previously determined models [10], providing a strong argument for using a targeted approach towards instrumentation rather than simply instrumenting full applications. The default Score-P filter does not instrument this function, leading to false-negative result in this case.

C *Validity*

The empirical approach we study always generates a performance model from a given input. We previously discussed in Section **B** how we can make sure that we generate the best possible model. There are situations, however, where the systemic influence of hardware or poor experiment design make the data unsuitable for understanding algorithmic performance. We identify such cases and provide guidance to identify the cause of the issue. We discuss two such examples: the effect of hardware contention in a multi-core

system (Section C1), and a qualitative change in the modeled function across the experiment (Section C2).

C1 *Detecting hardware contention*

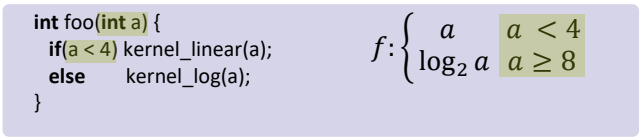


We evaluated the black-box and white-box modeling approaches with measurements of LULESH from Table 2. We observed a significant number of computational kernels, where the new model is worse at fitting the data even though it no longer contains false dependencies on p. Since the taint analysis proved that such functions cannot include such a dependency, yet it is visible in measurements, we conclude that that the resulting performance model must be affected by factors outside the application code itself. The taint-based modeling pipeline **detects** the presence of this perturbation while it was unknown to the black-box modeling approach.

We formulate the hypothesis that the co-location of MPI ranks on the same socket leads to hardware contention effects on functions with no dependence on MPI ranks in the source code. We test this hypothesis with a new experiment keeping the number of MPI ranks and problem size constant (p = 64 and size = 30) and varying the numbers or MPI ranks per node r, scaled from 2 to 18. By disabling multithreading, the larger number of cores available to each MPI rank should not affect the performance of compute kernels, and only communication routines might benefit from optimized MPI operations when processes are co-located. The expectation is that non-communication routines should have constant models. The entire application shows a significant increase in execution time, by 50%, from 130s to 195s, with the corresponding model $2.86 \cdot \log_2^2 \mathtt{rs} + 127$s. Out of 73 functions, 31 have an increasing model with statistically sound measurements. Figure 4 shows a few major examples.

Given the significant number of memory operations in the program, the saturation of memory bandwidth is the most likely culprit. Thanks to the inclusion of program information from taint analysis, we provide a type of insight that has not been available with purely black-box performance modeling. Modeling results that are independent of hardware effects and parallel allocations are possible for LULESH but only for certain levels of node saturation with MPI processes.

C2 *Validating the experiment design*



We evaluated the black-box and white-box modeling approaches with MILC test runs and noticed the largest difference between models of communication routines such as MPI_Isend and a MILC internal implementation of the gather collective operation.

Although the measurements are statistically valid, they fail to present a consistent behavior across the modeling domain. We notice a *qualitative*, not merely a quantitative difference between execution on 4, 8, 16 and larger numbers of ranks. As there is more than one behavior to be modeled in one interval, the parametric models estimated by Extra-P cannot represent the function accurately unless more measurement data is provided [25].

We have expanded our taint analysis to provide information regarding branches of code that are executed or not executed and therefore where application and/or library behavior can qualitatively change. This empowers the user to appropriately design his experiments to ensure there is only one behavior present in the data.

7 Conclusion

This work is the first to show that taint analysis, a method originally introduced to track the flow of sensitive information in computer programs, can be used to significantly advance the state of the art in empirical performance modeling for HPC applications. We showed various use-cases to improve cost, quality, and validity of the resulting models. Cost is reduced by lowering the number of necessary experiments as well as making individual experiments cheaper. Moreover, higher noise resilience and less instrumentation-induced intrusion render the models more accurate. Finally, with its ability to approximate the computational volume of program executions, taint analysis can help expose contention effects that prolong the runtime beyond what one would expect from considering computational volumes alone. Overall, our results show that for applications of realistic complexity empirical modeling must be carefully combined with static and compiler-assisted dynamic analyses to deliver high-quality and actionable performance models.

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A Artifact Appendix

A.1 Abstract

The artifact provides source code of our tool `perf-taint` and its major dependencies, tooling required to perform experiments described in Section 6, and data obtained on our systems to assist reproduction of results.

We provide detailed instructions in `README` and a set of shell scripts for conducting the experiments in the paper.

Besides, we include a "getting started" guide that demonstrates the application of our workflow to a dummy MPI application and section assisting with reusing our tool on another benchmarks and applications.

A.2 Artifact check-list (meta-information)

- **Algorithm:** taint-supported empirical performance modeling.
- **Program:** LULESH 2.0, MILC 7.8.1 (sources and LLVM IRs included).
- **Compilation:** GCC >= 5.1.0 to build included LLVM and Clang 10.0 from sources.
- **Transformations:** taint-based modeling implemented as an LLVM pass.
- **Binary:** source code and scripts to regenerate binaries, Docker containers for LLVM and Extra-P.
- **Run-time environment:** taint analysis runtime requires Linux x86. Using containers might require additional permissions.
- **Hardware:** a 16-core machine to run our analysis, a cluster of up to 729 cores is required to reproduce all results.
- **Run-time state:** modeling uses measurements from instrumented runs that can be affected by network contention and multi-tenant environments.
- **Output:** each experiment returns results independently. Results include text files with statistics, JSON models and matplotlib plots.
- **Experiments:** we provided shell scripts to prepare experiments, execute them locally or submit SLURM jobs and process results. Jupyter notebooks are provided for two experiments.
- **How much disk space required (approximately)?:** ca. 10-15 GB.
- **How much time is needed to complete experiments (approximately)?:** each experiment reports required compute time seperately.
- **Publicly available?:** Yes.

A.3 Description

A.3.1 How delivered

Our source code, software dependencies, benchmarks and scripts archived on Zenodo: `10.5281/zenodo.4381803`. The uncompressed artifact requires ca. 9 GB of disk space. The data provided with the artifact has been obtained on the following systems:

- Piz Daint: 36-core nodes with two Intel Xeon E5-2695 v4 2.10GHz, 128 GB memory. Local cluster: 36-core Intel Xeon 6154 3GHz, 384 GB memory
- Piz Daint: SUSE Linux Enterprise Server 15, kernel 4.12.14. Local cluster: CentOS Linux 7 kernel 3.10.0
- Compilers and versions: Taint analysis: Clang 10.0 development version, Piz Daint: GCC 8.3.0; Local cluster: GCC 8.3.0
- Applications and versions: Extra-P 3.0, Score-P 6.0, LLVM 10.0, libc++ 9.0.
- Libraries and versions: Cray MPICH 7.7.2, OpenMPI 4.0.3

A.3.2 Hardware dependencies

Cluster environment with MPI and SLURM scheduler should be sufficient. Each experiment has its own requirements regarding the number of CPU cores needed.

A.3.3 Software dependencies

There are three major software packages required to perform performance modeling, instrumented executions and tainted parameter modeling: Extra-P with Cube, Score-P, and perf-taint with LLVM, respectively. Each one requires Linux OS, and LLVM sanitizers used by perf-taint are known to work only on x86 systems. We provide three Docker images: `perf-taint` with our tool and LLVM framework, and `extrap` and `extrap3` with an Extra-P installation. In addition, we provide scripts performing automatic build of our code with major dependencies when Docker containers cannot be used.

A.4 Installation

Using Docker After downloading the artifact, please load archived Docker images from `docker` directory. Then, install Score-P using provided scripts in `sources` directory and initialize environmental variables:

```
source /path-to-artifact/scripts/initialize_env.sh
```

`README` describes which Docker images to use for different stages of experiments. To use Docker for experiments requiring perf-taint (image: `cfsan`) or Extra-P (image: `extrap` and `extrap3`), mount the artifact directory in the container:

```
docker run -it -v /path-artifact/:/home/docker/
    ↪ artifact perf-taint/perf-taint:IMAGE /bin/
    ↪ bash
```

Local Installation Docker images are the recommended way of reproducing results. When using Docker is not an option, our toolchain and its dependencies must be installed locally. After downloading the artifact, please install software dependencies using provided scripts in `sources` directory.

Before using the artifact, please initialize environmental variables that are necessary for scripts to work properly:

```
source /path-to-artifact/scripts/initialize_env.sh
```

For details, please check the corresponding sections in `README`.

A.5 Experiment workflow

The artifact consists of multiple experiments that correspond to various results obtained in Section 6 of the paper. For each one, we provide a suite of scripts and list of requirements to reproduce the result, placed in `modeling_results` directory. In the `README`,

we discuss in detail cluster hardware needed and compute time required to reproduce each experiment.

With the artifact, we provide the necessary data from the paper to repeat the analysis because the reproduction of Score-P runs requires an excessive number of corehours and large resources (up to 729 cores). Furthermore, we supply results to make each experiment independent of the other. Thus, one does not have to execute all steps sequentially. For example, if you execute A1, it will generate filters required by Score-P for A3 part. But if you skip A1, A3 is going to use filters provided with the artifact.

We evaluated our tool, `perf-taint`, on benchmarks LULESH and MILC. For each one of them, we generate LLVM IR with annotation for two parameters (B1, B2, A3) and with annotation of all major parameters (A1). We provide the original sources, patches implementing the manual parameter annotation and compiled IR bitcodes with LLVM 9.0. To regenerate the IR, please run the provided script:

```
cd modeling_results/{lulesh,milc}/sources
./generate_bitcodes.sh
```

Each experiment consists of three phases. For each one, we provide shell scripts to be executed consecutively.

Preparation This includes compilation of LLVM IRs and binaries, and copying necessary input files from previous experiments and data provided with the artifact.

Execution Results can be obtained locally or through a job submission to SLURM. Please adjust the provided SLURM jobscripts to ensure that they run correctly on your cluster.

Processing The final step includes generation of performance models and processing of time measurements.

A.6 Evaluation and expected result

Results of *A1* experiment provide the statistics presented in Table 2 and Table 3. Figures 3 and 4 are reproduced with experiments *A3* and *C1*, respectively, and the Jupyter notebooks supplied with them.

Results of experiments *A2*, *B1* and *B2* are reproduced as text files containing performance models discussed in the corresponding sections. Results from experiments *A2* and *C2* are not contained in the artifact, since they are based on a manual analysis of performance models obtained in other sections.

When reproducing instrumented runs with `Score-P`, the time measurements are going to change, affecting the performance models created by `Extra-P`. The models of MPI collectives will change when different MPI implementations are used. On the other hand, parametric dependencies of models should not change.

A.7 Experiment customization

Whenever possible, we discuss in the `README` how to modify the workflow to reduce the amount of work to verify only a fraction of data.

Our framework supports the analysis of MPI programs in C/C++. We don't provide a generic processing script, since the entire framework includes manual steps that are application-specific and cannot be automatized. If you would like to apply our toolchain to a new project, please follow the *Getting Started* guide of the `README` and perform the steps outlined below:

- Annotate program parameters that `perf-taint` should analyze by adding a call to `register_variable` immediately after variable definition and initialization.
- Compile the application to LLVM IR by using `clang` wrappers provided with our tool, obtaining a set of IRs for the project.
- `perf-taint` can be used exactly the same way as in the *Getting Started* guide. This step already provides the most important results: performance relevant functions, the impact of parameters on loops and functions, and files necessary for efficient instrumentation and modeling.
- Experiment design is always a manual process. We recommend the Extra-P publications as a good source of experiment design practices. Taking five samples per each parameter and five repetitions per sample is considered to be sufficient.
- Score-P instrumentation, instrumented runs and modeling steps work the same as in our experiments.

For details, please refer to *Reusability* section of the `README`.

A.8 Notes

While we aim to help users by automatizing the installation, it's not feasible to prevent all compatibility issues in cluster environments. `perf-taint` should always be built with the supplied `clang` compiler with support for taint analysis. To control which GCC installation is selected by `clang`, one should use the following `CMake` configuration flag for `perf-taint`:

```
-DPASS_COMPILER_FLAGS="--gcc-toolchain=${
    ↪ gcc_toolchain_location}"
```