Performance-Detective: Automatic Deduction of Cheap and Accurate Performance Models

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ABSTRACT
The many configuration options of modern applications make it difficult for users to select a performance-optimal configuration. Performance models help users in understanding system performance and choosing a fast configuration. Existing performance modeling approaches for applications and configurable systems either require a full-factorial experiment design or a sampling design based on heuristics. This results in high costs for achieving accurate models. Furthermore, they require repeated execution of experiments to account for measurement noise. We propose Performance-Detective, a novel code analysis tool that deduces insights on the interactions of program parameters. We use the insights to derive the smallest necessary experiment design and avoiding repetitions of measurements when possible, significantly lowering the cost of performance modeling. We evaluate Performance-Detective using two case studies where we reduce the number of measurements from up to 3125 to only 25, decreasing cost to only 2.9% of the previously needed core hours, while maintaining accuracy of the resulting model with 91.5% compared to 93.8% using all 3125 measurements.

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1 INTRODUCTION
The costs of operating high-performance systems are millions of euros per year [8, 10]. While computing centers do their best to design and run clusters economically, developers must ensure that their applications scale efficiently on computing clusters. Modern software systems are configurable and allow users to set many parameters according to their needs. For example, in the Pace3D material simulation [21], users select algorithm settings and properties to simulate, impacting performance metrics such as response time and throughput [40, 50]. Choosing a set of parameters that yields the best performance is challenging. Developers and users often do not know how configuration options interact or how a single configuration option influences performance [19, 39]. An example of such a challenge is understanding application
white-box modeling methodology that significantly lowers white-box approaches. The former suffers from high sampling optimizations that used imprecise heuristics, we use program information to deduce an optimized, minimal experiment design, removing measurement points that do not affect known interactions between non-functional parameters. We use parametric performance models obtained from the taint-based analysis [13] to understand the impact of parameters on program functions. Through a step-by-step analysis of parameter interactions, we derive conclusions on parameter interactions in the program’s control flow. Applying the deduced conclusions to the experiment design removes measuring points unnecessary to model parameter interactions. Thus, Performance-Detective can reduce the dimensionality of experiments from exponential to polynomial while avoiding the risk of excluding parameter dependencies from the experiment. The experiment design of Performance-Detective is orthogonal to the modeling approach and can be used with black-box and white-box performance modeling.

The deduced experiment design makes performance modeling more affordable and is easily applicable alongside modern performance modeling systems. To quantify the increased efficiency and validate model correctness, we empirically evaluate Performance-Detective using a multi-physics solver (see Figure 1) and a particle transport application. Performance-Detective maintains accuracy of 91.4% while reducing the costs of measurements by a factor of up to 34 times, compared against both the Extra-P empirical performance modeling tool [12, 36] and Performance-Influence Models [39].

Contributions:

- **Performance-Detective**, a white-box measurement methodology using a novel deductive analysis that uses the results of performance tainting to derive an optimized minimal subset of required measurements out of a multi-dimensional configuration space.
- An extensive evaluation against state-of-the-art modeling workflows, proving high accuracy and reduced experiment size.
- We identify main loops within applications using our deductive analysis, and leverage this to reduce the cost of experiments even further, in essence applying classical analytical performance modeling techniques to modern automatic modeling approaches.
- Two case studies of modeling and evaluating applications extrapolated and interpolated test points.

2 FOUNDATIONS

The deduction process of Performance-Detective is based on a program’s parametric profile obtained with taint-based performance modeling provided by Perf-Taint (Sec. 2.1). Performance-Detective overcomes the limitations of existing performance modeling tools (Sec. 2.2), enabling efficient and reliable white-box modeling.

2.1 Perf-Taint

Perf-Taint [13, 14] is a hybrid modeling tool that enhances the black-box and analytical modeling tools with program
information. Perf-Taint applies a sequence of static and dynamic analyses to the program to understand how its computational effort is affected by a change in input parameters. The result of the operation is a parametric profile of a program, consisting of a list of performance-relevant functions and parameters whose values can change the performance. Perf-Taint is built on top of LLVM [29] and supports distributed parallel applications implemented in C/C++ with MPI. Internally, the tool uses static LLVM loop analysis [16] and DFSan [15], a dataflow taint analysis library extended with support for control-flow tainting [49].

We present Perf-Taint on an example program with two functions in Figure 2. The function important is performance-relevant because its complexity changes with parameter x. Thus, both the parameter and the function are included in the performance profile on the right side. On the other hand, the function unimportant involves only a constant amount of computation. This information obtained from program analysis improves the overall modeling workflow by restricting the modeling to performance-relevant program elements. In practice, many short-running functions are particularly affected by noise and could otherwise generate false models that would make the modeling process more difficult and error-prone. These can be automatically excluded from the modeling process if Perf-Taint identified them as constant.

### 2.2 Limitations of modeling frameworks

The state-of-the-art modeling approaches do not allow for efficient modeling of computing applications with many parameters and numerical options.

Performance-Influence Models (PIMs) [48] derive performance models on the function level, but they do not use parameter dependencies and require expensive tracing instead of profiling. White-Box PIMs [45, 46] do not support numerical options. Though numerical options can be encoded and discretized [46], the approach does not use a learning method and, therefore, cannot predict inter- or extrapolating training configurations.

Extra-P [12] relies on the full-factorial experiment design where all parameter combinations must be considered, leading to a combinatorial explosion of the number of measurements. Heuristics have been proposed to optimize the experiment design [36], but they introduce a risk of missing parameter interactions and negatively affecting model quality. Furthermore, the impact of the noise present in measurements makes modeling with more than three parameters particularly challenging.

Perf-Taint [13] does not propose a deterministic and effective methodology for user analysis of the experiment design. While Perf-Taint detects no function depending on both x1 and x2 in the example in the listing below, it does not use parameter knowledge to reduce the sampling set.

```c
void f(int x) {
    for (int i = 0; i < iters; i++) {
        f(x1); g(x2);
    }
}
void g(int x) {
    for (int i : irange(0, x))
        calculate();
}
```

In the next code example, all functions are called in the main loop. If the main loop is executed often enough, repetitions of experiments are not necessary as the repetition of the calculations already accounts for measurement noise.

```c
for (int i = 0; i < iters; i++) {
    f(x1); g(x2);
}
```

However, Perf-Taint does not make use of this to suggest fewer experiments. Even though 25 and 5 measurements are sufficient to model the performance in these examples, Extra-P and Perf-Taint still require and suggest 125 measurements in both cases. Even though heuristics for sampling can lower experiment size, they do so at the cost of reducing model accuracy. While more samples can increase the accuracy, there is no strategy for selecting them, leading to a full-factorial experiment design.

### 3 APPROACH

Figure 3 depicts the overall workflow of performance modeling that we will detail in the following subsections. We start by analyzing the system to trace the influence of configuration options on single functions (Section 3.1). Performance-Detective then uses the insights about which parameter influences the performance of which function to deduce a minimal experiment design that exploits insights about the interplay of options (Section 3.2). After executing the experiments (Section 3.3), the performance of single functions can be modeled using any learning methodology. Finally, we derive a whole system model by summing up single models.

We assume that the system’s performance varies in functions that contain non-constant loops, i.e., a configuration option determines how often they are executed and how many iterations they include. First, we distinguish between functional and non-functional configuration options: while the functional options define the problem to be solved, non-functional options are free to vary. Then, we distinguish between configuration options that affect performance and those that do not.
modeling, we ignore options that affect neither the result nor the performance of a program. However, the exact distinction between functional and non-functional options is subjective and domain-specific [46].

We will use the example program in Figure 4 as a running example. It takes the three parameters x1, x2, and iters as configuration options and does calculations based on them.

### 3.1 System analysis

In the first step, we analyze the system to find out how configuration options influence its performance. We do this using the Perf-Taint approach introduced in Section 2.1. The analysis of Perf-Taint outputs parameter dependencies for each performance-relevant function: a function always depends on variables that determine the loop iteration count in the function.

**Example.** Figure 4 shows functions’ dependencies in the colored boxes. Function preCalculate is not influenced by the configuration options and is identified as constant. foo is dependent on x1, bar and baz iterate over the parameter z and depend on x2. We observe that iters has a multiplicative influence on the runtime of all functions and deduce that it linearly affects all computations. We do not consider foo to depend on x2 because we exclusively measure time spent in functions (cf. Section 3.3).

### 3.2 Experiment design

Based on the derived dependencies from the system analysis, Performance-Detective deduces the minimal experiment design. From a black-box view of the system in Figure 4, Performance-Detective starts with a full-factorial experiment design of the three parameters x1, x2, and iters. Since Performance-Detective detects that iters influences the runtime of foo, bar, and baz linearly, measuring variations of iters will not provide us additional insights into the system’s performance. Therefore, Performance-Detective can exclude this parameter from the experiment design. While the linear influence is easy to see in the example, this may not be the case for more complex real-world programs. To verify that the influence of the iters parameter is linear in such a case, we can measure execution times of loop iterations. If the runtime does not change significantly between them, i.e., the coefficient of variation is sufficiently small between iterations, we verify that the influence of the iters parameter is indeed linear.

Furthermore, we observe that x1 and x2 influence the performance of distinct functions and do not interact with each
other. Therefore, additional samples measuring their interactions will not provide further insights, and Performance-Detective can exclude them from the experiment design. In general, we assume that if options influence different sets of functions, they do not interact with each other, and Performance-Detective can vary them simultaneously. Also, we do not consider options linearly influencing system runtime, such as the number of main loop iterations.

Extra-P requires a full-factorial measurement setup [9] (Section 2.2). Even the sparse modeling approach with heuristics [36] requires at least five measurements per parameter to capture interactions between parameters. In contrast, Performance-Detective can detect the lack of interaction and strike out measurement configurations where only one parameter is changed, and the others are kept constant. This improvement reduces the dimensionality of the experiment compared to a full-factorial setup and provides further savings when compared to sparse modeling.

In the example above, Performance-Detective deterministically reduces the number of measurements from 125 in a full-factorial experiment design to only five measurement points without sacrificing accuracy.

3.3 Profiling

We use an instrumentation-based approach to capture the total time spent in a function during one execution of the program, summarizing time across all invocations. We measure time spent in a function exclusively, i.e., not including time spent in calls to other instrumented functions. We instrument functions identified as performance-relevant by Perf-Taint, i.e., containing loops dependent on configuration options and the main function. Previous works suggested repeating each sample five times to account for measurement noise. However, when Performance-Detective identifies a linear dependency of parameter on the main calculation, we can skip the repeated measurements and even halt execution after gathering at least five iterations of the main calculation loop. While this approach is common in analytical modeling, it has been outside the reach of automated modeling due to the difficulty of identifying configuration parameters that control the number of executions of the main loop.

Example. In Figure 4, Performance-Detective disregards the constant function preCalculate for instrumentation. We instrument foo, bar, and baz, as they depend on annotated input parameters, and main to capture the total runtime of the application. In exclusive measurement, the time obtained for foo does not include the time spent in bar. However, the time of baz includes the time spent in preCalculate.

3.4 Limitations

If all parameters are intertwined, no pruning of parameter combinations to measure is possible. Also, we do not regard binary options as switching between them results in performance jumps. We assume that performance-relevant behavior is located in computational loops and MPI communication routines. Modeling of recursion is not supported, but recursive computations are rare in HPC [13].

4 MODELING WORKFLOWS

Performance-Detective is orthogonal to the instrumentation and learning methodology, and it can reduce the costs of experiments in different performance modeling toolchains. We consider two state-of-the-art modeling workflows: the black-box, empirical Extra-P performance modeling tool (Sec. 4.1) and the white-box Performance-Influence Models (Sec. 4.2).

4.1 Extra-P

Extra-P [12] is a performance modeling tool that expresses the effect of configuration parameters $x_i, i \in \{1, \ldots, m\}$ on a performance metric $f(x_1, \ldots, x_m)$. The result, such as $t(n, p) = 10 \cdot n \cdot \log(p)$, is a familiar, human-readable function.

In practice, the configuration parameters most often analyzed are problem size and process count, and the metric of interest is usually the runtime. This allows developers to identify performance bottlenecks in their applications, especially when using it in conjunction with tools such as Score-P [26] that allows automatic instrumentation and measurement at the granularity of individual function calls.

The core assumption of the methods is that the complexity of most algorithms can be expressed using a small number of building blocks, summarized in Equation 1. The Performance Model Normal Form (PMNF) models a metric as a combination of polynomial and logarithmic expressions of configuration parameters. This limits the possible search space sufficiently to allow for a fast traversal while still being sufficiently flexible to cover the overwhelming majority of applications.

$$f(x_1, \ldots, x_m) = \sum_{k=1}^{n} c_k \cdot \prod_{i=1}^{m} x_i^{j \cdot k_i} \cdot \log^{i \cdot k_i}(x_i) \quad (1)$$

An issue not addressed in the state-of-the-art approaches is modeling more than three parameters. In practice, noise makes detecting parameters with a smaller impact on metrics of interest effectively impossible for even four parameters.

4.2 Performance-Influence Models

Performance-Influence Models (PIMs) [39] describe how configuration options and their interactions influence the performance of a system. They support a theoretically unlimited number of binary and numerical parameters. PIMs can be created using different sampling and learning techniques.
The models are learned in a black-box manner by providing the configurations used and measured total system runtime as inputs. Due to a high number of supported techniques, it is unclear which combination of methods will provide the best accuracy. However, there are works [17, 24] investigating the interplay of sampling and learning techniques and the influence of the sample size on model accuracy.

To further overcome these trade-offs between measurement effort and accuracy, Velez et al. [45, 46] proposed White-Box Performance-Influence Modeling for binary and binary-encoded configuration options. They analyze the options’ influence on the system’s execution and help find an optimal sample set. However, numerical options such as the problem size are not supported since continuous parameters would be tedious to encode. Weber et al. [48] present a two-step white-box process for creating PIMs on the function level. First, they use samples of the application execution to learn a PIM for every function. Then, they use tracing to derive more accurate models for functions that could not be learned with a specified accuracy. They use the extended Plackett-Burmann design [47] for sampling the numerical options and decision trees for learning models.

5 CASE STUDIES

We illustrate the deduction process of Performance-Detective presented in Section 3 with two case studies: Kripke, a 3D Sn particle-transport proxy application, and a real-world case study from Pace3D (Parallel Algorithms for Crystal Evolution) [21], a multi-physics framework that simulates how a material reacts to outside influences. For both case studies, we only consider the execution of the main calculation loops as this is where most of the work happens.

Pace3D: Pressure calculation with projected conjugate gradient method. The calculation consists of two steps: First, an approximate solution is calculated on a coarse grid. This approximate solution is then used to calculate the real solution on the fine grid. The grids represent the material, with each cell corresponding to one cube of the material. The solver iterates until it reaches a convergence criterion or a given maximum number of iterations. We consider the number of processes and the number of coarse grid cubes as non-functional parameters. We also use the size of the material to predict how much material each process should get to achieve the best performance. Additionally, we consider the maximum number of iterations.

Kripke. Angular fluxes are calculated using different numbers of directions and groups. Kripke was built to research how different data layouts, programming paradigms, and architectures influence performance [1]. We consider the number of direction sets as well as the number of processes as inputs. Due to a high number of supported techniques, it is unclear which combination of methods will provide the best accuracy. However, there are works [17, 24] investigating the interplay of sampling and learning techniques and the influence of the sample size on model accuracy.

To further overcome these trade-offs between measurement effort and accuracy, Velez et al. [45, 46] proposed White-Box Performance-Influence Modeling for binary and binary-encoded configuration options. They analyze the options’ influence on the system’s execution and help find an optimal sample set. However, numerical options such as the problem size are not supported since continuous parameters would be tedious to encode. Weber et al. [48] present a two-step white-box process for creating PIMs on the function level. First, they use samples of the application execution to learn a PIM for every function. Then, they use tracing to derive more accurate models for functions that could not be learned with a specified accuracy. They use the extended Plackett-Burmann design [47] for sampling the numerical options and decision trees for learning models.

5.1 System analysis

We analyze the scenarios with Perf-Taint [13]. The only necessary modifications to the source code are annotating and registering the variables corresponding to the parameters of interest. We run the analysis on a small problem size using only a few iterations, assuming that the computations and analysis results are representative, and validate the results with larger measurements in Section 6.2.

5.1.1 Pace3D. We annotate variables in the code corresponding to the number of processes (procs), material size (vol), coarse grid size (cubes), and spacing of the coarse grid (spacing). Additionally, we annotate the number of iterations for the fine as well as for the coarse grid. This results in a total of 21 lines of code added.

The coarse grid spacing is a dependent parameter (not linearly independent) and is calculated by dividing the material size by the coarse grid size (spacing = vol/cubes). Hence, we can replace the spacing by vol/cubes, substituting it by the independent parameters it is defined by. Listing 1 shows an example where we can conclude that the material size determines the performance of the loops.

From the results, Performance-Detective identifies that the maximum number of iterations on the fine grid determines the runtime of the main calculation. To verify that the influence is linear, we trace the iterations of the loop for one execution of the program and check whether the runtime of a single loop iteration changes. To do so, Performance-Detective calculates the coefficient of variation between them. In our

for (int i = 0; i < cubes; i++) {
    // spacing = vol / cubes
    for (int j = 0; j < spacing; j++) {
        // complexity = cubes · spacing
        // complexity = cubes · (vol / cubes)
    }
}

Listing 1: Program iterating over the spacing

(a) Pace3D
(b) Kripke

Figure 5: Number of functions depending on the annotated parameters per case study as Venn diagrams.
scenario, the coefficient of variation is 0.05 for 100 loop iterations. We conclude that the influence of iters is indeed linear.

Furthermore, the analysis results show that 12 functions are constant, and 54 are dependent on the annotated parameters. For the 2 functions dependent on the spacing, we can automatically assess that they in fact depend on the total volume, using replacement as shown in the example in Listing 1. The results, as shown in Figure 5a, show that the material size and the coarse grid size influence different functions.

5.1.2 Kripke. To annotate the number of processes (procs) as well as the number of direction sets (dirsets) and iterations (iters), we add a total of five lines of code. Using the analysis results, Performance-Detective analyzes that the number of iterations determines the runtime of the main calculation. As before, to verify that the influence is linear, we trace the loop iterations of one program execution. As the coefficient of variation between the measured 10 iterations is 0.0067, we conclude that the influence of iters is linear. Moreover, the analysis shows (cf. Figure 5b) that 19 functions are constant and 35 are dependent on procs, with 33 depending on dirsets and 2 on procs. The number of processes influences different functions than the number of direction sets.

5.2 Minimal Experiment Design

Figure 6 shows the process of Performance-Detective deducing the experiment design for Pace3D based on the insights gained from analyzing the system. From a black-box view at the system, Performance-Detective starts with four parameters and a full-factorial experiment design, leading to 625 measurement points. To account for measurement noise, each point has to be executed five times, leading to a total of 3125 experiment executions.

As we know that iters linearly influences the runtime of the main computation, Performance-Detective can exclude iters from the parameter space (Insight 1). Also, we can skip repetitions of the execution of measurement points and choose a sufficiently high value (≥ 5) for iters instead. This reduces the experiment design to 125 points that need to be executed only once. We also know that the functions affected by the coarse grid size are distinct from those affected by the total size. Thus, Performance-Detective can strike out configurations aiming to find interactions between them from the experiment design (Insight 2). This means that Performance-Detective varies vol and cubes simultaneously and only the number of processes independently of them. As procs interacts with vol and cubes according to the analysis, Performance-Detective includes procs as interacting parameter into the experiment design. Figure 7 (Sec. 6.2) shows the resulting training data points for Pace3D as crossed circles.

For Kripke, Performance-Detective deduces the experiment design similarly: As iters has a linear influence on the runtime of the main computation, it can exclude it from the parameter space (Insight 1) and we can skip repetitions of experiments. Furthermore, Performance-Detective can remove configurations aimed at finding interactions between procs and dirsets as they influence distinct sets of functions (Insight 2). Thus, Performance-Detective varies procs independently of dirsets, resulting in 5 measuring points with (procs, dirsets) = (8, 8), (16, 16), (32, 24), (64, 32), (128, 64).

Performance-Detective reduced the full experiment design space of 3125 experiment executions to only 25 executions needed for Pace3D, and from 625 to 5 for Kripke.

6 EVALUATION

To evaluate Performance-Detective, we assess the accuracy of the performance models generated for the case studies presented in Section 5. We evaluate the reduction of repetitions by inclusion of iterations and variation of independent parameters individually. Therefore, we formulate the following research questions:

RQ1 What is the model accuracy when generating it from a single measurement with a high number of iterations? RQ2 What is the model accuracy when generating it from a minimal experiment design by varying independent parameters simultaneously?

To answer the RQs, we compare our models with models generated following conventional experiment and sampling designs. The expected outcome of the evaluation is maintained accuracy while reducing the dimensionality of experiment design and not repeating experiment executions, resulting in significantly decreased cost for measurements.

6.1 Instrumented Experiments

Table 1 shows the hardware and software systems used for measuring. We instrument the application using the list of important functions generated by Perf-Taint and repeat the measurement of each configuration five times to assess RQ1 and RQ2 separately. The coefficient of variation between
CPU	Intel Xeon Gold 6230 2.1GHz
Cores	40 on 2 sockets
Memory	96 GB
MPI	OpenMPI 4.0.5 (Pace3D), OpenMPI 4.1.2 (Kripke)
Software	Score-P 7.0 [26] (Pace3D), Score-P 7.1 (Kripke), Perf-Taint, Extra-P

Table 1: Measurement environment

<table>
<thead>
<tr>
<th>Modeling approach</th>
<th>#executions</th>
<th>Mean error Pace3D</th>
<th>Mean error Kripke</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>interpolate</td>
<td>extrapolate</td>
</tr>
<tr>
<td>Extra-P</td>
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<td>8.31 %</td>
<td>9.31 %</td>
</tr>
<tr>
<td>Extra-P</td>
<td>1</td>
<td>8.05 %</td>
<td>8.74 %</td>
</tr>
<tr>
<td>Decision Trees</td>
<td>5</td>
<td>21.61 %</td>
<td>60.15 %</td>
</tr>
<tr>
<td>Decision Trees</td>
<td>1</td>
<td>22.62 %</td>
<td>62.80 %</td>
</tr>
</tbody>
</table>

Table 2: Mean error of models generated from Performance-Detective experiment design using a single application execution vs five repetitions

![Figure 7: Overview of training and test points on logarithmic scales. Training data Performance-Detective: ⊗, training data full-factorial: ○ and ⊖, Test data interpolated: ▲, test data extrapolated: ●.](image)

The results in Table 2 show that the accuracy remains about the same when using only one execution as for the models generated from the mean times of five repetitions. This suggests that it is sufficient to execute the measurement of each configuration point only once if the main calculation is executed sufficiently often. For Pace3D, we set the number of iterations of the main calculation to 100, and to 10 for Kripke. However, even five iterations per application run should be enough compared to one iteration per repetition of the experiment. While the total time measured in the main calculation stays the same for both variants, we can save the initialization overhead by executing it more often in only one execution.

6.2 RQ1: Modeling using a single measurement

To evaluate whether the inclusion of iterations in the model can simplify the experiment design, saving us repetitions of the measurements, we generate a model from a single execution of each measurement and compare the predictions of this model with test points. For evaluating the accuracy, we use the mean time of the five repeated executions of each test measurement point. To obtain a prediction of the total execution time, we sum up the predictions for the single functions and evaluate them against the execution time of the evaluation configurations.

We use two testing sets, containing either inter- or extrapolated measurement points. Figure 7 shows an overview of the test data sets used for Pace3D. For the interpolated test data of both case studies, we measure configurations in between the training data points. For Pace3D, we do not interpolate the number of processes as this would not provide insight into the quality of the minimal experiment design. We still treat the number of processes as a separate parameter and vary it separately from vol and cubes, as it interacts with both according to the analysis. For the respective independent parameters, we use points between each value used for training, as shown in Figure 7. This results in 80 measuring points for Pace3D and 16 for Kripke with the interpolated values \( \text{procs} = (12, 24, 48, 96) \) and \( \text{dirsets} = (12, 20, 28, 48) \).

For testing how well the model predicts extrapolated configuration points, we extrapolate parameters identified as independent and measure them together with the respective other parameter using a value used for the training set. This means that we measure the extrapolated values 54,000 and 108,000 for \( \text{cubes} \) together with the extrapolated values 3,456,000 and 5,184,000 for \( \text{vol} \) as well as with all the values for \( \text{vol} \) used for the training set, shown in Figure 7, for Pace3D. Following this approach results in 119 measuring points for the extrapolated test data set of Pace3D and 24 for Kripke, for which we extrapolate \( \text{procs} \) to 256 and 512 and \( \text{dirsets} \) to 96 and 128.

The results in Table 2 show that the accuracy remains about the same when using only one execution as for the models generated from the mean times of five repetitions. This suggests that it is sufficient to execute the measurement of each configuration point only once if the main calculation is executed sufficiently often. For Pace3D, we set the number of iterations of the main calculation to 100, and to 10 for Kripke. However, even five iterations per application run should be enough compared to one iteration per repetition of the experiment. While the total time measured in the main calculation stays the same for both variants, we can save the initialization overhead by executing it more often in only one execution.
To learn PIMs, we use the extended Plackett-Burman Design, resulting in 16 points for Pace3D and 10 for Kripke. For the Extra-P multi-parameter modeler [9], this means using a full-factorial setup with 125 measuring points for Pace3D and 25 for Kripke. For the Extra-P sparse modeler [36], we use 5 values for each parameter while keeping the others constant and one interaction point for each parameter combination, resulting in 16 points for Pace3D and 10 for Kripke. To learn PIMs, we use the extended Plackett-Burman Design [47] with 49 samples (Pace3D) or 10 samples (Kripke) and five levels, effectively being a subset of the full-factorial measuring points. We use the script of Weber et al. [48] to learn PIMs on a function level based on known parameter dependencies. However, we do not use their two-step process but only one profiling step using compiler instrumentation. In contrast to them, we use mean values derived from the repetitions of the experiment for modeling. They build a separate model for each repetition of the experiment.

As we showed in Section 6.2 that the accuracy of the models generated from a single application execution per measurement point is comparable to the accuracy of the model generated from repeating measurements five times for each point, we will continue with these models for Performance-Detective.

Table 3 shows the required number of measurements of each approach and the cost in total core hours. The cost of individual samples are not uniform across the configuration space, as the impact the parameters have on performance can mean some samples are orders of magnitude more expensive than others. We therefore consider the total core hours to be the more important metric. To evaluate the predictions’

### Table 3: Mean error of different models for interpolated and extrapolated test points.

<table>
<thead>
<tr>
<th>Experiment Design</th>
<th>Modeling approach</th>
<th>Perf-Taint?</th>
<th>Cost Pace3D</th>
<th>Mean error Pace3D</th>
<th>Cost Kripke</th>
<th>Mean error Kripke</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>core hours</td>
<td>#experiments</td>
<td>test set interpolated</td>
<td>test set extrapolated</td>
<td>core hours</td>
</tr>
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<td>25</td>
<td>8.05%</td>
<td>8.74%</td>
<td>5.3</td>
</tr>
<tr>
<td>Full-factorial Extra-P</td>
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<td>367.55</td>
<td>625</td>
<td>9.5%</td>
<td>10.7%</td>
<td>85.9</td>
</tr>
<tr>
<td>Full-factorial Extra-P</td>
<td>✓</td>
<td>367.55</td>
<td>625</td>
<td>6.2%</td>
<td>6.5%</td>
<td>85.9</td>
</tr>
<tr>
<td>Sparse Extra-P</td>
<td>✓</td>
<td>5.54</td>
<td>80</td>
<td>8.9%</td>
<td>17.7%</td>
<td>8.8</td>
</tr>
<tr>
<td>Sparse Extra-P</td>
<td>✓</td>
<td>5.54</td>
<td>80</td>
<td>15.0%</td>
<td>31.8%</td>
<td>8.8</td>
</tr>
<tr>
<td>Performance-Detective Decision Trees</td>
<td>✓</td>
<td>10.9</td>
<td>25</td>
<td>22.6%</td>
<td>47.7%</td>
<td>5.31</td>
</tr>
<tr>
<td>Plackett-Burman Decision Trees</td>
<td>✓</td>
<td>164.37</td>
<td>245</td>
<td>20.1%</td>
<td>45.4%</td>
<td>35.66</td>
</tr>
<tr>
<td>Plackett-Burman Decision Trees</td>
<td>✓</td>
<td>164.37</td>
<td>245</td>
<td>27.0%</td>
<td>44.2%</td>
<td>35.66</td>
</tr>
</tbody>
</table>

### Figure 8: Accuracy of different models for evaluation testing points.

(a) Accuracy of models for the Pace3D case study for excerpts of the interpolated and extrapolated data set with 64 processes.

(b) Accuracy of models for the Kripke case study for excerpts of the interpolated and extrapolated data set.

#### 6.3 RQ2: Varying independent parameters simultaneously

The central question in our evaluation is whether we can maintain accuracy of the model when generating it from a minimal experiment design. To answer this, we compare the accuracy of our Performance-Detective model to models created with conventional experiment or sampling designs. For the Extra-P multi-parameter modeler [9], this means using a full-factorial setup with 125 measuring points for Pace3D and 25 for Kripke. For the Extra-P sparse modeler [36], we use 5 values for each parameter while keeping the others constant and one interaction point for each parameter combination, resulting in 16 points for Pace3D and 10 for Kripke.
accuracy, we use the same test configurations as in Section 6.2, inter- and extrapolating the training data points. Table 3 depicts the mean error of the models from the different approaches.

6.3.1 Interpolated test data. Figure 8 shows the comparison of prediction error among models learned using Extra-P (depicted as [Cal16] and [Rit20]) and Decision Trees (depicted as [Web21]) both with and without the information about dependencies from Perf-Taint. We compare our approach to the full-factorial design and the sparse modeling approach.

One would expect all approaches to be reasonably effective at predicting configuration options within the range of measurements already available. In the case of Extra-P, using the full set of measurements leads to accurate models, with model errors seldom passing 10%, and the use of Perf-Taint has a relatively small impact on results. The results of the sparse modeler are worse overall, but for Pace3D, they are significantly improved by the use of Perf-Taint. Performance-Detective achieves results comparable to the full factorial experiment design of Extra-P, while requiring only a fraction (2.9% and 6.18%, respectively) of the cost.

The performance-influence models, however, show a consistently higher model error rate of over 20%. When using Performance-Detective, the quality of the models remains approximately the same, while the cost is reduced by a factor of 15 for Pace3D and 7 for Kripke.

6.3.2 Extrapolated test data. Figure 8 shows an overview of the accuracy of the different Extra-P (depicted as [Cal16] and [Rit20]) and PIM models ([Web21]), both using information about dependencies from Perf-Taint and without it.

When extrapolating, predicting the runtime is more challenging as any errors are quickly magnified. Overall, we observe the same trends as for interpolated evaluation points, with a couple of differences. For Pace3D, the sampling approach of Extra-P generates significantly higher errors when not used in conjunction with Perf-Taint. However, for Kripke, the errors of the sampling approach are increased when used together with Perf-Taint. The performance-influence models show a larger model error rate, this time of over 40% for Pace3D and over 30% for Kripke when using the Plackett-Burman sampling design. However, the approach for learning performance-influence models does not extrapolate, as we can see in our data: It only predicts the time measured for the highest training value of the respective extrapolated parameter.

While providing information about the dependencies derived by Perf-Taint can be beneficial to the accuracy of the sparse Extra-P modeler, it decreases accuracy for the full-factorial experiment design. This is because with a full-factorial design, there is a lot of measurement data and Perf-Taint only removes wrong dependencies that model noise. The accuracy of the sparse modeler increases because it has less measurement data and very few information about parameter interplay.

6.3.3 Discussion. For both case studies, we can maintain the accuracy of the model generated with the experiment design deduced by Performance-Detective (25 and 5 experiment executions) as compared to a full-factorial design (625 and 125 experiment executions) and Plackett-Burman sampling (245 and 50 experiment executions). While for Pace3D, the sparse modeler is even less expensive than Performance-Detective, it has a lower accuracy than Performance-Detective (mean accuracy of 85.9% and 74.9% with and without Perf-Taint as compared to 91.5%) with especially worse predictions for extrapolated test points (mean accuracy of 17.7% and 31.8% with and without Perf-Taint compared to 9.3%).

For the PIMs, we observe a generally significant prediction error in both evaluation sets, which does not change much depending on using our minimal experiment design or sampling, and usage of Perf-Taint. This indicates that the learning method decision trees is not well-suited to model the performance of these applications.

Across evaluation scenarios, we observe that Performance-Detective always dramatically decreases the cost of experiments, while not meaningfully degrading model quality.

6.4 Threats to validity

A threat to external validity is that we ran the taint analysis on a small problem size. This was possible for the scenarios shown because the calculations are the same and still representative. However, this is not guaranteed in the general case, as sometimes different branches can be active depending on problem size. We can detect this by using control-flow tainting, provided by Perf-Taint. The only impact this scenario would have is that the taint analysis will have a higher cost.

Regarding internal validity, not inlining functions defined as inline is a potential issue. Functions are not inlined if we detect them as being performance-relevant. This could distort the measurements, as not inlining might incur a performance penalty on the applications as a whole. The overhead introduced by the profiling itself is a further source of distortion. We mitigate this by only instrumenting functions detected as performance-relevant, and keep the overhead as low as possible.

7 RELATED WORK

Parametric Performance Models. The difficulty of modeling modern software systems with many parameters has been addressed by parametric software performance models [5, 28, 32, 35] and Performance-Influence Models (PIMs) [39].
The parametric software performance modelling approach Palladio [5, 35] allows the modelling of parametric dependencies. However, automated extraction of these models [28, 32] assumes that the system consists of software components with well-defined interfaces, which is usually not the case in HPC applications.

In white-box PIMs, machine learning and heuristic methods are used to iteratively learn models representing the influences and interactions of various application parameters. However, white-box PIMs are either limited to binary-encoded arguments or require expensive trace measurements (cf. Sections 2.2, 4.2). Other methods of learning efficient performance models for highly configurable systems use Fourier transformations to reduce the number of samples and parameter combinations [18, 51].

HPC Performance Modeling. Analytical performance models can be created manually through source code inspection and guidance by performance engineers [20, 25]. Unfortunately, such models require significant effort, and excluding empirical data makes the models prone to underestimate the effects of hardware congestion and network performance.

Extra-P [12] is the state-of-the-art workflow for empirical and parametric performance modeling, extended with multi-parameter modeling [9], validation of high-performance libraries [38], prototyping hardware requirements for HPC applications [11], and with white-box modeling [13, 14]. We present a wider discussion in Sections 2.1 and 4.1.

PALM [43] constructs performance models from annotated application source code and enhances them with user-provided insights, program analysis, and measurements. Aspen [41] is a domain-specific language for the manual specification of program operations. COMPASS [31] uses Aspen annotations to generate application models statically, but it requires user intervention when the kernels cannot be analyzed automatically. In contrast, Performance-Detective does not require user input and manual analysis steps.

Online learning improves the accuracy of static and compiler-based performance models [6, 7]. Machine learning methods have been applied successfully to model performance [22, 30, 42] and decrease the negative effects of measurement noise [37]. Performance-Detective provides a complete and white-box workflow that requires neither heuristics nor approximations to construct performance models, and we provide validated parametric dependencies of models.

Auto-tuning. Auto-tuning applies an optimization method to achieve one or more goals, such as minimizing runtime [2] or floating-point operations per second [44] of an application. To find the best configuration among the search space, global or local search methods are employed [3, 23, 33]. In contrast to auto-tuning approaches that find the best configuration for a given optimization goal, Performance-Detective enables efficient modeling of the whole configuration space and interactions among configuration options.

8 CONCLUSION

We have shown that we can significantly lower the cost of automatic performance modeling of applications with multiple configuration parameters. We deduce a minimal experiment design with Performance-Detective by exploiting automatically derived insights about parameter interplay and main loops and thus reduce the number and cost of required measurements while achieving comparable accuracy to methods costing more than an order of magnitude more compute hours. With Performance-Detective, we model the Pace3D real-world multi-physics solver using 25 rather than 3125 measurements, require 34 times fewer core hours and achieve and still maintain a model accuracy of 91.5% compared to 93.8% and 90.6% when all measurements are used. Furthermore, we model Kripke, reducing needed measurements from 125 to 5, leading to 16 times fewer core hours needed, while maintaining an accuracy of 89.2% compared to 90.6% using all measurements.

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