A benchmark suite and performance analysis of user-space provenance collectors

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1 INTRODUCTION

Within the computational science and engineering (CSE) community, there is a consensus that greater reproducibility is a pathway towards increased productivity and more impactful science [60]. In the past decade, this has inspired a diverse range of research and development efforts meant to give us greater control over our software, including containers and virtual machines to capture environments [14, 35, 58, 69], package managers for fine-grained management of dependencies [26, 43], interactive notebooks and workflows [11, 23, 42], and online platforms for archiving and sharing computational experiments [18, 28, 73, 74]. In this work, we focus our attention on **computational provenance** as another complementary strategy for managing reproducibility across the research software lifecycle. Computational provenance is the history of a computational task, describing the artifacts and processes that led to or influenced the end result [25]; the term encompasses a spectrum of tools and techniques ranging from simple logging to complex graphs decorated with sufficient detail to replay a computational experiment.

Provenance data can provide crucial information about the hardware and software environments in which a code is executed. The use cases for this data are numerous, and many different tools for collecting it have independently developed. What has been lacking, however, is a rigorous comparison of those available tools and the extent to which they are practically usable in CSE application contexts[1]. In an effort to summarize the state of the art and to establish goalposts for future research in this area, our paper makes the following contributions:

- *A rapid review on available system-level provenance collectors.* We identify 45 provenance collectors from prior work, identify their method-of-operation, and reproduce the ones that meet specific criteria. We successfully reproduced 9 out of 16[2] collectors that met our criteria.
- *A benchmark suite for system-level provenance collectors*: Prior work does not use a consistent set of benchmarks; often publications use an overlapping set of benchmarks from prior work. We find the superset of all benchmarks used in the prior work our rapid review identified, identify unrepresented areas, and find a statistically valid subset of the benchmark. Our benchmark subset is able to recover the original benchmark results within[3] 25% of the acutal value 95% of the time, assuming errors are iid and normally distributed.
- *We show that simple performance models are insufficient to capture the complexity of provenance collector overheads*: We use linear models for predicting the overhead of $X application in $Y provenance collector based on $X application's performance characteristics (e.g., number of file syscalls per second). Despite trying linear regression, with and without rank reduction, with and without feature selection, our best model is still quite inaccurate, showing performance overhead of application $X in provenance collector $Y is not as simple as features of $X times features of $Y.

The remainder of the paper is structured as follows. [ˆRMM: Outline paper structure here.]

Unpublished working draft. Not for distribution.

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[1]DSK: usable globally or perhaps in particular situations?
[2]TODO: update with data
[3]TODO: update with data

2 BACKGROUND

Provenance tools and data have many potential applications, including the following from Pimentel et al. [63] and Sar and Cao [68]:

1. **Reproducibility**. A description of the inputs and processes used to generate a specific output can aid manual and automatic reproduction of that output[4]. Empirical studies [20, 30, 78, 84] show that reproducibility is rarely achieved in practice, probably due to its difficulty under the short time budget that scientists have available to spend on reproducibility. If reproducibility was easier to attain, perhaps because of automatic provenance tracking, it may improve the reproducibility rate of computational research. Provenance data improves **manual reproducibility**, because users have a record of the inputs, outputs, and processes used to create a computational artifact. Provenance data also has the potential to enable **automatic reproducibility**, if the process trace is detailed enough to be "re-executed". This idea is also called "software record/replay". Automatic reproducibility opens itself up to other applications to, like saving space by deleting results, and regenerating them on-demand. However, not all provenance collectors make this their goal.

2. **Caching subsequent re-executions**. Computational science inquiries often involve changing some code and re-executing the workflows (e.g., testing different clustering algorithms). In these cases, the user has to keep track of what parts of the code they changed, and which process have to be re-executed. However, an automated system could read the computational provenance graphs produced by previous executions, look at what parts of the code changed, and safely decide what processes need to be re-executed. The dependency graph would be automatically deduced, leaving less chance for a dependency-misspecification, unlike Make and CMake, which require the user to manually specify a dependency graph.

3. **Comprehension**. Provenance helps the user understand and document workflows and workflow results. An automated tool that consumes provenance can answer queries like "What version of the data did I use for this figure?" and "Does this workflow include FERPA-protected data?". A user might have run dozens of different versions of their workflow, and they may want to ask an automated system, "show me the results I previously computed based on that data with this algorithm?".

There are three high-level methods by which one can capture computational provenance: 1) by modifying an application to report provenance data, 2) by leveraging a workflow engine or programming language to report provenance data, and 3) by leveraging an operating system to emit provenance data to report provenance data [25]. Application-level provenance is the most semantically rich, but the least general, since it only applies to particular applications which have been modified to disclose provenance. Workflow- and language-level provenance is a middle ground between semantic richness and generality, applying to all programs using a certain workflow or programming language. System-level provenance is the least semantically rich but most general, applying to all programs on that particular system.

The implementation cost of adopting system-level provenance in a project which currently has no provenance is low because the user need not change *anything* about their application or workflow; they merely need to install some provenance tracer onto their system and rerun their application. Although the user may eventually use a more semantically rich provenance, low-initial-cost system-level provenance would get provenance's "foot in the door". Since system-level provenance collection is a possibly valuable tradeoff between implementation cost and enabling provenance applications, system-level provenance will be the subject of this work.

In the context of system-level provenance, artifacts are usually files, processes, or strings of bytes. Operations are usually syscalls involving artifacts, e.g., `fork`, `exec`, `open`, `close`. For example, suppose a bash script runs a Python script that uses matplotlib to create a figure. A provenance collector may record the events in Section 2.

This collector could infer the required files (including executables, dynamic libraries, scripts, script libraries (e.g., matplotlib), data) *without* knowing anything about the program or programming language. We defer to the cited works for details on versioning artifacts [8] and cycles [55]. Some collectors may also record calls to network resources, the current time, process IPC, and other interactions.

While there is little additional programmer-time in using system-level provenance (no user code change), there is a non-trivial implicit overhead in monitoring and recording each computational process. Even a minor overhead per I/O operation would become significant when amplified over the tens of thousands of I/O operations that a program might execute per second. Prior publications in system-level provenance usually contains some benchmark programs to evaluate the overhead imposed by the system-level provenance tool. However, the set of chosen benchmark programs are not consistent from one publication to another, and overhead can be extremely sensitive to the exact choice of benchmark, so these results are totally incomparable between publications. Most publications only benchmark their new system against native/no-provenance, so prior work cannot easily establish which system-level provenance tool is the fastest.

2.1 Prior work

Each result of our rapid review (Table 2) is an obvious prior work on provenance collection in general. However, those prior works look at only one or maybe two competing provenance tools at a time. To the best of our knowledge, there has been no global comparison of provenance tools. ProvBench[5] uses 3 provenance collectors (CamFlow, SPADE, and OPUS), but they are solely concerned with the differences between representations of provenance, not performance.

On the other hand, benchmark subsetting is a well-studied area. This work mostly follows Yi et al. [82] paper which evaluates subsetting methodologies and determine that dimensionality reduction and clustering is broadly a good strategy. Phansalkar et al.[6] apply dimensionality reduction and clustering to SPEC CPU benchmarks.

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[4]"Reproduction", in the ACM sense, where a **different team** uses the **same artifacts** to generate the output artifact [6].

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[5]TODO: cite; also cite CARE
[6]TODO: Cite Subsetting the SPEC CPU2006 Benchmark Suite

(1) The user created a process, call it PID=1.

(2) The process PID=1 executed bash.

(3) The loader of process PID=1 loaded libc.so.6.

(4) The process PID=1 forked a process, call it PID=2.

(5) The process PID=2 executed python.

(6) The process PID=2 read matplotlib.py (script library).

(7) The process PID=2 opened database for reading and writing, which creates a new version of the node in th provenance graph.

(8) The process PID=2 wrote figure.png.

(a) Abridged list of events recorded by a hypothetical system-level provenance collector.
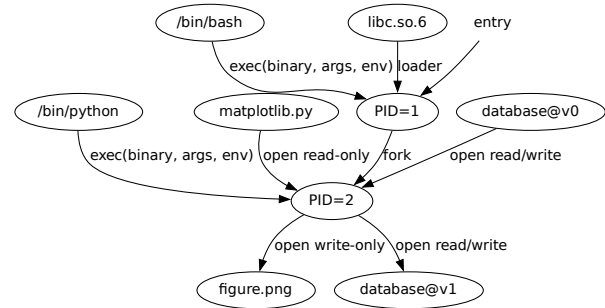
(b) Abridged graph of events recorded by a hypothetical system-level provenance collector. The arrows point in the direction of dataflow. Other authors use other conventions for what they render as nodes, edges, and arrow direction.

3 METHODS

3.1 Rapid Review

We began a rapid review to identify the research state-of-the-art tools for automatic system-level provenance.

Rapid Reviews are a lighter-weight alternative to systematic literature reviews with a focus on timely feedback for decision-making. Schünemann and Moja [70] show that Rapid Reviews can yield substantially similar results to a systematic literature review, albeit with less detail. Although developed in medicine, Cartaxo et al. show that Rapid Reviews are useful for informing software engineering design decisions [16, 17].

We conducted a rapid review with the following parameters:

- **Search terms**: "system-level AND provenance", "computational provenance"
- **Search engine**: Google Scholar
- **Number of results**: 50 of both searches. This threshold is the point of diminishing returns, as no new collectors came up in the 40th – 50th results.
- **Criteria**: A relevant publication would center on one or more operating system-level provenance collectors that capture file provenance. A tool requiring that the user use a specific application or platform would be irrelevant.

3.2 Benchmark Selection

Using the tools selected above, we identified all benchmarks that have been used in prior work. We excluded benchmarks for which we could not even find the original program (e.g., TextTransfer), benchmarks that were not available for Linux (e.g., Internet Explorer), benchmarks with a graphical component (e.g., Notepad++), and benchmarks with an interactive component (e.g., GNU Midnight Commander).

We implemented the benchmarks as packages for the Nix package manager[7], so they are runnable on many different platforms. Nix has official installers for Linux, Mac OS X, and Windows Subsystem for Linux on i686, x86_64, and aarch64 architectures, but

FreeBSD and OpenBSD both package Nix themselves, and it can likely be built from source on even more platforms.

We also added new benchmarks:

- **Data science**: None of the benchmarks resembled a typical data science program, so we added the most popular Notebooks from Kaggle.com, a data science competition website. Data science is a good use-case for provenance collection because because a user might want have a complex data science workflow and want to know from what data a certain result derives, and if it a certain result used the latest version of that data and code.
- **Compilations**: Prior work uses compilation of Apache or of Linux. We added compilation of several other packages (any package in Spack) to our benchmark. Compiling packages is a good use-case for a provenance collection because a user might trial-and-error multiple compile commands and not remember the exact sequence of "correct" commands; the provenance tracker would be able to recall the commands which did not get over-written, so the user can know what commands "actually worked".[8]

3.3 Performance Experiment

To get consistent measurements, we select as many benchmarks and provenance tracers as we reasonably can, and run a complete matrix (every tracer on every benchmark) 3 times in a random order[9]. Table 1 describes our experimental machine. We use BenchExec [12] to precisely measure the CPU time, wall time, memory utilization, and other attributes of the process (including child processes) in a Linux CGroup without networking, isolated from other processes. We disable ASLR, which does introduce non-determinism into the execution time, but it randomizes a variable that may otherwise have confounding effect [56]. We restrict the program to a single core in order to eliminate unpredictable scheduling and prevent other daemons from perturbing the experiment (they can run on the other N-1 cores). We wrap the programs that exit quickly in

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[7]See https://nixos.org/guides/how-nix-works

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[8]DSK: this reminds me of VisTrails from Utah.

[9]TODO: update with data

Table 1: Our experimental machine description.

Name	Value
CPU	11th Gen Intel(R) Core(TM) i7-1165G7 @ 2.80GHz
RAM	16 GiB of SODIMM DDR4 Synchronous 2400 MHz
Kernel	Linux 6.1.64

loops so they take about 10 seconds without any provenance system, isolating the cold-start costs. While cold-start costs can be significant, if the total program execution time is small, the user may not notice even the highest overhead of provenance collectors.

3.4 Benchmark Subsetting

We implemented and ran many different benchmarks, which may be costly for future researchers seeking to evaluate new provenance collector. A smaller, less-costly set of benchmarks may be sufficiently representative of the larger set.

Following Yi et al. [82], we evaluate the benchmark subset in two different ways:

- **Accuracy**. How closely do features of the subset resemble features of the original set? We will evaluate this by computing the root-mean squared error of a non-negative linear regression from the standardized features of selected benchmarks to the mean of features of the total set.
- **Representativeness.** How close are benchmarks in the original set to benchmarks in the subset? We will evaluate this by computing root mean squared error (RMSE) on the euclidean distance of standardized features from each benchmark in the original set to the closest benchmark in the selected subset.

We use a non-negative linear regression to account for the possibility that the total set has unequal proportions of benchmark clusters. We require the weights to be non-negative, so doing better on each benchmark in the subset implies a better performance on the total. Finally, we normalize these weights by adding several copies of the following an equation to the linear regression: $\text{weight}_A + \text{weight}_B + \cdots = 1$. Yi et al. [82] were attempting to subset with SPEC CPU 2006, which one can assume would already be balanced in these terms, so their analysis uses an unweighted average.

We standardize the features by mapping x to $z_x = (x - \bar{x})/\sigma_x$. While x is meaningful in absolute units, z_x is meaningful in relative terms (i.e., a value of 1 means "1 standard deviation greater than the mean"). Yi et al., by contrast, only normalize their features $x_{\text{norm}} = x/x_{\text{max}}$ which does not take into account the mean value. We want our features to be measured relative to the spread of those features in prior work.

We score by RMSE over mean absolute error (MAE), used by Yi et al. [82], because RMSE punishes outliers more. MAE would permits some distances to be large, so long it is made up for by other distances are small. RMSE would prefer a more equitable distribution, which might be worse on average, but better on the outliers. We think this aligns more with the intent of "representativeness."

For features, we will use features that are invariant between running a program ten times and running it once. This gives long

benchmarks and short benchmarks which exercise the same functionality similar feature vectors. In particular, we use:

1. The log overhead ratio of running the benchmark in each provenance collectors. We use the logarithm of the ratio, rather than the ratio directly because the logarithm is symmetric with respect to overshooting and undershooting. Suppose x provenance collector runs benchmark $y1$ twice as fast and benchmark $y2$ twice as slow; the average of the overhead would be $(2 + \frac{1}{2})/2 = 1.25$, whereas the average of the logarithms would be $\log 2 + \log \frac{1}{2} = \log 2 - \log 2 = 0$, meaning the 2x speedup "canceled out" the 2x slowdown on average). Note that the arithmetic mean of logarithms of a value is equivalent to the geometric mean of the value.
2. The ratio of CPU time to wall time.
3. The number of syscalls in each category per wall time second, where the categories consist of socket-related syscalls, syscalls that read file metadata, syscalls that write file metadata, syscalls that access the directory structure, syscalls that access file contents, exec-related syscalls, clone-related syscalls, exit-related syscalls, dup-related syscalls, pipe-related syscalls, close syscalls, pipe-related syscalls, and chdir syscalls.

In order to choose the subset, we will try clustering (k-means and agglomerative clustering with Ward linkage[10]), preceded by optional dimensionality reduction by principal component analysis (PCA). Once the benchmarks are grouped into clusters, we identify one benchmark from each of the k clusters to consist the benchmark subset. We will determine the best k experimentally.

3.5 Performance Model

A related problem to subsetting is inferring a performance model. There are two motivations for inferring a performance model:

- A sysadmin may wish to provide a computational provenance capturing system to their institution, but getting approval to run new software on their system may be expensive (e.g., on highly secure systems, the sysadmin may need to acquire a security audit of the code before it can be approved for use). They may want to prospectively estimate the overhead of provenance collectors without having to install all the provenance collectors on their system, so they can select the optimal collector for their use-case.
- Inferring a provenance model may improve our understanding of the bottlenecks in provenance collectors.

A performance model should input features of a prospective workload and output the approximate overhead under different systems. A priori, provenance collectors put a "tax" on certain syscalls (e.g., file I/O operations, process forks, process execs), because the system has to intercept and record these Therefore, we expect a low-dimensional linear model (perhaps number of I/O operations per second times a weight plus number of forks per second times another weight) would predict overhead optimally. To estimate this, we use the following models:

- **Ordinary least-squares (OLS) linear regression**. We estimate the runtime of each benchmark on each provenance collector as a linear regression of the features of each benchmark,

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[10]k-means and agglomerative/Ward both minimize within cluster variance, which is equivalent to minimizing our metric of "representativeness" defined earlier, although they minimize it in different ways: k-means minimizes by moving clusters laterally; Agglomerative/Ward minimizes by greedily joining clusters.

learning weights for each feature in each provenance collector using ordinary least-squares. This would create a model like $\text{weight}_1 \cdot \text{feature}_1 + \text{weight}_2 \cdot \text{feature}_2 + \cdots$ OLS requires a $n_{\text{bmarks}}n_{\text{feats}}$ parameters, but we can reduced its number of parameters, and thereby increase its out-of-domain generalizability, by the next two methods.

- **OLS compressed with SVD.** To further reduce the number of parameters, we apply singular value decomposition (SVD) to create a lossily-compressed representation of the learned weights. This model can be interpreted similarly to OLS, but using k "hidden" features which are linear combinations of n_{feats} "visible" features, where k is usually much less than n_{feats}. SVD uses $n_{\text{feats}}k + kn_{\text{bmarks}}$ parameters.
- **OLS on a greedy/random subset of features.** This method proceeds like the OLS regression, except it only uses a subset of the features, ignoring the rest. We tried two algorithms: greedy, which picks one additional feature that decreases loss the most until it has k features, and random, which selects a random k-sized subset, using kn_{bmarks} parameters.

We use the same features as in Section 3.4, but with the addition of a constant term, for a provenance collectors which have a fixed startup cost.

We use k-fold cross-validation to estimate generalizability of the predictor. While cross-validation does punish model-complexity and overfitting to some extent, we will still take the number of parameters into account when deciding the "best" model in the interest of epistemic modesty. Preferring fewer parameters makes the model more generalizable on out-of-domain data, since even our full cross-validation data is necessarily incomplete.

4 RESULTS

4.1 Selected Provenance Collectors

Table 2 shows the provenance collectors we collected and their qualitative features. Because there are not many open-source provenance collectors in prior work, we also include the following tools, which are not necessarily provenance collectors, but may be adapted as such: strace, ltrace, fsatrace, and RR. See **??** for more in-depth description of each collector. The second column shows the "collection method." See Appendix A for their exact definition.

The last column in the table categorizes the "state" of that provenance collector in this work into one of the following:

- **Not for Linux.** Our systems are Linux-based and Linux is used by many computational scientists. Therefore, we did not try to reproduce systems which were not Linux based.
- **VMs too slow.** Some provenance collectors require running the code in a virtual machine. We know a priori that these methods are prohibitively slow, with Panorama reporting 20x average overhead [83]. The provenance systems we are interested in have overheads in the 1.01x – 3x range. [ˆDSK: maybe say instead that we don't use prov systems that have VM overheads over 3x?]
- **Requires recompilation.** Some provenance collectors require the user to recompile their entire application and library stack. This is prohibitively onerous and negates the otherwise low cost of switching to system-level provenance we are pursuing.
- **Requires special hardware.** Some methods require certain CPUs, e.g., Intel CPUs for a dynamic instrumentation tool called

Intel PIN. Being limited to certain CPUs violates our goal of promulgating reproducibility to as many people as possible.
- **No source.**[11] We searched the original papers, GitHub, BitBucket, Google, and emailed the first author (CCing the others). If we still could not find the source code for a particular provenance collector, we cannot reproduce it. Note, however, that RecProv is implemented using rr, so we can use rr as a lower-bound for RecProv.
- **Requires custom kernel (Hi-Fi, LPM/ProvMon, CamFlow).** Collectors which modify Linux kernel code are out-of-scope for this work due to their increased maintenance overhead, security risk, and difficulty of system administration. Indeed, many of the systems are too old to be usable: LPM/ProvMon is a patch-set for Linux 2.6.32 (reached end-of-life 2016), Hi-Fi is a patch-set for Linux 3.2 (reached end-of-life in 2018). On the other hand, SingularityCE/Apptainer require Linux $\geq$ 3.8 for user namespaces.
- **Not reproducible (OPUS).** We tried to get this provenance system to run, with several weeks of effort: we emailed the original authors and other authors who used this system, and we left a GitHub issue describing the expected and actual results [12]. However, we still could not get the system to run properly.
- **Needs more time (DTrace, SPADE, eBPF/bpftrace).** We simply needed more time to implement these provenance collectors.
- **Reproduced/rejected (ltrace, CDE).** These are provenance collectors that we could reproduce on some workloads but not others (see Appendix D). Missing values would complicate the data analysis too much, so we had to exclude these from our running-time experiment.
- **Reproduced (strace, fsatrace, RR, ReproZip, PTU, Sciunit, CARE).** We reproduced this provenance collector on all of the benchmarks.

4.2 Implemented Benchmarks

Of these, Table 6 shows the benchmarks used to evaluate each tool, of which there are quite a few. We prioritized implementing frequently-used benchmarks, easy-to-implement benchmarks, and benchmarks that we believe have value in representing a computational science use-case.

- The most common benchmark classes from prior work are, **HTTP servers/traffic**, **HTTP servers/clients**, **FTP servers/traffic**, and **FTP servers/clients** are popular because prior work focuses overwhelmingly on provenance for the sake of security (auditing, intrusion detection, or digital forensics). While these benchmarks may not be specifically relevant for computational science workloads, we wanted to include them in our suite to improve our coverage of benchmarks used frequently in prior works. We implemented 5 HTTP servers (Apache, miniHTTP, Python's http.server, lighttpd, Nginx) running against traffic from Hey (successor to ApacheBench) and 2 HTTP clients (curl and

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[11]TODO: Evaluate this first, so "no source" AND "requires kernel changes" would be classified as "no source". Future work may be able to reproduce collectors which require kernel changes (or VMs), but has no chance of reproducing collectors which have no source.

[12]See https://github.com/dtg-FRESCO/opus/issues/1

[15]URSprung depends on IBM Spectrum Scale to get directory change notifications, so it is not for a *generic* Linux system.

Table 2: Provenance collectors from our search results and from experience.

Tool	Method	Status
strace	tracing	Reproduced
fsatrace	tracing	Reproduced
rr [59]	tracing	Reproduced
ReproZip [19]	tracing	Reproduced
Sciunit [62]	tracing	Reproduced
PTU [62][13]	tracing	Reproduced
CARE [34]	tracing	Reproduced
CDE [31]	tracing	Reproduced/rejected
ltrace	tracing	Reproduced/rejected
SPADE [27]	audit, FS, or compile-time	Needs more time
DTrace [1]	audit	Needs more time
eBPF/bpftrace	audit	Needs more time
SystemTap [65]	audit	Needs more time
Namiki et al. [57]	audit	Needs more time
PROV-IO [32]	lib. ins.	Needs more time
OPUS [8]	lib. ins.	Not reproducible
CamFlow [61]	kernel ins.	Requires custom kernel
Hi-Fi [64]	kernel ins.	Requires custom kernel
LPM/ProvMon [10]	kernel ins.	Requires custom kernel
Arnold[14]	kern ins.	Requires custom kernel
LPS [22]	kern ins.	Requires custom kernel
RecProv [38]	tracing	No source
LPROV [80]	kernel mod., lib. ins.	No source
S2Logger [75]	kernel mod.	No source
ProTracer [50]	kernel mod.	No source
FiPS [76]	FS	No source
PANDDE [24]	kernel ins., FS	No source
PASS/Pasta [55]	kernel ins., FS, lib. ins.	No source
PASSv2/Lasagna [54]	kernel ins.	No source
Lineage FS [68]	kernel ins.	No source
RTAG [37]	bin. ins.	No source
BEEP [47]	bin. ins.	Requires HW
libdft [40]	bin., kernel, lib. ins.	Requires HW
RAIN [36]	bin. ins.	Requires HW
DataTracker [72]	compile-time ins.	Requires HW
MPI[49]	compile-time ins.	Requires recompilation
LDX [44]	VM ins.	Requires recompilation
Panorama [83]	VM ins.	VMs are too slow
PROV-Tracer [71]	audit	VMs are too slow
ETW [5]	audit	Not for Linux
Sysmon [52]	audit	Not for Linux
TREC [79]	tracing	Not for Linux
URSprung [66]	audit	Not for Linux[15]
Ma et al. [48]	audit	Not for Linux
ULTra [15]	tracing	Not for Linux

Wget). We implemented 1 FTP server (ProFTPD) running against traffic from httpbench[16] and 3 FTP clients (curl, Wget, and lftp).

- **Compiling packages** from source is a common operation in computational science, so we implemented as many of these as we could and also implemented some of our own. However, compiling glibc and LLVM takes much longer than everything else in the benchmark suite, so we excluded LLVM and glibc. We implemented a pattern for compiling packages from Spack that discounts the time taken to download sources, counting only the time taken to unpack, patch, configure, compile, link, and install them. We implemented compiling Python, Boost, HDF5, Apache, git, and Perl.[17]

- Implementing headless for **browsers** in "batch-mode" without GUI interaction is not impossibly difficult, but non-trivial. Furthermore, we deprioritized this benchmark because few computational science applications resemble the workload of a web browser.
- **Archive** and **unarchiving** is a common task for retrieving data or source code. We benchmark un/archiving several archives with several compression algorithms. Choosing a compression algorithm may turn an otherwise I/O-bound workload to a CPU-bound workload, which would make the impact of provenance tracing smaller. We implemented archive and unarchiving a medium-sized project (7 MiB uncompressed) with no compression, gzip, pigz, bzip, and pbzip2.
- **I/O microbenchmarks** could be informative for explicating which I/O operations are most affected. Prior work uses lmbench [53], which benchmarks individual syscalls, Postmark [39], which focuses on many small I/O operations (typical for web servers), IOR[18], H5bench[19] and BT-IO[20], which are specialized for parallel I/O on high-performance machines, and custom benchmarks, for example running open/close in a tight loop. Since we did not have access to a high-performance machine, we used lmbench and Postmark. We further restrict lmbench to the test-cases relevant to I/O and used by prior work.
- **BLAST** [7] is a search for a fuzzy string in a protein database. However, unlike prior work, we split the benchmark into query groups described by Coulouris [21], since the queries have different performance characteristics: blastn (nucleotide-nucleotide BLAST), megablast (large numbers of query sequences) blastp (protein-protein BLAST), blastx (nucleotide query sequence against a protein sequence database), tblastn (protein query against the six-frame translations of a nucleotide sequence database), tblastx (nucleotide query against the six-frame translations of a nucleotide sequence database).
- Prior work uses several **CPU benchmarks**: SPEC CPU INT 2006 [33], SPLASH-3 [67], SPLASH-2[21] and HPCG[22]. While we do not expect CPU benchmarks to be particularly enlightening for provenance collectors, which usually only affect I/O performance, it was used in three prior works, so we tried to implement both. SPLASH-3 is an updated and fixed version of the same benchmarks in SPLASH-2. However, SPEC CPU INT 2006 is not free (as in beer), so we could only implement SPLASH-3.
- **Sendmail** is a quite old mail server program. Mail servers do not resemble a computational science workload, and it is unclear what workload we would run against the server. Therfore, we deprioritized this benchmark and did not implement it.
- **VCS checkouts** are a common computational science operation. We simply clone a repository (untimed) and run $vcs checkout $commit for random commits in the repository. CVS does not have a notion of global commits, so we use Mercurial and Git.
- VIC, FIE, ImageML, and Spark are real-world examples of **Data processing** and **machine-learning workflows**. We would like

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Table 3: Benchmarks implemented by this work. For brevity, we consider categories of benchmarks in Table 6

Prior works	This work	Benchmark group and examples from prior work
12	yes	HTTP server/traffic
10	yes	HTTP serer/client
10	yes	Compile user packages
9	yes	I/O microbenchmarks
9	no	Browsers
6	yes	FTP client
5	yes	FTP server/traffic
5	yes	Un/archive
5	yes	BLAST
5	yes	CPU benchmarks
5	yes	Coreutils + friends (bash, ls, procps)
3	yes	cp
2	yes	VCS checkouts
2	no	Sendmail
2	no	Machine learning workflows (CleanML, Spark, ImageML)
1	no	Data processing workflows (VIC, FIE)
1	no	RUBiS
1	no	x264
1	no	mysqld
1	no	gocr
1	no	Memcache
1	no	Redis
1	no	php
1	no	pybench
1	no	ping
1	no	mp3info
1	no	ngircd
1	no	CUPS

to implement these, but reproducing those workflows is non-trivial; they each require their own computational stack. For FIE, in particular, there is no script that glues all of the operations together; we would have to read the publication [13] which FIE supports to understand the workflow, and write our own script which glues the operations together.

- We did not see a huge representative value in **coreutils and friends (bash, cp, ls, procps)** that would not already be gleaned from lmbench, but due to its simplicity and use in prior work, we implemented it anyway. For bash, we do not know what exact workload prior works are using, but we test the speed of incrementing an integer and changing directories (cd).
- The **other** benchmark programs are mostly specific desktop applications used only in one prior work. These would likely not yield any insights not already yielded by the benchmarks we implemented, and for each one we would need to build it from source, find a workload for it, and take the time to run it. They weigh little in the argument that our benchmark suite represents prior work, since they are only used in one prior work.

Although SPLASH-3 CPU-oriented benchmarks contain mostly CPU-bound tasks, they often need to load data from a file, which does invoke the I/O subsystem. They are CPU benchmarks when the CPU is changed and the I/O subsystem remains constant, but

Table 4: This table shows percent overhead of the mean wall-time when running with a provenance collector versus running without provenance. A value of 1 means the new execution takes 1% longer than the old. "Noprov" refers to a system without any provenance collection (native), for which the slowdown is 0 by definition. fsatrace appears to have a negative slowdown in some cases due to random statistical noise. TODO: use the exact same label names as Table 3.

| collector / benchmark types	fsatrace	noprov	reprozip	rr	strace
archive	7	0	164	208	180
blast	-1	0	32	102	6
copy	48	0	7299	322	710
ftp client	-0	0	14	5	4
ftp server	1	0	58	-32	65
gcc	3	0	417	314	321
http client	-16	0	453	200	98
http server	6	0	791	965	516
lmbench	-14	0	31	15	5
notebook	-10	0	116	0	50
pdflatex	-10	0	290	19	79
postmark	9	0	2002	367	928
python	0	0	412	137	184
shell	18	0	4620	698	63
simple	23	0	977	1749	431
splash-3	-1	0	78	64	19
unarchive	6	0	179	190	177
vcs	3	0	453	169	185

when the CPU is constant and the I/O subsystem is changed, the total running time is influenced by I/O-related overhead.

4.3 Subsetted Benchmarks

Figure 2 shows the performance of various algorithms on benchmark susbetting. We observe:

1. The features are already standardized, so PCA has little to offer other than rotation and truncation. However, the truncation is throwing away potentially useful data. Since we have a large number of benchmarks, and the space of benchmarks is quite open-ended, the additional dimensions that PCA trims off appear be important for separating clusters of data.
2. K-means and agglomerative clustering yield nearly the same results. They both attempt to minimize within-cluster variance, although by different methods.
3. RMSE of the residual of linear regression will eventually hit zero because the k exceeds the rank of the matrix of features by benchmarks; The linear regression has enough degrees of freedom to perfectly map the inputs to their respective outputs.

It seems that agglomerative clustering with $k = 20$ has quite good performance, and further increases in k exhibit diminishing returns. At that point, the RMSE of the linear regression is about 1.12. Assuming the error is iid and normally distributed, we can estimate the standard error of the approximation of the total benchmark by linear regression is about 0.12 (log-space) or $e^{0.12} \approx 1.12$ (real-space). Within the sample, 68% of the data falls within one
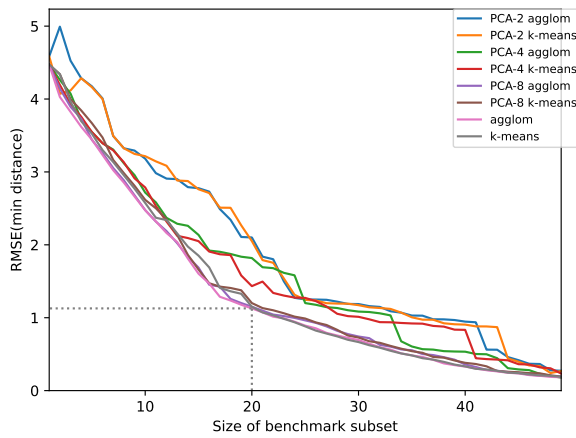
(a) Subsetting algorithms scored by the RMSE of the distance of each benchmark to the nearest selected benchmark. A dotted line shows the x- amd y-value of the point of diminishing return.
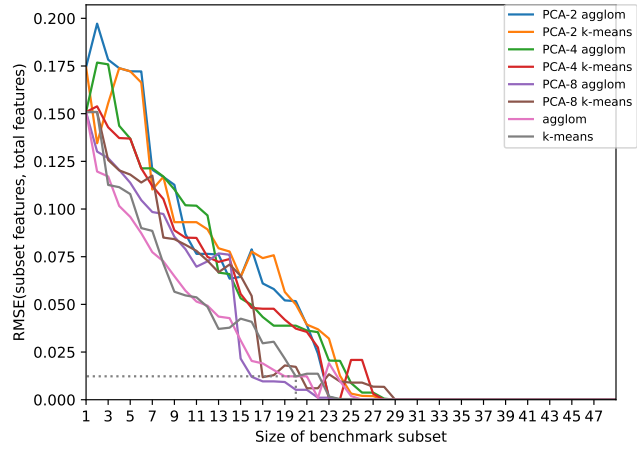
(b) Subsetting algorithms scored by the RMSE of the difference between (weighted) features of the subset and features of the original set. A dotted line shows the x- amd y-value of the point of diminishing return.

Figure 2: Competition for best benchmark subsetting algorithm, sweeping over subset size on the x-axis.

standard error (either multiplied or divided by a factor of 1.12x) and 95% of the data falls within two standard errors (a factor of $e^{2 \cdot 0.12}$ or 1.25x). We examine the generated clusters and benchmark subset in Table 5 and Figure 4.

Section 4.3 shows the a posteriori clusters with colors. Section 4.3 shows a priori benchmark "types", similar but more precise than those in Table 3. From these two, we offer the following observations:

1. It may appear that the algorithm did not select the benchmark closest to the cluster center, but this is because we are viewing a 2D projection of a high-dimensional space, like how three stars may appear next to each other in the sky, but in reality one pair may be much closer than the other, since we cannot perceive radial distance to each star.

2. Many of the clusters are singletons, for example the `python http.server` near $(5, 6)$; this is surprising, but given there are not any other points nearby, it seems reasonable.

3. We might expect that benchmarks of the same type would occupy nearby points in PCA space, but it seems they often do not. lmbench is particularly scattered with points at $(-1, 0)$ and $(0, 5)$, perhaps because it is a microbenchmark suite where each microbenchmark program tests a different subsystem.

4. Postmark is intended to simulate the file system traffic of a web server (many small file I/O). Indeed the Postmark at $(4, -2)$ falls near several of the HTTP servers at $(4, -2)$ and $(6, -2)$. Copy is also similar.

To elucidate the structure of the clusters, we plotted a dendrogram (Figure 4) and listed the members of each cluster (Table 5). We offer the following observations:

1. Fork and exec are close in feature-space, probably because programs usually do both.

2. cd and shell-echo are near each other. I is surprising that blastn is also near cd and shell-echo, but they both have similar cputime-to-walltime ratios.

Cluster representative	Weight (%)	Cluster members
unarchive pigz	26.4	git setuptools_scm, python-hello-world, unarchive, unarchive gzip, wget
lm-protection-fault	24.2	a-data-sci, blastp, blastx, lm-bw_file_rd, lm-bw_pipe, lm-bw_unix, lm-catch-signal, lm-getppid, lm-install-signal, lm-mmap, lm-page-fault, lm-read, lm-select-file, lm-select-tcp, lm-write, megabl, splash-cholesky, splash-lu, splash-ocean, splash-radiosity, splash-radix, splash-volrend, splash-water-nsquared, splash-water-spatial, tblast
latex-test	13.0	archive bzip2, archive gzip, blastn, comprehens, curl, latex-test2, lm-fstat, lm-stat, minihttp, python-import, titanic-da, unarchive bzip2
unarchive pbzip2	7.9	archive pbzip2, archive pigz, lighttpd
lm-fs	3.9	lm-open/close
lm-exec	3.7	
shell-incr	3.1	splash-fft
proftpd with ftpbench	2.5	
ftp-curl	2.4	ftp-wget, lftp
cp linux	2.0	
ls	1.7	echo, hello, ps, true
shell-echo	1.5	
nginx	1.5	
apache	1.4	
cd	1.4	
python http.server	1.3	
gcc-hello-world threads	0.7	gcc-hello-world
lm-fork	0.1	
postmark	0.0	archive, cp smaller
hg schema-validation	0.0	
all[23]	98.8	

Table 5: A table showing cluster membership and weights. The weights show one way of approximating the features in the original set, which is by multiplying the features of the cluster representative by the weight and summing over all clusters.

3. Many of the CPU-heavy workloads are grouped together, under lm-protection-fault.

4. Many of the un/archive benchmarks are grouped together with lighttpd, which also accesses many files.
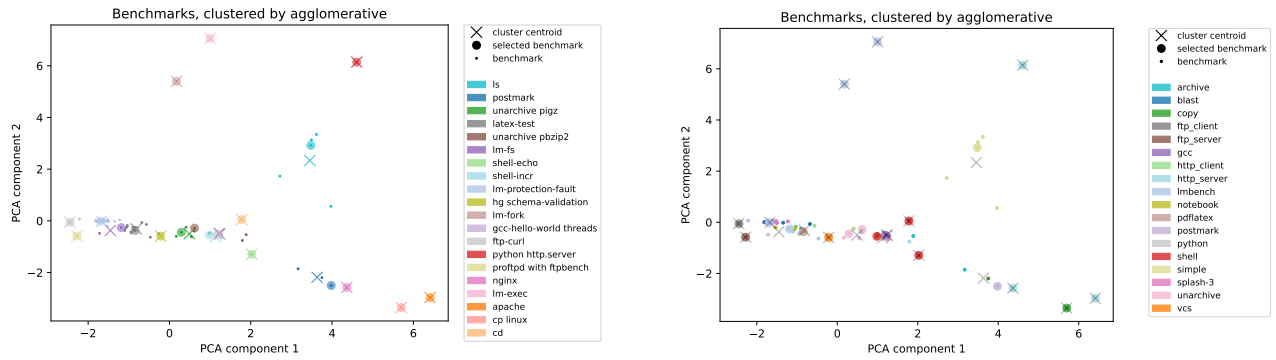
(a) Benchmark subset, where color shows resulting clusters. The same-color small dots are benchmarks in the same cluster, the "x" of that color is their hypothetical benchmark with their average features, and the big dot of that color is the closest actual benchmark to the average of their features. A benchmark subset replaces each cluster of small dots with just the single big dot.

(b) Benchmark subset, where color shows benchmark class (see Table 3). For example, archive-with-gzip and archive-with-bzip2 are two benchmarks of the same type, and therefore color. The "x" still shows a posteriori cluster centers as in Section 4.3.

Figure 3: Benchmarks, clustered agglomeratively into 20 subsets using standardized performance features. These axes show only two dimensions of a high-dimensional space. We apply PCA *after* computing the clusters, in order to project the data into a 2D plane.
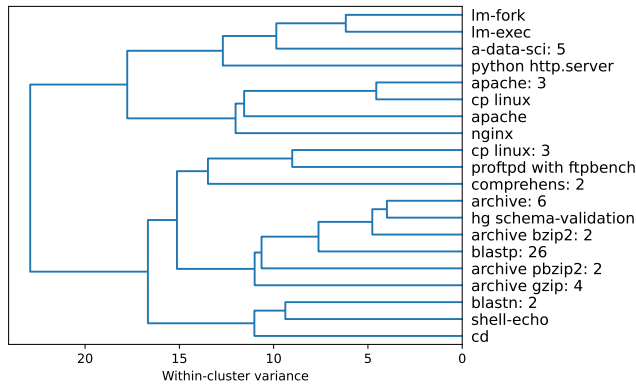

Figure 4: Dendrogram showing the distance between clusters. A fork at $x = x_0$ indicates that below that threshold of within-cluster variance, the two children clsuters are far away enough that they should be split into two; conversely, above that threshold they are close enough to be combined. We label each cluster by their "selected benchmark." If there is a colon and a number after the name, it indicates the number of benchmarks contained in that cluster. Otherwise, the cluster is a singleton.

4.3.1 Our suggestion. The programs in lmbench have very different performance characteristics (see Section 4.3). Due to their simplicity, their results are interpretable (e.g., testing latency of open() followed by close() in a tight loop). We report the total

time it takes to run a large number of iterations[24], rather than latency or throughput, in order to be consistent with benchmarks for which latency and throughput are not applicable terms. If one has to run part of lmbench, it is not too hard to run all of lmbench.

One should also include an application that does *some* CPU processing but manipulats many small files like Postmark. One need not go through the trouble of setting up Nginx, and although Apache appears a cluster representative, that cluster is also similar to Postmark.

TODO: Write more once we have better results.

There is an old adage, *the best benchmark is always the target application*. Benchmarking lmbench reveals how well certain aspects of performance, but benchmarking the target application reveals one the *actual* performance. If we may hazard a corollary, we might say, *the second best benchmark is one from the target domain*. Supposing one doens't know the exact application or inputs their audience will use, selecting applications from that domain is the next best option. This is why we are surprised why such a large domain, computational science, is underrepresented in benchmarks in prior work. Future work on system-level provenance for computational science should of course use a computational science benchmark, such as BLAST, compiling programs with Spack, or a workflow, whether or not they are selected by this clustering analysis. Likewise, work on security should include HTTP servers.

4.4 Predictive Model

Figure 5 shows us the competition between predictive performance models. We observe the following:

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[24]Users should set the environment variable ENOUGH to a large integer, otherwise lmbench will choose a number of iterations based on the observed speed of the machine which can vary between runs.
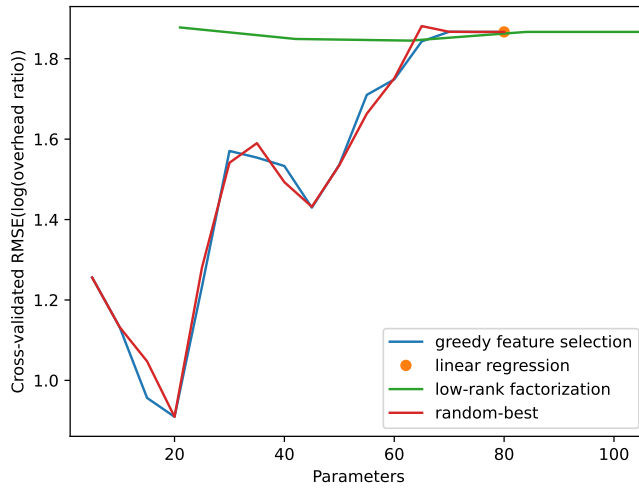
Figure 5: Competition between predictive performance models. Pure linear regression only has one instance with $n_{\text{feats}} \times n_{\text{bmarks}}$ parameters; the others have with varying numbers of parameters.

- When the number of parameters is large, all of the algorithms preform similarly; Even though greedy feature selection is more constrained than low-rank matrix factorization (every solution found by greedy is a candidate used by low-rank, but not vice versa), there are enough degrees of freedom to find similar enough candidates.
- Linear regression has equivalent goodness-of-fit to matrix factorization with a high k, as expected. When the compression factor is low, the compressed version is just as good as the original.
- Random-best usually does not do better than greedy feature selection. However, greedy is much easier to compute. Greedy is not necessarily optimal, but our problem domain may lack the complexity to generate these cases.

Greedy feature selection with 20 parameters (predicting the performance on 5 systems using only $k = 4$ of 16 features) seems to preform the best in cross-validation. Assuming the errors are iid and normally distributed, we find the standard error is about 0.95 in log-space or $e^{0.95} \approx 2.6$ in real-space. Within the sample, 68% of the data falls within a factor of 2.6 (one standard error) and 95% falls within a factor of $e^{2 \cdot 0.95} \approx 6.7$, which is quite bad. We view this result as saying, the performance overhead of provenance collectors is not easily predictable, even given our features (including the syscall-rates) of the program.

4.5 Discussion

Prior work focuses on security, not computational science. Table 3 shows the top-used benchmarks are server programs, followed by I/O benchmarks. Server programs access a lot of small files, with concurrency, which is a different file-access pattern than scientific applications. BLAST (used by 5 / 29 publications with benchmarks, see Table 6) is the only scientific program to be used

as a benchmark by more than one publication. Benchmark subsetting includes two[25] different BLAST programs, because they are sufficiently different than the rest.

One difference between security and computational science is that security-oriented provenance collectors have to work with adverserial programs: there should be no way for the program to circumvent the provenance tracing, e.g. PTRACE_DETACH. Computational science, on the other hand, may satisfied by a solution that *can* be intentionally circumvented by an uncooperative program, but would work most of the time, provided it can at least detect when provenance collection is potentially incomplete. Interposing standard libraries, although circumventable, has been used by other tools [81].

Provenance collectors vary in power and speed, but fast-and-powerful could be possible. While all bear the title, provenance collector, some are **monitoring**, merely recording a history of operations, while others are **interrupting**, interrupt the process when the program makes an operation. Fsatrace, Strace, and Ltrace are monitoring, while ReproZip, Sciunit, RR, CARE, and CDE are interrupting, using their interruption store a copy of the files that would be read or appended to by the process. We expect the monitoring collectors to be faster than the interrupting collectors, but the performance of strace is not that far off of the performance of RR[26]. Strace and RR both use ptrace, but strace does very little work while RR maintains may need to intercept and reinterpret the syscall, (see treatment of mmap in RR's publication [59]). This suggests most of the overhead actually be due to ptrace and its incurred context switches. None of the interrupting provenance collectors use library interposition or eBPF. Perhaps a faster underlying method would allow powerful features of interrupting collectors in a reasonable overhead budget.

Provenance collectors are too slow for "always on". One point of friciton when using system-level provenance collection is that users have to remember to turn it on, or else the system is useless. There may be advantage to be found in "always on" provenance system; for example, a user might change their login shell to start within a provenance collector. Unfortunately, the conventional provenance collectors exhibit an intolerably high overhead to be used always, with the exception of fsatrace. fsatrace is able to so much faster because it uses library interpositioning rather than ptrace (see "fast-and-powerful" discussion above), but fsatrace is one of the weakest collectors; it only collects file reads, writes, moves, deletes, queries, and touches (nothing on process forks and execs).

The space of benchmark performance in provenance systems is highly dimensional. The space of benchmarks is naturally embedded in a space with features as dimensions. If there were many linear relations between the features (e.g., CPU time per second = 1 - (file syscalls per second) * (file syscall latency)), then we would expect clustering to reveal fewer clusters than the number of features. Indeed, there are somewhat fewer clusters than the number of features ($20 < 21$)[27], it seems that most dimensions are not redundant or if they are, their redundancy is not expressible as linear relationship. This complexity is also present when trying to

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[25]TODO: update with data
[26]TODO: updaet with data.
[27]TODO: update with data

predict performance as a function of workload features; either the relationship is non-linear, or we are missing a relevant feature.

Computational scientists may already be using workflows. While system-level provenance is the easiest way to get provenance out of many applications, if the application is already written in a workflow engine, such as Pegasus[28], they can get provenance through the engine. Computational scientists may move to workflows for other reasons, because workflows make it easier to parallelize code on big machines and integrate loosely coupled components together. That may explain why prior work on system-level provenance focuses more on security applications.

4.6 Threats to Validity

Internal validity: We mitigate measurement noise by: - Isolating the sample machine Section 3.3 - Running the code in cgroups with a fixed allocation of CPU and RAM - Rewriting benchmarks that depend on internet resources to only depend on local resources - Averaging over 3[29] iterations helps mitigate noise. - Randomizing the order of each pair of collector and benchmark within each iteration We use cross-validation for the performance model

External validity: When measuring representativeness of our benchmark subset we use other characteristics of the workload, not just performance in each collector. Therefore, our set also maintains variety and representativeness in underlying characteristics, not just in the performance we observe. Rather than select the highest cluster value, we select the point of diminishing return, which is more likely to be generalizable.

Regarding the performance model, we use cross-validation to asses out-of-sample generalizability.

5 FUTURE WORK

In the future, we plan to implement compilation for more packages, in particular xSDK [9] packages. Compilation for these packages may be different than Apache and Linux because xSDK is organized into many dozens of loosely related packages. We also plan to implement computational workflows. Workflows likely have a different syscall access pattern unlike HTTP servers because the files may be quite large, unlike cp because workflows have CPU work blocked by I/O work, and unlike archiving because there are multiple "stages" to the computation.

We encourage future work that implements interrupting provenance collector using faster methods like library interposition or eBPF as opposed to ptrace. Between them, there are pros and cons: eBPF requires privileges, but could be exposed securely by a setuid/setgid binary; library interposition assumes the tracee only uses libc to make I/O operations. None of the interrupting collectors we know of exploit it, some of the interruption work may be "postponed"; if a file is read, it can be copied at any time unless/until it gets mutated ("copy-on-write-after-read"). Other reads can be safely copied after the program is done, and new file writes obviously do not need to be copied at all. Perhaps the performance overhead would be low enough to be "always on", however storage and querying cost need to be dispatched with as well.

28TODO: cite
29TODO: update

6 CONCLUSION

We intend this work to bridge from research to practical use of provenance collectors and an invitation for future research. In order to bridge research into practice, we identified reproducible and usable provenance collectors from prior work, and evaluated their performance on synthetic and real-world workloads. In order to invite future research, we collated and minimized a benchmark suite and identified gaps in prior work. We believe this work and the work it enables will address the practical concerns of a user wanting to use a provenance collector.

A COLLECTION METHODS

- **User-level tracing**: A provenance tool may use "debugging" or "tracing" features provided by the kernel, e.g., ptrace(2) [4], to trace another program's I/O operations.
- **Built-in auditing service**: A provenance tool may use auditing service built in to the kernel, e.g., Linux Auditing Framework [51], enhanced Berkeley Packet Filter (eBPF) [2], kprobes [41], and ETW [5] for Windows.
- **Filesystem instrumentation**: A provenance tool may set up a file system, so it can log I/O operations, e.g., using Filesystem in User SpacE (FUSE) interface [3], or Virtual File System (VFS) interface [29].
- **Dynamic library instrumentation**: A provenance tool may replace a library used to execute I/O operations (e.g., glibc) with one that logs the calls before executing them.
- **Binary instrumentation**: A provenance tool may use binary instrumentation (dynamic or static) to identify I/O operations in another program.
- **Compile-time instrumentation**: A provenance tool may be a compiler pass that modifies the program to emit provenance data, especially intra-program control flow.
- **Kernel instrumentation**: A provenance tool may be a modified kernel either by directly modifying and recompiling the kernel's source tree.
- **Kernel module**: Rather than directly modify the kernel's source, the provenance tool may simply require that the user load a custom kernel module.
- **VM instrumentation**: A provenance tool may execute the program in a virtual machine, where it can observe the program's I/O operations.

B TABLE OF BENCHMARKS BY PRIOR PUBLICATION

See Table 6 for a list of prior publications and what benchmarks they use, if, for example, one wishes to see the original contexts in which Firefox was used.

C SHORT DESCRIPTION OF NOTABLE PROVENANCE COLLECTORS

- **CDE** is a record/replay tool proposed by Guo and Engler [31]. During record, CDE uses ptrace to intercept its syscalls, and copy relevant files into an archive. During rerun, can use ptrace

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31LogGC measures the offline running time and size of garbage collected logs; there is no comparison to native would be applicable.

Table 6: Benchmarks used by prior works on provenance collectors (sorted by year of publication).

Publication	Benchmarks	Comparisons
TREC [79]	open/close, compile Apache, LaTeX	Native
ULTra [15]	getpid, LaTeX, Apache, compile package	Native, strace
PASS [55]	BLAST	Native ext2
Panorama [83]	curl, scp, gzip, bzip2	Native
PASSv2 [54]	BLAST, compile Linux, Postmark, Mercurial, Kepler	Native ext3, NFS
SPADEv2 [27]	BLAST, compile Apache, Apache	Native
Hi-Fi [64]	lmbench, compile Linux, Postmark	Native
libdft [40]	scp, {tar, gzip, bzip2} x {extract, compress}	PIN
PTU [62]	Workflows (PEEL0, TextAnalyzer)	Native
LogGC [46]	RUBiS, Firefox, MC, Pidgin, Pine, Proftpd, Sendmail, sshd, vim, w3m, wget, xpdf, yafc, Audacious, bash, Apache, mysqld	None[30]
CARE [34]	Compile perl, xz	Native
Arnold[31]	cp, CVS checkout, make libelf, LaTeX, Apache, gedit, Firefox, spreadsheet, SPLASH-2	Native
LPM/ProvMon [10]	lmbench, compile Linux, Postmark, BLAST	Native
Ma et al. [48]	TextTransfer, Chromium, DrawTool, NetFTP, AdvancedFTP, Apache, IE, Paint, Notepad, Notepad++, simplehttp, Sublime Text	Native
ProTracer [50]	Apache, miniHTTP, ProFTPD, Vim, Firefox, w3m, wget, mplayer, Pine, xpdf, MC, yafc	Auditd, BEEP
LDX [44]	SPEC CPU 2006, Firefox, lynx, nginx, tnftp, sysstat, gif2png, mp3info, prozilla, yopsweb, ngircd, gocr, Apache, pbzip2, pigz, axel, x264	Native
PANDDE [24]	ls, cp, cd, lpr	Native
MPI [49]	Apache, bash, Evince, Firefox, Krusader, wget, most, MC, mplayer, MPV, nano, Pine, ProFTPd, SKOD, TinyHTTPd, Transmission, Vim, w3m, xpdf, Yafc	Audit, LPM-HiFi
CamFlow [61]	lmbench, postmark, unpack kernel, compile Linux, Apache, Memcache, redis, php, pybench	Native
BEEP [47]	Apache, Vim, Firefox, wget, Cherokee, w3m, ProFTPd, yafc, Transmission, Pine, bash, mc, sshd, sendmail	Native
RAIN [36]	SPEC CPU 2006, cp linux, wget, compile libc, Firefox, SPLASH-3	Native
Sciunit [77]	Workflows (VIC, FIE)	Native
LPS [22]	IOR benchmark, read/write, MDTest, HPCG	Native
LPROV [80]	Apache, simplehttp, proftpd, sshd, firefox, filezilla, lynx, links, w3m, wget, ssh, pine, vim, emacs, xpdf	Native
MCI [45]	Firefox, Apache, Lighttpd, nginx, ProFTPD, CUPS, vim, elinks, alpine, zip, transmission, lftp, yafc, wget, ping, procps	BEEP
RTAG [37]	SPEC CPU 2006, scp, wget, compile llvm, Apache	RAIN
URSPRING [66]	open/close, fork/exec/exit, pipe/dup/close, socket/connect, CleanML, Vanderbilt, Spark, ImageML	Native, SPADE
PROV-IO [32]	Workflows (Top Reco, DASSA), I/O microbenchmark (H5bench)	Native
Namiki et al. [57]	I/O microbenchmark (BT-IO)	Native

to intercept syscalls and redirect them to files in the archive. PTU uses a modified version of CDE that works on all of our benchmarks, so we can use that as a proxy.

- **ltrace** similar to strace, but it traces dynamic library calls not necessarily syscalls. It still uses ptrace.
- **strace** is a well-known system program that uses Linux's ptrace functionality to record syscalls, their arguments, and their return code to a file. strace even parses datastructures to write strings and arrays rather than pointers. In this work, we use an strace configuration that captures all file-related syscalls but read/write[32], file-metadata realated syscalls, socket- and IPC-related sycalls but send/recv, and process-related syscalls.
- **fsatrace** reports file I/O using library-interpositioning, a technique where a program mimics the API of a standard library. Programs are written to call into the standard library, but the

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[32]We do not need to capture individual reads and writes, so long as we capture that the file was opened for reading/writing.

---

loader sends those calls to the interpositioning library instead. The interpositioning library can log the call and pass it to another library (possibly the "real" one), so the program's functionality is preserved. This avoids some context-switching overhead of ptrace, since the logging happens in the tracee's process.

- **CARE** is a record/replay tool inspired by CDE. However, CARE has optimizations enabling it to copy fewer files, and CARE archives can be replayed using chroot, lxc, or ptrace (by emulating chroot); CDE only supports ptrace, which is slower than the other two.
- **RR** [59] is a record/replay tool. It captures more syscalls than just file I/O, including getrandom and clock_gettime and it is able to replay its recordings in a debugger. Where other record/replay tools try to identify the relevant files, RR only memorizes the responses to each syscall, so it can only replay that exact code path. CDE, CARE, ReproZip, PTU, and Sciunit allow one to replay a different binary or supply different inputs in the filesystem of an existing recording.
- **ReproZip** is a record/replay inspired by CDE. ReproZip archives can be replayed in Vagrant, Docker, Chroot, or natively. Unlike other record/replay tools, ReproZip explicitly constructs the computational provenance graph.
- **PTU** (Provenance-To-Use) is an adaptation of CDE which explicitly constructs the computational provenance graph.
- **Sciunit** is a wrapper around PTU that also applies block-based deduplication.

D NOTE ON FAILED REPRODUCIBILITY

While we could run **ltrace** on some of our benchmarks, it crashed when processing on the more complex benchmarks. We localized the problem to the following code[33]:

```
/* FIXME: not good -- should use dynamic allocation. 19990703 mortene. */
if (proc->callstack_depth == MAX_CALLDEPTH - 1) {
  fprintf(stderr, "%s: Error: call nesting too deep!\n", __func__);
  abort();
  return;
}
```

CDE can run some of our benchmarks, but crashes when trying to copy from the tracee process to the tracer due to ret == NULL[34]:

```
static char* strcpy_from_child(struct tcb* tcp, long addr) {
  char* ret = strcpy_from_child_or_null(tcp, addr);
  EXITIF(ret == NULL);
  return ret;
}
```

The simplest explanation would be that the destination buffer is not large enough to store the data that strcpy wants to write. However, the destination buffer is PATHMAX.

E OPEN SOURCE CONTRIBUTIONS

The actual benchmark set and statistical analysis are open-source:
- https://github.com/charmoniumQ/prov-tracer/

This work necessitated modifying Spack, Sciunit, PTU, jupyter-contrib-nbextensions, Nixpkgs, ftpbench, and benchexec. Where appropriate, we submitted as pull-requests to the respective upstream projects.

The following were merged PRs developed as a result of this work:
- https://github.com/depaul-dice/sciunit/pull/35

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[33]See https://gitlab.com/cespedes/ltrace/-/blob/8eabf684ba6b11ae7a1a843aca3c0657c6329d73/handle_event.c#L775
[34]See https://github.com/usnistgov/corr-CDE/blob/v0.1/strace-4.6/cde.c#L2650

- https://github.com/spack/spack/pull/42159
- https://github.com/spack/spack/pull/42199
- https://github.com/spack/spack/pull/42114
- https://github.com/selectel/ftpbench/pull/5
- https://github.com/selectel/ftpbench/pull/4
- https://github.com/sosy-lab/benchexec/pull/984
- https://github.com/NixOS/nixpkgs/pull/263829
- https://github.com/NixOS/nixpkgs/pull/257396

The following are open PRs developed as a result of this work:

- https://github.com/spack/spack/pull/39902
- https://github.com/spack/spack/pull/42131
- https://github.com/spack/spack/pull/41048
- https://github.com/sosy-lab/benchexec/pull/990
- https://github.com/depaul-dice/sciunit/pull/36
- https://github.com/depaul-dice/provenance-to-use/pull/4
- https://github.com/depaul-dice/provenance-to-use/pull/5
- https://github.com/ipython-contrib/jupyter_contrib_nbextensions/pull/1649
- https://github.com/NixOS/nixpkgs/issues/268542

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