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

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ABSTRACT

Computational provenance has many important applications, especially to reproducibiliy. System-level provenance collectors claim to be able to track provenance data without requiring the user to change anything about their application. Anecdotally, however, system-level provenance collectors are not commonly used in computational science. This work aims to bring research in provenance collection closer to practice by evaluating prior work on a common benchmark subset and identifying gaps in prior work. This subset can be used a goalposts for future work on system-level 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 [67]. 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, 38, 65, 77], package managers for fine-grained management of dependencies [28, 47], interactive notebooks and workflows [11, 25, 46], and online platforms for archiving and sharing computational experiments [19, 30, 82, 83]. 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 [27]; 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, classify their method-of-operation, and reproduce the ones that meet specific criteria. We successfully reproduced 9 out of 15 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 5% 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 an application in particular provenance collector based on the application's performance characteristics (e.g., number of file syscalls per second). Despite trying linear regression, with and without rank reduction, with

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[1]DSK: usable globally or perhaps in particular situations?

and without feature selection, our best model is still quite inaccurate, showing performance overhead of provenance collector is not as simple.

The remainder of the paper is structured as follows. In Section 2, we motivate the value of provenance and the pros/cons of system-level provenance compared to application- and workflow-level provenance.

2 BACKGROUND

Provenance tools and data have many potential applications, including the following from Pimentel et al. [71] and Sar and Cao [76]:

1. **Reproducibility**. A description of the inputs and processes used to generate a specific output can aid manual and automatic reproduction of that output[2]. Empirical studies [21, 32, 87, 94] 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 reproduciblity 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 [27]. 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 Figure 1, including all file dependencies of the process without knowledge of the underlying program or programming language.

We defer to the cited works for details on versioning artifacts [8] and cycles [62]. 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 extermely 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.

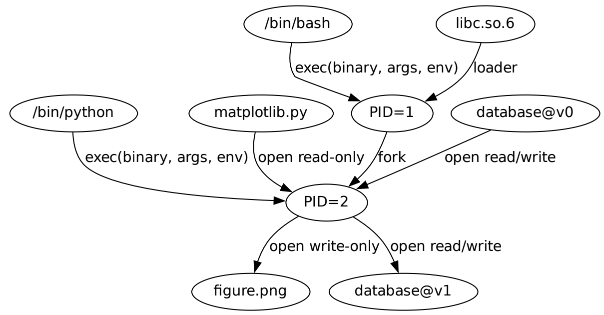
2.1 Prior work

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 [53] uses 3 provenance collectors (CamFlow, SPADE, and OPUS), but they are solely concerned with the differences betwen representations of provenance, not performance.

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

(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.



(b) Abridged graph of events. The arrows point in the direction of dataflow. Other authors use other conventions for what they render as nodes, edges, and arrow direction.

Figure 1: An abridged list and graph of events that a hypothetical system-level provenance collector would collect from a Bash script that invokes Python to plot some data. 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.

On the other hand, benchmark subsetting is a well-studied area. This work mostly follows Yi et al. [92] paper which evaluates subsetting methodologies and determine that dimensionality reduction and clustering is broadly a good strategy. Phansalkar et al. [70] apply dimensionality reduction and clustering to SPEC CPU benchmarks.

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 [78] 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 [17, 18].

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[3], 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 used in computational science 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 overwritten, so the user can know what commands actually worked [16].

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.

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

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

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 [63]. 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 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. [92], 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. [92] 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. [92], 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 ratio is be distributed symmetrically, but the logarithm may be. Suppose some provenance collector makes programs take roughly twice as long, but with a large amount of variance, so the expected value of the ratio is 2. A symmetric distribution would require the probability of observing a ratio of -1 for a particular program is equal to the probability of observing a ratio of 5, but a ratio of -1 is clearly impossible, while 5 is may possible due to the large variance. On the other hand, $\log x$ maps postive numbers (like ratios) to real numbers (which may be symmetrically distributed); $e^{0.3} \approx 2$, $e^{0.7} \approx 5$, and $e^{-0.1} = 0.9$ (negative logs indicate a speedup rather than slowdown, which are theoretically possible). Another reason: exp(arithmean(log(x))) is equal to geomean(x), which is preferred over arithmean(x) for performance ratios according to Mashey [59].
2. The ratio of CPU time to wall time. When limited to a single core on an unloaded system, wall time includes I/O but CPU time does not.
3. The number of syscalls in each category per wall time second, where the categories consist of socket-related, file-metadata-related, directory-related, file-related, exec-related, fork-related, exit-related syscalls, IPC-related syscalls, and chdir syscalls.

In order to choose the subset, we will try clustering (k-means and agglomerative clustering with Ward linkage[4]), 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

[4]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.

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, 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 $n_{\text{feats}} k + k n_{\text{bmarks}}$ 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 $k n_{\text{bmarks}}$ 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 Appendix A for more in-depth description of each collector. The second column shows the "collection method." See Appendix B 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 [93], which is too slow for practical use.
- **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 instrumention tool called Intel PIN. Being limited to certain CPUs violates our goal of promulgating reproducibility to as many people as possible.
- **No source.** 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 [5]. 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, Sciunit, PTU).** 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, 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.

From this we observe:

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

[6] 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 [66]	tracing	Reproduced
ReproZip [20]	tracing	Reproduced
CARE [37]	tracing	Reproduced
Sciunit [69]	tracing	Reproduced/rejected
PTU [69]	tracing	Reproduced/rejected
CDE [33]	tracing	Reproduced/rejected
ltrace	tracing	Reproduced/rejected
SPADE [29]	audit, FS, or compile-time	Needs more time
DTrace [1]	audit	Needs more time
eBPF/bpftrace	audit	Needs more time
SystemTap [73]	audit	Needs more time
PROV-IO [34]	lib. ins.	Needs more time
OPUS [8]	lib. ins.	Not reproducible
CamFlow [68]	kernel ins.	Requires custom kernel
Hi-Fi [72]	kernel ins.	Requires custom kernel
LPM/ProvMon [10]	kernel ins.	Requires custom kernel
Arnold[24]	kern ins.	Requires custom kernel
LPS [23]	kern ins.	Requires custom kernel
RecProv [41]	tracing	No source
FiPS [85]	FS	No source
Namiki et al. [64]	audit	No source
LPROV [89]	kernel mod., lib. ins.	No source
S2Logger [84]	kernel mod.	No source
ProTracer [56]	kernel mod.	No source
PANDDE [26]	kernel ins., FS	No source
PASS/Pasta [62]	kernel ins., FS, lib. ins.	No source
PASSv2/Lasagna [61]	kernel ins.	No source
Lineage FS [76]	kernel ins.	No source
RTAG [40]	bin. ins.	No source
BEEP [51]	bin. ins.	Requires HW
libdft [43]	bin., kernel, lib. ins.	Requires HW
RAIN [39]	bin. ins.	Requires HW
DataTracker [81]	compile-time ins.	Requires HW
MPI[55]	compile-time ins.	Requires recompilation
LDX [48]	VM ins.	Requires recompilation
Panorama [93]	VM ins.	VMs are too slow
PROV-Tracer [80]	audit	VMs are too slow
ETW [5]	audit	Not for Linux
Sysmon [58]	audit	Not for Linux
TREC [88]	tracing	Not for Linux
URSprung [74]	audit	Not for Linux[6]
Ma et al. [54]	audit	Not for Linux
ULTra [15]	tracing	Not for Linux

- 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 when the CPU is constant and the I/O subsystem is changed, the total running time is influenced by I/O-related overhead.
- cp is the slowest benchmark. It even induces a 45% overhead on fsatrace.

4.3 Subsetted Benchmarks

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

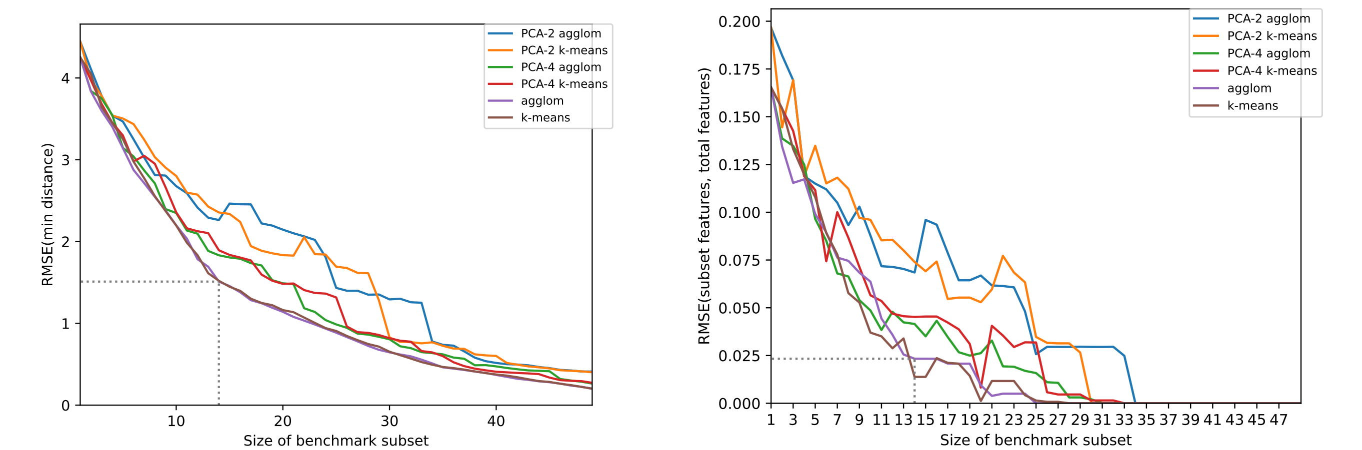
1. The features are already standardized, so PCA has little to offer other than rotation and truncation. However, the truncation is throwing away potentially useful data. Since we have a large number of benchmarks, and the space of benchmarks is quite

Table 3: Benchmarks implemented by this work. For brevity, we consider categories of benchmarks in Table 6. See Appendix E for a description of each benchmark group and how we implemented them.

Prior works	This work	Instances	Benchmark group and examples from prior work
12	yes	5	HTTP server/traffic
10	yes	2	HTTP server/client
10	yes	8	Compile user packages
9	yes	19 + 1	I/O microbenchmarks (lmbench + Postmark)
9	no		Browsers
6	yes	3	FTP client
5	yes	1	FTP server/traffic
5	yes	5×2	Un/archive
5	yes	5	BLAST
5	yes	10	CPU benchmarks (SPLASH-3)
5	yes	8	Coreutils and system utils
3	yes	2	cp
2	yes	2	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

Table 4: This table shows percent overhead of the mean walltime when running with a provenance collector versus running without provenance. A value of 1% means the execution in that cell takes 1.01 times the execution without provenance. Negative slowdown can occur sometimes due to random statistical noise. We aggregate values using geometric mean (which is associative).

	(none)	fsatrace	CARE	strace	RR	ReproZip
BLAST	0	-0	1	2	93	8
CPU bench SPLASH-3	0	2	7	18	47	74
Compile Spack	0	0	121	114	569	363
Compile gcc	0	4	135	222	316	342
Compile latex	0	5	70	39	19	288
Data science Notebook	0	1	15	33	21	192
Data science python	0	4	84	83	151	342
FTP srv/client	0	0	2	4	5	18
HTTP srv/client	0	-32	11	19	114	207
HTTP srv/traffic	0	5	138	421	1144	730
IO bench lmbench	0	-10	1	3	10	36
IO bench postmark	0	13	261	804	292	1962
Un/archive Archive	0	-2	75	121	180	139
Un/archive Unarchive	0	3	42	118	193	147
Utils	0	16	113	285	1366	693
Utils bash	0	22	121	45	567	3864
VCS checkout	0	6	73	188	178	428
cp	0	42	650	393	246	5895
Total (gmean)	0	0	45	69	145	196



(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.

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 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 Figure 4 and Table 5.

Figure 3a shows the a posteriori clusters with colors. Figure 3b 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.

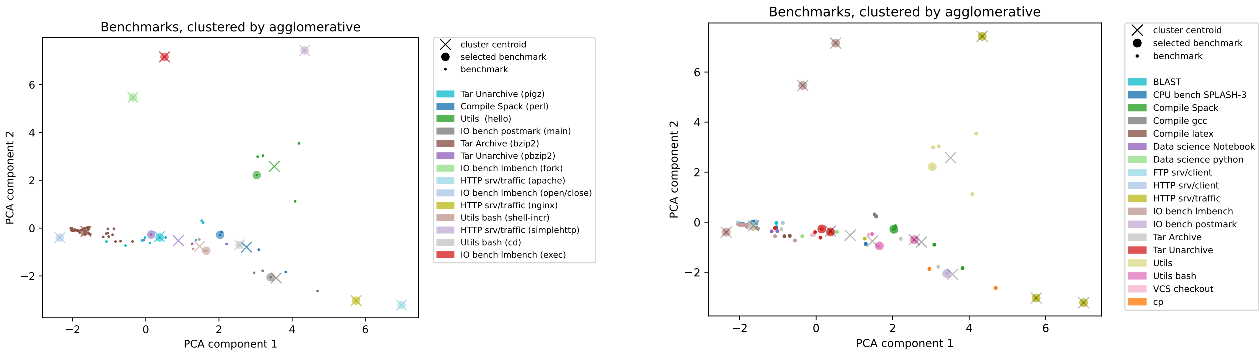
To elucidate the structure of the clusters, we plotted a dendrogram (Figure 4) and listed the members of each cluster (Table 5). We offer the following observations:

1. Fork and exec are close in feature-space, probably because programs usually do both.
2. cd and shell-echo are near each other. It is surprising that blastn is also near cd and shell-echo, but they both have similar cputime-to-walltime ratios.
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.

4.3.1 Our suggestion. The programs in lmbench have very different performance characteristics (see Figure 3b). 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[7], 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

[7]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.



(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 Figure 3a.

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.

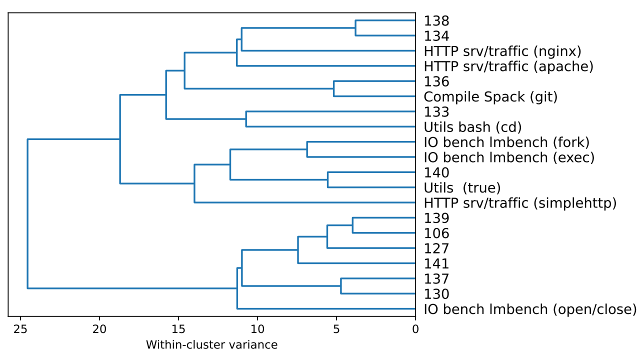


Figure 4: Dendrogram showing the distance between clusters. A fork at $x = x_0$ indicates that below that threshold of within-cluster variance, the two children clsuters are far away enough that they should be split into two; conversely, above that threshold they are close enough to be combined. We label 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.

need not go through the trouble of setting up Nginx, and although Apache appears a cluster representative, that cluster is also similar to Postmark.

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:

- 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

Tar Unarchive (pigz)	0.0	Compile gcc (hello-world), Compile gcc (threads), Data science python (python-hello-world), IO bench lmbench (fstat), IO bench lmbench (stat), Tar Unarchive (gzip), Tar Unarchive (unarchive), VCS checkout (git git-repo-1), VCS checkout (hg hg-repo-1)
Compile Spack (perl)	5.7	Compile Spack (git), Compile Spack (hdf5 mpi), Compile Spack (python)
Utils (hello)	8.0	Utils (echo), Utils (ls), Utils (ps), Utils (true)
IO bench postmark (main)	8.8	Tar Archive (archive), cp (linux), cp (smaller)
Tar Archive (bzip2)	55.0	BLAST (blastn), BLAST (blastp), BLAST (blastx), BLAST (mega), BLAST (tblastn), BLAST (tblastx), CPU bench SPLASH-3 (cholesky), CPU bench SPLASH-3 (lu), CPU bench SPLASH-3 (nsquared), CPU bench SPLASH-3 (ocean), CPU bench SPLASH-3 (radiosity), CPU bench SPLASH-3 (radix), CPU bench SPLASH-3 (raytrace), CPU bench SPLASH-3 (spatial), CPU bench SPLASH-3 (volrend), Compile latex (doc1), Compile latex (doc2), Data science Notebook (nb-1), Data science Notebook (nb-2), Data science Notebook (nb-3), Data science python (python-import), FTP srv/client (curl), FTP srv/client (lftp), FTP srv/client (wget), HTTP srv/client (curl), HTTP srv/client (wget), HTTP srv/traffic (minihttp), IO bench lmbench (bw_file_rd), IO bench lmbench (bw_pipe), IO bench lmbench (bw_unix), IO bench lmbench (catch-signal), IO bench lmbench (fs), IO bench lmbench (getppid), IO bench lmbench (install-signal), IO bench lmbench (mmap), IO bench lmbench (page-fault), IO bench lmbench (protection-fault), IO bench lmbench (read), IO bench lmbench (select-file), IO bench lmbench (select-tcp), IO bench lmbench (write), Tar Archive (gzip), Tar Unarchive (bzip2)
Tar Unarchive (pbzip2)	7.7	HTTP srv/traffic (lighttpd), Tar Archive (pbzip2), Tar Archive (pigz)
IO bench lmbench (fork)	1.0	
HTTP srv/traffic (apache)	0.7	
IO bench lmbench (open/close)	2.2	
HTTP srv/traffic (nginx)	2.0	
Utils bash (shell-incr)	4.5	CPU bench SPLASH-3 (fft), Utils bash (shell-echo)
HTTP srv/traffic (simplehttp)	1.5	
Utils bash (cd)	1.5	
IO bench lmbench (exec)	1.5	
all	100.2	

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.

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

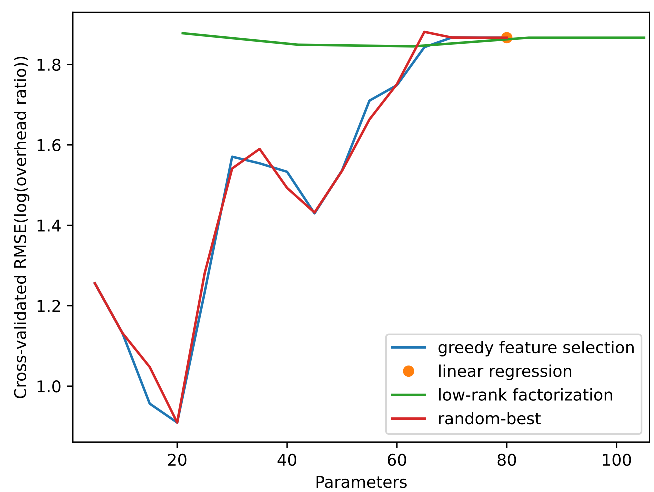


Figure 5: Competition between predictive performance models. Pure linear regression only has one instance with $n_{\text{feats}} \times n_{\text{bmarks}}$ parameters; the others have with varying numbers of parameters.

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 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 [91].

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. 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 [66]). 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), 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 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 [45], 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 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.

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 NOTABLE PROVENANCE COLLECTORS

- **CDE** is a record/replay tool proposed by Guo and Engler [33]. During record, CDE uses `ptrace` to intercept its syscalls, and copy relevant files into an archive. During rerun, can use `ptrace` 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[8], 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

[8] 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** [66] 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.

B 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 [57], enhanced Berkeley Packet Filter (eBPF) [2], kprobes [44], 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 [31].
- **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.

C 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.

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

Publication	Benchmarks	Comparisons
TREC [88]	open/close, compile Apache, LaTeX	Native
ULTra [15]	getpid, LaTeX, Apache, compile package	Native, strace
PASS [62]	BLAST	Native ext2
Panorama [93]	curl, scp, gzip, bzip2	Native
PASSv2 [61]	BLAST, compile Linux, Postmark, Mercurial, Kepler	Native ext3, NFS
SPADEv2 [29]	BLAST, compile Apache, Apache	Native
Hi-Fi [72]	lmbench, compile Linux, Postmark	Native
libdft [43]	scp, {tar, gzip, bzip2} x {extract, compress}	PIN
PTU [69]	Workflows (PEEL0, TextAnalyzer)	Native
LogGC [50]	RUBiS, Firefox, MC, Pidgin, Pine, Proftpd, Sendmail, sshd, vim, w3m, wget, xpdf, yafc, Audacious, bash, Apache, mysqld	None[9]
CARE [37]	Compile perl, xz	Native
Arnold[24]	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. [54]	TextTransfer, Chromium, DrawTool, NetFTP, AdvancedFTP, Apache, IE, Paint, Notepad, Notepad++, simplehttp, Sublime Text	Native
ProTracer [56]	Apache, miniHTTP, ProFTPD, Vim, Firefox, w3m, wget, mplayer, Pine, xpdf, MC, yafc	Auditd, BEEP
LDX [48]	SPEC CPU 2006, Firefox, lynx, nginx, tnftp, sysstat, gif2png, mp3info, prozilla, yopsweb, ngircd, gocr, Apache, pbzip2, pigz, axel, x264	Native
PANDDE [26]	ls, cp, cd, lpr	Native
MPI [55]	Apache, bash, Evince, Firefox, Krusader, wget, most, MC, mplayer, MPV, nano, Pine, ProFTPd, SKOD, TinyHTTPd, Transmission, Vim, w3m, xpdf, Yafc	Audit, LPM-HiFi
CamFlow [68]	lmbench, postmark, unpack kernel, compile Linux, Apache, Memcache, redis, php, pybench	Native
BEEP [51]	Apache, Vim, Firefox, wget, Cherokee, w3m, ProFTPd, yafc, Transmission, Pine, bash, mc, sshd, sendmail	Native
RAIN [39]	SPEC CPU 2006, cp linux, wget, compile libc, Firefox, SPLASH-3	Native
Sciunit [86]	Workflows (VIC, FIE)	Native
LPS [23]	IOR benchmark, read/write, MDTest, HPCG	Native
LPROV [89]	Apache, simplehttp, proftpd, sshd, firefox, filezilla, lynx, links, w3m, wget, ssh, pine, vim, emacs, xpdf	Native
MCI [49]	Firefox, Apache, Lighttpd, nginx, ProFTPd, CUPS, vim, elinks, alpine, zip, transmission, lftp, yafc, wget, ping, procps	BEEP
RTAG [40]	SPEC CPU 2006, scp, wget, compile llvm, Apache	RAIN
URSPRING [74]	open/close, fork/exec/exit, pipe/dup/close, socket/connect, CleanML, Vanderbilt, Spark, ImageML	Native, SPADE
PROV-IO [34]	Workflows (Top Reco, DASSA), I/O microbenchmark (H5bench)	Native
Namiki et al. [64]	I/O microbenchmark (BT-IO)	Native

D NOTE ON FAILED REPRODUCIBILITY

- While we could run **ltrace** on some of our benchmarks, it crashed when processing on the more complex benchmarks, for example

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

FTP server/client. We localized the problem to the following code[10]:

```
/* 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 on others, for example BLAST. THe crash occurs when trying to copy from the tracee process to the tracer due to `ret == NULL`[11]:

```
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`.
- **PTU** seemed to work outside of our container, but crashed strangely inside the container.
- **Sciunit** works on most benchmarks, but exhausts the memory of our system when processing FTP server/client and Spack compile package. We believe this is simply due to the benchmarks manipulating a large number of files and Sciunit trying to deduplicate them all.

E BENCHMARK DESCRIPTIONS

- 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 Wget). We implemented 1 FTP server (ProFTPD) running against traffic from httpbench[12] 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.
- 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 [60], which benchmarks individual syscalls, Postmark [42], which focuses on many small I/O operations (typical for web servers), IOR [79], H5bench [52] and BT-IO[13], 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 [22], 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 [35], SPLASH-3 [75], SPLASH-2 [90] and HPCG [36]. 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 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,

[10] See https://gitlab.com/cespedes/ltrace/-/blob/8eabf684ba6b11ae7a1a843aca3c0657c6329d73/handle_event.c#L775

[11] See https://github.com/usnistgov/corr-CDE/blob/v0.1/strace-4.6/cde.c#L2650

[12] See https://github.com/selectel/ftpbench

[13] See https://www.nas.nasa.gov/software/npb.html

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.

F 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 are merged PRs developed as a result of this work:

- https://github.com/depaul-dice/sciunit/pull/35
- 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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