Provenance-Aware Storage Systems

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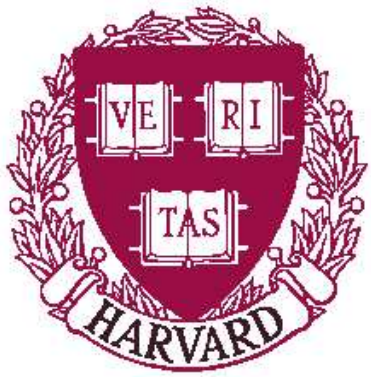
TR-05-06



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Abstract

A Provenance-Aware Storage System (PASS) is a storage system that automatically collects and maintains *provenance* or *lineage*, the complete history or ancestry of an item. We discuss the advantages of treating provenance as meta-data collected and maintained by the storage system, rather than as manual annotations stored in a separately administered database. We present a PASS implementation, discussing the challenges and performance cost, and the new functionality it enables. We show that with reasonable overhead, we can provide useful functionality not available in today's file systems or provenance management systems.

1 Introduction

Provenance is traditionally the ownership history of an object. In digital systems, ownership history includes a description of how the object was derived [4]. In software development, we express provenance in build rules and track it with source code control systems. Archivists maintain provenance meta-data to support document viability, renderability, understandability, authenticity, and identity in preservation contexts [20]. Scientific reproducibility requires provenance to precisely identify input data sets, experimental procedures, and parameterization. The business community uses "lineage" to refer to the history of a document. In all of these domains provenance increases an object's value.

Digital provenance is typically stored in standalone database systems, maintained in parallel with the data to which it refers. Separating provenance from its data introduces problems, such as: ensuring consistency between the provenance and the data, enforcing provenance maintenance, and preserving provenance during backup, restoration, copies, etc.

Provenance should be maintained by the storage system, since provenance is merely meta-data and storage systems manage meta-data. Managing provenance in the storage system provides many advantages:

- The storage system can generate system-level provenance automatically, freeing users from manually tracking provenance and tool designers from constructing application-specific provenance solutions.
- Provenance collection and management are transparent. Users take no special actions, so provenance collection is the norm rather than the exception.
- The tight coupling between data and provenance provided by the storage system avoids provenance loss both during normal activity and during management procedures such as backup, restoration, or data migration.
- System-level provenance produces a level of meta-data completeness difficult or impossible to achieve with application-level solutions.

A *provenance-aware storage system* (PASS) is a storage system that automatically collects, stores, manages, and provides search for provenance. Provenance-aware storage offers functionality unavailable in conventional systems. For example, comparing the provenance of two pieces of derived data, such as simulation results, can reveal changes between two program invocations. We can use provenance to identify the particular workflow that produced a document; this provides a tight coupling between workflow management and information life-cycle management (ILM). Searchable provenance enables queries like "Who is using my dataset?" or "On whose data am I depending when I run this experiment?" System-level provenance enables identification of configuration changes that affect applications.

We present the design and evaluation of a prototype PASS. A PASS is both a provenance solution and substrate upon which we can support other provenance systems. Domains characterized by command-line invocation of data transformations are well served by PASS and may not require any domain-specific solution. Domains that require GUI-driven applications or application environments still derive benefit from integration with provenance-aware storage. This paper contributes: An

approach to automatic provenance collection and maintenance; a prototype that demonstrates the efficacy and practicality of the PASS concept; an evaluation of PASS functionality and overhead; and a research agenda for future work on PASS.

The rest of this paper is organized as follows. In Section 2, we present several novel use cases that PASS enables. In Section 3, we compare PASS to existing provenance systems. In Section 4, we outline the requirements for PASS and explain how PASS interacts with existing provenance systems and file system utilities. In Section 5, we describe our PASS implementation. In Section 6, we quantify the overheads PASS introduces. We conclude in Section 7 with a discussion of open research issues and the long-term PASS agenda.

2 Novel Functionality

PASS provides novel features not available in other systems. In this section, we present use cases and examples that demonstrate the power of provenance-aware storage.

2.1 Understanding System Dependencies

Early experimentation with PASS presented some surprising results. We found that some objects we created unexpectedly included `/bin/mount` in their provenance. This was baffling, since we were executing relatively simple commands such as `sort a > b`.

We discovered that the Linux C library frequently reads the mount table, `/etc/mtab`, to determine where `procfs` is mounted before using it. `mount` and `umount` update `/etc/mtab`, so these programs quite correctly appeared in our sorted file's ancestry.

This behavior caused a slight problem. Since we have not been running with the operating system installed on a PASS volume, `/etc/mtab` has no persistent provenance. In such cases, we copy the object's provenance into the output file (`b`), where it is difficult to ignore. In the provenance displayed in this paper, we prune `/etc/mtab`'s ancestry using `ptrunc`, a provenance truncation utility. If `/etc/mtab` were on a PASS volume, only the `INPUT` record referencing `/etc/mtab` would appear in `b`'s provenance, and there would be no need for pruning.

2.2 Intrusion Detection

Since a PASS collects provenance inside the operating system and file system, it provides a detailed record of how objects change. This feature can be used in some cases both for intrusion detection and subsequent forensic analysis.

One of the authors uses a UNIX version of the Windows trash bin, aliasing `rm` (remove) to

```
mv !* ~/etc/garbage
```

which moves the target files to a garbage directory. Quite unexpectedly, several (private) recently deleted files appeared in `~/public_html`. This happened on a non-PASS system, so it took nearly a half hour to discover that `~/etc/garbage` had been symbolically linked to `~/public_html`. Had we had provenance for the files in `~/public_html`, we would have immediately observed that they had been explicitly moved from their original locations. Had we had application-specific provenance provided by the login shell, we would have known immediately that this arose from the `rm` alias.

2.3 Detecting System Changes

Because we collect provenance at the system level, we know the operating system and library versions and the environment present when an object was created. For example, the output of `sort a > b` depends on the value of the environment variable `LC_COLLATE`. This makes it easy to explain why two seemingly identical invocations produce different results, because the environment is encapsulated in the provenance. Tracking such changes in libraries and tools is similarly straightforward. PASS easily identifies changes in the environment, libraries, the operating system, or a tool.

2.4 Script Generation

Early users were most excited by PASS's potential to create scripts that reproduce a file originally created through trial and error. We find this one of the most compelling features of PASS.

Recently one of the authors was preparing a paper and discovered that one of the PostScript figures was being generated with the wrong bounding box. This produced a tiny figure surrounded by blank space. The solution (after several hours of experimental tinkering as the submission deadline approached) required creating a huge bitmap, cropping it with an image-manipulation tool, and then converting it to a different format for incorporation into the paper. This is a multistage process; using its provenance to capture the exact sequence of operations that produced the correct image would have been extremely useful. We discuss another example of script generation in Section 6.4.

2.5 Build Debugging

Large build environments are often missing elements of their dependency lists. These become apparent

when a build repeatedly produces a visibly flawed executable. The traditional solution (suggested explicitly for the Linux kernel) is simply to `make clean` after any change.

PASS easily identifies an inconsistent build: in nearly all build environments, it is incorrect for two different versions of the same source or intermediate file to simultaneously be ancestors of the same output. Examining the complete ancestry of an obsolete file reveals immediately the intermediate file that should have been rebuilt, identifying the missing dependency.

3 Provenance Solutions

Provenance is pervasive in scientific computing, business, and archival. Simmhan et al. categorize provenance solutions in terms of their architecture: database-oriented, service-oriented, and "other" [28]. We borrow and enrich this taxonomy. We extend database-oriented approaches to include file and file-system-oriented approaches such as PASS. The service-oriented architecture encompasses myriad grid-based solutions. Simmhan's "other" category refers to scripting architectures; we treat software development tools, i.e., source code control and build systems, as a specific instance of a scripting architecture. To these three categories, we add "environment architectures" where users perform all tasks in a unified environment that tracks provenance.

3.1 File, File System and Database Approaches

One obvious approach to provenance maintenance is to include provenance inside the corresponding data file. Astronomy's Flexible Image Transport (FITS) format [17] and the Spatial Data Transfer Standard (SDTS) [23] are examples of this approach. A FITS file header consists of a collection of tagged attribute/value pairs, some of which are provenance. Whenever a file is transformed, additional provenance is added to this header. This approach addresses the challenge of making the provenance and data inseparable, but it introduces other disadvantages. It is expensive to search the attribute space to find objects meeting some criteria. Tools that operate on such files must read and write the headers and be provenance-aware. The validity and completeness of the provenance is entirely dependent upon the tools that process the data. Worse yet, there is no way to determine if provenance is complete or accurate.

The Lineage File System (LinFS) [14] is most similar to PASS. LinFS is a file system that automatically tracks provenance at the file system level, focusing on executables, command lines and input files as the only source of provenance, ignoring the hardware and software environment in which such processes run. As shown in Section 2, complete system-level provenance provides functionality unavailable in other systems. A second, and perhaps more important, difference is that LinFS delays provenance collection, performing it at user-level by writing it to an external database. This loses the tight coupling we desire and introduces additional security challenges.

Trio [26] is to databases what a PASS is to file systems. Trio is a centralized database system that manages both data and its provenance. Trio extends SQL to support lineage and accuracy information when requested by a user or application. While PASS and LinFS operate at the granularity of files, Trio tracks provenance at tuple granularity. Unlike PASS, Trio's initial focus is on formalizing a query language and data model, and, to the best of our knowledge, has not yet been implemented.

Trio and PASS are complementary. Since PASS tracks provenance at file-level granularity, it will not be useful for tracking database updates. However, it is likely to be more efficient and useful for tracking provenance of file system objects.

3.2 Service-oriented Architectures

Many of the computational sciences use provenance systems designed for grid environments since provenance facilitates scientific verification, reproducibility, and collaboration. Most of these systems use a directed-acyclic-graph (DAG) representation to describe workflows. The tools that understand these workflows collect provenance and transmit it to a grid provenance service. For example, Globus [7] is used widely by high-energy physicists and includes the Metadata Catalog Service (MCS) [6] that stores metadata for logical data objects. MCS includes a set of common attributes and permits inclusion of domain- or application-specific attributes. San Diego SuperComputer's Storage Request Broker [2, 25] has a Metadata Catalog similar to the MCS.

Chimera [8] is a virtual data system that providing a virtual data language (VDL) and a virtual data catalog (VDC). The VDC implements a virtual data schema defining the objects and relations used to capture descriptions of program invocations and to record potential or actual invocations. The VDL is used for defining and manipulating data derivation procedures stored in the VDC. Chimera can be used to generate Grid workflows or plans from the derivations.

All these systems place the responsibility for provenance maintenance with the grid tools, storing provenance in a system parallel to the data storage. These systems create and maintain provenance only for data that is processed by provenance-aware tools, so there is no mechanism to capture provenance for local experimentation or

operations issued outside the bounds of these tools. Once again, PASS provides capabilities not found in these systems and is complimentary to their approaches. A grid-accessible PASS provides the advantages of both worlds.

3.3 Scripting Architectures

Software developers manage provenance manually using source code control and build systems. Though powerful, these systems rely more on manual intervention than PASS does. Build systems maintain dependencies *after* those dependencies have been specified; PASS derives dependencies based upon actual execution. Source code control systems track differences between manually-declared versions, but a manually-entered commit message is typically the only expression of the transformation between those two versions. Thus, the quality of provenance in these systems depends on the quality of commit messages and build configuration files. For example, makefiles that track include dependencies properly are considerably more useful than those that do not.

The source code control systems most similar to PASS are ClearCase (and its predecessor DSEE) and Vesta. ClearCase [5] is a source code control system, and like PASS, it is based on a custom file system. The file system serves as the source code repository, and the build system relies on the standard `make` utility. The custom file system tracks and maintains system dependencies to avoid work in future builds and to trigger rebuilds. PASS also captures these dependencies. As is the case with all build systems of which we are aware, ClearCase requires that critical dependencies be specified *a priori*; PASS derives dependencies by observation.

Vesta [11] is a second generation build system developed at DEC Systems Research Center (SRC). The key design goals were making builds repeatable, consistent, and incremental. As with DSEE, Vesta relies on a custom build environment that monitors the build process to extract dependencies and record complete environment information to facilitate repeatable builds. Like DSEE and other source code control systems, it relies on an *a priori* description of the derivation process. As a result, while extraordinarily useful for software development, it ignores the central PASS challenge: automatically generating the derivation rules as a system runs.

3.4 Environment Architectures

Other domains have environments that track work and record provenance as Vesta does for software development. GenePattern [10] is an environment for computational biologists, the Collaboratory for Multi-scale Chemical Sciences (CMCS) [19] is an environment for chemists, and the Earth System Science Workbench (ESSW) [9] is an environment for earth scientists. As long as a user modifies data exclusively in one of these environments, the environment can effectively track provenance. However, operating on data outside the environment or moving data between two different environments breaks the provenance chain. Traditional file system utilities, such as backup and restore, or regular utilities, such as remove and rename, can also break the provenance chain. The semantic information these environments provide is powerful; we propose PASS as a substrate under such environments. This hybrid architecture avoids disruptions in provenance and adds the ability to augment an environment's provenance with provenance about the operating system, libraries, and other system-level information.

3.5 Summary

Provenance-aware storage provides functionality not found in today's provenance solutions while being compatible with most of them. Ultimately, end-to-end provenance will require multiple approaches working in concert. As shown by our evaluation, using PASS as a substrate for the end-to-end solution provides significant benefits.

4 The PASS Vision

PASS collects and maintains provenance for all the objects stored in it. In service-oriented architectures, provenance is frequently captured in a DAG. This is also true in PASS. PASS automatically generates the DAG describing the relationship between processes running on it and the files stored in it. Our prototype tracks provenance at a file granularity, but this is not an inherent property of PASS; a system could track provenance at finer or coarser granularities [15] (e.g., bytes, lines, directories or whole volumes).

Data on a PASS is considered to be either new data or the output of some process. The provenance of a process' output must include:

- A unique reference to the particular instance of the program that created it.
- References to all input files.
- A complete description of the hardware platform on which the file was derived.
- A complete description of the operating system and system libraries that produced the output.
- The command line.
- The process environment.

- Parameters to the process (frequently encapsulated in the command line or input files)

- Other data (e.g., the random number generator seed) necessary to make pseudo-random computation repeatable.

Collecting all the information listed above poses challenges, but is possible. However, it is not possible to automatically collect provenance that the system never sees; we call such provenance *opaque provenance*. Opaque provenance arises when data originates from a non-PASS source, such as a user, another computer, or another file system that is not provenance-aware.

There are three approaches to opaque data. First, a PASS records any provenance it can deduce about an input, such as its creator, create time, its source (expressed as the URN for a networked object or the full path for a local, non-PASS object) and a unique fingerprint of the source (e.g., a hash value). Second, a PASS permits users to add annotations to files. Annotations can provide either provenance for opaque data or for semantic information, not available at the system-level. Third, a PASS allows storage and retrieval of application-specific provenance. Application-specific provenance records are like annotations, but provided programmatically from, for example, a driver for a remote data-producing device (e.g., a driver taking data from a telescope) or an application environment such as GenePattern [10]. A PASS distinguishes between internally-collected provenance, annotations, and application-generated provenance so queries can specify which attribute types are considered.

Field	Value
`FILE`	/b
`ARGV`	sort a
`NAME`	/bin/sort,/bin/cat
`INPUT`	*(pnode number of a)*
`OPENNAME`	/lib/i686/libc.so.6, /usr/share/locale/locale.alias, /etc/mtab,/proc/meminfo .#prov.mtab
`ENV`	PWD=/pass USER=root ...
`KERNEL`	Linux 2.4.29+autoprov #17 ...
`MODULE`	pasta,kbdb,autofs4,3c59x,...

Figure 1: Provenance of `sort a > b`. The `FILE` record is relative to the root of the PASS volume.

4.1 Requirements

In addition to automatically collecting provenance, PASS must provide the additional functionality outlined in this section.

PASS must support **application-generated provenance**, so that PASS can be used as a substrate for domain-specific provenance solutions. Applications that currently write to domain-specific provenance systems can instead write into a PASS's provenance database, producing an integrated view of application and system provenance. Our implementation uses a simple, low-level data representation that is easily mapped to XML, a relational schema, or any other data format used by an existing provenance solution.

PASS must provide **security for provenance**. Provenance can require different access controls than the data it describes. Consider an employee performance review that includes input from others: while the review itself must be readable by the employee, the provenance must not [14]. We conducted user studies to gather requirements for a provenance security model and determined that the security model for provenance can be divided into two pieces: one that protects access to ancestors and descendants and one that guards access to attributes. We are actively designing a security model for provenance, but its details are beyond the scope of this paper [3].

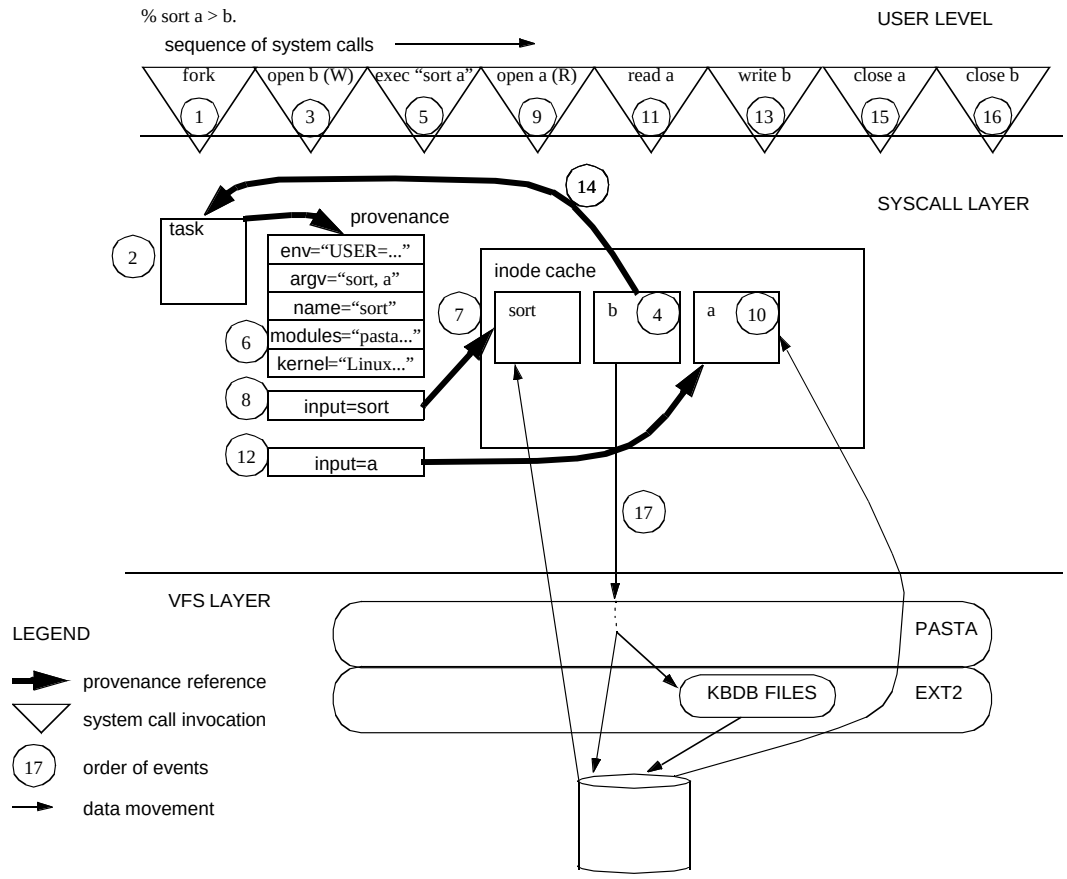
Finally, PASS must provide support for **queries on provenance**. Collecting provenance on data is not useful unless that provenance is easily accessed. Provenance queries fall into two categories: conventional attribute lookup and computation of transitive closures of ancestry (or descendancy) information. The latter are particularly challenging for most data management systems.

5 Implementation

We implemented PASS in Linux 2.4.29. To provide a framework for the implementation discussion, we begin with an example that describes how PASS collects and maintains provenance. We then present an overview of provenance collection followed by the details of its implementation. We conclude this section by evaluating our prototype relative to the requirements presented in the previous section.

Throughout the rest of this section, we use the example command line "`sort a > b`" to describe how PASS collects and stores provenance. Figure 1 shows the records that are added to the database, and Figure 2 shows the sequence of important system calls and the provenance collection steps performed while the command executes.

With this structure in mind, we present the details of our implementation in four parts. First, we present an overview of provenance collection. Second, we discuss the collector, which implements the activity shown in the the syscall layer in the figure. Third, we discuss our



1. Create a new process via `fork`.
2. Materialize a task_struct structure for the new process.
3. Open output file `b` as stdout.
4. Place `b`'s inode into the inode cache.
5. Exec `sort`
6. Create provenance records for the process.
7. Load the executable; place its inode in the inode cache.
8. Associate the executable's inode to the running process.
9. Open input file `a`.
10. Read `a`'s inode into the inode cache.
11. Read from `a`.
12. Add file `a's` provenance to the current process.
13. Write output to `b`.
14. Transfer process' provenance to `b`.
15. Close `a`.
16. Close `b`.
17. Write provenance to database.

Figure 2: Provenance Collection Example: We show the relevant system calls and provenance collection and maintenance steps for a simple command.

provenance-aware file system, which resides below the VFS layer. Last, we present our query system, which is not shown in the figure.

5.1 Overview

We maintain provenance information both in memory and on disk, and the two representations do not map one-to-one. On disk, file ancestry can be expressed as cross-references to other files. In memory, however, we must account for processes and for other objects such as pipes or sockets, which play important roles in provenance collection and derivation, but are not materialized in the file system.

We treat processes as provenanced objects, because processes produce files that must incorporate their creating process' provenance. Since we do not track explicit data flow within a process, *all* data a process accesses can potentially affect the process' outputs and must be included in its provenance.

In memory, we maintain an ancestry graph in which files reference processes, and processes reference PASS files, pipes, non-PASS files, and (transitively) even other processes. Many of these objects are never materialized on disk, and some that are written to disk cannot be readily cross-referenced. When we write provenance to disk we follow these references and copy the provenance into the database. Therefore, each object on disk may correspond to several in-memory objects, and some in-memory objects may appear on disk multiple times if they are ancestors of multiple files.

We collect provenance for every process on the system, because we cannot know in advance which processes might ultimately write to a PASS volume. We also collect provenance for non-PASS files, which is retained as long as their inodes are kept in memory.

5.2 The Collector

The collector generates in-memory provenance, intercepting system calls and translating them into provenance records, which are then attached as annotations to key kernel data structures. It also maintains the ancestry graph for in-memory objects. The final job of the collector is to map the in-memory graph to the on-disk provenance that is passed to the storage layer. We refer to on-disk provenance of an object via a unique *pnode number*.

In the `sort` example, the collector is relatively simple. For each provenance-related system call, the collector generates a suitable provenance record and binds the record to the appropriate structure. Figure 3 summarizes the system calls that the collector intercepts, the provenance records generated, and the structures to which records are attached.

Duplicate Elimination In the example, `sort` might issue many `read` system calls if its input file is large. The simple-minded collector creates a new provenance record for each read, even though the subsequent provenance records are exact duplicates of the first. Our collector tests for and eliminates duplicates at two points. When a record is collected, if it exactly duplicates an existing record already attached to the same kernel object, the new record is dropped. This does not eliminate all duplicates, however. Consider the shell command `(sort a; sort a) > b`, which writes two sorted copies of `a` into `b`. Both sort processes read `a` and have `a` as an ancestor. When the collector traverses the in-memory graph to write provenance for `b`, two references to `a` appear, so we also suppress duplicates during this traversal.

Versions Suppose that we executed `sort a > b` but `b` already existed. This truncates `b` and writes new data to it, logically creating a new version of `b`. We need to ensure that we also have a new version for the provenance of `b`, as the new `b` may have no relationship whatsoever to the old. Creating a new provenance version allocates a new pnode number. The collector intercepts the `truncate` operation to make sure this happens at the right time.

Because we are not running on a versioning file system, the data in the old `b` is lost. However, our file system does retain old versions of provenance, because the old `b` could be an ancestor of an important file, and we cannot remove that file's provenance.

In this example, it was easy to determine when to create new versions. However, declaring a new version is more complicated in the general case. Consider a sequence of write system calls. Does each write create a new version? What if we close and re-open the file after each write?

The simple approach of declaring a new version for every write suffers from *provenance explosion*, the creation of too much provenance and it does not suggest when to create new versions for processes. We must be able to group multiple writes together into a single version. In the simple case, it is sufficient to declare a new version, which we call *freezing*, on a file's last `close` and on any `sync`, The next section discusses the solution for more complicated ones.

Cycles Ideally, only versions that mean something to the user or the user's application should be given new pnode numbers. Versions generated by the system as a result of the way the application is written or as a result of properties of the collector implementation should be minimized. However, as the workload increases in complexity, reducing the number of versions introduces an even more daunting challenge: cycles. Consider the simple program that does:

System Call	Record Type	Description	Where attached
execve	ENV	environment	current process
	ARGV	command line arguments	current process
	NAME	process name	current process
	PID	process id	current process
	KERNEL	kernel version	current process
	MODULES	kernel modules loaded	current process
	INPUT	reference to program	current process
open	OPENNAME	pathname of file (non-PASS files only)	target file's inode
read	INPUT	reference to file	current process
write	INPUT	reference to current process	target file's inode

Figure 3: Basic provenance collection by system call.

```
read a
write a
```

When run, this program reads a, thereby becoming a descendant of a. Then it writes a, making itself also an ancestor of a. Unless the write to a causes a thaw of a, creating a new version that is not an ancestor of the process, we create a cycle.

This particular case is easily suppressed; however, the problem is considerably broader than this. Consider two processes P and Q:

```
  P             Q
read a
              read b
write b
              write a
close a       close a
close b       close b
```

If no new versions are created until close, Q's write of a creates a cycle; Q is an ancestor of a, which is an ancestor of P, which is an ancestor of b, which is an ancestor of Q. More complex examples include dozens of processes and intervening files.

Since we want to avoid declaring a new version on every write, there are at least three possible approaches to this problem:

1. Ignore it. Let cycles appear in the database and make the query tools deal with them. We consider this approach unacceptable.

2. Declare a new version only on writes that add new provenance information. In our current system, versions are too expensive to allow this, but we are pursuing more efficient version management in our V2 design that might allow this approach.

3. Detect and break cycles. This is our current solution.

Before adding an in-memory provenance record, the collector checks the in-memory ancestry graph for cycles. If the new record would create a cycle, we invoke our cycle-breaking algorithm.

The simplest way to break a cycle is to freeze the target of the operation that would create the cycle. (If a process were about to read from a file that was its own descendant, we would freeze the process; if a process were about to write a file that was its own ancestor, we would freeze the file.) This solution has two problems. First, the target might be a file, and creating extraneous versions of files is undesirable. Second, when data flows in a loop, it is often because of a circular operation (e.g., recompiling your compiler) and it is likely to repeat more than once. Creating a new version on every iteration causes a form of provenance explosion that we refer to as *version pumping*.

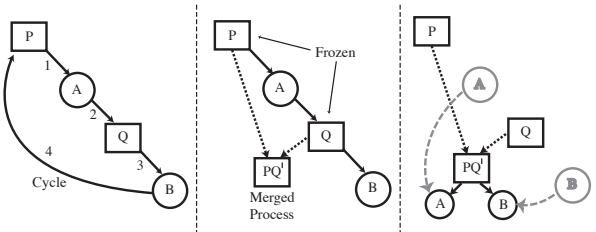
We developed *node-merging*, a more complicated algorithm to avoid these problems. Node-merging treats a set of processes that cycle data among themselves as a single entity for provenance purposes. The provenance of this shared entity is the union of the provenance of the processes that form it. Figure 4 illustrates this approach.

Specifically, if the cycle contains processes P_i and files F_j, we freeze all P_i and create a new "process" P_{new} descended from all P_i. (This "process" is really the data structure that holds in-memory provenance records; it hangs off the Linux task in such a way that it can be shared as necessary by this algorithm.) Then we change the parents of all F_j so they are all now descendants of P_{new}.

Implementation Details The implementation of the collector is approximately 4850 lines of code, plus approximately 250 lines of code to intercept system calls.

The collector communicates with the storage layer via five new VFS calls:

1. getpnid - returns a file's on-disk pnode number



1. Cycle Detected | 2. Freeze and Merge Processes | 3. Re-parent Files

Figure 4: Cycle breaking by node merging.

Database	Key	Values
MAP	inode number	pnode number
PROVENANCE	pnode number, record type	provenance data
ARGDATA	sequence number	command line text
ARGREVERSE	command line text	sequence number
ARGINDEX	words from `argv`	pnode number

Figure 5: Provenance databases.

2. `thaw` - bump the version of a file: allocate a new pnode number and prepare for writes

3. `freeze` - notification of file freeze

4. `write_prov_string` - write a "flat" (non-cross-reference) provenance record

5. `write_prov_xref` - write a provenance record that cross-references (by pnode number) another file on the same volume

5.3 The Storage Layer

The storage layer is composed of a stackable file system, called PASTA, that uses an in-kernel database engine to store its meta-data. Pasta uses the FiST [29] toolkit for Linux to layer itself on top of any conventional file system. We use `ext2fs` as our underlying file system.

We use an in-kernel port of the Berkeley DB embedded database library [18], called KBDB [13], to store and index provenance. Berkeley DB provides fast, indexed lookup and storage for key/value pairs. Berkeley DB does not provide a schema in the traditional sense. Instead, applications define their schema by creating indexed databases (tables in relational parlance), secondary indexes, and relationships between the tables. An entry in a Berkeley DB database consists of an indexed key and an opaque data item. The application determines how data items are interpreted.

We store provenance in five BDB databases, summarized in Figure 5. The PROVENANCE database is the primary repository of provenance records. The MAP database maps inode numbers to pnode numbers. A file's pnode number changes each time it is "unfrozen", which we call *thawed*. Command lines and environments are large relative to other provenance and are often repeated. The ARGDATA database implements an optimization, assigning (via BDB) a sequence number to each unique command line and environment. The ARGREVERSE database maps instances of an environment or command line to the sequence number assigned by ARGDATA. The ARGINDEX database is another secondary index, mapping components of command lines and environments (e.g., individual environment variables and their values) to pnode numbers.

5.4 The Query Tools

We make the provenance database accessible to users as a standard set of Berkeley DB databases. Making the provenance accessible as standard Berkeley DB files provides many advantages. We can use a variety of programming languages for building query tools (e.g., Python, Perl, Tcl, Java, C), and the standard DB utilities (e.g., dump, load) also work.

As we discuss in greater detail in Section 7.1, our prototype does not meet the security requirements identified earlier, but it does allow us to gain experience with PASS, deploy it in constrained situations, and extract as much information as possible to drive development of our later prototypes.

We built an easy-to-use query tool atop the Berkeley DB databases. The query tool has a built-in file system browser, the `provenance explorer`. Users navigate to the file of interest and run queries using the `provenance explorer`. The makefile query generates a set of commands corresponding to the sequence of events that led to the file's current state. Users can set various filters to, for example, remove commands that occurred before or after a given point in time. Another query, `dump_all`, retrieves the complete provenance for a selected file. The provenance explorer also allows users to add annotations to a file or to retrieve annotations for a file. We also support the command-line argument lookup query that allows users to search for files based on arguments to the processes that modified them. For example, a computational physicist can look up files that were modified by a process with an argument, `particle`, set to a particular value.

The `provenance explorer` is written in Java and uses JNI to access the Berkeley DB databases. To fa-

cilitate scripting, we also built command-line utilities that provide functionality equivalent to the `provenance explorer`.

5.5 Prototype versus Requirements

Our prototype has been a source of insight and source of future challenges, despite its limitations. We now analyze these limitations in light of the vision we outlined in Section 4.

The prototype accurately collects and maintains provenance. The provenance it collects for computations that are encapsulated in a process is complete. To the best of our knowledge, this is the first system that captures such information automatically and makes it generally accessible. Unlike many existing systems, it does so without requiring *a priori* specification of the workflow or DAG.

Although we create reasonable provenance for files copied from non-PASS file systems on the local machine, we do not yet create provenance for files that are transmitted across the net. We provide an API for user annotations and application-specific provenance, but this is still a manual process, and it is possible to do better with appropriate adapters on network connections.

A complete provenance solution requires provenance-aware applications, which are not yet available. However, as we demonstrated in Section 2, the functionality we currently provide does not exist in current systems and is complementary to domain-specific solutions. The interfaces we have defined for kernel provenance collection are models for interfaces for applications, and our preliminary investigation suggests that making applications provenance-aware will not be a significant obstacle. Building several provenance-aware applications is part of our next generation design process and will undoubtedly inform the future API. Although we have not yet integrated PASS with domain-specific solutions, the simplicity of our underlying schema makes the integration a straightforward programming exercise.

We have not yet implemented security. This functionality was not important to our first generation users. We wholeheartedly believe that we cannot add security to an already existing system, so we are intentionally designing our next generation PASS (V2) from scratch, incorporating what we have learned about provenance collection as well as what we have ascertained about appropriate security models for PASS [3].

A PASS provides query capabilities on provenance. The prototype provides simple query capabilities. These capabilities can be extended in a number of ways, but our first-generation users identified script-generation as a critical query capability. Our current script generation is primitive (it cannot reproduce pipelines without incurring huge overheads), but does meet the needs of our current users.

6 Evaluation

PASS requires in-kernel processing to track provenance, and it produces additional data that is ultimately written to disk. In this section, we demonstrate that these overheads are reasonable. We begin by discussing the system-wide disk space overhead needed for the provenance database, followed by a description of the evaluation platform. Next we present benchmark results illustrating both the disk-space and time overheads of our prototype. We then present query times for some sample queries run on the output of a Linux build. Finally, we present a sample application and its overhead.

6.1 System Overhead

We store provenance in five Berkeley DB databases. Each of the five Berkeley DB databases that store provenance has a 16 KB pagesize. Berkeley DB allocates a minimum of two pages for newly created databases. Thus, our PASS introduces 160 KB space overhead per file system (volume). This overhead is negligible, given today's enormous file systems.

6.2 Evaluation Platform

We evaluated our PASS prototype on a 500Mhz Pentium III machine with 768MB of RAM, running Redhat 7.3. We ran all experiments on a 40GB 7200 RPM Maxtor DiamondMax Plus 8 ATA disk drive. The results marked "PASS" were collected from our modified Linux 2.4.29 kernel (supporting provenance collection) and our provenance-aware file system, PASTA, running on top of ext2fs. The results marked "Ext2" were collected using the unmodified Linux 2.4.29 kernel and ext2fs.

To ensure a cold cache, we reformatted the file system on which the experiments took place between test runs. We used Auto-pilot [27] to run all our benchmarks. For all experiments, we measured system, user, and elapsed times, as well as the amount of disk space used for provenance. We compute wait time, which usually represents I/O time, as the difference between elapsed time and the sum of system and user times. We ran each experiment 10 times. In nearly all cases, the standard deviations were less than 5%. We do not discuss user time as our code is in the kernel and does not affect the user time.

6.3 Benchmark Performance

We begin with the large and small file microbenchmarks frequently used to evaluate file system performance [24].

These benchmarks exercise the `creat`, `read`, `write`, `fsync`, and `unlink` system calls for a large number of files spread over a directory hierarchy.

Phase	Ext2	PASS	% Overhead
create	10420	12180	16.89
read	10420	12180	16.89
write	10420	13476	29.33
write-sync	10420	13892	33.32
delete	24	3486	14,466

Figure 6: Space overhead (in KB) for the small file microbenchmark.

Phase	Ext2	PASS	% Overhead
create	0.91	3.02	232.41
read	0.71	1.51	111.90
write	1.62	4.42	172.09
write-sync	1.67	5.31	217.44
delete	1.13	1.22	7.56

Figure 7: Time overhead (in seconds) for the small file microbenchmark.

The small file test uses 2500 4 KB files with 25 files per directory. Figures 6 and 7 show that the overheads can be large, but are acceptable for two reasons: First, the absolute numbers are also quite small, so expressing the overhead as a percentage is misleading. Second, this is a particularly challenging benchmark for a PASS, because the files are small, and because the write phases of the benchmark overwrite existing files. (Only the create phase writes new files.) Thus the total data size remains unchanged while the provenance grows, suggesting that *provenance pruning*, discussed in Section 7.1, is an important area for further research.

Phase	Ext2	PASS	% Overhead
seq-write	6.16	7.11	15.47
seq-read	0.90	0.92	2.01
rand-write	6.20	7.04	13.58
rand-read	0.90	0.92	2.31
re-read	0.89	0.92	2.44

Figure 8: Time overhead (in seconds) for the large file microbenchmark.

The large file benchmark consists of five phases. First, it creates a 100MB file by sequential writing in units of 256KB; second, it reads the file sequentially; third, it writes 100MB to random locations in the existing file; fourth, it reads 100MB from random locations in the file; last, it re-reads the file again sequentially. The benchmark has virtually no space overhead, since it uses one file and adds only 10 new records to the provenance databases.

Figure 8 shows the time overhead. As a proportion of the running time, these are much better than the small file results, because the "application" is doing more work and the provenance collector proportionally less. The write overheads are still higher than is desirable due to the overwrite nature of the benchmark program. As shown in the next sections the large file results are more indicative of the overheads on realistic workloads.

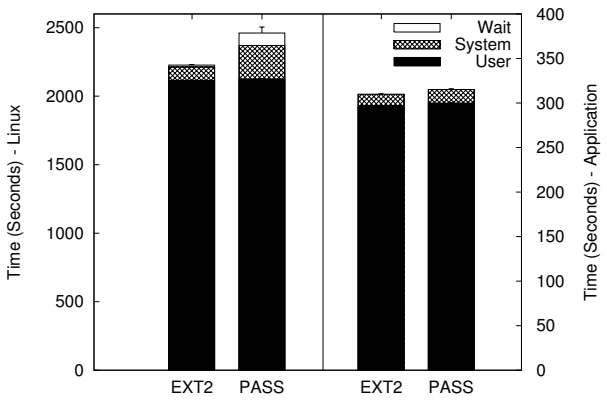


Figure 9: **Linux compile and Application benchmark results.** The left half of the graph shows the Linux compile result and uses the left axis. The right half of the graph shows the Application benchmark and uses the right axis.

	Makefile	Dump All
elapsed time	1055.09	91.90
system time	190.98	26.37
user time	817.12	17.57
average elapsed time per file	0.065	0.006
average db lookups per file	485	36

Figure 10: Query times, in seconds, for all files present after a Linux build.

For our last benchmark, we built the vanilla Linux 2.4.29 kernel. The left half of Figure 9 shows the results. This build generates 399 MB of data producing 11% space overhead and 10.5% execution time overhead. The time overheads are due to increases in system and wait times. The system time increases due to the work the collector does to maintain dependencies and detect cycles. The B-

tree comparisons by the database also contribute to the increase in system time. The increase in wait time can be attributed to the increased I/O due to database writes.

We then used the directory tree and files resulting from the Linux compile to measure provenance query times. For each file existing on PASS after the Linux build, we issued two queries: a makefile generation query and a dump_all query. Table 10 shows that the queries are fast: even though a makefile query performs nearly 500 lookups per file, it does so in only 65 ms due to the high performance of Berkeley DB. We create several Berkeley DB indices to facilitate rapid queries, but that results in higher write costs observed in the small-file benchmark.

6.4 Application Performance

One of our early users was a computational biologist who regularly uses `blast` [1] to find the protein sequences in one species that are closely related to the protein sequences in another species. She further tweaks the output of `blast` running Scriptome [22], a set of tools that filter, format, and merge data in tabular or common biological formats, on the output. Typically, she starts with two files containing the protein sequences of two different species of bacteria. A program, `formatdb`, formats the files and prepares them for `blast`. `Blast` determines the protein sequences in the first species that are most closely related to sequences in the other species. She then runs a series of Perl scripts from Scriptome. These scripts extract the relationships with the best scores and then relationally join the two files together to identify interesting cases, where the analysis shows that a protein in A is most closely related to a protein in B and the protein in B is found to be most closely related to the same protein in A. Finally, the scripts print out the relevant columns. The result is a list of proteins in the two species that might be related to each other evolutionarily. When the output is satisfactory, she uses the PASS query tools to generate a script containing the precise sequence of commands that produced the output file.

The right half of Figure 9 shows the overheads for a run of this workload. Although the kernel is collecting complete provenance, the overhead perceived by a user, 1.65% is sufficiently low that the new features appear to be available at no cost.

6.5 Evaluation Summary

PASS provides functionality unavailable in other systems, with moderate overhead. With the exception of the small file microbenchmark, our time and space overheads are small – typically less than 10% and always under 20%. We and our users are satisfied with these overheads. In addition, we found the system was useful in unanticipated ways such as its ability to generate scripts and its ability to uncover system mysteries.

7 Conclusion

Provenance-aware storage is a new research area that exposes myriad research challenges.

7.1 PASS Research Challenges

As we developed our prototype, we encountered problems with our initial design as well as problems that the design did not anticipate. Despite flaws in the prototype, we continued development so we could learn as much as possible before beginning the design of a second generation system. The current prototype is ready for deployment, and there are users eagerly awaiting its release. We are undertaking design of a second prototype based on the experience we have gained. In the following sections, we outline what we have learned and where there remains significant future research.

We began the PASS implementation with the simplest and lowest-level schema that could meet our query needs. In parallel with development of the prototype, we undertook an evaluation comparing different provenance storage solutions: our existing one, a relational database, XML-based representation, and LDAP-based representation [12]. We found that a Berkeley DB-based implementation provided the best run-time performance, but a relational implementation was more space-efficient[16]. For now, we have chosen to retain the KBDB-based implementation, while exploring ways to reduce its space utilization.

We recognized the security challenges early in the project, and that they are a source of myriad research opportunities. We conducted low fidelity user studies to gain insight into this area and identified the two-pronged security model that addresses provenance ancestry and attributes.

The cycle-breaking algorithm we described in Section 5.2 is complicated and has been the single greatest source of errors in the system. Cycle-free provenance collection is an explicit goal for our V2 design, but this remains a research challenge.

As currently implemented, the provenance databases are append-only, growing over time. Although this poses no more of a denial of service opportunity than does the ability to create files until disk space is depleted, it is wasteful and not viable in the long-term. Some provenance pruning is easy: deleting a file with no descendants should delete its provenance. However, deleting items with descendants may offer subtle opportunities for pruning. Tackling the general provenance pruning problem

requires synthesizing research in information flow and garbage collection and applying this work to this domain.

Provenance-aware storage will be more broadly accepted once we demonstrate integration with existing provenance solutions. Building provenance-aware applications is the first step in this direction. Discussions with users suggests that building a provenance-aware R environment [21] will make the platform attractive to biologists and social scientists. This is next on our agenda, but we hope that others will select tools to make provenance-aware as well.

Until all storage systems are provenance-capable, we face interoperability challenges. Moving files through a non-PASS system should not lose provenance, although it may prove difficult. Extended attributes have been in use for many years, yet there is still no safe way to move files and their extended attributes among systems with and without extended attribute support. Ultimately, we must develop provenance-aware network protocols so provenance can be atomically transmitted with data.

Finally, there remain difficult engineering issues. Our current handling of `mmap` is primitive and needs improvement. We built our PASS prototype to facilitate rapid implementation and deployment, but requiring a particular operating system is not a long-term solution. Instead, we need to develop network-attached PASS implementations complete with client-side plug-ins for NFS and CIFS clients. We will also build a versioning provenance-aware file system; exploring the considerations involved is another open research problem.

7.2 Acknowledgements

We thank our corporate sponsors, Network Appliance and IBM, for supporting this work in its early stages.

7.3 In Closing ...

We presented provenance management as a task for storage systems and described and evaluated the first prototype system that addresses this problem. While our PASS does not yet store application provenance, it provides a substrate offering significant provenance functionality and lends itself to unifying system and application provenance. We described several use cases where system provenance provides new capabilities and demonstrated that we can accomplish it with acceptable overhead.

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