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Mapping Out the HPC Dependency Chaos

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Abstract—High Performance Computing (HPC) software stacks have become complex, with the dependencies of some applications numbering in the hundreds. Packaging, distributing, and administering software stacks of that scale is a complex undertaking anywhere. HPC systems deal with esoteric compilers, hardware, and a panoply of uncommon combinations.

In this paper, we explore the mechanisms available for packaging software to find its own dependencies in the context of a taxonomy of software distribution, and discuss their benefits and pitfalls. We discuss workarounds for some common problems caused by using these composed stacks and introduce Shrinkwrap: A solution to producing binaries that directly load their dependencies from precise locations and in a precise order. Beyond simplifying the use of the binaries, this approach also speeds up loading as much as $7\times$ for a large dynamically-linked MPI application in our evaluation.

Index Terms—toolchains, package management, operating systems, filesystem hierarchy

I. INTRODUCTION

The Livermore Computing (LC) facility at Lawrence Livermore National Laboratory (LLNL) supports thousands of users on dozens of different clusters and hosts Sierra, ranked third on the Top500 [1] and is preparing for the upcoming deployment of El Capitan [2]. The simulation software written for these machines is complex and requires a large chain of dependencies that is continually growing. In 2015, it was significant to say that some applications required 70 dependencies, counted as packages which may contain one library or dozens depending on the packager. Today the Axom [3] library, a common support library for Livermore codes, can require more than 200 total dependencies. Each application and dependency can require specific compilers with specific runtime libraries and Message Passing Interface (MPI) implementations to achieve the best performance, or to work at all. Users may run several different codes or several different builds of the same code in the same environment as part of larger scientific workflows. Immense effort has gone into building complex software pipelines reliably, such as Spack [4] and EasyBuild [5] in HPC and in mainstream distributions as well, but far less work has gone into ensuring that the software will run consistently once it is built.

Part of the complexity in these systems comes from the fact that there is no single group or model in control of the package ecosystem on an HPC system. They are instead composed of layers managed by different domains of responsibility. As an example, a machine at LLNL will usually be based on RedHat

Enterprise Linux (RHEL) using the Tri-Lab Operating System Stack (TOSS), an extension of RHEL, and on capability systems extended further by vendor extensions. Most users will still not use compilers or much software from TOSS or the vendors directly, they use software from a separate site-specific development environment exposed by modules called TCE. If it were only these four layers, the problem might be reasonably tractable, but even TCE only provides the bare essentials. Each group then manages their own software stack, or stacks, built on top of some combination of the lower layers and possibly other groups's manually managed stacks. These are managed without any common infrastructure or planning, either manually or with one of the HPC package managers or some combination thereof.

The challenges faced at Livermore with regards to managing software complexity are a microcosm of what exists in the wider software ecosystem. Anywhere that multiple maintainers and versions of software stacks coexist these problems do as well. There has been an explosion in available software, packaging methodologies, and Linux distributions that compose them in an attempt to tame the chaos. The pursuit of creating software with increasingly complex dependencies reproducibly and portably is becoming a defining problem at large across all segments of the packaging and distribution community.

The primary differentiator between how packages find their dependencies in different packaging methodologies is whether they rely on established conventions or enforced search paths on each binary. The most common and well known method is to depend on a filesystem hierarchy similar to the FHS (Filesystem Hierarchy Standard) to determine the components linked into a binary at runtime. Some more recent systems use other mechanisms to locate binaries, libraries, or other necessary portions of an application. The first of these is the common mechanism used by nearly every Unix-like operating system and others throughout history. Everything from Multics, Darwin, Haiku, and BeOS, to modern hermetic root systems like CoreOS, search for binaries and libraries at well-known paths in the filesystem. The other main group we refer to as explicitly linked, or store-based. The major differentiator is that libraries loaded, and directories searched, by a given application are determined explicitly as part of build and distribution in the system, rather than being implicitly defined by the conventions of the distribution. This is accomplished in a number of ways and shows up in quite a few different places across the ecosystem. The trend

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toward containers like Podman or Singularity for distribution is one way to accomplish explicitly linking an application with all of its resources in a redistributable way. It can also mean directly referencing target libraries in a binary using RPATH or RUNPATH as package managers like Spack and most manual HPC installation trees do. It can even mean explicitly controlling or patching the loader as is done by systems such as Nix [6, 7] and Guix [8].

All of these non-traditional distribution mechanisms, package managers, and techniques are working on mitigating an underlying issue: The management of binary loading and interfaces is under-specified and managed all too often by pervasive arbitrary conventions. Our goal in this paper is to discuss the various approaches used today and in the past, explore some of the issues and workarounds commonly found in HPC systems today, and to present Shrinkwrap, our tool implementing a workaround that gives us the ability to run a program with little need to adhere to these arbitrary conventions. We present the following contributions:

- A survey of the state of practice in software distribution;
- A methodology, using existing loader mechanisms, to ensure binaries find their dependencies regardless of the user environment;
- Shrinkwrap: A novel solution to caching dependency resolution for binaries, implementing the methodology;
- An evaluation of Shrinkwrap and use cases detailing its use at LLNL and problems it has resolved.

II. COMMON PRACTICE OF SOFTWARE DISTRIBUTION

The taxonomy of packaging is synonymous with software deployment models. The nuance and variation across deployment models are often relegated to a small cohort across Linux distributions. Software complexity and the proliferation of software has made software deployment, specifically reproducibility, more relevant to the traditional user.

This section explores several common and rising software deployment models and discusses the tradeoffs of each. It ends with a discussion of how these models are composed to form the complete software ecosystem on an HPC system.

A. The Traditional Model: *Filesystem Hierarchy Standard*

Established in 1994, and in continuous refinement since, is the Filesystem Hierarchy Standard (FHS) [9], further extended with the XDG Base Directory specification (XDG) [10] in 2003 and the systemd file-hierarchy [11] specification. This is by *far* the most common layout used in modern Linux distributions, and is so pervasive that it is frequently replicated as a component of the other models. This is the familiar base directories such as `/bin`, `/etc`, `/lib` and others that we have all come to know. Using a consistent standard like this has huge advantages. Anyone can look at a system that is arranged this way and determine where to look for things. Package managers that target this model include some of the most venerable and well-tested in existence such as Debian's `apt` and the `rpm` ecosystems. These package managers work by

inserting software components into well-known locations on the system such as `/lib` or `/bin`.

The goal of a single unified directory structure like this is curating a system as a unified whole. It forms a single coherent set of packages that work together seamlessly, and only rarely allows more than one version of any given package. Since all software components must reside within a few key well-known directories, there is no easy way to support alternate versions of a component beyond appending suffixes. This aids in updating software components for security vulnerabilities, since there is only a single file that needs to be updated, and the need for rebuilds and expensive updates is minimized. Installation of a package is equivalent to writing files to this single root one at a time, potentially overwriting existing files of the same name. This multi-step approach to software delivery can leave the system in an inconsistent state if the process is interrupted, especially during distribution upgrades that replace critical base components like the C standard library. It is often difficult to undo a software deployment unless specific care is taken to create backups beforehand.

The lack of provenance of the files on disk is made worse by the fact that most packages declare their dependencies without any explicit version information. Figure 1 shows an analysis of the Debian package repository as of November 2021. Out of a total of roughly 209,000 packages, nearly 3/4 of them use completely unversioned dependency specifications. These packages work because, and only because, the maintainers of Debian diligently and manually ensure that the full graph of packages in a given distribution build, link, and *work* together. That is an extremely impressive feat, but means that an immense amount of knowledge about the needs of all of these packages is implicitly encoded and unenforceable in software. This cost is also paid repeatedly by different distributions such as Fedora [12]. While some may benefit as downstream consumers of packages from a parent distribution it is a fraction of the whole, leaving many distributions and package ecosystems duplicating the effort required to test, patch and compose packages.

B. *Self-Referential (Bundled) Model*

In an effort to make software applications more self-contained and easier to manage, software components can be bundled along with their dependencies. These are typically vendored within the same directory or in a specially-marked directory tree for the purpose. Bundled applications either rely on a modified search path that prioritizes local libraries, normal on Windows or Darwin and done by `AppImage` and `AppDir` formatted packages on Linux, or is replaced with a script that provides the appropriate options. To use a wrapper script, the values are passed in a variable like `LD_LIBRARY_PATH` to include the current working directory or a subdirectory. The ELF header is also able to imitate this setup through the use of the `$ORIGIN` expansion variable in `RPATH` and `RUNPATH` entries to refer to the location of the binary. The tradeoff to this approach is that there is a significant loss in the potential for deduplication across

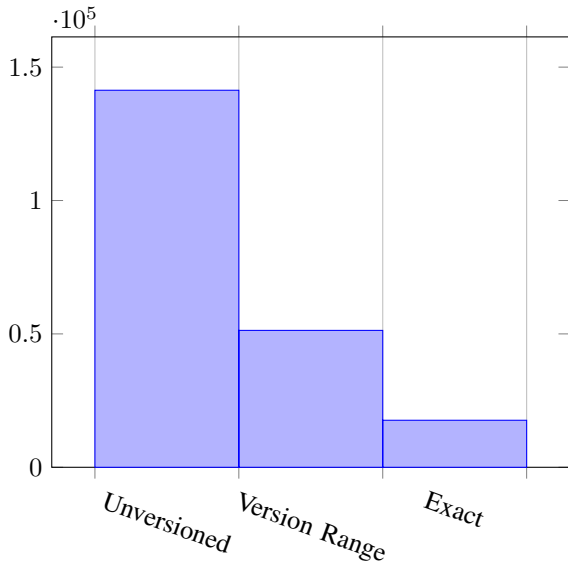


Fig. 1: Debian package dependencies by type

binaries employing the technique. Further, applying a security update for these embedded libraries will entail upgrading all of the bundles individually rather than updating a central location.

The benefit is a far simpler experience for users. This is one of the main reasons that Darwin applications can commonly be distributed in a click-and-drag-to-install manner for example. It further provides a relatively simple linking model that allows an application author to guarantee the libraries loaded are the ones they intended rather than system libraries chosen by a downstream maintainer or a user. The software package can reside anywhere on the filesystem and is not subject to the limited key space dilemma of FHS. Allowing multiple versions or minor changes of the same software package to exist on the system at the same time allows for the atomic installation and removal of the package as well. As a result, it is alluring for distributions of stand-alone scientific packages, especially graphical tools or others that are difficult to build and meant for novice end-users to install.

The challenge to this model is that it relies heavily on the software developer. Catching build dependencies is challenging unless the builds are always done in a sandbox environment. Because such a package uses its own vendored environment, it is very hard to extend, which poses significant challenges for packages that allow loading of user code or extensions. For example, including an embedded Python interpreter in an application is straightforward, but should it support installing packages into that vendored python? If so, where should they go? How should the user interact with them? It can also pose a security issue because the user can choose where to place the bundle. If the library path includes a writable directory, an attacker can leverage it to load unintended code.

In terms of compatibility, this is not the most familiar model to Unix devotees, but it is one of the best known to desktop users. Beyond that, this model is what allows almost

all packages for Windows and MacOS to be installed without extra dependencies outside of themselves. The lack of external dependencies, aside from the OS itself, is in fact so prevalent on Windows that the Microsoft WinGet package manager *does not support dependency specification or resolution at all* as of December 2021 [13]. From a user perspective, this model simplifies management and use but increases file size and increases the chances of libraries going unpatched because they are bundled with otherwise stable software that doesn't post updates to dependencies.

C. Hermetic Root Model

Hermetic Root systems are those whose goal it is to leverage many of the same implicit assumptions as the FHS model while improving upon the *atomicity* and *security* of the system. Given the pervasiveness of the FHS model for software packaging and administration, these systems benefit by providing a familiar and easy-to-target model. The key insight they provide is the creation of *layers* in constructing the filesystem, similar to those of *overlayfs*, with the added ability to deploy layers via a commit model that resembles *git*. The ability to commit a new layer or rollback to prior ones allows for the atomic delivery or rollback of installation or upgrade operations. The model does not seek to impose any restriction on how the data is laid out, and adopts any benefits or shortcomings of layouts used in addition to it. Although the creation of filesystem layers and the curation of working packages still represents a hurdle, once achieved the result can be distributed and reused providing a reproducible environment with which to run desired workloads. This model also easily supports making the entire operating system, and vast majority of package components, read-only with little effort making it resistant to many common classes of vulnerabilities.

The main challenge for this model in HPC is the slow move to support user namespaces in HPC centers. As restrictions relax and more centers deploy bubblewrap with FlatPack and Singularity or Podman-based solutions, this may become more practical, but for now the lack of capabilities to create images inside of normal compute resources, and inside of security domains, makes this difficult to use on many HPC systems.

D. Store Model

The *Store Model* refers to systems that install software components each in an individual directory under a specific filesystem root, usually with each individual package directory following the FHS. For example, Nix packages are installed under `/nix/store` and spack packages under `<spack-repo>/opt/spack`. This is a complete departure from the FHS model at the system level, moving nearly all directories from a single root-level location to one per package. References to dynamic libraries or shared code should only be done from other store locations, and only explicit references in the package descriptions should be respected. The explicit dependency linking between store paths creates a directed acyclic graph of software components and their dependencies. These systems often employ a consistent hash-naming scheme

to avoid conflicts, and allow arbitrary versions of the code to reside congruently, providing the ability to perform upgrades or rollbacks atomically by installing the whole new graph without invalidating the old one. In order to exert control over the linking process, shared objects are resolved by setting RPATH/RUNPATH during compilation, or through post-build actions that modify binaries using patchelf or similar tools.

Several new package managers and distributions employ this model, including Nix, Guix, and Spack. These originated from concepts first introduced through Nix [14]. The model requires package authors to canonicalize the build steps into the system's model so that the graph of all dependencies is explicit and complete. The consistent hashing scheme is often referred to as *pessimistic*, because it takes into account the package's full source, build steps, and the same for its complete transitive closure. Any minor change from source to compiler flags for any package in the build graph will cause a domino effect of rebuilds.

This model fares well from an atomicity and reproducibility standpoint, but security requires updates to propagate to all dependent packages, rewriting potentially large segments of a system's packages when a popular library like `libcurl` is patched. Even so, it is inherently no less secure than the others since those updates are provided in a similarly timely manner, they just happen to be larger. Where this model runs into problems is compatibility, familiarity and implementation given existing tools. A NixOS system cannot natively run a dynamic executable built on any other distribution even if the system has every single dependency used by that executable. There are projects that help deal with this such as Nix-LD [15], but the fact that everything in a Nix system is placed under the store means that even fundamental building blocks like the loader (`ld.so`) are not where an FHS system would expect them to be¹. It is done for good reason; this way a Nix system can use two different loaders with two C libraries side-by-side without issue, but the compatibility is poor by default.

While we normally don't conceive of it this way, the development tools, distributions and module directories of HPC systems tend to be a manually curated version of a Store Model system as well. This is hardly surprising, since that is a large part of the reason Spack builds the way it does, but when treated that way certain properties become clear. For consistency and usability, it is desirable to make each package in such a module directory *work* like a store model by ensuring that each package encodes all of its dependencies, rather than requiring environment variables loaded from a module.

Another issue that these models face is a model for loading of shared objects that was developed in and around the transition from SunOS to Solaris in the mid 1990s. Limited to using RPATH, RUNPATH, or environment variables they tend to use a combination of RPATH or RUNPATH and wrapper scripts to patch up the graph as best as they can to produce a working system. However, these methods were never meant

to be used for this purpose, and create their own problems. We'll discuss correctness issues further in Section III, but loading performance can be significantly impacted by using a store model even when the setup is correct. Since RPATH and RUNPATH only allow specifying paths to be searched, and they are all searched in order for each needed entry, applications with many dependencies end up searching many directories to find each library. Figure 2 depicts the dependency graph of the Ruby package in Nix with all 453 dependencies. It is so dense, and so many components that it's nigh illegible, but it itself is a *minor* dependency for many other packages. On a local filesystem, the overhead is usually small enough to be ignored, but when the dependencies are on a network filesystem it can be a significant performance issue.

E. HPC and the Module Model

We have eluded to the common setup of HPC systems in other parts of this section, but any given HPC system is usually comprised of layered instances of the FHS model and some form of the store model. Often the store model portion is less strictly structured and presented in the form of software modules handled by a module manager like *lmod*. As an example, the software stack on Lassen (the open compute version of Sierra), the base system is an FHS formed from a combination of RedHat, TOSS and IBM base packages. On top of that, there is a large set of developer environment packages available through modules in `/usr/tce`. As of this writing, 338 separate directories are managed by application teams, many of which provide built versions of their software or tools for downstream consumers to use in whatever way they have decided in their own tree.

Within any one component of this system, packages tend to be self-consistent, usable and stable. Difficulties arise from combining elements of multiple components, and the strategies used to compose them. Common issues include: one layer using RPATH to ensure all dependencies can be found while another uses RUNPATH which causes the RPATH to be ignored; runtime libraries injected by compilers without RPATH entries added relying on the environment; and difficulty identifying which packages are ABI compatible with one another or which compilers use which runtime library versions. Applications are composed from some combination of these components, and frequently more are pulled from package managers like Spack, `vcpkg`, `pip`, `conda`, as well as other sources. The chaos of these deployment strategies, tools, and requirements can confound even sophisticated application developers and dedicated HPC support teams, resulting in fragile software deployments.

III. DISCUSSION

The survey of packaging methodologies demonstrates that different means of bundling software within the Linux environment are possible and can achieve varied levels of atomicity, reproducibility, and security. In each classification, the system relies on a shared set of simple primitives controlling the loader to distinguish itself. These differences are subtle to all except the most well-versed in the space. For instance,

¹In fact, Nix patches away the ability for the linker to refer to default system locations or `ld.so.conf`



Fig. 2: A graph, or snarl, of the build and runtime package dependencies needed by Ruby in Nix.

the RPATH specified within the ELF header has precedence over all dynamic loading search locations *unless* RUNPATH is set, in which case it is *ignored*. Additionally complicating one’s understanding of how libraries are resolved is that RPATH entries in each ancestor are searched, whereas RUNPATH entries are not.

A. Issues with RPATH and RUNPATH

Understanding the link order of a binary is difficult in practice. Are needed libraries traversed breadth first or depth first? Using what mechanism are the libraries ultimately resolved? These questions may seem innocuous, but they are critical to what components load in a given environment. Issues can cause the link order, and thus the loaded dependencies, to subtly change long after installation and testing.

To answer some of these questions, mostly in the context of the glibc loader, shared objects are only loaded into memory a single time during traversal, usually based on their soname. If a shared object has already been visited and is needed by another dependency it will be provided without a lookup, and will not raise a warning or error if that library would not have been found otherwise. That is a useful performance optimization, but it also allows missing path entries to hide in working binaries that may surface later when the binary is run with a different set of flags or a new version of a library in the tree. Listing 1 shows an example of a library trace from a program called `dbwrap_tool` where the application and many of its libraries use RUNPATH to find what they need, but one library four levels down the tree has no RUNPATH. The `libsamba-modules-samba4` library finds three of its dependencies through default search paths, but the fourth wouldn’t be found at all if it hadn’t been loaded earlier in the tree by another library with a correct RUNPATH.

TABLE I: Properties of RPATH and RUNPATH

Property	RPATH	RUNPATH
Before LD_LIBRARY_PATH	Yes	No
After LD_LIBRARY_PATH	No	Yes
Propagates	Yes	No

The use of RUNPATH to instruct the linker, such as in the *Store Model*, is potentially problematic given that the granularity of the search path is at the directory level. Without a direct mapping of needed shared objects to their respective location, it is possible to find an incorrect object. The usual solution to this is to ensure that the order of items in the

```
$ libtree /usr/bin/dbwrap_tool
├─ libpopt-samba3-samba4.so [runpath]
│   └─ libccli-smb-common-samba4.so [runpath]
│       ├── libiovsbuf-samba4.so [runpath]
│       ├── libsmb-transport-samba4.so [runpath]
│       ├── libsamba-sockets-samba4.so [runpath]
│       └─ libgensec-samba4.so [runpath]
│           └─ libsamba-modules-samba4.so [runpath]
│               ├── libsamba-util.so.0 [default path]
│               ├── libtalloc.so.2 [default path]
│               ├── libsamba-errors.so.1 [default path]
│               └─ libsamba-debug-samba4.so not found
├─ libdbwrap-samba4.so [runpath]
├─ libutil-tdb-samba4.so [runpath]
├─ libsamba-debug-samba4.so [runpath]
├─ libpopt.so.0 [default path]
├─ libtalloc.so.2 [default path]
├─ libsamba-errors.so.1 [default path]
├─ libsmbconf.so.0 [default path]
└─ libsamba-util.so.0 [default path]
```

Listing 1: A demonstration that binaries can work due to shared objects being found by searching earlier paths

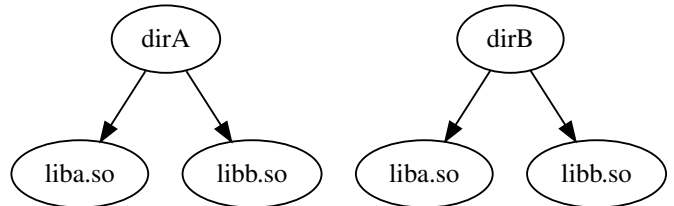


Fig. 3: A paradoxical setup for RUNPATH where the desired libraries are `dirA/liba.so` and `dirB/libb.so`

search path gives the correct result, but even simple conflicts can produce cases where this is no longer possible. Consider a system with libraries arranged as in Figure 3, in which `liba.so` is needed from `dirA` and `libb.so` is needed from `dirB`. In any ordering of any of the available search path options, there is no way to get the correct intended behavior without creating a new directory with the correct versions.

These issues have inspired a great deal of debate on the use of any of these mechanisms. The Debian community has publicly argued over policies in this space for many years; some of the resulting outcomes are now documented on their wiki [16]. The main concern centers around an application loading different versions of a library depending on loader order, arguing that the dynamic linker should solve this rather than RPATH or RUNPATH entries. That seems to be arguing for

use of `ld.so.conf` or similar to resolve these issues, which makes sense from the perspective of a distribution maintainer who can control that configuration easily and desires a single coherent FHS system. Some of the caution also comes from early use of `RPATH` by tools like `libtool`, which once included directories that also existed in `ld.so.conf` in the `RPATH`, locking system paths into the search out of order. The general desire to avoid `RPATH` is not new. In fact, the first version of the manpage for `ld.so` on Linux [17] included a statement that `RPATH` was deprecated and should be avoided.

On the other side, the Qt project published a recommendation [18] that authors of Qt applications should use `RPATH` and ensure `RUNPATH` isn't set. Given the distaste for `RPATH`, that may seem surprising, but Qt loads component libraries from code inside other libraries. As a result, an application that uses `QtGui` with an `RPATH` will provide its `RPATH` entries to the load issued in `QtGui`, allowing the system to find the correct version of the dependency. If the application has any `RUNPATH`, the search will only include those paths set on `QtGui` itself. Normally this is even treated as a feature rather than a bug, and the `QtGui` library should have a `RUNPATH` to find the dependency. That works as long as the dependency tree is strictly a tree, but if the application provides a plugin or a library that gets loaded, say by `dlopen`, in a different shared object, it has no way to provide search paths to that `dlopen` with `RUNPATH`. The only recourse at that point is `LD_LIBRARY_PATH`, which can cause even more damage in a `RUNPATH`-based system where more of the paths can be overridden in sub-applications, or adding an explicit API to load the library by absolute path.

From an administrator perspective, working with either `RUNPATH` or `RPATH` in an executable or library can cause pain points. If a library is locked to point to a library at `/opt/rocm-4.3.0` and that version is found to be buggy but binary compatible with 4.3.1 for example, then replacing 4.3.0 with 4.3.1 is more costly than without those paths set. They are forced to either recompile the library, symlink the new one into an inappropriate location, or override at the application level with `RPATH` or `LD_LIBRARY_PATH`. If the library uses `RUNPATH`, the `RPATH` solution on the application is insufficient as well, and can cause situations where parts of one version and parts of another are loaded due to two different search path orders with respect to `LD_LIBRARY_PATH`.

In the end, traditional search path management is fragile and poorly suited to store-based or module style package distribution, or separating packages by directory in general.

B. Questioning Dynamic Linking

The necessity for package curation in distributions is a point of contention as many language package managers trend towards vendoring dependencies to help improve reproducibility of the package [19] [20]. What at first became a solution to managing *dependency hell* soon became a *holy grail* to manage a single-unified graph of all software packages. The need for dependency-shared object resolution arose from a time when storage and bandwidth were expensive and in limited

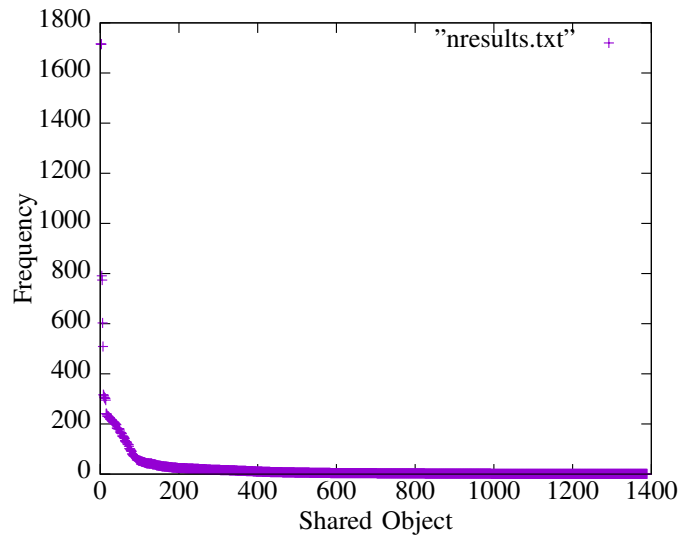


Fig. 4: Shared object reuse on a typical Debian installation with 3287 binaries. Only 4% of shared object files are used by more than 5% of the binaries

quantities or availability. The ability to upgrade a buggy or vulnerable package with as small a change as necessary to the dependency graph is a useful requirement of the past. There has been ongoing public discourse [21] [22] that demonstrates the total cost to re-download *all binaries* affected by CVEs in 2019 to be under 10 GiB (significantly smaller if you discount `glibc`). A survey of a local machine with 3,287 binaries demonstrates that the majority of libraries are used by relatively few binaries on the system as demonstrated in Figure 4. Why is dynamic linking continued given the lack of shared object reuse?

Much of this paper has been focused on the pitfalls and short-comings of dynamic linking, many of which are non-existent for a statically compiled executable. That said, in an HPC context, we have seen leadership class systems with only static linking that deduplicated statically linked binaries in memory, and a transition back to supporting dynamically linked binaries. The memory reuse benefits can be more noticeable when running the same application as one process per core and the same set of libraries loaded. In the wider community, Linux distributions have surfaced to explore the emerging pro-static philosophy [23], but have yet to gain meaningful traction.

Dynamic loading also provides one significant benefit we have not otherwise discussed. Many tools, especially prevalent in HPC, rely on dynamic linking to override or wrap symbols. For example, tools that use the `PMPI` interface are usually pre-loaded with `LD_PRELOAD`; same for performance or memory tools like `gperf`. Changing to fully static linking breaks *all* of these tools, rendering them unusable. That may still be worthwhile for final production release binaries in some cases, but it means that a great deal of work during development may need to use dynamic binaries.

C. Questioning the Loader Interface

In the mid-to-late 1990s, the tools provided by the linker allowed augmenting the search space for shared objects in well-intentioned ways, but these techniques have not aged well. RPATH was sufficiently misused and thus reviled on SunOS, Solaris, and later on Linux that it has been deprecated for 20 years. Yet, it is still supported and in active use in newly written systems to this day. Its replacement, RUNPATH, was meant to solve developers' issues by ensuring that LD_LIBRARY_PATH could override search paths in binaries, and that executables would not pollute their dependencies with their embedded search paths. While it succeeded in these goals, by not disallowing RPATH and RUNPATH from being used together and by eschewing propagation, it lost the ability to propagate search paths to dependencies when necessary.

The constraints we want to express are a combination of options to inject new paths into the library search path: *prepend*, *append*, and *whether to inherit*. All but one of the problems listed in Section III-A can be solved by offering prepend/append and a boolean propagation flag on each path added to the search space.

The desire to find all libraries within a few well-known directories from the FHS model has bled into the ability to specify the search space as a single list for all libraries. Allowing the ability to dictate the search space per shared object would give fine-grained control over the search semantics. This would also solve the final issue: the ability to load libraries with conflicting filenames from paths deterministically.

Having considered this direction, the other question that must be asked is why we must rely on a bare soname and a linear set of paths to search to do this job. The Fuchsia kernel and Zircon system loader implement a service to request dynamic libraries at load time, allowing load configurations to be changed between libraries during loading [24]. In the end, though, there is a standard ELF loader on top of it. Given the option to change the way dependencies are encoded in binaries could allow a system like Nix or Spack to store the hash of the library being requested, store the specification used to build it, or store enough information to be able to not just load it but determine with far greater detail which version is expected if it is not available. One can envision a system that would allow a user to take a binary set up that way and ask a tool to provide all of the dependencies it needs in place of distributing a static binary or a container.

D. Workarounds

While it's a pleasant thought experiment to imagine a world where we do not require backwards compatibility with established loaders, the state of the practice is that we must work within the limitations of ELF and the System V ABI model. Therefore, we propose a number of workarounds to allow packaging models to avoid some of these issues given the current capabilities of loaders. Additionally, we will discuss what seem to be the core features desired in a future loader to allow all of the package author, package maintainer, and the

end user to request the behavior they want without requiring massively long search paths and ambiguous lookups.

1) *Dependency Views*: This method is based on the concept of environment views from the Spack package manager, but could be used by any system that wants to do per-package resolution of dependencies. Rather than setting RPATH or RUNPATH entries on the executable and every library to all dependencies, each gains a single RPATH or RUNPATH to a package-local directory containing an FHS-styled filesystem populated with symlinks to the package's dependencies. Rather than a long list of RPATHs, there is now only one, and resolution should necessarily be much faster, especially on network filesystems where stating a file can be slow. An extra benefit to this is that it may work for resources other than dynamic libraries such as data or font packages, by providing the combined view of those dependencies a package may expect from a traditional FHS system. The downside is that this method requires both a tremendous number of symlinks, and thus filesystem inode resources, to represent a full system. It is also constrained to only allowing a package to depend on a single version of any dependency, since they cannot link on top of each other.

2) *Needy Executables*: A less costly workaround in terms of filesystem resources is to use the issue shown in Listing 1 to our advantage. Since libraries are cached by soname, and libraries are loaded in breadth-first-search order starting from those needed by the executable, we can fix the load order in the executable. We do this by directly linking all libraries required by the full transitive closure of dependencies into the executable. For example, consider an *executable* that depends on *liba* which depends on *libb*. Rather than having a normal needed list of just *a*, the binary would instead have a needed list of *a,b* and RPATH or RUNPATH entries to find both. The RUNPATH issue with propagating search paths to dependencies is partially mitigated here as well, since libraries are pulled to the top for resolution.

Despite working around some of the main issues of the traditional approach, this method still has flaws. If any pair of libraries in the set define the same strong symbol, the link will fail. Additionally, load paths for *dlopen* calls without a path are not directly resolved by this method. Since these are loaded programmatically, they are not part of any needed entry. We could envision a system that traces all such calls and adds the libraries to the needed list, but that could cause breakage due to initialization order or load parameters such as the local or global nature of symbols in the library.

IV. SHRINKWRAP

The introductions of Spack and similar store-like systems have added a much needed level of reproducibility and organization to managing the common combinatorial stacks required by the HPC community. The ability for a binary or shared object file to explicitly tell the dynamic linker through the use of RPATH to search specific content-addressable named locations is pivotal to this approach, as it is to the manual approaches described earlier.

Unfortunately, the ability to modify a dynamic linker’s search algorithm is very coarse. All of `RPATH`, `RUNPATH`, and `LD_LIBRARY_PATH` are simply lists of directories, and apply to all dependencies needed by the binary. As the number of dependencies for a shared object grows, so does the length of the list that must be searched, penalizing the startup time for the process. This *unnecessary* work has real consequences. Frings et al. have written how with sufficiently large dependency graphs, one can flood the filesystem with requests and have process startup times on the order of hours [25].

Based on our experiences, we have developed *Shrinkwrap*, an open-source implementation of the *Needy Executables* option presented in Section III-D2. Shrinkwrap provides the following features:

- Encodes dynamic dependencies in the binary by their absolute path;
- Lifts all transitive dependencies to the top shared object to simplify auditing and prevent `RPATH/RUNPATH` interference in transitive dependencies;
- Offers virtual resolution strategies to handle cross-platform binaries or alternative dynamic linkers;
- Available as open-source MIT licensed software.

When faced with a recurring problem, often the solution is to cache the previous answer to avoid unnecessary work. Shrinkwrap adopts this approach by *freezing* the required dependencies directly into the `DT_NEEDED` section of the binary. Rather than listing the soname each entry is an absolute path. Furthermore, the transitive dependency list is lifted to the top-level binary to simplify auditing the required dependencies. All of the needed dependencies, including transitive dependencies, are now listed by absolute paths on the top-level binary. Shrinkwrap is written in Python, leveraging the *lief* [26] library for parsing and writing ELF binaries. Lief was chosen for its clean interface, ability to work stand-alone, support for symbol analysis, and an option to support MachO and PE binaries to offer similar benefits on MacOS and Windows in the future.

The solution is conceptually simple, but applying the modifications to the binary in a general fashion is challenging. Our desire is to support all reasonably compliant linkers and loaders on Linux. In practice, Shrinkwrap currently supports *glibc* binaries and others that use the same loader behavior such as BSD *libc*s, but not *musl* [27]. Shrinkwrap relies on the dynamic linker deduplicating libraries with a common file basename or whose *soname* (ELF header value) are the same. Consider the example in Figure 5: Shrinkwrap elevated `libabc.so` to a direct absolute dependency of the binary, but relies on the dynamic linker deduplicating the resolution for `libxyz.so`, which does not refer to it absolutely. Referencing dependencies by their absolute path makes it impossible to swap out dependencies for alternative libraries using traditional methods like `LD_LIBRARY_PATH`. The use of `LD_PRELOAD` remains viable, so in cases where specific functionality would still be preferred to be overwritten, a backdoor into dynamic linking remains. This also means that traditional preloaded tools continue to work as normal.

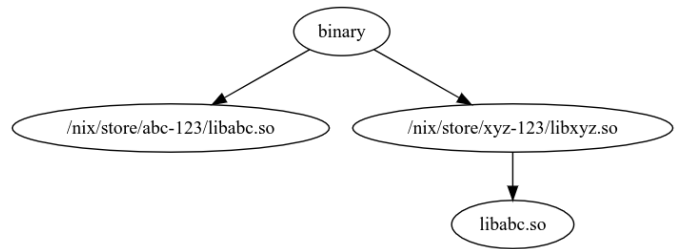


Fig. 5: Deduplication based on soname

When implementing Shrinkwrap against *glibc*, the deduplication is performed and the necessary libraries are resolved correctly. Unfortunately, other dynamic linkers such as *musl* do not exhibit the same behavior, causing the solution to not be compatible across other environments. The *musl* loader does not cache libraries loaded by their full path by soname, but by inode number, causing some load order issues with our scheme. They also do not implement the standard behavior of either `RPATH` or `RUNPATH`, but a meld of the two where paths are inherited by dependencies but are searched *after* `LD_LIBRARY_PATH`. This behavior would actually solve a number of problems with `RUNPATH`, but since it is non-standard it makes supporting *musl* more difficult for a tool like Shrinkwrap. This incompatibility was raised to the *musl* developers on their mailing list [28], however, the primary challenge is that while the System V ABI specification requires dynamic libraries to be deduplicated, or at least not to be loaded redundantly, it *does not* specify how they are to be matched to determine if they are duplicates.

Aside from dealing with divergent loader behaviors, Shrinkwrap must also identify which library on the filesystem each needed entry resolves to. In a simple case, using Shrinkwrap on the target system, we can use `ldd` or run the binary interpreter extracted from the binary with an option to list, as in `ld.so --list`, to get the actual behavior the loader would use given current conditions. When that works it gives Shrinkwrap exactly what we need and ensures consistent behavior. To handle cases where binaries are not executable on the current system, or where the loader is either not usable in this way or not executable itself, Shrinkwrap also offers a native strategy that traverses the filesystem the way that the loader would to find libraries. This is a useful option, but the number of corner cases is large. Mainly the issue is that the System V standard says libraries that do not match the architecture of the loading binary should be silently ignored, so we must detect these and avoid them since they are very common on systems with multiple native ABIs (x86 and x86_64 for example). Additionally, *glibc* supports loading more specialized versions based on the target architecture from subdirectories of each directory in the search path, and other expansions which must be faithfully replicated.

Shrinkwrap works strictly by replacing the `DT_NEEDED` libraries of the binary, however, dependencies may still be resolved via additional means such as `dlopen`. Binaries whose

runtime dependencies outnumber their static dependencies may not see optimal improvements. An area of future work as outlined in Section III-D2 would be to allow Shrinkwrap to audit all `dlopen` calls and lift them as `DT_NEEDED` so they can be easily referenced by absolute path. For cases where the user or packager knows what libraries will be dlopened, and the semantics allow, adding the names of these libraries to the needed section before using Shrinkwrap allows Shrinkwrap to resolve them as well. This works well for python modules for example, since they load cleanly and don't init until called. When the libraries are unknown however, perhaps plugins that aren't even installed in the same package, we will consider other mechanisms as future work.

All of that said, our tests across a varied array of binaries from Nix, Spack and hand-built HPC codes on a variety of architectures have given us confidence that Shrinkwrap is capable of handling most binaries found in the wild. Some example applications are discussed as part of Section V.

V. EVALUATION OF SHRINKWRAP

In order to evaluate Shrinkwrap as an approach to resolve practical issues with dynamic loading, we present evaluations of both the performance characteristics of a shrinkwrapped binary and case studies of applying Shrinkwrap to difficult library resolution problems. The performance of executing Shrinkwrap itself is bounded mostly by the time to traverse the filesystem, and if necessary, rewrite portions of the binary. To wrap a binary with 900 needed entries and an `RPATH` 900 entries long with a 213MiB main executable, took either four seconds on a Xeon E5-2695 system with the filesystem cache warm, or over a minute on a cold NFS cache. Since the operation is intended to be done only rarely, and usually on much smaller applications, its performance is sufficient. More important is the loading performance of binaries that have been shrinkwrapped, and the improvements in ergonomics of creating and using binaries on complex systems.

A. Loading Performance

The number of library dependencies needed by a particular binary and the number of entries in the `RUNPATH` can vary greatly. Consider a highly dynamic but common binary, the `emacs` editor, as built by Nix, lists **36** directories in its `RUNPATH` and requires **103** dependencies to be resolved. The result is that the dynamic linker could attempt nearly 3,600 filesystem operations to resolve the needed dependencies in the worst case, *every time the process is started*. This exorbitant cost can be made worse if the store itself resides on a shared filesystem such as NFS. This problem is not unique to Nix, and is present in other store-like systems. Courtès has written about this problem for the Guix system [29]. Table II shows the reduction to the `stat` and `openat` syscalls during process startup, and was captured using `strace`. The reduction in syscalls equates to a **36x** speedup.

While the total time is not long when considered as part of a single invocation, the effects magnify when applied in the context of even a modestly sized MPI application. To

	Calls (stat/openat)	Time (seconds)
emacs	1823	0.034121
emacs-wrapped	104	0.000950

TABLE II: Evaluation of emacs `stat/openat` syscalls

evaluate larger scale applications we use the Pynamic [30] dynamic application benchmark to measure the cost to launch and load a large MPI application at a modest scale. For our experiments, the benchmark is configured to match the general characteristics of a real LLNL application with approximately 900 shared libraries, using the "bigexe" configuration. All modules produced are listed as needed entries on the executable, modified slightly to place each of them in its own `rpath` directory. Figure 6 shows the results of running our Pynamic configuration on a system with two Xeon E5-2695 processors, loading the application and its libraries from NFS. Each test was run with a cold cache, and negative caching (caching the *non-existence* of a file) is disabled as it is by default on LLNL systems. At the smallest size, 512 processes on four nodes, the normal executable took 169 seconds to launch, while the wrapped executable took 30.5 for a speedup of $5.5\times$. At 2048 processes, the gap widens to $7.2\times$ for a total time-to-launch of 344.6 seconds for the normal executable. While this result is on the high end for what can be expected, the costs scale as the scale of the job increases, and the startup time benefits only grow. Shrinkwrap applies because even though the libraries and Python modules are loaded dynamically by the application, they are known at build time and included in the needed list. If there were more that were not known, it could be worthwhile to explore combining Shrinkwrap with an approach like Spindle to improve the load performance of those as well.

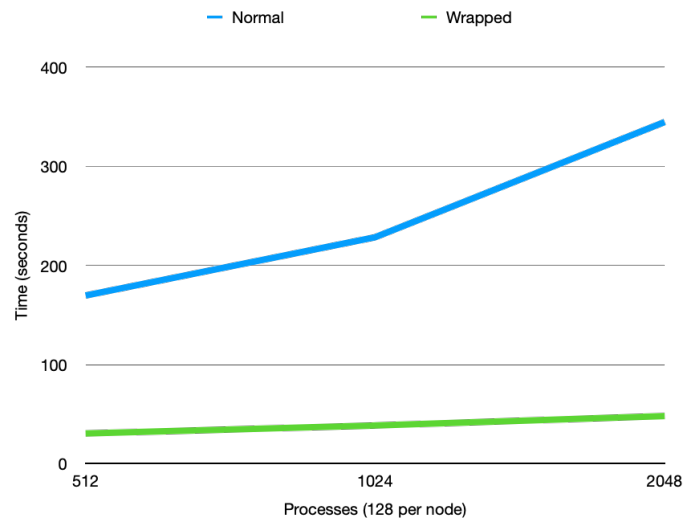


Fig. 6: Time-to-launch instances of Pynamic as built (Normal) and shrinkwrapped.

B. Use Cases

In the process of preparing for a new AMD-based super-computer, several software integration issues have arisen that resist traditional workarounds. The first of these is caused by a combination of three factors: RPATH entries in the main executable that point to all of the appropriate libraries, LD_LIBRARY_PATH set in modules to help with internal library search issues in ROCM packages, and those same ROCM packages using RUNPATH in place of RPATH. Any one of these would not be a problem by itself, even any two of them, but all three combined produces unfortunate effects. Specifically, an application built with ROCM version 4.5 will segfault if run when the module for a different ROCM version is loaded. This happens because after the first ROCM library is loaded, having been found by RPATH, the presence of a RUNPATH inside the library causes the loader to ignore the RPATH entries. The loader then prioritizes the now incorrect LD_LIBRARY_PATH, causing incorrect versions of the internal libraries used in ROCM to be loaded. Applying Shrinkwrap and linking all dependencies directly to the binary fixes this issue given a built binary inside a consistent environment.

The second issue comes from a workaround used inside a vendor library. When using the system compiler on an El Capitan Early Access system, compiling with OpenMP links in libomp.so, *without* OpenMP links libompstubs.so instead. This is perfectly reasonable, it means OpenMP runtime calls are always available. The downsides are twofold: the application is now dependent on load order to work correctly, and the linking approach to the Needy Executables workaround *does not work*. The load order is important because if libompstubs.so loads first the application will run with no threading or offload support. The workaround breaks because the stub library and the main OpenMP library are drop-in replacements, and define the same symbols. When both are loaded at runtime this is fine; whichever loads first wins. When both are specified on a link line, the link fails due to the duplicates. Since Shrinkwrap does not depend on manipulating the link line it can encode the required libraries without duplicate symbol conflicts. Once re-written to absolute paths, the initial load for all needed libraries is no longer environment dependent and can be inspected in the build environment and *relied upon* in the user's run environment. Though Shrinkwrap does not explicitly check symbol shadowing or load orders, it preserves the order the user set. This prevents a common class of errors in production codes on HPC systems, especially where multiple compiler stacks must be used and the results linked together.

VI. RELATED WORK

The labor, time, and *art* that goes into producing package distributions for Linux and the software packages that comprise them is not often a subject written about, at least publicly. This research seeks to begin to provide a common set of language and a survey of the current landscape to begin to foster continued discussion.

Recently, there has been a renewed interest in emerging platforms as the landscape of specialized hardware has grown. The quest for portability of software to multiple platforms is in the same effort to better understand the taxonomy of packages, their dependencies, and the ability to reproduce the software artifact. Khazem et al.'s research[31] into how portable software can be given changes to the toolchain (C/C++ compiler) or standard C library demonstrates the challenge of producing reproducible platform-independent software. In their effort to survey the portability of a large corpus of packages, the distribution's *dependency factor* was a constant hurdle. Many popular Linux distributions' packages (e.g., Debian, Fedora) have a large transitive closure, demonstrating how connected the package graph is. Research into the *Redirected Execution Daemon* was necessary to silently bypass failures, allowing builds to progress to completion and avoid the domino effect of failing packages to their upstream dependents.

The focus of our paper with respect to package taxonomies was focused at the lowest runnable unit within a Linux environment, an ELF file (executable or shared object), which often assumes that the language used was C/C++. This focus helps narrow the differences amongst package management solutions as they differ across distributions. The cornucopia of languages, however, is much larger than this narrower view, and many come with their own package management solution. Many of these languages reside atop a virtual machine and typically have their own concept of modules and resolution strategies. An interesting field of research is in the ability of this diaspora of language package management tooling to communicate amongst each other, potentially with that of the operating system, and avoid duplicating efforts[32].

VII. CONCLUSIONS

Package dependencies in HPC and across the ecosystem have increased drastically in recent years. As the dependencies between software have become increasingly interconnected, package management solutions have emerged to address new deployment models. In this paper, we surveyed the most well-known deployment models in use today in Unix-like environments and identified challenges each face as they make certain trade-offs for desired guarantees.

Distributions and package managers have begun to make leaps into greater atomicity, security, and reproducibility, but these goals are coming into conflict with the semantics of the ELF loader and incurring non-trivial costs as a result. We have presented some solutions that work around many of the common problems in this space within those options, and presented our tool for mapping out the chaos of dependencies: Shrinkwrap. Shrinkwrap is our solution to some of the common issues found in composing packages across models and from different sources into a reliable executable. In doing so, we have shown we can improve load times for some highly dynamic applications by a factor of seven, while making the application *easier* to launch for users.

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