Deployment of High Energy Physics software with a standard method

Thomas Hahn and Andrii Verbytskyi
Max-Planck Institute for Physics (Werner Heisenberg Institut), Föringer Ring 5, München 80805, DE
E-mail: andrii.verbytskyi@mpp.mpg.de

Abstract.
The installation and maintenance of scientific software for research in experimental, phenomenological, and theoretical High Energy Physics (HEP) requires a considerable amount of time and expertise. While many tools are available to make the task of installation and maintenance much easier, many of these tools require maintenance on their own, have little documentation and very few are used outside of HEP community.

For the installation and maintenance of the software, we rely on the well tested, extensively documented, and reliable stack of software management tools with the RPM Package Manager (RPM) at its core. The precompiled HEP software packages can be deployed easily and without detailed Linux system knowledge and are kept up-to-date through the regular system update process. The precompiled packages were tested on multiple installations of openSUSE, RHEL clones, and Fedora. As the RPM infrastructure is adopted by many Linux distributions, the approach can be used on more systems.

In this contribution, we discuss our approach to software deployment in detail, present the software repositories for multiple RPM-based Linux distributions to a wider public and call for a collaboration for all the interested parties.

1. Introduction
The modern studies in theoretical physics, experimental and phenomenology of High Energy physics (HEP) require a significant amount of specialised software. The creation of suitable computing environment and setup of required software requires significant efforts, time, which poses a barrier for newcomers even if the software is intended to be used unmodified.

In the recent years, these problems were attempted to be solved with a creation of different isolated environments, software managing tools or different combinations of those.

However, the available solutions have multiple disadvantages and practically not always result in a sufficient reduction of maintenance efforts, require users to learn each solution from a scratch and overwhelmingly lack of at least some important features.

Therefore, in our work, we present an approach which avoids implementation of custom software deployment system or isolated environments. Instead, we concentrate on the practical application and development of the existing “standard” solutions of the software deployment for the purposes of theoretical, experimental and phenomenology HEP computing.

In our contribution we show the application of this approach in the Linux/GNU OS distributives of RedHat and SUSE families using corresponding standard tools and present a repository with HEP software – HEPrpms.
2. Overview of software deployment techniques

In the recent years, a number of different approaches to the software deployment has been developed.

The most widely used are discussed below with advantages and disadvantages of each approach given for the use case of performing phenomenology studies in HEP-phenomenology/HEP-theory.

2.1. Scripted installation

The installation with scripts in isolated environments is, perhaps the oldest approach to the software installation. The installation is typically done with a shell ‘bootstrap’ script on Linux or MacOS with all the dependencies compiled on the spot. In the recent years this approach is often mixed with the Python virtual environments [1], which enhances the isolation of the resulting software from the standard environment of the host system.

The advantage of this approach is a relative simplicity of the setup and relatively uniform behaviour across different Unix-like operating systems. The approach also has a high reliability, as in most cases the ‘bootstrap’ scripts are created, documented and supported by the authors of the software. Typically, the installation does not require administrator privileges and multiple installations of the same software can exist.

The disadvantages include poor integration with the system installed software, the absence of binary packaging, debug information, version control, automatic updates, reproducibility of issues and tremendous real time/CPU costs.

2.2. LCG software stack

The second widespread approach to the software in the HEP community is the usage of LCG software stack [2]. In this approach the precompiled software is taken as is from the LCG stack installed in CVMFS [3]. The advantage of this approach is that the LCG software stack is quite complete, it is tested by the LHC experiments in collaboration with software developers, regularity obtains updates and no user maintenance is required beyond the availability of the CVMFS file system. The disadvantage is a need to maintain the complicated scripts that required to set-up any non-trivial environment, poor compatibility with non-LCG software, requirement of the presence of CVMFS, and absence of useful debug information. In some cases a specific knowledge of the internal details on the software configuration (e.g. applied patches) in LCG is needed.

2.3. “Universal” package managers

The third approach is the usage of different “universal” package managers. To this category one can include the installation of software with PyPi[4]/Anaconda[5] and the installation with Spack[6].

The main advantage of PyPi[4]/Anaconda[5] approach is cross-platforming of these package managers and the simplicity of usage – all those package managers concentrate on the installation experience of the users, nice documentation and the availability of binary packages in public repositories. The installation does not require administrator privileges and multiple installations of the same software can co-exist.

The disadvantages of this approach include the maintenance of the software stack is not centralised and quite often is semi-anonymous, the stack lacks debug packages and requires a maintenance of installations scripts/configurations etc. A sizeable disadvantage is also lack of important software functionality which arises from the lack of dependencies available in the PyPi/Anaconda repositories 1.

1 For instance, the recent tremendous effort to provide ROOT [7] in the Anaconda does not include the
The advantage of installation of software with Spack is the ability to easily specify all the dependencies that are used in the installation process, e.g. explicitly specify the exact version of the compiler and the dependency libraries and have multiple installations without exercising root privileges. From the non-technical point of view, an important advantage of Spack is the presence of large community.

The disadvantages include the absence of public binary repositories, missing debug information, a requirement to learn the Spack itself for using non-trivial software stacks, absence of automatic updates and the huge CPU costs for each and every installation from the sources.

2.4. Containers

A higher level of abstraction of the deployment approaches is the deployment of software in containers. We do not consider it an independent deployment approach, as in the end the installation process of software in a container uses one of the approaches already described above and has the same advantages/disadvantages.

2.5. The suggested approach – HEPrpm

The software deployment in the HEP phenomenology/theory/analysis studies outside of large collaborations process should have some specific properties. Most important should – it should have low maintenance costs – a dedicated effort for the development of group-specific tools for deployment is excluded. In the same time the approach should be reliable and the deployment should be reproducible. While the demands are high, the solution is quite simple. The task of software deployment is not new and was successfully solved in the software industry in multiple ways.

Therefore, we choose the approach of using the software deployment process as it is recommended by the OS vendors. Practically, this means one should implement the approach of the software deployment suggested by the OS vendors most widely used in HEP. The overwhelming majority of the computing systems used in HEP are the installations of RedHat, SUSE or Debian families of Linux with a small number of Windows and MacOS installations. Both RedHat and SUSE flavours of Linux have almost identical approaches to the installation of software which is based on the RedHat Package Manager (RPM) [9]. Therefore deployment of software with RPMs seems to be quite an attractive approach. The packaging process is explained in detail in the documentation of Fedora or SUSE and is briefly described below.

The packaging requires two components: the sources of the package and the .spec file. The later is a recipe how to build the package. It has a very standardised sections with meta-information on the package version, purpose, used sources, required software dependencies, the list of files to be installed. The .spec files (see Listing 1 as an example) are split into sections which correspond to the preparation for build, build, installation and which are executed separately after the expansion of the instructions in the .spec files. The instructions in .spec files are given with many convenience macros listed in the Fedora documentation [10], however many can be given as simple shell commands, e.g. the expansion of the sources can be done just with one command setup, see Listing 1. The .spec file and the corresponding sources are given to the standard rpmbuild command which is used to build a source RPM package .src.rpm or to build the source package and the the binary package. The resulting packages can be either directly installed to the desired system or put into a repository and the installed from the repository using YUM or DNF utilities.

functionality related to Grid, as the dependencies for this functionality rely on the stack of libraries native for RedHat and Debian systems [8] and an introduction of the stack in the anaconda would require a huge effort on itself.

In practice this advantage is very tiny, as many software packages relevant for HEP don't include support of operating systems other than Linux (or less frequently MacOS) and support of compilers other than GNU.
Listing 1. A spec file for the TheP8I package.

RPMBUILD, YUM and DNF are standard tools, with documentation on the build process provided by the RedHat and SUSE, therefore there is no burden of building tools maintenance and the preparation to the software packaging amounts to the creation of the .spec files.

The final product, HEPrpms software repository, is implemented as a set of .spec files prepared according to the standards of Fedora and SUSE. Those .spec files are available in a GIT repository https://github.com/andriish/HEPrpms to which any interested person can contribute. In addition, the git repository includes a trivial script that can grab the sources from the locations set in the .spec files, checks the MD5SUMS of the software sources and combines the sources with .spec files into .src.rpm packages. The software building can be done then from the .src.rpm files manually, however, a more attractive approach is to create the software packages in specialised services as CBS, COPR etc.

As of 2022 the set of the .spec files is used in the COPR build service to create a set of rpms. The corresponding repository is available at https://copr.fedorainfracloud.org/coprs/averbyts/HEPrpms. The repository requires quite little manpower to maintain, $O(\infty/\infty)$, however the updates of the repository are not regular and dedicated to updates of the software in the repository.

3. Advantages and disadvantages
The first obvious disadvantage of the suggested approach is the compatibility only with the RedHat and SUSE Linux systems. This stands in a contrast with the “universal” package managers approach which can provide support for multiple operating systems. However, practically many software packages are supported only for Linux and MacOS anyway.

Another perceived disadvantage could be the problems with building certain software with a specialised, i.e non-system compiler. The later capability is provided by e.g. SPACK. While using a different compiler chain could be easily implemented in the HEPrpms approach, we argue that often only GNU compilers are well supported. And while using a much newer GCC version could have some benefits, those benefits are negligible in case of modern operating systems. The other,
related disadvantages – the requirement of root privileges for the installation and ability to use only one particular version of software are discussed in the next section.

The advantages of the approach are that the package system is already maintained by the distributives for more than 20 years and is extremely reliable, stable and very well tested. The documentation is included in each and every release of RedHat/SUSE Linux distribution. It does not require extra maintenance manpower as the SPACK, NIXPKGS, etc. for the build infrastructure.

The second advantage is the availability of the binary repositories for the packages and the debug information. The binary packages can be provided by the PIP package manager and with some extra efforts by the SPACK/NIXPKG, however none of them provide the repositories with the debug information. Without the available binary repositories the usage of those installation methods for the CI is much more difficult in comparison to HEPrpms. The availability of the debug packages compatible with the system installed software makes the HEPrpms the only reliable option for the debug of applications.

The third most important advantage is that from the point of view of user, there is exactly zero maintenance time, knowledge requirements for the installation of software from HEPrpms. In this respect only the LCG stack stands on the same level as HEPrpms.

The fourth major advantage is the availability of cloud services that support the RPM approach: the very long standing OBS, CBS and COPR.

4. HEPrpms and containers

The two disadvantages of the RPMs based approach named in the previous section – the requirements of root privileges and the inability to have multiple versions of the same software are completely fixed with the capabilities provided by modern container engines. Consequently, standard packaging is the most practical approach to software deployment/maintenance for the continuous integration (CI) workloads. Using a standard container with precompiled packages from the HEPrpms repository does not require the creation of custom container images and therefore brings the costs of the CI containers creation and updates to zero. E.g. even the installation of software in a generic container from the vendors is fast enough for most of the CI workflows, see Listing 2.

```
stages:
  - test
  Fedora35-gcc-generic:
    image: fedora:35
    before_script:
      - uname -a
      - dnf -y install dnf-plugins-core
      - dnf -y copr enable averbyts/HEPrpms
      - dnf -y install TheP8I-TheP8I-devel
    script:
      #Here one can put all the commands that use TheP8I
      - ls
  stage: test
Listing 2. Example of GitLab CI configuration (in YAML) with a generic container from Fedora.
```

5. Conclusions

The idea to use the standard approach for the HEP-related software deployment is not new per se and was used many times in the past for the individual packages as well as for the larger projects [8]. However, the novelty of the presented work is that it shows an example how a reasonable large set of software can be packaged and prepared for a very easy deployment using the very well developed tools from the modern Linux/GNU OS and the available cloud services.

3 This example could be extended with a simple caching mechanism to reduce the network I/O.
6. Acknowledgments

Thanks to Matthias Ellert for a great example of HEP software packaging.

References

[1] Python developers 2022 https://docs.python.org/3/library/venv.html
[2] S Roiser et al 2010 J. Phys. Conf. Ser. 219 042022
[3] CVMFS developers 2022 https://cernvm.cern.ch/fs/
[4] The Python Package Index 2022 https://pypi.org/
[5] Anaconda 2022 https://www.anaconda.com/
[6] V Volkl et al 2021 EPJ Web Conf. 251 03056
[7] I Antcheva et al 2011 Comput. Phys. Commun. 182 1384–1385
[8] M Ellert et al 2007 Future Gener. Comput. Syst. 23 219–240
[9] RPM Package Manager 2022 https://rpm.org/
[10] Fedora project 2022 https://docs.fedoraproject.org/en-US/Fedora_Draft_Documentation/0.1/html/RPM_Guide/index.html