

HSF Packaging Working Group Update

Graeme A Stewart



HSF Packaging Group

Raison d'être:

- ...common issues, tools, and approaches to building and distributing the software stacks used by HEP experiments these are big stacks, e.g. 400 packages in LCG release used by ATLAS, LHCb, SWAN
- Continues to be a very active HSF group
- Published an <u>HSF Technical Note</u> looking at the main build tools
 - Community and FOSS main advantages and disadvantages summarised
 - Still valid, but tools evolve and change over time
- Last year...
 - We worked on a <u>Use Cases document</u> that elaborates the main requirements and desiderata for packaging in the HEP community
 - From librarians to developers
 - We also worked on some <u>Test Drive instructions</u>
 - Allowing people to rapidly test some of the different packaging solutions we know
 - Presentation at CHEP2018 summarising our work

TODOs for 2019

- Get main prototypes into a state where they solve most of the problems at a production level
 - "Continuous Delivery" system in place (build, make binary package, deploy to CVMFS, deploy to container)
 - Recall that CVMFS and containers are key features of the landscape now
 - We want these to aim at providing meaningful and testable solutions to the packaging problem for HEP
 - We have rolling updates and use the packaging group lists for discussion and sharing ideas and solutions
- Longer term goals and thoughts
 - CHEP2019 paper
 - Update of the packaging group technical note

CONDA



- Very popular package system
 - Language agnostic, Multi-platform, Multi-architecture, Binary installs
 - Data science and machine learning community use this extensively
- Deep rewrite in the last few years
 - Now supports multiple environments
 - These can be enabled and disabled easily, independent but share common components if they exist
 - o Builds quite deeply, having moved away from system libraries for internal consistency
- Official Anaconda packages (1400) supplemented by Conda Forge community support for 6000 more packages
 - Other channels: BioConda, AstroConda
- Conda package recipes easy to write in YAML
- Addition of ROOT packaging in Conda Forge (Chris Burr, Henry Schreiner) makes it very attractive for HEP analysis users
- Not clear it can so easily deliver full suite of production stacks to experiments

Nix



- Package manager based around deep rebuilds and a functional description of packages and their dependencies
 - Excels at build consistency and reproducibility
 - 40k Nixpkgs
- Support for multiple environments, with shared components
- Chris Burr was at <u>NixCon</u> in London, good survey of Nix community
 - Quite a popular solution in HPC world
- LHCb have a prototype with a significant number of projects building with Nix
- Main drawbacks for HEP are
 - Fixed build locations (not relocatable)
 - This is rather awkward for deployment (cvmfs) and development; not great for worldwide collaborations
 - Quite particular functional DSL for package descriptions
- Compute Canada do use Nix to build a base on which non-Nix development rests

Spack

- Package manager developed at LLNL, initially for HPCs
 - Builds rather deeply, but can be instructed to take system packages
 - Supports caches and relocation of binary artefacts
 - Strong support for scientific computing and from different science communities
 - Package descriptions written in Python
- We have had good contact with the development team for the last few years
 - FCC stack has been built using Spack for quite a few years
- Some really key features that support HEP use cases are in final development
 - Spack Chains allows different spack instances to build on top of each other
 - Better env setup for developers working from source added last year (spack setup)
- A few HEP people were added as developers in Spack GitHub
 - Help get HEP packages merged faster (review of these was slow in the past), e.g., ROOT
- We have our own channel in the Spack Slack workspace



Spack - Packaging Projects

FNAL MVP

- Provide builds to neutrino community, replacing outdated tools
- SpackDev project provides an easy development environment setup on top of Spack built packages
- o MVP (minimum viable product) can be <u>tested</u>, feedback encouraged
- A lot of useful HEP packages contributed (geant4, vecgeom, clhep, genie, log4cpp, lhapdf, ifdhc, ...)
- Discussion document on missing features and problem areas prepared for the community
 - e.g. sensitivity of package hashes to recipe changes

CERN FCC/LCG Stack

- Extending use of Spack from "higher level" FCC packages to deeper into the LCG stack
- About 200 packages targeted
- Will have a summer student to work on this

SuperNEMO

- In the process of migrating from homebrew to Spack
- First results very encouraging full report in next week's meeting

Conclusions

- Packaging remains a de facto area where working together as a community helps
- Group has remained active, informing the community and providing mutual support
- Prototypes are advanced and providing real solutions
 - Often now we are in the nitty-gritty and diabolical details
- Whether "one size fits all" remains to be seen
- My personal take:
 - Spack the most promising solution for production software builds
 - CONDA well liked and supported by end users could be a great way to provide analysis software