Evaluating SPACK for CMS offline Software

SFT Group Meeting

13th Mar 2023

CMS Software Stack

CMS Offline Software Stack

- CMSSW: Software and services needed by the simulation, calibration and alignment, and reconstruction
 - > 5.5M code lines:
 - 66% C/C++, 27% Python, 5% fortran and rest are build-rules/data files
 - > 17 active release cycles: 5.3, 8.0, 9.4 up to 13.0/13.1
 - 13.1.X development release cycle has 15 flavors
 - ROOT, GEANT, CLANG, LTO, Multi-Vectorization, ASAN, UBSAN etc.
 - Build for multiple OS/Arch/Compilers (cc7/el8/el9, x86_64/arm/power...)
 - > Build production: 2.5K shared libs/plugins, 1K binaries



CMS Offline Software Build/Packaging System

- CMS Offline Software Build/Packaging system consists of various components
 - > SCRAM: Software Configuration, Release and Management tool
 - <u>CMSSW-Config</u>: Build rules based on gmake
 - PKGTOOLS: Packaging system based on Redhat Package Manager (RPM)
 - > CMSPKG: Software distribution and Installation/Deletion tool
 - CMSDIST: The build recipes for building the package

All of these are though customized for CMS offline SW but can be used by

other projects

LCG Projects were using SCRAM in past to build POOL/CORAL.

CMC atill builds come of CODAL voice CCDAM

CMS still builds copy of CORAL using SCRAM

More details in backup slides

RPM external lz4 1.9.2

Source: https://github.com/%{n}/%{n}/archive/v%{realversion}.tar.gz

%prep

%setup -n %{n}-%{realversion}

%build

make %{makeprocesses}

%install

make PREFIX=%{i} install

CMS Package System: Summary

- All tools used for building/distribution/installation are independent of CMSSW releases/OS/archs/compilers
 - > Except for CMSDIST where though most of build recipes are shared between releases/OS/archs/compilers but we have separate git branches for each release/compiler
 - Build recipes do not depend of packaging/distribution tools so can be easily backported to older release cycles
- All tools are very stable and require low maintenance
 - Few commits per year (mostly for additional features)
 - > Over all 40K lines of code to maintain
 - 20K lines are stable and independent of CMSSW releases/OS/archs/compilers
 - 20K lines of build recipes gets most of the changes and mostly for development release cycles



SPACKLet's dive into SPACK world

SPACK

SPACK flexible package manager for HPC software

- ➤ A lot of development for/from **HEP** experiments in last 6 years
- Supports multiple version and configurations of software
- Single package file to have all supported versions, configurations and variants of the software

Just not a package manager but supports software distribution and installation

Binary relocatable packages

PKGTOOLS, CMSPKG and CMSDIST all in one

- Also covers part of SCRAM e.g package env setup (spack load/unload)
- Interferes with build rules too via its compiler wrappers

Why we looked in to SPACK

- Large community specially after 2016 when **HEP** exp start looking in to it
- HSF recommends SPACK for HEP community
 - ➤ **LCG/SPI** team looking in to it since 2020
- +6.5K built-in package recipes
- Out of the box RPATH/RUNPATH builds
 - ➤ No LD_LIBRARY_PATH required at runtime
- Python based simple package recipes
- Ivan Razumov, joined CMS in May 2021
 - > 1.5y of experience building LCG packages w/ SPACK
 - > A very active contributor of SPACK (>700 PRs)



```
class Cnmem(CMakePackage):
    """CNMem mempool for CUDA devices"""
    homepage = "https://github.com/NVIDIA/cnmem"
    git = "https://github.com/NVIDIA/cnmem.git"
    version("git", branch="master")
    depends_on("cmake@2.8.8:", type="build")
```

Building CMS Software stack using SPACK

- After 22 months long roller coaster ride, Ivan finally had managed to build CMSSW externals software stack
 - > Had to rewrite package recipes multiple time due to fast moving **SPACK** development
 - v0.16, v0.17, v0.18
 - > Final implementation uses inheritance
 - SPACK v0.19.0
- CMS SPACK env contains 650 packages | class Vdt(BuiltinVdt):
 - 350 package recipes from upstream SPACK
 - > 300 in cms-spack repository
 - **100** CMS specific (including +80 cms-data)
 - **140** use built-in package with CMS specific patches/sources/changes
 - 60 recipes are rewritten (mostly copied and changed according to CMS needs)

```
from spack import *
from spack.pkg.builtin.vdt import Vdt as BuiltinVdt
class Vdt(BuiltinVdt):
    __doc__ = BuiltinVdt.__doc__
    keep_archives = True
```

SPACKFew major design/scalability issues

Package recipes: are they really simple ...?

- Yes they are simple/readable for first version, single configuration
- **SPACK** package recipes contain all versions/configurations/variants/build systems in single file
 - Over the time these recipes become a nightmare to manage specially when you had to

backport changes to few years old software stack

10 to **50**+ lines **LZ4**:

ROOT: 60 to **650+** lines

Python: 25 to 1.5K lines

Boost: 60 to **740** lines

Package recipe grows only (unless someone does a cleanup)

1083 acc 127 autotools 134 tkonlinesw 1102 openfoam 148 alpgen 1103 py-tensorflow 1108 opency 148 rpm 1185 mfem 192 root 1309 openmpi 210 tensorflow 1579 python 284 acc cmsdist

spack

Package recipe: LZ4 package

```
class Lz4(MakefilePackage):
    """LZ4 is lossless compression algorithm, providing compression speed
    at 400 MB/s per core, scalable with multi-cores CPU. It also features
    an extremely fast decoder, with speed in multiple GB/s per core,
   typically reaching RAM speed limits on multi-core systems.""
   homepage = "https://lz4.github.io/lz4/"
   url = "https://github.com/lz4/lz4/archive/v1.9.2.tar.gz"
   version("1.9.4", sha256="0b0e3aa07c8c063ddf40b082bdf7e37a1562bda40a0ff5272957f3e987e0e54b")
   version("1.9.3", sha256="030644df4611007ff7dc962d981f390361e6c97a34e5cbc393ddfbe019ffe2c1")
   version("1.9.2", sha256="658ba6191fa44c92280d4aa2c271b0f4fbc0e34d249578dd05e50e76d0e5efcc")
   version("1.9.0", sha256="f8b6d5662fa534bd61227d313535721ae41a68c9d84058b7b7d86e143572dcfb")
   version("1.8.3", sha256="33af5936ac06536805f9745e0b6d61da606a1f8b4cc5c04dd3cbaca3b9b4fc43")
   version("1.8.1.2", sha256="12f3a9e776a923275b2dc78ae138b4967ad6280863b77ff733028ce89b8123f9"
   version("1.7.5", sha256="0190cacd63022ccb86f44fa5041dc6c3804407ad61550ca21c382827319e7e7e")
   version("1.3.1", sha256="9d4d00614d6b9dec3114b33d1224b6262b99ace24434c53487a0c8fd0b18cfed")
   depends_on("valgrind", type="test")
                     ### RPM external 174 1.9.2
   variant(
                     Source: https://github.com/%{n}/%{n}/archive/v%{realversion}.tar.gz
        "libs",
       default="shar
       values=("shar
       multi=True.
       description="%setup -n %{n}-%{realversion}
   def url for versi build
       url = "https: make %{makeprocesses}
       if version >
```

```
def build(self, spec, prefix):
                                par = True
                                if spec.compiler.name == "nvhpc":
                                    # relocation error when building shared and dynamic libs in
                                    # parallel
                                    par = False
                                    make("MOREFLAGS=-1rt", parallel=par) # fixes make error on CentOS6
With only one variant
make(parallel=par)
                            def install(self, spec, prefix):
                                make(
                                    "install",
                                    "PREFIX={0}".format(prefix).
                                    "BUILD_SHARED={0}".format("yes" if "libs=shared" in self.spec else "no"),
                                    "BUILD STATIC={0}".format("yes" if "libs=static" in self.spec else "no"),
                                        from spack import *
                            def patch(seiclass Lz4(Package):
                                            homepage = "http://cyan4973.github.io/land
                                # Remove
                                if self.
                                                     = "https://github.com/Cyan/973/lz4/archive/r131.tar.gz"
                                    filte
                                    filte
                                            version('131', '42b09fab423\\da9d3fb33bd5c560de9'
                                    filte
                                            def install(self
                            @run_after("
                            def darwin f:
                                if sys.p.
                                                make('install', 'PREFIX={0}'.format(prefix))
                                    fix darwin_install_name(self.prefix.llo,
```

Compiler Wrappers

- SPACK provide compiler wrappers (800 lines of bash script) which are added in to PATH before the build process
- Compiler wrappers are the heart and soul of SPACK and are the magic behind
 - > Injecting compilation flags
 - RPATH/RUNPATH
 - -Idirs for dependencies during building phase
 - -Ldirs for dependencies during link phase
 - Common flags: enabling debug mode, optimization etc.
 - Achieving the simple package recipes
 - Many packages recipes have misused this feature and do not pass the required parameters to build system (autoconf/make/cmake)
- Disabling include/library directories injection shows that many packages either failed to build or pick up system packages
 - My test only checked single version/configuration/variant

Compiler Wrappers: Injection of includes paths

- Build System generated command
 - > compiler options -{| isystem | finclude | dirs | system | dirs | options
- SPACK's compiler wrapper generated command
 - > compiler options -I{include dirs} -isystem{include dirs} \

Extra include paths of package dependencies

```
-I{SPACK_INCLUDE_DIRS} | -isystem{SPACK_INCLUDE_DIRS} \
```

- -I{system dirs} -isystem{system dirs} options
- Overall 25% increase in cmssw build time (2h25 vs 3h15)
 - > 16 Cores VM; building everything on SSD storage

Compiler Wrappers: Injecting -I/-L...

- CMSSW depends on large number of external packages
 - > 200 of these have include directories
 - > 325 have lib/lib64 directories
- Injecting over 200 -Idirs means compiler has to go through all these to find system/compiler headers
 - ➤ A lot of IO operations (specially if you are taking most of the externals from CVMFS or shared file system)

Strace: compiling a source file with just two includes i.e iostream/string

% time	seconds	usecs/call	calls	errors syscall
69.17	0.182506	60835	1.5K ₃	O errors 1 Wait4
19.24	0.050761	GCC 5	9371	586 lstat
5.53	0.014597	11	1272	1034 openat
1.84	0.004843	1614	3	execve

For actual CMSSW sources strace reported 100K-230K IO errors (see backup slides)

% time	seconds	usecs/call	calls	errors	syscall
64.85	0.677646	225882	36K ₃ I	O err	ors wait4
24.62	0.2572875	PACK?	35888	35642	openat
6.66	0.069584	GCC 7	9371	586	lstat
1.14	0.011958	2989	4		execve

Compiler Wrappers: Injecting -Idirs/-Ldirs...

- Extra -Idirs can override some system/compiler header
 - > CMSSW failed to build as one of external package provide a conflicting system header
 - There could be more externals doing this
 - ➤ Multiple packages providing the same header file can cause build/runtime issues
- Adding -Idirs/-Ldirs does not guarantee that you pick up externals from SPACK build
 - Many packages now a days bundle/download/build packages internally
 - **Tensorflow** does it for tons of externals
 - ONNXtime does the same
 - **Root** also has many internal built-in packages
 - > You either need to patch or configure the package to use your external or make sure that external package versions are identical (with same patches applied)

Compiler Wrappers: Debugging long commands

CMSSW compile/link command length comparison

gcc / spack	Compile	Link
Smallest	670 / 41K	2K / 165K
Longest	+40K 12K / 53K	+160K 44K / 207K

Long compile/link commands

- > Package build logs only contain compile/link commands generated by build system
 - Extra flags/optins added by spack are not visible

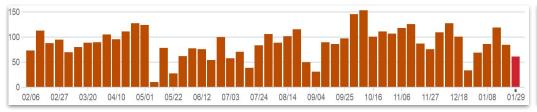
Really hard for developers of the package to debug the issue

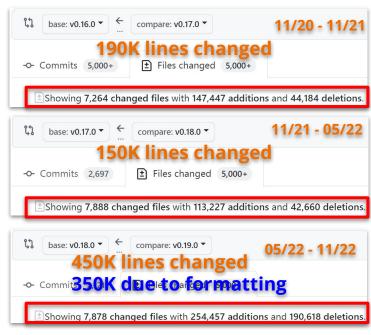
- > Developers use their build system to build a package.
 - They are only interested to know which configure and build options were used

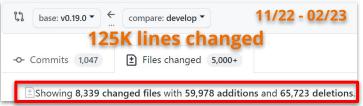
SPACK code base

- Very active projects
 - Gets many updates/fixes every week (avg 100 commits/week)
- 345K lines of python code
 - > 135K in core spack lib

SLOC Directory	SLOC-by-Language (Sorted)
209579 var	python=208372,
138267 lib	python=136512,
2920 share	sh=2561,csh=225,tcl=69,python=65

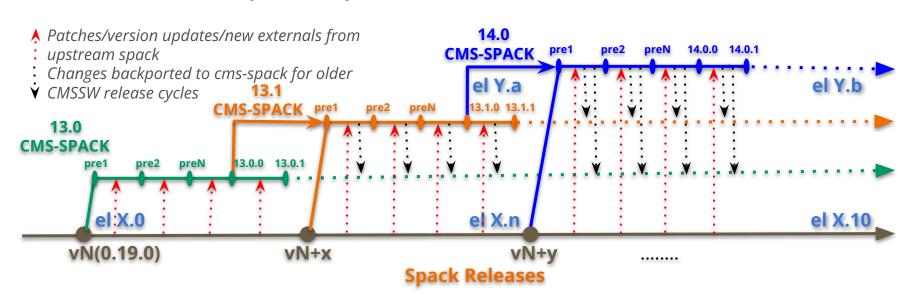






SPACK in large scale projects

- SPACK is moving target, so one can not use head of it
 - Projects needs to start with a tagged version and then
 - > Rest of the life of your release you have to maintain that SPACK code base



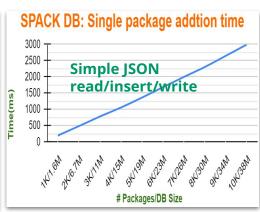
Software stack install time

- cmspkg takes 15mins to deploy full CMSSW software stack
 - CMSSW + dependencies (including bootstrap, GCC)
- SPACK takes 2hours to install CMS software stack (without GCC)
 - Installs one package at a time
 - For simple packages (with nothing to relocate) it takes (on average) 5-6s to download/install
 - For 650 packages it is already 1 hour
 - > For complex packages (with a lot of libraries/binaries) the install time is very high
 - CMSSW with over 4K binary products took 30 mins to install
 - It can easily add, at least, additional couple of hours for Pull Request testing

SPACK DB

- SPACK maintains a json file as DB to keep track of installed packages
 - Single package insertion at a time
- DB Insert time linearly increases based on DB size
- CMS Software for unique combination of OS/arch/Compiler goes under
 - single install path
 - slc7_amd64_gcc900: 8K packages in 2.5y
 - el8_amd64_gcc11: 2.1K packages in 9m
- Install time will only increase with time
- What if SPACK decided to change DB structure
 - > Sqlite implementation #34655
 - > We might not be able to use two different SPACK versions to install under same path

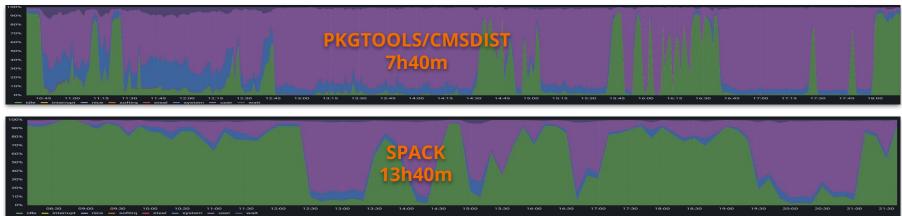




SPACK

Some minor issues which can be fixed in future releases

CMS Software stack: Build time w/o GCC and CMSSW



- Test were done on 16 Cores VM with 120GB memory with SSD
- SPACK builds single package at a time: Larger the machine bigger the waste
 - Parallel build support might improve but I was not able to tests it

Software stack install time: Parallel install

- SPACK parallel build/install fix applied
 - > Updated SPACK DB lock wait time to 60s (instead of 3s)
- SPACK install with -j16 failed
 - > For some unknown reason it start rebuilding packages
- SPACK install with -j2 worked but took more time than serial mode
 - > 2h40m to install cmssw + dependencies (without GCC)
 - 30mins to install CMSSW alone
 - Might take more time if cmssw was built with runpath

Environment setup

- SPACK provides various ways to use an installed package
 - spack load/unload
 - > spack environment
 - Bundle many related packages and activate all of them at once
 - > spack environment modules
 - SPACK generates module files which one can use with module load/purge
- All of these failed for large software stack
 - For large software stacks, the generated env is so large that it exceeds the max argument size (2MB)

Setting only the Python tools env (330 packages): slow as compared to CMSDIST: <1s vs >40s

```
> which python3 /usr/bin/python3
```

> spack load python-tools@3.0

> which python3

bash: /usr/bin/which: Argument list too long

> which python3
/usr/bin/python3

> module load python-tools-3.0-gcc-11.2.1-ovyelip

> which python3

bash: /usr/bin/which: Argument list too long

Package dependency on all Build systems

Every SPACK package loads all the build system known to SPACK

- Why we should care about it?
 - We have to either fix or remove the Build System if it fails due to python version updates within EL distros
 - EL8 has python 3.6, 3.8 and 3.9
 - EL9 has python 3.9 and 3.10

"""spack.util.package is a set of useful build tools and directives for packages. Everything in this module is automatically imported into Spack package files.

from spack.build_systems.perl import PerlPackage from spack.build_systems.python import PythonExtension, PythonPackage from spack.build_systems.qmake import QMakePackage from spack.build_systems.r import RPackage from spack.build_systems.racket import RacketPackage from spack.build_systems.rocm import ROCmPackage from spack.build_systems.ruby import RubyPackage

Missing system dependency checks

- ❖ PKGTOOLS/CMSDIST uses RPM to build CMS Offline packages
 - > We maintain our own RPM DB to control what our packages can pick up from system
 - > RPM post build checks make sure that packages we build do not accidentally depend on any thing which is not in our RPM DB
 - > This helped use control our system level dependencies and allowed CMS Offline SW to work (build/run) with in a major EL release cycle
- https://github.com/spack/spack/pull/28109 provides a partial implementation
 - Opened since Dec 2021
 - Uses Idd and hardcoded list of system libs
 - This functionality is not any way near to what rpmdeps provides
 - Shows that SPACK package can randomly pick up system libraries

Some other random things

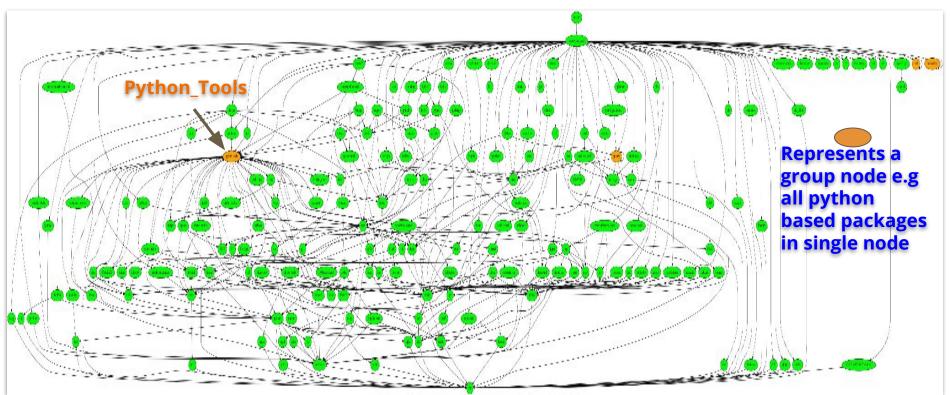
- SPACK concretize your whole env even if you want to build single package
 - > Copies all the patches of all the versions/variants for all packages in your env
 - Might be very annoying for developers
- SPACK compiles/generates byte code for all the packages known to it (6.7K)
 - > So you have to maintain all packages even if you do not use those
 - > Is var/spack/repos/builtin/packages/*/__pycache__/package.cpython-36.pyc |wc -l 6753
- No easy way to search binary caches for installation
 - We use tricks like copying a pre-concretized lock file (from the build step) to tell SPACK what to install
- We still have no experience with multiple parallel builds building/uploading same package
- Relatively large distribution size: +15% (45G vs 39G)

Summary

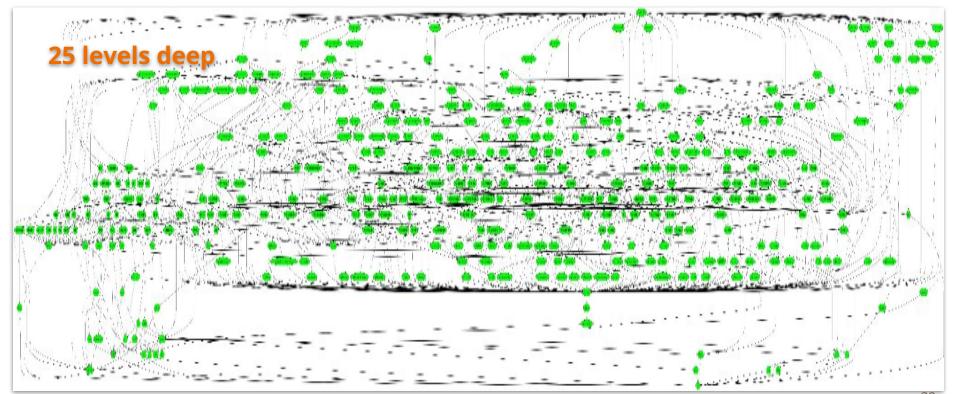
- SPACK is nice tool for small env with relatively small deps and life cycles
 - > CMS Software stack life cycle is even longer than EL distros
- Along with all the slowness/issues (as compare to existing CMS Packaging system), it also comes with high maintenance overhead
- Package recipes are not written with much care and will break any large software stack sooner or later
 - > Specially for SW stack with multiple ML tools which maintain/build their own deps
- I am sure I might have missed many nice features of SPACK but things which matters most for CMS software stack do not look good
- I am afraid it is not the right tool for packaging large software stacks

Backup

CMSSW: External Package Dependency



CMS Software stack: Python Packages Dependency



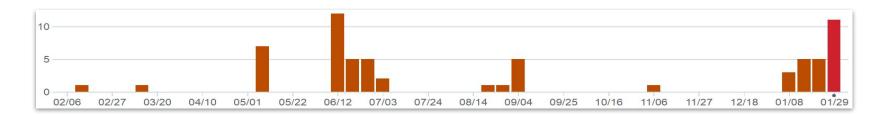
SCRAM

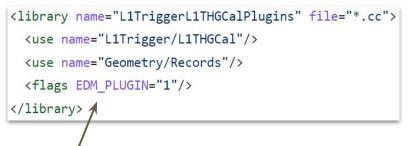
- CMS Software Configuration, Release and Management tool
 - Build System
 - Software Development and runtime environment setup
- Since 1998, this is the only tool CMS has used to build offline software
 - ➤ Initially written in **PERL** but in 2020/21 it was rewritten in **PYTHON**
 - Reduced code base: V2: 8.5K Perl, V3: 3.5K Python
- Backward compatibility within a SCRAM major version
 - SCRAM V2 latest version can still build and set env for 12 year old CMSSW_3_9
- It has been very stable and has not shown any sign of aging



CMSSW-Config

- Build rules for CMS offline software
 - gmake based rules
 - 3.5K lines of GMAKE
 - 3.3K of Python : To convert XML based rules in to gmake targets
 - SCRAM uses these rules to build CMSSW/FWLite/CORAL
- Provides hooks for SCRAM to dynamically set build/run time environment
 - CUDA Runtime
 - Micro-architectures





CMSSW-Config...

- **CMSSW** build rules are result of many years of work
- Build rules has been profiled multiple time to maximize the utilization of build and development resources
 - > We avoid long PATH, LD_LIBRARY_PATH, PYTHONPATH, CMSSW_SEARCH_PATH
 - libs, bins, data and python modules under single directory
 - Just like **view concept of LCG/Spack** but CMS has been using it since 2008
 - Running of all executables with full paths to avoid searching those in PATH
 - > Avoid duplication of *-lincdir, -Llibdir* to improve the compile/link time
 - > Proper (transitive) dependency handling to avoid passing of extra -ldir
 - Compact GMake rules in few files instead of many small ones
 - Smaller files (e.g. one per binary/library) takes a lot of time to load

PKGTOOLS

- CMS Offline Packaging tool
 - Build packages and their dependencies from sources
 - Written in PYTHON and uses Redhat Package Manager (RPM) as backend for building and installing packages
 - Nearly **200K binary packages** in the repository for various OS, archs and compilers
 - 6.7K CMSSW releases
- Very stable and requires low maintenance
 - 5K lines of PYTHON code
 - Single version to build full software stack of all CMSSW release cycles



<u>CMSPKG</u>

- Package distribution and installation tool. PKGTOOLS uses it to
 - download and install prebuilt packages
 - Upload newly build packages
- It was developed to replace apt/yum usage
- Uses RPM dependency information instead of maintaining its own dependency DB
- <15m to install full pre-build CMS-SW stack</p>
- One version to install any package
 - Used by all CMSSW release cycles/archs
 - > 2K Python, 2K bash lines of code (bootstrap

APT	CMSPKG
apt-get update	cmspkg -a arch update
apt-get -y install package	cmspkg -a arch -y install package
apt-get reinstall package	cmspkg -a arch reinstall package
apt-getreinstall install package	<pre>cmspkg -a archreinstall install package</pre>
apt-get remove package	cmspkg -a arch remove package
apt-get clean	cmspkg -a arch clean
apt-get upgrade	cmspkg -a arch upgrade



CMSDIST

- Collection of build recipes
 - > RPM Spec files to provide the actual build/install instructions and packages requirements
 - Uses BASH for build recipes
- 650 package recipes
 - > 320 Python packages
 - > 90 data packages
- One version/configuration per package
 - Multiple version supported via separate SPECs
- 20K lines of build recipes



Source: https://github.com/%{n}/%{n}/archive/v%{realversion}.tar.gz

RPM external 174 1.9.2



CMSDIST...

- Supports automatic generation of packages
 - Pip based packages
 - CMSSW Data packages

- [default]
- RecoTracker-MkR = V00-12-00
- RecoTauTag TaimingFiles=V00-07-00
- Physics Tools Mano AOD = V01 03 00
- CalibTracer-SiStripDCS=V01-01-00
- Non-root installation by creating a separate RPM DB **
 - Well controlled system package dependency
 - RPM post build dependency checks: To make sure we do not use anything outside our control **Pip based Python packages**

Multi-Vectorization packages zlib, zlib_haswell, zlib_skylake-avx512 etc.

- aiosignal==1.2.0 requirements.txt 17
- anyio==3.6.1 dependabot notifications 18
- **Security issues** 19 appdirs==1.4.4
- Requires: py3-cython py3-pkgconfig openmpi

- argon2-cffi==21.3.0 20
- argon2-cffi-bindings==21.2.0 21

%define PipPreBuild export HDF5_DIR=\${HDF5_ROOT} CC="mpicc"

Compiler Wrappers: Injecting -I/-L CMSSW sources

% time	seconds	usecs/ca	11	calls	errors	syscall
				5.	5K 10 6	errors wait4
70.91	0.430472	1434	90	3	1	wait4
16.83	0.102183	GCC	5	18638	1491	lstat
7.40	0.044904		9	4652	4219	onerat

	Alignn include	nent/ e few	Co	coaDa ot head	n q/src/Coc ders)	oaDaqRo	ဌ tEvent.	cc:1 incl		directly K IO errors
9	seconds	usecs/ca	all	calls	errors syscall	% tin	ne seconds	usecs/call	calls	errors syscall
1	0.430472	1434	190	5. .	KIO errors 1 wait4	63.4	6.561829	2187276	3	1 wait4
3	0.102183	GCC	5	18638	1491 lstat	32.2	.8 3.337334	SPACK 4	682340	52545 lstat
)	0.044904		9	4652	4219 operat	3.6	0.375959	GCC 6	55750	55309 openat

DQM/Physics/src/plughs.cc: 1055 includes

% time	seconds	usecs/	call	calls	errors	syscall
				42	K 10 e	rrors
85.45	5.872444	293	6222	2		wait4
6.97	0.478942	GCC	11	40275	37292	openat
5.33	0.366395		6	57083	4598	lstat

			23	0K IO ei	rors	
% time	seconds	usecs/call	calls	errors	syscall	
66.03	14.770776	7385388	2		wait4	
28.86	6.455500	SPACK	1266902	97661	lstat	
4.42	0.988656	GCC	133382	130391	openat	

rpath/runpath Issues

- **❖** RPATH/RUNPATH are great and works for most of the cases
 - > No need to set global **LD_LIBRARY_PATH** which can break other tools
 - CMSSW env breaks CMS Computing env
- Does not work for packages with stubs libraries which are suppose to be loaded from correct path at runtime
 - ➤ cuda
 - > dpm
 - > tkonlinesw
- Can not use RPATH if your software stack has packages with stubs libs
 - > RUNPATH works but then you need to set LD_LIBRARY_PATH to load the correct library at runtime

Life without LD_LIBRARY_PATH

- No CMSSW Patch release
 - CMSSW libraries loaded from full release will load all shared libraries from full release even if those are available in patch release
- No CMSSW developer area
 - > Same issue as patch release
- No usage of packages with stubs libraries
 - > cuda
- No multi micro-architectures builds
 - Which needs to load different vectorization library at runtime
- Lose the ability to build an external and test in developer area
 - Developers of externals e.g. root/geant4 etc. use their build system to build and use it directly in cmssw by updating the tool file
- ROOT dictionaries loading does not work