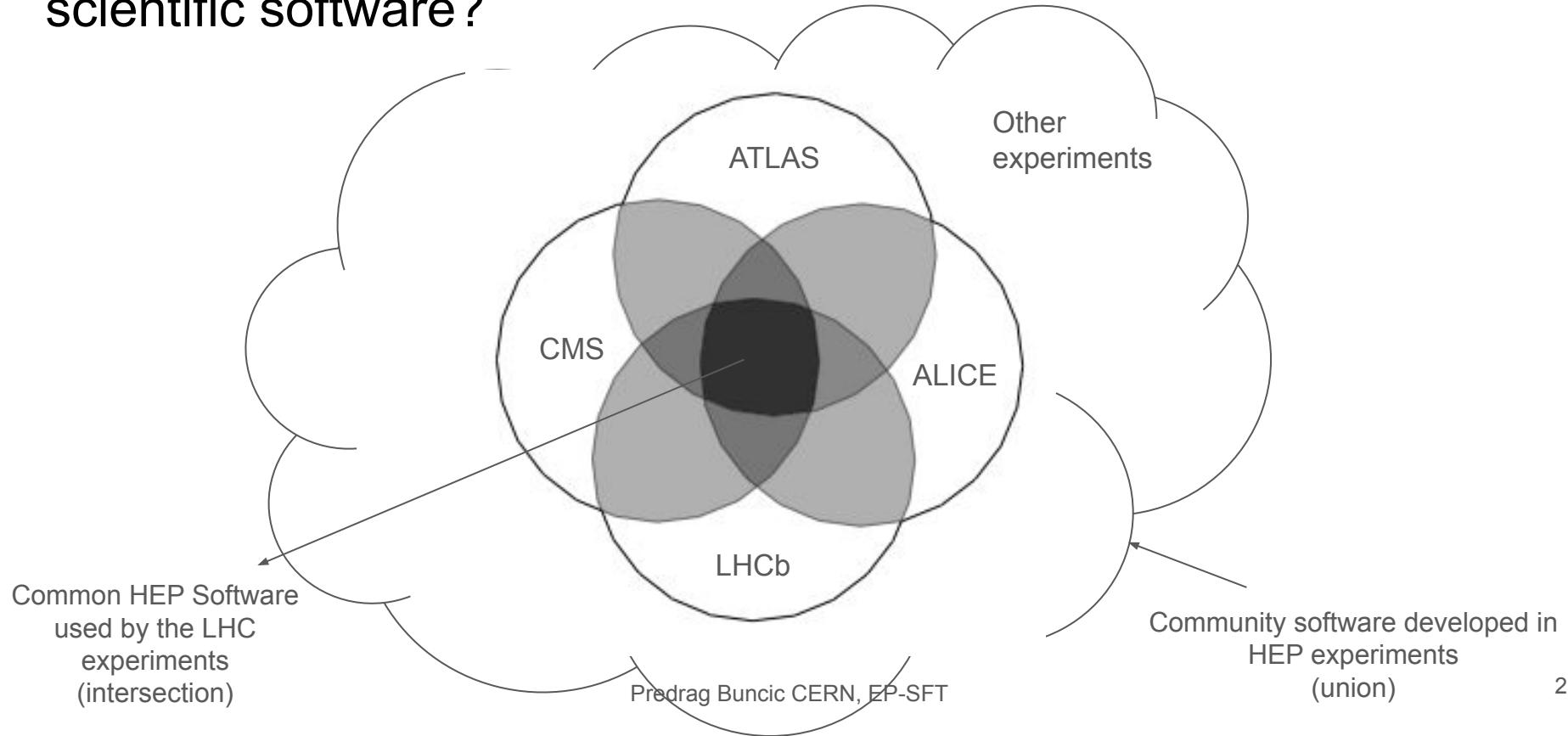


A path to convergence of build systems?

Predrag Buncic

How do we collaborate and work towards the success of common scientific software?



Current practices

- SFT/SPI Builds and tests software stacks for LHC experiments
 - Uses in-house LCGCMake system to build and test the software stacks and distribute build products via CVMFS and RPMs as consistent releases
 - 800+ packages on many platform {CPU, OS, compiler, flags} combinations
- LHCb and ATLAS use the same (or similar) CMake-based approach to complement the builds done by SFT (externals) with their software components.
- To some extent, others benefit from CI and testing but build the software using their tools.
 - ALICE uses aliBuild to build their entire software stack
 - CMS uses cmsBuild to build its entire software stack
- Everyone uses CVMFS to publish software releases and nightly builds for testing
- Everyone is reasonably happy with their setup

Why change anything?



Previous attempts to converge in a common tool

- HSF Software Packaging Working Group Report (03/2016) ?
 - <https://hepsoftwarefoundation.org/notes/HSF-TN-2016-03.pdf>
- Discussion in the Architects Forum (10/2023)
 - [Report from SPACK Working Group](#)

	Linux	MacOS X	Windows	Xcompiler
aliBuild	+	+	-	+
cmsBuild	+	+	-	+
Contractor	+	+	-	+
Homebrew	o	+	-	-
LCGCMake	+	+	o	o
Nix	+	+	o	o
SciSoft	+	+	-	-
Spack	+	+	-	+
Worch	+	+	-	o

	Multi-Rel	Multi-BuildVar	MultiShell-RTE	Relocation
aliBuild	+	+	+	+
cmsBuild	+	+	+	+
Contractor	+	+	NA	-
Homebrew	-	-	NA	-
LCGCMake	+	+	+	+
Nix	+	-	+	-
SciSoft	+	+	+	+
Spack	+	+	NA	-
Worch	+	+	+	+

	Depends-On	Ease-Add-Pkg	Ease-Bootstrap	Documentation
aliBuild	Python	spec-file	+	o
cmsBuild	Python,rpm,apt	spec-file	o	-
Contractor	Python	python file	git checkout	-
Homebrew	Ruby	Formula	+	+
LCGCMake	Python, Cmake	Cmake-macro	+	o
Nix	Perl	expression	-	+
SciSoft	Cmake	Cmake-macro	o	-
Spack	Python	auto template	git checkout	+
Worch	Waf,Python	Text-files	+	o

	Performance	Sys-Reuse	Community	Unique-IDs	VCS-Support
aliBuild	+	o	-	+	+
cmsBuild	+	o	-	+	+
Contractor	+	+	-	-	+
Homebrew	+	+	+	-	+
LCGCMake	+	+	+	+	+
Nix	+	-	+	+	?
SciSoft	o	o	+	+	+
Spack	o	o	+	+	+
Worch	+	+	-	o	+

aliBuild (by Giulio Eulisse and ALICE)

- It was reviewed by the HSF in 2016, many improvements and production experience since then
- Shares DNA with CMS
 - Giulio Eulisse designed cmsBuild before joining ALICE and adapting the lessons learned in cmsBuild to the ALICE environment.
- Written in Python and bash
- Package description in the form of .sh script
 - Easy to translate build instructions
 - Metadata in the form of a YAML preamble
- Support for
 - Local development, caching and reuse of build products system tools and libraries
 - Automatic relocation, parallel software installations
- Produces tar files, RPMs (via separate helper script).
- Runtime package configuration based on environment modules
- Used in production since 2015.

Predrag Buncic CERN, EP-SFT

The screenshot shows the GitHub homepage for the aliBuild repository. At the top, there's a navigation bar with 'Code' and 'Issues' tabs. Below the header, there's a brief introduction: 'A simple build tool for ALICE experiment software and its externals. Recipes for the externals and ALICE software are stored in alidist.' It provides instructions to 'git clone https://github.com/alisw/aliBuild.git' and 'aliBuild build O2Physics'. There are sections for 'Simple build recipes', 'Binary packages', 'Developer mode', and 'Docker support', each with a 'Read more' link. On the right, there's a sidebar with 'Reuses system tools', 'Integrates with modules', and another 'Docker support' section. At the bottom, there's a large 'https://alisw.github.io/aliBuild/' URL.

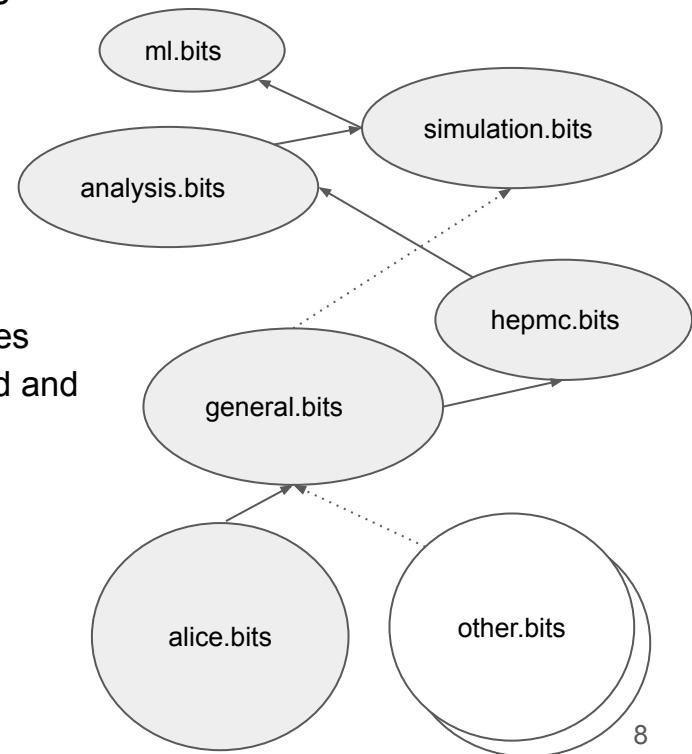
Lessons from the past

- AliEn BITS in 2003
 - It is possible to build and test ~200 (meta) packages with make driven tool (KDE Konstruct)
 - https://techbase.kde.org/Getting_Started/Build/Historic/Konstruct
- Grid Package Manager in 2004
 - It is better to use the file system than the package manager to distribute software (CVMFS)
- CernVM appliance in 2007
 - Built using Conary Package Manager by rPath
 - Had some great features
 - Could handle multiple repositories in search path
 - Reproducible builds in chroot environment
 - Relocating binary output to destination directory
 - Support for development and testing and release flows
 - Automated dependency discovery, parallel build (rMake, rBuilder)



BITS (demonstrator)

- BITS - A tool to Build, Integrate and Test Software packages
 - <https://github.com/bitsorg> on GitHub
 - Re-branded and extended aliBuild
 - Because names matter
 - As well as the backward compatibility
- Why start from aliBuild?
 - It covers most of the use cases
 - Simple and understandable recipes versioned in Git repositories
 - Written in Python and bash, it is relatively simple to understand and extend
- Extensions wrt aliBuild
 - Added support for multiple package repositories
 - Supports individually versioned package directories
 - Allows for parallel build flows on a single node and beyond
 - ~20% gain in build speed for ALICE case
 - Simplified build recipes



What about next 20 years?

- In an ideal world where all (LHC) experiments agree to use a common build tool
 - We work together to improve the common tool to meet all our requirements.
 - SFT builds general, hepmc, simulation, analysis and ml package groups and distributes them on CVMFS
 - The tool is specifically optimized to use CVMFS as an efficient distribution channel for software and reusable build products.
 - Experiments using the same tool add and maintain their repositories while benefiting from shared package build recipes.
 - Different CI pipelines run concurrently (possibly on the same shared build infrastructure), optimizing usage of personpower and computing resources.
 - Everyone is happy

Conclusions

- There are many package managers out there
 - Usually adapted to specific use cases
 - It is often easier to write a new one than to convince others to use the common one
- The software stacks of the LHC experiments differ
 - There are also significant overlaps
- The use cases must be almost identical
 - It should be possible to meet them in one tool
- Shouldn't we, as the community (LHC experiments, at least), finally start acting rationally, save effort and resources, agree on a homegrown tool, and, if needed, adapt it to match all our needs?
 - If so, SFT is willing to help.
 - But we need at least two experiments to sign up.
- BITS demo is a work in progress
 - This is the right moment to express interest and join the development

To BITS, or not to BITS, that is the question
[for discussion]

Backup

Summary of common software packages (in production)

- Common Software used and developed by the HEP Community:
 - **Geant4**, **ROOT**, fastjet, xrootd (4)
 - **VecGeom**, dd4hep, AIDA (2)
- MC Generators and tools:
 - hepmc, hepmc3, starlight, pythia6, lhapdf (4)
 - heppdt, rivet, thepeg, yoda, pythia8 (3)
 - evtgen, crmc, herwig3, hydjet, madgraph5amc, pyquen, sherpa, mctester (2)
- Scientific computing libraries (not strictly HEP):
 - boost, gsl (4)
 - blas, clhep, eigen, vdt (3)
 - onnxruntime, tensorflow, xgboost, matplotlib (2)
- Other commonly used libraries (not HEP specific)
 - tbb, fmt, freetype, jemalloc, libffi, libunwind, libxml2,sqlite, protobuf (4)

Input used for comparison

CMS

Input used for comparison

LHCB

aida boost cmake catch2 cppunit dd4hep davix edm4hep form gsl generator gitconddb graphics hepmc heppdt io jinja2 lcio machine markupsafe math other pyyaml python relax root sio simulation tool vc xml xercesc absl_py appdirs argon2_cffi asn1crypto assimp astor astunparse async_generator atomicwrites attrs babel backcall beautifulsoup4 beniget bison blas bleach bokeh build cachetools cairo capturer catboost certifi cffi cfitsio chardet charset_normalizer clhep click caketools collier coloredlogs contourpy coverage cppgsl crmc cryptography cycler cython debugpy decorator defusedxml dll distlib docutils doxygen eigen entrypoints et_xmlfile exceptiongroup fastjet fastjsonschema feynhiggs fftw filelock fcontrib flatbuffers flex fmt fontconfig fonttools freetype fribidi fs fsspec funcsigs future gast gdb geos gettext gl2ps glib go go_demangle go_liner go_readline go_runewidth google_auth google_auth_oauthlib google_pasta gosam gosam_contrib gperf gperftools graphviz grpcio h5py harfbuzz hdf5 hepmc3 herwig3 html5lib humanfriendly hypothesis idna importlib_metadata importlib_resources iniconfig ipykernel ipyparallel ipython ipython_genutils jax jaxlib jedi jemalloc joblib jsoncpp jsonschema jsonschema_specifications jupyter_client jupyter_core jupyterlab_pygments keras keras_applications keras_preprocessing kiwisolver lcgen libclang libffi libgit2 libsodium libtool libunwind libxml2 libxslt linkify_it_py looptools lxml madgraph5amc markdown markdown_it_py matplotlib matplotlib_inline mdit_py_plugins mdurl meson messaging mistune ml_dtypes mock more_itertools mpfr mpmath msgpackc multiprocess mypy mypy_extensions mysql nbclient nbconvert nbformat nest_asyncio networkx ninja njet nodejs nose notebook numpy oauthlib odfpy onnx onnxruntime openloops openpyxl opt_einsum oracle packaging pandas pandocfilters panel pango param parso pathlib2 pathos pbr pcre pcre2 pep517 pexpect photos++ pickleshare pillow pip pixman pkg_config platformdirs pluggy ply png podio powheg-box-v2 pox ppft pprof prometheus_client prompt_toolkit protobuf ptyprocess py pyasn1 pyasn1_modules pybind11 pycairo pycparser pyct pydantic pydot pydot_ng pygments pyparsing pyrPersistent pytest pytest_cov pythia6 pythia8 python_dateutil pythran pytz pyviz_comms pyzmq qd qgraf railroad_diagrams rangev3 referencing requests requests_oauthlib rivet rpds_py rsa ruamel_yaml ruamel_yaml_clib scandir scikitlearn scipy send2trash setuptools setuptools_scm shapely simplegeneric six sortedcontainers soupsieve spdlog sqlite starlight swig sympy syscalc tauola++ tbb tensorflow tensorflow_data_server tensorflow_plugin tensorflow_estimator tensorflow_io_gcs_filesystem termcolor terminado testpath texinfo theano thepeg threadpoolctl tinycc2 tomli torch tornado tqdm traitlets typed_ast typing_extensions uc_micro_py umesimd urllib3 valgrind vbfmlo vcversioner vdt veccore vectorclass verboseglogs virtualenv wcwidth webencodings werkzeug wheel wrapt xapian xgboost xlrd xqilla xrootd xyzservices yamlcpp yoda zeromq zipp

Input used for comparison

ATLAS

aida authlib boost cppunit davix form frontier_client gsl generator graphics hepmc heppdt io machine math other pyjwt pyaml python qt5 relax root sgen simulation tool vc xml xercesc absl apfel appdirs asn1crypto atomicwrites attrs auth_get_sso_cookie autopep8 backcall beautifulsoup4 beniget bison blas boto3 botocore build c_ares cairo ccache certifi cffi cfitsio chardet charset_normalizer clhep click cmaker tools coin3d collier configobj contourpy coverage cppgsl cppy crmc cryptography cuda cudnn cx_oracle cycler cython decorator defusedxml dill distlib distro doctopt doxygen eigen entrypoints et_xmlfile evtgen exceptiongroup fastjet feynhiggs fftw filelock fjcontrib flake8 flake8_bugbear flake8_builtins flex fmt fontconfig fonttools freetype fribidi fs funcsigs future gast gdb geneva gettext git gl2ps glib go go_demangle go_liner go_readline go_runewidth gosam gosam_contrib gperf gperftools graphviz greenlet grpc gssapi gtest harfbuzz hdf5 hdf5_mpi heaptrack hepmc hepmcanalysis heputils herwig3 highfive hijing hto4l hwloc hydjet hypothesis idna igprof importlib_metadata importlib_resources iniconfig ipython ipython_genutils java jedi jemalloc jmespath joblib jsoncpp kiwisolver kokkos lcenv lhapdf libffi libm_aocl libsodium libtool libunwind libxml2 libxslt looptools lxml madgraph5amc matplotlib maven mccabe mcfm mctester mcutils meson messaging mock more_itertools mpfr mpmath msgpackc multiprocess mypy mypy_extensions mysql ninja njet nose numpy odfpy openloops openmpi openpyxl oracle oracledb packaging pacparser pandas pango parso pathos pbr pcre pcre2 pep517 pepper_kokkos pexpect photos++ pickleshare pillow pip pixman pkg_config platformdirs pluggy ply png pox ppft pprof prompt_toolkit prophecy4f protobuf protobuf2 psutil ptyprocess py pybind11 pycairo pycodestyle pycparser pyflakes pygments pygraphviz pyparsing pypng pyqt5 pyqt5_sip pyqt_builder pyquen pylha pytest pytest_runner pythia6 pythia8 python_dateutil pythran pytz qd qgraf qrcode railroad_diagrams rangev3 re2 requests requests_gssapi rivet s3transfer scikitlearn scipy setuptools setuptools_scm sherpa sherpa-openmpi simplegeneric sip six sortedcontainers soupsieve sqlalchemy sqlite starlight stomppy superchic swig sympy syscalc tauola++ tbb texinfo thep8i thepeg threadpoolctl tiff toml tomli tornado tqdm traitlets typing_extensions tzdata urlib3 valgrind vbfmlo vdt virtualenv wcwidth wheel xapian xld xrootd yoda zeromq zipp

Input used for comparison

ALICE

bseil aegis alice-grid-utils alien-cas alien-runtime aliphysics aliroot apmon-cpp arrow base bookkeeping-api boost bz2 c-ares capstone cgal clang cmake common-o2 configuration control-occplugin curl datadistribution dds debuggui double-conversion dpmjet evtgen faircmakemodules fairlogger fairmq fairroot fastjet fftw3 flatbuffers fmt freetype gcc-toolchain geant3 geant4 geant4_vmc generators glfw gmp googlebenchmark grpc gsl hepmc hepmc3 igprof itsresponse jalien jalien-root jdk jemalloc jq json-c kfparticle lhapdf libffi libinfologger libjalieno2 libpng libunwind libuv libwebsockets libxml2 lz4 lzma mcsteplogger mlmodels monitoring mpfr ms_gsl o2 o2dpg o2pdpsuite o2physics o2sim odc onnxruntime openssl photos ppconsul protobuf pythia pythia6 python python-modules python-modules-list qualitycontrol rapidjson re2 root roounfold simulation sqlite starlight tauola tbb treelite utf8proc vc vecgeom vgm vmc xercesc xjalienfs xrootd xsimd zeromq zlib