# Open Source Build Tooling in High-Energy Physics Software

## Case studies of *Spack* and *CernVM-FS*

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Thomas Madlener (DESY), Valentin Volkl (CERN)

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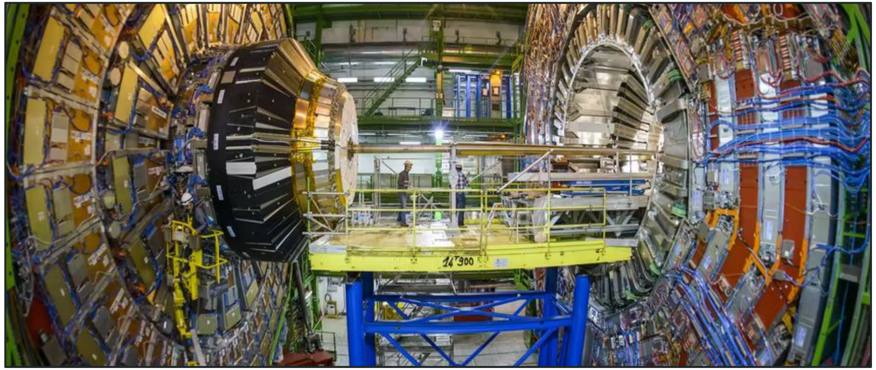
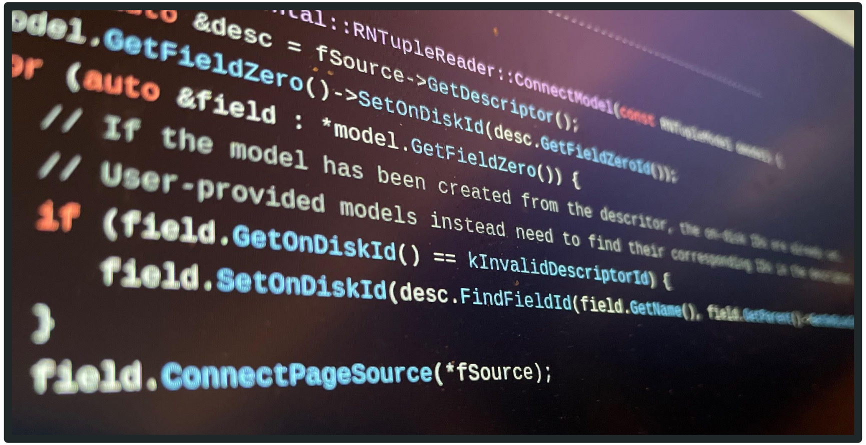
# HEP Software and Computing



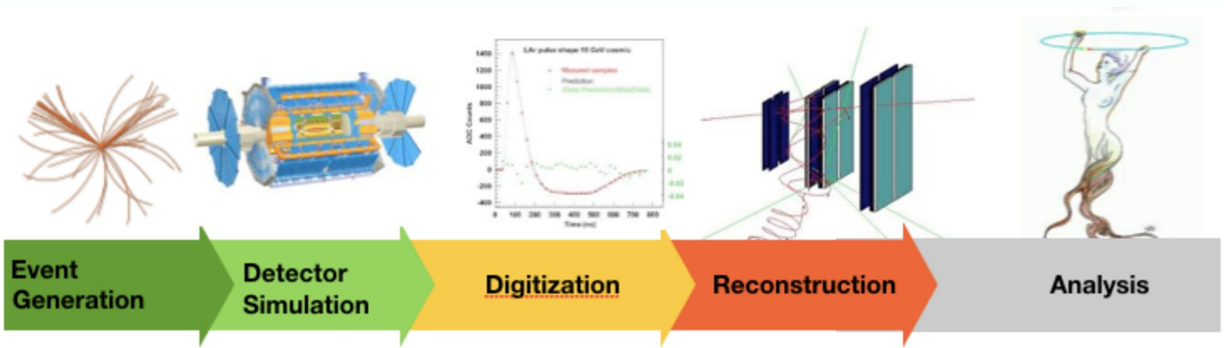


# Computing Workloads in HEP

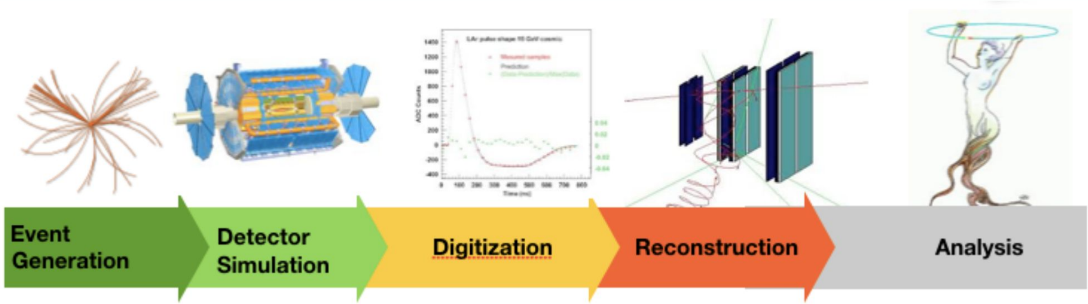
- **Accelerator** vs. **Detector**
- **Online** vs. **Offline**

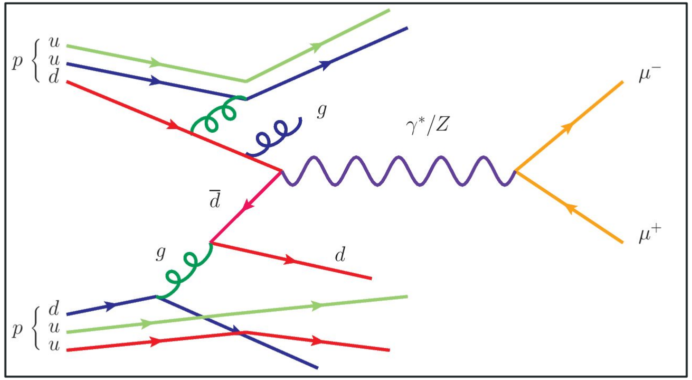
**Offline Data Processing:**

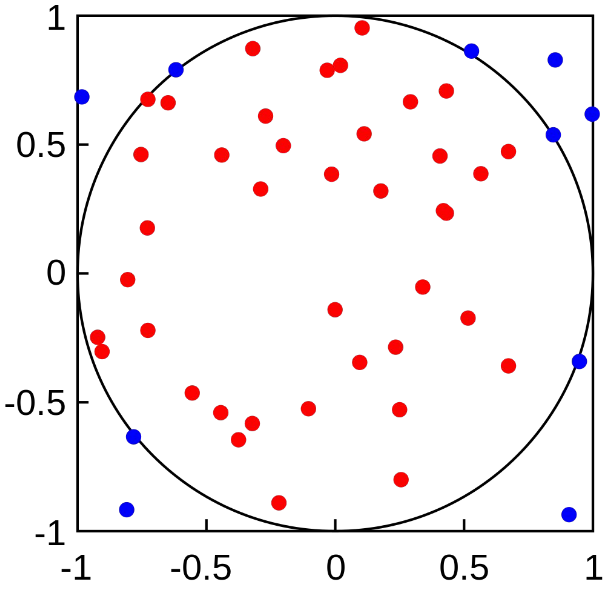
- Generation
- Simulation
- Digitization
- Reconstruction
- Analysis



# Event Generation

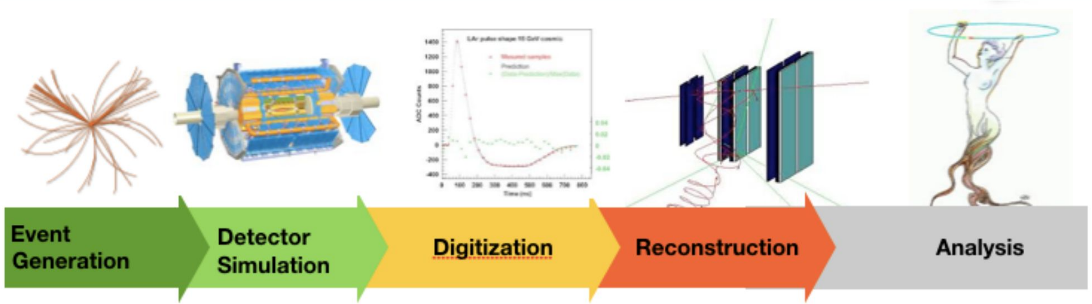


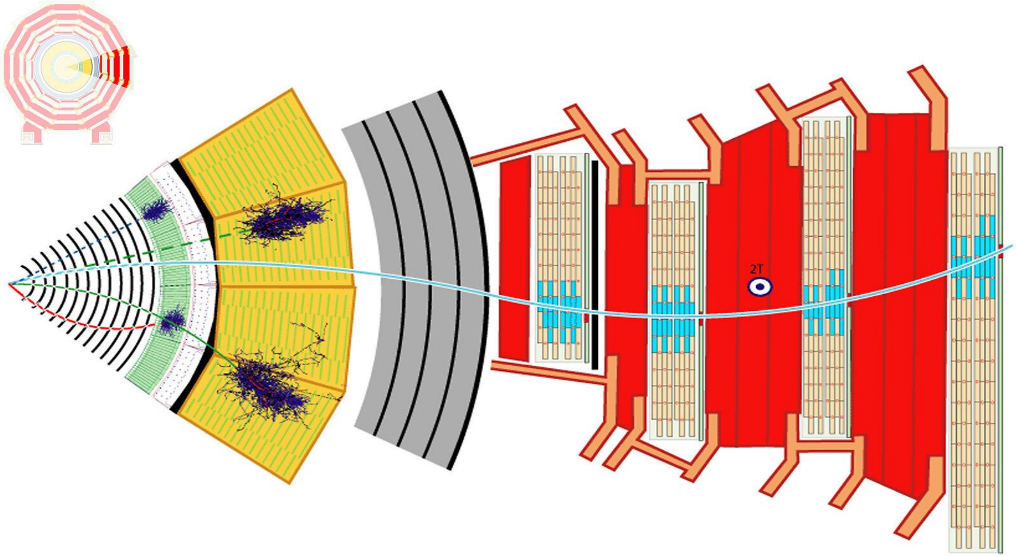



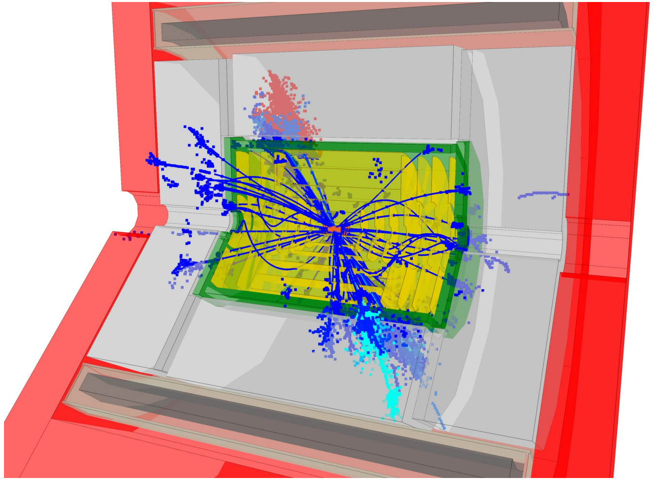




$$\sigma_{ab\to N} = \int_0^1 \mathrm{d}x_a\,\mathrm{d}x_b\, f_a(x_a,\mu_F) f_b(x_b,\mu_F) \int_{\text{cuts}} \mathrm{d}\Phi_N\, \frac{1}{2\hat{s}} |\mathcal{M}(\Phi_N,\mu_F,\mu_R)|^2$$

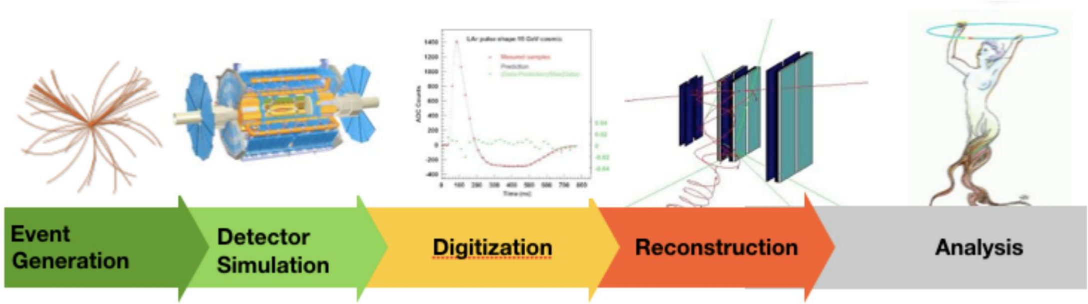
# Detector Simulation

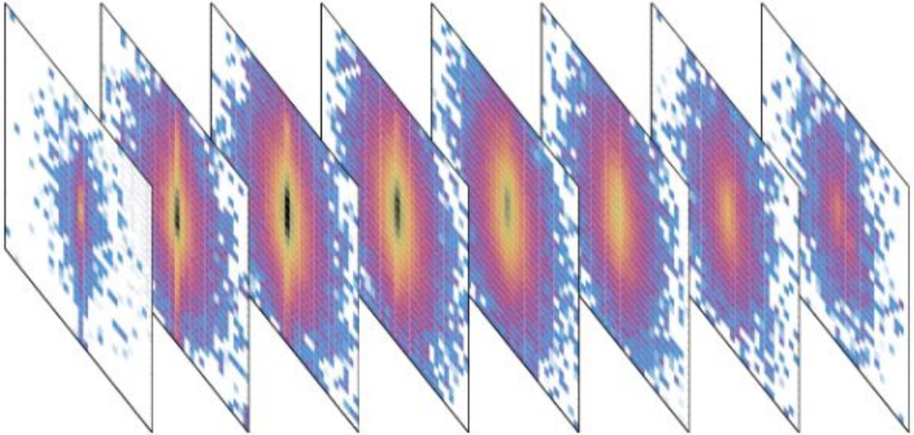


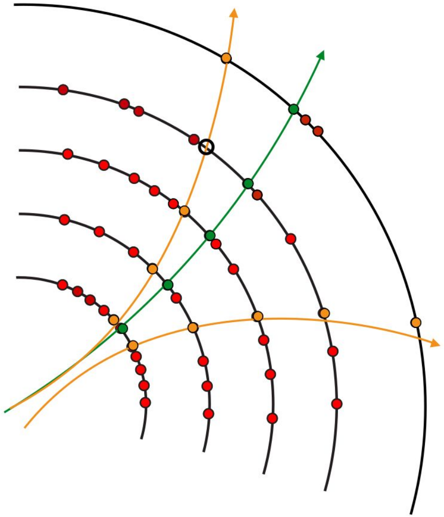



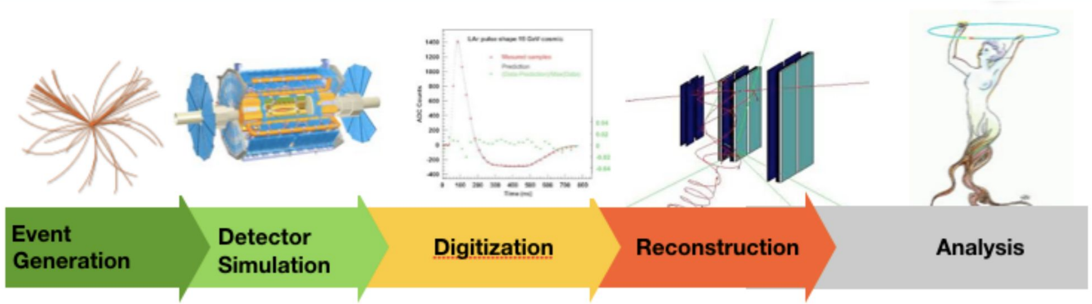
# Reconstruction

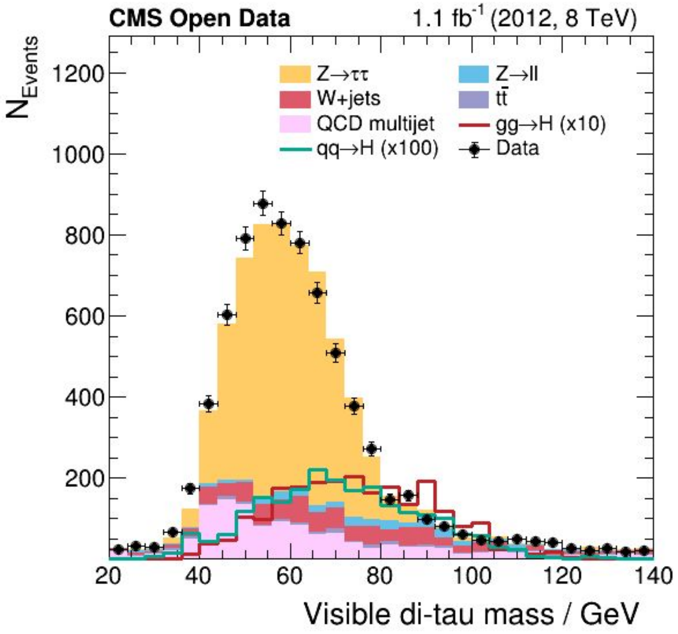


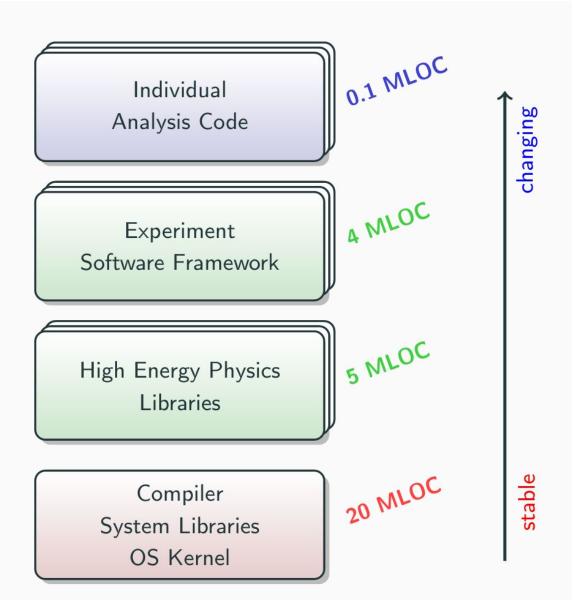


# Analysis


Event Generation
Detector Simulation
Digitization
Reconstruction
Analysis

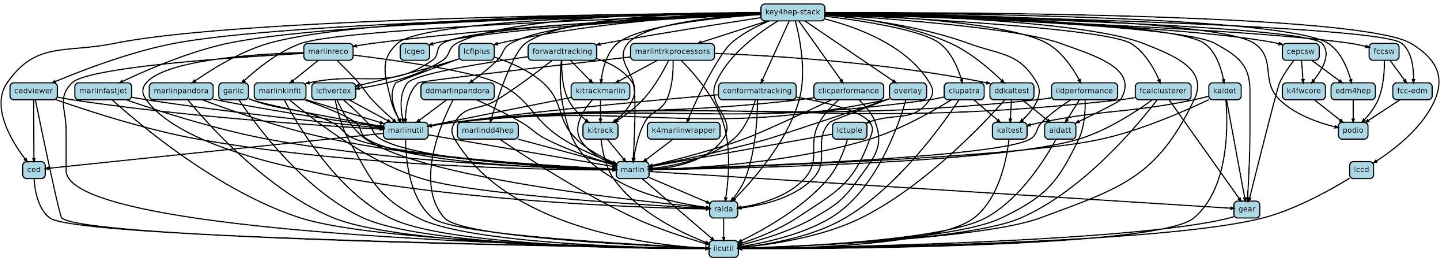

CMS Open Data
1.1 fb-1 (2012, 8 TeV)
N_Events
Z→ττ
Z→ll
W+jets
tt̄
QCD multijet
gg→H (x10)
qq→H (x100)
Data
1200
1000
800
600
400
200
20
40
60
80
100
120
140
Visible di-tau mass / GeV

# The HEP Software Stack



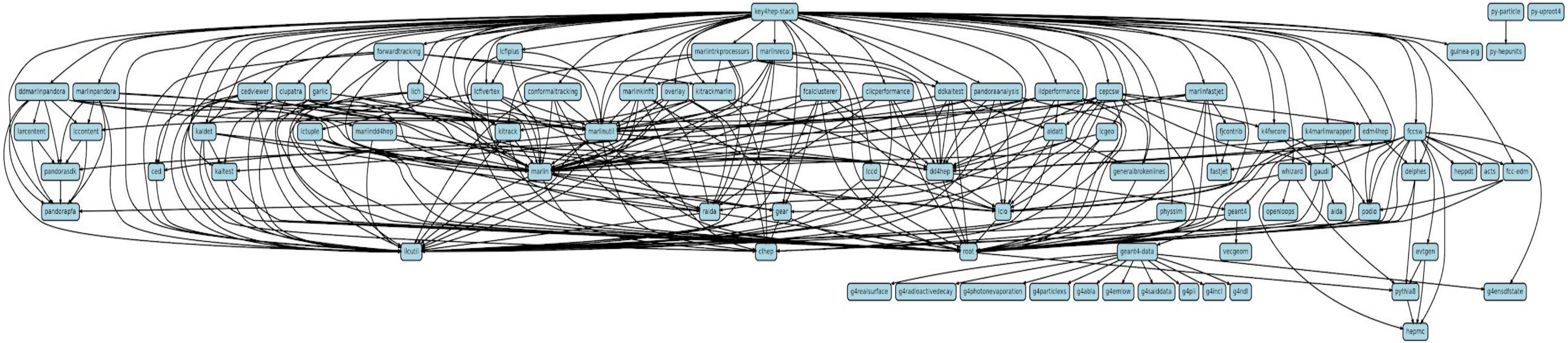
# Dependency Graph of HEP software Stack

Experiment-specific Packages



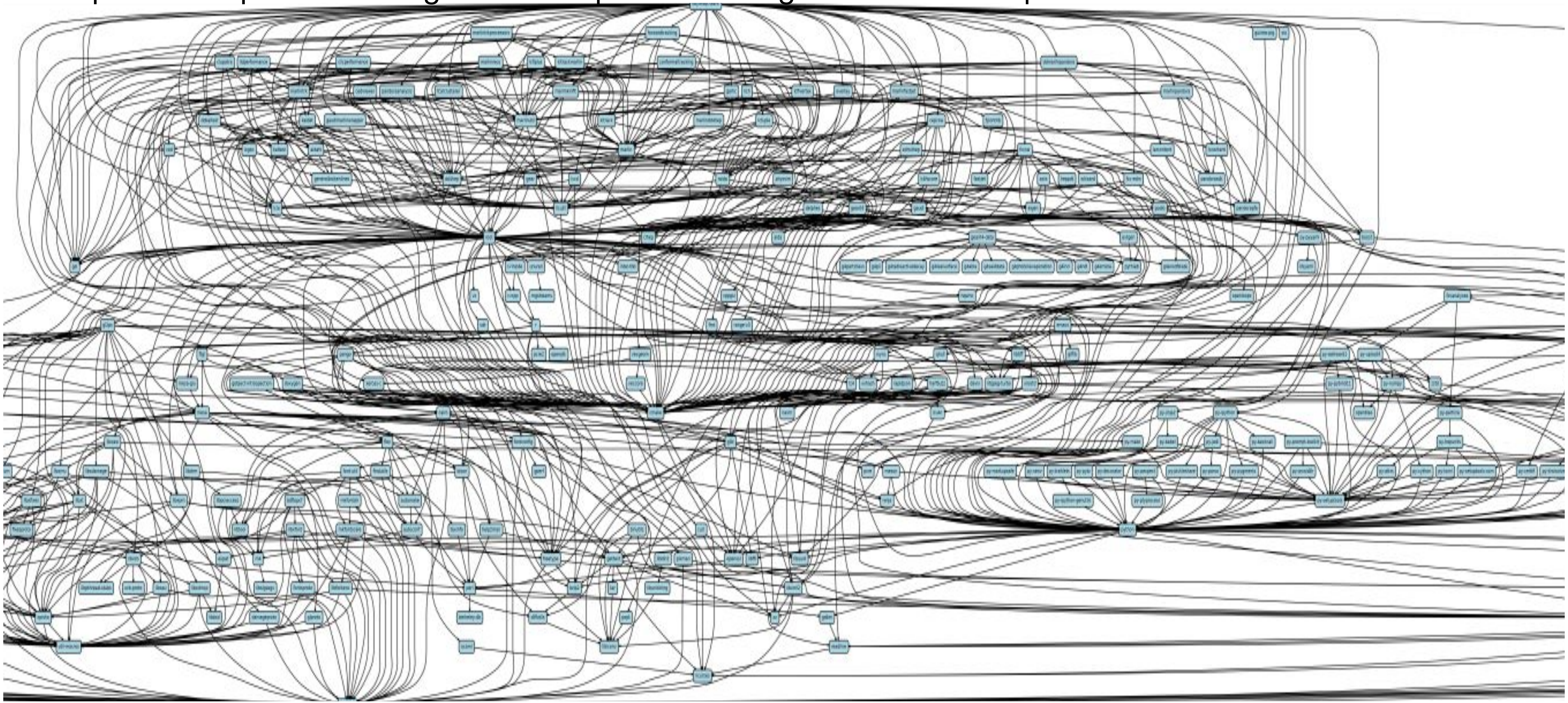
# Dependency Graph of HEP software stack

Experiment-specific Packages + HEP-specific packages



# Dependency Graph of HEP software stack

Experiment-specific Packages + HEP-specific Packages + General Purpose Libraries



# Requirements for a Build System

[ ] Need to be able to scale to a typical experiment software stack

A typical HEP stack contains some 300 packages

- 60 Experiment-specific
- 50 HEP-specific
- 200 System/General Purpose

14 GB install size, some 6h to build on single 4-core machine

[ ] Combinatorics of multiple versions, platforms, Release/Debug ...

[ ] Easy central deployment

[ ] Reproducibility

[ ] Support software development usecases

# Build systems - previously...

- Often custom experiment-specific tools
- Fairly opaque, few transferable skills
- Difficult to maintain
- Need for a community-wide solution!
- Best practices in using build systems (Modern CMake ...)

# Spack for HEP

- Originally written for/by HPC community
  - Emphasis on dealing with **multiple configurations** of the same packages
    - Different versions, compilers, external library versions ...
    - ... may coexist on the same system
- Not the only solution in this problem space:
  - EasyBuild
  - Nix/Guix
  - Conda
  - Gentoo Prefix



See https://hepsoftwarefoundation.org/notes/HSF-TN-2016-03.pdf for a comparison

And: previous FOSDEM talks about Spack by T. Gamblin!

# Spack packages are simple Python

```
from spack import *

class Dyninst(Package):
    """API for dynamic binary instrumentation.  Modify programs while they
       are executing without recompiling, re-linking, or re-executing."""

    homepage = "https://paradyn.org"

    version('8.2.1', 'abf60b7faabe7a2e', url="http://www.paradyn.org/release8.2/DyninstAPI-8.2.1.tgz")
    version('8.1.2', 'bf03b33375afa66f', url="http://www.paradyn.org/release8.1.2/DyninstAPI-8.1.2.tgz")
    version('8.1.1', 'd1a04e995b7aa709', url="http://www.paradyn.org/release8.1/DyninstAPI-8.1.1.tgz")

    depends_on("libelf")
    depends_on("libdwarf")
    depends_on("boost@1.42:")


    # new version uses cmake
    def install(self, spec, prefix):
        libelf = spec['libelf'].prefix
        libdwarf = spec['libdwarf'].prefix

        with working_dir('spack-build', create=True):
            cmake('..',
                  '-DBoost_INCLUDE_DIR=%s' % spec['boost'].prefix.include,
                  '-DBoost_LIBRARY_DIR=%s' % spec['boost'].prefix.lib,
                  '-DBoost_NO_SYSTEM_PATHS=TRUE',
                  '-DLIBELF_INCLUDE_DIR=%s'   % join_path(libelf.include, 'libelf'),
                  '-DLIBELF_LIBRARIES=%s'     % join_path(libelf.lib, 'libelf.so'),
                  '-DLIBDWARF_INCLUDE_DIR=%s' % libdwarf.include,
                  '-DLIBDWARF_LIBRARIES=%s'   % join_path(libdwarf.lib, 'libdwarf.so'),
                  *std_cmake_args)
            make()
            make("install")

    # Old version uses configure
    @when('@:8.1')
    def install(self, spec, prefix):
        configure("--prefix=" + prefix)
        make()
        make("install")
```

Metadata

Version/URLs

Dependencies

Patches (not shown)

Commands for install

Access build config through *spec.*

# Spack basics

- Spack handles combinatorial version complexity by assigning hashes `/a83xd43`
- Concretization fills in missing configuration details when the user is not explicit

```
spack install root

spack install root@6.20.04

spack install root@6.20.04 % gcc@9.3.0

spack install root@6.20.04 % gcc@9.3.0 target=broadwell

spack install root@6.20.04 % gcc@9.3.0 ^python@3.8.2
```

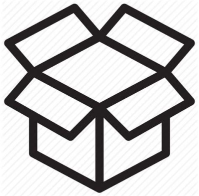
# Status of HEP software in Spack

- Around 80 package recipes with `hep` tag

```
pythia8 photos syscalc madgraph5amc g4emlow lcio heputils vbfnlo g4incl lhapdf sherpa py-particle openloops herwigpp
heppdt tauola lhapdfsets root collier garfieldpp py-uproot geant4 evtgen clhep gaudi geant4-data vgm alpgen relax
g4tendl g4realsurface genfit py-hepdata-validator g4ndl cool recola fjcontrib delphes dd4hep whizard hepmc3 pythia6
g4ensdfstate coral g4photonevaporation kassiopeia yoda acts chaplin simsipm mcutils recola-sm py-hepunits herwig3
hepmc py-gosam ccs-qcd g4saiddata g4neutronxs aida g4radioactivedecay podio edm4hep g4abla njet apfel fastjet qd
thepeg rivet vecgeom gosam-contrib unigen hepmcanalysis geant4-vmc genie g4pii py-uproot4 hoppet qgraf g4particlexs
dire
```

- Many (> 25) active maintainers from different experiments
- 3rd party repositories for full experiment stacks
  - CMS: https://github.com/iarspider/cms-spack-repo
  - EIC: https://github.com/eic/eic-spack
  - Key4hep: https://github.com/key4hep/key4hep-spack
  - LCG-releases: https://gitlab.cern.ch/sft/sft-spack-repo

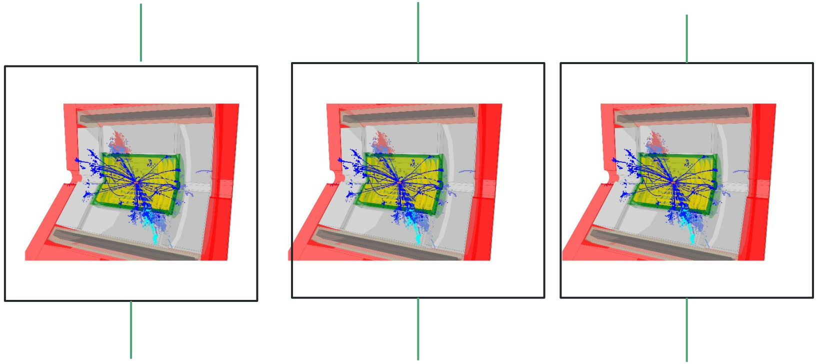
# Open Issues and Wishlist

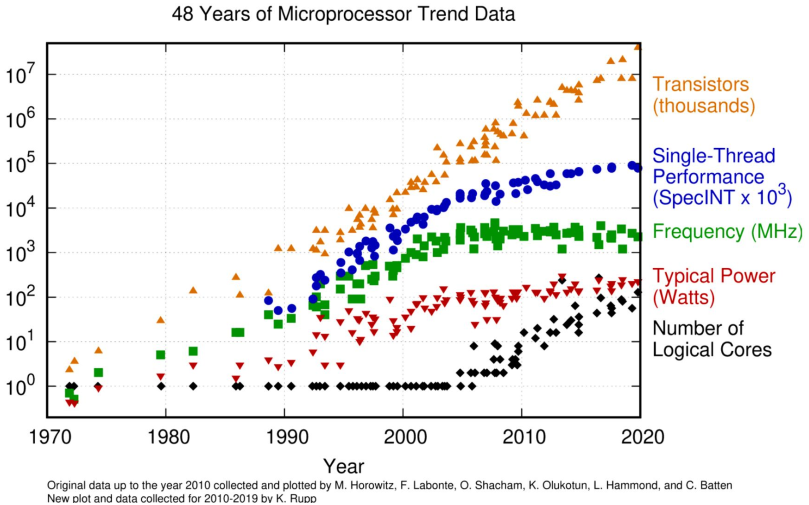


- Data packages
  - Implies compiler dependency
- Avoid rebuilding ROOT! (thank you for `spack install -reuse`)
- Building glibc
- Nightly builds from git master
- Relocation and build path
- Setup script generation

# Software Deployment with CVMFS

# HPC for HEP





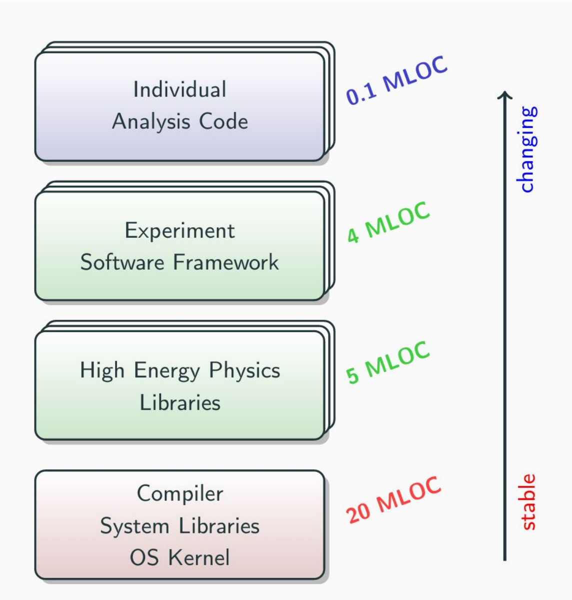

- Many workloads in HEP are embarrassingly parallel!
- Off-line, single events can usually be processed on modest hardware
  - Nevertheless large volume - truly Big Data!
  - Distributed computing and  “Computing Grid”

- Still much potential to use heterogeneous computing and HPC resources.

# The LHC Computing Grid

Started in 2002
Provide processing power and data access to physicists
~170 centres in 42 countries
Running 24/7/365

# The Anatomy of a HEP Software Stack




Key Figures for LHC Experiments

- Hundreds of (novice) developers
- > 100 000 files per release
- 1TB / day of nightly builds
- ~100 000 machines world-wide
- Daily production releases, remain available “eternally”

# Software distribution - CernVM-FS

- Read-only, globally distributed file system optimized for software delivery
- Provides uniform, consistent and versioned POSIX file system access to /cvmfs

```
$ ls /cvmfs/cms.cern.ch
slc7_amd64_gcc700  slc7_ppc64le_gcc530  slc7_aarch64_gcc700  slc6_mic_gcc481
...
```

- Populate and propagate new and updated content
  - A few “software librarians” can publish into /cvmfs
  - All content in /cvmfs is cryptographically signed
  - Transactional writes as in git commit/push
- More details under [https://cernvm.cern.ch/fs/](https://cernvm.cern.ch/fs/)

# CVMFS Deployment

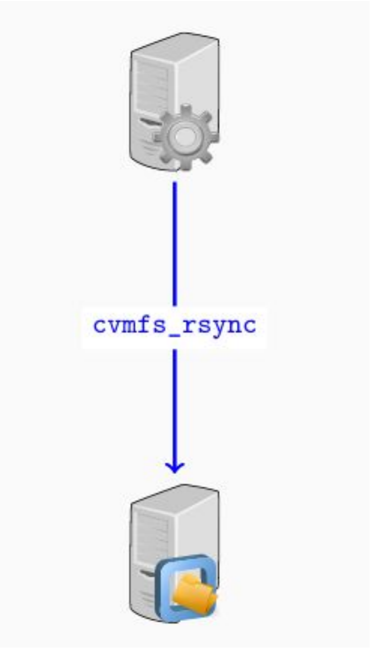
Several possible workflows (see presentation by Jakob Blomer)

1. The Postscript relocation approach
2. The rsync approach
3. The Gateway approach
4. The Container approach

The rsync approach:

- Builder mounts a read/write copy of the /cvmfs tree
- Builder changes/installs software in place
- Publisher uses rsync to pull changes from the builder

Non-trivial to maintain multiple, synchronized publishers



# Conclusions

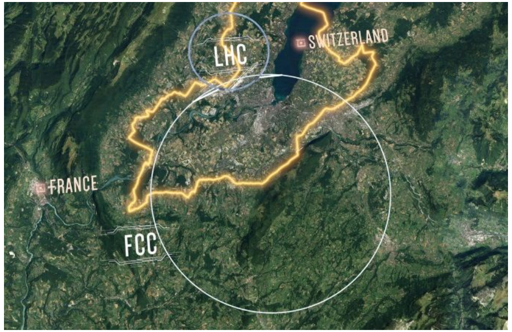
High Energy Physics faces some fairly unique challenges...

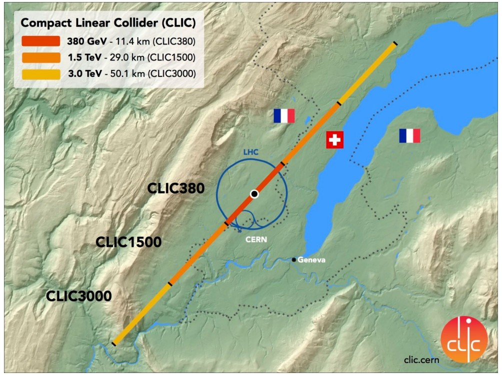
- And innovated on tools to solve them (see CVMFS in this presentation)

... but also many common ones, and would probably not be possible without the wider OSS ecosystem.

- HEP 💙 Open Source!
  - Open Data projects
  - Software Projects:
    - ROOT
    - Geant4
    - Indico
    - ...

Future Collider Projects are collaborating on Software (Key4hep)!




FCC, CLIC, ILC, CEPC, ...