Key4hep - Turnkey Software for Future Colliders

2021 International Workshop on Future Linear Colliders (LCWS2021)

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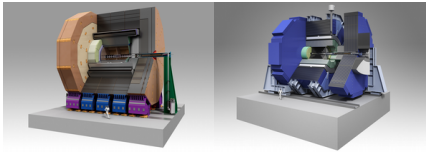
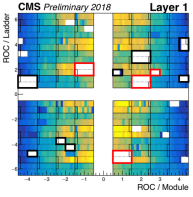
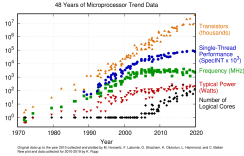
Mar 15, 2021

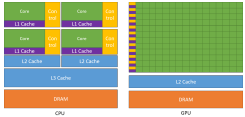
Software Challenges in HEP

- Future detector studies rely on well maintained software to properly study possible detector concepts and their physics reach and limitations
- Long Lifetimes – Shift of priorities throughout the evolution of an experiment
  - Conceptual and design work with quick iterations relying on simulation
  - Production and dealing with the real world requires stability but also continual updates
  - Data preservation
  - Upgrade to better (sub-)detectors
  - Avoid amassing “technical debt”
  - New technological developments and paradigms

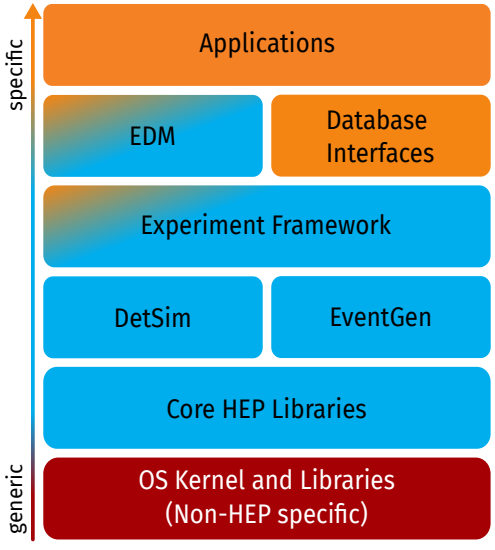








HEP Software Stack



Application layer of modules / algorithms / processors performing physics tasks
(PandoraPFA, FastJet, ACTS, ...)

Data access and representation layer including Event Data Model

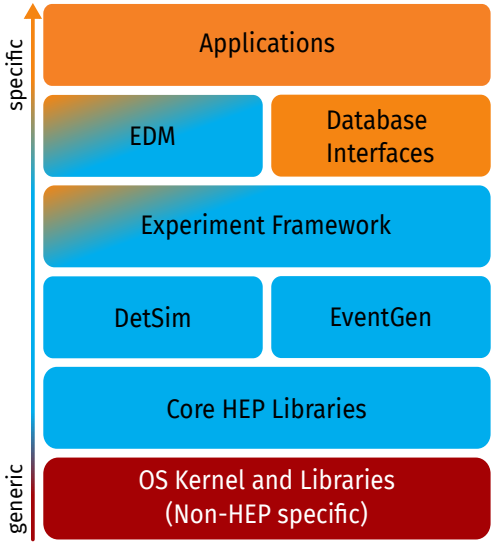
Experiment core orchestration layer
(Marlin, Gaudi, CMSSW, ...)

Specific components reused by many experiments
(DD4hep, Delphes, Pythia, ...)

Commonly used HEP core libraries
(ROOT, Geant4, CLHEP, ...)

Commonly used tools and libraries
(Python, CMake, boost, ...)

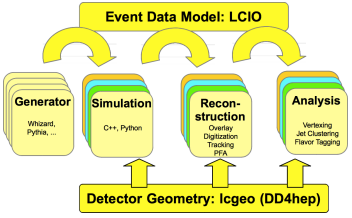
HEP Software Stack



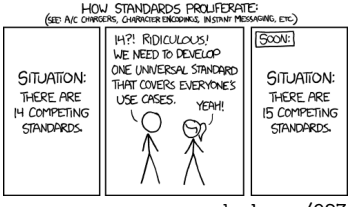
- Pieces of software are not living in isolation
- Ecosystem of interacting components
- Compatibility between different elements doesn't come for free
  - Common standards can help a lot
- Choosing the right interoperability point between packages correctly is one of the main challenges
- Building a consistent stack of software for an experiment is highly non-trivial
  - Benefits can be gained from using common approaches

Key4hep Goals

- Connect and extend individual packages towards a complete data processing framework
  - Convert a set of disconnected packages into a **turnkey** system
  - Share as many components as possible to reduce overhead for all users
- Re-use existing tools as much as possible
  - e.g. from ILC/CLIC and FCC studies
- Easy to use for librarians, developers and users
  - Easy to deploy (e.g. CVMFS, containers)
  - Easy to set up
  - Easy to extend
- Provide full functionality for different use cases
- Provide examples and documentation for simulation, reconstruction, ...

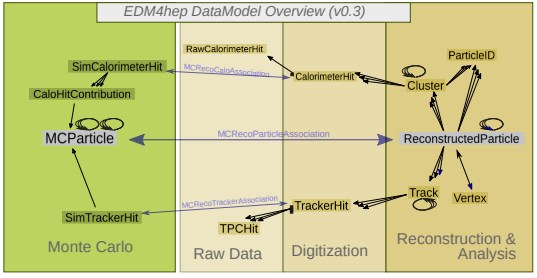


iLCSoft components here, but general scheme applies



xkcd.com/927

EDM4HEP



key4hep/EDM4Hep

cern.ch/edm4hep

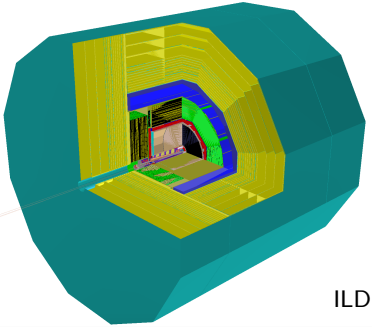
- To facilitate interoperability, different components should talk the same language
- In HEP this is the **Event Data Model**
  - Describes the structure of HEP Data
- See talk by T. Madlener in this workshop

DD4hep - Detector Description Toolkit for HEP

- Originally developed for ILC and CLIC but with all of HEP in mind
- Provides a complete detector description
  - Geometry, materials, visualization, readout, alignment, calibration, ...
- From a **single source of information**
  - Used in simulation, reconstruction, analysis
- Comes with a powerful plug-in mechanism that allows customization
- More or less "industry standard" by now
  - ILC, CLIC, FCC, CEPC, LHCb, ...
  - CMS is switching to DD4hep
- `ddsim` already directly outputs EDM4hep
  - when writing `...emd4hep.root` files

AIDASoft/DD4hep

dd4hep.web.cern.ch



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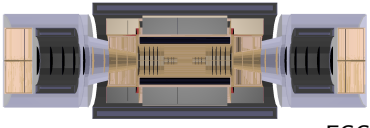
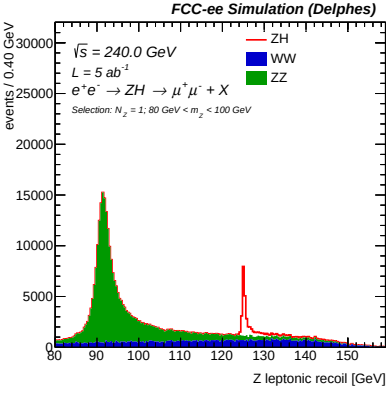


FCC

k4SimDelphes - First steps towards physics

DELPHES
fast simulation

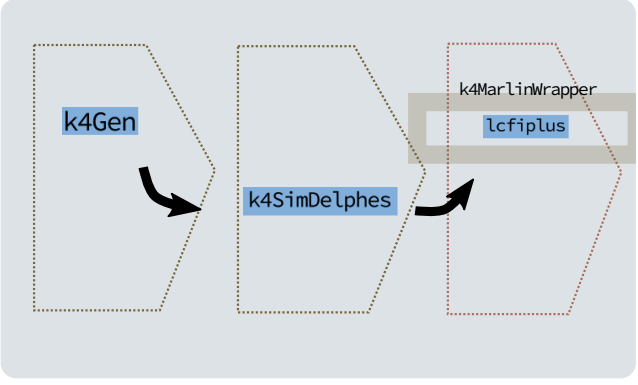
- key4hep/k4SimDelphes uses delphes to do the simulation and reconstruction and creates output files in EDM4HEP format
- **Quick way to get your hands dirty and do some physics with EDM4HEP**
- Currently available as standalone executables
  - E.g. `DelphesPythia8_EDM4HEP`, `DelphesSTDHEP_EDM4HEP`, ...
- Part of a coherent approach to generation / simulation in Key4hep
  - Ideally no difference between the different approaches of simulating a detector response
  - Work on full integration is ongoing



courtesy of C. Helsens

Experiment Framework

- Frameworks are the ideal solution in terms of modularity and consistency across components.



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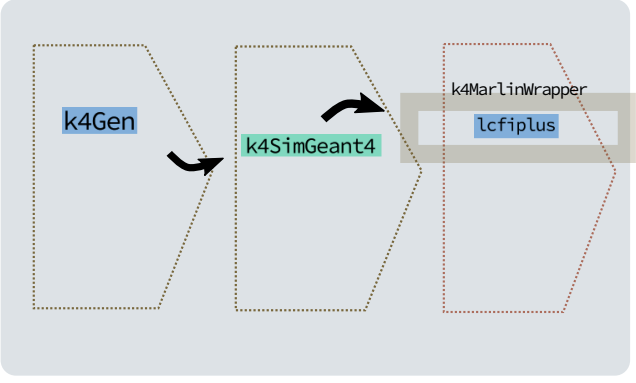


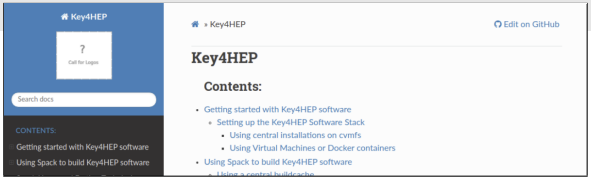
Experiment Framework

- Traditionally HEP has not done too well with sharing efforts towards a common experiment framework
  - Notable exception is `Marlin` used by ILC and CLIC
- `Gaudi`, originally developed by LHCb, now also used by ATLAS, FCCSW and smaller experiments
  - Supports concurrency
  - "Battle-proven" from data taking during LHC operations
  - Currently undergoing a modernization
- Key4hep has decided to adapt `Gaudi` as its experiment framework
  - Contribute to its development where necessary
- Integration and migration of iLCSoft algorithms into Key4hep with the help of a `Marlin`→`Gaudi` wrapper
  - Allows to use `Marlin` processors within the `Gaudi` framework
  - See talk by P. Fernandez in this workshop

Key4hep Framework - k4FWCore

- k4FWCore — key4hep/k4FWCore
  - Core Key4hep framework providing core functionality, e.g.
    - Data Service for podio collections
    - Overlay for backgrounds
  - Recently switched to Gaudi v35
- k4-project-template — key4hep/k4-project-template
  - Template repository showing how to build new components on top of the core Key4hep framework
- Ongoing work to collaborate more with Gaudi ecosystem (Gaussino)
- Ongoing work to integrate more components (ACTS, ...)

Software Infrastructure



- Documentation
  - key4hep.github.io/key4hep-doc
    (main documentation)
  - cern.ch/edm4hep
    (doxygen code reference)
- Modern CMake configuration for the individual components
  - Facilitates their usage as dependencies for other components
- Automated builds and continuous integration (CI) where possible
  - Regular nightly builds of the complete stack
  - Use of the spack package manager
- Distribution via CVMFS
  - Latest release can be found at `/cvmfs/sw.hsf.org/key4hep`
- **Release early and release often**
  - Make fixes available early
  - Discover problems and collect feedback as early as possible

Spack for Key4hep

- Spack is a package manager
  - Does not replace CMake, Autotools, ...
  - Comparable to apt, yum, homebrew, ...
  - Independent of operating system
  - Builds all packages from source
- Originaly developed by the HPC community
  - Emphasis on dealing with **multiple configurations** of the same package
    - Different versions, compilers, external library versions, ...
  - Several versions of the same package can coexist on the same system
- The whole Key4hep software stack can be built from scratch using spack
- Spack allows different workflows for setting up consistent software stacks
  - Currently testing which one fits our purposes the best

Spack for developers

- Spack itself is now also available after sourcing the setup script and can be used to install packages on top of the CVMFS installation

```
source /cvmfs/sw.hsf.org/key4hep/setup.sh
spack dev-build conformaltracking@master
```

- With only a few configuration changes (key4hep/key4hep-spack), Spack can be used to install ilcsoft from scratch on a wide range of systems

```
spack install ilcsoft arch=linux-centos7-skylake
spack install ilcsoft arch=darwin-catalina-ivybridge
```

- Complete guide to Spack for software developers: `http://cern.ch/key4hep`

Testing Strategies

- Testing is crucial for any non-trivial software
- For Key4hep, try to add tests to build system with CTest
- Use `Catch2` for unittests – to be expanded.
- Install tests now added to release workflow
- Documentation pages with code now also automatically converted to notebooks and tested.

Citing Software

zenodo

- Important to credit authors and for reproducibility
- Zenodo can automatically create a **DOI** (Digital Object Identifier) for each release

DOI 10.5281/zenodo.4564683

- Another **DOI** always points to the latest version of the software
- Now enabled for all Key4hep packages

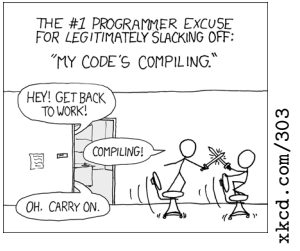
```
@software{thomas_madlener_2021_4564683,
  author       = {Thomas Madlener and
                  Valentin Volkl and
                  clementhelsens and
                  Frank Gaede and
                  Marcin Chrzaszcz},
  title        = {key4hep/k4SimDelphes: Zenodo Release},
  year         = 2021,
  publisher    = {Zenodo},
  version      = {v00-01-04},
  doi          = {10.5281/zenodo.4564683},
  url          = {https://doi.org/10.5281/zenodo.4564683} }
```

At the moment more work than people!

- Active weekly meetings, alternating between EDM4HEP and Key4hep
  https://indico.cern.ch/category/11461/
- Check out documentation at https://cern.ch/key4hep
  - Also contains some examples
- **Any feedback is welcome**, this should not just be an academic exercise!
- If you find any issues, **do not hesitate to report them**
  - Documentation not up to date?
  - Examples not working?
- **We also greatly appreciate pull requests**

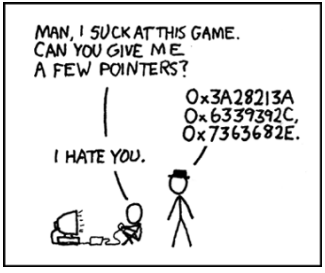
Summary & Outlook

- Setting up a consistent and working HEP software stack is non-trivial
- **General agreement to move to a common HEP software stack** for future experiments
  - Re-use existing tools where possible and ensure their interoperability
  - Make everybody benefit from new developments
- `Gaudi` will be used as core framework, but integration / migration strategy for `Marlin` and iLCSoft exists
- A lot of work has been invested to get working prototypes for the core components and a **common EDM4HEP**
- A lot of work still ahead!



Pointers to Resources

- Key4hep
  - key4hep.github.io/key4hep-doc
  - key4hep
- EDM4HEP
  - key4hep/EDM4hep
  - cern.ch/edm4hep
- k4SimDelphes
  - key4hep/k4SimDelphes
  - delphes/delphes
  - cp3.irmp.ucl.ac.be/projects/delphes
- podio
  - AIDASoft/podio
- DD4hep
  - AIDASoft/DD4hep
  - dd4hep.web.cern.ch



xkcd.com/138

Supplementary Material

k4SimDelphes

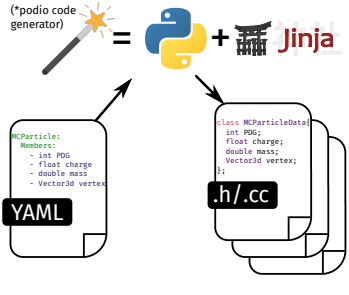
- Produces several output collections
  - One collection of `edm4hep::ReconstructedParticle` that comprise all reconstructed particles of an event
    - Photon, Muon, Electron collections that *point* into this collection
    - Jet collection with constituents from this collection
  - One collection of `edm4hep::MCParticle` for the generated particles
  - Associations between MC and reco particles
- Configurable output contents
  - Which delphes collections should be considered?
- No changes to delphes cards necessary
- Conversion is done on the contents of the delphes `TreeWriter`
  - Could be used to convert already generated files
  - Least invasive method, that does require only minimal changes to the Delhpes code

Delphes - Overview

- Delphes is a fast detector simulation response tool based on a parameterized description of the detector
- Understands several commom HEP input formats and produces output files using its own EDM
- Needs a "delphes card" that describes the detector
  - Parameterized efficiencies, resolutions, ...
  - Available for ILC, CLIC, FCC-ee/hh (and others)
- Can do basic reconstruction
  - Jet finding, b-tagging, isolated object finding, ...
  - Again based on the parameterized inputs

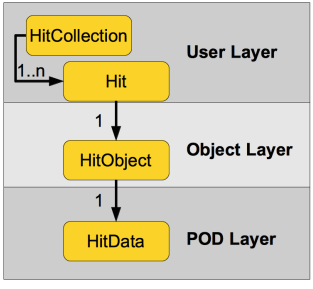
podio as Generator for EDM4HEP

- Original HEP c++ EDMs are heavily Object Oriented
  - Deep inheritance structures
  - Objects scattered in memory
  - Hard to deal with in multi-threaded environments
- Data access can be very slow with these approaches
- Use `podio` to generate thread safe code starting from a high level description of the desired EDM
  - Target different I/O backends for persistency
  - Users are isolated from implementation details
- Treating python as first class citizen and allow "pythonic" usage
- Recently has experienced revitalisation but to become production ready some work is still needed



AIDASoft/podio

The Philosophy of podio



- **User Layer** consists of handles to the EDM objects and offers the full functionality
- The **Object Layer** handles resources and references to other layers
- The actual POD data live in the **POD Layer**
- Easy to use through a clear design of ownership
  - Users should not have to care about this
- Layered design allows for efficient memory layout and performant I/O implementation
  - ROOT I/O is used by default
  - An SIO based implementation is available

Building the Key4hep stack from source using spack

- Setting up the central spack repository

```
git clone https://github.com/spack/spack.git
source spack/share/spack/setup-env.sh
```

- Add Key4hep specific packages not yet present in the central repository

```
git clone https://github.com/key4hep/key4hep-spack.git
spack repo add key4hep-spack
```

- In order to have consistent stack, some packages need some additional configuration
  - e.g. pinning versions, or specifying build options

```
cp key4hep-spack/config/packages.yaml spack/etc/spack
```

- Install it

```
spack install key4hep-stack
```

- See also: the documentation

Some Experiences with Spack

- Collaboration with spack developers pretty smooth
  - Some HEP colleagues have merging rights for the central spack repository
  - Some HEP packages actively maintain their package recipes (ACTS)
- Rapid development in central spack repository
  - Stable builds need to pin the used spack version
  - Potentially miss latest features
  - Documentation in general very good, but sometimes not completely up-to-date
- Spack developers very responsive, but roadmap is sometimes a bit opaque
  - E.g. the *concretizer* development have taken very long to be integrated
- The build recipes are very nice to persistify build-system know-how

```
conflicts("%gcc@8.3.1",
          msg="There are known issues with compilers from redhat's devtoolsets"
          "which are therefore not supported."
          "See
https://root-forum.cern.ch/t/devtoolset-gcc-toolset-compatibility/38286")
```

Spack - Usage for Developers

- Usage of spack for developing software is pushing spacks intended purpose, but it is possible
  - Spack can build directly from git branches
  - Development can be done “as usual” after using spack to build dependencies
  - Spack can be used to setup *environments*
  - Spack *dev-build* compiles local code according to recipe
- Development workflows are also being worked on by spack developers
- Mixing sytem libraries and spack installed libraries can lead to some unexpected issues
  - Missing version information for some libraries that is expected by system packages (usually no problem)
  - Reproducible environments from setup scripts need some work
- Many packages from LCG releases already available as spack recipes