

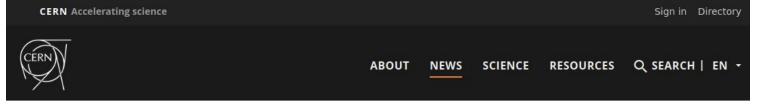


The LHCb Open Data Project

Sebastian Neubert¹

¹HISKP Bonn

HEP Seminar, Dortmund 12.01.23

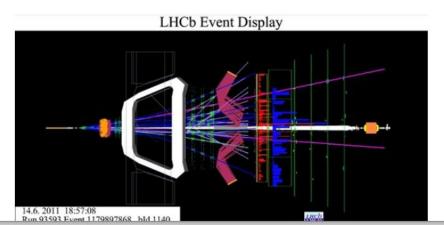


News > News > Topic: Knowledge sharing

LHCb releases first set of data to the public

The LHCb collaboration has released data from Run 1 of the LHC to the public for the first time, allowing research to be conducted by anyone in the world

⁸ DECEMBER, 2022 | By LHCb collaboration



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LHCb 2011 Beam3500GeV MagDown LEPTONIC Stream Stripping21r1

proton-proton (pp) collision data collected by the LHCb experiment in the year 2011 of Run1 of the LHC....

Dataset Collision LHCb

The Open Science Philosophy (at CERN)

Recognize the universal importance of the fundamental scientific knowledge produced at CERN and the key role of openness in the pursuit of CERN organisational mission.

Commits to the advancement of science and wide dissemination of knowledge by adopting practices to make scientific research more open, global, collaborative and responsive to societal changes.

In fulfilment of the collective moral and fiduciary responsibility to member states and the broader global scientific community Data collected at the LHC is a heritage to humanity.

It has been obtained through collaborative work using public funds.

Therefore, CERN is committed to preserve, curate, steward and share the data with the public.

Goals of Open Data - Maximizing Scientific Value

- Validation / reproduction of published results
- Reinterpretation of the data
 - test future theories
 - refine phenomenological models
 - use different statistical tools
- Reuse of data sets
 - Combined analyses
 - Use collected data as input for future studies
 - Algorithm development (e.g. machine learning community)

• Data mining

- \circ ~ search for interesting physics in unexplored parts of the data
- use new techniques to (re-)select data

We cannot anticipate the questions future generations might ask of this data. require different levels of data complexity

Open Science Landscape - Recent Trends

- Funding agencies: requests for data management plans
- Publishers: requests for data products allowing to
 - validate / reproduce results
 - reuse data for further studies

Science Community: "Data is not enough":

- Papers with code https://paperswithcode.com/
- Interactive publications
- Federated infrastructures and computing/science portals (e.g. NFDI)
- Not a new realization (see e.g. DPHEP study group <u>2013 status report</u>) but technology (esp cloud computing, containerization) has made progress!
- Development driven especially through bioinformatics and machine learning / AI community

Policies

the CERN experiments have given themselves

CERN Open Data Policy 2020

Initiated beginning 2020 by the chair of the European Commission

CERN director of research: Mandate for a working group to draft a common policy for all LHC experiments

Endorsed by the Collaboration Boards of ALICE, ATLAS, CMS and LHCb

CERN Open Science Policy 2022

Includes all experiments at CERN

Working group formed https://openscience.cern/

Includes a wider scope of topics:

- Open access, open data, open source, open hardware
- Research integrity, research assessment
- Open infrastructure
- Training and outreach, citizen science

Open data policy

The CERN Open Data Policy reflects values that have been enshrined in the CERN Convention for more than sixty years that were reaffirmed in the European Strategy for Particle Physics (2020)¹, and aims to empower the LHC experiments to adopt a consistent approach towards the openness and preservation of experimental data. Making data available responsibly (applying FAIR standards²), at different levels of abstraction and at different points in time, allows the maximum realisation of their scientific potential and the fulfillment of the collective moral and fiduciary responsibility to member states and the broader global scientific community. CERN understands that in order to optimise reuse opportunities, immediate and continued resources are needed. The level of support that CERN and the experiments will be able to provide to external users will depend on available resources.

FAIR Data Principles

[The FAIR Guiding Principles for scientific data management and stewardship. Nature *Sci Data* **3**, 160018 (2016). https://doi.org/10.1038/sdata.2016.18]



Findable: Metadata and data should be easy to find for both humans and computers.



Accessible: The exact conditions under which the data is accessible should be provided in such a way that humans and machines can understand them.



Interoperable: The (meta)data should be based on standardized vocabularies, ontologies, thesauri etc. so that it integrates with existing applications or workflows.



Reusable: Metadata and data should be well-described so that they can be replicated and/or combined in different research settings. https://go-fair.org Solved by

https://opendata.cern.ch

Needs dedicated work by the experimental collaborations (here efforts in HEP are in their infancy)

DPHEP Levels of Data Complexity

https://arxiv.org/abs/1205.4667

1. Published results

+ additional information

- supplemental data tables, ntuples
- HEPData entries, rivet plugins
- notes, technical information
- \circ documentation, slides
- analysis code, jupyter notebooks

2. Education and Outreach

 simplified data formats, e.g. highly preprocessed ntuples

- 3. Reconstructed data + analysis level software
 - Calibrated reconstructed data with the level of detail useful for algorithmic, performance and physics studies
 - preservation of analysis level experiment-specific software
- 4. Raw data + reconstruction software
 - \circ $\,$ Not released for LHC data

Open data policy: Level 3 data releases

Reconstructed Data (Level 3) Policy: The LHC experiments will release calibrated reconstructed data with the level of detail useful for algorithmic, performance and physics studies. The release of these data will be accompanied by provenance metadata, and by a concurrent release of appropriate simulated data samples, software, reproducible example analysis workflows, and documentation. Virtual computing environments that are compatible with the data and software will be made available. The information provided will be sufficient to allow high-quality analysis of the data including, where practical, application of the main correction factors and corresponding systematic uncertainties related to calibrations, detector reconstruction and identification. A limited level of support for users of the Level 3 Open Data will be provided on a best-effort basis by the collaborations.

Level 3 data is addressed at professional researchers

Level 3 open data release policy

Policy since 27th Feb 2013 updated in <u>CERN Open Data Policy 2020</u> and <u>CERN Open Science Policy 2022</u>

- Level 3 open data: reconstructed events (DPHEP definition)
 - \circ $\;$ LHCb: Output of stripping / turbo / sprucing $\;$
 - MC on demand
- 50 % of data 5 years after end of running period (a.e.r.)
 - Run I: End of 2017
 - Run II: End of 2023
- 100 % of data 10 years a.e.r.
 - Run I: End of 2022

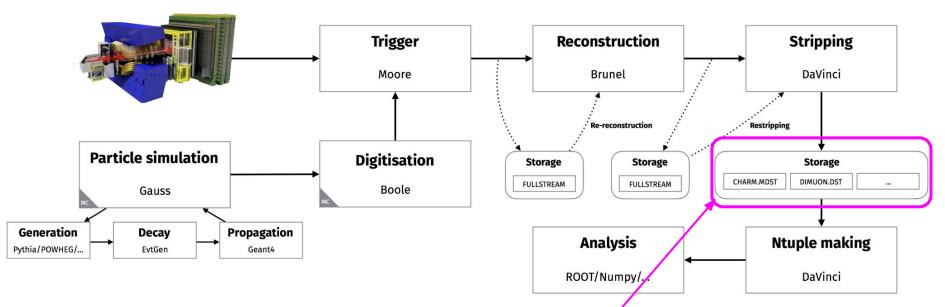
This model differs from the astrophysics model of open data.

Reason: incentive structures for instrument/detector builders vs data analysts, differy widely between the two fields

- Goal of the OD release is to enable scientific research by 3rd parties
- Level 3 data releases are addressed at professional users

LHCb Level 3 Data

Release policy: 50% @ 5yrs, 100% @ 10yrs after end of running period



- Level 3 data in LHCb defined as the output of the stripping
- Same level of abstraction accessed by LHCb members
- Contains comprehensive set of selections (1620 selections in v21)
- Organized in ~10 streams, according to physics signature
- Software needed to access data (DaVinci) is open source, available via CVMFS (or container)
- Documentation: <u>LHCb Starterkit</u> openly available

LHCb Run I open data release

- Released 3 Streams:
 - Electroweak EW,
 - Leptonic,
 - Radiative
- ~ 200TB (roughly 20% of RUN I data)
- Data released in LHCb MDST and DST formats
- Needs DaVinci application to read
- Detailed description of stripping selections
- Glossary of 960 LHCb specific terms
- Monte Carlo samples on demand

http://opendata.cern.ch/

Data to be released next: full 2011/12 Stripping Output

BHADRON.MDST BHADRONCOMPLETEEVENT.DST CHARM.MDST CHARMCOMPLETEEVENT.DST DIMUON.DST EW.DST LEPTONIC.MDST RADIATIVE.DST SEMILEPTONIC.DST

We create one OD record per stream/year/MagSetting

Metadata is exported from Dirac BKK

Documentation: https://lhcb-dpa.web.cern.ch/lhcb-dpa/wp6/open-data-release.html

Data can only be withheld on a stream by stream basis. Withholding release of data because of ongoing analyses.

Level 3 Data - Resources

	ALICE	ATLAS	CMS	LHCb
Run 2	2 PB	0.5 PB	2 PB	10 PB (including Run 1)
Run 3	4 PB	1 PB	4 PB	45 PB
Total	6 PB	1.5 PB	6 PB	55 PB

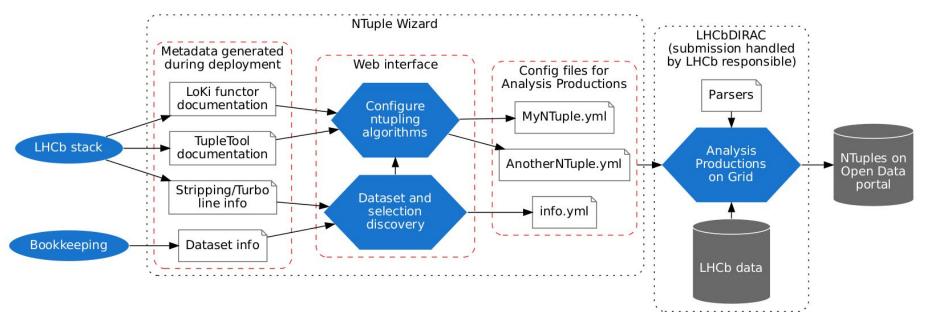
Mitigation Strategies:

- Provide protected access to existing copies of stripping/turbo output via WG-production slots. Needs "ntupling wizard"
- Provide direct access to data on grid storage

Future development: NtupleWizard

Please test and provide feedback! (mattermost)

- NtupleWizard is functional <u>https://lbwizard.web.cern.ch/</u>
- Idea: only keep existing replicas of the data, allow OD users access via dedicated analysis production jobs



Paper in preparation

Decay search

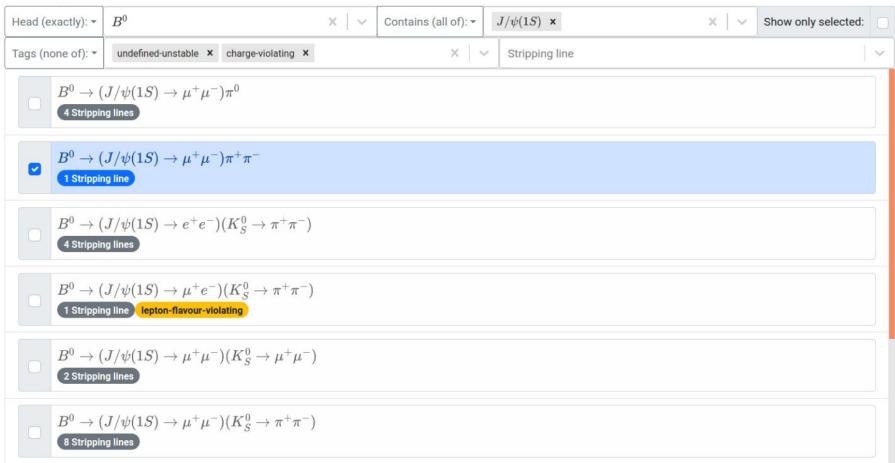


Fig. 3 Example of the decay candidate search function of the Ntuple Wizard.

NTuple Wizard

Production configuration

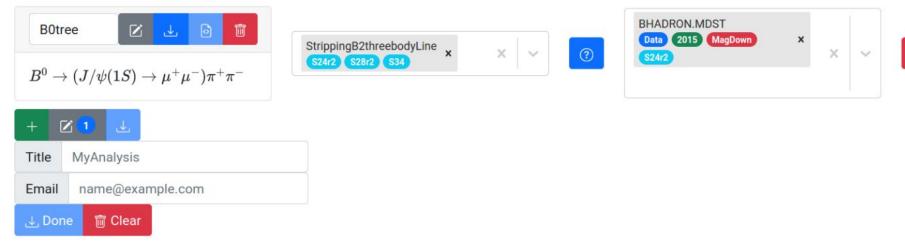
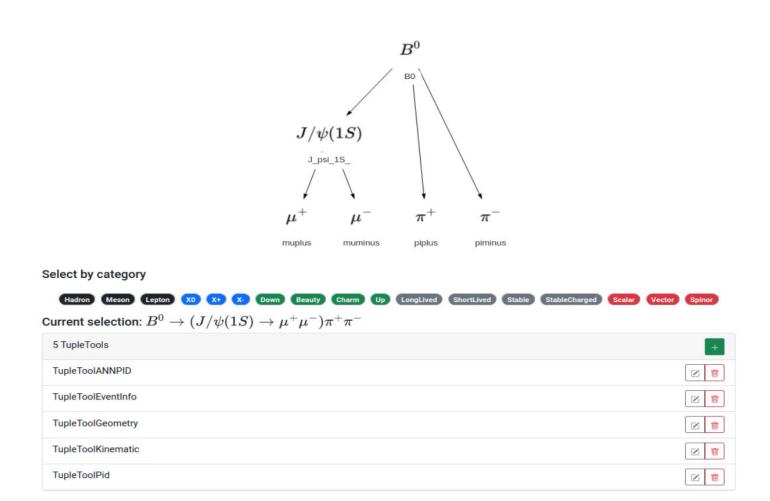


Fig. 4 Example of the data set selection and production configuration step of the Ntuple Wizard.

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 Configure $B^0
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BQ

We are just getting started

Challenges with LHCb Open Data release

Things to improve or add

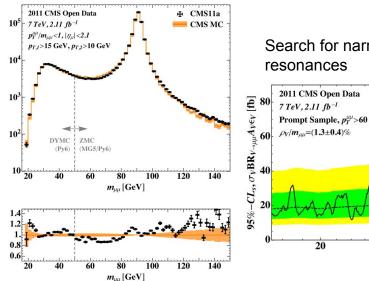
- Calibration samples + tools
- Documentation on available MC samples
- Analysis example + runtime environment
- MDST and DST are very specialized data formats
 - NTuple wizard will write plain ROOT ntuples
 - \circ NTuple wizard provides much clearer representation of the content of the data
- Integrate NTuple Wizard with Open Data Portal (activity starting now)
- Training for outside users (see CMS Open Data workshops)
- All activity currently severely limited by available resource within LHCb

How is LHC Open Data going to be used?

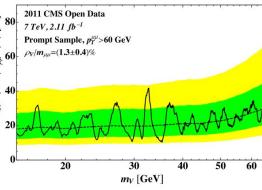
No experience for LHCb data, yet.

But various studies done on CMS open data. Overview: arXiv:2106.05726

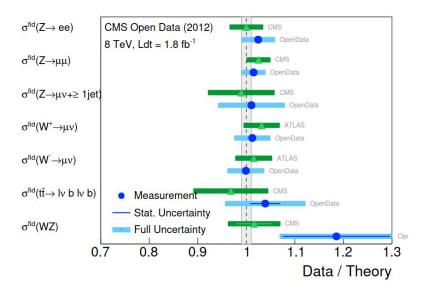
Dimuon spectrum [PRD100(2019)015021]:



Search for narrow dimuon



SM cross section measurements on CMS open data [1907.08197]



Going beyond level 3 data

Open science and Open data policies:

5. Research integrity, reuse and reproducibility

We should publish ntuples and statistical models to make our results more impactful

CERN is committed to ensuring the integrity of research. In order to facilitate the reuse of its research products, CERN provides infrastructures to accommodate the scale and complexity of its research outputs. Reuse and reproducibility are facilitated by practising comprehensive analysis preservation to capture relevant research objects, such as research data releases with supporting metadata, auxiliary data, linked software, reproducible analysis workflows, documentation, etc.

• • •

what to publish depends
 on individual analysis

Published Results (Level 1) Policy: Peer-reviewed publications represent the primary scientific output from the experiments. In compliance with the CERN Open Access Policy, all such publications are available with Open Access, and so are available to the public. To maximise the scientific value of their publications, the experiments will make public additional information and data at the time of publication, stored in collaboration with portals such as HEPData,⁴ with selection routines stored in specialised tools. The data made available may include simplified or full binned likelihoods, as well as unbinned likelihoods based on datasets of event-level observables extracted by the analyses. Reinterpretation of published results is also made possible through analysis preservation and direct collaboration with external researchers.





LHCb publications

[to restricted-access page]

PUBLICATIONS PER WORKING GROUP	L
B DECAYS TO CHARMONIUM	Г
B DECAYS TO OPEN CHARM	
CHARMLESS b-HADRON DECAYS	
b-HADRONS AND QUARKONIA	
CHARM PHYSICS	
FLAVOUR TAGGING	
LUMINOSITY	
QCD, ELECTROWEAK AND EXOTICA	
RARE DECAYS	

SEMILEPTONIC B DECAYS

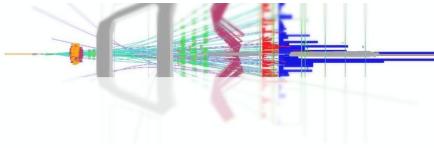
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ist of papers (Total of 655 papers and 50538 citations)

TITLE	DOCUMENT NUMBER	JOURNAL	SUBMITTED ON	CITED
Measurement of Υ production in pp collisions at $\sqrt{s}=5~{ m TeV}$	PAPER-2022-036 arXiv:2212.12664 [PDF]	JHEP	24 Dec 2022	
First observation and branching fraction measurement of the $\Lambda_b^0 o D_s^- p$ decay	PAPER-2022-038 arXiv:2212.12574 [PDF]	JHEP	23 Dec 2022	
Search for rare decays of D^0 mesons into two muons	PAPER-2022-029 arXiv:2212.11203 [PDF]	PRL	21 Dec 2022	
Measurement of lepton universality parameters in $B^+\to K^+\ell^+\ell^-$ and $B^0\to K^{*0}\ell^+\ell^-$ decays	PAPER-2022-045 arXiv:2212.09153 [PDF]	PRD	18 Dec 2022	10
Test of lepton universality in $b o s \ell^+ \ell^-$ decays	PAPER-2022-046 arXiv:2212.09152 [PDF]	PRL	18 Dec 2022	9
Search for the rare decays $W^+ o D^+_s \gamma$ and $Z o D^0 \gamma$ at LHCb	PAPER-2022-033 arXiv:2212.07120 [PDF]	Chin. Phys. C	14 Dec 2022	
Search for $K^0_{\mathrm{S(L)}} ightarrow \mu^+ \mu^- \mu^+ \mu^-$ decays at LHCb	PAPER-2022-035 arXiv:2212.04977 [PDF]	PRD	09 Dec 2022	
Amplitude analysis of $B^0 o \overline{D}^0 D_s^+ \pi^-$ and $B^+ o D^- D_s^+ \pi^+$ decays	PAPER-2022-027 arXiv:2212.02717 [PDF]	PRD	06 Dec 2022	
First observation of a doubly charged tetraquark and its neutral partner	PAPER-2022-026 arXiv:2212.02716 [PDF]	PRL	06 Dec 2022	
$J\!h\!\psi$ and D^0 production in $\sqrt{s_{ m NN}}$ = 68.5 GeV PbNe collisions	PAPER-2022-011 arXiv:2211.11652 [PDF]	EPJC	21 Nov 2022	
Charmonium production in p Ne collisions at $\sqrt{s_{ m NN}}=68.5~{ m GeV}$	PAPER-2022-014 arXiv:2211.11645 [PDF]	EPJC	21 Nov 2022	
Open charm production and asymmetry in <i>p</i> Ne collisions at $\sqrt{s_{ m NN}}$ = 68.5 GeV	PAPER-2022-015 arXiv:2211.11633 [PDF]	EPJC	21 Nov 2022	
Searches for the rare hadronic decays $B^0 o par p par p$ and $B^0_s o par p par p$	PAPER-2022-032 arXiv:2211.08847 [PDF]	PRL	16 Nov 2022	





Search for rare decays of D^0 mesons into two muons

[to restricted-access page] INFORMATION Abstract LHCB-PAPER-2022-029 A search for the very rare $D^0 \rightarrow \mu^+\mu^-$ decay is performed using data collected by the LHCb experiment in proton-proton collisions at $\sqrt{s} = 7$, 8 and 13TeV, corresponding to an integrated luminosity of 9fb⁻¹. The search is optimised for D^0 mesons from $D^{*+} \rightarrow D^0 \pi^+$ decays but is also sensitive to D^0 mesons from other sources. No evidence for an excess of events over the expected background is observed. An upper CERN-EP-2022-273 limit on the branching fraction of this decay is set at $\mathcal{B}(D^0 \to \mu^+\mu^-) < 3.1 \times 10^{-9}$ at a 90% CL. This represents the world's most stringent limit, constraining models of physics beyond the Standard Model. ARXIV:2212.11203 [PDF] Figures and captions (SUBMITTED ON 21 DEC 2022) Distributions of Δm for (left) $D^0 \rightarrow K^- \pi^+$ and (right) $D^0 \rightarrow \pi^+ \pi^-$ normalisation Figla.pdf [32 KiB] ×10⁻ PRL HiDef png [192 KiB] channels candidates for (top) Run 1 and (bottom) Run 2 data. The distributions are Thumbnail [154 KiB] Candidates / ($0.1 \text{ MeV}/c^2$) superimposed with the fit. 50 LHCb **INSPIRE 2616985** $3 \, \text{fb}^{-1}$ TOOLS 40 Data ÷. **GET BIBTEX** ----- Fitted model 30 $\cdots D^0 \rightarrow K^- \pi^+$ ----- Comb. background 20 142 144 146 148 150 140 $\Delta m [MeV/c^2]$ Fig1b.pdf [32 KiB] ×10 HiDef png [195 KiB] (c^{2}) Thumbnail [154 KiB]

LHCb Analysis LifeCycle Management tool

Database tool:

- Organizes complete review workflow
 - Workflow tracker connected to membership database
 - Overview tables for management
- Collect all kinds of additional information belonging to an analysis
- Extracts of collected material can be exported
 - Public pages
 - Open science portals, etc
- Will unify/replace WG-databases, EB-database, public pages, ...

First Implementation: new LHCb Public FIGURES pages



FAQ 💄 LOGIN Help 🗸

Old LHCb Public Figures page 🛽

Title	Report number	Keywords	Submitted on \checkmark
First LHCb upgrade reconstruction results on fixed-target data 🖸	LHCb-FIGURE-2023-001	SMOG Tracking Real Time Analysis LHC Run 3	2023-01-04
Di-photon invariant mass 🖸	LHCb-FIGURE-2022-019	ECal calibration Real Time Analysis LHC Run 3	2022-12-08
Tracking alignment with LHCb Run 3 commissioning data 🔀	LHCb-FIGURE-2022-018	SciFi Tracking Alignment and Vertexing VELO Real Time Analysis LHC Run 3	2022-11-29
Coarse Time Alignment of the SciFi - Run253101 - LHCb Commissioning [2]	LHCb-FIGURE-2022-017	SciFi Tracking LHC Run 3 and 4 LHC Run 3	2022-11-24
VELO alignment with LHCb Run 3 commissioning data 🛯	LHCb-FIGURE-2022-016	LHC Run 3 Real Time Analysis Alignment and Vertexing ACAT2022 VEL0 Tracking	2022-11-14
Recent updates from PV-finder for ACAT 2022 🗾	LHCb-FIGURE-2022-015	Alignment and Vertexing Real Time Analysis	2022-11-14

➡ DOWNLOAD PLOTS

Di-photon invariant mass from early Run~3 data

Report Number LHCb-FIGURE-2022-019

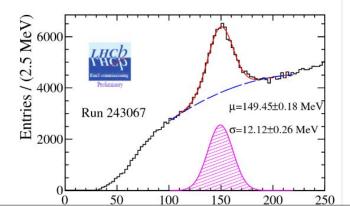
 $\label{eq:short abstract} \blacksquare \qquad Short abstract \\ Mass distributions of π^0 candidates reconstructed from $Run 243067$ and $Run 253597$. }$

CDS Link

G Additional information (only available for LHCb members)

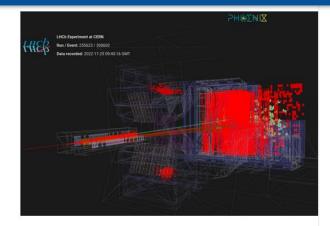
Figures and captions

Distribution of the invariant mass of the π^0 candidates (black histogram) reconstructed in Run 243067. The total PDF (red solid line), signal PDF (pink hatched area) and background PDF (blue dashed line) of the fit results are also shown.



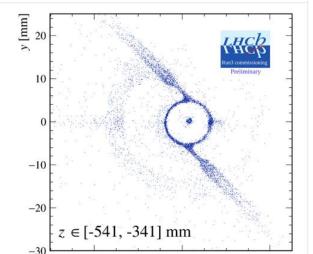
 $\equiv \frac{HCb}{HCp}$ ALCM ~

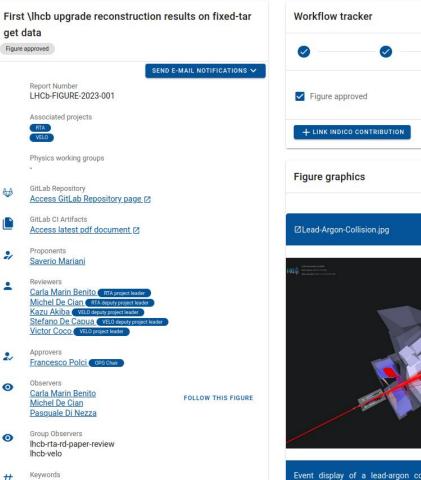
Event display of a proton-argon collision recorded on the 25/11/2022. Data acquired with \velo open with 1 mm gap, Ar injected in the \smogtwo cell and the reconstruction sequence under commissioning. The same picture with a non-dark theme, different views or different settings for the detector display can be obtained by running on the ProtonArgon.json file in \href{https://lhcb-eventdisplay.web.cern.ch} {phoenix}.

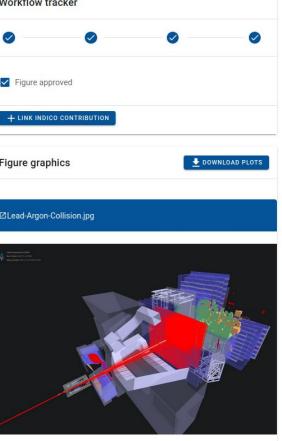


Proton-Argon-zoom_dark.png

Vertices with $z \in [-541, -341] \,\mathrm{mm}$ from beam collisions on the residual gas in \lhc and secondary interactions in the material reconstructed by the \velo open with 1 mm gap in a run with no injected gas in the \smogtwo cell. The beamspot, the \smogtwo cell in its fully closed position and the support of the injection capillary (right side of the cell) can be clearly distinguished. Note that the \smogtwo closure occurs before that of the \velo, possibly with a misalignment with respect to the beam that cancels when the \velo is also fully closed. Run number 250356.







 $\equiv \frac{l H c b}{l H c p}$ ALCM ~

with injected hydrogen, helium and argon obtained during the commissioning of the LHCb experiment are discussed.

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CDS Link

Workflow history

modified on 2023-01-04 10:17

Figure approved by Francesco Polci

modified on 2023-01-02 20:44

Figure marked as ready for approval by Victor Coco

modified on 2022-12-14 17:52

Figure marked as ready for review by Saverio Mariani

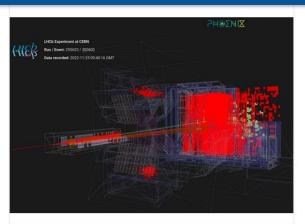
modified on 2022-12-14 14:31

Figure registered by Saverio Mariani

Figure information history

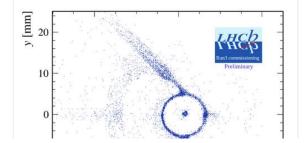
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Event display of a proton-argon collision recorded on the 25/11/2022. Data acquired with lvelo open with 1 mm gap, Ar injected in the \smogtwo cell and the reconstruction sequence under commissioning. The same picture with a non-dark theme, different views or different settings for the detector display can be obtained by running on the ProtonArgon, ison file in \href(https://lhcb-eventdisplay.web.cern.ch}{phoenix}.

SMOG2_cell_material_interactions.png



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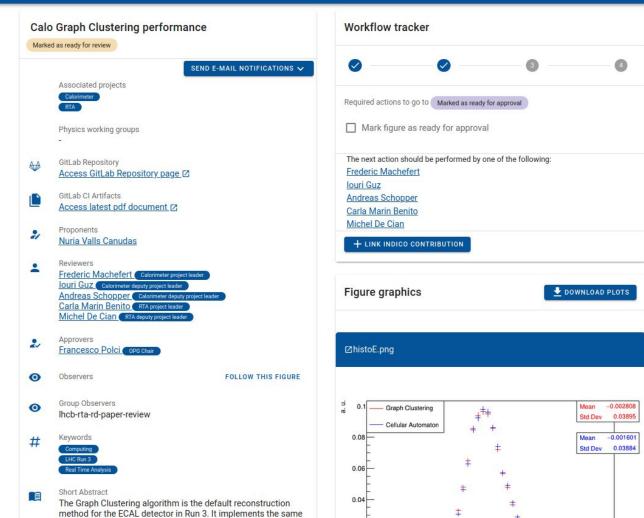
Figure

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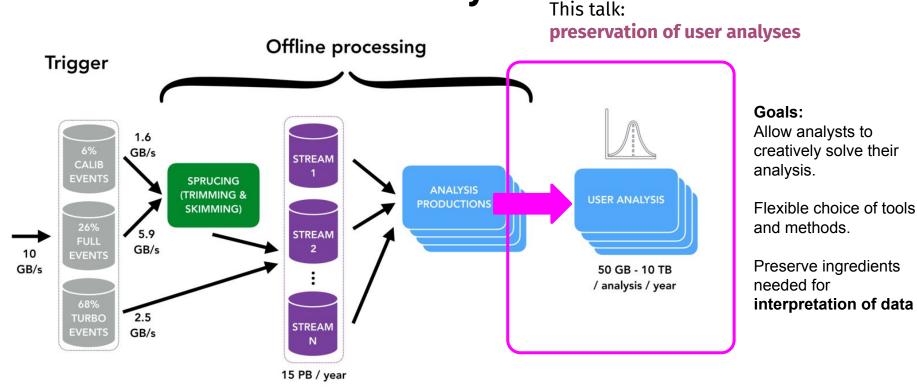
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Title	Report number 个	Stage	Keywords	Registration date 🗸	GitLab
Machine-Learnt parametrizations for the Ultra-Fast Simulation of the LHCb detector	LHCb-FIGURE-2022-004	Figure imported	Imported figure	2022-12-19	https://gitlab docs/FIGUR FIGURE-2022
First LHCb upgrade reconstruction results on fixed-target data 🖸	LHCb-FIGURE-2023-001	Figure approved	SMOG Tracking Real Time Analysis LHC Run 3	2022-12-14	<u>https://gitla docs/FIGUF 2023-001</u>
Di-photon invariant mass [2]	LHCb-FIGURE-2022-019	Figure approved	ECal calibration Real Time Analysis LHC Run 3	2022-11-30	<u>https://gitla</u> docs/FIGUR 2022-019
Mass plots with early Run\3 data 🔀	draft-LHCb-FIGURE- 2022-034	Drafting	Real Time Analysis Trigger LHC Run 3	2022-11-28	https://gitla docs/FIGUF /draft-lhcb-1
Coarse Time Alignment of the SciFi - Run253101 - LHCb Commissioning [2]	LHCb-FIGURE-2022-017	Figure approved	SciFi Tracking LHC Run 3 and 4 LHC Run 3	2022-11-24	https://gitla docs/FIGUF 2022-017
Tracking alignment with LHCb Run 3 commissioning data 🔀	LHCb-FIGURE-2022-018	Figure approved	SciFi Tracking Alignment and Vertexing VELO Real Time Analysis LHC Run 3	2022-11-22	https://gitla docs/FIGU 2022-018
Calo Graph Clustering performance 🛽	draft-LHCb-FIGURE- 2022-031	Marked as ready for review	Real Time Analysis Computing LHC Run 3	2022-11-18	https://gitla docs/FIGUF /draft-lhcb-
Performance of the Run 3 HLT2 topological triggers [2]	draft-LHCb-FIGURE- 2022-030	Drafting	Real Time Analysis Physics LHC Run 3 ACAT2022	2022-10-26	<u>https://gitla docs/FIGUF /draft-lhcb-</u>
VELO alignment with LHCb Run 3	LHCb-FIGURE-2022-016	Figure approved	Tracking Alignment and Vertexing VELO	2022-10-12	<u>https://gitla</u> docs/FIGUF

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Preservation of User Analyses,



centrally managed and preserved

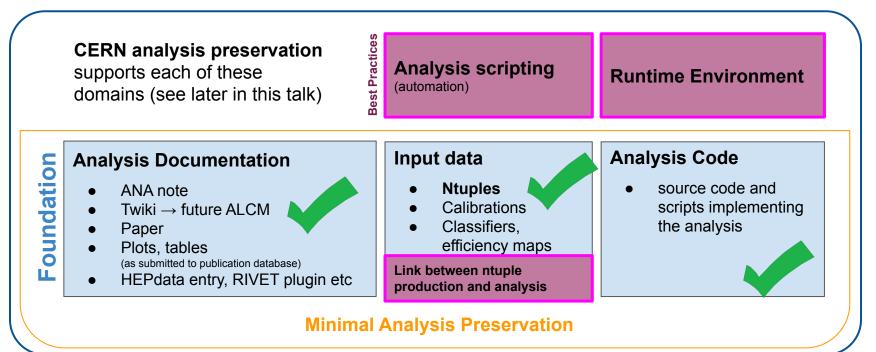
managed by proponents / PWG

data preparation

data interpretation

Analysis preservation domains

Full Analysis Preservation



Who should use full analysis preservation (AP)?

Data fluidity

- updating analysis with new data
 - e.g. early measurements
- control channels and their analysis for
 calibrations and officioncios

calibrations and efficiencies

- during commissioning
- precision measurements
- combining measurements

Data fluidity AP for updating **AP essential part** with new data, of the scientific or during analysis product development AP as "CI" for Enable analysis reinterpretation development to maximize and review scientific value

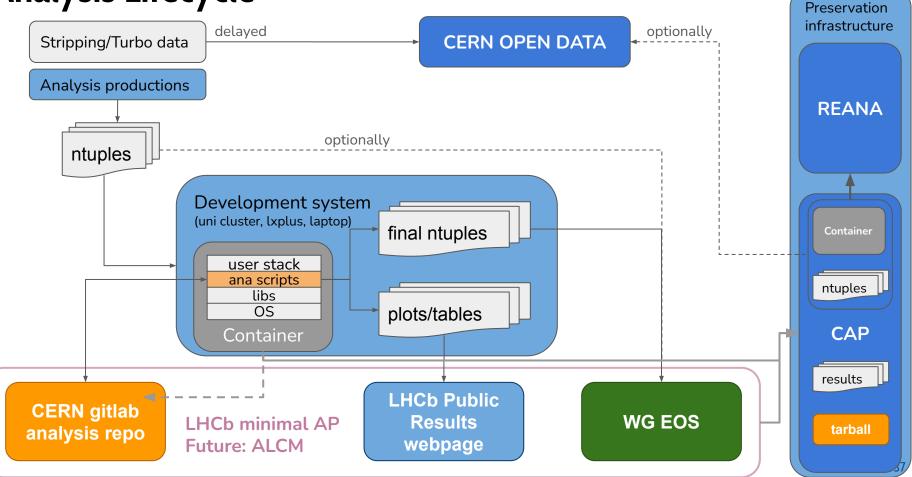
Model dependence

Model dependence

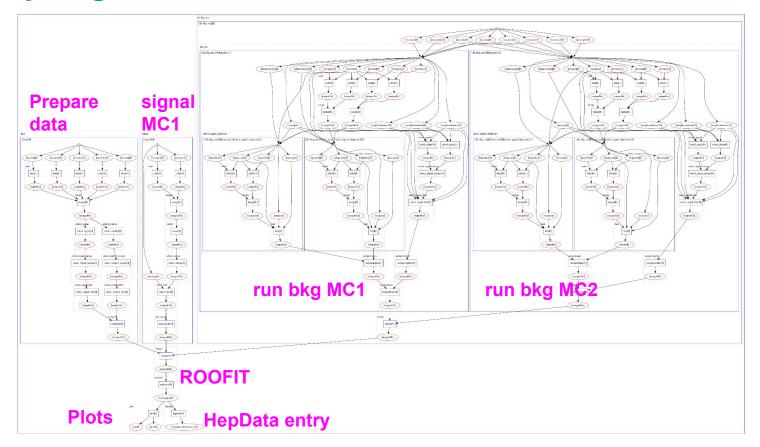
- significant phenomenology input
 - amplitude analyses!
- choice of observables based on theory input
- **auxiliary inputs**: e.g. Formfactors
- MC generators / samples
- statistical methodology

The level of detail of analysis preservation and published research products need to be decided case-by-case

Analysis Lifecycle



https://github.com/reanahub/reana-demo-bsm-search



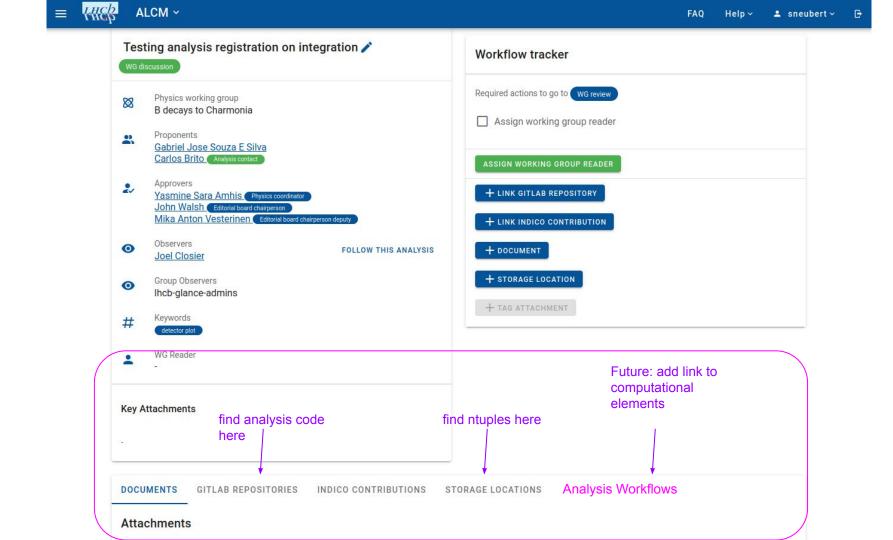
Analysis Productions Starterkit Lesson

- Ntuple production metadata preserved automatically!
- Not yet supporting Run 3 DaVinci
 - Conversion will be simple from lb-run DaVinci/vXrY \ gaudirun.py my_options.py

- Need to maintain link between ntuple production and analysis
- Will be able to use <u>apd</u> (Analysis Production Data)
- Provides PFN(s) for datasets
 - Designed to allow analyses to be rerunnable long-term

```
import apd
     datasets = apd.AnalysisData("MyWG", "MyAnalysis")
 3
     rule train_bdt:
 4
          input:
              data = datasets(datatype="2022", mc=False),
 6
              mc = datasets(datatype="2022", mc=True)
          output:
              fn = "classifier.pkl"
 9
10
         shell:
11
              "scripts/train_bdt.py --data {' '.join(input.data)} --mc {' '.join(input.mc)}"
```

ALCM for Papers and Analysis Preservation



LHCb Analysis Workflow Template

- Basic skeleton snakemake workflow (not a snakemake tutorial)
- Demonstrates **snakemake reports**
- Demonstrates running analysis in the gitlab-ci
- Runtime environment config through
 lb-conda
- Demonstrates deploy to <u>REANA</u>
- Can be used to initialize a new analysis repo
- or as tutorial what to add to your existing project

https://gitlab.cern.ch/lhcb-dpa/wp6-analysis-pr eservation-and-open-data/analysis-workflowtemplate

A Analysis Workflow Template ⊕ Project ID: 115835 €

-0- 46 Commits 🖇 1 Branch 🖉 0 Tags 🕒 399 KB Files 🗔 3.7 MB Storage

This repository demonstrates best practices for designing a user-analysis workflow. It contains an example, how to use snakemake and the CI. It can serve as a template for new analyses.

master	~ analysis-workflow-	emplate / + ~	History Find file	Web IDE	
	e branch 'master' into 'master' stian Neubert authored 1 day ag				
↑ Upload File ★ Add Kuber		configuration Add LICENSE	Add CHANGELOG	d CONTRIBUTING	
Name		Last commit		Last update	
🗅 report		Expanded Hello World workflo	w with a filteri	3 weeks ago	
E scripts		Ready for REANA	Ready for REANA		
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l ₩.gitlab-ci.	yml	Update .gitlab-ci.yml	Update .gitlab-ci.yml		
🌣 .krb5.con	f	Update krb5.conf		11 months ago	
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M environm	ent.md	Update environment.md		3 months ago	
} reana.yar	nl	Configure analysis on REANA	Configure analysis on REANA using lhcb-doc		
🖂 run.sh		refactor workflow directories		3 weeks ago	

Snakemake workflow description

Set of analysis scripts, input data, and parameters + tacit knowledge how and in what order to run them

Machine readable description of workflow (similar to Makefile for software build)

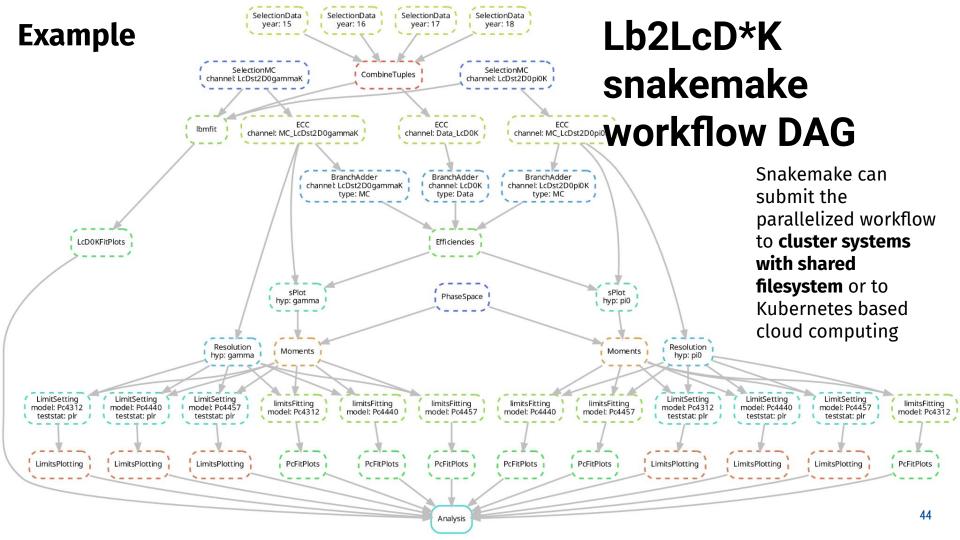
- Snakemake selected as top recommendation after comparative review in 2017 (see LHCb-INT-2017-021)
- Wide use inside collaboration
- Feature complete
- Easy to get started
- Supported by CERN REANA

Snakemake is very well documented

https://snakemake.readthedocs.io/en/stabl e/

https://snakemake.readthedocs.io/en/stabl e/snakefiles/best_practices.html

https://hsf-training.github.io/analysis-esse ntials/snakemake/README.html



Provenance tracking: snakemake reports

Static html generated by snakemake

Register important results for reporting

Shows rules, and parameters how each plot was produced

Snakemake Report				Fri Apr 29 17:35:15 2022 CET Snakemake 6.8.0
° Workflow	Legendre Moments			
II Statistics	Show 10 🗢 entries			Search:
Configuration				
RESULTS	File Descri	ption 🕕 Job properties		11 Thumbnail
Efficiencies	Moments_DstK_ECCgamma_4.png	Rule	MomentsPlotting	
Fits_LcD0K		Wildcards	hyp=gamma, max_order=4	
Legendre Moments		Parameters	2	Z T
Resolution				7 * * * * * * * * * * * * * * * * * * *
	Moments_DstK_ECCpi0_4.png	Rule	MomentsPlotting	
		Wildcards	hyp=pi0, max_order=4	and the second s
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		Wildcards	hyp=gamma, max_order=4	
		Parameters	-	a
				Z have been
	Moments_LcDst_ECCpi0_4.png	Rule	MomentsPlotting	2 20.0 2
		Wildcards	hyp=pi0, max_order=4	
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				2 <u>1</u> 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
	Moments_LcK_ECCgamma_4.png	Rule	MomentsPlotting	5 m
		Wildcards	hyp=gamma, max_order=4	
		Parameters	-	

https://snakemake.readthedocs.io/en/stable/snakefiles/reporting.html



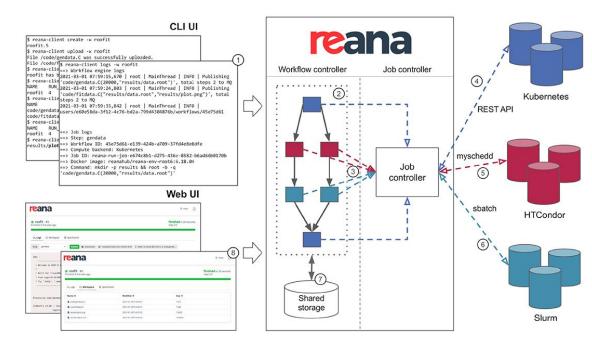
How to make sure the workflow can be run later?

- Capture all dependencies: docker or singularity container
 - Recommended: standard CERN / LHCb containers
 - e.g. gitlab-registry.cern.ch/lhcb-docker/os-base/centos7-devel
- Configure additional software from CVMFS
- For non-LHCb software use lb-conda to load environments from cvmfs
 - <u>https://gitlab.cern.ch/lhcb-core/lbcondawrappers</u>
 - default environment provides: Python 3, ROOT, Snakemake, jupyterlab, matplotlib, scikit-learn, tensorflow and many more.
- **Deploy analysis to REANA** to test if everything is preserved appropriately
- EMTF analysis are natural candidates for early adopters!

REANA: https://docs.reana.io/

Scalable Declarative HEP Analysis Workflows for Containerised Compute Clouds" published in Frontiers in Big Data (2021).

[PJ Web Conf 2014 (2019) 06034]



Supported:

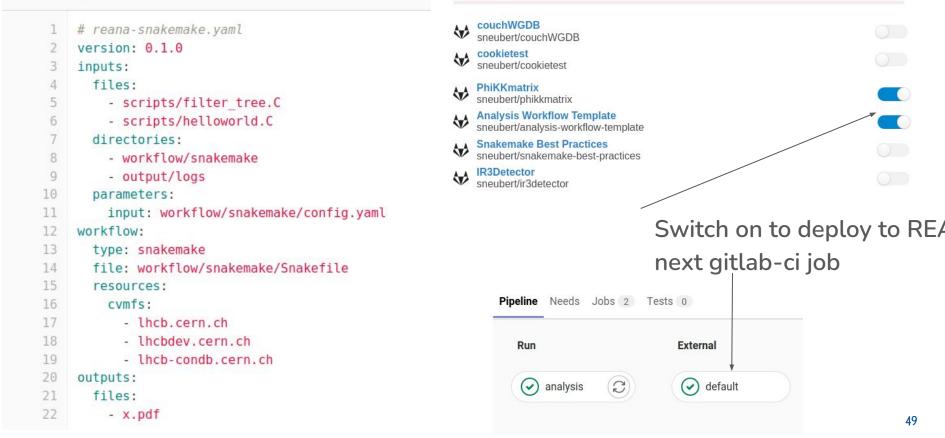
Workflow description: Snakemake, Common Workflow Language, Yadage

Compute backends: Kubernetes, HTCondor, Slurm

Deploy analysis to REANA via gitlab https://reana.cern.ch/profile

Your GitLab projects

reana.yaml 🚰 415 Bytes



REANA Webinterface <u>https://reana.cern.ch</u>

Analysis Workflow Template #17 Finished 5 days ago	finished in 2 min 42 sec step 2/2	1
		Open Jupyter Notebook 🛛 🍯
Logs 🗅 Workspace 🗟 Specification		Delete workflow
Step hello_world • finished • Kubernetes • gitlab-registry.cern.ch/lhcb-docker/os \$ ZSH_VERSION= VIR	TUAL_ENV= PYT	
job: :		
Welcome to ROOT 6.26/00 https://root.cern (c) 1995-2021, The ROOT Team; conception: R. Brun, F. Rademakers		Interactive session
Built for linuxx8664gcc on Mar 05 2022, 12:03:00		
From tag , 3 March 2022		possible via Jupyter
With		
Try '.help', '.demo', '.license', '.credits', '.quit'/'.q'		
Processing scripts/helloworld.C("filtered_tree.root")		
RooRealVar::Hello World from Sebastian Neubert = 0 L(-42 - 42)		
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TFile* filtered_tree.root		
KEY: TTree tree;1 tree		
Info in <tcanvas::print>: pdf file x.pdf has been created</tcanvas::print>		
(int) 0		

Don't make perfect the enemy of good

Ideally:

Produce every plot and (result) number in the ANA note in a workflow on REANA and document their provenance in a snakemake report.

but a more realistic goal might be to ensure that:

The central value of the result can be computed in a (snakemake) workflow running on REANA.

It is also possible to split the analysis into several smaller workflows. In this case it would be good to preserve intermediate data products.

Concluding remarks: Curating Research Products

- Different scientific questions require different levels of detail in the empirical evidence.
 - Level of model-dependence will influence how much the experimental data can be "compressed" into a few numbers.
 - Techniques that allow reinterpretation of the data are the same as those needed to adapt to a fluid dataset
- Decisions on the level of detail of analysis preservation have to be tuned to the individual study IMHO: avoid one-fits-all solutions
 - It is possible to support this with a small number of generic tools, practices, and standards
- This data curation requires dedicated resources.
 - Maximizing scientific value is not for free
- The technologies used to support the effort are very useful beyond fundamental science. Come join us!

Backup

Analysis workflow template documentation

The repository is designed to be used as a template and only contains basic building blocks. For more complex examples how to use snakemake see https://snakemake.readthedocs.io/en/stable/snakefiles/best_practices.html.

- Analysis Workflow Template
 - Hello-World example
 - Running the example on lxplus
 - Running the example in the CI
 - Setting up authentication via the Ibanadat account
 - Downloading CI Artifacts
 - Running the example on REANA
 - Setting up authentication on REANA
 - Configuring snakemake rules for delopy to REANA
 - Running the workflow on REANA using the command line interface
 - Using an Ihcb container and Ib-conda to configure the runtime environment
 - A closer look at reana.yaml
 - Snakemake tricks

LHCb analyses using snakemake (examples)

- https://gitlab.cern.ch/LHCb-QEE/WmassMeasurement
- <u>https://gitlab.cern.ch/LHCb-RD/rad-lb2pkgamma</u>
- https://gitlab.cern.ch/lhcb-b2cc/sin2beta_b2ccks_run2
- https://gitlab.cern.ch/LHCb-RD/ewp-rkstz
- <u>https://gitlab.cern.ch/lhcb-b2cc/Bs2JpsiPhi-FullRun2</u>
- https://gitlab.cern.ch/mstahl/LcD0KRun2
- https://gitlab.cern.ch/LHCb-RD/rad-lb2l0gamma-angular
- <u>https://gitlab.cern.ch/RECEPT/Semileptonics</u>
- <u>https://gitlab.cern.ch/LHCb-RD/vrd-b2xemu-aachen</u>
- <u>https://gitlab.cern.ch/lhcb-b2oc/analyses/b2oc-deltams-run2</u>
- <u>https://gitlab.cern.ch/lhcb-slb/rdstar-hadronic-run2</u>
- https://gitlab.cern.ch/lhcb-charm/charm-production-run-3
- https://gitlab.cern.ch/lhcb-charm/d2hll-analysis