The vision for the

PUNCH Science Data Platform

PUNCH

PUNCH LUNCH, 14 January 2021

Particles, Universe, NuClei and Hadrons for the NFDI

S. Neubert, P. Bechtle (U Bonn)

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- PUNCH4NFDI & Motivation
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- Why PUNCH is the right community to engage in a challenging new idea
 - Examples for complex integrated analysis workflows in our fields
 - Open data in PUNCH
 - The interplay of open workflows and analysis preservation
- Some components and capabilities of the PUNCH SDP
 - The idea of the (Dynamic) Research Product, and the catalogue behind it
 - The use cases and a few exemplifications



PUNCH4NFDI: Particles, Universe, NuClei, Hadrons for the NFDI

Particle physics (Higgs event in CMS)



PUNCH data are diverse

- in size and rate
- in complexity and purpose
- in abstraction level

Hadron&Nuclear physics (Heavy-ion collision, Alice)

PUNCH4NFDI expertise

- Big data and open data
- Data irreversibility and reduction

S-DALIN

 Highly collaborative globally distributed data management

Astronomy (Black hole, Event Horizon Telescope)

JUWELS@FZJ, GridKa ...

Astroparticle physics (Neutrino event, IceCube)

Disclaimer:

Both authors of this talk are particle/hadron physicists. Almost all examples are borrowed from our own respective areas, but the **design of the tools** designed here is inspired by and will serve a **wide variety of sciences, even beyond PUNCH**



The PUNCH Science Data Platform SDP



Emphasize the ability to Find Understand Combine Create A web of knowledge between Data, Metadata, Simulation Code, Tools Results from different fields Discover Develop Store Connect to other repositories On the PUNCH SDP

Research product contains executable workflow

The Genesis of the PUNCH SDP



The Layer model of data abstractions

(TA3)

Transformations





The planned PUNCH SDP is not alone: ESCAPE and EOSC

MANAGEMENT INNOVATION NETWORKING DISSEMINATION



Contacts: Mark Allen Added benefits of the PUNCH SDP:

- 1.) In close collaboration with developments for ESCAPE and the EOSC, bring the technology behind individual parts of ESCAPE and the EOSC to all of PUNCH, and then to more science
- 2.) Add important functionality development: RP and their catalogue

What is it?

The Virtual Observatory (VO) for astronomy integrates distributed infrastructures into one single virtual astronomy facility. ESCAPE supports the integration of the various multi-messenger ESFRI facilities and other research infrastructures into the EOSC through the VO framework, to ensure that their high-level scientific products and big data sets are openly accessible.

The VO is an essential component for the astronomy data landscape, it facilitates interoperability and re-use of data. ESCAPE will ensures that VO data are accessible to the European and international communities through EOSC. It sets the path for a new era of cross-disciplinary interoperability and connections to the necessary computing resources, as well as enabling the use of VO data in scientific analysis platforms. The ESCAPE enabled VO services aim to be a key for discovery and reuse, using common disciplinary IVOA standards and fostering good practices for data access, deposition and sharing of data, as well as for data management curation and preservation.

Who are the Target Users?

ESFRI, Research Infrastructures and other data providers, Research scientists, and Virtual Observatory builders

What is the value added / impact?

The VO provides interoperable access to European and international astronomical data and services. It is a pioneer of data sharing with a well established alliance of international partners who cooperate to build the necessary interoperability standards.



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Explore Virtual Research Environments

Infrastructure Monitor

About Catalogue

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The planned PUNCH SDP is different



The foreseen components of the PUNCH SDP

- Access Control, Accounting: Authentication and Authorization Infrastructure
- Searchable **catalogue** of **RP**s ((combination of) data, metadata, simulation, code, tools, example workflows, ...)
- **Metadata** representation of the role of individual components in the RPs, and of metadata conversions
- Links to **other repositories** and catalogues (arxiv, inspirehep, VO, HepData, DOIs,...)
- Different **user interfaces** to choose from -- web, work in a terminal on your computer, ...
- Interface to job execution
- Data, (parts of the) Metadata and Simulation can be stored in the data lakes of the platform or on external repositories

Finding open data / code from papers (current status) https://arxiv.org/abs/1701.05927v2

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Mendeley Data

Electromagnetic Calorimeter Shower Images

Published: 09-05-2017 | Version 1 | DOI: 10.17632/pvn3xc3wy5.1 Contributors: Benjamin Nachman, Luke de Oliveira, Michela Paganini

Description

Each HDF5 file has the following structure: `energy Dataset {100000, 1}`

| `layer_0 | Dataset {100000, 3, 96}` |
|-----------|---------------------------|
| `layer_1 | Dataset {100000, 12, 12}` |
| `layer_2 | Dataset {100000, 12, 6}` |
| `overflow | Dataset {100000, 3}` |

In practice, each file is a collection of 100,000 calorimeter showers corresponding to the particle specified in the file name (eplus = positrons, gamma = photons, piplus = charged pions).

The calorimeter we built is segmented longitudinally into three layer with different depths and granularities. In units of mm, the three layers have the following (eta, phi, z) dimensions: Layer 0: (5, 160, 90) | Layer 1: (40, 40, 347) | Layer 2: (80, 40, 43)

In the HDFS files, the 'energy' entry specifies the true energy of the incoming particle in units of GeV. 'layer_0', 'layer_1', and 'layer_2' represents the energy deposited in each layer of the calorimeter in an image data format. Given the segmentation of each calorimeter layer, these images have dimensions 3x96 (in layer 0), 12x12 (in layer 1), and 12x6 (in layer 3). The 'overflow' contains the amount of energy that was deposited outside of the calorimeter section we are considering.

Download All (541 MB)

| Files | |
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| eplus.hdf5 | 388 MB 🖄 🥑 Cite |
| gamma.hdf5 | 388 MB 🖄 🥑 Cite |
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Citations Views Downloads

Latest version

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Version 1 Published: 09-05-2017 DOI: 10.17632/pm3xc3wy5.1 Cite this dataset Nachman, Benjamin; de Oliveira, Luke; Paganini, Michela (2017), "Electromagnetic Calorimeter Shower Images", Mendeley Data, V1, doi: 10.17632/pm3xc3wy5.1 http://dx.doi.org/10.17632/pm3xc3wy5.1

O Cite this dataset

Institutions

Yale University

Categories

Particle Physics, Machine Learning, High Energy Detector

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HEPData https://www.hepdata.net/

- mainly used to publish
 high level observables / analysis results
 - \circ cross sections
 - particle properties
 - SM parameters
 - limits and confidence regions
- machine readable format for observables and uncertainties





CERN Open Data example entry

opendata.cern.ch

allows to reproduce the Higgs discovery

| Search or jump to ms-opendata-analyses / | Pull requests issues Marketplace Explore HiggsExample20112012 | | 100 |
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HiggsExample20112012

adapted for github by F. Blekman, @frevablekman

This example guides the user to reproducing the discovery of the Higgs boson using the 2011 and 2012 datasets, in the four-lepton final states. It contains multiple levels of examples, from very simple to a full analysis, all with CMS Open Data.

This documentation and tutorial can also be found on the CMS opendata portal, in a slightly modified configuration. It is based on the original code in [http://opendata.cem.ch/record/5500] on the CERN Open Data portal (Jomhari, Nur Zulaiha; Geiser, Achim; Bin Anuar, Afiq Aizuddin; (2017). Higgs-to-four-lepton analysis example using 2011-2012 data CERN Open Data Portal. DOI:10.7483/OPENDATA.CMS.JKB8.RR42) and modified here for direct download from aithub.



 $\sqrt{s} = 7$ TeV, L = 5.1 fb⁻¹ $\sqrt{s} = 8$ TeV, L = 5.3 fb⁻¹

 $K_0 > 0.5$

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CMS

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Data

Z+X

Root files for Higgs-to-four-lepton analysis example using 2011-2012 data

💿 lomhari, Nur Zulaiha ; 💿 Geiser, Achim ; 🌀 Bin Anuar, Afiq Aizuddin

Cite as: Jomhari, Nur Zulaiha; Geiser, Achim; Bin Anuar, Afiq Alzuddin; (2017). Root files for Higgs-to-four-lepton analysis example using 2011-2012 data. CERN Open Data Portal. DOI:10.7483/OPENDATA.CMS.IKB8.D634

Derived CMS CERN-LHC

Description

This record contains root files that were processed for the Higgs analysis example on the CMS 2011-2012 Open Data.

Dataset characteristics

24 files, 1.6 MB in total.

How can you use these data?

These datasets are provided as part of the Higgs-to-four-lepton analysis example using 2011-2012 data. You can download all root files needed for the Level 3 exercise to your working area by downloading first the file list rootfilelist.txt and then the root files with wget -i rootfilelist.txt.

Please note that the following files are not needed to produce the plot but are only the products of intermittent processing steps:

- DY101Jets12.root
- DY50Mag12.root
- DYTo2mu12.root
- TTJets11.root
- TTJets12.root

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| DY1012.r | oot | | | | | | | | 66.1 kB | ▲ Download |
| DY101Jet | s12.root | | | | | | | | 63.9 kB | ⊥ Download |
| DY50Mag | 12.root | | | | | | | | 69.7 kB | ± Download |
| First | Previous | 1 | 2 | 3 | 4 | 5 | Next | Last | | |

Disclaimer

GNU General Public License (GPL) version 3

New CERN Open Data Policy published December 2020

https://cds.cern.ch/record/2745133 endorsed by all LHC collaborations

Lays out policy for 4 levels of complexity [arXiv:1205.4667]

- 1. Public results -
- 2. Outreach and education
- 3. Reconstructed data -
- 4. Raw data (will not be made 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, 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."

"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 [..]" The REANA Project https://reanahub.io/

reana

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Reproducible research data analysis platform



REANA architecture https://reanahub.io/



Tibor Simko, poster presented at eScience IEEE 2019

restored many of the laws w

Example Analysis

Search for physics beyond the standard model at ATLAS <u>https://github.com/reanahub/reana-demo-bsm-search</u> Input data is simulated from statistical models as part of workflow here Workflow described by a directed acyclic graph (DAG) using the **yadage** engine

 automatic parallelisation of workflow graph



REANA interactive session https://reanahub.io/

- REANA manages projects in so called "workspaces" (basically a directory)
- Data and code are uploaded into the workspace
- Workspaces can be examined interactively using Jupyter Notebooks



Current Paradigm

Publications may be supported by

- open data sets (various repositories)
- code, workflows (github)

High level results available in machine readable form

Data catalogues (e.g VO)

PUNCH4NFDI

development

Items loosely linked

- hyperlinks in project descriptions / abstracts
- "papers with code" links (arXiv)
- Inspired by how we reference papers
- no standard way of linking / interfacing

Executing computational elements left to users

DSP and the role of the Research Product (RP)

RPs provide a common concept to talk about the output of research. An RP can be a

- paper
- (meta)data set
- scientific code
- workflow
- computational element

Building a catalogue of RPs establishes a common standard to link RPs

papers, data and code as first class citizens

RPs facilitate composition => reuse previous work to create new scientific value

RPs can be active computational elements (Dynamic RPs)

- Workflows + execution environment
- Statistical analysis, combination with other results, ...

PUNCH Science Catalogue

- Collect available material from across PUNCH community in a common, searchable catalogue
 - publications, code, datasets/sources, existing catalogues
 - Common interface to establish links
- Catalogue entries are the **research products** (RPs)
- Use these collections to develop meta-data schemes, describing the RPs
 - building on existing developments in particular in astrophysics
 - establish schemata to allow composition of RPs
- **Portal Entry point** for user searches

Platform SDP

Research product contains executable workflow



Many options for the user

The Use Cases: How and where our work might improve



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The Use Cases: An example from a global analysis



Now: Every analyst must download, compile, interface every code, read results from tables, ...

Data taking and reduction (TA5)

The Use Cases: An example from a hadron spectroscopy analysis



Summary

- The **PUNCH Science Data Platform SDP** is an important part of the PUNCH4NFDI consortium's plans for advancing the computing of the PUNCH sciences and the whole NFDI
- It builds on the collaboration with other platform developments, and on the improvement of platform use through a continuation of the developments of **techniques available in our communities**
- The **Research Product** is a central part of the PUNCH-SDP: It can add an important representation of *knowledge in the interaction and integration* of *data, metadata, simulation, tools and code*, which is especially strong in our communities due to the one-off nature of our experiments: Big Data and unique one-off experiments place common challenges for (Astro)Particle-, Hadron-Physics and Astronomy

Backup

[sneubert@lxplus7106 REANA-test]\$ rm -rf reana-demo-bsm-search/ [sneubert@lxplus7106 REANA-test]\$ git clone https://github.com/reanahub/reana-demo-bsm-search.git Cloning into 'reana-demo-bsm-search'... remote: Enumerating objects: 45, done. remote: Counting objects: 100% (45/45), done. remote: Compressing objects: 100% (28/28), done. remote: Total 126 (delta 15), reused 36 (delta 11), pack-reused 81 Receiving objects: 100% (126/126), 6.17 MiB | 9.11 MiB/s, done. Resolving deltas: 100% (49/49), done. [sneubert@lxplus7106 REANA-test]\$ cd reana-demo-bsm-search/ [sneubert@lxplus7106 reana-demo-bsm-search]\$ ls code docs environments LICENSE README.rst reana.yaml workflow [sneubert@lxplus7106 reana-demo-bsm-search]\$

[sneubert@lxplus7106 REANA-test]\$ rm -rf reana-demo-bsm-search/ [sneubert@lxplus7106 REANA-test]\$ git clone https://github.com/reanahub/reana-demo-bsm-search.git Cloning into 'reana-demo-bsm-search'... remote: Enumerating objects: 45. done. remote: Counting objects: 100% (45/45), done. remote: Compressing objects: 100% (28/28). done. remote: Total 126 (delta 15), reused 36 (delta 11), pack-reused 81 Receiving objects: 100% (126/126), 6.17 MiB | 9.11 MiB/s, done. Resolving deltas: 100% (49/49), done. [sneubert@lxplus7106 REANA-test]\$ cd reana-demo-bsm-search/ [sneubert@lxplus7106 reana-demo-bsm-search]\$ ls code docs environments LICENSE README.rst reana.yaml workflow [sneubert@lxplus7106 reana-demo-bsm-search]\$ reana-client create -n myanalysis [sneubert@lxplus7106 reana-demo-bsm-search]\$ export REANA WORKON=myanalysis [sneubert@lxplus7106 reana-demo-bsm-search]\$ reana-client upload File /workflow/allmc input.vml was successfully uploaded. File /workflow/databkgmc.yml was successfully uploaded. File /workflow/inputsig.vml was successfully uploaded. File /workflow/inputsm.yml was successfully uploaded. File /workflow/steps.yml was successfully uploaded. File /workflow/wflow all mc.yml was successfully uploaded. File /workflow/workflow data.yml was successfully uploaded. File /workflow/workflow mc.yml was successfully uploaded. File /workflow/workflow select shape.yml was successfully uploaded. File /workflow/workflow sig.yml was successfully uploaded. [sneubert@lxplus7106 reana-demo-bsm-search]\$

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